DIMSEMs — Diagonally Implicit Single-Eigenvalue Methods for the Numerical Solution of Stiff ODEs on Parallel Computers: A Preliminary Report

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Abstract

We describe a new class of General Linear Methods (GLMs) with the following properties: the methods are strictly diagonally implicit, allowing efficient parallel implementation; the stability matrix has no spurious eigenvalues (i.e., only one eigenvalue of the stability matrix is non-zero); the methods have high stage order, allowing them to retain their order on problems for which order reduction might otherwise be a problem; the methods are L-stable, making them suitable for the solution of stiff problems. As well as presenting some order barriers, we derive and test methods of orders 2–6.

Key words. Parallel, Numerical Solution, Initial Value Problem, IVP, Ordinary Differential Equation, ODE, General Linear Method, GLM, Order, Stability.

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1 Introduction and Background

This is a preliminary report on numerical methods for the parallel solution of stiff initial-value problems (IVPs) for ordinary differential equations (ODEs) of the form

$$\begin{aligned} u'(x) &= f(u(x)) \quad \forall x \in [x_0, x_{end}], \\ u(x_0) &= u_0, \end{aligned}$$

where $u : \mathbb{R} \to \mathbb{R}^K$. For notational convenience we assume a scalar equation ($K = 1$) unless otherwise noted, but the results generalise to vectors by the use of tensor product notation. Methods for solving IVPs typically compute approximations to $u(x_n), n = 1, \ldots, N$ on some mesh $x_0 < x_1 < \cdots < x_N = x_{end}$, where the approximation at each successive step depends on one or more of the approximations at previous steps. We seek methods which permit parallel computation within each step of the solver, rather than attempting to replace the entire sequential step-by-step integration with a parallel process. Our methods will therefore be suitable for machines with a few processors, such as shared-memory machines, rather than the hundreds or thousands of processors available with local-memory, message-passing architectures.

1.1 General Linear Methods

The methods developed here are members of the class of general linear methods (GLMs) introduced by Butcher. (See [6] for a survey.) They are also known as multivalue methods (MVMs). Given a vector y_n of external stages on the current step, they first compute a vector of internal stages,

$$Y_n = A_1 y_n + hB_1 F(Y_n) \in \mathbb{R}^s,$$

and then compute y_{n+1} from it by

$$y_{n+1} = A_2 y_n + hB_2 F(Y_n) \in \mathbb{R}^r.$$

Here h is the stepsize, $F(Y_n)$ is the vector formed by applying f to each component of Y_n, and A_1, B_1, A_2 and B_2 are matrices of constant coefficients which determine the method. The components of the external stages y_n may in different methods represent approximations to the solution at various points, derivatives of the solution, or other quantities. The internal stages are approximations to the solution at points determined by the internal abscissae $c_1, \ldots, c_s$,

$$Y_{n,i} \approx u(x_n + c_i h), \quad i = 1, \ldots, s.$$

A starting method is required to provide the initial approximation y_0, and, if the solution itself is not a component of y_n, a finishing method is needed to recover it [2, 6].

Two common types of GLM are Nordsieck methods, in which the external stages ap-

proximate scaled derivatives of the solution of the ODE, and multistep Runge-Kutta (MRK) methods, in which they approximate the solution itself at various points. That is, for a Nordsieck GLM,

$$y_{n,i} \approx \frac{h^{i-1}}{(i-1)!} u^{(i-1)}(x_n), \quad i = 1, \ldots, r, \tag{1}$$

while for an MRK,

$$y_{n,i} \approx u(x_n + d_i h), \quad i = 1, \ldots, r, \tag{2}$$

where $d_i = i - r$ are the external abscissae,

$$A_2 = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & 1 & 0 \\ 0 & \cdots & \cdots & 0 & 1 \\ \alpha_1 & & \cdots & & \alpha_r \end{bmatrix}, \tag{3}$$

and

$$B_2 = \begin{bmatrix} 0 & \cdots & 0 \\ & \vdots & \\ 0 & \cdots & 0 \\ \gamma_1 & \cdots & \gamma_r \end{bmatrix}, \tag{4}$$

for some α_i's and γ_i's.

A GLM is called explicit if B_1 is strictly lower triangular, that is, lower triangular with zeroes on the diagonal. Otherwise it is implicit. Although the computation of the internal stages Y_n is considerably less expensive in an explicit method, only implicit methods are suitable for the solution of stiff problems. In an implicit method, computing Y_n at each step requires the solution of a system of generally nonlinear equations,

$$Y_n = A_1 y_n + h B_1 F(Y_n).$$

This is typically performed using a Newton iteration,

$$\begin{aligned} (I_s - h B_1 F'(Y_n^{(k)}))\Delta^{(k)} &= -R(Y_n^{(k)}) \\ Y_n^{(k+1)} &= Y_n^{(k)} + \Delta^{(k)}, \end{aligned} \tag{5}$$

(or some variant in which $F'(Y_n^{(k)})$ is replaced by an approximation) where

$$R(Y) = Y - A_1 y_n - h B_1 F(Y)$$

is the function whose zero is the internal stage vector Y_n, and $Y_n^{(k)}$ is the k-th iterate approximating Y_n.

1.2 Parallelism in Implicit GLMs

The parallelism inherent in an implicit GLM depends on the structure of B_1. (Note that, in the following, the names given to GLMs of various structures vary with different authors.)

A *diagonally implicit* GLM has

$$B_1 = \begin{bmatrix} \lambda_1 & & & & \\ b_{21} & \lambda_2 & & & \\ b_{31} & b_{32} & \lambda_3 & & \\ \vdots & \vdots & & \ddots & \\ b_{s1} & b_{s2} & \cdots & b_{s,s-1} & \lambda_s \end{bmatrix}.$$

With this structure, each internal stage value $Y_{n,i}$ is coupled only to those before it, so that the $Y_{n,i}$'s may be solved for in sequence. If $\lambda_1 = \cdots = \lambda_s$, the method is called *singly diagonally implicit*. Such methods have been investigated, for instance, by Burrage and Chipman [3] for use on sequential machines.

In a *strictly diagonally implicit* GLM, B_1 is a diagonal matrix,

$$B_1 = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_s \end{bmatrix}.$$

This decouples the component equations of the Newton iteration (5) into

$$(1 - h\lambda_i f'(Y_{n,i}^{(k)}))\Delta_i^{(k)} = -R(Y_n^{(k)})_i, \quad i = 1, \ldots, s,$$

with the effect that $\Delta_i^{(k)}$, $i = 1, \ldots, s$, can be solved for independently. For a K-dimensional IVP, (5) becomes

$$(I_K - h\lambda_i f'(Y_{n,i}^{(k)}))\Delta_i^{(k)} = -R(Y_n^{(k)})_i, \quad i = 1, \ldots, s, \tag{6}$$

with $\Delta_i^{(k)} \in \mathbb{R}^K$, and a separate factorisation of each

$$(I_K - h\lambda_i f'(Y_{n,i}^{(k)}))$$

is required for each distinct λ_i. (Or, some other scheme must be used to accommodate the distinct λ_i's, such as Enright's factorisation [13] or an iterative linear solver.) The s factorisations however can be done in parallel, as can the s solves for $\Delta_i^{(k)}$, $i = 1, \ldots, s$.

If we restrict B_1 to be a multiple of the identity, $B_1 = \lambda I$, the result is a *singly strictly diagonally implicit* GLM. For a K-dimensional problem, (5) becomes

$$(I_K - h\lambda f'(Y_{n,i}^{(k)}))\Delta_i^{(k)} = -R(Y_n^{(k)})_i, \quad i = 1, \ldots, s,$$

where $\Delta_i^{(k)} \in \mathbb{R}^K$. On a sequential machine, it is common to approximate each $(I_K - h\lambda f'(Y_{n,i}^{(k)}))$, $i = 1, \ldots, s$, by a single matrix $N^{(k)}$, to avoid having to perform s factorisations per iteration. The constant diagonal λ in a singly implicit method is therefore an advantage on a sequential machine. On a parallel machine, however, each factorisation, as well as each of the subsequent solves, can be assigned to a different processor, so there is less incentive to limit the structure of B_1 in this way.

Butcher recently introduced a class of methods called DIMSIMs [8, 9, 10, 11] which contains methods with each of the above structures. Because of their particular relevance to our work, these methods will be discussed separately later.

1.3 Error Coefficients

An important property of a method is the accuracy of the generated solution, and the dependence of this accuracy on the stepsize. This leads to the concepts of local and global error, error coefficients and order of accuracy. Local error is the error in the solution produced at the end of a single step started with exact information, while global error is the error after a sequence of steps, only the first of which is started with exact information. Error coefficients are a problem-independent characterisation of the local error.

A valuable tool for the analysis of numerical methods for ODEs is the form of Taylor series known as a Butcher series,

$$B(\varphi, u) = \sum_{t \in T} \varphi(t) \frac{h^{\rho(t)}}{\rho(t)!} D(t)(u). \tag{7}$$

Here T is the set of monotonically labeled rooted trees, $\varphi : T \to \mathbb{R}^m$ for some m, $\rho(t)$ is the order of tree t (that is, the number of nodes in t), and $D(t)$ is the elementary differential associated with the ODE for the tree t. Let ϕ be the empty tree, which is the tree with no nodes, and let $\bullet$ be the tree with only a root node. Let $t = [t_1, \ldots, t_m]$ represent the tree formed by joining each of the trees $t_1, \ldots, t_m$ with a new branch from each of their respective root nodes to a new node, which becomes the root of t. Then for the ODE $u'(x) = f(u(x))$, $D(t)$ is defined recursively by

$$D(\phi)(u) = u,$$

$$D(\bullet)(u) = f(u),$$

and

$$D(t)(u) = f^{(m)}(u)(D(t_1)(u) \cdots D(t_m)(u)) \quad \text{for} \quad t = [t_1, \ldots, t_m].$$

If $K > 1$, the multiplication of vectors is done componentwise. More on Butcher series may be found in [2, 7, 15, 16, 17, 19]. As an example, if $\varphi(t) = c^{\rho(t)}$, then $B(\varphi, u(x_n))$ is the Taylor series for $u(x_n + ch)$ expanded about the point x_n.

We now summarise the result of using Butcher series to analyse the local error in a GLM stepping from y_n to y_{n+1}. Let $\hat{y}_k$ be the vector of exact values to which the external stage

vector y_k is an approximation, for every step k. By appropriate choice of what is known as the true-value function, $q : T \to \mathbb{R}^r$, we can expand $\hat{y}_k$ in a Butcher series around x_k,

$$\hat{y}_k = B(q, u(x_k)) \quad \forall k, \tag{8}$$

where $u : \mathbb{R} \to \mathbb{R}$ is the true solution of the IVP. Let $y_n = \hat{y}_n$, so that the method starts the n-th step with exact information. The local error l_n then satisfies

$$\begin{aligned} l_n &= y_{n+1} - \hat{y}_{n+1} && (9) \\ &= B(e, u(x_n)), && (10) \end{aligned}$$

for an appropriate choice of $e(t) \in \mathbb{R}^r$, the vector of local error coefficients of the method for the tree t. Using the theorem of Hairer and Wanner [16] on the composition of Butcher series, we can express $e(t)$ recursively in terms of local error coefficients of trees of lower order, the true-value function q, and the coefficient matrices A_1, B_1, A_2, B_2 of the method. The resulting expressions are the basis for the computer programs we wrote to find error coefficients for the methods we developed.

1.4 Order of Accuracy and Simplifying Assumptions

The order of a method, as mentioned in the previous section, is a characterisation of the sensitivity of the error to changes in stepsize. The global error is defined as

$$g_n = y_{n+1} - \hat{y}_{n+1},$$

where

$$y_0 = \hat{y}_0.$$

A method is said to have global order p (or, simply, order p) if p is the largest value such that $g_n = O(h^p)$. Similarly a method is said to have local order $p+1$ if p is the largest value such that $l_n = O(h^{p+1})$. A global error of order p usually corresponds to a local error of order $p+1$, although it is possible in certain situations to have local and global errors of the same order [12, 22]. When classifying methods according to their accuracy, the order of the method is typically the most significant, while the size of the local error coefficients distinguishes between methods of the same order.

The equations which must be satisfied for a method to have a certain local order are called the order conditions. For a method of local order $p+1$, we require that $e(t) = 0$ for all trees t of order $\rho(t) \leq p$, where $e(t)$ are the error coefficients. This results in global order at least p, provided the method is stable. Solving these order conditions directly for methods of non-trivial order is extremely difficult, however, as they consist of large systems of nonlinear equations. For this reason it is customary to employ simplified order conditions, also known as simplifying assumptions, which are sufficient, but not necessary, conditions for the order

conditions to hold.

The methods developed in this report make use of the A, B and C simplifying assumptions of Burrage and Moss [4]. These are defined as

$$A(w) \quad : \quad q(t) = q(\tau^{\rho(t)}), \quad \forall t \ni \rho(t) \leq w, \tag{11}$$

$$B(w) \quad : \quad A_2 q(\tau^k) + kB_2 c^{k-1} = \sum_{i=0}^{k} \left(\begin{array}{c} k \\ i \end{array} \right) q(\tau^i), \quad k = 0, \ldots, w, \tag{12}$$

$$C(w) \quad : \quad A_1 q(\tau^k) + kB_1 c^{k-1} = c^k, \quad k = 0, \ldots, w, \tag{13}$$

where kB_1c^{k-1} and kB_2c^{k-1} are taken as 0 when $k = 0$, and $\tau^k = [\bullet, \ldots, \bullet]$ is what is known as the *bushy* tree of order k. The importance of these simplifying assumptions is given by a theorem of Burrage and Moss [4], which states that a GLM satisfying $A(p)$, $B(p)$, and $C(p-1)$ has order at least p, provided the method is stable. Furthermore, the stage order (the order of the internal stages) is at least $p-1$, and if $C(p)$ is satisfied, it is at least p. The solution of these simplified order conditions, while by no means trivial, is much easier than that of the raw order conditions described earlier. More on simplifying assumptions for GLMs may be found in [1, 2, 4].

1.5 Stability Regions of GLMs

When a GLM is used with a sufficiently large fixed stepsize, the computed solution may become unstable, that is, may grow without bound, even though the true solution remains bounded or decays. For certain methods applied to so-called *stiff* problems, the stepsize necessary for stability may be much smaller than that necessary to produce a sufficiently accurate solution with a more appropriate method. An important indication of the suitability of a method is the size of the stability region,

$$\begin{aligned} R \quad = \quad & \{h\mu : \exists c \in \mathbb{R} \ni \text{the method applied with stepsize } h \text{ to the test problem} \\ & u' = \mu u, \text{ where } \mu \in \mathbb{C}, \text{ produces a solution } u_n \text{ satisfying } |u_n| \leq c|u_0| \ \forall n\}. \end{aligned}$$

This can be shown to be equivalent to

$$R = \{z \in \mathbb{C} : \|M(z)^n\| \text{ is bounded } \forall n \geq 1\},$$

where

$$M(z) = A_2 + zB_2(I - zB_1)^{-1}A_1$$

is the *stability matrix* associated with the GLM. A third equivalent definition of R is

$$\begin{aligned} R \quad = \quad & \{z \in \mathbb{C} : \|\gamma\| \leq 1 \text{ for all nondefective eigenvalues } \gamma \text{ of } M(z) \\ & \text{and } \|\gamma\| < 1 \text{ for all defective eigenvalues } \gamma \text{ of } M(z).\} \end{aligned}$$

It is known that explicit GLMs can have only finite stability regions: to achieve infinite stability regions an implicit method is required. This means explicit methods are suitable only for non-stiff problems, and stiff problems require the use of an implicit method to avoid the penalty of stability imposed restrictions on the stepsize.

A desirable property for a method intended for the solution of stiff problems is that its stability region R include the whole left complex half-plane. A method with this property is called A-stable, and has the favourable characteristic that the stepsize is never restricted by stability on linear constant-coefficient problems, regardless of stiffness.

The previous discussion has considered stability for the scalar test problem

$$u' = \mu u, \quad \mu \in \mathbb{C}.$$

However, stability for the vector problem

$$u' = Cu, \quad C \in \mathbb{R}^{K \times K},$$

where C is diagonalisable, can be shown to follow from stability on each of the scalar problems

$$u' = \mu_i u, \quad i = 1, \ldots, K,$$

where $\mu_1, \ldots, \mu_K$ are the eigenvalues of C. This, as well as a weaker result which holds when C is not diagonalisable, are given by Theorem 4 in Appendix A.

2 How We Came to DIMSEMs

The goal of our research is to produce A-stable GLMs with diagonal B_1. Such methods are suitable for solving stiff problems on a parallel machine. A second goal is to find a whole class of such methods, together with a methodology for generating methods of any desired order. The first subclass of GLMs which we considered was Diagonally Implicit Multistep Runge Kutta methods (DIMRKs), which are MRKs with diagonal B_1. Two classes of these methods, arising from modifications to the methods of Burrage and Chipman [3], were investigated initially. The first satisfies $B(r+s-1)$ and $C(r-1)$, and hence has order at least r, with $c_1, \ldots, c_s$ and $\lambda_1, \ldots, \lambda_s$ as free parameters. The second satisfies $B(r)$ and $C(r)$, also has order at least r, and has $\gamma_1, \ldots, \gamma_{s-1}$ (defined in (4)) as free parameters. The simplified order conditions were solved algebraically using Maple [23], and the free parameter space was searched numerically for methods that appeared to be A-stable. The A-stability of these candidate methods was then verified theoretically using a technique based on the Schur criterion and the maximum principle of complex analysis [3]. Although methods of orders 2 to 5 were found this way, this simple approach does not appear to be extensible to higher orders due to the rapidly increasing cost, as order increases, of solving the order conditions by brute force. Another disadvantage of this approach is that it requires trial-

and-error numerical searching to find A-stable methods. Little insight is available into the nature of A-stable choices of the parameters, as algebraic expressions for objects such as the characteristic polynomial of the stability matrix, or the eigenvalues, are too expensive to compute.

Our eventual concentration on a new class of methods for which A-stability is much easier to analyse grew out of a seminar [5] given by Butcher, in which he introduced his work on DIMSIM methods. Although Butcher's subsequent development of these methods takes a different direction from ours, the two classes are sufficiently related to warrant discussing DIMSIMs in the next section.

2.1 DIMSIMs — Diagonally Implicit Multi-Stage Integration Methods

Although our introduction to the GLMs known as DIMSIMs was through an early seminar by Butcher, they have now been described in published work [8, 9, 10, 11]. The methods are classified into four types, depending on the structure of B_1. These are defined in Fig. 1, which also indicates the type of problem and kind of architecture for which each type is suitable. Types 1 and 3 are explicit methods, intended for non-stiff problems, while type 2 is singly diagonally implicit, and type 4 is singly strictly diagonally implicit.

The DIMSIMs described in [9, 10, 11] are constructed with $r = s$, $A_1 = I$, $A_2 e = e$, where e is an r-vector of all 1's, and B_2 is determined from the order conditions $A(r)$, $B(r)$, and $C(r)$ in terms of the c_i's, B_1, and A_2. This gives an order and a stage order of r. Although Butcher gives his order conditions in terms of the exponential function and integrals of interpolating polynomials instead of the expressions (11), (12), and (13), the two representations can be shown to be equivalent. Additional DIMSIMs in which various combinations of r, s, the order, and the stage order differ by one from the values above, are developed by Butcher and Jackiewicz in [8].

In his seminar, Butcher exhibited a type-2, order-2 DIMSIM which had been constructed to have the same stability region as a certain diagonally implicit Runge-Kutta (DIRK) method. This was achieved by making one eigenvalue of the stability matrix $M(z)$ zero for all z, and making the other eigenvalue equal to the stability function of the DIRK method. A generalisation of this example leads to the idea of *Single-Eigenvalue Methods* (SEMs), in which all but one eigenvalue of $M(z)$ is zero for all z. We use the term DIMSEM — *Diagonally IMplicit Single-Eigenvalue Method* — to describe a SEM having a diagonal B_1 matrix. Although Butcher [9] mentions it as a useful property, Butcher's, and Butcher and Jackiewicz's, DIMSIMs, do not possess the single-eigenvalue property. We have found it useful however for the simplification it provides in the search for A-stable methods. Aside from facilitating the search for A-stable methods, single-eigenvalue methods might have better numerical properties, as there are no spurious solutions arising from the non-principal eigenvalues which contribute to the solution until they die out. Butcher [9] points out that

DIMSIM	B_1 Structure	Problem	Machine
Type 1	$\begin{bmatrix} 0 & & & & \\ b_{21} & 0 & & & \\ b_{31} & b_{32} & \ddots & & \\ \vdots & \vdots & \ddots & 0 & \\ b_{s1} & b_{s2} & \cdots & b_{ss} & 0 \end{bmatrix}$	non stiff	serial
Type 2	$\begin{bmatrix} \lambda & & & & \\ b_{21} & \lambda & & & \\ b_{31} & b_{32} & \ddots & & \\ \vdots & \vdots & \ddots & \lambda & \\ b_{s1} & b_{s2} & \cdots & b_{ss} & \lambda \end{bmatrix}$	stiff	serial
Type 3	$\begin{bmatrix} 0 & & & & \\ 0 & 0 & & & \\ 0 & 0 & \ddots & & \\ \vdots & \vdots & \ddots & 0 & \\ 0 & 0 & \cdots & 0 & 0 \end{bmatrix}$	non stiff	parallel
Type 4	$\begin{bmatrix} \lambda & & & & \\ & \lambda & & & \\ & & \ddots & & \\ & & & \lambda & \\ & & & & \lambda \end{bmatrix}$	stiff	parallel

Figure 1: Butcher's four DIMSIM types [9]

this desirable property is also possessed by Runge-Kutta methods. Indeed, this is likely a better justification for SEMs than our original one, the ease of determining A-stability, as Butcher and Jackiewicz [8, 11, 10] have since been able to find elegant mathematical expressions for the eigenvalues of their stability matrices, from which A-stable methods can be derived without resorting to numerical searching or computationally intractable algebraic manipulation.

2.2 Application to Proving A- and L-Stability

The problem of determining A- and L-stability of a GLM simplifies considerably if the stability matrix has only one nonzero eigenvalue. If we let

$$\text{eig}(M(z)) = \{e_1(z), \ldots, e_r(z)\},$$

and suppose that

$$e_2(z) = \cdots = e_r(z) = 0 \quad \forall z \in \mathbb{C},$$

then

$$\mathrm{tr}(M(z)) = \sum_{i=1}^{r} e_i(z) = e_1(z).$$

Now recall that

$$M(z) = A_2 + zB_2(I - zB_1)^{-1}A_1,$$

so that the trace is a rational function of z, say

$$e_1(z) = \frac{P(z)}{Q(z)}. \tag{14}$$

For a strictly diagonal method, where

$$B_1 = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_s \end{bmatrix},$$

it follows easily that

$$Q(z) = \prod_{i=1}^{s}(1 - \lambda_i z), \tag{15}$$

so that $e_1(z)$ is analytic and has no poles in $\mathbb{C}^-$ provided all the λ_i's have positive real parts. (For general B_1, (15) holds if $\lambda_1, \ldots, \lambda_s$ are the eigenvalues of B_1. This follows from (19).) By the maximum principle, it suffices to check that $|e_1(iy)| \leq 1 \; \forall y \in \mathbb{R}$ to ensure A-stability. Now, if we define the *E-polynomial*

$$E(y) = |P(iy)|^2 - |Q(iy)|^2, \tag{16}$$

then

$$|e_1(iy)| \leq 1 \Leftrightarrow E(y) \leq 0,$$

and, assuming the polynomials P and Q have real coefficients, a sufficient condition for A-stability is that $\lambda_i \in \mathbb{C}^+$ for $i = 1, \ldots, s$ and $E(y)$ has all nonpositive coefficients. (This follows from the observation that, if P and Q are real polynomials, then $E(y)$ is an even polynomial, that is, the coefficients of each odd power of y in $E(y)$ is zero.) An A-stable SEM is also L-stable iff $|e_1(z)| \to 0$ as $|z| \to \infty$. From (14), this is equivalent to $\deg(P) < \deg(Q)$. Given the coefficient matrices of a candidate method, not only can these conditions be easily checked, but they are often simple enough to provide insight into what choices of the free parameters are required to ensure A- and L-stability.

3 Maximal Order of Single-Eigenvalue GLMs

Before beginning the construction of DIMSEMs, we develop an upper bound on the order they might attain. The following three theorems and two corollaries apply to a larger class of methods than DIMSEMs, in that B_1 need not be diagonal. They extend to single-eigenvalue GLMs the corresponding result of Jackson and Nørsett for Runge-Kutta methods [20, Theorem 2.1].

Theorem 1 *Let $e_1(z), \ldots, e_r(z)$ be the eigenvalues of the stability matrix $M(z)$ of a GLM. Assume $e_1(z) = e^z + O(z^{p+1})$, and $e_2(z) = \cdots = e_r(z) = 0$ for all z. Then*

$$p \leq d + \delta + \sum_{i=1}^{k} r_i,$$

where B_1 has eigenvalues $\gamma_1, \ldots, \gamma_k$ with no repetitions, r_i is the size of the largest Jordan block associated with γ_i, d is the number of distinct complex nonreal eigenvalues of B_1, and δ is 1 if B_1 has at least one nonzero real eigenvalue and 0 otherwise.

Remark. We have not assumed B_1 is diagonal in the theorem above.

Proof. Let S be a matrix that transforms B_1 to its Jordan canonical form:

$$\hat{B}_1 = S^{-1} B_1 S = \operatorname{diag}(J_i),$$

where the Jordan blocks can be written as

$$J_i = \gamma_i I + E_i, \quad E_i^{r_i} = 0, \quad i = 1, \ldots, k.$$

Then the stability matrix is

$$\begin{aligned} M(z) &= A_2 + zB_2(I - zB_1)^{-1} A_1 \\ &= A_2 + z\hat{B}_2(I - z\hat{B}_1)^{-1} \hat{A}_1 \\ &= A_2 + z\hat{B}_2 X(z) \hat{A}_1, \end{aligned}$$

where $\hat{B}_2 = B_2 S$, $\hat{A}_1 = S^{-1} A_1$ and $X(z) = (I - z\hat{B}_1)^{-1}$. Also,

$$\begin{aligned} I - z\hat{B}_1 &= I - z \operatorname{diag}(\gamma_i I + E_i) \\ &= \operatorname{diag}\left((1 - \gamma_i z) I - z E_i\right), \end{aligned}$$

so that

$$X(z) = \begin{bmatrix} X_1(z) & & \\ & \ddots & \\ & & X_k(z) \end{bmatrix},$$

where

$$\begin{aligned} X_i(z) &= ((1-\gamma_i z)I - zE_i)^{-1} \\ &= \left((1-\gamma_i z)\left(I - \frac{z}{1-\gamma_i z}E_i\right)\right)^{-1} \\ &= \frac{1}{1-\gamma_i z}\left(I - \frac{z}{1-\gamma_i z}E_i\right)^{-1} \\ &= \frac{1}{1-\gamma_i z}\sum_{l=0}^{r_i-1}\left(\frac{z}{1-\gamma_i z}E_i\right)^l \end{aligned} \tag{17}$$

for $i = 1, \ldots, k$, since $E_i^{r_i} = 0$. Then the nonzero eigenvalue of $M(z)$ is

$$\begin{aligned} e_1(z) &= \mathrm{tr}(M(z)) \\ &= \mathrm{tr}(A_2) + \mathrm{tr}(z\hat{B}_2 X(z)\hat{A}_1), \end{aligned}$$

and

$$\begin{aligned} \left(z\hat{B}_2 X(z)\hat{A}_1\right)_{ll} &= z\sum_m (\hat{B}_2)_{lm}(X(z)\hat{A}_1)_{ml} \\ &= z\sum_m (\hat{B}_2)_{lm}\sum_n X(z)_{mn}(\hat{A}_1)_{nl} \\ &= z\sum_m\sum_n \alpha_{mnl}X(z)_{mn} \end{aligned} \tag{18}$$

for suitable α_{mnl}'s. From (17) however it follows that

$$zX_{mn}(z) = \sum_{q=0}^{r_m-1}\frac{z^{q+1}(1-\gamma_m z)^{r_m-(q+1)}}{(1-\gamma_m z)^{r_m}}E_{mn}^q,$$

and, using this in (18), we get

$$(z\hat{B}_2 X(z)\hat{A}_1)_{ll} = \sum_m\sum_n \alpha_{mnl}\sum_{q=0}^{r_m-1}E_{mn}^q\frac{z^{q+1}(1-\gamma_m z)^{r_m-(q+1)}}{(1-\gamma_m z)^{r_m}}.$$

Therefore, for suitable α_{iq}'s,

$$\mathrm{tr}(z\hat{B}_2 X(z)\hat{A}_1) = \sum_{i=1}^{k}\sum_{q=0}^{r_i-1}\alpha_{iq}\frac{z^{q+1}(1-\gamma_i z)^{r_i-(q+1)}}{(1-\gamma_i z)^{r_i}}$$

$$= \sum_{i=1}^{k} \frac{P_i(z)}{Q_i(z)},$$

where

$$P_i(z) = \sum_{q=0}^{r_i-1} \alpha_{iq} z^{q+1} (1-\gamma_i z)^{r_i-(q+1)}$$

has degree at most r_i, and

$$Q_i(z) = (1-\gamma_i z)^{r_i}.$$

Thus

$$e_1(z) = \mathrm{tr}(A_2) + \sum_{i=1}^{k} \frac{P_i(z)}{Q_i(z)}. \tag{19}$$

Letting $a = \mathrm{tr}(A_2)$ ($a = 1$ for a consistent method) gives

$$\begin{aligned} e_1(z) &= a + \sum_{i=1}^{k} \frac{P_i(z)}{Q_i(z)} \\ &= \frac{a \prod_i Q_i(z) + \sum_j \left(P_j(z) \prod_{i \neq j} Q_i(z) \right)}{\prod_i Q_i(z)} \\ &= \frac{P(z)}{Q(z)}, \end{aligned}$$

where

$$\deg(P(z)) \leq \sum_{i=1}^{k} r_i.$$

It then follows from Theorem 8 in [18] that, if

$$e_1(z) = e^z + O(z^{p+1}), \tag{20}$$

then

$$p \leq d + \delta + \sum_{i=1}^{k} r_i$$

as required. □

This result is used in the next theorem to bound the order of the local error of the method.

Theorem 2 *Let $e_1(z), \ldots, e_r(z)$ be the eigenvalues of the stability matrix $M(z)$ of a GLM for which $q(\phi) \neq 0$. Assume $e_2(z) = \cdots = e_r(z) = 0$ for all z and $p \geq 0$ is the largest value such that $e_1(z) = e^z + O(z^{p+1})$. Then the order of the local error of the method is at most $p+1$.*

Remark. The assumption $q(\phi) \neq 0$ is used to exclude methods for which $\hat{y}_n = 0$ for all n. This exclusion is not unreasonable, as such methods are likely to lack a suitable finishing method [6] for recovering the solution of the IVP.

Proof. We apply the method to the linear test problem $u' = \mu u$, $u(0) = 1$, for which $u(x) = e^{\mu x}$ and

$$y_{n+1} = M(z)y_n, \tag{21}$$

where $z = h\mu$. The local error is

$$l_n = y_{n+1} - \hat{y}_{n+1}, \tag{22}$$

where $y_n = \hat{y}_n$ and, for all k, $\hat{y}_k = B(q, u(x_k))$. For $u' = \mu u$, however, the elementary differentials satisfy $D(t)(u) = \mu^k u$ when $t = \tau_k$, the *tall* tree $[\cdots[\bullet]\cdots]$ of order k, and $D(t)(u) = 0$ otherwise. Therefore,

$$\hat{y}_k = \sum_{i=0}^{\infty} q(\tau_i)\frac{h^i}{i!}\mu^i u(x_k). \tag{23}$$

But $u(x_{n+1}) = e^z u(x_n)$, so that comparing (23) for $k = n$ and $k = n + 1$ gives

$$\hat{y}_{n+1} = e^z \hat{y}_n. \tag{24}$$

Combining this with (21) and (22) gives

$$l_n = M(z)\hat{y}_n - e^z \hat{y}_n. \tag{25}$$

Suppose $l_n = O(z^{q+1})$ for some $q \geq 0$. To show $q \leq p$, we require $\hat{y}_n \neq 0$. This follows from the definition of the test problem $u' = \mu u$, $u(0) = 1$, and the assumption that $q(\phi) \neq 0$, since, by (23), $\hat{y}_n = q(\phi)u(x_n) + O(z)$, so that $\hat{y}_n \neq 0$ for h (and hence z) sufficiently small. Therefore, from (25), there is a matrix $E_n = O(z^{q+1})$ such that

$$(M(z) + E_n)\,\hat{y}_n = e^z \hat{y}_n. \tag{26}$$

Since $e_1(z) = e^z + O(z^{p+1})$ with $p \geq 0$, and $e_2(z) = \cdots = e_r(z) = 0$ for all z, $e_1(z)$ is a simple eigenvalue of $M(z)$ for all z sufficiently small. From (26) and a result of Wilkinson [24, Chapter 2, Section 5], it follows that $M(z)$ has an eigenvalue $e^z + O(z^{q+1})$, which must be $e_1(z)$, the one nonzero eigenvalue of $M(z)$. That is,

$$e_1(z) = e^z + O(z^{q+1}). \tag{27}$$

But p is the largest value such that $e_1(z) = e^z + O(z^{p+1})$, so $q \leq p$, and therefore the order of the local error of the GLM is at most $p + 1$. □

The next result follows immediately from Theorems 1 and 2.

Corollary 1 *Let $e_1(z), \ldots, e_r(z)$ be the eigenvalues of the stability matrix $M(z)$ of a GLM for which $q(\phi) \neq 0$ and assume $e_2(z) = \cdots = e_r(z) = 0$ for all z. Then the order of the local error of the GLM is at most $p+1$, where*

$$p = d + \delta + \sum_{i=1}^{k} r_i,$$

B_1 has eigenvalues $\gamma_1, \ldots, \gamma_k$ with no repetitions, r_i is the size of the largest Jordan block associated with γ_i, d is the number of distinct complex nonreal eigenvalues of B_1, and δ is 1 if B_1 has at least one nonzero real eigenvalue and 0 otherwise.

We now state a theorem that bounds the order of the global error of a SEM.

Theorem 3 *Let $e_1(z), \ldots, e_r(z)$ be the eigenvalues of the stability matrix $M(z)$ of a GLM for which $q(\phi) \neq 0$. Assume $e_2(z) = \cdots = e_r(z) = 0$ for all z and $p \geq 0$ is the largest value such that $e_1(z) = e^z + O(z^{p+1})$. Then the order of the global error of the method is at most p.*

Proof. By Theorem 2, the order of the local error of the method is at most $p+1$. By [22, Theorem 5.3] for example, it follows that the order of the global error is at most $p+1$ also. We prove below by contradiction that the order of the global error is not $p+1$, so it is at most p.

To this end, apply the method to the linear test problem $u' = \mu u$, $u(0) = 1$, for which $u(x) = e^{\mu x}$ and $y_{n+1} = M(z)y_n$ for $z = h\mu$. Let $e_1(z)$ be the nonzero eigenvalue of $M(z)$. For now fix $z = h\mu$ and let $M = M(z)$ and $e_1 = e_1(z)$. Let T be a matrix which transforms M to its Jordan canonical form, $J = T^{-1}MT$, where

$$J = \begin{bmatrix} e_1 & & & & \\ & 0 & \delta_2 & & \\ & & \ddots & \ddots & \\ & & & \ddots & \delta_{r-1} \\ & & & & 0 \end{bmatrix}, \qquad \delta_i = 0 \text{ or } 1.$$

Let T_i, $i = 1, \ldots, r$, be the columns of T, known as generalised eigenvectors. Then $MT = TJ$ implies

$$\begin{aligned} MT_1 &= e_1 T_1 \\ MT_2 &= 0 \\ MT_3 &= \delta_2 T_2 \Longrightarrow M^2 T_3 = \delta_2 M T_2 = 0 \\ &\vdots \\ MT_r &= \delta_{r-1} T_{r-1} \Longrightarrow M^{r-1} T_r = \delta_{r-1} \cdots \delta_2 M T_2 = 0, \end{aligned} \tag{28}$$

so that

$$M^{k-1}T_k = 0, \quad \text{for } k = 2, \ldots, r. \tag{29}$$

Since T is nonsingular, $T_1, \ldots, T_r$ are linearly independent, so there exist scalars $\alpha_1, \ldots, \alpha_r$ such that

$$y_0 = \sum_{i=1}^{r} \alpha_i T_i.$$

Since we may multiply T by a constant, we may assume without loss of generality that $\alpha_1 = 1$. Then

$$\begin{aligned} y_n &= M^n y_0 \\ &= \sum_{i=1}^{r} \alpha_i M^n T_i \\ &= e_1^n T_1, \quad \text{for } n \geq r-1, \end{aligned} \tag{30}$$

by (28) and (29). From (24) we have $\hat{y}_{n+1} = e^z \hat{y}_n$, so that

$$\hat{y}_n = e^{nz} \hat{y}_0. \tag{31}$$

Then, for $y_0 = \hat{y}_0$, the global error is

$$\begin{aligned} g_{n-1} &= y_n - \hat{y}_n, \\ &= e_1^n T_1 - e^{nz} \hat{y}_0, \quad \text{for } n \geq r-1, \end{aligned}$$

from (30) and (31). Now allowing z to vary again and making explicit the dependencies on z gives

$$g_{n-1}(z) = e_1(z)^n T_1(z) - e^{nz} \hat{y}_0(z), \quad \text{for } n \geq r-1. \tag{32}$$

Recall that p is the largest integer such that

$$e_1(z) = e^z + O(z^{p+1}). \tag{33}$$

It therefore follows that p is the largest integer such that the following two relations hold:

$$e_1(z)^r = e^{rz} + O(z^{p+1}), \tag{34}$$

$$e_1(z)^n = e^{nz} + O(z^p), \tag{35}$$

where r is the number of external stages of the method and $nz = C$ for some constant $C > 0$ in (35).

Now we assume that the order of the global error is $p+1$ and show that this leads to a contradiction, from which it follows that the order of the global error is at most p.

To begin, let $n = r$. If the order of the global error were $p+1$ for $p \geq 0$, then it follows from (32) that

$$g_{r-1}(z) = e_1(z)^r T_1(z) - e^{rz}\hat{y}_0(z) = O(z^{p+1}). \tag{36}$$

So, as $z \to 0$, $g_{r-1}(z) \to 0$, $e^{rz} \to 1$, $e_1(z)^r \to 1$ by (34) and $\hat{y}_0(z) = B(q, u(0)) = q(\phi)u(0) + O(z) \to q(\phi)$, since $u(0) = 1$. Therefore, $T_1(z) \to q(\phi)$ also. So, in particular, $T_1(z)$ is bounded away from both 0 and ∞ as $z \to 0$, since, by the hypothesis of the theorem, $q(\phi) \neq 0$.

We can refine the last result by rewriting (36) as

$$g_{r-1}(z) = \left[e_1(z)^r - e^{rz}\right] T_1(z) + e^{rz}\left[T_1(z) - \hat{y}_0(z)\right] = O(z^{p+1}) \tag{37}$$

and by noting that, as $z \to 0$, $e_1(z)^r - e^{rz} = O(z^{p+1})$ by (34), $T_1(z)$ is bounded as $z \to 0$ and $e^{rz} \to 1$, so that

$$T_1(z) - \hat{y}_0(z) = O(z^{p+1}). \tag{38}$$

Note that (38) does not depend on n, and so holds even when the assumption that $n = r$ is removed.

Now let $nz = C$ for some constant $C > 0$ as $z \to 0$ and rewrite (32) as

$$g_{n-1}(z) = \left[e_1(z)^n - e^{nz}\right] T_1(z) + e^{nz}\left[T_1(z) - \hat{y}_0(z)\right] = O(z^{p+1}), \tag{39}$$

where we have again assumed that the order of the global error is $p+1$. Since $e^{nz} = e^C$ and, as $z \to 0$, $T_1(z)$ is bounded away from 0 and $T_1(z) - \hat{y}_0(z) = O(z^{p+1})$ by (38), (39) implies that $e_1(z)^n - e^{nz} = O(z^{p+1})$ also, contradicting (35) and thereby completing the proof. □

The next result follows immediately from Theorems 1 and 3.

Corollary 2 *Let $e_1(z), \ldots, e_r(z)$ be the eigenvalues of the stability matrix $M(z)$ of a GLM for which $q(\phi) \neq 0$ and assume $e_2(z) = \cdots = e_r(z) = 0$ for all z. Then the order of the global error of the GLM is at most p, where*

$$p = d + \delta + \sum_{i=1}^{k} r_i,$$

B_1 has eigenvalues $\gamma_1, \ldots, \gamma_k$ with no repetitions, r_i is the size of the largest Jordan block associated with γ_i, d is the number of distinct complex nonreal eigenvalues of B_1, and δ is 1 if B_1 has at least one nonzero real eigenvalue and 0 otherwise.

4 Singly Implicit DIMSEMs and DIMSEM-MRKs — Some Negative Results

Applying Corollaries 1 and 2 to DIMSEMs, for which $B_1 = \mathrm{diag}(\lambda_i)$ with $\lambda_i \in \mathbb{R}$ for $i = 1, \ldots, s$, we see that the orders of the local and global errors are at most $s+2$ and $s+1$, respectively, since $d = 0$, $\delta = 1$, each $r_i = 1$ and $k \leq s$ imply $p \leq s+1$. Moreover, the maximal values $s+2$ and $s+1$ occur only if all the λ_i's are distinct. It remains to be seen whether this order is attainable for general s.

These corollaries also show that high order, singly implicit DIMSEMs do not exist. In particular, the orders of the local and global errors of a DIMSEM with $B_1 = \lambda I$, where $\lambda \in \mathbb{R}$, are at most 3 and 2, respectively, since $d = 0$, $\delta = 1$, $k = 1$ and $r_1 = 1$ imply $p = 2$.

A consequence of these results is that we need to allow a general diagonal matrix B_1 in DIMSEMs. Our search for such methods began with the class of MRKs with $r = s$, and satisfying the simplifying assumptions $B(r)$ and $C(r-1)$. These methods have order at least r. It turns out, however, that such a DIMSEM with $r = 3$ cannot be A-stable. In fact, as we show in the remainder of this section, it has a finite stability region.

We begin by solving the order conditions. $C(r-1)$ imposes r^2 conditions on A_1, which determine it in terms of B_1, the c_i's and $q : T \to \mathbb{R}^r$, which are free parameters. (This follows rigorously from (45), and the nonsingularity of the matrix Q for MRKs in Section 8.) $B(r)$ imposes $r(r+1)$ conditions on A_2 and B_2, which determine the γ_i's and α_r in (3) and (4) in terms of the free parameters. The remaining α_i's in A_2 are determined by the requirement that the stability matrix has $r-1$ zero eigenvalues, as follows.

Because of the special form of A_2 and B_2, the stability matrix,

$$M(z) = A_2 + zB_2(I - zB_1)^{-1}A_1,$$

of an MRK has a particularly simple characteristic polynomial:

$$\begin{aligned} \varphi(w,z) &= \det(wI - M(z)) \\ &= w^r - \beta_{r-1}(z)w^{r-2} - \cdots - \beta_1(z)w - \beta_0(z), \end{aligned} \tag{40}$$

where

$$\beta_{i-1}(z) = \alpha_i + \sum_{j=1}^{s} \frac{\gamma_j a_{ji} z}{1 - \lambda_j z}, \quad i = 1, \ldots, r, \tag{41}$$

and $a_{ji} = (A_1)_{ji}$. The requirement that $M(z)$ has $r-1$ zero eigenvalues implies that φ has w^{r-1} as a factor. This requires $\beta_i(z) = 0$ for all z for $i = 0, \ldots, r-2$, from which it immediately follows from (41) that $\alpha_i = 0$ for $i = 1, \ldots, r-1$. Thus all the coefficient matrices of the method are determined in terms of c_i's and λ_i's, which are still free.

We now examine further the implications of the zero-eigenvalue condition. Substituting

$$\frac{1}{1-\lambda_j z} = \sum_{k=0}^{\infty} \lambda_j^k z^k, \quad |z| < \frac{1}{|\lambda_j|},$$

into (41) and re-arranging terms, we get

$$\beta_{i-1}(z) = \sum_{k=0}^{\infty} z^{k+1} \sum_{j=1}^{s} \gamma_j a_{ji} \lambda_j^k = 0 \quad \forall |z| < \frac{1}{\max_j |\lambda_j|}, \quad i = 1, \ldots, r-1,$$

from which it follows that

$$\sum_{j=1}^{s} \gamma_j a_{ji} \lambda_j^k = 0, \quad i = 1, \ldots, r-1, \quad k = 0, 1, 2, \ldots \tag{42}$$

Now let n be the number of distinct λ_i's, that is,

$$S = \{\lambda_1, \ldots, \lambda_s\} = \{\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n\},$$

where the $\tilde{\lambda}_i$'s are distinct. Let

$$S_i = \left\{ j : \lambda_j = \tilde{\lambda}_i \right\}.$$

Then

$$\bigcup_{i=1}^{n} S_i = \{1, \ldots, s\},$$

and it follows from (42) that

$$\begin{aligned} 0 &= \sum_{l=1}^{n} \sum_{j \in S_l} \gamma_j a_{ji} \lambda_j^k \\ &= \sum_{l=1}^{n} \tilde{\lambda}_l^k w_{il}, \quad i = 1, \ldots, r-1, \quad k = 0, 1, 2, \ldots, \end{aligned}$$

where

$$w_{il} = \sum_{j \in S_l}^{s} \gamma_j a_{ji}.$$

This implies that, for $i = 1, \ldots, r-1$,

$$\begin{bmatrix} 1 & \cdots & 1 \\ \tilde{\lambda}_1 & \cdots & \tilde{\lambda}_n \\ & \vdots & \\ \tilde{\lambda}_1^{n-1} & \cdots & \tilde{\lambda}_n^{n-1} \end{bmatrix} \begin{bmatrix} w_{i1} \\ \vdots \\ \vdots \\ w_{in} \end{bmatrix} = 0.$$

Since the $\tilde{\lambda}_i$'s are distinct, the Vandermonde matrix is non-singular, and hence the w_{ij}'s

must be zero. Thus we have that

$$\sum_{j \in S_l}^{s} \gamma_j a_{ji} = 0, \quad i = 1, \ldots, r-1, \quad l = 1, \ldots, n. \tag{43}$$

We now consider the consequences of this for various numbers of distinct λ_i's.

In particular, if all the λ_i's are distinct, then

$$\gamma_j a_{ji} = 0, \quad i = 1, \ldots, r-1, \quad j = 1, \ldots, s,$$

so that for each $j = 1, \ldots, s$, either $\gamma_j = 0$ or $a_{ji} = 0$, $i = 1, \ldots, r-1$. In the case $r = s = 3$, there is no method that satisfies these conditions. (Recall that the γ_j's and a_{ji}'s are already determined in terms of the λ_i's and c_i's.)

As noted at the beginning of this section, a DIMSEM with all λ_i's equal can be of order at most 2. Since this MRK is of order at least 3, the λ_i's cannot all be equal.

The only remaining choice is two λ_i's equal and one different. Suppose $\lambda_1 = \lambda_2 \neq \lambda_3$. (Because of symmetry, the other permutations turn out to behave identically.) In this case $S_1 = \{1, 2\}$, $S_2 = \{3\}$, and (43) has the unique solution

$$\begin{aligned} \lambda_1 &= \lambda_2 = 1/3, & \lambda_3 &= 0, \\ c_1 &= \frac{1}{3}\,\frac{21c_2 - 50}{3c_2 - 7}, & c_3 &= 2, \end{aligned}$$

with c_2 free. The remaining non-zero eigenvalue however is

$$\beta_{r-1}(z) = \frac{1}{2}\,\frac{6 + 4z + z^2}{3 - z},$$

for which $|\beta_{r-1}(z)| \to \infty$ as $|z| \to \infty$. Therefore the method has a finite stability region.

In conclusion, singly implicit DIMSEMs, as well as the subclass of DIMSEM-MRKs considered above, cannot form the basis for a class of A-stable DIMSEMs of high order. It is necessary to relax the conditions imposed in this section to find a suitable class of DIMSEMs for solving stiff problems. We chose to look next at general DIMSEM-GLMs.

5 Linking Stability and Order Conditions

To produce a method with $r - 1$ zero eigenvalues, it is necessary to zero the coefficient functions $\beta_i(z)$ of w^i in the characteristic polynomial $\varphi(w, z)$ in (40), for $i = 0, \ldots, r-2$. As each $\beta_i(z)$ is a rational function of z, this amounts to zeroing the numerator polynomial, which involves setting all the coefficients of each polynomial to zero. These coefficients are complicated nonlinear functions in the coefficients of the method. Solving these equations, together with the simplified order conditions, is a costly process when done algebraically

to facilitate later choice of the remaining free parameters for A-stability. The process is eased somewhat by transforming the stability matrix in such a way that the simplified order conditions can be incorporated into it. Then the $r-1$ eigenvalues can be set to zero, with the assurance that a method of the desired order can be recovered later. To do this, we choose the simplifying assumptions $A(r-1)$, $B(r-1)$ and $C(r-1)$, because, from (12) and (13), $B(r-1)$ and $C(r-1)$ can be conveniently written in matrix form as follows.

$$B(r-1) \quad : \quad A_2Q + B_2W = QP, \tag{44}$$

$$C(r-1) \quad : \quad A_1Q + B_1W = V, \tag{45}$$

where

$$\begin{aligned}
Q &= [q_0, \ldots, q_{r-1}] \in \mathbb{R}^{r \times r}, \\
q_k &= q(\tau^k) = q(t) \quad \forall t \ni \rho(t) = k, \quad k = 0, \ldots, r-1, \\
V_{ij} &= c_i^{j-1}, \quad V \in \mathbb{R}^{s \times r}, \\
W_{ij} &= (j-1)c_i^{j-2}, \quad W \in \mathbb{R}^{s \times r}, \\
P_{ij} &= \left\{ \begin{array}{cc} \left(\begin{array}{c} j-1 \\ i-1 \end{array} \right), & j \geq i \\ 0, & \text{otherwise} \end{array} \right\}, \quad P \in \mathbb{R}^{r \times r},
\end{aligned}$$

and 0^0 is taken to be 1. In the following, we need to assume that Q is nonsingular. Let $\bar{B}_2 = Q^{-1}B_2$, and consider the transformed stability matrix

$$\begin{aligned}
\bar{M}(z) &= Q^{-1}M(z)Q \\
&= Q^{-1}\left(A_2 + zB_2(I - zB_1)^{-1}A_1\right)Q \\
&= Q^{-1}(QP - B_2W) + zQ^{-1}B_2(I - zB_1)^{-1}(V - B_1W) \\
&= P - \bar{B}_2W + z\bar{B}_2(I - zB_1)^{-1}(V - B_1W) \\
&= P + \bar{B}_2\left[z(I - zB_1)^{-1}(V - B_1W) - W\right] \\
&= P + \bar{B}_2\left[(I - zB_1)^{-1}\left(zV - zB_1W - (I - zB_1)W\right)\right] \\
&= P + \bar{B}_2(I - zB_1)^{-1}(zV - W).
\end{aligned} \tag{46}$$

If we define

$$U = \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & r-1 \\ & & & 0 \end{bmatrix},$$

then $VU = W$ and

$$\bar{M}(z) = P + \bar{B}_2(I - zB_1)^{-1}V(zI - U). \tag{47}$$

The matrix $\bar{M}(z)$ has the same eigenvalues as $M(z)$, but, by incorporating the order conditions (44) and (45), the A_1 and A_2 matrices have been eliminated. The problem of finding a DIMSEM has now been reduced to

- picking values for the free parameters λ_i, c_i, and $\bar{B}_2$, so that $\bar{M}(z)$ has $r-1$ zero eigenvalues, and
- recovering the remaining method coefficients using $B_2 = Q\bar{B}_2$ and the order conditions

$$A_1 = (V - B_1 W)Q^{-1} \tag{48}$$
$$A_2 = (QP - B_2 W)Q^{-1}. \tag{49}$$

The resulting method (if it exists and is stable) has order at least $r-1$ and stage order at least $r-1$.

6 A Class of A-stable Diagonal Methods (ADMs)

We now describe an interesting class of methods which, although not DIMSEMs, are singly strictly diagonally implicit and A-stable. (In Butcher's classification, Fig. 2.1, they are type-4 DIMSIMs.)

If $\lambda_i = \lambda$ for $i = 1, \ldots, s$, then the transformed stability matrix (47) simplifies to

$$\bar{M}(z) = P + \frac{1}{1-\lambda z} T(zI - U),$$

where $T = \bar{B}_2 V$. We choose T below and then recover $\bar{B}_2 = TV^{-1}$. This requires that $r = s$ and the c_i's are distinct so that V is nonsingular. If we let T be upper triangular, $\bar{M}(z)$ is also upper triangular, and so the eigenvalues are simply the diagonal elements

$$e_i(z) = 1 + \frac{T_{ii} z}{1-\lambda z}, \quad i = 1, \ldots, r. \tag{50}$$

For $\lambda \in \mathbb{R}^+$ and any choice of

$$T_{ii} \in (0, 2\lambda), \quad i = 1, \ldots, r, \tag{51}$$

it follows that

$$|e_i(z)| < 1 \quad \forall z \in \mathbb{C}^- \setminus \{0\}, \quad i = 1, \ldots, r.$$

However, $e_i(0) = 1$ for $i = 1, \ldots, r$, so the method will be A-stable if and only if $\bar{M}(0)$ is diagonalisable. If we choose

$$T_{ij} = \frac{1}{j} \begin{pmatrix} j \\ i-1 \end{pmatrix}, \quad i = 1, \ldots, r-1, \quad j = i, \ldots, r-1, \tag{52}$$

then $\bar{M}(0) = P - TU = I$ is diagonal. Moreover, since $T_{ii} = 1$ for $i = 1, \ldots, r-1$, (51) is satisfied if

$$\lambda > \max(1/2, T_{rr}/2).$$

Thus, we have found a class of A-stable, singly strictly diagonally implicit GLMs of order and stage order $r-1$ for any $r \geq 1$. The c_i's, λ, T_{rr}, and q are still free. If we choose $\lambda = T_{rr} = 1$, then (50) reduces to

$$e_i(z) = \frac{1}{1-z}, \quad i = 1, \ldots, r,$$

from which it follows immediately that $|e_i(z)| \to 0$ as $|z| \to \infty$. This L-stable class of ADMs has the c_i's and q free.

Interestingly, recovering the original coefficient matrix A_2 using (49) gives

$$\begin{aligned} A_2 &= (QP - Q\bar{B}_2 W)Q^{-1} \\ &= (QP - QTV^{-1}VU)Q^{-1} \\ &= Q(P - TU)Q^{-1} \\ &= QIQ^{-1} \\ &= I. \end{aligned}$$

This is also the design choice made in the DIMSIMs of [8, 9, 10, 11], of which the type-4 variants are also singly strictly diagonally implicit. The DIMSIMs however have higher orders and the remaining coefficients are chosen differently.

7 A Class of DIMSEMs

This section contains the main contribution of this report. We introduce two theorems — Theorems 5 and 6 — which define a class of DIMSEMs of order $r-1$, for any $r \geq 2$. (The proofs of these theorems, because they are so long, appear separately in Appendices B and C, respectively.) The choice of method coefficients made in Theorem 5 arose as a generalisation of patterns observed in methods of orders 2–6, which were derived by solving the zero-eigenvalue equations in Maple. The computational feasibility of solving these equations depended on the simplification achieved by taking all the internal abscissae c_i's to be equal. Although this results in the Vandermonde matrix V being singular, this choice is acceptable, since our technique described in Section 5 for determining the coefficients of a GLM satisfying the zero-eigenvalue equations does not require V to be nonsingular.

We initially applied this somewhat unusual choice of parameters with all the c_i's equal to one, resulting in the creation of A-stable DIMSEMs up to order four, but greater success was obtained by setting all the c_i's to zero. In this case, the Vandermonde matrix V simplifies

to

$$V = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ \vdots & & \vdots & \\ 1 & 0 & \cdots & 0 \end{bmatrix},$$

so that the quantity $V(zI - U)$ appearing in the transformed stability matrix

$$\bar{M}(z) = P + \bar{B}_2(I - zB_1)^{-1}V(zI - U)$$

becomes

$$V(zI - U) = \begin{bmatrix} z & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots & \\ z & -1 & 0 & \cdots & 0 \end{bmatrix}.$$

The transformed stability matrix itself becomes

$$\bar{M}(z) = P + \begin{bmatrix} za_1(z) & -a_1(z) & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots & \\ za_r(z) & -a_r(z) & 0 & \cdots & 0 \end{bmatrix}, \tag{53}$$

where

$$a_i(z) = \sum_{k=1}^{s} \frac{b_{ik}}{1 - \lambda_k z}, \quad i = 1, \ldots, r, \tag{54}$$

$b_{ik} = (\bar{B}_2)_{ik}$ and $B_1 = \mathrm{diag}(\lambda_1, \ldots, \lambda_s)$. This form of $\bar{M}(z)$ is simple enough to enable direct algebraic computation of the characteristic polynomial up to $r = 5$ (corresponding to order $r - 1 = 4$) using Maple. The advantage of this technique, however, is that relationships between elements of the $\bar{B}_2$ matrix of the resulting DIMSEMs allow extension to methods of higher order.

When solving the zero-eigenvalue equations using Maple, certain patterns were observed. When $s = r - 1$, it appeared that there is always a unique solution which leaves the λ_i's free. There also appeared to be a powerful recurrence expressing the rest of the $\bar{B}_2$ matrix in terms of its last row. These observations gave rise to Theorem 5 in Appendix B, the proof of which relies on an expression for the characteristic polynomial of the transformed stability matrix given by Theorem 6 in Appendix C.

As explained in Section 4, the characteristic polynomial associated with a DIMSEM has the form

$$\begin{aligned} \varphi(w, z) &= \det(wI - M(z)) \\ &= w^r - e_1(z)w^{r-1} - \beta_{r-2}(z)w^{r-2} - \cdots - \beta_1(z)w - \beta_0(z), \end{aligned}$$

where

$$\beta_i(z) = \frac{P_i(z)}{Q_i(z)} = 0 \quad \text{for } i = 0, \ldots, r-2 \text{ and all } z,$$

P_i and Q_i are polynomials and $e_1(z)$ is a rational function of z. The requirement that $M(z)$ have $r-1$ zero eigenvalues is equivalent to $\beta_0(z) = \cdots = \beta_{r-2}(z) = 0$ for all z, which in turn is equivalent to $P_0(z) = \cdots = P_{r-2}(z) = 0$ for all z, which in turn is equivalent to having all the coefficients of $P_i(z)$ equal to zero for $i = 0, \ldots, r-2$. This last condition is what we have been calling the zero-eigenvalue equations. Note $e_1(z)$ is the remaining nonzero eigenvalue of $M(z)$, so it governs the stability of the method.

A-stability is easy to check, even without computing $e_1(z)$ from the characteristic polynomial. This is important, because algebraic computation of the characteristic polynomial is too complicated to be feasible for high orders. From (53), (54), and the zero-eigenvalue property, it follows that

$$\begin{aligned} e_1(z) &= \operatorname{tr}(\bar{M}(z)) \\ &= r + z a_1(z) - a_2(z) \\ &= r + \sum_{k=1}^{s} \frac{z b_{1k} - b_{2k}}{1 - \lambda_k z}. \end{aligned}$$

This can be expressed in the form

$$e_1(z) = \frac{P(z)}{Q(z)}, \tag{55}$$

and the associated E-polynomial (16) constructed. Recall that a sufficient condition for A-stability is that the coefficients of the E-polynomial are negative and the λ_i's are positive. It is sometimes possible to solve these inequalities directly for the remaining free parameters in the low-order methods. The procedure followed to construct L-stable DIMSEMs up to order 6 for numerical testing is described in the next two sections.

8 A Class of L-Stable DIMSEMs

Until now, it has not been necessary to specify the true-value function q. The only restrictions on q have been the simplifying assumption $A(r-1)$, which states that $q(t)$ depends only on the order of the tree t, up to order $r-1$, and the requirement that the matrix Q be nonsingular. Both of the common choices of true-value function, based on Nordsieck and multistep implementations, satisfy these requirements. Because our methods satisfy $A(r-1)$, we will write q_k for $q(t)$, where t is any tree of order $k \leq r-1$. Also, let e_k be the vector in $\mathbb{R}^r$ with 1 as the k-th component and 0 elsewhere. Then in Nordsieck-type methods (1), q is given by

$$q_k = e_{k+1}, \quad k = 0, \ldots, r-1,$$

so that

$$Q = I_r \in \mathbb{R}^{r \times r}.$$

For multistep GLMs,

$$q_k = d^k, \quad k = 0, \ldots, r-1,$$

where $d \in \mathbb{R}^r$ is the vector of external abscissae, and d^k is taken componentwise with $0^0 = 1$. The corresponding matrix Q is

$$Q = [d^0, d^1, \ldots, d^{r-1}] \in \mathbb{R}^{r \times r}.$$

This corresponds to the external stages approximating the solution at various points,

$$y_{n,i} \approx u(x_n + d_i h), \quad i = 1, \ldots, r.$$

In deriving specific methods from our classes for testing purposes, we chose the multistep-type true-value function, and used the same external abscissae

$$d_i = i - r, \quad i = 1, \ldots, r$$

as used in MRKs. Unlike MRKs, however, our A_2 and B_2 are general matrices, and not the restricted forms (3) and (4).

The first step in the creation of the methods was the algebraic solution of the zero-eigenvalue equations using the techniques of the previous section. This produced classes of DIMSEMs of order $p = 2, \ldots, 6$, $p = r - 1 = s$, with the λ_i's as free parameters. Then the E-polynomial was formed and A- and L-stability investigated.

8.1 Choice of Free Parameters for the DIMSEMs

The DIMSEMs of order $s = r - 1$ defined by Theorem 5 have free parameters $\lambda_1, \ldots, \lambda_s$, where $B_1 = \mathrm{diag}(\lambda_1, \ldots, \lambda_s)$. The values of $\lambda_1, \ldots, \lambda_s$ were chosen to make the methods L-stable and to achieve a good compromise between small error coefficients and reasonable-sized entries in the coefficient matrices A_1, A_2, and B_2.

The error coefficient function $e(t)$ defined in (10) is a vector-valued function, the i-th component of which gives the local error associated with the tree t for the i-th external stage. To optimize the method, we used the quantities T_1, T_2 and T_3, where

$$T_k = \frac{1}{(p+k)!} \max \{ \| e(t) \|_\infty : \rho(t) = p + k \}, \quad k = 1, 2, 3, \ldots$$

and p is the order of the method. These are the principal, secondary, tertiary etc. normalised, maximum-norm error coefficients associated with the method. We wrote a Maple program, incorporating a data structure for rooted trees, to compute algebraic expressions for the

error coefficients. All computation involved in the choice of the free parameters was done algebraically using Maple.

The first step in the procedure was to determine λ_s in terms of $\lambda_1, \ldots, \lambda_{s-1}$ so that $\deg(P) < \deg(Q)$, where the one nonzero eigenvalue of $M(z)$ is $e_1(z) = P(z)/Q(z)$. This ensures that, if the method is A-stable, it will also be L-stable. The next step was to heuristically choose values for $\lambda_3, \ldots, \lambda_{s-1}$, leaving at most λ_1 and λ_2 to be selected based on the 3-dimensional plots described below. To achieve A-stability, the region where all the coefficients of the E-polynomial (16) are negative, and the region where $\lambda_i > 0$, $i = 1, \ldots, s$, were plotted. The intersection of these regions indicates choices of the free parameters which result in an A-stable method, and hence an L-stable one, because of the earlier choice of λ_s. Then the error coefficients T_1, T_2 and T_3, and the maxcf function were plotted, where

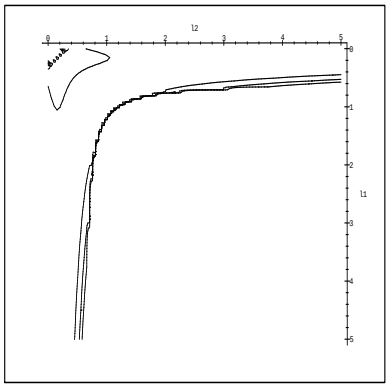
$$\text{maxcf} = \max\{\|A_1\|, \|B_1\|, \|A_2\|, \|B_2\|\}, \tag{56}$$

$$\|A\| = \{\max|A_{ij}| : i, j\}. \tag{57}$$

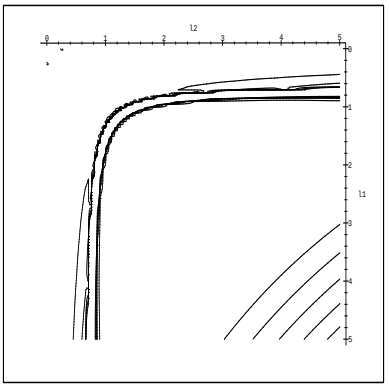
Finally, a line in (λ_1,λ_2)-space was selected which appeared to pass through an L-stable region with a favourable compromise between error coefficients and maxcf. Plots of the various functions along this line were then made, from which the final values for λ_1 and λ_2 were chosen. Often, with the high-order methods, the initial heuristic choice of λ_i's did not permit all the objectives to be satisfied, in which case the λ_i's were modified and further plots made. This was repeated if necessary until a suitable choice was found.

Fig. 2 shows a series of plots for the fifth order DIMSEM. Because they have been reduced from their original large size and rendered as monochrome contour plots instead of interactively viewable, colour, 3-dimensional surfaces, it is not likely that much quantitative information can be derived from them. They are included only to illustrate the parameter-selection process. The first three rows are contour plots with λ_1 on the vertical axis and λ_2 on the horizontal axis. In the first and second rows, $\lambda_1, \lambda_2 \in [0, 5]$, while in the third row (a magnified view of the second row), $\lambda_1, \lambda_2 \in [0, 1]$. For this method, T_1, T_2, and T_3 (first row) show only small variation, which is fortunate because keeping maxcf reasonable while achieving L-stability is quite restrictive on λ_1 and λ_2. The dark areas in the maxcf plots are steep increases in maxcf due to singularities in the method coefficients corresponding to a confluence of two λ_i's. The method is L-stable at the intersection of the shaded regions in the second and third plots in the third line. The value $\lambda_2 = 0.29$ was chosen as the line passing through the L-stable region as well as through an area of small maxcf. The plots in the last row have $\lambda_1 \in [0, 1]$ on the horizontal axis, while λ_2 is fixed at 0.29. The T_i's are the essentially constant lines in the left plot. We then chose $\lambda_1 = 0.37$ for the smallest maxcf in the L-stable interval shown in the right plot.

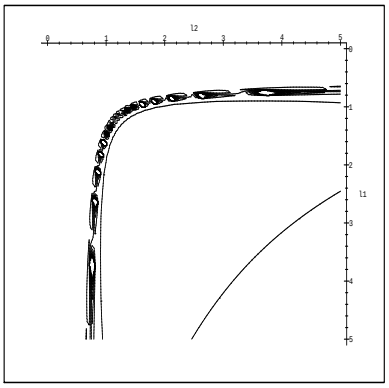
The chosen values for the free parameters, along with the resulting error coefficients and maxcf (56) are given in Table 1. The λ_i's shown are exact, while the T_i's and maxcf are rounded.



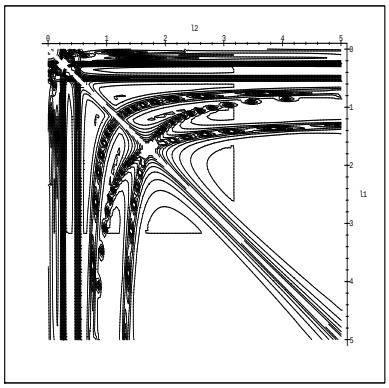
T_1 vs. (λ_2, λ_1)



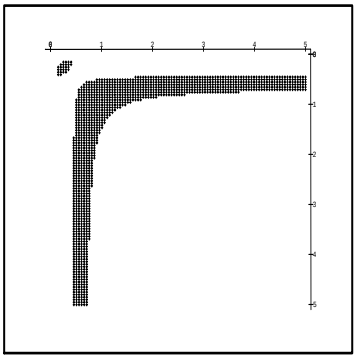
T_2 vs. (λ_2, λ_1)



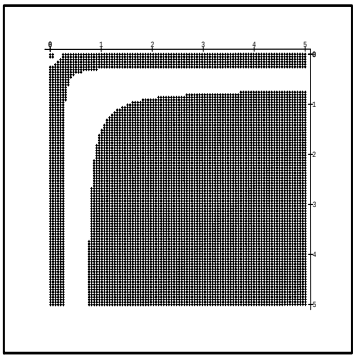
T_3 vs. (λ_2, λ_1)



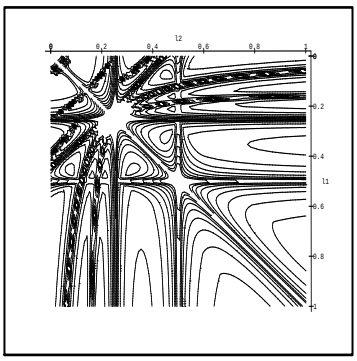
$\log_{10}$ maxcf vs. (λ_2, λ_1)



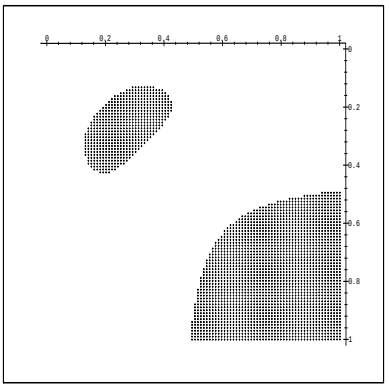
E-poly coeffs < 0 vs. (λ_2, λ_1)



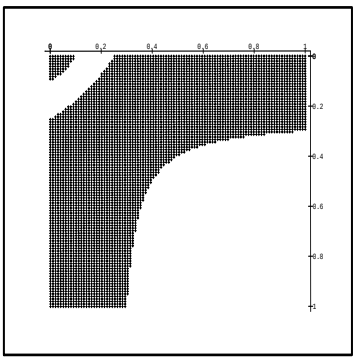
$\lambda_5 > 0$ vs. (λ_2, λ_1)



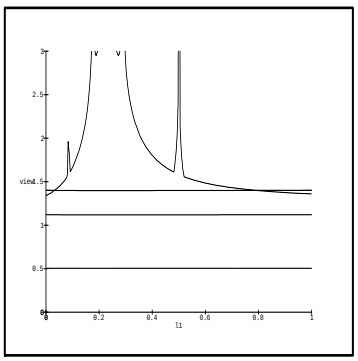
$\log_{10}$ maxcf vs. (λ_2, λ_1)



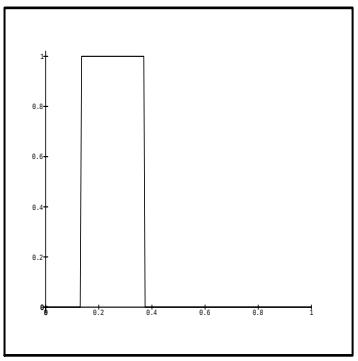
E-poly coeffs < 0 vs. (λ_2, λ_1)



$\lambda_5 > 0$ vs. (λ_2, λ_1)



T_1, T_2, T_3, $\log_{10}$ maxcf vs. λ_1



L-Stable vs. λ_1

Figure 2: Graphs for Choosing the Free Parameters for the Fifth Order DIMSEM.

order	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	T_1	T_2	T_3	T_4	T_5	T_6	maxcf
2	.49	$\frac{1}{51}$					.33	.33	.26	.12	.045	.020	2
3	.25	.43	$\frac{79}{87}$				.44	.51	.44	.27	.14	.13	5
4	1.3	.27	1.0	$\frac{1337}{2710}$			.46	.87	.95	.80	.92		8
5	.37	.29	.25	.50	$\frac{654}{4981}$		.50	1.1	1.4	1.3			85
6	.71	.095	.25	.50	.75	$\frac{5086}{15879}$	.53	1.4	2.1				33

Table 1: Choice of Free Parameters and Error Coefficients for the DIMSEM Class.

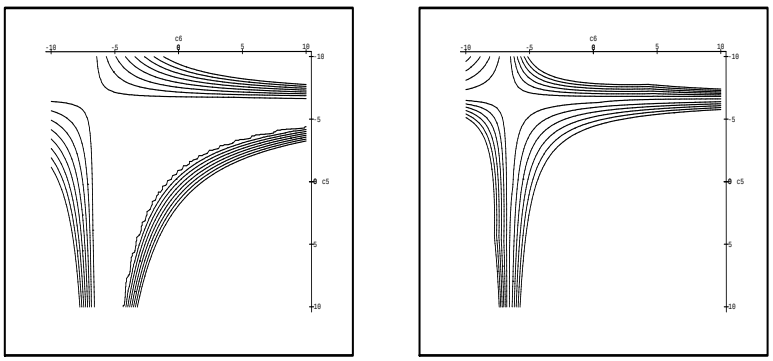
	DIMSEMs					Burrage's MRKs					Gauss/Radau-IA IRKs				
order	r	s	T_1	T_2	T_3	r	s	T_1	T_2	T_3	r	s	T_1	T_2	T_3
2	3	2	.33	.33	.26	2	1	.33	.33	.23	1	1	.083	.17	.18
3	4	3	.44	.51	.44	2	2	.37	1.1	2.1	1	2	.014	.031	.037
4	5	4	.46	.87	.95	3	2	.45	1.4	2.8	1	2	1.3E-3	2.8E-3	2.9E-3
5	6	5	.50	1.1	1.4	4	3	1.4	9.7	39	1	3	1.4E-4	3.0E-4	3.3E-4
6	7	6	.53	1.4	2.1	5	4	.49	5.3	30	1	3	9.9E-6	2.0E-5	7.9E-5

Table 2: Comparison of Error Coefficients of DIMSEMs, Burrage and Chipman's MRKs, and Gauss/Radau-IA IRKs.

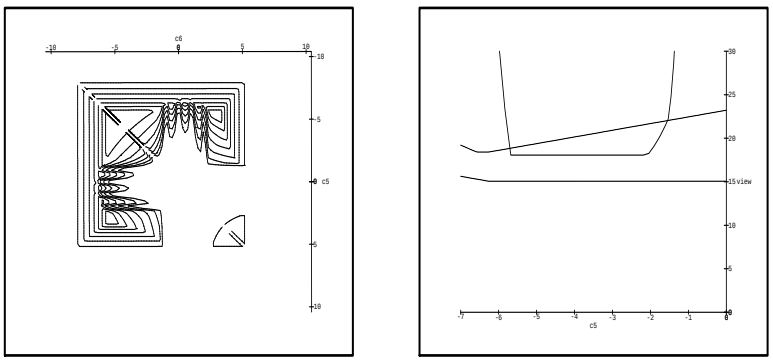
The error coefficients of the L-stable DIMSEMs were then compared with those of two other classes of A-stable methods, the MRKs of Burrage and Chipman [3] and the Gauss and Radau-IA IRKs (see, for example, [7]). The MRKs are implicit with a lower-triangular B_1 matrix, while the Gauss/Radau formulas are fully implicit Runge-Kutta methods. In Burrage and Chipman's methods, the choices of the free parameters used were those given on page 410 of their paper, which were used in their numerical testing. The results are shown in Table 2. Most of the error coefficients of the DIMSEMs are an improvement over those of the MRKs, and the ones which are not are only slightly worse. The improvements in T_2 and T_3 are quite significant. Both the DIMSEMs and MRKs have much larger error coefficients than the corresponding Gauss or Radau IRKs, however.

9 Choice of Free Parameters for the ADMs

ADMs of order $r-1$ with $r=s$ are described in Section 6. Like the DIMSEMs derived in the previous section, the specific ADMs given in this section are based on a multivalue-type true-value function. The free parameters λ and T_{rr} are both set to 1, giving ADMs which are L-stable for all values of $c_1, \ldots, c_s$. It turns out that the principal error coefficients, and hence T_1, are fixed for each method, independent of the free parameters. The selection of the c_i's was performed in a manner similar to that of the λ_i's for the DIMSEMs (Section 8.1),



T_1 vs. (c_6, c_5) T_2 vs. (c_6, c_5)



$\log_{10}$ maxcf vs. (c_6, c_5) T_2, T_3, maxcf / 2 vs. c_5

Figure 3: Graphs for Choosing the Free Parameters of the Fifth Order ADM.

except that only T_2, T_3, and the maxcf function (56) had to be considered due to the fixed T_1 and inherent L-stability.

To illustrate the process, Fig. 3 shows a series of plots for the fifth order ADM. The first three are contour plots with c_5 on the vertical axis and c_6 on the horizontal axis, covering the interval $[-10, 10]$. The contours in T_1 and T_2 show hills rising from a central valley. The line $c_6 = -5.7$ was chosen as passing near the minima of the T_i's and maxcf. The final plot has $c_5 \in [-7, 0]$ on the horizontal axis with $c_6 = -5.7$. The U-shaped function is maxcf/2 and the others are T_1 and T_2. We chose $c_5 = -5.67$ to minimise (roughly) T_1 and T_2 in the plateau region of maxcf.

The results of the optimisation are shown in Table 3. The values given for the c_i's are exact, while those for the T_i's are rounded. Observe that the error coefficients of these ADM methods are very large in comparison to the other methods considered. The size of the coefficient matrix entries, maxcf, also seems to increase more quickly with the order of the method for ADMs than for DIMSEMs. This might limit the maximum order of practical methods of this class, unless a way is found to reduce this coefficient growth. Nevertheless, the ADM methods found perform well in numerical testing.

order	c_1	c_2	c_3	c_4	c_5	c_6	c_7	T_1	T_2	T_3	T_4	T_5	T_6	maxcf
2	0	1	-1.6					.83	.63	.49	.43	.37	.39	2
3	0	1	-2.26	-1.2				1.8	.92	1.36	.96	.65	.57	5
4	0	1	-1	-2.85	-3.81			4.2	5.6	5.3	3.7	2.6		10
5	0	1	-1	2	-5.67	-5.7		10	15	19	15			36
6	0	1	-1	2	-2	-6.66	-3	25	50	68				224

Table 3: Choice of Free Parameters and Error Coefficients for the ADM Class.

10 Numerical Testing

Preliminary numerical testing was performed to verify the accuracy and stability of the methods derived in the previous sections. Because we have yet to develop error estimators and stepsize-changing strategies for these methods, the testing was carried out with fixed-stepsize implementations. As this is not ideal for methods intended for stiff problems, the testing was not exhaustive, but rather was intended to guard against errors and oversights in the theoretical work.

Testing was done using double precision in FORTRAN on a Sun4. The coefficient matrices of the methods were computed exactly using Maple, and then converted into floating point numbers of sufficient accuracy for the testing. A Newton iteration (6) was used to solve for the internal stages. For the DIMSEMs, $c_1 = \cdots = c_s = d_r = 0$, so that $y_{n,r}$ provides a good initial guess for each $Y_{n+1,i}$. The ADM class, however, has nonzero c_i's, so the $y_{n,i}$ with the smallest distance $|d_i - (c_j + 1)|$ was used as an initial guess for $Y_{n+1,j}$, $j = 1, \ldots, s$. In many cases this is not as good an initial guess as the DIMSEM one, but it proved to be adequate for convergence provided the stepsize was not too large. The convergence criterion used for the Newton iteration was

$$||Y_n^{(k-1)} - Y_n^{(k)}||_\infty \leq 10^{-15},$$

where $Y_n^{(k)}$ is the k-th iterate approximating Y_n.

The integrations were started with the exact solution to the problem, and both local and global errors were measured. The test problems were integrated several times, halving the stepsize each time, and the apparent (local or global) order $\tilde{p}$ was computed from each pair of consecutive runs using the formula

$$\tilde{p} = \log_2(e_{2h}/e_h),$$

where e_h is the (local or global) error corresponding to stepsize h. The local error measured was the maximum over all n of $||l_n||_\infty$, where l_n is defined in (9). This was only possible because an analytic solution was available for the computation of $\hat{y}_{n+1}$. This measurement of the local error was used only to verify agreement with the theory, and is not possible in a practical solver. The maximum global error measured was the maximum of the global errors

on each step for each external stage, and the endpoint global error was the maximum of the global errors on the last step for each external stage.

Two types of test problems were used. The first is a nonlinear problem chosen for the presence of all the elementary differentials $D(t)$ in the Butcher series, as well as the availability of an analytic solution. It is

$$y' = \omega \sin y,$$

which for the initial condition $y(x_0) = y_0$ satisfies

$$y(x) = 2 \arctan \left(e^{\omega(x-x_0)} \tan \frac{y_0}{2} \right).$$

This problem was integrated on both $[0, 1]$ and $[0, 100]$ with initial condition $y(0) = 1$ and $\omega = -1$. The short interval was used to demonstrate correct order behaviour, while the long interval was used to verify stability on a stiff problem.

The results for the DIMSEMs on $[0, 1]$ are shown in Section 10.1.1. All the DIMSEM methods produce the expected local order on this problem. The order 2, 3, and 4 DIMSEMs show a global order one less than the local order, while the order 5 and 6 DIMSEMs exhibit a global order one higher than expected in general, and equal to the local order. The results for the DIMSEMs on $[0, 100]$ are shown in Section 10.1.2. The results are similar to those for the interval $[0, 1]$, except that the endpoint global order for the sixth order DIMSEM is rather erratic. The endpoint global errors remain extremely small for all the DIMSEMs. This demonstrates that the methods are stable, and the stepsize is not being significantly restricted by the stiffness of the problem.

The results for the ADM methods on $[0, 1]$ are shown in Section 10.2.1. Possibly due to their larger error coefficients, the ADM methods approach their expected local and global orders more clearly before the error becomes limited by roundoff. All the ADMs produce the expected local order, and show a global order one less than the local order. The results for the ADM methods on $[0, 100]$ are shown in Section 10.2.2. The methods again produce the expected local order, and a maximum global order one less than the local order. The endpoint global errors appear to be roundoff-limited, and so the corresponding orders are not meaningful. The small endpoint global errors however indicate the methods are stable.

The second test problem is that of Prothero and Robinson [21],

$$y' = g'(x) + \omega \left(y - g(x) \right),$$

where g is a given function. With the initial condition $y(0) = g(0)$, it has the solution $y(x) = g(x)$, but can be made arbitrarily stiff by choosing $\omega \ll 0$. We used $g(x) = \sin(x)$ and $\omega = -10^6$, making the problem stiff but non-dissipative, allowing the computation of meaningful apparent orders. This problem is used to investigate the phenomenon of order-reduction, which tends to make methods perform with less than their asymptotic order if

larger stepsizes are used. There is evidence that the observed order of a GLM can be expected to approximate its stage order [3].

The results for the DIMSEMs on this problem are shown in Section 10.1.3. Each DIMSEM shows the expected local order. The global order on this problem is one higher than expected in general, and equal to the local order. The order-6 DIMSEM endpoint global order suffers roundoff contamination, but all other observed orders are quite clear. Order-reduction (a reduced order with larger stepsizes) is not evident.

The results for the ADM methods on this problem are shown in Section 10.2.3. The ADMs behave similarly to the DIMSEMs on this problem, with the local order as expected and the global order equal to the local order. Except for the endpoint global order of the fifth order ADM, all the observed orders are quite clear.

10.1 Test Results for the DIMSEMs

10.1.1 Problem 1

This subsection gives the test results for the problem

$$y' = -\sin y, \quad y(0) = 1,$$

on the interval $[0, 1]$, for each of the DIMSEM methods. These results are discussed at the start of Section 10.

METHOD DIMSEM2L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	2.21e-01		2.21e-01		2.21e-01	
5.00e-01	2.31e-02	3.26e+00	2.31e-02	3.26e+00	1.45e-02	3.93e+00
2.50e-01	2.26e-03	3.35e+00	2.26e-03	3.35e+00	2.17e-03	2.74e+00
1.25e-01	2.51e-04	3.17e+00	2.54e-04	3.15e+00	2.17e-04	3.32e+00
6.25e-02	2.98e-05	3.07e+00	3.22e-05	2.98e+00	1.64e-05	3.72e+00
3.12e-02	3.65e-06	3.03e+00	5.66e-06	2.51e+00	5.66e-06	1.54e+00
1.56e-02	4.51e-07	3.01e+00	1.59e-06	1.83e+00	1.59e-06	1.83e+00
7.81e-03	5.62e-08	3.01e+00	4.17e-07	1.93e+00	4.17e-07	1.93e+00
3.91e-03	7.01e-09	3.00e+00	1.07e-07	1.97e+00	1.07e-07	1.97e+00
1.95e-03	8.75e-10	3.00e+00	2.70e-08	1.98e+00	2.70e-08	1.98e+00
9.77e-04	1.09e-10	3.00e+00	6.79e-09	1.99e+00	6.79e-09	1.99e+00

METHOD DIMSEM3L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	1.00e-01		1.00e-01		1.00e-01	
5.00e-01	3.46e-02	1.54e+00	2.71e-02	1.89e+00	2.71e-02	1.89e+00
2.50e-01	2.44e-03	3.82e+00	2.41e-03	3.49e+00	7.09e-04	5.26e+00
1.25e-01	1.64e-04	3.90e+00	1.64e-04	3.87e+00	3.64e-05	4.28e+00
6.25e-02	1.02e-05	4.01e+00	1.02e-05	4.01e+00	4.11e-06	3.15e+00
3.12e-02	6.28e-07	4.02e+00	7.24e-07	3.81e+00	4.82e-07	3.09e+00
1.56e-02	3.89e-08	4.01e+00	7.74e-08	3.22e+00	5.79e-08	3.06e+00
7.81e-03	2.42e-09	4.01e+00	9.11e-09	3.09e+00	7.08e-09	3.03e+00
3.91e-03	1.51e-10	4.00e+00	1.11e-09	3.04e+00	8.76e-10	3.02e+00
1.95e-03	9.42e-12	4.00e+00	1.37e-10	3.02e+00	1.09e-10	3.01e+00
9.77e-04	5.88e-13	4.00e+00	1.68e-11	3.03e+00	1.32e-11	3.04e+00

METHOD DIMSEM4L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	1.17e-01		1.17e-01		1.17e-01	
5.00e-01	4.47e-02	1.39e+00	4.47e-02	1.39e+00	5.58e-03	4.39e+00
2.50e-01	1.31e-03	5.09e+00	1.31e-03	5.09e+00	6.80e-04	3.04e+00
1.25e-01	3.04e-05	5.43e+00	2.04e-05	6.00e+00	1.05e-05	6.02e+00
6.25e-02	9.48e-07	5.00e+00	9.25e-07	4.46e+00	9.25e-07	3.50e+00
3.12e-02	2.94e-08	5.01e+00	6.02e-08	3.94e+00	5.99e-08	3.95e+00
1.56e-02	9.15e-10	5.01e+00	3.78e-09	3.99e+00	3.73e-09	4.01e+00
7.81e-03	2.85e-11	5.00e+00	2.36e-10	4.00e+00	2.31e-10	4.01e+00
3.91e-03	8.90e-13	5.00e+00	1.47e-11	4.00e+00	1.44e-11	4.01e+00
1.95e-03	2.80e-14	4.99e+00	9.19e-13	4.00e+00	8.95e-13	4.01e+00
9.77e-04	1.33e-15	4.39e+00	6.33e-14	3.86e+00	6.09e-14	3.88e+00

METHOD DIMSEM5L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	3.68e-01		3.68e-01		3.68e-01	
5.00e-01	4.28e-02	3.10e+00	5.09e-02	2.85e+00	5.09e-02	2.85e+00
2.50e-01	1.35e-03	4.99e+00	7.98e-04	6.00e+00	3.11e-05	1.07e+01
1.25e-01	2.46e-05	5.77e+00	2.46e-05	5.02e+00	3.99e-06	2.96e+00
6.25e-02	3.54e-07	6.12e+00	3.54e-07	6.12e+00	5.52e-08	6.17e+00
3.12e-02	4.84e-09	6.19e+00	4.84e-09	6.19e+00	7.51e-10	6.20e+00
1.56e-02	6.92e-11	6.13e+00	6.92e-11	6.13e+00	1.06e-11	6.15e+00
7.81e-03	1.03e-12	6.07e+00	1.03e-12	6.07e+00	1.52e-13	6.12e+00
3.91e-03	1.73e-14	5.89e+00	1.68e-14	5.94e+00	1.29e-14	3.56e+00
1.95e-03	1.55e-15	3.48e+00	2.95e-14	-8.17e-01	2.68e-14	-1.06e+00
9.77e-04	2.00e-15	-3.63e-01	4.36e-14	-5.63e-01	4.16e-14	-6.35e-01

METHOD DIMSEM6L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	6.21e-01		6.21e-01		6.21e-01	
5.00e-01	7.23e-02	3.10e+00	7.84e-02	2.99e+00	7.84e-02	2.99e+00
2.50e-01	1.37e-03	5.72e+00	1.37e-03	5.84e+00	5.55e-04	7.14e+00
1.25e-01	7.67e-06	7.48e+00	5.28e-06	8.02e+00	3.21e-07	1.08e+01
6.25e-02	6.33e-08	6.92e+00	4.17e-08	6.98e+00	3.38e-09	6.57e+00
3.12e-02	5.01e-10	6.98e+00	4.18e-10	6.64e+00	3.16e-11	6.74e+00
1.56e-02	3.92e-12	7.00e+00	3.62e-12	6.85e+00	1.94e-13	7.35e+00
7.81e-03	3.16e-14	6.95e+00	2.93e-14	6.95e+00	1.57e-14	3.62e+00
3.91e-03	3.11e-15	3.35e+00	3.20e-14	-1.26e-01	2.50e-14	-6.69e-01
1.95e-03	3.33e-15	-9.95e-02	7.22e-14	-1.18e+00	6.77e-14	-1.44e+00
9.77e-04	5.00e-15	-5.85e-01	1.14e-13	-6.62e-01	1.12e-13	-7.21e-01

10.1.2 Problem 2

This subsection gives the test results for the problem

$$y' = -\sin y, \quad y(0) = 1,$$

on the interval $[0, 100]$, for each of the DIMSEM methods. These results are discussed at the start of Section 10.

METHOD DIMSEM2L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
2.50e+00	1.84e+00		1.84e+00		2.64e-15	
1.25e+00	4.13e-01	2.16e+00	4.13e-01	2.16e+00	3.03e-15	-1.97e-01
6.25e-01	4.92e-02	3.07e+00	4.92e-02	3.07e+00	9.82e-16	1.62e+00
3.12e-01	4.71e-03	3.38e+00	4.71e-03	3.38e+00	6.88e-44	9.35e+01
1.56e-01	5.04e-04	3.23e+00	5.06e-04	3.22e+00	1.64e-44	2.07e+00
7.81e-02	5.89e-05	3.10e+00	7.22e-05	2.81e+00	3.04e-45	2.43e+00
3.91e-02	7.16e-06	3.04e+00	1.89e-05	1.93e+00	6.19e-46	2.30e+00
1.95e-02	8.84e-07	3.02e+00	4.82e-06	1.97e+00	1.37e-46	2.17e+00
9.77e-03	1.10e-07	3.01e+00	1.22e-06	1.99e+00	3.23e-47	2.09e+00
4.88e-03	1.37e-08	3.00e+00	3.05e-07	1.99e+00	7.81e-48	2.05e+00
2.44e-03	1.71e-09	3.00e+00	7.65e-08	2.00e+00	1.92e-48	2.02e+00
1.22e-03	2.13e-10	3.00e+00	1.91e-08	2.00e+00	4.76e-49	2.01e+00
6.10e-04	2.67e-11	3.00e+00	4.79e-09	2.00e+00	1.18e-49	2.01e+00

METHOD DIMSEM3L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
2.50e+00	NEWTON ITERATION FAILED TO CONVERGE					
1.25e+00	6.09e-01		5.85e-01		1.27e-15	
6.25e-01	7.68e-02	2.99e+00	6.36e-02	3.20e+00	1.52e-15	-2.66e-01
3.12e-01	5.83e-03	3.72e+00	5.31e-03	3.58e+00	4.19e-17	5.19e+00
1.56e-01	3.97e-04	3.88e+00	3.97e-04	3.74e+00	2.22e-47	1.01e+02
7.81e-02	2.50e-05	3.99e+00	2.50e-05	3.99e+00	5.36e-47	-1.27e+00
3.91e-02	1.54e-06	4.02e+00	1.55e-06	4.01e+00	8.63e-48	2.64e+00
1.95e-02	9.52e-08	4.02e+00	1.57e-07	3.31e+00	1.16e-48	2.89e+00
9.77e-03	5.92e-09	4.01e+00	1.81e-08	3.12e+00	1.50e-49	2.95e+00
4.88e-03	3.69e-10	4.00e+00	2.18e-09	3.05e+00	1.91e-50	2.98e+00
2.44e-03	2.30e-11	4.00e+00	2.69e-10	3.02e+00	2.40e-51	2.99e+00
1.22e-03	1.44e-12	4.00e+00	3.31e-11	3.02e+00	3.04e-52	2.98e+00
6.10e-04	8.94e-14	4.01e+00	3.66e-12	3.18e+00	4.33e-53	2.81e+00

METHOD DIMSEM4L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
2.50e+00	NEWTON ITERATION FAILED TO CONVERGE					
1.25e+00	1.13e+00		8.60e-01		3.85e-15	
6.25e-01	9.29e-02	3.60e+00	9.29e-02	3.21e+00	3.84e-15	2.74e-03
3.12e-01	4.78e-03	4.28e+00	4.78e-03	4.28e+00	7.31e-16	2.39e+00
1.56e-01	9.05e-05	5.72e+00	6.70e-05	6.16e+00	3.53e-16	1.05e+00
7.81e-02	2.90e-06	4.97e+00	2.18e-06	4.94e+00	1.98e-47	1.04e+02
3.91e-02	9.00e-08	5.01e+00	1.46e-07	3.90e+00	8.50e-49	4.54e+00
1.95e-02	2.80e-09	5.01e+00	9.23e-09	3.98e+00	4.41e-50	4.27e+00
9.77e-03	8.71e-11	5.01e+00	5.77e-10	4.00e+00	2.50e-51	4.14e+00
4.88e-03	2.72e-12	5.00e+00	3.60e-11	4.00e+00	1.49e-52	4.07e+00
2.44e-03	8.49e-14	5.00e+00	2.25e-12	4.00e+00	9.02e-54	4.04e+00
1.22e-03	3.11e-15	4.77e+00	1.46e-13	3.95e+00	5.17e-55	4.13e+00
6.10e-04	7.77e-16	2.00e+00	2.05e-14	2.83e+00	4.98e-56	3.38e+00

METHOD DIMSEM5L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
2.50e+00	NEWTON ITERATION FAILED TO CONVERGE					
1.25e+00	1.69e+00		1.41e+00		2.05e-15	
6.25e-01	1.31e-01	3.69e+00	1.30e-01	3.44e+00	2.22e-15	-1.18e-01
3.12e-01	4.38e-03	4.90e+00	3.84e-03	5.08e+00	2.24e-15	-1.18e-02
1.56e-01	8.84e-05	5.63e+00	8.84e-05	5.44e+00	5.30e-16	2.08e+00
7.81e-02	1.41e-06	5.97e+00	1.41e-06	5.97e+00	3.20e-37	7.05e+01
3.91e-02	1.92e-08	6.20e+00	1.92e-08	6.20e+00	5.56e-51	4.57e+01
1.95e-02	2.70e-10	6.15e+00	2.70e-10	6.15e+00	8.56e-53	6.02e+00
9.77e-03	3.98e-12	6.09e+00	3.98e-12	6.09e+00	1.51e-54	5.83e+00
4.88e-03	6.05e-14	6.04e+00	6.05e-14	6.04e+00	1.32e-55	3.51e+00
2.44e-03	2.33e-15	4.70e+00	1.83e-14	1.73e+00	1.98e-55	-5.86e-01
1.22e-03	2.00e-15	2.22e-01	3.87e-14	-1.09e+00	3.89e-55	-9.71e-01

METHOD DIMSEM6L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
2.50e+00	NEWTON ITERATION FAILED TO CONVERGE					
1.25e+00	NEWTON ITERATION FAILED TO CONVERGE					
6.25e-01	1.52e-01		2.37e-01		9.37e-15	
3.12e-01	4.53e-03	5.07e+00	4.53e-03	5.71e+00	3.98e-15	1.23e+00
1.56e-01	3.50e-05	7.02e+00	3.36e-05	7.08e+00	1.00e-15	1.99e+00
7.81e-02	2.99e-07	6.87e+00	1.80e-07	7.55e+00	1.04e-15	-5.26e-02
3.91e-02	2.38e-09	6.97e+00	1.85e-09	6.60e+00	4.73e-51	1.17e+02
1.95e-02	1.87e-11	6.99e+00	1.69e-11	6.77e+00	1.08e-54	1.21e+01
9.77e-03	1.46e-13	6.99e+00	1.38e-13	6.94e+00	1.25e-55	3.11e+00
4.88e-03	3.66e-15	5.32e+00	3.92e-14	1.82e+00	2.46e-55	-9.77e-01
2.44e-03	4.44e-15	-2.78e-01	5.02e-14	-3.57e-01	4.77e-55	-9.55e-01

10.1.3 Problem 3

This subsection gives the test results for the problem

$$y' = g'(x) + \omega\left(y - g(x)\right), \quad y(0) = g(0),$$

with $g(x) = \sin(x)$ and $\omega = -10^6$, on the interval $[0, 10]$, for each of the DIMSEM methods. These results are discussed at the start of Section 10.

METHOD DIMSEM2L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	8.61e-01		8.61e-01		5.31e-01	
5.00e-01	1.21e-01	2.83e+00	1.21e-01	2.83e+00	1.19e-01	2.15e+00
2.50e-01	1.55e-02	2.97e+00	1.55e-02	2.97e+00	1.52e-02	2.97e+00
1.25e-01	1.95e-03	2.99e+00	1.95e-03	2.99e+00	1.80e-03	3.07e+00
6.25e-02	2.44e-04	3.00e+00	2.44e-04	3.00e+00	2.16e-04	3.06e+00
3.12e-02	3.05e-05	3.00e+00	3.05e-05	3.00e+00	2.63e-05	3.04e+00
1.56e-02	3.81e-06	3.00e+00	3.81e-06	3.00e+00	3.24e-06	3.02e+00
7.81e-03	4.77e-07	3.00e+00	4.77e-07	3.00e+00	4.00e-07	3.02e+00
3.91e-03	5.96e-08	3.00e+00	5.96e-08	3.00e+00	4.95e-08	3.01e+00
1.95e-03	7.45e-09	3.00e+00	7.45e-09	3.00e+00	6.10e-09	3.02e+00
9.77e-04	9.30e-10	3.00e+00	9.30e-10	3.00e+00	7.44e-10	3.04e+00
4.88e-04	1.16e-10	3.00e+00	1.16e-10	3.00e+00	8.90e-11	3.06e+00
2.44e-04	1.45e-11	3.00e+00	1.45e-11	3.00e+00	1.04e-11	3.10e+00
1.22e-04	1.80e-12	3.01e+00	1.80e-12	3.01e+00	1.16e-12	3.16e+00
6.10e-05	2.24e-13	3.01e+00	2.24e-13	3.01e+00	1.36e-13	3.09e+00

METHOD DIMSEM3L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	8.36e-01		8.36e-01		8.36e-01	
5.00e-01	5.98e-02	3.81e+00	5.98e-02	3.81e+00	2.47e-02	5.08e+00
2.50e-01	3.86e-03	3.95e+00	3.86e-03	3.95e+00	2.91e-04	6.41e+00
1.25e-01	2.43e-04	3.99e+00	2.43e-04	3.99e+00	7.78e-05	1.90e+00
6.25e-02	1.52e-05	4.00e+00	1.52e-05	4.00e+00	6.64e-06	3.55e+00
3.12e-02	9.53e-07	4.00e+00	9.53e-07	4.00e+00	4.68e-07	3.83e+00
1.56e-02	5.96e-08	4.00e+00	5.96e-08	4.00e+00	3.08e-08	3.92e+00
7.81e-03	3.72e-09	4.00e+00	3.73e-09	4.00e+00	1.98e-09	3.96e+00
3.91e-03	2.33e-10	4.00e+00	2.35e-10	3.99e+00	1.27e-10	3.96e+00
1.95e-03	1.49e-11	3.97e+00	1.61e-11	3.86e+00	8.87e-12	3.84e+00
9.77e-04	3.99e-13	5.22e+00	2.30e-12	2.81e+00	2.84e-13	4.97e+00
4.88e-04	2.56e-14	3.96e+00	1.14e-12	1.01e+00	1.10e-13	1.36e+00
2.44e-04	7.11e-15	1.85e+00	1.06e-12	1.15e-01	2.78e-14	1.99e+00
1.22e-04	7.11e-15	0.00e+00	5.50e-13	9.42e-01	5.37e-14	-9.53e-01

METHOD DIMSEM4L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	7.92e-01		7.92e-01		2.81e-01	
5.00e-01	2.96e-02	4.74e+00	2.96e-02	4.74e+00	2.32e-02	3.60e+00
2.50e-01	9.64e-04	4.94e+00	9.64e-04	4.94e+00	9.63e-04	4.59e+00
1.25e-01	3.04e-05	4.99e+00	3.04e-05	4.99e+00	2.94e-05	5.03e+00
6.25e-02	9.53e-07	5.00e+00	9.53e-07	5.00e+00	8.70e-07	5.08e+00
3.12e-02	2.98e-08	5.00e+00	2.98e-08	5.00e+00	2.62e-08	5.05e+00
1.56e-02	9.31e-10	5.00e+00	9.33e-10	5.00e+00	8.42e-10	4.96e+00
7.81e-03	1.34e-11	6.12e+00	6.09e-11	3.94e+00	3.84e-11	4.46e+00
3.91e-03	4.18e-13	5.00e+00	1.96e-11	1.64e+00	3.53e-12	3.44e+00
1.95e-03	1.31e-14	5.00e+00	9.76e-12	1.00e+00	9.34e-13	1.92e+00
9.77e-04	1.00e-15	3.71e+00	5.45e-12	8.40e-01	1.70e-13	2.46e+00
4.88e-04	7.77e-16	3.63e-01	2.72e-12	1.00e+00	1.78e-13	-6.45e-02

METHOD DIMSEM5L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	7.45e-01		7.45e-01		5.11e-01	
5.00e-01	1.46e-02	5.67e+00	1.46e-02	5.67e+00	1.17e-02	5.45e+00
2.50e-01	2.40e-04	5.93e+00	2.40e-04	5.93e+00	4.18e-05	8.13e+00
1.25e-01	3.80e-06	5.98e+00	3.80e-06	5.98e+00	7.56e-07	5.79e+00
6.25e-02	5.95e-08	6.00e+00	6.09e-08	5.96e+00	2.28e-08	5.05e+00
3.12e-02	9.34e-10	5.99e+00	1.67e-09	5.19e+00	2.35e-10	6.59e+00
1.56e-02	7.35e-12	6.99e+00	4.86e-10	1.78e+00	5.07e-11	2.21e+00
7.81e-03	1.15e-13	6.00e+00	2.51e-10	9.55e-01	1.11e-10	-1.13e+00
3.91e-03	2.66e-15	5.43e+00	1.25e-10	1.01e+00	1.25e-10	-1.70e-01
1.95e-03	1.89e-15	4.97e-01	6.58e-11	9.22e-01	1.05e-11	3.57e+00
9.77e-04	1.89e-15	0.00e+00	3.03e-11	1.12e+00	2.40e-12	2.13e+00
4.88e-04	2.11e-15	-1.60e-01	1.74e-11	8.04e-01	6.61e-12	-1.46e+00

METHOD DIMSEM6L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	7.28e-01		7.28e-01		7.28e-01	
5.00e-01	7.26e-03	6.65e+00	7.26e-03	6.65e+00	2.80e-03	8.02e+00
2.50e-01	5.99e-05	6.92e+00	5.99e-05	6.92e+00	5.73e-05	5.61e+00
1.25e-01	4.75e-07	6.98e+00	4.75e-07	6.98e+00	4.71e-07	6.93e+00
6.25e-02	3.72e-09	7.00e+00	5.29e-09	6.49e+00	2.75e-09	7.42e+00
3.12e-02	1.54e-11	7.91e+00	1.34e-09	1.98e+00	5.38e-11	5.68e+00
1.56e-02	1.21e-13	7.00e+00	6.54e-10	1.04e+00	1.56e-10	-1.53e+00
7.81e-03	3.44e-15	5.14e+00	3.72e-10	8.13e-01	2.24e-10	-5.23e-01
3.91e-03	3.22e-15	9.62e-02	2.07e-10	8.46e-01	1.06e-10	1.07e+00
1.95e-03	3.66e-15	-1.86e-01	9.47e-11	1.13e+00	2.60e-11	2.04e+00
9.77e-04	4.11e-15	-1.65e-01	5.71e-11	7.31e-01	2.14e-11	2.77e-01

10.2 Test Results for the ADM Methods

10.2.1 Problem 1

This subsection gives the test results for the problem

$$y' = -\sin y, \quad y(0) = 1,$$

on the interval $[0, 1]$, for each of the ADM methods. These results are discussed at the start of Section 10.

METHOD ADM2L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	3.51e-01		3.51e-01		3.51e-01	
5.00e-01	4.91e-02	2.84e+00	5.06e-02	2.80e+00	5.06e-02	2.80e+00
2.50e-01	5.53e-03	3.15e+00	6.65e-03	2.93e+00	2.49e-03	4.35e+00
1.25e-01	6.31e-04	3.13e+00	9.84e-04	2.76e+00	6.28e-04	1.99e+00
6.25e-02	7.49e-05	3.07e+00	2.33e-04	2.08e+00	2.33e-04	1.43e+00
3.12e-02	9.13e-06	3.04e+00	6.57e-05	1.83e+00	6.57e-05	1.83e+00
1.56e-02	1.13e-06	3.02e+00	1.72e-05	1.93e+00	1.72e-05	1.93e+00
7.81e-03	1.40e-07	3.01e+00	4.40e-06	1.97e+00	4.40e-06	1.97e+00
3.91e-03	1.74e-08	3.00e+00	1.11e-06	1.99e+00	1.11e-06	1.99e+00
1.95e-03	2.18e-09	3.00e+00	2.79e-07	1.99e+00	2.79e-07	1.99e+00
9.77e-04	2.72e-10	3.00e+00	6.99e-08	2.00e+00	6.99e-08	2.00e+00

METHOD ADM3L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	3.20e+00		3.20e+00		3.20e+00	
5.00e-01	1.10e-01	4.86e+00	2.47e-01	3.70e+00	2.47e-01	3.70e+00
2.50e-01	9.49e-03	3.54e+00	2.26e-02	3.45e+00	2.24e-02	3.46e+00
1.25e-01	6.47e-04	3.87e+00	2.09e-03	3.43e+00	1.83e-03	3.61e+00
6.25e-02	4.08e-05	3.99e+00	2.18e-04	3.26e+00	1.75e-04	3.39e+00
3.12e-02	2.54e-06	4.00e+00	2.47e-05	3.15e+00	1.89e-05	3.21e+00
1.56e-02	1.58e-07	4.00e+00	2.93e-06	3.08e+00	2.19e-06	3.11e+00
7.81e-03	9.88e-09	4.00e+00	3.56e-07	3.04e+00	2.63e-07	3.06e+00
3.91e-03	6.17e-10	4.00e+00	4.40e-08	3.02e+00	3.22e-08	3.03e+00
1.95e-03	3.85e-11	4.00e+00	5.46e-09	3.01e+00	3.99e-09	3.01e+00
9.77e-04	2.41e-12	4.00e+00	6.80e-10	3.00e+00	4.96e-10	3.01e+00

METHOD ADM4L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	NEWTON ITERATION FAILED TO CONVERGE					
5.00e-01	2.87e-01		6.21e-01		6.21e-01	
2.50e-01	1.06e-02	4.76e+00	1.36e-02	5.51e+00	2.63e-03	7.88e+00
1.25e-01	2.51e-04	5.40e+00	9.39e-04	3.86e+00	9.39e-04	1.48e+00
6.25e-02	8.22e-06	4.93e+00	6.17e-05	3.93e+00	6.12e-05	3.94e+00
3.12e-02	2.61e-07	4.98e+00	3.76e-06	4.04e+00	3.65e-06	4.07e+00
1.56e-02	8.20e-09	4.99e+00	2.30e-07	4.03e+00	2.21e-07	4.05e+00
7.81e-03	2.57e-10	5.00e+00	1.42e-08	4.02e+00	1.35e-08	4.03e+00
3.91e-03	8.04e-12	5.00e+00	8.82e-10	4.01e+00	8.36e-10	4.01e+00
1.95e-03	2.51e-13	5.00e+00	5.49e-11	4.01e+00	5.20e-11	4.01e+00
9.77e-04	7.99e-15	4.97e+00	3.42e-12	4.00e+00	3.24e-12	4.00e+00

METHOD ADM5L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	NEWTON ITERATION FAILED TO CONVERGE					
5.00e-01	2.51e-01		2.51e-01		2.00e-01	
2.50e-01	1.95e-02	3.68e+00	5.62e-02	2.16e+00	5.62e-02	1.83e+00
1.25e-01	4.39e-04	5.48e+00	1.18e-03	5.58e+00	7.35e-04	6.26e+00
6.25e-02	6.54e-06	6.07e+00	2.12e-05	5.79e+00	3.48e-06	7.72e+00
3.12e-02	9.21e-08	6.15e+00	4.62e-07	5.52e+00	7.48e-08	5.54e+00
1.56e-02	1.34e-09	6.10e+00	1.18e-08	5.29e+00	4.41e-09	4.09e+00
7.81e-03	2.02e-11	6.06e+00	3.31e-10	5.15e+00	1.64e-10	4.74e+00
3.91e-03	3.12e-13	6.02e+00	9.89e-12	5.06e+00	5.48e-12	4.91e+00
1.95e-03	6.22e-15	5.65e+00	4.78e-13	4.37e+00	9.90e-14	5.79e+00
9.77e-04	1.11e-15	2.49e+00	1.23e-13	1.96e+00	1.23e-13	-3.08e-01

METHOD ADM6L DBLE PROBLEM 1 X0 = 0.00e+00 XEND = 1.00e+00

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	NEWTON ITERATION FAILED TO CONVERGE					
5.00e-01	1.43e+00		1.43e+00		3.79e-01	
2.50e-01	3.43e-02	5.39e+00	5.25e-02	4.77e+00	5.25e-02	2.85e+00
1.25e-01	3.39e-04	6.66e+00	1.17e-03	5.49e+00	1.05e-03	5.64e+00
6.25e-02	2.91e-06	6.86e+00	1.73e-05	6.08e+00	1.25e-05	6.40e+00
3.12e-02	2.33e-08	6.96e+00	2.35e-07	6.20e+00	1.45e-07	6.43e+00
1.56e-02	1.83e-10	7.00e+00	3.35e-09	6.13e+00	1.87e-09	6.27e+00
7.81e-03	1.43e-12	7.00e+00	4.99e-11	6.07e+00	2.66e-11	6.14e+00
3.91e-03	1.43e-14	6.64e+00	1.02e-12	5.61e+00	8.98e-13	4.89e+00
1.95e-03	2.11e-15	2.76e+00	1.41e-13	2.85e+00	1.41e-13	2.67e+00
9.77e-04	1.22e-15	7.88e-01	1.21e-12	-3.10e+00	1.21e-12	-3.10e+00

10.2.2 Problem 2

This subsection gives the test results for the problem

$$y' = -\sin y, \quad y(0) = 1,$$

on the interval $[0, 100]$, for each of the ADM methods. These results are discussed at the start of Section 10.

METHOD ADM2L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
6.25e-01	9.62e-02		1.03e-01		1.83e-16	
3.12e-01	1.12e-02	3.10e+00	1.25e-02	3.03e+00	5.36e-18	5.09e+00
1.56e-01	1.26e-03	3.15e+00	2.82e-03	2.15e+00	1.66e-16	-4.95e+00
7.81e-02	1.48e-04	3.09e+00	7.17e-04	1.98e+00	3.28e-16	-9.84e-01
3.91e-02	1.80e-05	3.05e+00	1.79e-04	2.00e+00	1.31e-16	1.32e+00
1.95e-02	2.21e-06	3.02e+00	4.47e-05	2.00e+00	1.96e-16	-5.77e-01
9.77e-03	2.74e-07	3.01e+00	1.11e-05	2.00e+00	4.74e-16	-1.28e+00
4.88e-03	3.41e-08	3.01e+00	2.78e-06	2.00e+00	4.72e-16	4.38e-03
2.44e-03	4.25e-09	3.00e+00	6.96e-07	2.00e+00	4.72e-16	2.71e-03
1.22e-03	5.31e-10	3.00e+00	1.74e-07	2.00e+00	4.72e-16	-5.40e-04
6.10e-04	6.64e-11	3.00e+00	4.35e-08	2.00e+00	4.72e-16	-1.63e-03

METHOD ADM3L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
6.25e-01	2.39e-01		7.38e-01		1.31e-15	
3.12e-01	2.15e-02	3.48e+00	5.09e-02	3.86e+00	4.34e-16	1.60e+00
1.56e-01	1.56e-03	3.79e+00	4.46e-03	3.51e+00	8.37e-16	-9.47e-01
7.81e-02	9.96e-05	3.97e+00	4.48e-04	3.32e+00	5.93e-16	4.97e-01
3.91e-02	6.22e-06	4.00e+00	4.94e-05	3.18e+00	7.21e-16	-2.81e-01
1.95e-02	3.87e-07	4.01e+00	5.79e-06	3.09e+00	7.19e-16	4.72e-03
9.77e-03	2.41e-08	4.00e+00	7.01e-07	3.05e+00	7.18e-16	2.68e-03
4.88e-03	1.51e-09	4.00e+00	8.61e-08	3.02e+00	7.16e-16	2.90e-03
2.44e-03	9.41e-11	4.00e+00	1.07e-08	3.01e+00	7.15e-16	3.07e-03
1.22e-03	5.88e-12	4.00e+00	1.33e-09	3.01e+00	7.14e-16	7.21e-04
6.10e-04	3.67e-13	4.00e+00	1.66e-10	3.00e+00	7.14e-16	-6.26e-05

METHOD ADM4L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
6.25e-01	5.15e-01		1.19e+00		2.38e-15	
3.12e-01	3.67e-02	3.81e+00	5.63e-02	4.40e+00	5.48e-16	2.12e+00
1.56e-01	7.29e-04	5.65e+00	2.14e-03	4.72e+00	6.55e-16	-2.59e-01
7.81e-02	2.48e-05	4.88e+00	1.51e-04	3.83e+00	1.58e-15	-1.27e+00
3.91e-02	7.94e-07	4.97e+00	9.26e-06	4.03e+00	6.97e-16	1.18e+00
1.95e-02	2.50e-08	4.99e+00	5.65e-07	4.03e+00	8.00e-16	-1.99e-01
9.77e-03	7.84e-10	5.00e+00	3.48e-08	4.02e+00	7.13e-16	1.65e-01
4.88e-03	2.45e-11	5.00e+00	2.16e-09	4.01e+00	5.98e-16	2.55e-01
2.44e-03	7.67e-13	5.00e+00	1.34e-10	4.01e+00	6.23e-16	-6.07e-02
1.22e-03	2.42e-14	4.99e+00	8.36e-12	4.01e+00	6.50e-16	-6.00e-02
6.10e-04	1.00e-15	4.60e+00	4.99e-13	4.06e+00	6.78e-16	-6.05e-02

METHOD ADM5L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
6.25e-01	NEWTON ITERATION FAILED TO CONVERGE					
3.12e-01	5.82e-02		1.24e-01		1.08e-15	
1.56e-01	1.57e-03	5.21e+00	4.40e-03	4.81e+00	2.05e-15	-9.30e-01
7.81e-02	2.58e-05	5.93e+00	7.58e-05	5.86e+00	1.00e-15	1.03e+00
3.91e-02	3.62e-07	6.15e+00	1.55e-06	5.61e+00	1.12e-15	-1.59e-01
1.95e-02	5.22e-09	6.12e+00	3.79e-08	5.35e+00	8.45e-16	4.05e-01
9.77e-03	7.78e-11	6.07e+00	1.04e-09	5.19e+00	8.49e-16	-5.71e-03
4.88e-03	1.19e-12	6.03e+00	3.04e-11	5.09e+00	8.50e-16	-2.44e-03
2.44e-03	2.00e-14	5.89e+00	1.07e-12	4.83e+00	8.49e-16	2.61e-03
1.22e-03	1.33e-15	3.91e+00	2.55e-13	2.07e+00	8.44e-16	8.81e-03
6.10e-04	8.88e-16	5.85e-01	1.93e-13	4.05e-01	8.44e-16	-8.93e-04

METHOD ADM6L DBLE PROBLEM 2 X0 = 0.00e+00 XEND = 1.00e+02

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
6.25e-01	NEWTON ITERATION FAILED TO CONVERGE					
3.12e-01	NEWTON ITERATION FAILED TO CONVERGE					
1.56e-01	1.50e-03		3.75e-03		1.14e-14	
7.81e-02	1.37e-05	6.78e+00	6.95e-05	5.75e+00	2.85e-14	-1.32e+00
3.91e-02	1.11e-07	6.95e+00	9.36e-07	6.21e+00	1.43e-14	1.00e+00
1.95e-02	8.72e-10	6.99e+00	1.31e-08	6.16e+00	3.34e-14	-1.23e+00
9.77e-03	6.82e-12	7.00e+00	1.93e-10	6.09e+00	1.21e-15	4.78e+00
4.88e-03	5.67e-14	6.91e+00	3.14e-12	5.94e+00	1.44e-15	-2.49e-01
2.44e-03	2.66e-15	4.41e+00	9.24e-13	1.77e+00	1.59e-15	-1.44e-01
1.22e-03	1.22e-15	1.13e+00	5.25e-13	8.16e-01	1.70e-15	-9.55e-02
6.10e-04	7.77e-16	6.52e-01	9.08e-13	-7.92e-01	1.88e-15	-1.45e-01

10.2.3 Problem 3

This subsection gives the test results for the problem

$$y' = g'(x) + \omega\left(y - g(x)\right), \quad y(0) = g(0),$$

with $g(x) = \sin(x)$ and $\omega = -10^6$, on the interval $[0, 10]$, for each of the ADM methods. These results are discussed at the start of Section 10.

METHOD ADM2L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	6.03e-01		9.73e-01		4.85e-01	
5.00e-01	8.47e-02	2.83e+00	1.54e-01	2.66e+00	1.41e-01	1.78e+00
2.50e-01	1.08e-02	2.96e+00	2.07e-02	2.90e+00	2.07e-02	2.77e+00
1.25e-01	1.36e-03	2.99e+00	2.62e-03	2.98e+00	2.49e-03	3.05e+00
6.25e-02	1.71e-04	3.00e+00	3.29e-04	2.99e+00	2.97e-04	3.07e+00
3.12e-02	2.14e-05	3.00e+00	4.12e-05	3.00e+00	3.59e-05	3.05e+00
1.56e-02	2.67e-06	3.00e+00	5.15e-06	3.00e+00	4.41e-06	3.03e+00
7.81e-03	3.34e-07	3.00e+00	6.44e-07	3.00e+00	5.46e-07	3.01e+00
3.91e-03	4.17e-08	3.00e+00	8.05e-08	3.00e+00	6.79e-08	3.01e+00
1.95e-03	5.22e-09	3.00e+00	1.01e-08	3.00e+00	8.46e-09	3.00e+00
9.77e-04	6.52e-10	3.00e+00	1.26e-09	3.00e+00	1.06e-09	3.00e+00

METHOD ADM3L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	1.50e+00		1.30e+00		1.29e+00	
5.00e-01	1.07e-01	3.81e+00	1.04e-01	3.64e+00	7.76e-02	4.05e+00
2.50e-01	6.91e-03	3.95e+00	7.06e-03	3.88e+00	9.44e-04	6.36e+00
1.25e-01	4.36e-04	3.99e+00	4.50e-04	3.97e+00	1.25e-04	2.92e+00
6.25e-02	2.73e-05	4.00e+00	2.83e-05	3.99e+00	1.10e-05	3.51e+00
3.12e-02	1.71e-06	4.00e+00	1.77e-06	4.00e+00	8.27e-07	3.73e+00
1.56e-02	1.07e-07	4.00e+00	1.11e-07	4.00e+00	5.60e-08	3.88e+00
7.81e-03	6.67e-09	4.00e+00	6.92e-09	4.00e+00	3.63e-09	3.95e+00
3.91e-03	4.17e-10	4.00e+00	4.33e-10	4.00e+00	2.32e-10	3.97e+00
1.95e-03	2.64e-11	3.98e+00	2.75e-11	3.98e+00	1.42e-11	4.03e+00
9.77e-04	9.25e-13	4.84e+00	2.65e-12	3.37e+00	8.91e-13	3.99e+00

METHOD ADM4L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	2.18e+00		2.63e+00		1.54e+00	
5.00e-01	8.18e-02	4.74e+00	9.64e-02	4.77e+00	7.27e-02	4.41e+00
2.50e-01	2.66e-03	4.94e+00	3.22e-03	4.90e+00	3.09e-03	4.55e+00
1.25e-01	8.41e-05	4.99e+00	1.03e-04	4.97e+00	9.43e-05	5.04e+00
6.25e-02	2.64e-06	5.00e+00	3.24e-06	4.99e+00	2.79e-06	5.08e+00
3.12e-02	8.24e-08	5.00e+00	1.01e-07	5.00e+00	8.39e-08	5.06e+00
1.56e-02	2.58e-09	5.00e+00	3.17e-09	5.00e+00	2.56e-09	5.03e+00
7.81e-03	2.84e-11	6.50e+00	1.66e-10	4.25e+00	7.60e-11	5.08e+00
3.91e-03	1.23e-12	4.53e+00	1.07e-11	3.96e+00	7.43e-12	3.35e+00
1.95e-03	1.15e-13	3.43e+00	2.05e-11	-9.42e-01	2.04e-13	5.18e+00
9.77e-04	1.15e-14	3.31e+00	1.05e-11	9.68e-01	2.78e-13	-4.44e-01

METHOD ADM5L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	7.57e+00		7.57e+00		3.82e+00	
5.00e-01	1.51e-01	5.64e+00	1.19e-01	5.99e+00	8.90e-02	5.42e+00
2.50e-01	2.51e-03	5.91e+00	2.09e-03	5.83e+00	3.55e-04	7.97e+00
1.25e-01	3.98e-05	5.98e+00	3.37e-05	5.96e+00	7.31e-06	5.60e+00
6.25e-02	6.24e-07	5.99e+00	5.31e-07	5.99e+00	2.05e-07	5.16e+00
3.12e-02	9.77e-09	6.00e+00	8.49e-09	5.97e+00	3.89e-09	5.72e+00
1.56e-02	2.31e-10	5.40e+00	2.10e-10	5.34e+00	9.43e-11	5.37e+00
7.81e-03	1.31e-11	4.15e+00	1.57e-10	4.16e-01	3.29e-11	1.52e+00
3.91e-03	7.52e-13	4.12e+00	8.30e-11	9.23e-01	3.88e-12	3.08e+00
1.95e-03	1.86e-13	2.02e+00	5.20e-11	6.73e-01	1.68e-12	1.21e+00
9.77e-04	9.26e-14	1.00e+00	2.28e-11	1.19e+00	3.84e-13	2.13e+00
4.88e-04	4.63e-14	1.00e+00	1.28e-11	8.32e-01	1.21e-12	-1.66e+00

METHOD ADM6L DBLE PROBLEM 3 X0 = 0.00e+00 XEND = 1.00e+01

H	MAXIMUM--LOCAL ERROR	ORDER	MAXIMUM-GLOBAL ERROR	ORDER	ENDPOINT--GLOBAL ERROR	ORDER
1.00e+00	2.49e+01		1.29e+01		5.38e+00	
5.00e-01	2.66e-01	6.54e+00	1.35e-01	6.58e+00	9.12e-02	5.88e+00
2.50e-01	2.25e-03	6.89e+00	1.95e-03	6.11e+00	1.05e-03	6.44e+00
1.25e-01	1.79e-05	6.97e+00	1.73e-05	6.82e+00	8.13e-06	7.01e+00
6.25e-02	1.41e-07	6.99e+00	1.39e-07	6.96e+00	6.07e-08	7.07e+00
3.12e-02	2.09e-09	6.08e+00	1.94e-09	6.16e+00	5.22e-10	6.86e+00
1.56e-02	3.42e-11	5.93e+00	1.04e-09	9.02e-01	1.52e-10	1.78e+00
7.81e-03	4.33e-12	2.98e+00	4.58e-10	1.18e+00	7.80e-11	9.62e-01
3.91e-03	2.03e-12	1.09e+00	1.02e-09	-1.15e+00	5.18e-11	5.90e-01
1.95e-03	5.92e-13	1.78e+00	2.69e-10	1.92e+00	4.04e-11	3.61e-01
9.77e-04	5.91e-13	2.71e-04	2.59e-10	5.70e-02	9.27e-12	2.12e+00
4.88e-04	5.92e-13	-2.71e-04	1.33e-10	9.58e-01	7.66e-12	2.75e-01

11 Conclusions and Future Work

In this report, we have introduced two new classes of methods which show promise for the solution of stiff problems on parallel computers. Both the ADM and DIMSEM classes contain methods of all orders ≥ 2. L-stable methods of orders 2–6 from each of these classes have been derived, and have behaved satisfactorily in fixed-stepsize numerical testing.

We plan to develop a variable-stepsize implementation of each of the methods and test it. To implement the methods in variable-stepsize form, suitable error estimators and a technique for changing stepsize during the integration will have to be devised. We also intend to conduct some performance testing on a parallel machine.

There is much further research to do on DIMSEMs. A desirable generalisation would be to remove the requirement that $c_1 = \cdots = c_s = 0$, since we believe this ought to lead to better methods. Further generalisations might be to use the Nordsieck-type of true-value function, or some other more general type, in place of the multistep-type true-value function employed here. Also, the nonlinear stability of the methods should be investigated.

A Theorem 4

Theorem 4 *A GLM is stable on the vector linear problem*

$$u'(t) = Cu(t), \quad C \in \mathbb{R}^{K \times K},$$

if it is stable on each of the scalar problems

$$u'(t) = \mu_i u(t), \quad i = 1, \ldots, K,$$

if C is diagonalisable, or

$$u'(t) = \mu_i u(t) + d_i(t), \quad i = 1, \ldots, K,$$

otherwise, where $\mu_1, \ldots, \mu_K$ are the eigenvalues of C and all the d_i's are analytic.

Proof. Write the vector method as

$$\begin{aligned} Y_n &= (A_1 \otimes I_K) y_n + h(B_1 \otimes I_K) F(Y_n), \\ y_{n+1} &= (A_2 \otimes I_K) y_n + h(B_2 \otimes I_K) F(Y_n). \end{aligned}$$

For the ODE $u'(t) = Cu(t)$, $F(Y_n) = (I_s \otimes C)Y_n$, so that the method becomes

$$\begin{aligned} Y_n &= (A_1 \otimes I_K) y_n + h(B_1 \otimes C) Y_n, \\ y_{n+1} &= (A_2 \otimes I_K) y_n + h(B_2 \otimes C) Y_n. \end{aligned}$$

First, assume that C is diagonalisable and let T be a matrix such that

$$T^{-1} C T = D = \begin{pmatrix} \mu_1 & & \\ & \ddots & \\ & & \mu_K \end{pmatrix}.$$

Using

$$\begin{aligned} z_n &= (I_r \otimes T) y_n, \\ z_{n+1} &= (I_r \otimes T) y_{n+1}, \\ Z_n &= (I_s \otimes T) Y_n, \end{aligned}$$

we can rewrite the method as

$$z_{n+1} = (A_2 \otimes I_K) z_n + h(B_2 \otimes D) Z_n.$$

Now define

$$e_{l,k} = (0, \ldots, 0, 1, 0, \ldots, 0) \in \mathbb{R}^l,$$

where the 1 occurs in the k-th component. Then $z_{n+1,k}$, the sub-vector of z_{n+1} consisting of the k-th component of each of the r block components in $\mathbb{R}^K$, is given by

$$\begin{aligned}
z_{n+1,k} &= (I_r \otimes e_{K,k}) z_{n+1} \\
&= (I_r \otimes e_{K,k})(A_2 \otimes I_K) z_n + h(I_r \otimes e_{K,k})(B_2 \otimes D) Z_n \\
&= (A_2 \otimes e_{K,k}) z_n + h(B_2 \otimes e_{K,k} D) Z_n \\
&= (A_2 \otimes I_1)(I_r \otimes e_{K,k}) z_n + h(B_2 \otimes \mu_k e_{K,k}) Z_n \\
&= A_2 z_{n,k} + h\mu_k (B_2 \otimes I_1)(I_s \otimes e_{K,k}) Z_n \\
&= A_2 z_{n,k} + h\mu_k B_2 Z_{n,k}.
\end{aligned}$$

Similarly,

$$Z_{n,k} = A_1 z_{n,k} + h\mu_k B_1 Z_{n,k}.$$

Thus $z_{n+1,k}$ is the result of applying the method to the scalar problem $u' = \mu_k u$. Since the method is stable on each of these scalar problems,

$$\|z_{n+1}\| \leq \alpha \|z_0\|$$

for some constant α independent of n, so

$$\begin{aligned}
\|y_{n+1}\| &= \|(I_r \otimes T^{-1}) z_{n+1}\| \\
&\leq \|I_r \otimes T^{-1}\| \|z_{n+1}\| \\
&\leq \|I_r \otimes T^{-1}\| \alpha \|z_0\| \\
&= \alpha \|I_r \otimes T^{-1}\| \|(I_r \otimes T) y_0\|, \\
&\leq \alpha \|I_r \otimes T^{-1}\| \|I_r \otimes T\| \|y_0\|,
\end{aligned}$$

which shows the method is stable on the vector problem too.

If C is not diagonalisable, consider the Jordan Canonical Form J of C. Without loss of generality, we may assume J consists of one Jordan block only (corresponding to μ, say), because the separate blocks decouple in a manner similar to the diagonalisable case considered above. Therefore assume

$$T^{-1} C T = J = \begin{pmatrix} \mu & & & \\ 1 & \ddots & & \\ & \ddots & \ddots & \\ & & 1 & \mu \end{pmatrix}.$$

An argument similar to that for the diagonalisable case shows that

$$Z_{n,k} = A_1 z_{n,k} + h\mu_k B_1 Z_{n,k} + hB_1 Z_{n,k-1} \in \mathbb{R}^s,$$
$$z_{n+1,k} = A_2 z_{n,k} + h\mu_k B_2 Z_{n,k} + hB_2 Z_{n,k-1} \in \mathbb{R}^r,$$

where the $Z_{n-1,k}$ terms are omitted for $k = 1$. Thus $z_{n+1,k}$ is the result of applying the original method to the scalar problem $u'(t) = \mu u(t) + d(t)$, where $d(t_n) = Z_{n,k-1}$. Since the scalar method is stable on such a problem for any analytic d, it follows, as in the diagonalisable case, that the vector method is also stable. □

B Theorem 5

Theorem 5 *Let $b_{ij} = (\bar{B}_2)_{ij}$ and set*

$$b_{rj} = \frac{1}{s!} \frac{\sum_{k=0}^{s-1} \frac{\theta_{kj}^{(s)}}{(s-k)!}}{\prod_{\substack{l=1 \\ l \neq j}}^{s} (\lambda_l - \lambda_j)} \tag{58}$$

$$= \frac{1}{s! \lambda_j^{s-1} p_j(\frac{1}{\lambda_j})} \sum_{k=0}^{s-1} \frac{\theta_{kj}^{(s)}}{(s-k)!}, \tag{59}$$

where

$$\theta_{kj}^{(s)} \text{ is the coefficient of } x^k \text{ in } p_j(x) \tag{60}$$

and

$$p_j(x) = \prod_{\substack{l=1 \\ l \neq j}}^{s} (\lambda_l x - 1). \tag{61}$$

Also set

$$b_{ij} = T_{ij}(\lambda) b_{rj}, \quad i = 1, \ldots, r-1, \tag{62}$$

where $\lambda = (\lambda_1, \ldots, \lambda_s)$ and $\{\lambda_i : i = 1, \ldots, s\}$ are distinct and nonzero,

$$T_{ij}(\lambda) = \frac{1}{(i-1)!} \sum_{l=0}^{r-i} \left[(i-1+l)! \gamma_{s-i-l+1}^{(s)} \lambda_j^l \right], \tag{63}$$

and

$$\gamma_k^{(s)} = \begin{cases} \sum_{1 \leq i_1 < \cdots < i_k \leq s} i_1 \cdots i_k, & k \geq 1, \\ 1, & k = 0. \end{cases} \tag{64}$$

Then the transformed stability matrix $\bar{M}_r(z)$ has $r-1$ zero eigenvalues for all $z \neq 1/\lambda_i$, $i = 1, \ldots, s$.

Remark. The requirement that $z \neq 1/\lambda_i$ for $i = 1, \ldots, s$ is a necessary restriction, since the factor $(I - zB_1)$ that occurs in both $M(z)$ and $\bar{M}(z)$ is singular if and only if $z = 1/\lambda_i$ for some $i = 1, \ldots, s$. Note that, if we choose $\lambda_i > 0$ for $i = 1, \ldots, s$, then $M(z)$ and $\bar{M}(z)$ are well defined and the single eigenvalue property holds for all $z \in \mathbb{C}^-$.

Proof. Theorem 6 in Appendix C gives the following expression for the characteristic polynomial of the transformed stability matrix $\bar{M}_r(z)$:

$$\phi_r(w, z) = \sum_{k=0}^{r} \phi_k^{(r)}(z) w^k, \tag{65}$$

where

$$\phi_k^{(r)}(z) = \begin{cases} \delta_k^{(s)} + \sum_{i=1}^{r} \left[(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z) a_i(z) \right], & k = 0, \ldots, r-1, \\ 1, & k = r, \end{cases} \tag{66}$$

and

$$a_i(z) = \sum_{k=1}^{s} \frac{b_{ik}}{1 - \lambda_k z}. \tag{67}$$

(The other quantities are defined in Theorem 6.) We will show that $\phi_r(w, z)$ has all but one of its w-roots at zero for all $z \neq 1/\lambda_i$, $i = 1, \ldots, s$. This is equivalent to

$$\phi_k^{(r)}(z) = 0, \quad \text{for } k = 0, \ldots, r-2 \text{ and } z \neq 1/\lambda_i \text{ for } i = 1, \ldots, s, \tag{68}$$

for then

$$\begin{aligned} \phi_r(w, z) &= \phi_r^{(r)}(z) w^r + \phi_{r-1}^{(r)}(z) w^{r-1} \\ &= \left[\phi_r^{(r)}(z) w + \phi_{r-1}^{(r)}(z) \right] w^{r-1}, \end{aligned}$$

which has a root of multiplicity $r - 1$ at $w = 0$.

From (66) and (67), we have

$$\begin{aligned} \phi_k^{(r)}(z) &= \delta_k^{(s)} + \sum_{i=1}^{r} \left[(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z) \sum_{j=1}^{s} \frac{b_{ij}}{1 - \lambda_j z} \right] \\ &= \delta_k^{(s)} + \sum_{i=1}^{r} \sum_{j=1}^{s} \left(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z \right) \frac{b_{ij}}{1 - \lambda_j z} \\ &= \delta_k^{(s)} + \sum_{i=1}^{r} \frac{\sum_{j=1}^{s} \left(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z \right) \prod_{\substack{l=1 \\ l \neq j}}^{s} (1 - \lambda_l z)}{\prod_{j=1}^{s} (1 - \lambda_j z)} b_{ij} \\ &= \delta_k^{(s)} + \sum_{i=1}^{r} \frac{\sum_{j=1}^{s} \left(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z \right) (-1)^{s-1} p_j(z)}{(-1)^s p(z)} b_{ij} \end{aligned}$$

$$= \frac{\delta_k^{(s)} p(z) - \sum_{i=1}^{r} \sum_{j=1}^{s} \left(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z\right) p_j(z) b_{ij}}{p(z)}$$

$$= \frac{q_k(z)}{p(z)}, \tag{69}$$

where

$$q_k(z) = \delta_k^{(s)} p(z) - \sum_{i=1}^{r} \sum_{j=1}^{s} \left(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z\right) p_j(z) b_{ij}, \tag{70}$$

$$p(z) = \prod_{j=1}^{s} (\lambda_j z - 1). \tag{71}$$

Note that $q_k(z)$ is a polynomial of degree s. To prove (68) then, it suffices to show $q_k(z) = 0$ at $s+1$ different z's. Then,

$$\begin{aligned} & q_k(z) = 0 \quad \forall z \\ \Longrightarrow \quad & \phi_k^{(r)}(z) = q_k(z)/p(z) = 0 \quad \forall z \ni p(z) \neq 0 \\ \Longrightarrow \quad & \phi_k^{(r)}(z) = 0 \quad \forall z \neq \frac{1}{\lambda_i}, \quad i = 1, \ldots, s, \end{aligned}$$

which is (68). The values we choose for z to prove $q_k(z) = 0$ are

$$z = \frac{1}{\lambda_1}, \ldots, \frac{1}{\lambda_s}, 0, \tag{72}$$

which are distinct and well-defined because the λ_i's are distinct and nonzero. Then from (61) and (71) we have

$$\begin{aligned} p\left(\frac{1}{\lambda_j}\right) &= 0, \quad j = 1, \ldots, s, \\ p_j\left(\frac{1}{\lambda_m}\right) &= 0, \quad m \neq j. \end{aligned}$$

Consider $z = 1/\lambda_j$ first. Applying the above expressions to (70) gives

$$q_k\left(\frac{1}{\lambda_j}\right) = -\psi_{kj}, \tag{73}$$

where

$$\psi_{kj} = \sum_{i=1}^{r} \left(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} \frac{1}{\lambda_j}\right) p_j\left(\frac{1}{\lambda_j}\right) b_{ij}. \tag{74}$$

Now we have, using (74) and (62),

$$\begin{aligned}\psi_{kj} &= \sum_{i=1}^{r}\left(\alpha_{k,i}^{(s)}+\beta_{k,i}^{(s)}\frac{1}{\lambda_j}\right)p_j\left(\frac{1}{\lambda_j}\right)T_{ij}b_{rj}\\ &= \frac{1}{\lambda_j}p_j\left(\frac{1}{\lambda_j}\right)b_{rj}\sum_{i=1}^{r}\left(\lambda_j\alpha_{k,i}^{(s)}+\beta_{k,i}^{(s)}\right)T_{ij}. \qquad (75)\end{aligned}$$

Thus

$$\psi_{kj}=0 \Longleftrightarrow \begin{cases} \frac{1}{\lambda_j}p_j\left(\frac{1}{\lambda_j}\right)b_{rj}=0, \text{ or} \\ \sum_{i=1}^{r}\left(\lambda_j\alpha_{k,i}^{(s)}+\beta_{k,i}^{(s)}\right)T_{ij}=0. \end{cases} \qquad (76)$$

Consider the first alternative in (76). The first factor $1/\lambda_j \neq 0$. Also,

$$p_j\left(\frac{1}{\lambda_j}\right)=\prod_{\substack{l=1\\ l\neq j}}^{s}\left(\frac{\lambda_l}{\lambda_j}-1\right)\neq 0,$$

because the λ_j's are distinct. We could have $b_{rj}=0$, but, by (58), this requires

$$\sum_{k=0}^{s-1}\frac{\theta_{kj}^{(s)}}{(s-k)!}=0$$

which imposes a condition on the λ_j's (through $\theta_{kj}^{(s)}$), and we prefer to keep the λ_j's as free parameters. It turns out that the second alternative in (76) is always true, so we will prove

$$\sum_{i=1}^{r}\left(\lambda_j\alpha_{k,i}^{(s)}+\beta_{k,i}^{(s)}\right)T_{ij}=0, \quad j=1,\ldots,s, \quad k=0,\ldots,r-2. \qquad (77)$$

From (72), we must also show $q_k(0)=0$. Now $p(0)=(-1)^s$ and $p_j(0)=(-1)^{s-1}$, so by (70), $q_k(0)=0$ is equivalent to

$$\delta_k^{(s)}+\sum_{i=1}^{r}\sum_{j=1}^{s}\alpha_{k,i}^{(s)}b_{ij}=0, \quad k=0,\ldots,r-2. \qquad (78)$$

Therefore we will show (77) and (78). Consider (77) first. Using (95) gives

$$\begin{aligned}(77) &\Longleftrightarrow \sum_{i=1}^{r}\left(-(i-1)\lambda_j\beta_{k,i-1}^{(s)}T_{ij}\right)+\sum_{i=1}^{r}\beta_{k,i}^{(s)}T_{ij}=0\\ &\Longleftrightarrow \sum_{i=1}^{r-1}(-\lambda_j iT_{i+1,j}+T_{ij})\beta_{k,i}^{(s)}+\beta_{k,r}^{(s)}=0. \qquad (79)\end{aligned}$$

From (63) and (64), we have

$$\begin{aligned}
& -\lambda_j i T_{i+1,j} + T_{ij} \\
= \; & -\lambda_j i \sum_{l=0}^{r-i-1} \frac{(i+l)!}{i!} \gamma_{s-i-l}^{(s)} \lambda_j^l + \sum_{l=0}^{r-i} \frac{(i-1+l)!}{(i-1)!} \gamma_{s-i-l+1}^{(s)} \lambda_j^l \\
= \; & -\sum_{l=1}^{r-i} \frac{(i-1+l)!}{(i-1)!} \gamma_{s-i-l+1}^{(s)} \lambda_j^l + \sum_{l=0}^{r-i} \frac{(i-1+l)!}{(i-1)!} \gamma_{s-i-l+1}^{(s)} \lambda_j^l \\
= \; & \gamma_{s-i+1}^{(s)},
\end{aligned}$$

because all but the $l = 0$ term cancels. Using this in (79) reduces what we must prove to

$$\sum_{i=1}^{r-1} \gamma_{s-i+1}^{(s)} \beta_{k,i}^{(s)} + \beta_{k,r}^{(s)} = 0, \quad k = 0, \ldots, r-2,$$

or

$$\sum_{i=1}^{r} \gamma_{s-i+1}^{(s)} \beta_{k,i}^{(s)} = 0, \quad k = 0, \ldots, r-2, \tag{80}$$

since $\gamma_0^{(s)} = 1$ by (64). Using (97), we rewrite (96) as

$$\beta_{k,i}^{(s)} = \begin{cases} (-1)^{s+1-k} \begin{pmatrix} s \\ k \end{pmatrix}, & i = 1, \\ (-1)^{s-k} \left[\sum_{l=0}^{s-k-1} (-1)^l \begin{pmatrix} s-l-1 \\ k \end{pmatrix} \Sigma_l^{i-1} \right], & i \geq 2. \end{cases} \tag{81}$$

Applying (81) to (80) further reduces what we must prove to

$$\begin{aligned}
& \gamma_s^{(s)} \beta_{k,1}^{(s)} + \sum_{i=2}^{r} \gamma_{s-i+1}^{(s)} \beta_{k,i}^{(s)} = 0 \\
\iff \; & \gamma_s^{(s)} \beta_{k,1}^{(s)} + \sum_{i=1}^{s} \gamma_{s-i}^{(s)} \beta_{k,i+1}^{(s)} = 0 \\
\iff \; & (-1)^{s+1-k} \gamma_s^{(s)} \begin{pmatrix} s \\ k \end{pmatrix} + (-1)^{s-k} \sum_{i=1}^{s} \gamma_{s-i}^{(s)} \sum_{l=0}^{s-k-1} (-1)^l \begin{pmatrix} s-l-1 \\ k \end{pmatrix} \Sigma_l^i = 0 \\
\iff \; & \gamma_s^{(s)} \begin{pmatrix} s \\ k \end{pmatrix} + \sum_{i=1}^{s} \gamma_{s-i}^{(s)} \sum_{l=1}^{s-k} (-1)^l \begin{pmatrix} s-l \\ k \end{pmatrix} \Sigma_{l-1}^i = 0.
\end{aligned} \tag{82}$$

By Lemma 4 in Appendix D.4,

$$\Sigma_{l-1}^i = (-1)^l \sum_{m=1}^{l} (-1)^m \begin{pmatrix} l \\ m \end{pmatrix} m^i.$$

Using this in (82), we must show

$$\begin{aligned}
&\gamma_s^{(s)} \left(\begin{array}{c} s \\ k \end{array} \right) + \sum_{l=1}^{s-k} (-1)^l \left(\begin{array}{c} s-l \\ k \end{array} \right) \sum_{i=1}^{s} \gamma_{s-i}^{(s)} \Sigma_{l-1}^i = 0 \\
\iff\ &\gamma_s^{(s)} \left(\begin{array}{c} s \\ k \end{array} \right) + \sum_{l=1}^{s-k} (-1)^l \left(\begin{array}{c} s-l \\ k \end{array} \right) \sum_{i=1}^{s} \gamma_{s-i}^{(s)} (-1)^l \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) m^i = 0 \\
\iff\ &\gamma_s^{(s)} \left(\begin{array}{c} s \\ k \end{array} \right) + \sum_{l=1}^{s-k} \left(\begin{array}{c} s-l \\ k \end{array} \right) \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) U_m^{(s)}, \qquad (83)
\end{aligned}$$

where

$$U_m^{(s)} = \sum_{i=1}^{s} \gamma_{s-i}^{(s)} m^i. \qquad (84)$$

Lemma 5 in Appendix D.5 gives an expression for $U_m^{(s)}$. This together with $\gamma_s^{(s)} = s!$ from (64) reduces (83) to

$$\begin{aligned}
&s! \left(\begin{array}{c} s \\ k \end{array} \right) + \sum_{l=1}^{s-k} \left(\begin{array}{c} s-l \\ k \end{array} \right) \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) s! \left[\left(\begin{array}{c} m+s \\ s \end{array} \right) - 1 \right] = 0 \\
\iff\ &\left(\begin{array}{c} s \\ k \end{array} \right) + \sum_{l=1}^{s-k} \left(\begin{array}{c} s-l \\ k \end{array} \right) \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) \left[\left(\begin{array}{c} m+s \\ s \end{array} \right) - 1 \right] = 0. \qquad (85)
\end{aligned}$$

Now

$$\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) = \sum_{m=0}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) - 1 = -1, \quad l \neq 0, \qquad (86)$$

by (452). Also,

$$\begin{aligned}
\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) \left(\begin{array}{c} m+s \\ s \end{array} \right) &= \sum_{m=0}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) \left(\begin{array}{c} m+s \\ s \end{array} \right) - 1 \\
&= (-1)^l \left(\begin{array}{c} s \\ s-l \end{array} \right) - 1 = (-1)^l \left(\begin{array}{c} s \\ l \end{array} \right) - 1, \qquad (87)
\end{aligned}$$

by (456). Using (86) and (87) in (85), we need to show

$$\left(\begin{array}{c} s \\ k \end{array} \right) + \sum_{l=1}^{s-k} \left(\begin{array}{c} s-l \\ k \end{array} \right) \left[(-1)^l \left(\begin{array}{c} s \\ l \end{array} \right) - 1 - (-1) \right] = 0, \quad k = 0, \ldots, r-2,$$

which is equivalent to Lemma 6 in Appendix D.6, completing the proof of (77).

Now consider (78). Letting

$$S_i^{(s)} = \sum_{j=1}^{s} b_{ij}, \qquad (88)$$

and using (95) and (94), we rewrite (78) as

$$
\begin{aligned}
& -\sum_{i=1}^{r} \alpha_{k,i}^{(s)} \sum_{j=1}^{s} b_{ij} = \delta_k^{(s)}, \quad k = 0, \ldots, r-2 \\
\iff & \sum_{i=2}^{r} (i-1) \beta_{k,i-1}^{(s)} \sum_{j=1}^{s} b_{ij} = \delta_k^{(s)}, \quad k = 0, \ldots, r-2 \\
\iff & \sum_{i=1}^{s} i \beta_{k,i}^{(s)} S_{i+1}^{(s)} = (-1)^{s+1-k} \left(\begin{array}{c} s+1 \\ k \end{array} \right), \quad k = 0, \ldots, s-1. \qquad (89)
\end{aligned}
$$

Using (81) in (89), we rewrite the left side as

$$
\begin{aligned}
& (-1)^{s+1-k} \left(\begin{array}{c} s \\ k \end{array} \right) S_2^{(s)} + (-1)^{s-k} \sum_{i=2}^{s} i \sum_{l=0}^{s-k-1} (-1)^l \left(\begin{array}{c} s-l-1 \\ k \end{array} \right) \Sigma_l^{i-1} S_{i+1}^{(s)} \\
= & (-1)^{s+1-k} \left(\begin{array}{c} s \\ k \end{array} \right) S_2^{(s)} + (-1)^{s-k} \sum_{l=0}^{s-k-1} (-1)^l \left(\begin{array}{c} s-l-1 \\ k \end{array} \right) \sum_{i=2}^{s} i \Sigma_l^{i-1} S_{i+1}^{(s)} \\
= & (-1)^{s+1-k} \left(\begin{array}{c} s \\ k \end{array} \right) S_2^{(s)} + (-1)^{s-k} \sum_{l=0}^{s-k-1} (-1)^l \left(\begin{array}{c} s-l-1 \\ k \end{array} \right) M_l^{(s)}, \qquad (90)
\end{aligned}
$$

where

$$
M_l^{(s)} = \sum_{i=2}^{s} i \Sigma_l^{i-1} S_{i+1}^{(s)}. \qquad (91)
$$

We now make use of Lemmas 5 and 6 in Appendices D.5 and D.6. When $s = 1$, $k = 0, \ldots, s-1$ reduces to $k = 0$, and $M_l^{(s)} = 0$. So (90) becomes

$$
(-1)^{s+1-k} \left(\begin{array}{c} s \\ k \end{array} \right) 1 = (-1)^{s+1-k} \left(\begin{array}{c} s+1 \\ k \end{array} \right),
$$

which equals the right side of (89), as required. When $s \geq 2$, (90) becomes

$$
\begin{aligned}
& (-1)^{s-k} \left[- \left(\begin{array}{c} s \\ k \end{array} \right) s + \sum_{l=0}^{s-k-1} (-1)^l \left(\begin{array}{c} s-l-1 \\ k \end{array} \right) \left(\begin{array}{c} s \\ l+2 \end{array} \right) \right] \\
= & (-1)^{s-k} \left[- \left(\begin{array}{c} s \\ k \end{array} \right) s + \sum_{l=2}^{s-k+1} (-1)^l \left(\begin{array}{c} s-l+1 \\ k \end{array} \right) \left(\begin{array}{c} s \\ l \end{array} \right) \right] \\
= & (-1)^{s-k} \sum_{l=1}^{s-k+1} (-1)^l \left(\begin{array}{c} s-l+1 \\ k \end{array} \right) \left(\begin{array}{c} s \\ l \end{array} \right) \\
= & (-1)^{s-k+1} \sum_{l=0}^{s-k} (-1)^l \left(\begin{array}{c} s-l \\ k \end{array} \right) \left(\begin{array}{c} s \\ l+1 \end{array} \right),
\end{aligned}
$$

so that (89) becomes

$$\sum_{l=0}^{s-k}(-1)^l \left(\begin{array}{c} s-l \\ k \end{array} \right) \left(\begin{array}{c} s \\ l+1 \end{array} \right) = \left(\begin{array}{c} s+1 \\ k \end{array} \right), \quad k = 0, \ldots, s-1.$$

Letting $N = s-k$, $0 \le k \le s-1 \Rightarrow 1 \le s-k \le s$, so Lemma 9 in Appendix D.9 suffices. This completes the proof of (78), and so we have proven Theorem 5. □

C Theorem 6

Theorem 6 *Assume $z \neq 1/\lambda_i$ for $i = 1, \ldots, s$ and let*

$$\phi_r(w,z) = det(wI - \bar{M}_r(z)),$$

where $\bar{M}_r(z) = \bar{M}(z)$ defined in (47). Also let $c_i = 0$ for $i = 1, \ldots, s$. Then

$$\phi_r(w,z) = \sum_{k=0}^{r} \phi_k^{(r)}(z) w^k, \tag{92}$$

where

$$\phi_k^{(r)}(z) = \left\{ \begin{array}{ll} \delta_k^{(s)} + \sum_{i=1}^{r} \left[(\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z) a_i(z) \right], & k = 0, \ldots, r-1, \\ 1, & k = r, \end{array} \right. \tag{93}$$

$$s = r - 1 \ge 1,$$

$$\delta_k^{(s)} = (-1)^{s+1-k} \left(\begin{array}{c} s+1 \\ k \end{array} \right), \tag{94}$$

$$\alpha_{k,i}^{(s)} = \left\{ \begin{array}{ll} 0, & i = 1, \\ -(i-1)\beta_{k,i-1}^{(s)}, & i \ge 2, \end{array} \right. \tag{95}$$

$$\beta_{k,i}^{(s)} = \left\{ \begin{array}{ll} (-1)^{s+1-k} \left(\begin{array}{c} s \\ k \end{array} \right), & i = 1, \\ (-1)^{s-k} \left[\left(\begin{array}{c} s-1 \\ k \end{array} \right) + \sum_{l=1}^{s-k-1} (-1)^l \left(\begin{array}{c} s-l-1 \\ k \end{array} \right) \Sigma_l^{i-1} \right], & i \ge 2, \end{array} \right. \tag{96}$$

$$a_i(z) = \sum_{k=1}^{s} \frac{b_{ik}}{1 - \lambda_k z},$$

and

$$\Sigma_l^n = \left\{ \begin{array}{ll} \sum_{1 \le i_1 < \cdots < i_l \le n-1} \left(\begin{array}{c} i_2 \\ i_1 \end{array} \right) \left(\begin{array}{c} i_3 \\ i_2 \end{array} \right) \cdots \left(\begin{array}{c} i_l \\ i_{l-1} \end{array} \right) \left(\begin{array}{c} n \\ i_l \end{array} \right), & l \ge 1, \\ 1, & l = 0. \end{array} \right. \tag{97}$$

Remark. Again note that the requirement that $z \neq 1/\lambda_i$ for $i = 1, \ldots, s$ is a necessary restriction, since the factor $(I - zB_1)$ that occurs in both $M(z)$ and $\bar{M}(z)$ is singular if and only if $z = 1/\lambda_i$ for some $i = 1, \ldots, s$. If we choose $\lambda_i > 0$ for $i = 1, \ldots, s$, then $M(z)$ and $\bar{M}(z)$ are well defined and the single-eigenvalue property obtained by Theorem 5 holds for all $z \in \mathbb{C}^-$.

Proof. The proof is by induction on r. From (47), our $r \times r$ transformed stability matrix is

$$\bar{M}_r(z) = P + \bar{B}_2(I - zB_1)^{-1}V(zI - U),$$

where

$$P_{ij} = \begin{cases} \begin{pmatrix} j-1 \\ i-1 \end{pmatrix}, & j \geq i \\ 0, & j < i \end{cases},$$

$$B_1 = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_s \end{bmatrix},$$

$$s = r - 1,$$

and $V_{ij} = c_i^{j-1}$, but since all the c_i's are zero,

$$V = \begin{bmatrix} 1 & \\ \vdots & \bigcirc \\ 1 & \end{bmatrix}.$$

Then

$$V(zI - U) = \begin{bmatrix} 1 & \\ \vdots & \bigcirc \\ 1 & \end{bmatrix} \begin{bmatrix} z & -1 & & \\ & \ddots & \ddots & \\ & & \ddots & -(r-1) \\ & & & z \end{bmatrix} = \begin{bmatrix} z, & -1 & \\ \vdots & \vdots & \bigcirc \\ z, & -1 & \end{bmatrix},$$

and

$$(I - zB_1)^{-1}V(zI - U) = \begin{bmatrix} \frac{1}{1-\lambda_1 z} & & \\ & \ddots & \\ & & \frac{1}{1-\lambda_s z} \end{bmatrix} \begin{bmatrix} z, & -1 & \\ \vdots & \vdots & \bigcirc \\ z, & -1 & \end{bmatrix} = \begin{bmatrix} \frac{z}{1-\lambda_1 z}, & \frac{-1}{1-\lambda_1 z} & \\ \vdots & \vdots & \bigcirc \\ \frac{z}{1-\lambda_s z}, & \frac{-1}{1-\lambda_s z} & \end{bmatrix}.$$

Thus, letting $b_{ij} = (\bar{B}_2)_{ij}$ gives

$$\bar{M}_r(z)_{ij} = \begin{cases} P_{ij} + z\sum_{k=1}^{s} \frac{b_{ik}}{1-\lambda_k z}, & j = 1 \\ P_{ij} - \sum_{k=1}^{s} \frac{b_{ik}}{1-\lambda_k z}, & j = 2 \\ P_{ij}, & j \geq 3 \end{cases}$$

or

$$\bar{M}_r(z) = P + \begin{bmatrix} za_1(z), & -a_1(z) & \\ \vdots & \vdots & \bigcirc \\ za_r(z), & -a_r(z) & \end{bmatrix},$$

where

$$a_i(z) = \sum_{k=1}^{s} \frac{b_{ik}}{1-\lambda_k z}.$$

Then

$$\phi_r(w,z) = \det(wI - \bar{M}_r(z)) = (-1)^r \det(\bar{M}_r(z) - wI),$$

so that

$$(-1)^r \phi_r(w,z) = \det(\bar{M}_r(z) - wI) =$$

$$\begin{vmatrix} za_1 + \binom{0}{0} - w & -a_1 + \binom{1}{0} & \binom{2}{0} & \cdots & \binom{r-2}{0} & \binom{r-1}{0} \\ za_2 & -a_2 + \binom{1}{1} - w & \binom{2}{1} & \cdots & \binom{r-2}{1} & \binom{r-1}{1} \\ za_3 & -a_3 & \binom{2}{2} - w & \cdots & \binom{r-2}{2} & \binom{r-1}{2} \\ \vdots & \vdots & & \ddots & \vdots & \vdots \\ za_{r-1} & -a_{r-1} & \bigcirc & & \binom{r-2}{r-2} - w & \binom{r-1}{r-2} \\ za_r & -a_r & & & & \binom{r-1}{r-1} - w \end{vmatrix}, \tag{98}$$

an $r \times r$ matrix.

As noted earlier, the proof is by induction on $r \geq 2$. First consider the base case $r = 2$ ($s = 1$), for which (98) reduces to

$$\begin{aligned} (-1)^2 \phi_2(w,z) &= \begin{vmatrix} za_1 + 1 - w & -a_1 + 1 \\ za_2 & -a_2 + 1 - w \end{vmatrix} \\ &= (za_1 + 1 - w)(-a_2 + 1 - w) - (za_2)(-a_1 + 1) \\ &= (1-w)^2 + (1-w)za_1 - (1-w)a_2 - za_2 \\ &= 1 + za_1 - (1+z)a_2 + (-2 + a_2 - za_1)w + w^2. \end{aligned}$$

Therefore, from (92), we must show that

$$\begin{aligned} \phi_0^{(2)} &= 1 + za_1 - (1+z)a_2, \\ \phi_1^{(2)} &= -2 + a_2 - za_1, \\ \phi_2^{(2)} &= 1. \end{aligned}$$

From (94), (95), and (96),

$$\begin{aligned}
\delta_0^{(1)} &= (-1)^2 \left(\begin{array}{c} 2 \\ 0 \end{array} \right) = 1, \\
\delta_1^{(1)} &= (-1)^1 \left(\begin{array}{c} 2 \\ 1 \end{array} \right) = -2, \\
\alpha_{0,1}^{(1)} &= \alpha_{1,1}^{(1)} = 0, \\
\beta_{0,1}^{(1)} &= (-1)^2 \left(\begin{array}{c} 1 \\ 0 \end{array} \right) = 1, \\
\beta_{1,1}^{(1)} &= (-1)^1 \left(\begin{array}{c} 1 \\ 1 \end{array} \right) = -1, \\
\alpha_{0,2}^{(1)} &= -\beta_{0,1}^{(1)} = -1, \\
\alpha_{1,2}^{(1)} &= -\beta_{1,1}^{(1)} = 1, \\
\beta_{0,2}^{(1)} &= (-1)^1 \left[\left(\begin{array}{c} 0 \\ 0 \end{array} \right) + 0 \right] = -1, \\
\beta_{1,2}^{(1)} &= (-1)^0 \left[\left(\begin{array}{c} 0 \\ 1 \end{array} \right) + 0 \right] = 0.
\end{aligned}$$

Using these expressions in (93), we get

$$\begin{aligned}
\phi_0^{(2)} &= 1 + (0 + 1z)a_1 + (-1 - 1z)a_2 = 1 + za_1 - (1 + z)a_2, \\
\phi_1^{(2)} &= -2 + (0 - 1z)a_1 + (1 + 0z)a_2 = -2 + a_2 - za_1, \\
\phi_2^{(2)} &= 1,
\end{aligned}$$

as required.

The rest of the proof is devoted to the general case, $r \geq 3$ ($s \geq 2$). Expanding (98) along the last row gives

$$(-1)^r \phi_r(w,z) = (-1)^{r-1} z a_r \begin{vmatrix} -a_1 + \left(\begin{array}{c} 1 \\ 0 \end{array} \right) & \left(\begin{array}{c} 2 \\ 0 \end{array} \right) & \cdots & \left(\begin{array}{c} r-2 \\ 0 \end{array} \right) & \left(\begin{array}{c} r-1 \\ 0 \end{array} \right) \\ -a_2 + \left(\begin{array}{c} 1 \\ 1 \end{array} \right) - w & \left(\begin{array}{c} 2 \\ 1 \end{array} \right) & \cdots & \left(\begin{array}{c} r-2 \\ 1 \end{array} \right) & \left(\begin{array}{c} r-1 \\ 1 \end{array} \right) \\ -a_3 & \left(\begin{array}{c} 2 \\ 2 \end{array} \right) - w & \cdots & \left(\begin{array}{c} r-2 \\ 2 \end{array} \right) & \left(\begin{array}{c} r-1 \\ 2 \end{array} \right) \\ \vdots & \bigcirc & \ddots & \vdots & \vdots \\ -a_{r-1} & & & \left(\begin{array}{c} r-2 \\ r-2 \end{array} \right) - w & \left(\begin{array}{c} r-1 \\ r-2 \end{array} \right) \end{vmatrix}$$

$$+ \quad (-1)^r(-a_r)\begin{vmatrix} za_1+\binom{0}{0}-w & \binom{2}{0} & \cdots & \binom{r-2}{0} & \binom{r-1}{0} \\ za_2 & \binom{2}{1} & \cdots & \binom{r-2}{1} & \binom{r-1}{1} \\ za_3 & \binom{2}{2}-w & \cdots & \binom{r-2}{2} & \binom{r-1}{2} \\ \vdots & & \ddots & \vdots & \vdots \\ za_{r-1} & \bigcirc & & \binom{r-2}{r-2}-w & \binom{r-1}{r-2} \end{vmatrix} \tag{99}$$

$$+ \quad \left[\binom{r-1}{r-1}-w\right]\begin{vmatrix} za_1+\binom{0}{0}-w & -a_1+\binom{1}{0} & \binom{2}{0} & \cdots & \binom{r-2}{0} \\ za_2 & -a_2+\binom{1}{1}-w & \binom{2}{1} & \cdots & \binom{r-2}{1} \\ za_3 & -a_3 & \binom{2}{2}-w & \cdots & \binom{r-2}{2} \\ \vdots & \vdots & & \ddots & \vdots \\ za_{r-1} & -a_{r-1} & \bigcirc & & \binom{r-2}{r-2}-w \end{vmatrix}.$$

Let us call the three determinants above A, B and C, respectively, so that

$$(-1)^r\phi_r(w,z) = (-1)^{r-1}za_rA + (-1)^r(-a_r)B + \left[\binom{r-1}{r-1}-w\right]C. \tag{100}$$

Now $C = (-1)^{r-1}\phi_{r-1}(w,z)$ is known by induction, and A and B differ only in the first column. Let

$$D^{(s)} = \begin{vmatrix} \binom{2}{0} & \binom{3}{0} & \cdots & \binom{r-2}{0} & \binom{r-1}{0} \\ \binom{2}{1} & \binom{3}{1} & \cdots & \binom{r-2}{1} & \binom{r-1}{1} \\ \binom{2}{2}-w & \binom{3}{2} & \cdots & \binom{r-2}{2} & \binom{r-1}{2} \\ & & \ddots & \vdots & \vdots \\ \bigcirc & & & \binom{r-2}{r-2}-w & \binom{r-1}{r-2} \end{vmatrix},$$

and define

$$D^{(s)}_k = D^{(s)} \text{ with the } k\text{-th row crossed out.} \tag{101}$$

This gives an $(r-2)\times(r-2)$ determinant equal to columns 2 to $r-1$ of A and B. Expanding

A and B down the first column gives

$$A = \left[-a_1 + \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right] D_1^{(s)} - \left[-a_2 + \begin{pmatrix} 1 \\ 1 \end{pmatrix} - w\right] D_2^{(s)} - \sum_{i=3}^{r} (-1)^{(i-1)} a_i D_i^{(s)},$$

and

$$B = \left[z a_1 + \begin{pmatrix} 0 \\ 0 \end{pmatrix} - w\right] D_1^{(s)} - z a_2 D_2^{(s)} + \sum_{i=3}^{r} (-1)^{(i-1)} z a_i D_i^{(s)}.$$

Then (100) becomes

$$\begin{aligned}
& (-1)^r \phi_r(w,z) \\
= \; & (-1)^{r-1} z a_r A + (-1)^r (-a_r) B + \left[\begin{pmatrix} r-1 \\ r-1 \end{pmatrix} - w\right] (-1)^{r-1} \phi_{r-1}(w,z) \\
= \; & (-1)^{r-1} \left\{ a_r [zA + B] + \left[\begin{pmatrix} r-1 \\ r-1 \end{pmatrix} - w\right] \phi_{r-1}(w,z) \right\} \\
= \; & (-1)^{r-1} \left\{ a_r \left[z \left(-a_1 + \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) D_1^{(s)} - z \left(-a_2 + \begin{pmatrix} 1 \\ 1 \end{pmatrix} - w\right) D_2^{(s)} - z \sum_{i=3}^{r} (-1)^{i-1} a_i D_i^{(s)} \right.\right. \\
& \left. + \left(z a_1 + \begin{pmatrix} 0 \\ 0 \end{pmatrix} - w \right) D_1^{(s)} - z a_2 D_2^{(s)} + \sum_{i=3}^{r} (-1)^{i-1} z a_i D_i^{(s)} \right] \\
& \left. + \left[\begin{pmatrix} r-1 \\ r-1 \end{pmatrix} - w\right] \phi_{r-1}(w,z) \right\} \\
= \; & (-1)^{r-1} \left\{ a_r \left[(z+1-w) D_1^{(s)} + (zw - z) D_2^{(s)} \right] + (1-w) \phi_{r-1}(w,z) \right\},
\end{aligned}$$

which implies

$$\phi_r(w,z) = -a_r \left\{ (z+1-w) D_1^{(s)} + (zw - z) D_2^{(s)} \right\} - (1-w) \phi_{r-1}(w,z). \tag{102}$$

Our goal is to show that (93) = (102), so we need expressions for $D_1^{(s)}$ and $D_2^{(s)}$. We have from (101),

$$D_1^{(s)} = \begin{vmatrix}
\begin{pmatrix} 2 \\ 1 \end{pmatrix} & \begin{pmatrix} 3 \\ 1 \end{pmatrix} & \cdots & \cdots & \begin{pmatrix} r-1 \\ 1 \end{pmatrix} \\
1-w & \begin{pmatrix} 3 \\ 2 \end{pmatrix} & \cdots & \cdots & \begin{pmatrix} r-1 \\ 2 \end{pmatrix} \\
 & 1-w & \begin{pmatrix} 4 \\ 3 \end{pmatrix} & \cdots & \begin{pmatrix} r-1 \\ 3 \end{pmatrix} \\
 & & \ddots & & \vdots \\
 & \bigcirc & & 1-w & \begin{pmatrix} r-1 \\ r-2 \end{pmatrix}
\end{vmatrix},$$

and

$$D_2^{(s)} = \begin{vmatrix} 1 & 1 & \cdots & \cdots & 1 \\ 1-w & \binom{3}{2} & \cdots & \cdots & \binom{r-1}{2} \\ & 1-w & \binom{4}{3} & \cdots & \binom{r-1}{3} \\ & & \ddots & & \vdots \\ & \bigcirc & & 1-w & \binom{r-1}{r-2} \end{vmatrix}.$$

Note that $D_1^{(s)}$ and $D_2^{(s)}$ differ only in the first row, so we will expand them along that row. To do this we need to know the $(r-3)\times(r-3)$ determinants $\bar{M}_k^{(s)}$, which are defined by letting

$$\bar{M}^{(s)} = \begin{vmatrix} 1-w & \binom{3}{2} & \cdots & \cdots & \cdots & \binom{r-1}{2} \\ & 1-w & \binom{4}{3} & \cdots & \cdots & \binom{r-1}{3} \\ & & 1-w & \binom{5}{4} & \cdots & \binom{r-1}{4} \\ & \bigcirc & & \ddots & & \vdots \\ & & & & 1-w & \binom{r-1}{r-2} \end{vmatrix},$$

and

$$\bar{M}_k^{(s)} = \bar{M}^{(s)} \text{ with the } k\text{-th column crossed out.}$$

Then,

$$D_1^{(s)} = \sum_{k=1}^{s-1} (-1)^{k-1} \binom{k+1}{1} \bar{M}_k^{(s)}, \tag{103}$$

$$D_2^{(s)} = \sum_{k=1}^{s-1} (-1)^{k-1} \bar{M}_k^{(s)}. \tag{104}$$

Note that $\bar{M}_k^{(s)}$ is a block upper-triangular determinant, with the top-left block being itself upper triangular. Thus

$$\bar{M}_k^{(s)} = (1-w)^{k-1} M_{s-k-1}^{(s)}, \tag{105}$$

where for $n \geq 1$,

$$M_n^{(s)} = \begin{vmatrix} \binom{s-n+1}{s-n} & \cdots & \cdots & \binom{s}{s-n} \\ 1-w & \binom{s-n+2}{s-n+1} & \cdots & \binom{s}{s-n+1} \\ & \ddots & & \vdots \\ \bigcirc & & 1-w & \binom{s}{s-1} \end{vmatrix}, \tag{106}$$

an $n \times n$ determinant, and $M_0^{(s)} = 1$. Then from (103), (104), and (105),

$$D_1^{(s)} = \sum_{k=1}^{s-1} (-1)^{k-1}(k+1)(1-w)^{k-1} M_{s-k-1}^{(s)}, \tag{107}$$

$$D_2^{(s)} = \sum_{k=1}^{s-1} (-1)^{k-1}(1-w)^{k-1} M_{s-k-1}^{(s)}. \tag{108}$$

We now define a transformation on the arguments of the binomial coefficients in $M_n^{(s)}$, under which properties of the binomial coefficients are not invariant. Therefore, we will consider the binomial coefficient $\binom{i}{j}$ as an ordered pair $\begin{bmatrix} i \\ j \end{bmatrix}$ while we are using the transformation. We begin by writing (106) as

$$M_n^{(s)} = \begin{vmatrix} \begin{bmatrix} s-n+1 \\ s-n \end{bmatrix} & \cdots & \cdots & \begin{bmatrix} s \\ s-n \end{bmatrix} \\ 1-w & \begin{bmatrix} s-n+2 \\ s-n+1 \end{bmatrix} & \cdots & \begin{bmatrix} s \\ s-n+1 \end{bmatrix} \\ & \ddots & & \vdots \\ \bigcirc & & 1-w & \begin{bmatrix} s \\ s-1 \end{bmatrix} \end{vmatrix}. \tag{109}$$

We now define the transformation $\psi_n^{(s)}$ as follows. For any expression E, $\psi_n^{(s)}(E)$ is found by replacing every occurrence of $\begin{bmatrix} i \\ j \end{bmatrix}$ according to the mapping

$$\begin{bmatrix} i \\ j \end{bmatrix} \longmapsto \begin{bmatrix} i-(s-n) \\ j-(s-n-1) \end{bmatrix} = \begin{bmatrix} i-s+n \\ j-s+n+1 \end{bmatrix}.$$

Then $\psi_n^{(s)}(M_n^{(s)}) = M_n$, where

$$M_n = \begin{vmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} & \begin{bmatrix} 2 \\ 1 \end{bmatrix} & \cdots & \cdots & \begin{bmatrix} n \\ 1 \end{bmatrix} \\ 1-w & \begin{bmatrix} 2 \\ 2 \end{bmatrix} & \cdots & \cdots & \begin{bmatrix} n \\ 2 \end{bmatrix} \\ & 1-w & \begin{bmatrix} 3 \\ 3 \end{bmatrix} & \cdots & \begin{bmatrix} n \\ 3 \end{bmatrix} \\ & & \ddots & & \vdots \\ & \bigcirc & & 1-w & \begin{bmatrix} n \\ n \end{bmatrix} \end{vmatrix}, \tag{110}$$

and $\psi_n^{(s)^{-1}}(M_n) = M_n^{(s)}$, where $\psi_n^{(s)^{-1}}$ replaces every occurrence of $\begin{bmatrix} i \\ j \end{bmatrix}$ according to the inverse mapping

$$\begin{bmatrix} i \\ j \end{bmatrix} \longmapsto \begin{bmatrix} s-n+i \\ s-n+j-1 \end{bmatrix}.$$

Now we can work with the simple determinant M_n and then recover $M_n^{(s)}$ later. We now find an expression for M_n using Lemma 1 in Appendix D.1. Recall we are trying to show that (93) = (102). So far, we can write (102) in terms of $M_n^{(s)}$ using (107) and (108). Since Lemma 1 gives us an expression for M_n, we will now express $M_n^{(s)} = \psi_n^{(s)^{-1}}(M_n)$ in terms of M_n. Looking at (347), we define

$$\tilde{\Sigma}_l^{s,n} = \psi_n^{(s)^{-1}}(\bar{\Sigma}_l^n) = \bar{\Sigma}_l^n \Big|_{\begin{bmatrix} i \\ j \end{bmatrix} \leftarrow \begin{pmatrix} s-n+i \\ s-n+j-1 \end{pmatrix}}, \tag{111}$$

undoing the transformation and recovering the binomial coefficients from the ordered pairs. We can then write

$$M_n^{(s)} = \psi_n^{(s)^{-1}}(M_n) = \begin{cases} \sum_{k=0}^{n-1}(-1)^{n-k} w^k \sum_{l=1}^{n-k}(-1)^l \begin{pmatrix} n-l \\ k \end{pmatrix} \tilde{\Sigma}_l^{s,n}, & n \geq 1, \\ 1, & n = 0. \end{cases} \tag{112}$$

The special case $M_0^{(s)}$ comes from (105). Now, using (111) and (348), we find that

$$\tilde{\Sigma}_l^{s,n} = \begin{cases} \sum_{1 \leq i_1 < \cdots < i_{l-1} \leq n-1} \begin{pmatrix} s-n+i_1 \\ s-n \end{pmatrix} \begin{pmatrix} s-n+i_2 \\ s-n+i_1 \end{pmatrix} \cdots \\ \qquad \begin{pmatrix} s-n+i_{l-1} \\ s-n+i_{l-2} \end{pmatrix} \begin{pmatrix} s \\ s-n+i_{l-1} \end{pmatrix}, & l \geq 2 \\ \begin{pmatrix} s \\ s-n \end{pmatrix}, & l = 1 \end{cases}$$

$$= \begin{cases} \sum_{s-n+1\le i_1<\cdots<i_{l-1}\le s-1} \left(\begin{array}{c} i_1 \\ s-n \end{array} \right) \left(\begin{array}{c} i_2 \\ i_1 \end{array} \right) \cdots \left(\begin{array}{c} i_{l-1} \\ i_{l-2} \end{array} \right) \left(\begin{array}{c} s \\ i_{l-1} \end{array} \right), & l \ge 2 \\ \left(\begin{array}{c} s \\ n \end{array} \right), & l = 1. \end{cases} \tag{113}$$

We now use (102) together with (92) by induction to get

$$\phi_r(w,z) = -a_r(z)\left[(z+1-w)D_1^{(s)} + (zw-z)D_2^{(s)}\right] - (1-w)\sum_{k=0}^{r-1} w^k \phi_k^{(r-1)}. \tag{114}$$

Our goal now is to show that (114) = (92). We do this by comparing the terms involving $a_i(z)$ in both expressions, for $i = 1, \ldots, r$, and also the terms independent of any $a_i(z)$. First, note that, since no $D_k^{(s)}$ contains any $a_i(z)$, the coefficient of $a_r(z)$ in (114) is

$$-\left[(z+1-w)D_1^{(s)} + (zw-z)D_2^{(s)}\right], \tag{115}$$

and the terms involving $a_i(z)$, $i = 1, \ldots, r-1$, must be

$$\begin{aligned} & -(1-w)\sum_{k=0}^{r-1} w^k \phi_k^{(r-1)} \\ = & -\sum_{k=0}^{r-1} w^k \phi_k^{(r-1)} + \sum_{k=0}^{r-1} w^{k+1} \phi_k^{(r-1)} \\ = & -\sum_{k=0}^{r-1} w^k \phi_k^{(r-1)} + \sum_{k=1}^{r} w^k \phi_{k-1}^{(r-1)} \\ = & -\phi_0^{(r-1)} - \sum_{k=1}^{r-1} w^k (\phi_k^{(r-1)} - \phi_{k-1}^{(r-1)}) + w^r \phi_{r-1}^{(r-1)}. \end{aligned} \tag{116}$$

Therefore, we must show that the coefficients of $a_i(z)$, $i = 1, \ldots, r-1$, as well as the term independent of any $a_i(z)$ in (116) and (92) agree. First, consider the term with no $a_i(z)$'s. Using (93) and (94), we see that in (92) this term is

$$\begin{aligned} \sum_{k=0}^{r} w^k \delta_k^{(s)} &= \sum_{k=0}^{r} (-1)^{s+1-k} \left(\begin{array}{c} s+1 \\ k \end{array} \right) w^k \\ &= (-1)^{s+1} \sum_{k=0}^{s+1} (-1)^k \left(\begin{array}{c} s+1 \\ k \end{array} \right) w^k \end{aligned} \tag{117}$$

Using (93) and (94) in (116), we see that the term with no $a_i(z)$'s is

$$-\left[\delta_0^{(s-1)} + \sum_{k=1}^{r-1} w^k (\delta_k^{(s-1)} - \delta_{k-1}^{(s-1)}) - w^r \delta_{r-1}^{(s-1)}\right]$$

$$
\begin{aligned}
&= -(-1)^s \left[(-1)^0 \begin{pmatrix} s \\ 0 \end{pmatrix} + \sum_{k=1}^{s} (-1)^k \left(\begin{pmatrix} s \\ k \end{pmatrix} + \begin{pmatrix} s \\ k-1 \end{pmatrix} \right) w^k - (-1)^0 \begin{pmatrix} s \\ s \end{pmatrix} w^r \right] \\
&= (-1)^{s+1} \left[\begin{pmatrix} s+1 \\ 0 \end{pmatrix} + \sum_{k=1}^{s} (-1)^k \begin{pmatrix} s+1 \\ k \end{pmatrix} w^k - \begin{pmatrix} s+1 \\ s+1 \end{pmatrix} w^r \right] \\
&= (-1)^{s+1} \sum_{k=0}^{s+1} (-1)^k \begin{pmatrix} s+1 \\ k \end{pmatrix} w^k = (117),
\end{aligned}
$$

as required. Now let $i = 1, \ldots, r-1$ and consider the coefficients of $w^k a_i(z)$ in (116) and (92). In (92), we have for $k = 0, \ldots, r-1$

$$
\alpha_{k,i}^{(s)} + \beta_{k,i}^{(s)} z, \tag{118}
$$

and for $k = r$ the coefficient of $w^k a_i(z)$ is 0. In (116) there are 3 cases: First, when $k = 0$, the coefficient of $w^k a_i(z)$ in (116) is

$$
-\left(\alpha_{0,i}^{(s-1)} + \beta_{0,i}^{(s-1)} z \right), \tag{119}
$$

in which case we need to show

$$
\begin{aligned}
\alpha_{0,i}^{(s)} &= -\alpha_{0,i}^{(s-1)}, && (120) \\
\beta_{0,i}^{(s)} &= -\beta_{0,i}^{(s-1)}, && (121)
\end{aligned}
$$

for $i = 1, \ldots, r-1$. Second, when $k = 1, \ldots, r-1$, the coefficient of $w^k a_i(z)$ in (116) is

$$
-\left[\alpha_{k,i}^{(s-1)} + \beta_{k,i}^{(s-1)} z - \left(\alpha_{k-1,i}^{(s-1)} + \beta_{k-1,i}^{(s-1)} z \right) \right], \tag{122}
$$

in which case we need to show

$$
\begin{aligned}
\alpha_{k,i}^{(s)} &= -\alpha_{k,i}^{(s-1)} + \alpha_{k-1,i}^{(s-1)}, && (123) \\
\beta_{k,i}^{(s)} &= -\beta_{k,i}^{(s-1)} + \beta_{k-1,i}^{(s-1)}, && (124)
\end{aligned}
$$

for $k = 1, \ldots, r-1$ and $i = 1, \ldots, r-1$. Third, when $k = r$, the coefficient of $w^k a_i(z)$ in (116) is 0 as required, since $\phi_{r-1}^{(r-1)} = 1$ by (93). Consider the second equation (121) of the first case. Using (96), we have, for $i = 1$,

$$
LS = (-1)^{s+1} \begin{pmatrix} s \\ 0 \end{pmatrix} = (-1)^{s+1} = -(-1)^s \begin{pmatrix} s-1 \\ 0 \end{pmatrix} = RS.
$$

For $i > 1$,

$$\begin{aligned} LS &= (-1)^s \left[\begin{pmatrix} s-1 \\ 0 \end{pmatrix} + \sum_{l=1}^{s-1} (-1)^l \begin{pmatrix} s-l-1 \\ 0 \end{pmatrix} \Sigma_l^{i-1} \right] \\ &= (-1)^s \left[1 + \sum_{l=1}^{s-1} (-1)^l \Sigma_l^{i-1} \right], \\ RS &= -(-1)^{s-1} \left[\begin{pmatrix} s-2 \\ 0 \end{pmatrix} + \sum_{l=1}^{s-2} (-1)^l \begin{pmatrix} s-l-2 \\ 0 \end{pmatrix} \Sigma_l^{i-1} \right] \\ &= (-1)^s \left[1 + \sum_{l=1}^{s-2} (-1)^l \Sigma_l^{i-1} \right] \end{aligned}$$

and $LS = RS$ because, by (97), $i \leq r - 1 = s$ implies $\Sigma_{s-1}^{i-1} = 0$.

For (120), when $i = 1$, $LS = RS = 0$ by (95). When $i > 1$, using (95) together with (121), which we already proved, we get

$$LS = -(i-1)\beta_{0,i-1}^{(s)} = (i-1)\beta_{0,i-1}^{(s-1)} = RS.$$

Now consider the second equation (124) of the second case. Using (96), we have, for $i = 1$,

$$\begin{aligned} LS &= (-1)^{s+1-k} \begin{pmatrix} s \\ k \end{pmatrix}, \\ RS &= -\left[(-1)^{s-k} \begin{pmatrix} s-1 \\ k \end{pmatrix} - (-1)^{s-k+1} \begin{pmatrix} s-1 \\ k-1 \end{pmatrix} \right] \\ &= (-1)^{s+1-k} \left[\begin{pmatrix} s-1 \\ k \end{pmatrix} + \begin{pmatrix} s-1 \\ k-1 \end{pmatrix} \right] \\ &= (-1)^{s+1-k} \begin{pmatrix} s \\ k \end{pmatrix} = LS. \end{aligned}$$

For $i > 1$,

$$\begin{aligned} LS &= (-1)^{s-k} \left[\begin{pmatrix} s-1 \\ k \end{pmatrix} + \sum_{l=1}^{s-k-1} (-1)^l \begin{pmatrix} s-l-1 \\ k \end{pmatrix} \Sigma_l^{i-1} \right] \\ RS &= -\left\{ (-1)^{s-1-k} \left[\begin{pmatrix} s-2 \\ k \end{pmatrix} + \sum_{l=1}^{s-k-2} (-1)^l \begin{pmatrix} s-l-2 \\ k \end{pmatrix} \Sigma_l^{i-1} \right] \right. \\ &\quad \left. -(-1)^{s-k} \left[\begin{pmatrix} s-2 \\ k-1 \end{pmatrix} + \sum_{l=1}^{s-k-1} (-1)^l \begin{pmatrix} s-l-2 \\ k-1 \end{pmatrix} \Sigma_l^{i-1} \right] \right\} \\ &= (-1)^{s-k} \left\{ \begin{pmatrix} s-2 \\ k \end{pmatrix} + \begin{pmatrix} s-2 \\ k-1 \end{pmatrix} + \sum_{l=1}^{s-k-2} (-1)^l \left[\begin{pmatrix} s-l-2 \\ k \end{pmatrix} + \begin{pmatrix} s-l-2 \\ k-1 \end{pmatrix} \right] \Sigma_l^{i-1} \right. \end{aligned}$$

$$
\begin{aligned}
&+(-1)^{s-k-1}\left(\begin{array}{c} s-(s-k-1)-2 \\ k-1 \end{array}\right)\Sigma_{s-k-1}^{i-1}\Bigg\} \\
&= (-1)^{s-k}\left\{\left(\begin{array}{c} s-1 \\ k \end{array}\right)+\sum_{l=1}^{s-k-2}(-1)^l\left(\begin{array}{c} s-l-1 \\ k \end{array}\right)\Sigma_l^{i-1}+(-1)^{s-k-1}\left(\begin{array}{c} k-1 \\ k-1 \end{array}\right)\Sigma_{s-k-1}^{i-1}\right\} \\
&= (-1)^{s-k}\left\{\left(\begin{array}{c} s-1 \\ k \end{array}\right)+\sum_{l=1}^{s-k-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ k \end{array}\right)\Sigma_l^{i-1}\right\} \\
&= LS.
\end{aligned}
$$

For (123), when $i=1$, $LS=RS=0$. When $i>1$, using (95) together with (124), which we already proved, we get

$$
LS=-(i-1)\beta_{k,i-1}^{(s)}=-\left[-(i-1)\beta_{k,i-1}^{(s-1)}+(i-1)\beta_{k-1,i-1}^{(s-1)}\right]=RS.
$$

So we have established the agreement of all the terms in (114) and (92) except the $a_r(z)$ term, which we consider now.

The coefficient of $a_r(z)$ in (92) is

$$
\sum_{k=0}^{r}w^k\left(\alpha_{k,r}^{(s)}+\beta_{k,r}^{(s)}z\right), \tag{125}
$$

while that in (114) is

$$
-\left[(z+1-w)D_1^{(s)}+(zw-z)D_2^{(s)}\right]=-\left[z\left(D_1^{(s)}+(w-1)D_2^{(s)}\right)+(1-w)D_1^{(s)}\right].
$$

Thus we must show that

$$
\sum_{k=0}^{r}w^k\alpha_{k,r}^{(s)}=-(1-w)D_1^{(s)}, \tag{126}
$$

and

$$
\sum_{k=0}^{r}w^k\beta_{k,r}^{(s)}=-\left[D_1^{(s)}+(w-1)D_2^{(s)}\right]. \tag{127}
$$

Note first that the left sides of (126) and (127) have no terms with $k>s-1=r-2$. This is because, from (96),

$$
\beta_{k,r}^{(s)}=(-1)^{s-k}\left[\left(\begin{array}{c} s-1 \\ k \end{array}\right)+\sum_{l=1}^{s-k-1}\cdots\right],
$$

which is zero for $k>s-1$. It then follows from (95) that

$$
\alpha_{k,r}^{(s)}=-(r-1)\beta_{k,r-1}^{(s)}=-(r-1)(-1)^{s-k}\left[\left(\begin{array}{c} s-2 \\ k \end{array}\right)+\sum_{l=1}^{s-k-2}\cdots\right],
$$

which is zero for $k > s-2$. Thus we can replace (126) and (127) by

$$\sum_{k=0}^{r-2} w^k \alpha_{k,r}^{(s)} = -(1-w)D_1^{(s)}, \tag{128}$$

and

$$\sum_{k=0}^{r-2} w^k \beta_{k,r}^{(s)} = -\left[D_1^{(s)} + (w-1)D_2^{(s)}\right]. \tag{129}$$

From (112) we have

$$M_n^{(s)} = \begin{cases} \sum_{k=0}^{n-1}(-1)^{n-k} w^k T_{n,k}^{(s)}, & n \geq 1, \\ 1, & n = 0, \end{cases} \tag{130}$$

where

$$T_{n,k}^{(s)} = \sum_{l=1}^{n-k}(-1)^l \begin{pmatrix} n-l \\ k \end{pmatrix} \tilde{\Sigma}_l^{s,n}. \tag{131}$$

Using this in (107) and (108), we get

$$D_1^{(s)} = \sum_{n=1}^{s-2}(n+1)(1-w)^{n-1} \sum_{k=0}^{s-n-2}(-1)^{s-k} w^k T_{s-n-1,k}^{(s)} + (-1)^s s(1-w)^{s-2}, \tag{132}$$

$$D_2^{(s)} = \sum_{n=1}^{s-2}(1-w)^{n-1} \sum_{k=0}^{s-n-2}(-1)^{s-k} w^k T_{s-n-1,k}^{(s)} + (-1)^s (1-w)^{s-2}. \tag{133}$$

Looking at (132) and (133), we see that the highest power of w in $D_1^{(s)}$ and $D_2^{(s)}$ is $s-2$. So

$$D_1^{(s)} = \sum_{k=0}^{s-2} t_k w^k \tag{134}$$

$$D_2^{(s)} = \sum_{k=0}^{s-2} u_k w^k \tag{135}$$

for suitable t_k's and u_k's. Then (128) and (129) reduce to

$$\alpha_{k,r}^{(s)} = -t_k + t_{k-1}, \quad k = 0, \ldots, r-2, \tag{136}$$

$$\beta_{k,r}^{(s)} = -t_k - u_{k-1} + u_k, \quad k = 0, \ldots, r-2, \tag{137}$$

where

$$t_{-1} = u_{-1} = t_{r-2} = u_{r-2} = 0. \tag{138}$$

All that remains is to prove (136) and (137) subject to (138).

To this end, we now find expressions for the t_k's and u_k's. Consider the expression (133)

for $D_2^{(s)}$ first. The argument of the n-sum is

$$\begin{aligned}
& (1-w)^{n-1} \sum_{k=0}^{s-n-2} (-1)^{s-k} w^k T^{(s)}_{s-n-1,k} \\
= & \sum_{l=0}^{n-1} (-1)^l \left(\begin{array}{c} n-1 \\ l \end{array} \right) w^l \sum_{k=0}^{s-n-2} (-1)^{s-k} w^k T^{(s)}_{s-n-1,k} \\
= & (-1)^s \sum_{l=0}^{n-1} \sum_{k=0}^{s-n-2} (-1)^{l+k} \left(\begin{array}{c} n-1 \\ l \end{array} \right) T^{(s)}_{s-n-1,k} w^{l+k} \\
= & (-1)^s \sum_{k=0}^{s-n-2} \sum_{l=0}^{n-1} \alpha(k,l) w^{l+k}, \qquad (139)
\end{aligned}$$

where

$$\alpha(k,l) = (-1)^{l+k} \left(\begin{array}{c} n-1 \\ l \end{array} \right) T^{(s)}_{s-n-1,k}.$$

We want to express (139) as powers of w. Consider the general case

$$\sum_{k=0}^{a} \sum_{l=0}^{b} \alpha(k,l) w^{k+l}.$$

Let $p = k + l$, so that $l = p - k$. Then $0 \le p - k \le b \Longrightarrow p - b \le k \le p$, so that

$$\sum_{k=0}^{a} \sum_{l=0}^{b} \alpha(k,l) w^{k+l} = \sum_{p=0}^{a+b} \sum_{k=\max\{0,p-b\}}^{\min\{a,p\}} \alpha(k,p-k) w^p. \qquad (140)$$

In (139), $a = s-n-2$, $b = n-1$, and $a+b = s-3$. Therefore

$$(139) = (-1)^s \sum_{p=0}^{s-3} \sum_{k=\max\{0,p-n+1\}}^{\min\{s-n-2,p\}} (-1)^p w^p \left(\begin{array}{c} n-1 \\ p-k \end{array} \right) T^{(s)}_{s-n-1,k},$$

and so from (133),

$$\begin{aligned}
D_2^{(s)} &= (-1)^s \sum_{n=1}^{s-2} \sum_{p=0}^{s-3} (-1)^p w^p \sum_{k=\max\{0,p-n+1\}}^{\min\{s-n-2,p\}} \left(\begin{array}{c} n-1 \\ p-k \end{array} \right) T^{(s)}_{s-n-1,k} + (-1)^s \sum_{p=0}^{s-2} (-1)^p \left(\begin{array}{c} s-2 \\ p \end{array} \right) w^p \\
&= (-1)^s \left\{ \sum_{p=0}^{s-3} (-1)^p w^p \left[\sum_{n=1}^{s-2} \sum_{k=\max\{0,p-n+1\}}^{\min\{s-n-2,p\}} \left(\begin{array}{c} n-1 \\ p-k \end{array} \right) T^{(s)}_{s-n-1,k} + \left(\begin{array}{c} s-2 \\ p \end{array} \right) \right] + (-1)^s w^{s-2} \right\}.
\end{aligned}$$

Thus we have

$$u_p = \begin{cases} (-1)^{s+p}\left[\sum_{n=1}^{s-2}\sum_{k=\max\{0,p-n+1\}}^{\min\{s-n-2,p\}}\left(\begin{array}{c} n-1 \\ p-k \end{array}\right) T^{(s)}_{s-n-1,k} + \left(\begin{array}{c} s-2 \\ p \end{array}\right)\right], & p \le s-3, \\ 1, & p = s-2. \end{cases} \tag{141}$$

Similarly, for $D_1^{(s)}$,

$$t_p = \begin{cases} (-1)^{s+p}\left[\sum_{n=1}^{s-2}(n+1)\sum_{k=\max\{0,p-n+1\}}^{\min\{s-n-2,p\}}\left(\begin{array}{c} n-1 \\ p-k \end{array}\right) T^{(s)}_{s-n-1,k} + \left(\begin{array}{c} s-2 \\ p \end{array}\right) s\right], & p \le s-3, \\ s, & p = s-2. \end{cases} \tag{142}$$

Now we use (141) and (142) to prove (136) and (137). Consider (137) first. There are 3 cases: $k = 0$, $k = 1, \ldots, r-3$, and $k = r-2$. If $k = 0$, (137) requires

$$\beta^{(s)}_{0,r} = -t_0 + u_0. \tag{143}$$

If $s = 2$, the right side is $-s + 1 = -1$. From (96), the left side is

$$(-1)^2\left[\left(\begin{array}{c} 1 \\ 0 \end{array}\right) + (-1)^1\left(\begin{array}{c} 0 \\ 0 \end{array}\right)\Sigma_1^2\right] = 1 - \Sigma_1^2 = -1$$

by (97), as required. When $s \ge 3$, we see from (141), (142) and (131) that the right side of (143) is

$$\begin{aligned} -t_0 + u_0 &= -(-1)^s\left[\sum_{n=1}^{s-2} n \sum_{k=\max\{0,-n+1\}}^{\min\{s-n-2,0\}}\left(\begin{array}{c} n-1 \\ -k \end{array}\right) T^{(s)}_{s-n-1,k} + \left(\begin{array}{c} s-2 \\ 0 \end{array}\right)(s-1)\right] \\ &= -(-1)^s\left[\sum_{n=1}^{s-2} n T^{(s)}_{s-n-1,0} + (s-1)\right] \\ &= -(-1)^s\left[\sum_{n=1}^{s-2} n \sum_{l=1}^{s-n-1}(-1)^l\left(\begin{array}{c} s-n-1-l \\ 0 \end{array}\right)\tilde{\Sigma}_l^{s,s-n-1} + (s-1)\right] \\ &= -(-1)^s\left[\sum_{n=1}^{s-2} n \sum_{l=1}^{s-n-1}(-1)^l\tilde{\Sigma}_l^{s,s-n-1} + (s-1)\right]. \end{aligned}$$

Using (96), we see that the left side is

$$\begin{aligned} \beta^{(s)}_{0,r} &= (-1)^s\left[\left(\begin{array}{c} s-1 \\ 0 \end{array}\right) + \sum_{l=1}^{s-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ 0 \end{array}\right)\Sigma_l^{r-1}\right] \\ &= (-1)^s\left[1 + \sum_{l=1}^{s-1}(-1)^l\Sigma_l^{r-1}\right]. \end{aligned}$$

Therefore, (143) is equivalent to

$$\sum_{l=1}^{s-1}(-1)^l\Sigma_l^s = -s - \sum_{n=1}^{s-2} n \sum_{l=1}^{s-n-1}(-1)^l\tilde{\Sigma}_l^{s,s-n-1}$$

which in turn is equivalent to

$$\sum_{l=1}^{s-1}(-1)^l\Sigma_l^s = -s - \sum_{n=1}^{s-2}(s-n-1)\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n}. \tag{144}$$

Since the left side of (144) involves Σ_l^s and the right side involves $\tilde{\Sigma}_l^{s,n}$, we need to find a relationship between these two quantities. From (97),

$$\begin{aligned}
\Sigma_l^s &= \sum_{1\le i_1<\cdots<i_l\le s-1}\binom{i_2}{i_1}\binom{i_3}{i_2}\cdots\binom{i_l}{i_{l-1}}\binom{s}{i_l} \\
&= \sum_{i_1=1}^{s-l}\sum_{i_1<i_2<\cdots<i_l\le s-1}\binom{i_2}{i_1}\binom{i_3}{i_2}\cdots\binom{i_l}{i_{l-1}}\binom{s}{i_l} \\
&= \sum_{i=1}^{s-l}\sum_{i+1\le i_2<\cdots<i_l\le s-1}\binom{i_2}{i_1}\binom{i_3}{i_2}\cdots\binom{i_l}{i_{l-1}}\binom{s}{i_l} \\
&= \sum_{i=1}^{s-l}\tilde{\Sigma}_l^{s,s-i},
\end{aligned}$$

by (111). Thus

$$\Sigma_l^s = \sum_{n=1}^{s-l}\tilde{\Sigma}_l^{s,s-n}. \tag{145}$$

Using this in (144) reduces what we need to prove to

$$\sum_{l=1}^{s-1}(-1)^l\sum_{n=1}^{s-l}\tilde{\Sigma}_l^{s,s-n} = -s - \sum_{n=1}^{s-2}(s-n-1)\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n}. \tag{146}$$

Now switch the order of the sums on the left side of (146) to agree with those on the right side. When $l=1$, $n=1,\ldots,s-1$. When $l=s-1$, $n=1$. Thus, $l=1,\ldots,s-n$ and $n=1,\ldots,s-1$. So (146) is equivalent to

$$\begin{aligned}
&\sum_{n=1}^{s-1}\sum_{l=1}^{s-n}(-1)^l\tilde{\Sigma}_l^{s,s-n} = -s - \sum_{n=1}^{s-2}(s-n-1)\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n} \\
\iff\ &\sum_{n=1}^{s-1}\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n} = -s - \sum_{n=1}^{s-2}(s-n-1)\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n} \\
\iff\ &\sum_{n=1}^{s-2}\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n} + \sum_{l=1}^{s-1}(-1)^l\tilde{\Sigma}_l^{s,s-1} = -s - \sum_{n=1}^{s-2}(s-n-1)\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n}
\end{aligned}$$

$$\iff \sum_{n=1}^{s-2}(s-n)\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n}+\sum_{l=1}^{s-1}(-1)^l\tilde{\Sigma}_l^{s,s-1}+s=0 \tag{147}$$

Using Lemma 2 in Appendix D.2, we reduce the left side of (147) to

$$\begin{aligned}
&\sum_{n=1}^{s-2}(s-n)(-1)^n\begin{pmatrix} s \\ n \end{pmatrix}+(-1)^{s-1}\begin{pmatrix} s \\ s-1 \end{pmatrix}+s \\
= \;& s\sum_{n=1}^{s-2}(-1)^n\begin{pmatrix} s \\ n \end{pmatrix}-\sum_{n=1}^{s-2}(-1)^n n\begin{pmatrix} s \\ n \end{pmatrix}+(-1)^{s-1}s+s \\
= \;& s\left[\sum_{n=0}^{s}(-1)^n\begin{pmatrix} s \\ n \end{pmatrix}-(-1)^0\begin{pmatrix} s \\ 0 \end{pmatrix}-(-1)^{s-1}\begin{pmatrix} s \\ s-1 \end{pmatrix}-(-1)^s\begin{pmatrix} s \\ s \end{pmatrix}\right] \\
& -\left[\sum_{n=0}^{s}(-1)^n n\begin{pmatrix} s \\ n \end{pmatrix}-(-1)^0 0\begin{pmatrix} s \\ 0 \end{pmatrix}-(-1)^{s-1}(s-1)\begin{pmatrix} s \\ s-1 \end{pmatrix}-(-1)^s s\begin{pmatrix} s \\ s \end{pmatrix}\right] \\
& +(-1)^{s-1}s+s \\
= \;& s\left[0-1+(-1)^s s-(-1)^s\right]-\left[0-0+(-1)^s(s-1)s-(-1)^s s\right]-(-1)^s s+s=0,
\end{aligned}$$

since $s \geq 2$ implies

$$\sum_{n=0}^{s}(-1)^n\begin{pmatrix} s \\ n \end{pmatrix}=0$$

by (452) and

$$\sum_{n=0}^{s}(-1)^n n\begin{pmatrix} s \\ n \end{pmatrix}=0$$

by (450). This completes the proof of (143), the $k=0$ case of (137).

Now consider $k=r-2=s-1$, in which case (137) becomes

$$\beta_{s-1,r}^{(s)}=-t_{s-1}-u_{s-2}+u_{s-1}. \tag{148}$$

Using (141) and (138), we see that the right side of (148) equals $0-1+0=-1$, while, from (96), the left side equals $-(1+0)=-1$ also. Therefore, (148) holds, as required.

All that remains is to show that (137) holds for $k=1,\ldots,r-3=s-2$, which is equivalent to showing that

$$\beta_{k,r}^{(s)}=-t_k-u_{k-1}+u_k,$$

or, on substituting p for k,

$$\beta_{p,r}^{(s)}=-t_p-u_{p-1}+u_p, \quad \text{for } p=1,\ldots,s-2. \tag{149}$$

First consider $p=s-2$. Then, using (142), (141) and (131), we have

$$-t_p-u_{p-1}+u_p \;=\; -s-u_{s-3}+1$$

$$
\begin{aligned}
&= 1 - s + \left[\sum_{n=1}^{s-2} \left(\begin{array}{c} n-1 \\ n-1 \end{array} \right) T^{(s)}_{s-n-1,s-n-2} + \left(\begin{array}{c} s-2 \\ s-3 \end{array} \right) \right] \\
&= -1 + \sum_{n=1}^{s-2} T^{(s)}_{s-n-1,s-n-2} \\
&= -1 - \sum_{n=1}^{s-2} \left(\begin{array}{c} s-n-2 \\ s-n-2 \end{array} \right) \tilde{\Sigma}_1^{s,s-n-1} \\
&= -1 - \sum_{n=1}^{s-2} \tilde{\Sigma}_1^{s,n}, \qquad (150)
\end{aligned}
$$

where (150) follows from the line above it by reversing the order of the sum. We now apply (145) with $l = 1$ and (113) to get

$$
\sum_{n=1}^{s-2} \tilde{\Sigma}_1^{s,n} = \Sigma_1^s - \tilde{\Sigma}_1^{s,s-1} = \Sigma_1^s - \left(\begin{array}{c} s \\ s-1 \end{array} \right) = \Sigma_1^s - s.
$$

Using this in (150) gives $-1 - (\Sigma_1^s - s)$ for the right side of (149). From (96), the left side of (149) is

$$
\begin{aligned}
\beta^{(s)}_{s-2,r} &= \left(\begin{array}{c} s-1 \\ s-2 \end{array} \right) - \left(\begin{array}{c} s-2 \\ s-2 \end{array} \right) \Sigma_1^{r-1} \\
&= s - 1 - \Sigma_1^s,
\end{aligned}
$$

as required.

It remains to show (149) for $p = 1, \ldots, s-3$. The next large portion of the proof is devoted to this. For the right side of (149), we have

$$
\begin{aligned}
u_p - t_p - u_{p-1} &= (-1)^{s+p} \left[\sum_{n=1}^{s-2} (-n) \sum_{k=\max\{0,p-n+1\}}^{\min\{s-n-2,p\}} \left(\begin{array}{c} n-1 \\ p-k \end{array} \right) T^{(s)}_{s-n-1,k} + \left(\begin{array}{c} s-2 \\ p \end{array} \right) (1-s) \right] \\
&\quad -(-1)^{s+p-1} \left[\sum_{n=1}^{s-2} \sum_{k=\max\{0,p-n\}}^{\min\{s-n-2,p-1\}} \left(\begin{array}{c} n-1 \\ p-k-1 \end{array} \right) T^{(s)}_{s-n-1,k} + \left(\begin{array}{c} s-2 \\ p-1 \end{array} \right) \right]. \qquad (151)
\end{aligned}
$$

We handle the *min* and *max* occurring in the sums by splitting the range of n as follows.

$$
1 \le n \le p \implies \left\{ \begin{array}{l} \max\{0, p-n\} = p-n, \\ \max\{0, p-n+1\} = p-n+1, \end{array} \right. \qquad (152)
$$

$$
p+1 \le n \le s-2 \implies \left\{ \begin{array}{l} \max\{0, p-n\} = 0, \\ \max\{0, p-n+1\} = 0, \end{array} \right. \qquad (153)
$$

$$1 \le n \le s-p-2 \implies \begin{cases} \min\{s-n-2, p\} = p, \\ \min\{s-n-2, p-1\} = p-1, \end{cases} \tag{154}$$

$$s-p-1 \le n \le s-2 \implies \begin{cases} \min\{s-n-2, p\} = s-n-2, \\ \min\{s-n-2, p-1\} = s-n-2. \end{cases} \tag{155}$$

Are any of these ranges incompatible?

$$\text{(152) and (154)} \implies \begin{cases} p \ge 1, \\ s-p-2 \ge 1 \end{cases} \implies p \le s-3 \quad \text{(which is always true)},$$

$$\text{(152) and (155)} \implies s-p-1 \le p \Longrightarrow p \ge \frac{s-1}{2},$$

$$\text{(153) and (154)} \implies p+1 \le s-p-2 \Longrightarrow p \le \frac{s-3}{2},$$

$$\text{(153) and (155)} \implies \begin{cases} p+1 \le s-2, \\ s-p-1 \le s-2 \end{cases} \implies p \le s-3 \quad \text{(which is always true)}.$$

Thus, when $p \le (s-3)/2$, we have (152) and (154), (153) and (154), and (153) and (155); and when $p \ge (s-3)/2$, we have (152) and (154), (152) and (155), and (153) and (155).

First, assume

$$1 \le p \le \frac{s-3}{2}. \tag{156}$$

In this case, (151) becomes

$$\begin{aligned} & (-1)^{s+p} \left[\binom{s-2}{p} (1-s) + \binom{s-2}{p-1} \right] \\ + \; & (-1)^{s+p} \left\{ \sum_{n=1}^{p} \left[-n \sum_{k=p-n+1}^{p} \binom{n-1}{p-k} T^{(s)}_{s-n-1,k} + \sum_{k=p-n}^{p-1} \binom{n-1}{p-k-1} T^{(s)}_{s-n-1,k} \right] \right. \\ + \; & \sum_{n=p+1}^{s-p-2} \left[-n \sum_{k=0}^{p} \binom{n-1}{p-k} T^{(s)}_{s-n-1,k} + \sum_{k=0}^{p-1} \binom{n-1}{p-k-1} T^{(s)}_{s-n-1,k} \right] \\ + \; & \left. \sum_{n=s-p-1}^{s-2} \left[-n \sum_{k=0}^{s-n-2} \binom{n-1}{p-k} T^{(s)}_{s-n-1,k} + \sum_{k=0}^{s-n-2} \binom{n-1}{p-k-1} T^{(s)}_{s-n-1,k} \right] \right\} \end{aligned}$$

By (131), this is equivalent to

$$(-1)^{s+p} \left\{ \binom{s-2}{p} (1-s) + \binom{s-2}{p-1} \right. \tag{157}$$

$$\left. - \sum_{n=1}^{p} \sum_{k=p-n+1}^{p} \sum_{l=1}^{s-n-k-1} (-1)^l n \binom{n-1}{p-k} \binom{s-n-l-1}{k} \tilde{\Sigma}^{s,s-n-1}_{l} \right. \tag{158}$$

$$+ \sum_{n=1}^{p} \sum_{k=p-n}^{p-1} \sum_{l=1}^{s-n-k-1} (-1)^l \binom{n-1}{p-k-1} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \tag{159}$$

$$- \sum_{n=p+1}^{s-p-2} \sum_{k=0}^{p} \sum_{l=1}^{s-n-k-1} (-1)^l n \binom{n-1}{p-k} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \tag{160}$$

$$+ \sum_{n=p+1}^{s-p-2} \sum_{k=0}^{p-1} \sum_{l=1}^{s-n-k-1} (-1)^l \binom{n-1}{p-k-1} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \tag{161}$$

$$- \sum_{n=s-p-1}^{s-2} \sum_{k=0}^{s-n-2} \sum_{l=1}^{s-n-k-1} (-1)^l n \binom{n-1}{p-k} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \tag{162}$$

$$+ \sum_{n=s-p-1}^{s-2} \sum_{k=0}^{s-n-2} \sum_{l=1}^{s-n-k-1} (-1)^l \binom{n-1}{p-k-1} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \Bigg\} \tag{163}$$

From (96), the left side of (149) is

$$\beta_{p,r}^{(s)} = (-1)^{s+p} \left[\binom{s-1}{p} + \sum_{l=1}^{s-p-1} (-1)^l \binom{s-l-1}{p} \Sigma_l^s \right] \tag{164}$$

since $r \geq 3$. To show the left and right sides of (149) are indeed equal, we will switch the order of the sums in (157) to (163) from n, k, l to l, k, n and then evaluate the k sum, since $\tilde{\Sigma}_l^{s,s-n-1}$ is independent of k. We first derive some general formulas for switching sums and then use them in specific instances.

First, consider the sums

$$\sum_{k=a}^{b} \sum_{l=1}^{c-k},$$

where a, b, c are free. When $k = a$, $l = 1, \ldots, c-a$. When $k = b$, $l = 1, \ldots, c-b$. Thus, for $l = 1, \ldots, c-b$, $k = a, \ldots, b$, and for $l = c-b, \ldots, c-a$, $k = a, \ldots, c-l$. Therefore,

$$\sum_{k=a}^{b} \sum_{l=1}^{c-k} = \sum_{l=1}^{c-b} \sum_{k=a}^{b} + \sum_{l=c-b+1}^{c-a} \sum_{k=a}^{c-l}. \tag{165}$$

Next, consider the sums

$$\sum_{n=1}^{p} \sum_{l=a-n}^{b},$$

where a, b, p are free. When $n = 1$, $l = a-1, \ldots, b$. When $n = p$, $l = a-p, \ldots, b$. Thus, for $l = a-1, \ldots, b$, $n = 1, \ldots, p$, and for $l = a-p, \ldots, a-1$, $n = a-l, \ldots, p$. Therefore,

$$\sum_{n=1}^{p} \sum_{l=a-n}^{b} = \sum_{l=a-p}^{a-1} \sum_{n=a-l}^{p} + \sum_{l=a}^{b} \sum_{n=1}^{p}. \tag{166}$$

Now consider the sums

$$\sum_{n=a}^{b}\sum_{l=c-n}^{d},$$

where a, b, c, d are free. When $n = a$, $l = c - a, \ldots, d$. When $n = b$, $l = c - b, \ldots, d$. Thus, for $l = c - a, \ldots, d$, $n = a, \ldots, b$, and for $l = c - b, \ldots, c - a$, $n = c - l, \ldots, b$. Therefore,

$$\sum_{n=a}^{b}\sum_{l=c-n}^{d} = \sum_{l=c-b}^{c-a}\sum_{n=c-l}^{b} + \sum_{l=c-a+1}^{d}\sum_{n=a}^{b}. \tag{167}$$

Finally, consider the sums

$$\sum_{n=a}^{b}\sum_{l=c-n}^{d-n},$$

where a, b, c, d are free. When $n = a$, $l = c - a, \ldots, d - a$. When $n = b$, $l = c - b, \ldots, d - b$. Here we need to consider 2 cases. First, if $c-a \le d-b$, for $l = c-b, \ldots, c-a$, $n = c-l, \ldots, b$, for $l = c - a, \ldots, d - b$, $n = a, \ldots, b$, and for $l = d - b, \ldots, d - a$, $n = a, \ldots, d - l$. Second, if $d-b \le c-a$, for $l = c-b, \ldots, d-b$, $n = c-l, \ldots, b$, for $l = d-b, \ldots, c-a$, $n = c-l, \ldots, d-l$, and for $l = c - a, \ldots, d - a$, $n = a, \ldots, d - l$. Therefore, when $c - a \le d - b$,

$$\sum_{n=a}^{b}\sum_{l=c-n}^{d-n} = \sum_{l=c-b}^{c-a}\sum_{n=c-l}^{b} + \sum_{l=c-a+1}^{d-b}\sum_{n=a}^{b} + \sum_{l=d-b+1}^{d-a}\sum_{n=a}^{d-l}, \tag{168}$$

and when $d - b \le c - a$,

$$\sum_{n=a}^{b}\sum_{l=c-n}^{d-n} = \sum_{l=c-b}^{d-b}\sum_{n=c-l}^{b} + \sum_{l=d-b+1}^{c-a}\sum_{n=c-l}^{d-l} + \sum_{l=c-a+1}^{d-a}\sum_{n=a}^{d-l}. \tag{169}$$

This completes the general sum-reversal formulas. We now apply them.

It is convenient to work without the sum arguments, when possible, to avoid unnecessary clutter. Applying (165) to the k and l sums in (158) gives $a = p - n - 1$, $b = p$, $c = s - n - 1$, $c - b = s - n - p - 1$ and $c - a = s - p - 2$, so that

$$\begin{aligned}(158) &= -\sum_{n=1}^{p}\sum_{k=p-n+1}^{p}\sum_{l=1}^{s-n-k-1} \\ &= -\sum_{n=1}^{p}\sum_{l=1}^{s-n-p-1}\sum_{k=p-n+1}^{p} - \sum_{n=1}^{p}\sum_{l=s-n-p}^{s-p-2}\sum_{k=p-n+1}^{s-n-l-1}. \end{aligned}\tag{170}$$

Applying (165) again to the first n and l sums in (170) gives $a = 1$, $b = p$, $c = s - p - 1$, $c - b = s - 2p - 1$ and $c - a = s - p - 2$. Applying (166) to the second n and l sums in (170)

gives $a = s-p$ and $b = s-p-2$. Therefore,

$$\begin{aligned}(158) &= -\sum_{l=1}^{s-2p-1}\sum_{n=1}^{p}\sum_{k=p-n+1}^{p} - \sum_{l=s-2p}^{s-p-2}\sum_{n=1}^{s-p-l-1}\sum_{k=p-n+1}^{p} \\ &\quad - \sum_{l=s-2p}^{s-p-1}\sum_{n=s-l-p}^{p}\sum_{k=p-n+1}^{s-n-l-1} - \sum_{l=s-p}^{s-p-2}\sum_{n=1}^{p}\sum_{k=p-n+1}^{s-n-l-1}. \qquad (171)\end{aligned}$$

(Note that the last l sum is empty). Recovering the arguments from (158), we now evaluate the k sums appearing in (171). The first one is

$$\begin{aligned}\sum_{k=p-n+1}^{p}\binom{n-1}{p-k}\binom{s-n-l-1}{k} &= \sum_{k=0}^{n-1}\binom{n-1}{n-1-k}\binom{s-n-l-1}{k+p-n+1} \\ &= \binom{n-1+s-n-l-1}{n-1+p-n+1} \\ &= \binom{s-l-2}{p}, \qquad (172)\end{aligned}$$

by (455). The second k sum is

$$\begin{aligned}&\sum_{k=p-n+1}^{s-n-l-1}\binom{n-1}{p-k}\binom{s-n-l-1}{k} \\ =\ &\sum_{k=0}^{s-p-l-2}\binom{n-1}{n-1-k}\binom{s-n-l-1}{k+p-n+1} \\ =\ &\sum_{k=0}^{s-p-l-2}\binom{n-1}{k}\binom{s-n-l-1}{k+p-n+1} \\ =\ &\sum_{k=0}^{N}\binom{x}{k}\binom{N+r}{k+r} \quad \text{for } N=s-p-l-2,\ x=n-1,\ r=p-n+1 \\ =\ &\sum_{k=0}^{N}\binom{x}{k}\binom{N+r}{N-k} \\ =\ &\binom{x+N+r}{N} = \binom{x+N+r}{x+r} = \binom{s-l-2}{p}, \qquad (173)\end{aligned}$$

by (453). Then, from (158), (171), (172) and (173), we have

$$\begin{aligned}(158) &= -\sum_{l=1}^{s-2p-1}(-1)^l\binom{s-l-2}{p}\sum_{n=1}^{p} n\tilde{\Sigma}_l^{s,s-n-1} \\ &\quad -\sum_{l=s-2p}^{s-p-2}(-1)^l\binom{s-l-2}{p}\sum_{n=1}^{s-p-l-1} n\tilde{\Sigma}_l^{s,s-n-1}\end{aligned}$$

$$-\sum_{l=s-2p}^{s-p-1}(-1)^l\binom{s-l-2}{p}\sum_{n=s-l-p}^{p} n\tilde{\Sigma}_l^{s,s-n-1}. \tag{174}$$

Applying (165) to the k and l sums in (159) gives $a=p-n$, $b=p-1$, $c=s-n-1$, $c-b=s-p-n$ and $c-a=s-p-1$, so that

$$\begin{aligned}(159) &= \sum_{n=1}^{p}\sum_{k=p-n}^{p-1}\sum_{l=1}^{s-n-k-1}\\ &= \sum_{n=1}^{p}\sum_{l=1}^{s-p-n}\sum_{k=p-n}^{p-1}+\sum_{n=1}^{p}\sum_{l=s-p-n-1}^{s-p-1}\sum_{k=p-n}^{s-n-l-1}.\end{aligned} \tag{175}$$

Applying (165) again to the first n and l sums in (175) gives $a=1$, $b=p$, $c=s-p$, $c-b=s-2p$ and $c-a=s-p-1$. Applying (166) to the second n and l sums in (175) gives $a=s-p+1$ and $b=s-p-1$. Therefore,

$$\begin{aligned}(159) &= \sum_{l=1}^{s-2p}\sum_{n=1}^{p}\sum_{k=p-n}^{p-1}+\sum_{l=s-2p+1}^{s-p-1}\sum_{n=1}^{s-p-l}\sum_{k=p-n}^{p-1}\\ &\quad+\sum_{l=s-2p+1}^{s-p}\sum_{n=s-l-p+1}^{p}\sum_{k=p-n}^{s-n-l-1}+\sum_{l=s-p+1}^{s-p-2}.\end{aligned} \tag{176}$$

(Note that the last sum is empty). Recovering the arguments from (159), we now evaluate the k sums appearing in (176). The first one is

$$\begin{aligned}\sum_{k=p-n}^{p-1}\binom{n-1}{p-k-1}\binom{s-n-l-1}{k} &= \sum_{k=0}^{n-1}\binom{n-1}{n-k-1}\binom{s-n-l-1}{k+p-n}\\ &= \binom{n-1+s-n-l-1}{n-1+p-n}\\ &= \binom{s-l-2}{p-1},\end{aligned} \tag{177}$$

by (455). The second k sum is

$$\begin{aligned}&\sum_{k=p-n}^{s-n-l-1}\binom{n-1}{p-k-1}\binom{s-n-l-1}{k}\\ =\ &\sum_{k=0}^{s-p-l-1}\binom{n-1}{n-1-k}\binom{s-n-l-1}{k+p-n}\\ =\ &\sum_{k=0}^{s-p-l-1}\binom{n-1}{k}\binom{s-n-l-1}{k+p-n}\end{aligned}$$

$$= \sum_{k=0}^{N} \left(\begin{array}{c} x \\ k \end{array} \right) \left(\begin{array}{c} N+r \\ k+r \end{array} \right) \quad \text{for } N = s-p-l-1, x = n-1, r = p-n$$
$$= \sum_{k=0}^{N} \left(\begin{array}{c} x \\ k \end{array} \right) \left(\begin{array}{c} N+r \\ N-k \end{array} \right)$$
$$= \left(\begin{array}{c} x+N+r \\ N \end{array} \right) = \left(\begin{array}{c} x+N+r \\ x+r \end{array} \right) = \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right), \tag{178}$$

by (453). Then, from (159), (176), (177) and (178), we have

$$\begin{aligned} (159) &= \sum_{l=1}^{s-2p} (-1)^l \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right) \sum_{n=1}^{p} \tilde{\Sigma}_l^{s,s-n-1} \\ &+ \sum_{l=s-2p+1}^{s-p-1} (-1)^l \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right) \sum_{n=1}^{s-p-l} \tilde{\Sigma}_l^{s,s-n-1} \\ &+ \sum_{l=s-2p+1}^{s-p} (-1)^l \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right) \sum_{n=s-l-p+1}^{p} \tilde{\Sigma}_l^{s,s-n-1}. \end{aligned} \tag{179}$$

Applying (165) to the k and l sums in (162) gives $a = 0$, $b = s-n-2$, $c = s-n-1$, $c-b = 1$ and $c-a = s-n-1$, so that

$$\begin{aligned} (162) &= -\sum_{n=s-p-1}^{s-2} \sum_{k=0}^{s-n-2} \sum_{l=1}^{s-n-k-1} \\ &= -\sum_{n=s-p-1}^{s-2} \sum_{l=1}^{s-n-1} \sum_{k=0}^{s-n-l-1}. \end{aligned} \tag{180}$$

Applying (165) again to the n and l sums in (180) gives $a = s-p-1$, $b = s-2$, $c = s-1$, $c-b = 1$ and $c-a = p$. Therefore,

$$(162) = -\sum_{l=1}^{p} \sum_{n=s-p-1}^{s-l-1} \sum_{k=0}^{s-n-l-1} \tag{181}$$

Recovering the arguments from (162), we now evaluate the k sum appearing in (181).

$$\sum_{k=0}^{s-n-l-1} \left(\begin{array}{c} n-1 \\ p-k \end{array} \right) \left(\begin{array}{c} s-n-l-1 \\ k \end{array} \right)$$
$$= \sum_{k=0}^{N} \left(\begin{array}{c} n-1 \\ p-k \end{array} \right) \left(\begin{array}{c} N \\ k \end{array} \right) \quad \text{for } N = s-n-l-1$$
$$= \sum_{k=0}^{N} \left(\begin{array}{c} n-1 \\ n-1-p+k \end{array} \right) \left(\begin{array}{c} N \\ k \end{array} \right)$$

$$
\begin{aligned}
&= \begin{pmatrix} N+n-1 \\ N+n-1-p \end{pmatrix} \\
&= \begin{pmatrix} N+n-1 \\ p \end{pmatrix} \\
&= \begin{pmatrix} s-l-2 \\ p \end{pmatrix}, \qquad (182)
\end{aligned}
$$

by (455). Then, from (162), (181) and (182), we have

$$
(162) \;=\; -\sum_{l=1}^{p}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=s-p-1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1}. \qquad (183)
$$

For (163), the same sums as for (162) appear, so that (181) applies. Recovering the arguments from (163), we now evaluate the k sum appearing in (181).

$$
\begin{aligned}
&\sum_{k=0}^{s-n-l-1} \begin{pmatrix} n-1 \\ p-k-1 \end{pmatrix} \begin{pmatrix} s-n-l-1 \\ k \end{pmatrix} \\
&= \sum_{k=0}^{N} \begin{pmatrix} n-1 \\ p-k-1 \end{pmatrix} \begin{pmatrix} N \\ k \end{pmatrix} \\
&= \sum_{k=0}^{N} \begin{pmatrix} n-1 \\ n-p+k \end{pmatrix} \begin{pmatrix} N \\ k \end{pmatrix} \quad \text{for } N = s-n-l-1 \\
&= \begin{pmatrix} N+n-1 \\ N+n-p \end{pmatrix} \\
&= \begin{pmatrix} N+n-1 \\ p-1 \end{pmatrix} \\
&= \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix}, \qquad (184)
\end{aligned}
$$

by (455). Then, from (163), (181) and (184), we have

$$
(163) \;=\; \sum_{l=1}^{p}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=s-p-1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1}. \qquad (185)
$$

Now consider (160), which is somewhat more involved. Applying (165) to the k and l sums in (160) gives $a = 0$, $b = p$, $c = s-n-1$, $c-b = s-n-p-1$ and $c-a = s-n-1$, so that

$$
(160) \;=\; -\sum_{n=p+1}^{s-p-2} \sum_{k=0}^{p} \sum_{l=1}^{s-n-k-1}
$$

$$= -\sum_{n=p+1}^{s-p-2}\sum_{l=1}^{s-p-n-1}\sum_{k=0}^{p} - \sum_{n=p+1}^{s-p-2}\sum_{l=s-p-n}^{s-n-1}\sum_{k=0}^{s-n-l-1}. \tag{186}$$

Applying (165) again to the first n and l sums in (186) gives $a = p+1$, $b = s-p-2$, $c = s-p-1$, $c-b = 1$ and $c-a = s-2p-2$, so that

$$\sum_{n=p+1}^{s-p-2}\sum_{l=1}^{s-p-n-1} = \sum_{l=1}^{s-2p-2}\sum_{n=p+1}^{s-p-l-1}. \tag{187}$$

For the second n and l sums in (186), we must consider whether (168) or (169) applies. We have $a = p+1$, $b = s-p-2$, $c = s-p$, and $d = s-1$, hence

$$c-a = s-2p-1, \quad c-b = 2, \quad d-a = s-p-2, \quad d-b = p+1. \tag{188}$$

(168) applies when

$$\begin{aligned} c-a \le d-b &\iff s-2p-1 \le p+1 \\ &\iff p \ge \frac{s-2}{3}, \end{aligned} \tag{189}$$

and (169) applies when

$$\begin{aligned} d-b \le c-a &\iff s-2p-1 \ge p+1 \\ &\iff p \le \frac{s-2}{3}. \end{aligned} \tag{190}$$

We are currently assuming $1 \le p \le (s-3)/2$ from (156), which implies $s \ge 5$. However,

$$\frac{s-3}{2} \ge \frac{s-2}{3} \iff 3s-9 \ge 2s-4 \iff s \ge 5,$$

so that

$$\frac{s-3}{2} \ge \frac{s-2}{3}.$$

This means, for $1 \le p \le (s-3)/2$, both cases (189) and (190) occur. So we need to consider two sub-cases:

$$1 \le \quad p \quad \le \frac{s-2}{3}, \tag{191}$$

$$\frac{s-2}{3} \le \quad p \quad \le \frac{s-3}{2}, \tag{192}$$

for which (169) and (168) apply, respectively.

Consider (191) first. Using (188) in (169), we find that the second n and l sums in (186)

become

$$\sum_{n=p+1}^{s-p-2}\sum_{l=s-p-n}^{s-n-1} = \sum_{l=2}^{p}\sum_{n=s-p-l}^{s-p-2} + \sum_{l=p+1}^{s-2p-1}\sum_{n=s-p-l}^{s-l-1} + \sum_{l=s-2p}^{s-p-2}\sum_{n=p+1}^{s-l-1}. \tag{193}$$

Now consider (192). Using (188) in (168), we find that the second n and l sums in (186) become

$$\sum_{n=p+1}^{s-p-2}\sum_{l=s-p-n}^{s-n-1} = \sum_{l=2}^{s-2p-1}\sum_{n=s-p-l}^{s-p-2} + \sum_{l=s-2p}^{p}\sum_{n=p+1}^{s-p-2} + \sum_{l=p+1}^{s-p-2}\sum_{n=p+1}^{s-l-1}. \tag{194}$$

Recovering the arguments from (160), we now evaluate the k sum appearing in (186).

$$\begin{aligned}
&\sum_{k=0}^{s-n-l-1}\binom{n-1}{p-k}\binom{s-n-l-1}{k}\\
&= \sum_{k=0}^{N}\binom{n-1}{n-1-p+k}\binom{N}{k} \quad \text{for } N = s-n-l-1\\
&= \binom{N+n-1}{N+n-1-p}\\
&= \binom{N+n-1}{p}\\
&= \binom{s-l-2}{p}, \qquad (195)
\end{aligned}$$

by (455). Then, from (160), (187), (193) and (195), we have

$$\begin{aligned}
(160) \;=\; &-\sum_{l=2}^{p}(-1)^l\binom{s-l-2}{p}\sum_{n=s-p-l}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1}\\
&-\sum_{l=p+1}^{s-2p-1}(-1)^l\binom{s-l-2}{p}\sum_{n=s-p-l}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1}\\
&-\sum_{l=s-2p}^{s-p-2}(-1)^l\binom{s-l-2}{p}\sum_{n=p+1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1}\\
&-\sum_{l=1}^{s-2p-2}(-1)^l\binom{s-l-2}{p}\sum_{n=p+1}^{s-p-l-1} n\tilde{\Sigma}_l^{s,s-n-1}, \qquad (196)
\end{aligned}$$

for $1 \le p \le \frac{s-2}{3}$. Similarly, from (160), (187), (194) and (195), we have

$$\begin{aligned}
(160) \;=\; &-\sum_{l=2}^{s-2p-1}(-1)^l\binom{s-l-2}{p}\sum_{n=s-p-l}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1}\\
&-\sum_{l=s-2p}^{p}(-1)^l\binom{s-l-2}{p}\sum_{n=p+1}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1}
\end{aligned}$$

$$
\begin{aligned}
&- \sum_{l=p+1}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=p+1}^{s-l-1} n \tilde{\Sigma}_l^{s,s-n-1} \\
&- \sum_{l=1}^{s-2p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=p+1}^{s-p-l-1} n \tilde{\Sigma}_l^{s,s-n-1},
\end{aligned} \tag{197}
$$

for $\frac{s-2}{3} \leq p \leq \frac{s-3}{2}$.

Now consider (161). Applying (165) to the k and l sums in (161) gives $a = 0$, $b = p-1$, $c = s-n-1$, $c-b = s-p-n$ and $c-a = s-n-1$, so that

$$
(161) = \sum_{n=p+1}^{s-p-2} \sum_{k=0}^{p-1} \sum_{l=1}^{s-n-k-1} = \sum_{n=p+1}^{s-p-2} \sum_{l=1}^{s-p-n} \sum_{k=0}^{p-1} + \sum_{n=p+1}^{s-p-2} \sum_{l=s-p-n+1}^{s-n-1} \sum_{k=0}^{s-n-l-1}. \tag{198}
$$

Applying (165) again to the first n and l sums in (198) gives $a = p+1$, $b = s-p-2$, $c = s-p$, $c-b = 2$ and $c-a = s-2p-1$, so that

$$
\sum_{n=p+1}^{s-p-2} \sum_{l=1}^{s-p-n} = \sum_{l=1}^{2} \sum_{n=p+1}^{s-p-2} + \sum_{l=3}^{s-2p-1} \sum_{n=p+1}^{s-p-l}. \tag{199}
$$

For the second n and l sums in (198), we must again consider whether (168) or (169) applies. We have $a = p+1$, $b = s-p-2$, $c = s-p+1$, and $d = s-1$, hence

$$
c-a = s-2p, \quad c-b = 3, \quad d-a = s-p-2, \quad d-b = p+1. \tag{200}
$$

(168) applies when

$$
\begin{aligned}
c-a \leq d-b &\iff s-2p \leq p+1 \\
&\iff p \geq \frac{s-1}{3},
\end{aligned} \tag{201}
$$

and (169) applies when

$$
\begin{aligned}
d-b \leq c-a &\iff s-2p \geq p+1 \\
&\iff p \leq \frac{s-1}{3}.
\end{aligned} \tag{202}
$$

We are currently assuming $1 \leq p \leq (s-3)/2$ (156), which implies $s \geq 5$. However,

$$
\frac{s-1}{3} \geq \frac{s-3}{2} \iff 2s-2 \geq 3s-9 \iff s \geq 7,
$$

so that

$$
\frac{s-3}{2} \geq \frac{s-2}{3}.
$$

Again this means, for $1 \leq p \leq (s-3)/2$, both cases (201) and (202) occur. So we need to

consider two sub-cases:

$$1 \leq \quad p \quad \leq \frac{s-1}{3}, \tag{203}$$

$$\frac{s-1}{3} \leq \quad p \quad \leq \frac{s-3}{2}, \tag{204}$$

for which (169) and (168) apply, respectively.

Consider (203) first. Using (200) in (169), we see that the second n and l sums in (198) become

$$\sum_{n=p+1}^{s-p-2} \sum_{l=s-p-n+1}^{s-n-1} = \sum_{l=3}^{p} \sum_{n=s-p-l+1}^{s-p-2} + \sum_{l=p+1}^{s-2p} \sum_{n=s-p-l+1}^{s-l-1} + \sum_{l=s-2p+1}^{s-p-2} \sum_{n=p+1}^{s-l-1}. \tag{205}$$

Now consider (204). Using (200) in (168), we see that the second n and l sums in (198) become

$$\sum_{n=p+1}^{s-p-2} \sum_{l=s-p-n+1}^{s-n-1} = \sum_{l=3}^{s-2p} \sum_{n=s-p-l+1}^{s-p-2} + \sum_{l=s-2p+1}^{p} \sum_{n=p+1}^{s-p-2} + \sum_{l=p+1}^{s-p-2} \sum_{n=p+1}^{s-l-1}. \tag{206}$$

Recovering the arguments from (161), we now evaluate the k sums appearing in (198). For the first k sum, we have

$$\sum_{k=0}^{p-1} \left(\begin{array}{c} n-1 \\ p-k-1 \end{array} \right) \left(\begin{array}{c} s-n-l-1 \\ k \end{array} \right) = \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right), \tag{207}$$

by (453). For the second k sum,

$$\begin{aligned} & \sum_{k=0}^{s-n-l-1} \left(\begin{array}{c} n-1 \\ p-k-1 \end{array} \right) \left(\begin{array}{c} s-n-l-1 \\ k \end{array} \right) \\ = & \sum_{k=0}^{N} \left(\begin{array}{c} n-1 \\ n-p+k \end{array} \right) \left(\begin{array}{c} N \\ k \end{array} \right) \quad \text{for } N = s-n-l-1 \\ = & \left(\begin{array}{c} N+n-1 \\ N+n-p \end{array} \right) \\ = & \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right), \end{aligned} \tag{208}$$

by (455). Then, from (161), (199), (205), (207) and (208), we have

$$\begin{aligned} (161) \quad = \quad & \sum_{l=3}^{p} (-1)^l \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right) \sum_{n=s-p-l+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \\ + \quad & \sum_{l=p+1}^{s-2p} (-1)^l \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right) \sum_{n=s-p-l+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \end{aligned}$$

$$
\begin{aligned}
&+ \sum_{l=s-2p+1}^{s-p-2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \\
&+ \sum_{l=1}^{2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \\
&+ \sum_{l=3}^{s-2p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-l} \tilde{\Sigma}_l^{s,s-n-1}, \qquad (209)
\end{aligned}
$$

for $1 \le p \le \frac{s-1}{3}$. Similarly, from (161), (199), (206), (207) and (208), we have

$$
\begin{aligned}
(161) &= \sum_{l=3}^{s-2p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-l+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \\
&+ \sum_{l=s-2p+1}^{p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \\
&+ \sum_{l=p+1}^{s-p-2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \\
&+ \sum_{l=1}^{2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \\
&= \sum_{l=3}^{s-2p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-l} \tilde{\Sigma}_l^{s,s-n-1}, \qquad (210)
\end{aligned}
$$

for $\frac{s-1}{3} \le p \le \frac{s-3}{2}$.

Recall that we are trying to show (149) for $p = 1, \ldots, s-3$. So far, we have all the cases for $1 \le p \le (s-3)/2$, and this interval is handled in two parts, $1 \le p \le (s-2)/3$ and $(s-1)/3 \le p \le (s-3)/2$. The left side of (149) is (164). When $1 \le p \le (s-2)/3$, the right side is assembled from (157), (174), (179), (196), (209), (183) and (185). This equals

$$
\begin{aligned}
&(-1)^{s+p} \left[\binom{s-2}{p} (1-s) + \binom{s-2}{p-1} \right. && (211) \\
&- \sum_{l=1}^{s-2p-1} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{p} n \tilde{\Sigma}_l^{s,s-n-1} && (212) \\
&- \sum_{l=s-2p}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{s-p-l-1} n \tilde{\Sigma}_l^{s,s-n-1} && (213) \\
&- \sum_{l=s-2p}^{s-p-1} (-1)^l \binom{s-l-2}{p} \sum_{n=s-l-p}^{p} n \tilde{\Sigma}_l^{s,s-n-1} && (214) \\
&+ \sum_{l=1}^{s-2p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=1}^{p} \tilde{\Sigma}_l^{s,s-n-1} && (215)
\end{aligned}
$$

$$+ \quad \sum_{l=s-2p+1}^{s-p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=1}^{s-p-l} \tilde{\Sigma}_l^{s,s-n-1} \tag{216}$$

$$+ \quad \sum_{l=s-2p+1}^{s-p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-l-p+1}^{p} \tilde{\Sigma}_l^{s,s-n-1} \tag{217}$$

$$- \quad \sum_{l=2}^{p} (-1)^l \binom{s-l-2}{p} \sum_{n=s-p-l}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1} \tag{218}$$

$$- \quad \sum_{l=p+1}^{s-2p-1} (-1)^l \binom{s-l-2}{p} \sum_{n=s-p-l}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{219}$$

$$- \quad \sum_{l=s-2p}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=p+1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{220}$$

$$- \quad \sum_{l=1}^{s-2p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=p+1}^{s-p-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{221}$$

$$+ \quad \sum_{l=3}^{p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-l+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{222}$$

$$+ \quad \sum_{l=p+1}^{s-2p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-l+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \tag{223}$$

$$+ \quad \sum_{l=s-2p+1}^{s-p-2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \tag{224}$$

$$+ \quad \sum_{l=1}^{2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{225}$$

$$+ \quad \sum_{l=3}^{s-2p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-l} \tilde{\Sigma}_l^{s,s-n-1} \tag{226}$$

$$- \quad \sum_{l=1}^{p} (-1)^l \binom{s-l-2}{p} \sum_{n=s-p-1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{227}$$

$$+ \quad \sum_{l=1}^{p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \Bigg]. \tag{228}$$

We need to simplify this large expression to show it equals (164). The first step is to coalesce sums with adjacent ranges. It may help when reading this to check off each expression as it is used. In (214), we may take the upper limit on l to be $s-p-2$, since the $l = s-p-1$ term is zero. Then

$$(213) + (214) \quad = \quad - \sum_{l=s-2p}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{p} n\tilde{\Sigma}_l^{s,s-n-1} \tag{229}$$

$$(227)+(218) = -\sum_{l=2}^{p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=s-p-l}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \quad (230)$$

$$-(-1)\left(\begin{array}{c} s-3 \\ p \end{array}\right)\sum_{n=s-p-1}^{s-2} n\tilde{\Sigma}_1^{s,s-n-1} \quad (231)$$

$$(228)+(222) = \sum_{l=3}^{p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=s-p-l+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (232)$$

$$+\sum_{l=1}^{2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=s-p-1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (233)$$

$$(212)+(221) = -\sum_{l=1}^{s-2p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-p-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \quad (234)$$

$$-(-1)^{s-2p-1}\left(\begin{array}{c} 2p-1 \\ p \end{array}\right)\sum_{n=1}^{p} n\tilde{\Sigma}_{s-2p-1}^{s,s-n-1} \quad (235)$$

$$(225)+(233) = \sum_{l=1}^{2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (236)$$

$$(229)+(220) = -\sum_{l=s-2p}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \quad (237)$$

$$(230)+(219) = -\sum_{l=2}^{s-2p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=s-p-l}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \quad (238)$$

$$(232)+(223) = \sum_{l=3}^{s-2p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=s-p-l+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (239)$$

$$(226)+(239) = \sum_{l=3}^{s-2p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (240)$$

$$+(-1)^{s-2p}\left(\begin{array}{c} 2p-2 \\ p-1 \end{array}\right)\sum_{n=p+1}^{2p-1} \tilde{\Sigma}_{s-2p}^{s,s-n-1} \quad (241)$$

$$(234) + (235) + (238) + (231) \;=\; -\sum_{l=1}^{s-2p-1}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \quad (242)$$

$$(237) + (242) \;=\; -\sum_{l=1}^{s-p-2}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \quad (243)$$

$$(236) + (240) \;=\; \sum_{l=1}^{s-2p-1}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (244)$$

$$(244) + (241) \;=\; \sum_{l=1}^{s-2p}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (245)$$

$$(245) + (224) \;=\; \sum_{l=1}^{s-p-2}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (246)$$

In (217), we may take the upper limit on l to be $s-p-1$, since the $l = s-p$ term is zero. Then,

$$(216) + (217) \;=\; \sum_{l=s-2p+1}^{s-p-1}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=1}^{p} \tilde{\Sigma}_l^{s,s-n-1} \quad (247)$$

$$(247) + (215) \;=\; \sum_{l=1}^{s-p-1}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=1}^{p} \tilde{\Sigma}_l^{s,s-n-1} \quad (248)$$

$$(246) + (248) \;=\; \sum_{l=1}^{s-p-2}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (249)$$

$$+(-1)^{s-p-1} \begin{pmatrix} p-1 \\ p-1 \end{pmatrix} \sum_{n=1}^{p} \tilde{\Sigma}_{s-p-1}^{s,s-n-1} \quad (250)$$

$$(249) + (250) \;=\; \sum_{l=1}^{s-p-1}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \quad (251)$$

The only remaining expressions that have not yet been used are (211), (243) and (251).

Therefore we have established that the right side of (137) is their sum,

$$\begin{aligned}
& (-1)^{s+p}\left[\left(\begin{array}{c} s-2 \\ p \end{array}\right)(1-s)+\left(\begin{array}{c} s-2 \\ p-1 \end{array}\right)\right. \\
+ & \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \\
- & \left.\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1}\right]. \qquad (252)
\end{aligned}$$

We must show this equals (164). Note that in (252),

$$\begin{aligned}
\left(\begin{array}{c} s-2 \\ p \end{array}\right)(1-s)+\left(\begin{array}{c} s-2 \\ p-1 \end{array}\right) &= \left(\begin{array}{c} s-2 \\ p \end{array}\right)+\left(\begin{array}{c} s-2 \\ p-1 \end{array}\right)-s\left(\begin{array}{c} s-2 \\ p \end{array}\right) \\
&= \left(\begin{array}{c} s-1 \\ p \end{array}\right)-s\left(\begin{array}{c} s-2 \\ p \end{array}\right).
\end{aligned}$$

Since the first of these terms also appears in (164), what we need to show is

$$\begin{aligned}
& \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\Sigma_l^s+s\left(\begin{array}{c} s-2 \\ p \end{array}\right) \\
- & \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \\
+ & \sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \\
= & \ 0 \qquad (253)
\end{aligned}$$

We now express the Σ_l^s in terms of $\tilde{\Sigma}_l^{s,s-n}$. Applying (145) to the first line of (253), we get

$$\begin{aligned}
& \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\Sigma_l^s \\
= & \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\sum_{n=1}^{s-l}\tilde{\Sigma}_l^{s,s-n} \\
= & \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\sum_{n=0}^{s-l-1}\tilde{\Sigma}_l^{s,s-(n+1)} \\
= & \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1}+\sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\tilde{\Sigma}_l^{s,s-1}.
\end{aligned}$$

Substituting this into (253), we now need to show

$$\begin{aligned}
&\sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\tilde{\Sigma}_l^{s,s-1} + s\left(\begin{array}{c} s-2 \\ p \end{array}\right) \\
&+\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \\
&+\sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \\
&=0, \qquad (254)
\end{aligned}$$

which is equivalent to

$$\begin{aligned}
&\sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\tilde{\Sigma}_l^{s,s-1} + s\left(\begin{array}{c} s-2 \\ p \end{array}\right) \\
&+\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1}(n+1)\tilde{\Sigma}_l^{s,s-n-1} \\
&=0, \qquad (255)
\end{aligned}$$

because the $l = s-p-1$ term in the third line of (254) is zero. Now the $l=1$ term in the first sum of (255) is

$$-\left(\begin{array}{c} s-2 \\ p \end{array}\right)\tilde{\Sigma}_1^{s,s-1} = -\left(\begin{array}{c} s-2 \\ p \end{array}\right)\left(\begin{array}{c} s \\ s-1 \end{array}\right) = -s\left(\begin{array}{c} s-2 \\ p \end{array}\right),$$

by (113). Thus the first line of (255) becomes

$$\sum_{l=2}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ p \end{array}\right)\tilde{\Sigma}_l^{s,s-1} = -\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\tilde{\Sigma}_{l+1}^{s,s-1}.$$

So what we want to prove, (255), reduces to

$$\begin{aligned}
&-\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\tilde{\Sigma}_{l+1}^{s,s-1} \\
&+\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1}(n+1)\tilde{\Sigma}_l^{s,s-n-1} \\
&=0,
\end{aligned}$$

which is equivalent to

$$\sum_{l=1}^{s-p-2} (-1)^l \left(\begin{array}{c} s-l-2 \\ p \end{array} \right) \left[\sum_{n=1}^{s-l-1} (n+1) \tilde{\Sigma}_l^{s,s-n-1} - \tilde{\Sigma}_{l+1}^{s,s-1} \right] = 0,$$

which in turn holds if

$$\sum_{n=1}^{s-l-1} (n+1) \tilde{\Sigma}_l^{s,s-n-1} - \tilde{\Sigma}_{l+1}^{s,s-1} = 0, \quad \text{for } l = 1, \ldots, s-p-2. \tag{256}$$

To establish (256), first consider $l \geq 2$. Using (113), we see that

$$\begin{aligned} & \sum_{n=1}^{s-l-1} (n+1) \tilde{\Sigma}_l^{s,s-n-1} \\ = & \sum_{n=1}^{s-l-1} (n+1) \sum_{n+2 \leq i_1 < \cdots < i_{l-1} \leq s-1} \left(\begin{array}{c} i_1 \\ n+1 \end{array} \right) \left(\begin{array}{c} i_2 \\ i_1 \end{array} \right) \cdots \left(\begin{array}{c} i_{l-1} \\ i_{l-2} \end{array} \right) \left(\begin{array}{c} s \\ i_{l-1} \end{array} \right) \\ = & \sum_{n=1}^{s-l-1} (n+1) \sum_{n+2 \leq i_2 < \cdots < i_l \leq s-1} \left(\begin{array}{c} i_2 \\ n+1 \end{array} \right) \left(\begin{array}{c} i_3 \\ i_2 \end{array} \right) \cdots \left(\begin{array}{c} i_l \\ i_{l-1} \end{array} \right) \left(\begin{array}{c} s \\ i_l \end{array} \right). \end{aligned} \tag{257}$$

On the other hand, $l \geq 2$ implies $l+1 \geq 2$, so

$$\begin{aligned} \tilde{\Sigma}_{l+1}^{s,s-1} &= \sum_{2 \leq i_1 < \cdots < i_l \leq s-1} \left(\begin{array}{c} i_1 \\ 1 \end{array} \right) \left(\begin{array}{c} i_2 \\ i_1 \end{array} \right) \cdots \left(\begin{array}{c} i_l \\ i_{l-1} \end{array} \right) \left(\begin{array}{c} s \\ i_l \end{array} \right) \\ &= \sum_{i_1=2}^{s-l} \sum_{i_1 < i_2 < \cdots < i_l \leq s-1} \left(\begin{array}{c} i_1 \\ 1 \end{array} \right) \left(\begin{array}{c} i_2 \\ i_1 \end{array} \right) \cdots \left(\begin{array}{c} i_l \\ i_{l-1} \end{array} \right) \left(\begin{array}{c} s \\ i_l \end{array} \right) \\ &= \sum_{i_1=3}^{s-l+1} \sum_{i_1 \leq i_2 < \cdots < i_l \leq s-1} \left(\begin{array}{c} i_1 - 1 \\ 1 \end{array} \right) \left(\begin{array}{c} i_2 \\ i_1 - 1 \end{array} \right) \cdots \left(\begin{array}{c} i_l \\ i_{l-1} \end{array} \right) \left(\begin{array}{c} s \\ i_l \end{array} \right) \\ &= \sum_{n=1}^{s-l-1} \sum_{n+2 \leq i_2 < \cdots < i_l \leq s-1} \left(\begin{array}{c} n+1 \\ 1 \end{array} \right) \left(\begin{array}{c} i_2 \\ n+1 \end{array} \right) \cdots \left(\begin{array}{c} i_l \\ i_{l-1} \end{array} \right) \left(\begin{array}{c} s \\ i_l \end{array} \right) \\ &= (257). \end{aligned}$$

Now consider $l = 1$. Using (113), we have

$$\begin{aligned} \sum_{n=1}^{s-l-1} (n+1) \tilde{\Sigma}_l^{s,s-n-1} &= \sum_{n=1}^{s-2} (n+1) \tilde{\Sigma}_1^{s,s-n-1} \\ &= \sum_{n=1}^{s-2} (n+1) \left(\begin{array}{c} s \\ s-n-1 \end{array} \right) \\ &= \sum_{n=1}^{s-2} (n+1) \left(\begin{array}{c} s \\ n+1 \end{array} \right). \end{aligned} \tag{258}$$

Also,

$$\begin{aligned}
\tilde{\Sigma}_{l+1}^{s,s-1} &= \tilde{\Sigma}_{2}^{s,s-1} \\
&= \sum_{2 \le i_1 \le s-1} \left(\begin{array}{c} i_1 \\ 1 \end{array} \right) \left(\begin{array}{c} s \\ i_1 \end{array} \right) \\
&= \sum_{n=2}^{s-1} n \left(\begin{array}{c} s \\ n \end{array} \right) \\
&= \sum_{n=1}^{s-2} (n+1) \left(\begin{array}{c} s \\ n+1 \end{array} \right) \\
&= (257).
\end{aligned}$$

Therefore (256) is proven, as required.

Recall that we are in the process of showing (149) for $1 \le p \le (s-3)/2$, and have just completed the case (156), where $1 \le p \le (s-2)/3$. We now address the case where $(s-2)/3 < p \le (s-3)/2$, that is, $(s-1)/3 \le p \le (s-3)/2$. In this case (197) and (210) apply, so that the right side of (149) is assembled from (157), (174), (179), (197), (210), (183) and (185). This equals

$$(-1)^{s+p} \left[\left(\begin{array}{c} s-2 \\ p \end{array} \right) (1-s) + \left(\begin{array}{c} s-2 \\ p-1 \end{array} \right) \right] \tag{259}$$

$$- \sum_{l=1}^{s-2p-1} (-1)^l \left(\begin{array}{c} s-l-2 \\ p \end{array} \right) \sum_{n=1}^{p} n \tilde{\Sigma}_{l}^{s,s-n-1} \tag{260}$$

$$- \sum_{l=s-2p}^{s-p-2} (-1)^l \left(\begin{array}{c} s-l-2 \\ p \end{array} \right) \sum_{n=1}^{s-p-l-1} n \tilde{\Sigma}_{l}^{s,s-n-1} \tag{261}$$

$$- \sum_{l=s-2p}^{s-p-1} (-1)^l \left(\begin{array}{c} s-l-2 \\ p \end{array} \right) \sum_{n=s-l-p}^{p} n \tilde{\Sigma}_{l}^{s,s-n-1} \tag{262}$$

$$+ \sum_{l=1}^{s-2p} (-1)^l \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right) \sum_{n=1}^{p} \tilde{\Sigma}_{l}^{s,s-n-1} \tag{263}$$

$$+ \sum_{l=s-2p+1}^{s-p-1} (-1)^l \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right) \sum_{n=1}^{s-p-l} \tilde{\Sigma}_{l}^{s,s-n-1} \tag{264}$$

$$+ \sum_{l=s-2p+1}^{s-p} (-1)^l \left(\begin{array}{c} s-l-2 \\ p-1 \end{array} \right) \sum_{n=s-l-p+1}^{p} \tilde{\Sigma}_{l}^{s,s-n-1} \tag{265}$$

$$- \sum_{l=2}^{s-2p-1} (-1)^l \left(\begin{array}{c} s-l-2 \\ p \end{array} \right) \sum_{n=s-p-l}^{s-p-2} n \tilde{\Sigma}_{l}^{s,s-n-1} \tag{266}$$

$$- \sum_{l=s-2p}^{p} (-1)^l \left(\begin{array}{c} s-l-2 \\ p \end{array} \right) \sum_{n=p+1}^{s-p-2} n \tilde{\Sigma}_{l}^{s,s-n-1} \tag{267}$$

$$- \sum_{l=p+1}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=p+1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{268}$$

$$- \sum_{l=1}^{s-2p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=p+1}^{s-p-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{269}$$

$$+ \sum_{l=3}^{s-2p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-l+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{270}$$

$$+ \sum_{l=s-2p+1}^{p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{271}$$

$$+ \sum_{l=p+1}^{s-p-2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \tag{272}$$

$$+ \sum_{l=1}^{2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{273}$$

$$+ \sum_{l=3}^{s-2p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-p-l} \tilde{\Sigma}_l^{s,s-n-1} \tag{274}$$

$$- \sum_{l=1}^{p} (-1)^l \binom{s-l-2}{p} \sum_{n=s-p-1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{275}$$

$$+ \sum_{l=1}^{p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \Bigg]. \tag{276}$$

We now simplify this large expression to show it equals (164). We first coalesce sums with adjacent ranges. Again, it may help when reading this to check off each expression as it is used. This time, we'll do all the negative sums first, and then the positive ones. In (262), we may take the upper limit on l to be $s-p-2$, since the $l = s-p-1$ term is zero. Then

$$(261) + (262) = - \sum_{l=s-2p}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{p} n\tilde{\Sigma}_l^{s,s-n-1} \tag{277}$$

$$(260) + (269) = - \sum_{l=1}^{s-2p-1} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{s-p-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{278}$$

$$(266) + (278) = - \sum_{l=2}^{s-2p-1} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1} - (-1) \binom{s-3}{p} \sum_{n=1}^{s-p-2} n\tilde{\Sigma}_1^{s,s-n-1}$$

$$= \quad -\sum_{l=1}^{s-2p-1}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1} \tag{279}$$

Now $p \leq (s-3)/2 \Longrightarrow p \leq (s-2)/2 \Longrightarrow p \leq s-p-2$, so that

$$(267) + (277) \quad = \quad -\sum_{l=s-2p}^{p}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1} \tag{280}$$

$$-\sum_{l=p+1}^{s-p-2}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{p} n\tilde{\Sigma}_l^{s,s-n-1} \tag{281}$$

$$(281) + (268) \quad = \quad -\sum_{l=p+1}^{s-p-2}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{282}$$

$$(279) + (280) \quad = \quad -\sum_{l=1}^{p}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1} \tag{283}$$

$$(275) + (283) \quad = \quad -\sum_{l=1}^{p}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{284}$$

$$(282) + (284) \quad = \quad -\sum_{l=1}^{s-p-2}(-1)^l \begin{pmatrix} s-l-2 \\ p \end{pmatrix} \sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{285}$$

Now we do the positive sums.

$$(263) + (274) + (270) \quad = \quad \sum_{l=3}^{s-2p-1}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{286}$$

$$+\sum_{l=1}^{2}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=1}^{p} \tilde{\Sigma}_l^{s,s-n-1} \tag{287}$$

$$(-1)^{s-2p} \begin{pmatrix} 2p-2 \\ p-1 \end{pmatrix} \sum_{n=1}^{p} \tilde{\Sigma}_{s-2p}^{s,s-n-1} \tag{288}$$

$$(-1)^{s-2p} \begin{pmatrix} 2p-2 \\ p-1 \end{pmatrix} \sum_{n=p+1}^{s-p-2} \tilde{\Sigma}_{s-2p}^{s,s-n-1} \tag{289}$$

$$(287) + (273) \quad = \quad \sum_{l=1}^{2}(-1)^l \begin{pmatrix} s-l-2 \\ p-1 \end{pmatrix} \sum_{n=1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{290}$$

$$(286)+(290) \;=\; \sum_{l=1}^{s-2p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-p-2}\tilde{\Sigma}_l^{s,s-n-1} \tag{291}$$

$$(271)+(289) \;=\; \sum_{l=s-2p}^{p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=p+1}^{s-p-2}\tilde{\Sigma}_l^{s,s-n-1} \tag{292}$$

$$(291)+(292) \;=\; \sum_{l=1}^{p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=p+1}^{s-p-2}\tilde{\Sigma}_l^{s,s-n-1} \tag{293}$$

$$+\sum_{l=1}^{s-2p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_l^{s,s-n-1} \tag{294}$$

$$(264)+(265) \;=\; \sum_{l=s-2p+1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_l^{s,s-n-1} \tag{295}$$

$$(294)+(288)+(295) \;=\; \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_l^{s,s-n-1} \tag{296}$$

$$(272)+(296) \;=\; \sum_{l=p+1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \tag{297}$$

$$+\sum_{l=1}^{p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_l^{s,s-n-1} \tag{298}$$

$$(-1)^{s-p-1}\left(\begin{array}{c} p-1 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_{s-p-1}^{s,s-n-1} \tag{299}$$

$$(293)+(298) \;=\; \sum_{l=1}^{p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-p-2}\tilde{\Sigma}_l^{s,s-n-1} \tag{300}$$

$$(300)+(276) \;=\; \sum_{l=1}^{p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \tag{301}$$

$$(301)+(297)+(299) \;=\; \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \tag{302}$$

The only remaining expressions that have not yet been used are (259), (285) and (302). Therefore we have established that the right side of (137) is their sum,

$$\begin{aligned}
& (-1)^{s+p}\left[\left(\begin{array}{c} s-2 \\ p \end{array}\right)(1-s)+\left(\begin{array}{c} s-2 \\ p-1 \end{array}\right)\right. \\
+ & \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \\
- & \left.\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1}\right].
\end{aligned}$$

This is exactly the same as (252), which we have already shown to be equal to (164). Therefore we have completed the entire range of $1 \le p \le (s-3)/2$. Now we assume that

$$\frac{s-1}{2} \le p \le s-3.$$

As in the case of (156), we have (152) and (154), (152) and (155), and (153) and (155). Thus (151) becomes

$$(-1)^{s+p}\left[\left(\begin{array}{c} s-2 \\ p \end{array}\right)(1-s)+\left(\begin{array}{c} s-2 \\ p-1 \end{array}\right)\right] \tag{303}$$

$$\begin{aligned}
+ \quad & (-1)^{s+p}\left\{\sum_{n=1}^{s-p-2}\left[-n\sum_{k=p-n+1}^{p}\left(\begin{array}{c} n-1 \\ p-k \end{array}\right)T^{(s)}_{s-n-1,k}\right.\right. \\
& \left.\left.+\sum_{k=p-n}^{p-1}\left(\begin{array}{c} n-1 \\ p-k-1 \end{array}\right)T^{(s)}_{s-n-1,k}\right]\right.
\end{aligned} \tag{304}$$

$$+ \quad \sum_{n=s-p-1}^{p}\left[-n\sum_{k=p-n+1}^{s-n-2}\left(\begin{array}{c} n-1 \\ p-k \end{array}\right)T^{(s)}_{s-n-1,k}+\sum_{k=p-n}^{s-n-2}\left(\begin{array}{c} n-1 \\ p-k-1 \end{array}\right)T^{(s)}_{s-n-1,k}\right] \tag{305}$$

$$\left. + \quad \sum_{n=p+1}^{s-2}\left[-n\sum_{k=0}^{s-n-2}\left(\begin{array}{c} n-1 \\ p-k \end{array}\right)T^{(s)}_{s-n-1,k}+\sum_{k=0}^{s-n-2}\left(\begin{array}{c} n-1 \\ p-k-1 \end{array}\right)T^{(s)}_{s-n-1,k}\right]\right\}. \tag{306}$$

Using (131), we see that this reduces to

$$(-1)^{s+p}\left\{\left(\begin{array}{c} s-2 \\ p \end{array}\right)(1-s)+\left(\begin{array}{c} s-2 \\ p-1 \end{array}\right)\right. \tag{307}$$

$$- \quad \sum_{n=1}^{s-p-2}\sum_{k=p-n+1}^{p}\sum_{l=1}^{s-n-k-1}(-1)^l n\left(\begin{array}{c} n-1 \\ p-k \end{array}\right)\left(\begin{array}{c} s-n-l-1 \\ k \end{array}\right)\tilde{\Sigma}_l^{s,s-n-1} \tag{308}$$

$$\left. + \quad \sum_{n=1}^{s-p-2}\sum_{k=p-n}^{p-1}\sum_{l=1}^{s-n-k-1}(-1)^l\left(\begin{array}{c} n-1 \\ p-k-1 \end{array}\right)\left(\begin{array}{c} s-n-l-1 \\ k \end{array}\right)\tilde{\Sigma}_l^{s,s-n-1}\right. \tag{309}$$

$$- \sum_{n=s-p-1}^{p} \sum_{k=p-n-1}^{s-n-2} \sum_{l=1}^{s-n-k-1} (-1)^l n \binom{n-1}{p-k} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \tag{310}$$

$$+ \sum_{n=s-p-1}^{p} \sum_{k=p-n}^{s-n-2} \sum_{l=1}^{s-n-k-1} (-1)^l \binom{n-1}{p-k-1} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \tag{311}$$

$$- \sum_{n=p+1}^{s-2} \sum_{k=0}^{s-n-2} \sum_{l=1}^{s-n-k-1} (-1)^l n \binom{n-1}{p-k} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \tag{312}$$

$$+ \sum_{n=p+1}^{s-2} \sum_{k=0}^{s-n-2} \sum_{l=1}^{s-n-k-1} (-1)^l \binom{n-1}{p-k-1} \binom{s-n-l-1}{k} \tilde{\Sigma}_l^{s,s-n-1} \Bigg\}. \tag{313}$$

Comparing this to (164), we again see that an appropriate strategy is to switch the order of the sums from n, k, l to l, k, n and then to evaluate the k sum, since $\tilde{\Sigma}_l^{s,s-n-1}$ is independent of k. Note that the k and l sums of (308), (309), (312) and (313) are the same as in (158), (159), (162) and (163), respectively, so we can use the same reversals as before, namely (170), (175) and (180). Therefore we have from (170), using a different range on the n sum,

$$(308) \;=\; -\sum_{n=1}^{s-p-2} \sum_{l=1}^{s-n-p-1} \sum_{k=p-n+1}^{p} - \sum_{n=1}^{s-p-2} \sum_{l=s-n-p}^{s-p-2} \sum_{k=p-n+1}^{s-n-l-1}. \tag{314}$$

Applying (165) to the first n and l sums in (314), we have $a = 1$, $b = s-p-2$, $c = s-p-1$, $c-b = 1$ and $c-a = s-p-2$. Applying (166) to the second n and l sums in (314), we have $a = s-p$ and $b = s-p-2$, $p \leftarrow s-p-2$. Therefore,

$$(308) \;=\; -\sum_{l=1}^{0} - \sum_{l=1}^{s-p-2} \sum_{n=1}^{s-p-l-1} \sum_{k=p-n+1}^{p} - \sum_{l=2}^{s-p-1} \sum_{n=s-p-l}^{s-p-2} \sum_{k=p-n+1}^{s-n-l-1} - \sum_{l=s-p}^{s-p-2}. \tag{315}$$

(Note that the first and last sums are empty). The k sums are the same as (172) and (173), so we have

$$\begin{aligned} (308) \;=\; & - \sum_{l=1}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{s-p-l-1} n \tilde{\Sigma}_l^{s,s-n-1} \\ & - \sum_{l=2}^{s-p-1} (-1)^l \binom{s-l-2}{p} \sum_{n=s-p-l}^{s-p-2} n \tilde{\Sigma}_l^{s,s-n-1}. \end{aligned} \tag{316}$$

From (175), only changing the ranges on the n sums, we have

$$(309) \;=\; \sum_{n=1}^{s-p-2} \sum_{l=1}^{s-p-n} \sum_{k=p-n}^{p-1} + \sum_{n=1}^{s-p-2} \sum_{l=s-p-n+1}^{s-p-1} \sum_{k=p-n}^{s-n-l-1}. \tag{317}$$

Applying (165) to the first n and l sums in (317), we have $a = 1$, $b = s-p-2$, $c = s-p$, $c-b = 2$ and $c-a = s-p-1$. Applying (166) to the second n and l sums in (317), we

have $a = s-p+1$ and $b = s-p-1$, $p \leftarrow s-p-2$. Therefore,

$$(309) \quad = \quad \sum_{l=1}^{2} \sum_{n=1}^{s-p-2} \sum_{k=p-n}^{p-1} + \sum_{l=3}^{s-p-1} \sum_{n=1}^{s-p-l} \sum_{k=p-n}^{p-1} + \sum_{l=3}^{s-p} \sum_{n=s-p-l+1}^{s-p-2} \sum_{k=p-n}^{s-n-l-1} + \sum_{l=s-p+1}^{s-p-1} . \quad (318)$$

(Note that the last sum is empty). The k sums are the same as (177) and (178), so we have

$$\begin{aligned}(309) \quad = \quad & \sum_{l=1}^{2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=1}^{s-p-1} \tilde{\Sigma}_l^{s,s-n-1} \\ & + \sum_{l=3}^{s-p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=1}^{s-p-l} \tilde{\Sigma}_l^{s,s-n-1} \\ & + \sum_{l=3}^{s-p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-l+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} . \end{aligned} \quad (319)$$

From (180), only changing the range on the n sum, we have

$$(312) \quad = \quad - \sum_{n=p+1}^{s-2} \sum_{l=1}^{s-n-1} \sum_{k=0}^{s-n-l-1} . \quad (320)$$

Applying a slight variation of (165) to the n and l sums in (320), we have $a = p+1$, $b = s-2$, $c = s-1$, $c-b = 1$ and $c-a = s-p-2$. Therefore,

$$(312) \quad = \quad - \sum_{l=1}^{0} - \sum_{l=1}^{s-p-2} \sum_{n=p+1}^{s-l-1} \sum_{k=0}^{s-n-l-1} . \quad (321)$$

(Note that the first sum is empty). The k sum is the same as (182), so we have

$$(312) \quad = \quad - \sum_{l=1}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=p+1}^{s-l-1} n \tilde{\Sigma}_l^{s,s-n-1} . \quad (322)$$

Now (313) has the same k and l sums as (312), and its k sum is (184), so we have

$$(313) \quad = \quad \sum_{l=1}^{s-p-2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} . \quad (323)$$

Expressions (310) and (311) cannot be recycled, so we compute them from scratch. Applying a slight variation of (165) to (310), we have $a = p-n-1$, $b = s-n-2$, $c = s-n-1$, $c-b = 1$ and $c-a = s-p$. Therefore

$$(310) \quad = \quad - \sum_{n=s-p-1}^{p} \sum_{k=p-n-1}^{s-n-2} \sum_{l=1}^{s-n-k-1}$$

$$
\begin{aligned}
&= -\sum_{n=s-p-1}^{p}\sum_{l=1}^{s-p}\sum_{k=p-n-1}^{s-n-l-1} \\
&= -\sum_{l=1}^{s-p}\sum_{n=s-p-1}^{p}\sum_{k=p-n-1}^{s-n-l-1}. \qquad (324)
\end{aligned}
$$

The k sum is

$$
\begin{aligned}
&\sum_{k=p-n-1}^{s-n-l-1}\binom{n-1}{p-k}\binom{s-n-l-1}{k} \\
&= \sum_{k=0}^{s-p-l}\binom{n-1}{n-k+1}\binom{s-n-l-1}{p-n+k-1} \\
&= \sum_{k=0}^{s-p-l-2}\binom{n-1}{n-k+1}\binom{s-n-l-1}{p-n+k-1} \\
&= \sum_{k=0}^{s-p-l-2}\binom{n-1}{k}\binom{s-n-l-1}{s-p-l-k-2} \\
&= \sum_{k=0}^{N}\binom{n-1}{k}\binom{s-n-l-1}{N-k} \quad \text{for } N = s-p-l-2 \\
&= \binom{s-l-2}{s-p-l-2} \\
&= \binom{s-l-2}{p}, \qquad (325)
\end{aligned}
$$

by (453). Thus we have

$$
(310) = -\sum_{l=1}^{s-p}(-1)^l\binom{s-l-2}{p}\sum_{n=s-p-1}^{p} n\tilde{\Sigma}_l^{s,s-n-1}. \qquad (326)
$$

Applying a slight variation of (165) to (311), we have $a = p-n$, $b = s-n-2$, $c = s-n-1$, $c-b = 1$ and $c-a = s-p-1$. Therefore

$$
\begin{aligned}
(311) &= \sum_{n=s-p-1}^{p}\sum_{k=p-n}^{s-n-2}\sum_{l=1}^{s-n-k-1} \\
&= \sum_{n=s-p-1}^{p}\sum_{l=1}^{s-p-1}\sum_{k=p-n}^{s-n-l-1} \\
&= \sum_{l=1}^{s-p-1}\sum_{n=s-p-1}^{p}\sum_{k=p-n}^{s-n-l-1}. \qquad (327)
\end{aligned}
$$

The k sum is (178), so we have

$$(311) \;=\; \sum_{l=1}^{s-p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-1}^{p} \tilde{\Sigma}_l^{s,s-n-1}. \tag{328}$$

We can now assemble the right side of (149) from (303), (316), (319), (326), (328), (322) and (323). This equals

$$(-1)^{s+p} \left[\binom{s-2}{p} (1-s) + \binom{s-2}{p-1} \right. \tag{329}$$

$$- \sum_{l=1}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{s-p-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{330}$$

$$- \sum_{l=2}^{s-p-1} (-1)^l \binom{s-l-2}{p} \sum_{n=s-p-l}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1} \tag{331}$$

$$+ \sum_{l=1}^{2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{332}$$

$$+ \sum_{l=3}^{s-p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=1}^{s-p-l} \tilde{\Sigma}_l^{s,s-n-1} \tag{333}$$

$$+ \sum_{l=3}^{s-p} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-l+1}^{s-p-2} \tilde{\Sigma}_l^{s,s-n-1} \tag{334}$$

$$- \sum_{l=1}^{s-p} (-1)^l \binom{s-l-2}{p} \sum_{n=s-p-1}^{p} n\tilde{\Sigma}_l^{s,s-n-1} \tag{335}$$

$$+ \sum_{l=1}^{s-p-1} (-1)^l \binom{s-l-2}{p-1} \sum_{n=s-p-1}^{p} \tilde{\Sigma}_l^{s,s-n-1} \tag{336}$$

$$- \sum_{l=1}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=p+1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \tag{337}$$

$$\left. + \sum_{l=1}^{s-p-2} (-1)^l \binom{s-l-2}{p-1} \sum_{n=p+1}^{s-l-1} \tilde{\Sigma}_l^{s,s-n-1} \right]. \tag{338}$$

We now simplify this large expression to show it equals (164). We first coalesce sums with adjacent ranges. As before, it may help when reading this to check off each expression as it is used.

$$\begin{aligned} (330) + (331) \;=\; & - \sum_{l=2}^{s-p-2} (-1)^l \binom{s-l-2}{p} \sum_{n=1}^{s-p-2} n\tilde{\Sigma}_l^{s,s-n-1} \\ & -(-1) \binom{s-3}{p} \sum_{n=1}^{s-p-2} n\tilde{\Sigma}_1^{s,s-n-1} \end{aligned}$$

$$-(-1)^{s-p-1}\left(\begin{array}{c} p-1 \\ p \end{array}\right)\sum_{n=1}^{s-p-2} n\tilde{\Sigma}_{s-p-1}^{s,s-n-1} \tag{339}$$

$$\begin{aligned}(333)+(334) &= \sum_{l=3}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-p-2}\tilde{\Sigma}_l^{s,s-n-1} \\ &\quad +(-1)^{s-p}\left(\begin{array}{c} p-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-p-2}\tilde{\Sigma}_{s-p}^{s,s-n-1} \\ &= \sum_{l=3}^{s-p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-p-2}\tilde{\Sigma}_l^{s,s-n-1} \end{aligned} \tag{340}$$

$$(332)+(340) = \sum_{l=1}^{s-p}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-p-2}\tilde{\Sigma}_l^{s,s-n-1} \tag{341}$$

$$\begin{aligned}(335)+(339) &= -\sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{p} n\tilde{\Sigma}_l^{s,s-n-1} \\ &\quad -(-1)^{s-p}\left(\begin{array}{c} p-2 \\ p \end{array}\right)\sum_{n=1}^{p} n\tilde{\Sigma}_{s-p}^{s,s-n-1} \\ &= -\sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{p} n\tilde{\Sigma}_l^{s,s-n-1} \end{aligned} \tag{342}$$

$$\begin{aligned}(336)+(341) &= \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_l^{s,s-n-1} \\ &\quad +(-1)^{s-p}\left(\begin{array}{c} p-2 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_{s-p}^{s,s-n-1} \\ &= \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_l^{s,s-n-1} \end{aligned} \tag{343}$$

$$\begin{aligned}(337)+(342) &= -\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \\ &\quad -(-1)^{s-p-1}\left(\begin{array}{c} p-1 \\ p \end{array}\right)\sum_{n=1}^{p} n\tilde{\Sigma}_{s-p}^{s,s-n-1} \\ &= -\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1} n\tilde{\Sigma}_l^{s,s-n-1} \end{aligned} \tag{344}$$

$$
\begin{aligned}
(338)+(343) &= \sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \\
&\quad +(-1)^{s-p-1}\left(\begin{array}{c} p-2 \\ p-1 \end{array}\right)\sum_{n=1}^{p}\tilde{\Sigma}_{s-p-1}^{s,s-n-1} \\
&= \sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \qquad (345)
\end{aligned}
$$

The only remaining expressions that have not yet been used are (329), (344) and (345). Therefore we have established that the right side of (137) is their sum,

$$
\begin{aligned}
& (-1)^{s+p}\left[\left(\begin{array}{c} s-2 \\ p \end{array}\right)(1-s)+\left(\begin{array}{c} s-2 \\ p-1 \end{array}\right)\right. \\
+ & \sum_{l=1}^{s-p-1}(-1)^l\left(\begin{array}{c} s-l-2 \\ p-1 \end{array}\right)\sum_{n=1}^{s-l-1}\tilde{\Sigma}_l^{s,s-n-1} \\
- & \left.\sum_{l=1}^{s-p-2}(-1)^l\left(\begin{array}{c} s-l-2 \\ p \end{array}\right)\sum_{n=1}^{s-l-1}n\tilde{\Sigma}_l^{s,s-n-1}\right]. \qquad (346)
\end{aligned}
$$

This is exactly the same as (252), which we have already shown to be equal to (164). Therefore we have shown that (252) = (164) for $1 \le p \le s-3$, completing the proof of Theorem 6. □

D Lemmas

The following lemmas are used in the proofs of Theorems B and C.

D.1 Lemma 1

Lemma 1 *Let M_n be defined as in (110). Recall that the notation $\left[\begin{array}{c} i \\ j \end{array}\right]$ is being used as a scalar function of 2 variables, which will eventually be substituted for the binomial coefficient $\left(\begin{array}{c} i \\ j \end{array}\right)$. Then, for $n \ge 1$,*

$$
M_n = \sum_{k=0}^{n-1}(-1)^{n-k}w^k\sum_{l=1}^{n-k}(-1)^l\left(\begin{array}{c} n-l \\ k \end{array}\right)\bar{\Sigma}_l^n, \qquad (347)
$$

where

$$\bar{\Sigma}_l^n = \begin{cases} \sum_{1\le i_1<\cdots<i_{l-1}\le n-1} \left[\begin{array}{c} i_1 \\ 1 \end{array}\right] \left[\begin{array}{c} i_2 \\ i_1+1 \end{array}\right] \cdots \left[\begin{array}{c} i_{l-1} \\ i_{l-2}+1 \end{array}\right] \left[\begin{array}{c} n \\ i_{l-1}+1 \end{array}\right], & l \ge 2 \\ \left[\begin{array}{c} n \\ 1 \end{array}\right], & l = 1. \end{cases} \tag{348}$$

Proof. Expanding M_n along the top row gives

$$M_n = \sum_{i=1}^{n} (-1)^{i-1} \left[\begin{array}{c} i \\ 1 \end{array}\right] M_{n,i}, \tag{349}$$

where $M_{n,i}$ is the determinant of the $(n-1)\times(n-1)$ matrix formed from M_n by crossing out the top row and the i-th column. Note $M_{n,i}$ is block upper-triangular and the top left block is upper triangular. So $M_{n,n}$ is upper triangular, and $M_{n,n} = (1-w)^{n-1}$. If $1 \le i < n$, then

$$M_{n,i} = (1-w)^{i-1} \begin{vmatrix} \left[\begin{array}{c} i+1 \\ i+1 \end{array}\right] & \cdots & \cdots & \left[\begin{array}{c} n \\ i+1 \end{array}\right] \\ 1-w & \left[\begin{array}{c} i+2 \\ i+2 \end{array}\right] & \cdots & \left[\begin{array}{c} n \\ i+2 \end{array}\right] \\ & \ddots & \ddots & \vdots \\ \bigcirc & & 1-w & \left[\begin{array}{c} n \\ n \end{array}\right] \end{vmatrix},$$

where the matrix on the right side is $(n-i)\times(n-i)$. Now note that

$$M_{n-i} = \begin{vmatrix} \left[\begin{array}{c} 1 \\ 1 \end{array}\right] & \cdots & \cdots & \left[\begin{array}{c} n-i \\ 1 \end{array}\right] \\ 1-w & \left[\begin{array}{c} 2 \\ 2 \end{array}\right] & \cdots & \left[\begin{array}{c} n-i \\ 2 \end{array}\right] \\ & \ddots & & \vdots \\ \bigcirc & & 1-w & \left[\begin{array}{c} n-i \\ n-i \end{array}\right] \end{vmatrix},$$

is also the determinant of a $(n-i)\times(n-i)$ matrix and that

$$M_{n,i} = (1-w)^{i-1} M_{n-i} \Big|_{\left[\begin{array}{c} u \\ v \end{array}\right] \leftarrow \left[\begin{array}{c} u+i \\ v+i \end{array}\right]} \tag{350}$$

for $i = 1, \ldots, n-1$.

Since $i \geq 1$ in (349) and (350), we can apply induction on (347). The base case, $n = 1$, states that

$$M_1 = (-1)^1 w^0 (-1)^1 \left(\begin{array}{c} 1 \\ 1 \end{array} \right) \bar{\Sigma}_1^1,$$

which follows immediately from (348) and (110). Induction then gives

$$M_{n-i} = \sum_{k=0}^{n-i-1} (-1)^{n-i-k} w^k \sum_{l=1}^{n-i-k} (-1)^l \left(\begin{array}{c} n-i-l \\ k \end{array} \right) \bar{\Sigma}_l^{n-i}$$

for $i = 1, \ldots, n-1$. So

$$M_{n-i} \Big| \left[\begin{array}{c} u \\ v \end{array} \right] \leftarrow \left[\begin{array}{c} u+i \\ v+i \end{array} \right] = \sum_{k=0}^{n-i-1} (-1)^{n-i-k} w^k \sum_{l=1}^{n-i-k} (-1)^l \left(\begin{array}{c} n-i-l \\ k \end{array} \right) \hat{\Sigma}_l^{n,i} \tag{351}$$

for $i = 1, \ldots, n-1$, where

$$\hat{\Sigma}_k^{n,i} = \bar{\Sigma}_l^{n-i} \Big| \left[\begin{array}{c} u \\ v \end{array} \right] \leftarrow \left[\begin{array}{c} u+i \\ v+i \end{array} \right].$$

Using (348) to evaluate $\hat{\Sigma}_k^{n,i}$ gives

$$\begin{aligned} &\hat{\Sigma}_k^{n,i} \\ &= \begin{cases} \sum_{1 \leq i_1 < \cdots < i_{l-1} \leq n-i-1} \left[\begin{array}{c} i_1 + i \\ i+1 \end{array} \right] \left[\begin{array}{c} i_2 + i \\ i_1 + i + 1 \end{array} \right] \cdots \left[\begin{array}{c} i_{l-1} + i \\ i_{l-2} + i + 1 \end{array} \right] \left[\begin{array}{c} n \\ i_{l-1} + i + 1 \end{array} \right], & l \geq 2 \\ \left[\begin{array}{c} n \\ i+1 \end{array} \right], & l = 1 \end{cases} \\ &= \begin{cases} \sum_{i+1 \leq i_1 < \cdots < i_{l-1} \leq n-1} \left[\begin{array}{c} i_1 \\ i+1 \end{array} \right] \left[\begin{array}{c} i_2 \\ i_1 + 1 \end{array} \right] \cdots \left[\begin{array}{c} i_{l-1} \\ i_{l-2} + 1 \end{array} \right] \left[\begin{array}{c} n \\ i_{l-1} + 1 \end{array} \right], & l \geq 2 \\ \left[\begin{array}{c} n \\ i+1 \end{array} \right], & l = 1. \end{cases} \end{aligned} \tag{352}$$

Now (350), (351) and (352) imply

$$M_{n,i} = (1-w)^{i-1} \sum_{k=0}^{n-i-1} (-1)^{n-i-k} w^k S_k^{n,i} \tag{353}$$

for $i = 1, \ldots, n-1$, where

$$S_k^{n,i} = \sum_{l=1}^{n-i-k} (-1)^l \left(\begin{array}{c} n-i-l \\ k \end{array} \right) \hat{\Sigma}_l^{n,i}.$$

Then, from (349) and (353), we have

$$\begin{aligned}
M_n &= \sum_{i=1}^{n}(-1)^{i-1}\left[\begin{array}{c} i \\ 1 \end{array}\right] M_{n,i} \\
&= \sum_{i=1}^{n-1}(-1)^{i-1}\left[\begin{array}{c} i \\ 1 \end{array}\right](1-w)^{i-1}\sum_{k=0}^{n-i-1}(-1)^{n-i-k}S_k^{n,i}w^k \\
&\quad +(-1)^{n-1}\left[\begin{array}{c} n \\ 1 \end{array}\right](1-w)^{n-1} \\
&= (-1)^{n-1}\left[\sum_{i=1}^{n-1}\left[\begin{array}{c} i \\ 1 \end{array}\right](1-w)^{i-1}\sum_{k=0}^{n-i-1}(-1)^{k}S_k^{n,i}w^k + \left[\begin{array}{c} n \\ 1 \end{array}\right](1-w)^{n-1}\right] \\
&= (-1)^{n-1}\left[\sum_{i=1}^{n-1}\left[\begin{array}{c} i \\ 1 \end{array}\right](1-w)^{i-1}\sum_{k=0}^{n-i-1}(-1)^{k}\sum_{l=1}^{n-i-k}(-1)^{l}\left(\begin{array}{c} n-i-l \\ k \end{array}\right)\hat{\Sigma}_l^{n,i}w^k\right. \\
&\quad \left. + \left[\begin{array}{c} n \\ 1 \end{array}\right](1-w)^{n-1}\right]. \qquad (354)
\end{aligned}$$

We must now show that (354) agrees with (347). Since (354) contains $\hat{\Sigma}_l^{n,i}$ and (347) is written in terms of $\bar{\Sigma}_l^n$, we need to find a relationship between these quantities. From (352),

$$\hat{\Sigma}_l^{n,i} = \begin{cases} \sum_{i+1\le i_1<\cdots<i_{l-1}\le n-1}\left[\begin{array}{c} i_1 \\ i+1 \end{array}\right]\left[\begin{array}{c} i_2 \\ i_1+1 \end{array}\right]\cdots\left[\begin{array}{c} i_{l-1} \\ i_{l-2}+1 \end{array}\right]\left[\begin{array}{c} n \\ i_{l-1}+1 \end{array}\right], & l\ge 2 \\ \left[\begin{array}{c} n \\ i+1 \end{array}\right], & l=1, \end{cases}$$

and, for $l \ge 1$, we see from (348) that

$$\begin{aligned}
\bar{\Sigma}_{l+1}^n &= \sum_{1\le i_1<\cdots<i_l\le n-1}\left[\begin{array}{c} i_1 \\ 1 \end{array}\right]\left[\begin{array}{c} i_2 \\ i_1+1 \end{array}\right]\cdots\left[\begin{array}{c} i_l \\ i_{l-1}+1 \end{array}\right]\left[\begin{array}{c} n \\ i_l+1 \end{array}\right] \\
&= \sum_{i_1=1}^{n-l}\left[\begin{array}{c} i_1 \\ 1 \end{array}\right]\sum_{i_1<i_2<\cdots<i_l\le n-1}\left[\begin{array}{c} i_2 \\ i_1+1 \end{array}\right]\cdots\left[\begin{array}{c} n \\ i_l+1 \end{array}\right] \\
&= \sum_{i=1}^{n-l}\left[\begin{array}{c} i \\ 1 \end{array}\right]\sum_{i+1\le i_1<\cdots<i_{l-1}\le n-1}\left[\begin{array}{c} i_1 \\ i+1 \end{array}\right]\cdots\left[\begin{array}{c} n \\ i_{l-1}+1 \end{array}\right] \\
&= \sum_{i=1}^{n-l}\left[\begin{array}{c} i \\ 1 \end{array}\right]\hat{\Sigma}_l^{n,i}.
\end{aligned}$$

Thus we have that

$$\bar{\Sigma}_l^n = \sum_{i=1}^{n-l+1}\left[\begin{array}{c} i \\ 1 \end{array}\right]\hat{\Sigma}_{l-1}^{n,i} \qquad (355)$$

for $l \geq 2$, while, for $l = 1$,

$$\bar{\Sigma}_1^n = \left[\begin{array}{c} n \\ 1 \end{array} \right] \quad \text{and} \quad \hat{\Sigma}_1^{n,i} = \left[\begin{array}{c} n \\ i+1 \end{array} \right].$$

We now return to showing that (347) equals (354). Using (355) gives

$$\begin{aligned}
(347) &= \sum_{k=0}^{n-1} (-1)^{n-k} w^k \left[\sum_{l=2}^{n-k} (-1)^l \left(\begin{array}{c} n-l \\ k \end{array} \right) \sum_{i=1}^{n-l+1} \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_{l-1}^{n,i} - \left(\begin{array}{c} n-1 \\ k \end{array} \right) \left[\begin{array}{c} n \\ 1 \end{array} \right] \right] \\
&= \sum_{k=0}^{n-1} (-1)^{n-k} w^k \left[- \sum_{l=1}^{n-k-1} (-1)^l \left(\begin{array}{c} n-l-1 \\ k \end{array} \right) \sum_{i=1}^{n-l} \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} - \left(\begin{array}{c} n-1 \\ k \end{array} \right) \left[\begin{array}{c} n \\ 1 \end{array} \right] \right] \\
&= (-1)^{n-1} \sum_{k=0}^{n-1} (-1)^k w^k \left[\sum_{l=1}^{n-k-1} (-1)^l \left(\begin{array}{c} n-l-1 \\ k \end{array} \right) \sum_{i=1}^{n-l} \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} + \left(\begin{array}{c} n-1 \\ k \end{array} \right) \left[\begin{array}{c} n \\ 1 \end{array} \right] \right] \\
&= (-1)^{n-1} \left[\sum_{k=0}^{n-1} \sum_{l=1}^{n-k-1} \sum_{i=1}^{n-l} (-1)^{k+l} w^k \left(\begin{array}{c} n-l-1 \\ k \end{array} \right) \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \right. \\
&\qquad \left. + \left[\begin{array}{c} n \\ 1 \end{array} \right] \sum_{k=0}^{n-1} (-1)^k \left(\begin{array}{c} n-1 \\ k \end{array} \right) w^k \right].
\end{aligned}$$

On the other hand,

$$\begin{aligned}
(354) &= (-1)^{n-1} \left[\sum_{i=1}^{n-1} \left[\begin{array}{c} i \\ 1 \end{array} \right] (1-w)^{i-1} \sum_{k=0}^{n-i-1} (-1)^k \sum_{l=1}^{n-i-k} (-1)^l \left(\begin{array}{c} n-i-l \\ k \end{array} \right) \hat{\Sigma}_l^{n,i} w^k \right. \\
&\qquad \left. + \left[\begin{array}{c} n \\ 1 \end{array} \right] (1-w)^{n-1} \right].
\end{aligned}$$

Comparing these expressions, we see that they both begin with the factor $(-1)^{n-1}$, so we can ignore that part. Also, the term after the + sign in both expressions agrees, so that too can be ignored. Therefore we must prove that

$$\sum_{i=1}^{n-1} \left[\begin{array}{c} i \\ 1 \end{array} \right] (1-w)^{i-1} \sum_{k=0}^{n-i-1} (-1)^k \sum_{l=1}^{n-i-k} (-1)^l \left(\begin{array}{c} n-i-l \\ k \end{array} \right) \hat{\Sigma}_l^{n,i} w^k \tag{356}$$

$$= \sum_{k=0}^{n-1} \sum_{l=1}^{n-k-1} \sum_{i=1}^{n-l} (-1)^{k+l} w^k \left(\begin{array}{c} n-l-1 \\ k \end{array} \right) \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i}. \tag{357}$$

Expanding the $(1-w)^{i-1}$ in (356) gives

$$\begin{aligned}
&\sum_{i=1}^{n-1} \left[\begin{array}{c} i \\ 1 \end{array} \right] \sum_{m=0}^{i-1} (-1)^m \left(\begin{array}{c} i-1 \\ m \end{array} \right) w^m \sum_{k=0}^{n-i-1} (-1)^k \sum_{l=1}^{n-i-k} (-1)^l \left(\begin{array}{c} n-i-l \\ k \end{array} \right) \hat{\Sigma}_l^{n,i} w^k \\
&= \sum_{i=1}^{n-1} \sum_{m=0}^{i-1} \sum_{k=0}^{n-i-1} \sum_{l=1}^{n-i-k} (-1)^{k+l+m} \left[\begin{array}{c} i \\ 1 \end{array} \right] \left(\begin{array}{c} i-1 \\ m \end{array} \right) \left(\begin{array}{c} n-i-l \\ k \end{array} \right) \hat{\Sigma}_l^{n,i} w^{k+m}.
\end{aligned} \tag{358}$$

Now, to compare (358) and (357), express (358) as a sum of powers of w. The part of (358) after the i sum has the form

$$\sum_{k=0}^{n-i-1} \sum_{m=0}^{i-1} \alpha(m,k) w^{m+k}. \tag{359}$$

Let $p = m+k$, so that $k = p-m$. Then $0 \le k \le n-i-1$ and $0 \le m \le i-1 \Rightarrow 0 \le p \le n-2$. Therefore, we want to write (359) as

$$\sum_{p=0}^{n-2} \beta_p w^p,$$

for suitable β_p's. Given p, we find the restrictions on m: $0 \le m \le i-1$ and $k = p-m$ with $0 \le k \le n-i-1 \Rightarrow p-n+i+1 \le m \le p \Rightarrow \max\{0, p-n+i+1\} \le m \le \min\{i-1, p\}$. Therefore,

$$(359) = \sum_{p=0}^{n-2} \sum_{m=\max\{0,p-n+i-1\}}^{\min\{i-1,p\}} \alpha(m, p-m) w^p.$$

Applying this to (358) gives

$$\sum_{i=1}^{n-1} \sum_{p=0}^{n-2} \sum_{m=\max\{0,p-n+i-1\}}^{\min\{i-1,p\}} \sum_{l=1}^{n-i-p+m} (-1)^{p+l} \left[\begin{array}{c} i \\ 1 \end{array} \right] \left(\begin{array}{c} i-1 \\ m \end{array} \right) \left(\begin{array}{c} n-i-l \\ p-m \end{array} \right) \hat{\Sigma}_l^{n,i} w^p,$$

which, upon exchanging the first two sums, becomes

$$\sum_{p=0}^{n-2} \sum_{i=1}^{n-1} \sum_{m=\max\{0,p-n+i-1\}}^{\min\{i-1,p\}} \sum_{l=1}^{n-i-p+m} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \left(\begin{array}{c} i-1 \\ m \end{array} \right) \left(\begin{array}{c} n-i-l \\ p-m \end{array} \right) \hat{\Sigma}_l^{n,i}. \tag{360}$$

In (357), we may take the first sum from $k = 0$ to $n-2$, since for $k = n-1$ the second sum is empty. This, as well as replacing k by p, gives

$$(357) = \sum_{p=0}^{n-2} \sum_{l=1}^{n-p-1} \sum_{i=1}^{n-l} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \hat{\Sigma}_l^{n,i}. \tag{361}$$

We must show (360) and (361) are equal. First, we eliminate the max and min occurring in (360) by considering several cases. We have

$$\begin{aligned} 0 \ge p-n+i-1 &\iff i \le n-p+1, \\ i-1 \le p &\iff i \le p+1. \end{aligned}$$

Thus,

$$\begin{aligned} 1 \le i \le n-p &\implies \max\{0, p-n+i-1\} = 0, \\ n-p+1 \le i \le n-1 &\implies \max\{0, p-n+i-1\} = p-n+i-1, \\ 1 \le i \le p &\implies \min\{i-1, p\} = i-1, \end{aligned}$$

$$p+1 \le i \le n-1 \implies \min\{i-1,p\} = p.$$

When $p \le n/2$, $p \le n-p$, so that

$$\begin{array}{lll}
1 \le i \le p & \implies \max\{0,p-n+i-1\} = 0, & \min\{i-1,p\} = i-1, \\
p+1 \le i \le n-p & \implies \max\{0,p-n+i-1\} = 0, & \min\{i-1,p\} = p, \\
n-p+1 \le i \le n-1 & \implies \max\{0,p-n+i-1\} = p-n+i-1, & \min\{i-1,p\} = p,
\end{array}$$

and when $n/2 \le p$, $p \ge n-p$, so that

$$\begin{array}{lll}
1 \le i \le n-p & \implies \max\{0,p-n+i-1\} = 0, & \min\{i-1,p\} = i-1, \\
n-p+1 \le i \le p & \implies \max\{0,p-n+i-1\} = p-n+i-1, & \min\{i-1,p\} = i-1, \\
p+1 \le i \le n-1 & \implies \max\{0,p-n+i-1\} = p-n+i-1, & \min\{i-1,p\} = p.
\end{array}$$

Using the relations above and omitting the arguments to the sums for brevity, we can rewrite (360) as

$$\begin{aligned}
(360) \quad = & \sum_{p=0}^{\lfloor n/2 \rfloor} \sum_{i=1}^{p} \sum_{m=0}^{i-1} \sum_{l=1}^{n-i-p+m} && (362) \\
+ & \sum_{p=0}^{\lfloor n/2 \rfloor} \sum_{i=p+1}^{n-p} \sum_{m=0}^{p} \sum_{l=1}^{n-i-p+m} && (363) \\
+ & \sum_{p=0}^{\lfloor n/2 \rfloor} \sum_{i=n-p+1}^{n-1} \sum_{m=p-n+i-1}^{p} \sum_{l=1}^{n-i-p+m} && (364) \\
+ & \sum_{p=\lfloor n/2 \rfloor+1}^{n-2} \sum_{i=1}^{n-p} \sum_{m=0}^{i-1} \sum_{l=1}^{n-i-p+m} && (365) \\
+ & \sum_{p=\lfloor n/2 \rfloor+1}^{n-2} \sum_{i=n-p+1}^{p} \sum_{m=p-n+i-1}^{i-1} \sum_{l=1}^{n-i-p+m} && (366) \\
+ & \sum_{p=\lfloor n/2 \rfloor+1}^{n-2} \sum_{i=p+1}^{n-1} \sum_{m=p-n+i-1}^{p} \sum_{l=1}^{n-i-p+m} . && (367)
\end{aligned}$$

Comparing (361) with (362) to (367), we find that the m and l sums in (362) to (367) must be exchanged. We first derive a general method for switching sums of this form and then apply it to each case.

Consider the sums

$$\sum_{m=a}^{b} \sum_{l=1}^{c+m},$$

where a, b, c are free. When $m = a$, $l = 1, \ldots, c + a$. When $m = b$, $l = 1, \ldots, c + b$. Thus, for $l = 1, \ldots, c + a$, $m = a, \ldots, b$, and for $l = c + a, \ldots, c + b$, $m = l - c, \ldots, b$. Therefore,

$$\sum_{m=a}^{b} \sum_{l=1}^{c+m} = \sum_{l=1}^{c+a} \sum_{m=a}^{b} + \sum_{l=c+a+1}^{c+b} \sum_{m=l-c}^{b} . \tag{368}$$

Applying (368) to (366) gives $a = p - n + i + 1$ (because the l sum in (366) is empty when $m < p - n + i + 1$), $b = i - 1$ and $c = n - i - p \Rightarrow c + a = 1$ and $c + b = n - p - 1$. Therefore,

$$\begin{aligned} \sum_{m=p-n+i-1}^{i-1} \sum_{l=1}^{n-i-p+m} &= \sum_{m=p-n+i+1}^{i-1} \sum_{l=1}^{n-i-p+m} \\ &= \sum_{l=1}^{1} \sum_{m=p-n+i+1}^{i-1} + \sum_{l=2}^{n-p-1} \sum_{m=l-n+i+p}^{i-1} \\ &= \sum_{l=1}^{n-p-1} \sum_{m=l-n+i+p}^{i-1} . \end{aligned} \tag{369}$$

Applying (368) to (362) and (365) gives $a = 0$, $b = i - 1$, and $c = n - i - p \Rightarrow c + a = n - i - p$ and $c + b = n - p - 1$. Therefore,

$$\sum_{m=0}^{i-1} \sum_{l=1}^{n-i-p+m} = \sum_{l=1}^{n-i-p} \sum_{m=0}^{i-1} + \sum_{l=n-i-p+1}^{n-p-1} \sum_{m=l-n+i+p}^{i-1} . \tag{370}$$

Applying (368) to (364) and (367) gives $a = p - n + i + 1$ (because the l sum in (364) and (367) is empty when $m < p - n + i + 1$), $b = p$ and $c = n - i - p \Rightarrow c + a = 1$ and $c + b = n - i$. Therefore,

$$\begin{aligned} \sum_{m=p-n+i-1}^{p} \sum_{l=1}^{n-i-p+m} &= \sum_{m=p-n+i+1}^{p} \sum_{l=1}^{n-i-p+m} \\ &= \sum_{l=1}^{1} \sum_{m=p-n+i+1}^{p} + \sum_{l=2}^{n-i} \sum_{m=l-n+i+p}^{p} \\ &= \sum_{l=1}^{n-i} \sum_{m=l-n+i+p}^{p} . \end{aligned} \tag{371}$$

Applying (368) to (363) gives $a = 0$, $b = p$, and $c = n - i - p \Rightarrow c + a = n - i - p$ and $c + b = n - i$. Therefore,

$$\sum_{m=0}^{p} \sum_{l=1}^{n-i-p+m} = \sum_{l=1}^{n-i-p} \sum_{m=0}^{p} + \sum_{l=n-i-p+1}^{n-i} \sum_{m=l-n+i+p}^{p} . \tag{372}$$

Now, using (369) to (372) in (362) to (367) and inserting the arguments to the sums from (360), we find that (360) =

$$\sum_{p=0}^{\lfloor n/2\rfloor}\sum_{i=1}^{p}\sum_{l=1}^{n-i-p}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=0}^{i-1}\binom{i-1}{m}\binom{n-i-l}{p-m} \tag{373}$$

$$+\sum_{p=0}^{\lfloor n/2\rfloor}\sum_{i=1}^{p}\sum_{l=n-i-p+1}^{n-p-1}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=l-n+i+p}^{i-1}\binom{i-1}{m}\binom{n-i-l}{p-m} \tag{374}$$

$$+\sum_{p=0}^{\lfloor n/2\rfloor}\sum_{i=p+1}^{n-p}\sum_{l=1}^{n-i-p}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=0}^{p}\binom{i-1}{m}\binom{n-i-l}{p-m} \tag{375}$$

$$+\sum_{p=0}^{\lfloor n/2\rfloor}\sum_{i=p+1}^{n-p}\sum_{l=n-i-p+1}^{n-i}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=l-n+i+p}^{p}\binom{i-1}{m}\binom{n-i-l}{p-m} \tag{376}$$

$$+\sum_{p=0}^{\lfloor n/2\rfloor}\sum_{i=n-p+1}^{n-1}\sum_{l=1}^{n-i}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=l-n+i+p}^{p}\binom{i-1}{m}\binom{n-i-l}{p-m} \tag{377}$$

$$+\sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{i=1}^{n-p}\sum_{l=1}^{n-i-p}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=0}^{i-1}\binom{i-1}{m}\binom{n-i-l}{p-m} \tag{378}$$

$$+\sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{i=1}^{n-p}\sum_{l=n-i-p+1}^{n-p-1}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=l-n+i+p}^{i-1}\binom{i-1}{m}\binom{n-i-l}{p-m} \tag{379}$$

$$+\sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{i=n-p+1}^{p}\sum_{l=1}^{n-p-1}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=l-n+i+p}^{i-1}\binom{i-1}{m}\binom{n-i-l}{p-m} \tag{380}$$

$$+\sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{i=p+1}^{n-1}\sum_{l=1}^{n-i}(-1)^{p+l}w^p\begin{bmatrix} i \\ 1 \end{bmatrix}\hat{\Sigma}_l^{n,i}\sum_{m=l-n+i+p}^{p}\binom{i-1}{m}\binom{n-i-l}{p-m}. \tag{381}$$

We now simplify the m-sums in the above expression. Using (454) in (373) and (378), we have

$$\sum_{m=0}^{i-1}\binom{i-1}{m}\binom{n-i-l}{p-m}=\binom{n-l-1}{p}.$$

In (374), (379) and (380), we have

$$\begin{aligned}\sum_{m=l-n+i+p}^{i-1}\binom{i-1}{m}\binom{n-i-l}{p-m} &= \sum_{m=u}^{i-1}\binom{i-1}{m}\binom{p-u}{p-m}, \quad \text{for } u=l-n+i+p\\ &= \sum_{k=0}^{i-1-u}\binom{i-1}{k+u}\binom{p-u}{p-(k+u)}\\ &= \sum_{k=0}^{a}\binom{a+u}{k+u}\binom{p-u}{p-k-u}, \quad \text{for } a=i-1-u\end{aligned}$$

$$
\begin{aligned}
&= \sum_{k=0}^{a} \left(\begin{array}{c} a+u \\ a-k \end{array} \right) \left(\begin{array}{c} p-u \\ k \end{array} \right) \\
&= \left(\begin{array}{c} a+p \\ a \end{array} \right) \\
&= \left(\begin{array}{c} n-l-1 \\ p \end{array} \right)
\end{aligned}
$$

by (453). In (375), using (453), we have

$$
\sum_{m=0}^{p} \left(\begin{array}{c} i-1 \\ m \end{array} \right) \left(\begin{array}{c} n-i-l \\ p-m \end{array} \right) = \left(\begin{array}{c} n-l-1 \\ p \end{array} \right).
$$

In (377) and (381), we have

$$
\begin{aligned}
\sum_{m=l-n+i+p}^{p} \left(\begin{array}{c} i-1 \\ m \end{array} \right) \left(\begin{array}{c} n-i-l \\ p-m \end{array} \right) &= \sum_{m=p-u}^{p} \left(\begin{array}{c} i-1 \\ m \end{array} \right) \left(\begin{array}{c} u \\ p-m \end{array} \right), \quad \text{for } u = n-i-l \\
&= \sum_{k=0}^{u} \left(\begin{array}{c} i-1 \\ k+p-u \end{array} \right) \left(\begin{array}{c} u \\ u-k \end{array} \right) \\
&= \sum_{k=0}^{u} \left(\begin{array}{c} i-1 \\ k+p-u \end{array} \right) \left(\begin{array}{c} u \\ k \end{array} \right) \\
&= \left(\begin{array}{c} u+i-1 \\ u+p-u \end{array} \right) \\
&= \left(\begin{array}{c} n-l-1 \\ p \end{array} \right)
\end{aligned}
$$

by (455). Replacing the m-sums in (373) to (381) with the above expressions gives

$$
\begin{aligned}
(360) \quad &= \sum_{p=0}^{\lfloor n/2 \rfloor} \sum_{i=1}^{p} \sum_{l=1}^{n-i-p} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \\
&+ \sum_{p=0}^{\lfloor n/2 \rfloor} \sum_{i=1}^{p} \sum_{l=n-i-p+1}^{n-p-1} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \\
&+ \sum_{p=0}^{\lfloor n/2 \rfloor} \sum_{i=p+1}^{n-p} \sum_{l=1}^{n-i-p} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \\
&+ \sum_{p=0}^{\lfloor n/2 \rfloor} \sum_{i=p+1}^{n-p} \sum_{l=n-i-p+1}^{n-i} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \\
&+ \sum_{p=0}^{\lfloor n/2 \rfloor} \sum_{i=n-p+1}^{n-1} \sum_{l=1}^{n-i} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right)
\end{aligned}
$$

$$+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2} \sum_{i=1}^{n-p} \sum_{l=1}^{n-i-p} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right)$$

$$+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2} \sum_{i=1}^{n-p} \sum_{l=n-i-p+1}^{n-p-1} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right)$$

$$+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2} \sum_{i=n-p+1}^{p} \sum_{l=1}^{n-p-1} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right)$$

$$+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2} \sum_{i=p+1}^{n-1} \sum_{l=1}^{n-i} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right),$$

and, by coalescing adjacent sums, we get

$$(360) = \sum_{p=0}^{\lfloor n/2\rfloor} \sum_{i=1}^{p} \sum_{l=1}^{n-p-1} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \quad (382)$$

$$+ \sum_{p=0}^{\lfloor n/2\rfloor} \sum_{i=p+1}^{n-p} \sum_{l=1}^{n-i} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \quad (383)$$

$$+ \sum_{p=0}^{\lfloor n/2\rfloor} \sum_{i=n-p+1}^{n-1} \sum_{l=1}^{n-i} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \quad (384)$$

$$+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2} \sum_{i=1}^{n-p} \sum_{l=1}^{n-p-1} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \quad (385)$$

$$+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2} \sum_{i=n-p+1}^{p} \sum_{l=1}^{n-p-1} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right) \quad (386)$$

$$+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2} \sum_{i=p+1}^{n-1} \sum_{l=1}^{n-i} (-1)^{p+l} w^p \left[\begin{array}{c} i \\ 1 \end{array} \right] \hat{\Sigma}_l^{n,i} \left(\begin{array}{c} n-l-1 \\ p \end{array} \right). \quad (387)$$

Now switch the i and l sums in (382) to (387). The ones in (382), (385) and (386) are independent, so they just exchange. The remaining ones have the form

$$\sum_{i=a}^{b} \sum_{l=1}^{c-i},$$

where a, b, c are free. When $i = a$, $l = 1, \ldots, c-a$. When $i = b$, $l = 1, \ldots, c-b$. Thus, for $l = 1, \ldots, c-b$, $i = a, \ldots, b$, and, for $l = c-b, \ldots, c-a$, $i = a, \ldots, c-l$. Therefore,

$$\sum_{i=a}^{b} \sum_{l=1}^{c-i} = \sum_{l=1}^{c-b} \sum_{i=a}^{b} + \sum_{l=c-b+1}^{c-a} \sum_{i=a}^{c-l}. \quad (388)$$

Applying (388) to (383) gives $a = p+1$, $b = n-p$ and $c = n \Rightarrow c-b = p$ and $c-a = n-p-1$. Therefore,

$$\sum_{i=p+1}^{n-p}\sum_{l=1}^{n-i} = \sum_{l=1}^{p}\sum_{i=p+1}^{n-p} + \sum_{l=p+1}^{n-p-1}\sum_{i=p+1}^{n-l}. \tag{389}$$

Applying (388) to (384) gives $a = n-p+1$, $b = n-1$ and $c = n \Rightarrow c-b = 1$ and $c-a = p-1$. Therefore,

$$\begin{aligned}\sum_{i=n-p+1}^{n-1}\sum_{l=1}^{n-i} &= \sum_{l=1}^{1}\sum_{i=n-p+1}^{n-1} + \sum_{l=2}^{p-1}\sum_{i=n-p+1}^{n-l} \\ &= \sum_{l=1}^{p-1}\sum_{i=n-p+1}^{n-l}.\end{aligned} \tag{390}$$

Applying (388) to (387) gives $a = p+1$, $b = n-1$ and $c = n \Rightarrow c-b = 1$ and $c-a = n-p-1$. Therefore,

$$\begin{aligned}\sum_{i=p+1}^{n-1}\sum_{l=1}^{n-i} &= \sum_{l=1}^{1}\sum_{i=p+1}^{n-1} + \sum_{l=2}^{n-p-1}\sum_{i=p+1}^{n-l} \\ &= \sum_{l=1}^{n-p-1}\sum_{i=p+1}^{n-l}.\end{aligned} \tag{391}$$

Now, switching the i and l sums in (382), (385) and (386) and applying (389), (390) and (391) to (383), (384) and (387), respectively, as well as removing the sum arguments for clarity, gives

$$\begin{aligned}(360) &= \sum_{p=0}^{\lfloor n/2\rfloor}\sum_{l=1}^{n-p-1}\sum_{i=1}^{p} + \sum_{p=0}^{\lfloor n/2\rfloor}\sum_{l=1}^{p}\sum_{i=p+1}^{n-p} + \sum_{p=0}^{\lfloor n/2\rfloor}\sum_{l=p+1}^{n-p-1}\sum_{i=p+1}^{n-l} + \sum_{p=0}^{\lfloor n/2\rfloor}\sum_{l=1}^{p-1}\sum_{i=n-p+1}^{n-l} \\ &+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{l=1}^{n-p-1}\sum_{i=1}^{n-p} + \sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{l=1}^{n-p-1}\sum_{i=n-p+1}^{p} + \sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{l=1}^{n-p-1}\sum_{i=p+1}^{n-l} \\ &= \sum_{p=0}^{\lfloor n/2\rfloor}\left[\sum_{l=1}^{n-p-1}\sum_{i=1}^{p} + \sum_{l=1}^{p}\sum_{i=p+1}^{n-p} + \sum_{l=p+1}^{n-p-1}\sum_{i=p+1}^{n-l} + \sum_{l=1}^{p-1}\sum_{i=n-p+1}^{n-l}\right] \\ &+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2}\left[\sum_{l=1}^{n-p-1}\sum_{i=1}^{n-p} + \sum_{l=1}^{n-p-1}\sum_{i=n-p+1}^{p} + \sum_{l=1}^{n-p-1}\sum_{i=p+1}^{n-l}\right] \\ &= \sum_{p=0}^{\lfloor n/2\rfloor}\left[\sum_{l=1}^{n-p-1}\sum_{i=1}^{p} + \sum_{l=1}^{p}\sum_{i=p+1}^{n-p} + \sum_{l=p+1}^{n-p-1}\sum_{i=p+1}^{n-l} + \sum_{l=1}^{p-1}\sum_{i=n-p+1}^{n-l}\right] \\ &+ \sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{l=1}^{n-p-1}\sum_{i=1}^{n-l}.\end{aligned} \tag{392}$$

It turns out that the arguments to both of the p sums are in fact equal. That is,

$$\begin{aligned}
&\sum_{l=1}^{n-p-1}\sum_{i=1}^{p}+\sum_{l=1}^{p}\sum_{i=p+1}^{n-p}+\sum_{l=p+1}^{n-p-1}\sum_{i=p+1}^{n-l}+\sum_{l=1}^{p-1}\sum_{i=n-p+1}^{n-l}\\
=&\sum_{l=1}^{n-p-1}\sum_{i=1}^{p}+\sum_{l=1}^{p}\sum_{i=p+1}^{n-p}+\sum_{l=p+1}^{n-p-1}\sum_{i=p+1}^{n-l}+\sum_{l=1}^{p}\sum_{i=n-p+1}^{n-l}\\
=&\sum_{l=1}^{n-p-1}\sum_{i=1}^{p}+\sum_{l=p+1}^{n-p-1}\sum_{i=p+1}^{n-l}+\sum_{l=1}^{p}\sum_{i=p+1}^{n-l}, \quad \text{since } l\le p\Rightarrow n-l\ge n-p,\\
=&\sum_{l=1}^{n-p-1}\sum_{i=1}^{p}+\sum_{l=1}^{n-p-1}\sum_{i=p+1}^{n-l}, \quad \text{since } l\le n-p-1\Rightarrow n-l\ge p+1,\\
=&\sum_{l=1}^{n-p-1}\sum_{i=1}^{n-l}.
\end{aligned}$$

Using this in (392), we finally have that

$$(360)=\sum_{p=0}^{\lfloor n/2\rfloor}\sum_{l=1}^{n-p-1}\sum_{i=1}^{n-l}+\sum_{p=\lfloor n/2\rfloor+1}^{n-2}\sum_{l=1}^{n-p-1}\sum_{i=1}^{n-l}=\sum_{p=0}^{n-2}\sum_{l=1}^{n-p-1}\sum_{i=1}^{n-l}.$$

Putting the sum arguments from (382) to (387) back in, we get

$$(360)=\sum_{p=0}^{n-2}\sum_{l=1}^{n-p-1}\sum_{i=1}^{n-l}(-1)^{p+l}w^p\left[\begin{array}{c} i \\ 1 \end{array}\right]\left(\begin{array}{c} n-l-1 \\ p \end{array}\right)\hat{\Sigma}_l^{n,i},$$

which equals (361), completing the proof of Lemma 1. □

D.2 Lemma 2

Lemma 2

$$\sum_{l=1}^{n}(-1)^l\tilde{\Sigma}_l^{s,n}=(-1)^n\left(\begin{array}{c} s \\ n \end{array}\right), \quad \textit{for } n=1,\ldots,s-1,\ s\ge 1. \tag{393}$$

Proof. For $l\ge 2$, we see from (113) that

$$\begin{aligned}
\tilde{\Sigma}_l^{s,n} &= \sum_{s-n+1\le i_1<\cdots<i_{l-1}\le s-1}\left(\begin{array}{c} i_1 \\ s-n \end{array}\right)\left(\begin{array}{c} i_2 \\ i_1 \end{array}\right)\cdots\left(\begin{array}{c} i_{l-1} \\ i_{l-2} \end{array}\right)\left(\begin{array}{c} s \\ i_{l-1} \end{array}\right)\\
&= \sum_{i_1=s-n+1}^{s-l+1}\left(\begin{array}{c} i_1 \\ s-n \end{array}\right)\sum_{i_1<i_2<\cdots<i_{l-1}\le s-1}\left(\begin{array}{c} i_2 \\ i_1 \end{array}\right)\cdots\left(\begin{array}{c} i_{l-1} \\ i_{l-2} \end{array}\right)\left(\begin{array}{c} s \\ i_{l-1} \end{array}\right)
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{k=s-n+1}^{s-l+1} \binom{k}{s-n} \sum_{k<i_1<i_2\cdots<i_{l-2}\le s-1} \binom{i_1}{k}\binom{i_2}{i_1}\cdots\binom{i_{l-2}}{i_{l-3}}\binom{s}{i_{l-2}} \\
&= \sum_{k=s-n+2}^{s-l+2} \binom{k-1}{s-n} \sum_{k\le i_1<i_2\cdots<i_{l-2}\le s-1} \binom{i_1}{k-1}\binom{i_2}{i_1}\cdots\binom{i_{l-2}}{i_{l-3}}\binom{s}{i_{l-2}} \\
&= \sum_{N=l-1}^{n-1} \binom{s-N}{s-n} \tilde{\Sigma}_{l-1}^{s,N}
\end{aligned}
$$

while, for $l = 1$,

$$\tilde{\Sigma}_1^{s,n} = \binom{s}{n}.$$

So the left side of (393) reduces to

$$-\binom{s}{n} + \sum_{l=2}^{n}(-1)^l \sum_{N=l-1}^{n-1} \binom{s-N}{s-n} \tilde{\Sigma}_{l-1}^{s,N}. \tag{394}$$

Now switch the l and N sums. For $l = 2$, $N = 1, \ldots, n-1$. For $l = n$, $N = n-1$. Thus $N = 1, \ldots, n-1$ and $l = 2, \ldots, N+1$. Thus, continuing from (394), we find that the left side of (393) becomes

$$
\begin{aligned}
&-\binom{s}{n} + \sum_{N=1}^{n-1}\sum_{l=2}^{N+1}(-1)^l \binom{s-N}{s-n} \tilde{\Sigma}_{l-1}^{s,N} \\
&= -\binom{s}{n} - \sum_{N=1}^{n-1} \binom{s-N}{s-n} \sum_{l=1}^{N}(-1)^l \tilde{\Sigma}_l^{s,N} \\
&= -\binom{s}{n} - \sum_{N=1}^{n-1} \binom{s-N}{s-n} (-1)^N \binom{s}{N} \quad \text{by induction, since } N \le n-1 \\
&= -\sum_{N=0}^{n-1} \binom{s-N}{s-n} (-1)^N \binom{s}{N} \\
&= -(-1)^{n-1}\binom{s}{n} \quad \text{by Lemma 3 in Appendix D.3} \\
&= (-1)^n \binom{s}{n},
\end{aligned}
$$

completing the proof of the lemma. □

D.3 Lemma 3

Lemma 3

$$\sum_{k=0}^{n}(-1)^k \binom{s-k}{s-n-1}\binom{s}{k} = (-1)^n \binom{s}{n+1}, \quad \textit{for } n = 0,\ldots,s-1,\ s \geq 1. \tag{395}$$

Proof. We use induction on s and n. The base cases are as follows. If $n = 0$,

$$LS = \binom{s}{s-1}\binom{s}{0} = s = \binom{s}{1} = RS.$$

If $s = 1$, then $n = 0$, so we have already proved this case above.

Now consider the general case, $n \geq 1$, $s \geq 2$. Let S_n^s be the left side of (395). Then

$$\begin{aligned}
S_n^s &= \sum_{k=1}^{n}(-1)^k \binom{s-k}{s-n-1}\binom{s}{k} + \binom{s}{s-n-1}\binom{s}{0} \\
&= \sum_{k=1}^{n}(-1)^k \binom{s-k}{s-n-1}\binom{s-1}{k} && (396)\\
&\quad + \sum_{k=1}^{n}(-1)^k \binom{s-k}{s-n-1}\binom{s-1}{k-1} && (397)\\
&\quad + \binom{s}{s-n-1}.
\end{aligned}$$

Lines (396) and (397) can be expanded as follows.

$$\begin{aligned}
(396) &= \sum_{k=1}^{n}(-1)^k \binom{s-k-1}{s-n-1}\binom{s-1}{k} && (398)\\
&\quad + \sum_{k=1}^{n}(-1)^k \binom{s-k-1}{s-n-2}\binom{s-1}{k}. && (399)\\
(397) &= \sum_{k=1}^{n}(-1)^k \binom{s-1-(k-1)}{s-1-(n-1)-1}\binom{s-1}{k-1} \\
&= -\sum_{k=0}^{n-1}(-1)^k \binom{s-1-k}{s-1-(n-1)-1}\binom{s-1}{k} \\
&= -S_{n-1}^{s-1} \\
&= (-1)^n \binom{s-1}{n},
\end{aligned}$$

where the last line follows from (395) by induction on n and s. Furthermore,

$$(398) = \sum_{k=1}^{n-1}(-1)^k \binom{s-1-k}{s-1-(n-1)-1}\binom{s-1}{k} + (-1)^n \binom{s-n-1}{s-n-1}\binom{s-1}{n}$$

$$
\begin{aligned}
&= \sum_{k=0}^{n-1}(-1)^k \left(\begin{array}{c} s-1-k \\ s-1-(n-1)-1 \end{array} \right) \left(\begin{array}{c} s-1 \\ k \end{array} \right) \\
&\quad - \left(\begin{array}{c} s-1 \\ s-n-1 \end{array} \right) \left(\begin{array}{c} s-1 \\ 0 \end{array} \right) + (-1)^n \left(\begin{array}{c} s-1 \\ n \end{array} \right) \\
&= S_{n-1}^{s-1} - \left(\begin{array}{c} s-1 \\ s-n-1 \end{array} \right) + (-1)^n \left(\begin{array}{c} s-1 \\ n \end{array} \right) \\
&= (-1)^{n-1} \left(\begin{array}{c} s-1 \\ n \end{array} \right) - \left(\begin{array}{c} s-1 \\ s-n-1 \end{array} \right) + (-1)^n \left(\begin{array}{c} s-1 \\ n \end{array} \right) \\
&= - \left(\begin{array}{c} s-1 \\ s-n-1 \end{array} \right),
\end{aligned}
$$

where the second to last line follows from (395) by induction on n and s. Also,

$$
\begin{aligned}
(399) &= \sum_{k=0}^{n}(-1)^k \left(\begin{array}{c} s-k-1 \\ s-n-2 \end{array} \right) \left(\begin{array}{c} s-1 \\ k \end{array} \right) - \left(\begin{array}{c} s-1 \\ s-n-2 \end{array} \right) \left(\begin{array}{c} s-1 \\ 0 \end{array} \right) \\
&= \sum_{k=0}^{n}(-1)^k \left(\begin{array}{c} (s-1)-k \\ (s-1)-n-1 \end{array} \right) \left(\begin{array}{c} s-1 \\ k \end{array} \right) - \left(\begin{array}{c} s-1 \\ s-n-2 \end{array} \right) \\
&= S_n^{s-1} - \left(\begin{array}{c} s-1 \\ s-n-2 \end{array} \right) \\
&= (-1)^n \left(\begin{array}{c} s-1 \\ n+1 \end{array} \right) - \left(\begin{array}{c} s-1 \\ s-n-2 \end{array} \right),
\end{aligned}
$$

where the last line follows from (395) by induction on s. Finally,

$$
\begin{aligned}
S_n^s &= (397) + (398) + (399) + \left(\begin{array}{c} s \\ s-n-1 \end{array} \right) \\
&= (-1)^n \left(\begin{array}{c} s-1 \\ n \end{array} \right) \\
&\quad - \left(\begin{array}{c} s-1 \\ s-n-1 \end{array} \right) + (-1)^n \left(\begin{array}{c} s-1 \\ n+1 \end{array} \right) - \left(\begin{array}{c} s-1 \\ s-n-2 \end{array} \right) \\
&\quad + \left(\begin{array}{c} s \\ s-n-1 \end{array} \right) \\
&= (-1)^n \left[\left(\begin{array}{c} s-1 \\ n \end{array} \right) + \left(\begin{array}{c} s-1 \\ n+1 \end{array} \right) \right] \\
&\quad - \left(\begin{array}{c} s-1 \\ s-n-1 \end{array} \right) + \left(\begin{array}{c} s \\ s-n-1 \end{array} \right) - \left(\begin{array}{c} s-1 \\ s-n-2 \end{array} \right)
\end{aligned}
$$

$$
\begin{aligned}
&= (-1)^n \binom{s}{n+1} - \binom{s}{s-n-1} + \binom{s}{s-n-1} \\
&= (-1)^n \binom{s}{n+1}
\end{aligned}
$$

as required, completing the proof of Lemma 3. □

D.4 Lemma 4

Lemma 4

$$
\Sigma_l^n = (-1)^{l+1} \sum_{m=1}^{l+1} (-1)^m \binom{l+1}{m} m^n, \quad \textit{for } l = 0, \ldots, n-1,\ n \geq 1. \tag{400}
$$

Proof. The proof is by induction on l. We first handle the base cases. For $l = 0$,

$$
RS = (-1)^1 (-1)^1 \binom{1}{1} 1^n = 1 = \Sigma_0^n = LS
$$

by (97). For $l = 1$,

$$
RS = -\binom{2}{1} 1^n + \binom{2}{2} 2^n = 2^n - 2,
$$

while

$$
LS = \Sigma_1^n = \sum_{j=1}^{n-1} \binom{n}{j},
$$

by (97). However, (451) gives

$$
\sum_{j=0}^{n} \binom{n}{j} = 2^n,
$$

from which it follows that

$$
LS = 2^n - \binom{n}{0} - \binom{n}{n} = 2^n - 2 = RS.
$$

Now consider the general case, $l \geq 2$ (hence $n \geq 3$). We use the recursive expression for Σ_l^n given by Lemma 10 in Appendix D.10, which, together with (400) by induction, gives

$$
\begin{aligned}
\Sigma_l^n &= \sum_{j=1}^{n-1} \binom{n}{j} (-1)^l \sum_{m=1}^{l} (-1)^m \binom{l}{m} m^j \\
&= (-1)^l \sum_{m=1}^{l} (-1)^m \binom{l}{m} \sum_{j=1}^{n-1} \binom{n}{j} m^j
\end{aligned}
$$

$$
\begin{aligned}
&= (-1)^l \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) [(1+m)^n - m^n - 1] \\
&= (-1)^l \left[\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) (1+m)^n \right. \\
&\qquad \left. - \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) m^n - \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) \right] \\
&= (-1)^l \left[\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) (1+m)^n - \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) m^n + 1 \right], \qquad (401)
\end{aligned}
$$

by (452), since in the general inductive step $l \geq 1$. For the right side of (400), we have

$$
\begin{aligned}
&(-1)^{l+1} \sum_{m=1}^{l+1} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) m^n \\
&= (-1)^{l+1} \left[\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) m^n + (-1)^{l+1} (l+1)^n \right] \\
&= (-1)^{l+1} \left[\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) m^n + \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m-1 \end{array} \right) m^n + (-1)^{l+1} (l+1)^n \right] \\
&= (-1)^{l+1} \left[\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) m^n - \sum_{m=0}^{l-1} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) (1+m)^n + (-1)^{l+1} (l+1)^n \right] \\
&= (-1)^{l+1} \left[\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) m^n - \sum_{m=0}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) (1+m)^n \right] \\
&= (-1)^{l+1} \left[\sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) m^n - \sum_{m=1}^{l} (-1)^m \left(\begin{array}{c} l \\ m \end{array} \right) (1+m)^n + 1 \right],
\end{aligned}
$$

which equals (401), as required. □

D.5 Lemma 5

Lemma 5

$$
\begin{aligned}
U_m^{(s)} &= \sum_{i=1}^{s} \gamma_{s-i}^{(s)} m^i \quad \textit{from (84)} \qquad (402) \\
&= s! \left[\left(\begin{array}{c} m+s \\ s \end{array} \right) - 1 \right], \quad \textit{for } s \geq 1,\ m \geq 0. \qquad (403)
\end{aligned}
$$

Proof. We first establish a recursive relationship for $\gamma_k^{(s)}$. For $k \geq 2$, it follows from (64) that

$$\begin{aligned}
\gamma_k^{(s)} &= \sum_{1 \leq i_1 < \cdots < i_k \leq s} i_1 \cdots i_k \\
&= \sum_{1 \leq i_1 < \cdots < i_k < s} i_1 \cdots i_k + \sum_{1 \leq i_1 < \cdots < i_k = s} i_1 \cdots i_k \\
&= \sum_{1 \leq i_1 < \cdots < i_k \leq s-1} i_1 \cdots i_k + s \sum_{1 \leq i_1 < \cdots < i_{k-1} \leq s-1} i_1 \cdots i_k \\
&= s\gamma_{k-1}^{(s-1)} + \gamma_k^{(s-1)}.
\end{aligned}$$

It is easy to see from (64) that this recursive relationship holds for $k = 1$ also. Therefore we have shown that

$$\gamma_k^{(s)} = s\gamma_{k-1}^{(s-1)} + \gamma_k^{(s-1)} \tag{404}$$

for $k \geq 1$.

We now prove the lemma by induction on s. For $s = 1$, it follows from (402) and (64) that

$$LS = \gamma_0^{(1)} m^1 = m = 1! \left[\begin{pmatrix} m+1 \\ 1 \end{pmatrix} - 1 \right] = RS.$$

For $s > 1$, we get by using (404) in (402) and then by using (64) that

$$\begin{aligned}
U_m^{(s)} &= \sum_{i=1}^{s} \gamma_{s-i}^{(s)} m^i \\
&= \sum_{i=1}^{s-1} \gamma_{s-i}^{(s)} m^i + \gamma_0^{(s)} m^s \\
&= \sum_{i=1}^{s-1} \left(\gamma_{s-i}^{(s-1)} + s\gamma_{s-i-1}^{(s-1)} \right) m^i + \gamma_0^{(s)} m^s \\
&= \sum_{i=1}^{s-1} \gamma_{s-i}^{(s-1)} m^i + \sum_{i=1}^{s-1} s\gamma_{s-i-1}^{(s-1)} m^i + m^s \\
&= m \sum_{i=0}^{s-2} \gamma_{s-i-1}^{(s-1)} m^i + s \sum_{i=1}^{s-1} \gamma_{s-i-1}^{(s-1)} m^i + m^s \\
&= m \left(U_m^{(s-1)} + \gamma_{s-1}^{(s-1)} m^0 - \gamma_0^{(s-1)} m^{s-1} \right) + sU_m^{(s-1)} + m^s \\
&= mU_m^{(s-1)} + m(s-1)! - mm^{s-1} + sU_m^{(s-1)} + m^s \\
&= (m+s)U_m^{(s-1)} + m(s-1)! \\
&= (m+s)(s-1)! \left[\begin{pmatrix} m+s-1 \\ s-1 \end{pmatrix} - 1 \right] + m(s-1)! \quad \text{by induction on (403)} \\
&= (s-1)! \left[(m+s) \begin{pmatrix} m+s-1 \\ s-1 \end{pmatrix} - (m+s) + m \right]
\end{aligned}$$

$$
\begin{aligned}
&= s!\left[\frac{(m+s)}{s}\left(\begin{array}{c} m+s-1 \\ s-1 \end{array}\right)-1\right] \\
&= s!\left[\frac{(m+s)(m+s-1)!}{s(s-1)!m!}-1\right] \\
&= s!\left[\frac{(m+s)!}{s!m!}-1\right] \\
&= s!\left[\left(\begin{array}{c} m+s \\ s \end{array}\right)-1\right],
\end{aligned}
$$

as required. □

D.6 Lemma 6

Lemma 6

$$
\sum_{l=1}^{s-k}(-1)^l\left(\begin{array}{c} s \\ l \end{array}\right)\left(\begin{array}{c} s-l \\ k \end{array}\right) = -\left(\begin{array}{c} s \\ k \end{array}\right), \quad \textit{for } k=0,\ldots,s-1,\ s\geq 1. \tag{405}
$$

Proof. The proof is by induction on k and s. We first check the base cases. If $k=0$, then

$$
LS = \sum_{l=0}^{s}(-1)^l\left(\begin{array}{c} s \\ l \end{array}\right)-1 = 0-1 = -1 = RS
$$

by (452), since $s\neq 0$. If $s=1$, then $k=0$, so we have already proved this case above.

Now consider the general case, $s\geq 2$ and $k=1,\ldots,s-1$.

$$
\begin{aligned}
\text{LS} &= \sum_{l=1}^{s-k}(-1)^l\left(\begin{array}{c} s \\ l \end{array}\right)\left(\begin{array}{c} s-l \\ k \end{array}\right) \\
&= \sum_{l=1}^{s-k}(-1)^l\left\{\left[\left(\begin{array}{c} s-1 \\ l \end{array}\right)+\left(\begin{array}{c} s-1 \\ l-1 \end{array}\right)\right]\left(\begin{array}{c} s-l \\ k \end{array}\right)\right\} \\
&= \sum_{l=1}^{s-k}(-1)^l\left\{\left(\begin{array}{c} s-1 \\ l \end{array}\right)\left[\left(\begin{array}{c} s-l-1 \\ k \end{array}\right)+\left(\begin{array}{c} s-l-1 \\ k-1 \end{array}\right)\right]+\left(\begin{array}{c} s-1 \\ l-1 \end{array}\right)\left(\begin{array}{c} s-l \\ k \end{array}\right)\right\} \\
&= \sum_{l=1}^{s-k}(-1)^l\left(\begin{array}{c} s-1 \\ l \end{array}\right)\left(\begin{array}{c} s-l-1 \\ k \end{array}\right)+\sum_{l=1}^{s-k}(-1)^l\left(\begin{array}{c} s-1 \\ l \end{array}\right)\left(\begin{array}{c} s-l-1 \\ k-1 \end{array}\right) \\
&\quad +\sum_{l=1}^{s-k}(-1)^l\left(\begin{array}{c} s-1 \\ l-1 \end{array}\right)\left(\begin{array}{c} s-l \\ k \end{array}\right) \\
&= \sum_{l=1}^{s-k-1}(-1)^l\left(\begin{array}{c} s-1 \\ l \end{array}\right)\left(\begin{array}{c} s-l-1 \\ k \end{array}\right)+(-1)^{s-k}\left(\begin{array}{c} s-1 \\ s-k \end{array}\right)\left(\begin{array}{c} k-1 \\ k \end{array}\right)
\end{aligned}
$$

$$
\begin{aligned}
&+\sum_{l=1}^{s-k}(-1)^l\binom{s-1}{l}\binom{s-l-1}{k-1}\\
&+\sum_{l=1}^{s-k-1}(-1)^l\binom{s-1}{l-1}\binom{s-l}{k}+(-1)^{s-k}\binom{s-1}{s-k-1}\binom{k}{k}\\
=\;&\sum_{l=1}^{s-k-2}(-1)^l\binom{s-1}{l}\binom{s-l-1}{k}+(-1)^{s-k-1}\binom{s-1}{s-k-1}\binom{s-(s-k-1)-1}{k}\\
&+0+\sum_{l=1}^{s-k}(-1)^l\binom{s-1}{l}\binom{s-l-1}{k-1}\\
&-\sum_{l=0}^{s-k-2}(-1)^l\binom{s-1}{l}\binom{s-l-1}{k}+(-1)^{s-k}\binom{s-1}{k}\\
=\;&\sum_{l=1}^{s-k-2}(-1)^l\binom{s-1}{l}\binom{s-l-1}{k}+(-1)^{s-k-1}\binom{s-1}{k}\binom{k}{k}\\
&-\binom{s-1}{k-1}\quad\text{by induction on (405)}\\
&-\sum_{l=1}^{s-k-2}(-1)^l\binom{s-1}{l}\binom{s-l-1}{k}-\binom{s-1}{0}\binom{s-1}{k}+(-1)^{s-k}\binom{s-1}{k}\\
=\;&-\binom{s-1}{k-1}-\binom{s-1}{k}+(-1)^{s-k-1}\binom{s-1}{k}+(-1)^{s-k}\binom{s-1}{k}\\
=\;&-\binom{s}{k},
\end{aligned}
$$

as required. □

D.7 Lemma 7

Lemma 7

$$
\begin{aligned}
M_l^{(s)} &= \sum_{i=2}^{s} i\Sigma_l^{i-1}S_{i+1}^{(s)} \quad \textit{from (91)} &(406)\\
&= \binom{s}{l+2}, \quad \textit{for } l=0,\ldots,s-1,\ s\geq 2. &(407)
\end{aligned}
$$

In particular, for $l=s-1$ we have

$$M_{s-1}^{(s)}=\binom{s}{s+1}=0.$$

Proof. From (406),

$$M_l^{(s)} = \sum_{i=2}^{s} i\Sigma_l^{i-1} S_{i+1}^{(s)}. \tag{408}$$

We begin by finding a convenient expression for $S_{i+1}^{(s)}$. From (418) of Lemma 12, we have

$$\begin{aligned} S_{i+1}^{(s)} &= \frac{1}{s!i!} L_{i+1}^{(s)} \\ &= \frac{1}{s!i!} \sum_{k=0}^{s-i} \frac{(i+k)!}{(k+1)!} \gamma_{s-i-k}^{(s)} \\ &= \frac{1}{s!i!} \sum_{k=0}^{s-i} \frac{(s-k)!}{(s-i-k+1)!} \gamma_k^{(s)} \\ &= \frac{1}{s!i} \sum_{k=0}^{s-i} \left(\begin{array}{c} s-k \\ i-1 \end{array} \right) \gamma_k^{(s)}. \end{aligned}$$

Using this in (408) and then using (400) of Lemma 4 for Σ_l^{i-1}, we get

$$\begin{aligned} M_l^{(s)} &= \sum_{i=2}^{s} i\Sigma_l^{i-1} \frac{1}{s!i} \sum_{k=0}^{s-i} \left(\begin{array}{c} s-k \\ i-1 \end{array} \right) \gamma_k^{(s)} \\ &= \frac{1}{s!} \sum_{i=2}^{s} \Sigma_l^{i-1} \sum_{k=0}^{s-i} \left(\begin{array}{c} s-k \\ i-1 \end{array} \right) \gamma_k^{(s)} \\ &= \frac{1}{s!} \sum_{i=2}^{s} (-1)^{l+1} \sum_{m=1}^{l+1} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) m^{i-1} \sum_{k=0}^{s-i} \left(\begin{array}{c} s-k \\ i-1 \end{array} \right) \gamma_k^{(s)} \\ &= \frac{1}{s!} (-1)^{l+1} \sum_{m=1}^{l+1} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) \sum_{i=2}^{s} m^{i-1} \sum_{k=0}^{s-i} \left(\begin{array}{c} s-k \\ i-1 \end{array} \right) \gamma_k^{(s)} \\ &= (-1)^{l+1} \sum_{m=1}^{l+1} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) V_m^{(s)}, \end{aligned} \tag{409}$$

where

$$V_m^{(s)} = \frac{1}{s!} \sum_{i=2}^{s} m^{i-1} \sum_{k=0}^{s-i} \left(\begin{array}{c} s-k \\ i-1 \end{array} \right) \gamma_k^{(s)}. \tag{410}$$

Substituting the expression for $V_m^{(s)}$ given by Lemma 11 in Appendix D.11 into (409), we get

$$\begin{aligned} M_l^{(s)} &= (-1)^{l+1} \sum_{m=1}^{l+1} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) \left[\left(\begin{array}{c} s+m \\ 1+m \end{array} \right) - s \right] \\ &= (-1)^{l+1} \left\{ \sum_{m=1}^{l+1} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) \left(\begin{array}{c} s+m \\ 1+m \end{array} \right) - s \sum_{m=1}^{l+1} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) \right\} \\ &= (-1)^{l+1} \left\{ \sum_{m=0}^{l+1} (-1)^m \left(\begin{array}{c} l+1 \\ m \end{array} \right) \left(\begin{array}{c} s+m \\ 1+m \end{array} \right) - \left(\begin{array}{c} l+1 \\ 0 \end{array} \right) \left(\begin{array}{c} s \\ 1 \end{array} \right) \right. \end{aligned}$$

$$
\begin{aligned}
& -s\left[\sum_{m=0}^{l+1}(-1)^m\binom{l+1}{m}-\binom{l+1}{0}\right]\Bigg\} \\
= \;& (-1)^{l+1}\left\{(-1)^{l+1}\binom{s}{l+2}-s-s(0-1)\right\} \\
= \;& \binom{s}{l+2},
\end{aligned}
$$

by (457) and (452), completing the proof of the lemma. □

D.8 Lemma 8

Lemma 8

$$S_2^{(s)} = s, \quad \textit{for } s \geq 1. \tag{411}$$

Proof. From the expression for $S_i^{(s)}$ given by Lemma 12 in Appendix D.12, it follows that

$$S_2^{(s)} = \frac{1}{s!}L_2^{(s)} = \frac{1}{s!}\sum_{l=0}^{s-1}\gamma_{s-l-1}^{(s)} = \frac{1}{s!}\sum_{l=0}^{s-1}\gamma_l^{(s)}.$$

So we must prove

$$\sum_{l=0}^{s-1}\gamma_l^{(s)} = ss!, \quad \text{for } s \geq 1,$$

which is equivalent to

$$\sum_{l=0}^{s}\gamma_l^{(s)} = ss! + s! = (s+1)!, \quad \text{for } s \geq 1, \tag{412}$$

since $\gamma_s^{(s)} = s!$ by (64). The relation (412) follows from Lemma 13 in Appendix D.13. □

D.9 Lemma 9

Lemma 9

$$\sum_{l=0}^{N}(-1)^l\binom{s-l}{N-l}\binom{s}{l+1} = \binom{s+1}{s-N}, \quad \textit{for } N = 1,\ldots,s,\ s \geq 1. \tag{413}$$

Proof. The proof is by induction on s. We first check the base case, $s = 1$. For $s = 1$, $1 \le N \le s$ implies $N = 1$ and so

$$LS = \left(\begin{array}{c} 1 \\ 1 \end{array} \right) \left(\begin{array}{c} 1 \\ 1 \end{array} \right) - \left(\begin{array}{c} 0 \\ 0 \end{array} \right) \left(\begin{array}{c} 1 \\ 2 \end{array} \right) = 1 = \left(\begin{array}{c} 2 \\ 0 \end{array} \right) = RS.$$

Now consider the general case, $s \ge 2$. The left side of (413) is

$$\begin{aligned}
LS &= \sum_{l=0}^{N} (-1)^l \left(\begin{array}{c} s-l \\ N-l \end{array} \right) \left(\begin{array}{c} s \\ l+1 \end{array} \right) \\
&= \sum_{l=0}^{N} (-1)^l \left(\begin{array}{c} s-l \\ N-l \end{array} \right) \left[\left(\begin{array}{c} s-1 \\ l+1 \end{array} \right) + \left(\begin{array}{c} s-1 \\ l \end{array} \right) \right] \\
&= \sum_{l=0}^{N} (-1)^l \left[\left(\begin{array}{c} s-l \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l+1 \end{array} \right) + \left(\begin{array}{c} s-l \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l \end{array} \right) \right] \\
&= \sum_{l=0}^{N-1} (-1)^l \left[\left(\begin{array}{c} s-l-1 \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l+1 \end{array} \right) + \left(\begin{array}{c} s-l-1 \\ N-l-1 \end{array} \right) \left(\begin{array}{c} s-1 \\ l+1 \end{array} \right) \right] \\
&\quad + (-1)^N \left(\begin{array}{c} s-N \\ N-N \end{array} \right) \left(\begin{array}{c} s-1 \\ N+1 \end{array} \right) + \sum_{l=0}^{N} (-1)^l \left(\begin{array}{c} s-l \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l \end{array} \right) \\
&= \sum_{l=0}^{N-1} (-1)^l \left(\begin{array}{c} s-l-1 \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l+1 \end{array} \right) \\
&\quad + \sum_{l=0}^{N-1} (-1)^l \left(\begin{array}{c} s-l-1 \\ N-l-1 \end{array} \right) \left(\begin{array}{c} s-1 \\ l+1 \end{array} \right) \\
&\quad + (-1)^N \left(\begin{array}{c} s-1 \\ N+1 \end{array} \right) \\
&\quad + \sum_{l=0}^{N} (-1)^l \left(\begin{array}{c} s-l \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l \end{array} \right) \\
&= \sum_{l=0}^{N} (-1)^l \left(\begin{array}{c} s-l-1 \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l+1 \end{array} \right) - (-1)^N \left(\begin{array}{c} s-N-1 \\ N-N \end{array} \right) \left(\begin{array}{c} s-1 \\ N+1 \end{array} \right) \\
&\quad + \sum_{l=0}^{N-1} (-1)^l \left(\begin{array}{c} s-l-1 \\ N-l-1 \end{array} \right) \left(\begin{array}{c} s-1 \\ l+1 \end{array} \right) \\
&\quad + (-1)^N \left(\begin{array}{c} s-1 \\ N+1 \end{array} \right) \\
&\quad + \sum_{l=1}^{N} (-1)^l \left(\begin{array}{c} s-l \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l \end{array} \right) + \left(\begin{array}{c} s \\ N \end{array} \right) \left(\begin{array}{c} s-1 \\ 0 \end{array} \right) \\
&= \sum_{l=0}^{N} (-1)^l \left(\begin{array}{c} s-l-1 \\ N-l \end{array} \right) \left(\begin{array}{c} s-1 \\ l+1 \end{array} \right)
\end{aligned}$$

$$+\sum_{l=0}^{N-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ N-l-1 \end{array}\right)\left(\begin{array}{c} s-1 \\ l+1 \end{array}\right)$$
$$-\sum_{l=0}^{N-1}(-1)^l\left(\begin{array}{c} s-l-1 \\ N-l-1 \end{array}\right)\left(\begin{array}{c} s-1 \\ l+1 \end{array}\right)+\left(\begin{array}{c} s \\ N \end{array}\right).$$

For $N = 1, \ldots, s-1$, this becomes

$$\begin{aligned} LS &= \left(\begin{array}{c} s \\ s-N-1 \end{array}\right) \quad \text{from (413) by induction on } s \\ &\quad +\left(\begin{array}{c} s \\ N \end{array}\right) \\ &= \left(\begin{array}{c} s \\ N+1 \end{array}\right)+\left(\begin{array}{c} s \\ N \end{array}\right) \\ &= \left(\begin{array}{c} s+1 \\ N+1 \end{array}\right) \\ &= \left(\begin{array}{c} s+1 \\ s-N \end{array}\right) \\ &= RS, \end{aligned}$$

as required. When $N = s$, (413) satisfies

$$\begin{aligned} LS &= \sum_{l=0}^{s-1}(-1)^l\left(\begin{array}{c} s \\ l+1 \end{array}\right) \\ &= -\sum_{l=1}^{s}(-1)^l\left(\begin{array}{c} s \\ l \end{array}\right) \\ &= -\sum_{l=0}^{s}(-1)^l\left(\begin{array}{c} s \\ l \end{array}\right)+1 \\ &= 1 \quad \text{by (452), since } s \neq 0 \\ &= \left(\begin{array}{c} s+1 \\ 0 \end{array}\right) \\ &= RS. \end{aligned}$$

□

D.10 Lemma 10

Lemma 10

$$\Sigma_l^n = \sum_{j=1}^{n-1} \left(\begin{array}{c} n \\ j \end{array} \right) \Sigma_{l-1}^j = \sum_{j=l}^{n-1} \left(\begin{array}{c} n \\ j \end{array} \right) \Sigma_{l-1}^j, \quad \textit{for } l = 2, \ldots, n-1,\ n \geq 3. \tag{414}$$

Proof. Since $l \geq 2$, it follows from (97) that

$$\begin{aligned}
\Sigma_l^n &= \sum_{1 \leq i_1 < \cdots < i_l \leq n-1} \left(\begin{array}{c} i_2 \\ i_1 \end{array} \right) \left(\begin{array}{c} i_3 \\ i_2 \end{array} \right) \cdots \left(\begin{array}{c} i_l \\ i_{l-1} \end{array} \right) \left(\begin{array}{c} n \\ i_l \end{array} \right) \\
&= \sum_{i_l=l}^{n-1} \left(\begin{array}{c} n \\ i_l \end{array} \right) \sum_{1 \leq i_1 < \cdots < i_{l-1} < i_l} \left(\begin{array}{c} i_2 \\ i_1 \end{array} \right) \left(\begin{array}{c} i_3 \\ i_2 \end{array} \right) \cdots \left(\begin{array}{c} i_l \\ i_{l-1} \end{array} \right) \\
&= \sum_{j=l}^{n-1} \left(\begin{array}{c} n \\ j \end{array} \right) \sum_{1 \leq i_1 < \cdots < i_{l-1} \leq j-1} \left(\begin{array}{c} i_2 \\ i_1 \end{array} \right) \left(\begin{array}{c} i_3 \\ i_2 \end{array} \right) \cdots \left(\begin{array}{c} i_{l-1} \\ i_{l-2} \end{array} \right) \left(\begin{array}{c} j \\ i_{l-1} \end{array} \right) \\
&= \sum_{j=l}^{n-1} \left(\begin{array}{c} n \\ j \end{array} \right) \Sigma_{l-1}^j,
\end{aligned}$$

as required. This also equals

$$\sum_{j=1}^{n-1} \left(\begin{array}{c} n \\ j \end{array} \right) \Sigma_{l-1}^j,$$

because $\Sigma_l^j = 0$ for $j \leq l-1$ by (97). □

D.11 Lemma 11

Lemma 11

$$V_m^{(s)} = \frac{1}{s!} \sum_{i=2}^{s} m^{i-1} \sum_{k=0}^{s-i} \left(\begin{array}{c} s-k \\ i-1 \end{array} \right) \gamma_k^{(s)} \quad \textit{from (410)} \tag{415}$$

$$= \left(\begin{array}{c} s+m \\ 1+m \end{array} \right) - s, \quad \textit{for } s \geq 1,\ m \geq 0. \tag{416}$$

Proof. We first switch the i and k sums in (415). When $i = 2$, $k = 0, \ldots, s-2$. When $i = s$, $k = 0$. Therefore, for $k = 0, \ldots, s-2$, $i = 2, \ldots, s-k$. This gives

$$\begin{aligned}
V_m^{(s)} &= \frac{1}{s!} \sum_{k=0}^{s-2} \gamma_k^{(s)} \sum_{i=2}^{s-k} \left(\begin{array}{c} s-k \\ i-1 \end{array} \right) m^{i-1} \\
&= \frac{1}{s!} \sum_{k=0}^{s-2} \gamma_k^{(s)} \sum_{i=1}^{s-k-1} \left(\begin{array}{c} s-k \\ i \end{array} \right) m^i
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{s!}\sum_{k=0}^{s-2}\gamma_k^{(s)}\left[\sum_{i=0}^{s-k}\left(\begin{array}{c} s-k \\ i \end{array}\right)m^i - m^{s-k} - 1\right] \\
&= \frac{1}{s!}\left[\sum_{k=0}^{s-2}\gamma_k^{(s)}(1+m)^{s-k} - \sum_{k=0}^{s-2}\gamma_k^{(s)}m^{s-k} - \sum_{k=0}^{s-2}\gamma_k^{(s)}\right]. \qquad (417)
\end{aligned}
$$

We now find expressions for the individual sums. From Lemma 5 in Appendix D.5, we have

$$
\begin{aligned}
&\sum_{i=1}^{s}\gamma_{s-i}^{(s)}m^i = s!\left(\begin{array}{c} m+s \\ s \end{array}\right) - s! \\
&\Longrightarrow \quad \sum_{i=0}^{s}\gamma_{s-i}^{(s)}m^i = s!\left(\begin{array}{c} m+s \\ s \end{array}\right), \quad \text{since } \gamma_s^{(s)} = s! \text{ by (64)} \\
&\Longrightarrow \quad \sum_{i=0}^{s}\gamma_i^{(s)}m^{s-i} = s!\left(\begin{array}{c} m+s \\ s \end{array}\right) \\
&\Longrightarrow \quad \sum_{i=0}^{s-2}\gamma_i^{(s)}m^{s-i} = s!\left(\begin{array}{c} m+s \\ s \end{array}\right) - s! - \gamma_{s-1}^{(s)}m,
\end{aligned}
$$

and, replacing m by $m+1$, we get

$$
\sum_{i=0}^{s-2}\gamma_i^{(s)}(m+1)^{s-i} = s!\left(\begin{array}{c} s+m+1 \\ s \end{array}\right) - s! - \gamma_{s-1}^{(s)}(m+1).
$$

Using these relations, together with (424) of Lemma 13, in (417), we find that

$$
\begin{aligned}
V_m^{(s)} &= \frac{1}{s!}\left\{\left[s!\left(\begin{array}{c} s+m+1 \\ s \end{array}\right) - s! - (m+1)\gamma_{s-1}^{(s)}\right]\right. \\
&\quad - \left[s!\left(\begin{array}{c} m+s \\ s \end{array}\right) - s! - m\gamma_{s-1}^{(s)}\right] \\
&\quad \left. - \left[(s+1)! - \gamma_s^{(s)} - \gamma_{s-1}^{(s)}\right]\right\} \\
&= \frac{1}{s!}\left\{s!\left[\left(\begin{array}{c} s+m+1 \\ s \end{array}\right) - \left(\begin{array}{c} m+s \\ s \end{array}\right)\right] - (s+1)! + \gamma_s^{(s)}\right\} \\
&= \left(\begin{array}{c} s+m+1 \\ s \end{array}\right) - \left(\begin{array}{c} m+s \\ s \end{array}\right) - (s+1) + 1 \quad \text{by (64)} \\
&= \left(\begin{array}{c} s+m \\ s-1 \end{array}\right) - s \\
&= \left(\begin{array}{c} s+m \\ 1+m \end{array}\right) - s,
\end{aligned}
$$

as required. □

D.12 Lemma 12

Lemma 12

$$S_i^{(s)} = \sum_{j=1}^{s} b_{ij} = \frac{1}{s!(i-1)!} L_i^{(s)}, \quad \textit{for } i = 2, \ldots, r, \ s \geq 1, \tag{418}$$

where

$$L_i^{(s)} = \sum_{l=0}^{r-i} \frac{(i+l-1)!}{(l+1)!} \gamma_{s-i-l+1}^{(s)}. \tag{419}$$

Proof. Using (62), (63) and (58), we see for $i = 1, \ldots, r$ that

$$\begin{aligned}
S_i^{(s)} &= \sum_{j=1}^{s} b_{ij} \\
&= \sum_{j=1}^{s} T_{ij}(\lambda) b_{rj} \\
&= \sum_{j=1}^{s} \left[\left(\frac{1}{(i-1)!} \sum_{l=0}^{r-i} (i-1+l)! \gamma_{s-i-l+1}^{(s)} \lambda_j^l \right) \left(\frac{1}{s!} \frac{\sum_{k=0}^{s-1} \frac{\theta_{kj}^{(s)}}{(s-k)!}}{\prod_{\substack{m=1 \\ m \neq j}}^{s} (\lambda_m - \lambda_j)} \right) \right] \\
&= \frac{1}{s!(i-1)!} \sum_{l=0}^{r-i} (i-1+l)! \gamma_{s-i-l+1}^{(s)} \sum_{k=0}^{s-1} \frac{1}{(s-k)!} \sum_{j=1}^{s} \frac{\lambda_j^l \theta_{kj}^{(s)}}{\prod_{\substack{m=1 \\ m \neq j}}^{s} (\lambda_m - \lambda_j)} \\
&= \frac{1}{s!(i-1)!} \sum_{l=0}^{r-i} (i-1+l)! \gamma_{s-i-l+1}^{(s)} K_l^{(s)}, \qquad (420)
\end{aligned}$$

where

$$K_l^{(s)} = \sum_{k=0}^{s-1} \frac{1}{(s-k)!} J_{l,k}^{(s)} \tag{421}$$

and

$$J_{l,k}^{(s)} = \sum_{j=1}^{s} \frac{\lambda_j^l \theta_{kj}^{(s)}}{\prod_{\substack{m=1 \\ m \neq j}}^{s} (\lambda_m - \lambda_j)}. \tag{422}$$

Using Lemma 14 of Appendix D.14 together with (421), we find that

$$K_l^{(s)} = \frac{1}{[(s-(s-l-1)]!} = \frac{1}{(l+1)!}, \quad \text{for } l = 0, \ldots, s. \tag{423}$$

Therefore, from (420),

$$\begin{aligned}
S_i^{(s)} &= \frac{1}{s!(i-1)!} \sum_{l=0}^{r-i} \frac{(i-1+l)!}{(l+1)!} \gamma_{s-i-l+1}^{(s)} \\
&= \frac{1}{s!(i-1)!} L_i^{(s)},
\end{aligned}$$

as required. □

D.13 Lemma 13

Lemma 13

$$\sum_{k=0}^{s} \gamma_k^{(s)} = (s+1)!, \quad \textit{for } s \geq 0. \tag{424}$$

Proof. The proof is by induction on s. For base case, $s = 0$, so

$$LS = \gamma_0^{(s)} = 1 = RS$$

by (64).

Before considering the general case, $s \geq 1$, we first prove the following recurrence for $\gamma_l^{(s)}$ for $l \geq 1$ by induction on l:

$$\gamma_l^{(s)} = \sum_{n=l-1}^{s-1} (n+1)\gamma_{l-1}^{(n)}. \tag{425}$$

In the base case, $l = 1$,

$$RS = \sum_{n=0}^{s-1} (n+1)\gamma_0^{(n)} = \sum_{n=1}^{s} n = \gamma_1^{(s)} = LS$$

by (64). For the general case, $l \geq 2$, we use (404) to show

$$\begin{aligned}
\gamma_l^{(s)} &= s\gamma_{l-1}^{(s-1)} + \gamma_l^{(s-1)} \\
&= s\gamma_{l-1}^{(s-1)} + \sum_{n=l-1}^{s-2} (n+1)\gamma_{l-1}^{(n)} \quad \text{by induction on (425)} \\
&= \sum_{n=l-1}^{s-1} (n+1)\gamma_{l-1}^{(n)} \\
&= RS,
\end{aligned}$$

which proves the recurrence (425).

To prove the general case of (424) for $s \geq 1$, we use (425) in (424) to get

$$LS = \gamma_0^{(s)} + \sum_{l=1}^{s} \sum_{n=l-1}^{s-1} (n+1)\gamma_{l-1}^{(n)}.$$

Now switch the l and n sums. When $l = 1$, $n = 0, \ldots, s-1$. When $l = s$, $n = s-1$. Thus, for $n = 0, \ldots, s-1$, $l = 1, \ldots, n+1$. Therefore,

$$\begin{aligned} LS &= 1 + \sum_{n=0}^{s-1} \sum_{l=1}^{n+1} (n+1)\gamma_{l-1}^{(n)} \\ &= 1 + \sum_{n=0}^{s-1} (n+1) \sum_{l=0}^{n} \gamma_l^{(n)} \\ &= 1 + \sum_{n=0}^{s-1} (n+1)(n+1)! \qquad (426) \end{aligned}$$

where (426) follows by induction on (424), since $n < s$. To prove (426) equals the right side of (424), we need to show

$$\sum_{n=0}^{s-1} (n+1)(n+1)! = (s+1)! - 1,$$

which is equivalent to

$$\sum_{n=1}^{s} nn! = (s+1)! - 1. \qquad (427)$$

We prove (427) by induction on $s \geq 1$.

In the base case, $s = 1$,

$$LS = 1 = 2 - 1 = RS.$$

In the general case, $s \geq 2$,

$$\begin{aligned} \sum_{n=1}^{s} nn! &= \sum_{n=1}^{s-1} nn! + ss! \\ &= s! - 1 + ss! \quad \text{by induction on (427)} \\ &= s!(1+s) - 1 \\ &= (s+1)! - 1, \end{aligned}$$

as required. □

D.14 Lemma 14

Lemma 14

$$J_{l,k}^{(s)} = \sum_{j=1}^{s} \frac{\lambda_j^l \theta_{kj}^{(s)}}{\prod_{\substack{m=1 \\ m \neq j}}^{s} (\lambda_m - \lambda_j)} \quad \textit{from (422)}$$

$$= \left\{ \begin{array}{ll} 0, & k = 0, \ldots, s-l-2, \\ 1, & k = s-l-1, \\ 0, & k \geq s-l, \end{array} \right\} \quad \textit{for } l = 0, \ldots, s-1,\ s \geq 1. \tag{428}$$

Proof. Fix s, l, k for now and let

$$a_j = \lambda_j^l \theta_{kj}^{(s)}. \tag{429}$$

Then

$$J_{l,k}^{(s)} = \sum_{j=1}^{s} \frac{a_j}{\prod_{\substack{m=1 \\ m \neq j}}^{s} (\lambda_m - \lambda_j)}. \tag{430}$$

Consider the common denominator

$$d = \prod_{1 \leq i < m \leq s} (\lambda_i - \lambda_m),$$

and let

$$n_j = (-1)^{s-j} \prod_{\substack{1 \leq i < m \leq s \\ i, m \neq j}} (\lambda_i - \lambda_m).$$

Then

$$\begin{aligned} \frac{n_j}{d} &= \frac{(-1)^{s-j} \prod_{\substack{1 \leq i < m \leq s \\ i, m \neq j}} (\lambda_i - \lambda_m)}{\prod_{1 \leq i < m \leq s} (\lambda_i - \lambda_m)} \\ &= \frac{(-1)^{s-j} \prod_{\substack{1 \leq i < m \leq s \\ i, m \neq j}} (\lambda_i - \lambda_m)}{\prod_{\substack{1 \leq i < m \leq s \\ i, m \neq j}} (\lambda_i - \lambda_m) \prod_{\substack{1 \leq i < m \leq s \\ i = j}} (\lambda_i - \lambda_m) \prod_{\substack{1 \leq i < m \leq s \\ m = j}} (\lambda_i - \lambda_m)} \\ &= \frac{(-1)^{s-j}}{\prod_{\substack{1 \leq i < m \leq s \\ i = j}} (\lambda_i - \lambda_m) \prod_{\substack{1 \leq i < m \leq s \\ m = j}} (\lambda_i - \lambda_m)} \\ &= \frac{(-1)^{s-j}}{\prod_{1 \leq j < m \leq s} (\lambda_j - \lambda_m) \prod_{1 \leq i < j \leq s} (\lambda_i - \lambda_j)} \\ &= \frac{1}{\prod_{1 \leq j < m \leq s} (\lambda_m - \lambda_j) \prod_{1 \leq m < j \leq s} (\lambda_m - \lambda_j)} \\ &= \frac{1}{\prod_{\substack{m=1 \\ m \neq j}}^{s} (\lambda_m - \lambda_j).} \end{aligned}$$

Therefore, from (430), we have

$$J_{l,k}^{(s)} = \frac{\sum_{j=1}^{s} a_j n_j}{d}$$

$$= \frac{\sum_{j=1}^{s} \lambda_j^l \theta_{kj}^{(s)} (-1)^{s-j} \prod_{\substack{1 \le i<m \le s \\ i,m \ne j}} (\lambda_i - \lambda_m)}{\prod_{1 \le i<j \le s} (\lambda_i - \lambda_j)}$$

$$= \frac{(-1)^s A_{l,k}^{(s)}}{\prod_{1 \le i<j \le s} (\lambda_i - \lambda_j)}, \tag{431}$$

where

$$A_{l,k}^{(s)} = \sum_{j=1}^{s} \lambda_j^l \theta_{kj}^{(s)} (-1)^j \prod_{\substack{1 \le i<m \le s \\ i,m \ne j}} (\lambda_i - \lambda_m). \tag{432}$$

So (428) is equivalent to

$$A_{l,k}^{(s)} = \left\{ \begin{array}{ll} 0, & k \ge 0,\ k \ne s-l-1, \\ (-1)^s \prod_{1 \le i<j \le s} (\lambda_i - \lambda_j), & k = s-l-1, \end{array} \right\} \quad \text{for } l = 0, \ldots, s,\ s \ge 1. \tag{433}$$

From (60) and (61), it follows that

$$\theta_{kj}^{(s)} = \left\{ \begin{array}{ll} (-1)^{s-1-k} \sum_{\substack{1 \le i_1 < \cdots < i_k \le s \\ i_1, \ldots, i_k \ne j}} \lambda_{i_1} \cdots \lambda_{i_k}, & k \ne 0, \\ (-1)^{s-1}, & k = 0. \end{array} \right. \tag{434}$$

Therefore, for any fixed k, both the left side and the right side of (433) may be considered as polynomials in λ_s, say. The degree of the $j = s$ term of $A_{l,k}^{(s)}$ in λ_s is $l + 0 + 0 \le s - 1$. The degree of any $j < s$ term is $0 + 1 + (s-2) = s - 1$. Thus, it suffices to show (433) is true for s distinct values of λ_s, for example, $\lambda_s = 0, \lambda_1, \ldots, \lambda_{s-1}$.

We begin with the case of $\lambda_s = \lambda_n$, for some $n = 1, \ldots, s-1$. Consider $j \ne n$ and $j \ne s$ in (432). In this case, $\lambda_n - \lambda_s$ occurs in the product, so the only possibly nonzero terms of the sum occur when $j = n$ or $j = s$. That is,

$$A_{l,k}^{(s)} = \lambda_n^l \theta_{kn}^{(s)} (-1)^n \prod_{\substack{1 \le i<m \le s \\ i,m \ne n}} (\lambda_i - \lambda_m) + \lambda_s^l \theta_{ks}^{(s)} (-1)^s \prod_{\substack{1 \le i<m \le s \\ i,m \ne s}} (\lambda_i - \lambda_m). \tag{435}$$

Note that, from (434), $\theta_{k,n}^{(s)} = \theta_{k,s}^{(s)}$, since $\lambda_n = \lambda_s$. Also,

$$\begin{aligned} & \prod_{\substack{1 \le i<m \le s \\ i,m \ne n}} (\lambda_i - \lambda_m) \\ &= \prod_{\substack{1 \le i<m<s \\ i,m \ne n}} (\lambda_i - \lambda_m) \prod_{\substack{1 \le i<s \\ i \ne n}} (\lambda_i - \lambda_s) \\ &= \prod_{\substack{1 \le i<m<s \\ i,m \ne n}} (\lambda_i - \lambda_m) \prod_{\substack{1 \le i<s \\ i \ne n}} (\lambda_i - \lambda_n) \end{aligned}$$

$$
\begin{aligned}
&= \prod_{\substack{1\le i<m<s\\ i,m\neq n}} (\lambda_i-\lambda_m) \prod_{1\le i<n} (\lambda_i-\lambda_n) \prod_{n<i<s} (\lambda_i-\lambda_n)\\
&= \prod_{\substack{1\le i<m<s\\ i,m\neq n}} (\lambda_i-\lambda_m) \prod_{1\le i<n} (\lambda_i-\lambda_n)(-1)^{s-n-1} \prod_{n<i<s} (\lambda_n-\lambda_i)\\
&= (-1)^{s-n-1} \prod_{1\le i<m<s} (\lambda_i-\lambda_m)\\
&= (-1)^{s-n-1} \prod_{\substack{1\le i<m\le s\\ i,m\neq s}} (\lambda_i-\lambda_m). \qquad (436)
\end{aligned}
$$

Thus, continuing from (435), we find that

$$
\begin{aligned}
A^{(s)}_{l,k} &= \lambda_n^l \theta^{(s)}_{ks} (-1)^n (-1)^{s-n-1} \prod_{\substack{1\le i<m\le s\\ i,m\neq s}} (\lambda_i-\lambda_m) + \lambda_s^l \theta^{(s)}_{ks} (-1)^s \prod_{\substack{1\le i<m\le s\\ i,m\neq s}} (\lambda_i-\lambda_m)\\
&= 0 \qquad (437)
\end{aligned}
$$

We must now show that this agrees with the right side of (433). When $k \neq s-l-1$, the right side is 0. When $k = s-l-1$, it is

$$
(-1)^s \prod_{1\le i<j\le s} (\lambda_i-\lambda_j) = 0,
$$

because $\lambda_n = \lambda_s$. We have just shown (433) for $\lambda_s = \lambda_n$, $n = 1,\ldots,s-1$.

It remains to show (433) for $\lambda_s = 0$, which we do by induction on s and l. First we show the general case, $s > 1$ and $l > 0$. From (432),

$$
\begin{aligned}
A^{(s)}_{l,k} &= \sum_{j=1}^{s-1} \lambda_j^l \theta^{(s)}_{kj} (-1)^j \prod_{\substack{1\le i<m\le s\\ i,m\neq j}} (\lambda_i-\lambda_m) + (-1)^s \lambda_s^l \theta^{(s)}_{ks} \prod_{\substack{1\le i<m\le s\\ i,m\neq s}} (\lambda_i-\lambda_m)\\
&= \sum_{j=1}^{s-1} \lambda_j^l \theta^{(s)}_{kj} (-1)^j \prod_{\substack{1\le i<m\le s\\ i,m\neq j}} (\lambda_i-\lambda_m), \qquad (438)
\end{aligned}
$$

because $l > 0$ implies $\lambda_s^l = 0^l = 0$. We now find recursive relationships for the expressions in (438). When $\lambda_s = 0$, (434) implies that

$$
\begin{aligned}
\theta^{(s)}_{kj} &= (-1)^{s-k-1} \sum_{\substack{1\le i_1<\cdots<i_k\le s\\ i_1,\ldots,i_k\neq j}} \lambda_{i_1}\cdots\lambda_{i_k}, \quad k\neq 0\\
&= (-1)^{s-k-1} \left(\sum_{\substack{1\le i_1<\cdots<i_k=s\\ i_1,\ldots,i_k\neq j}} \lambda_{i_1}\cdots\lambda_{i_k} + \sum_{\substack{1\le i_1<\cdots<i_k\le s-1\\ i_1,\ldots,i_k\neq j}} \lambda_{i_1}\cdots\lambda_{i_k} \right)
\end{aligned}
$$

$$= (-1)^{s-k-1} \sum_{\substack{1\le i_1<\cdots<i_k\le s-1 \\ i_1,\ldots,i_k\neq j}} \lambda_{i_1}\cdots\lambda_{i_k}, \quad j\neq s,$$
$$= -\theta_{kj}^{(s-1)}, \quad j\neq s, \tag{439}$$

since $\lambda_s = 0$. (This holds when $k = 0$ too, by (434).) Also, since $\lambda_s = 0$,

$$\prod_{\substack{1\le i<m\le s \\ i,m\neq j}} (\lambda_i-\lambda_m) = \prod_{\substack{1\le i<m=s \\ i\neq j}} (\lambda_i-\lambda_m) \prod_{\substack{1\le i<m\le s-1 \\ i,m\neq j}} (\lambda_i-\lambda_m)$$
$$= \prod_{\substack{i=1 \\ i\neq j}}^{s-1} \lambda_i \prod_{\substack{1\le i<m\le s-1 \\ i,m\neq j}} (\lambda_i-\lambda_m), \quad j\neq s. \tag{440}$$

Using (439) and (440) in (438) gives

$$A_{l,k}^{(s)} = \sum_{j=1}^{s-1}(-1)^j\lambda_j^l(-\theta_{kj}^{(s-1)}) \prod_{\substack{i=1 \\ i\neq j}}^{s-1}\lambda_i \prod_{\substack{1\le i<m\le s-1 \\ i,m\neq j}} (\lambda_i-\lambda_m)$$
$$= -\prod_{i=1}^{s-1}\lambda_i \sum_{j=1}^{s-1}(-1)^j\lambda_j^{l-1}\theta_{kj}^{(s-1)} \prod_{\substack{1\le i<m\le s-1 \\ i,m\neq j}} (\lambda_i-\lambda_m)$$
$$= -A_{l-1,k}^{(s-1)} \prod_{i=1}^{s-1}\lambda_i, \tag{441}$$

by (432). From (433) by induction on s and l,

$$A_{l-1,k}^{(s-1)} = \left\{ \begin{array}{l} 0, \quad k\ge 0, \quad k\neq (s-1)-(l-1)-1 = s-l-1, \\ (-1)^{s-1}\prod_{1\le i<j\le s-1}(\lambda_i-\lambda_j), \quad k = s-l-1, \end{array} \right\} \quad l = 0,\ldots,s. \tag{442}$$

We now use this in (441). If $k\neq s-l-1$ then $A_{l,k}^{(s)} = 0$, as required by (433). If $k = s-l-1$, then

$$A_{l,k}^{(s)} = -(-1)^{s-1} \prod_{1\le i<j\le s-1}(\lambda_i-\lambda_j) \prod_{i=1}^{s-1}\lambda_i = (-1)^s \prod_{1\le i<j\le s}(\lambda_i-\lambda_j),$$

(since $\lambda_s = 0$) also as required.

All that remains is to check the base cases of (433). When $s = 1$, $LS = -\lambda_1^l\theta_{k1}^{(1)}$ by (432). From (434), $\theta_{k1}^{(1)} = 0$, since the sum is empty. So $LS = 0$. But $RS = 0$ also, if $k\neq s-l-1 = -l$. If $k = -l$, then $k = l = 0$, which is handled in the next case.

When $l = 0$,

$$LS = \sum_{j=1}^{s}\theta_{kj}^{(s)}(-1)^j \prod_{\substack{1\le i<m\le s \\ i,m\neq j}} (\lambda_i-\lambda_m), \tag{443}$$

and

$$RS = \begin{cases} 0, & k \geq 0,\ k \neq s-1, \\ (-1)^s \prod_{1 \leq i < j \leq s} (\lambda_i - \lambda_j), & k = s-1. \end{cases} \tag{444}$$

We will show that $LS = RS$ by induction on k. First, the base case, $k = 0$. From (434), $\theta_{0j}^{(s)} = (-1)^{s-1}$. Thus,

$$LS = (-1)^{s-1} \sum_{j=1}^{s} (-1)^j \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq j}} (\lambda_i - \lambda_m). \tag{445}$$

If $k < s-1$, that is, $s > 1$, then $RS = 0$ by (444). To show $LS = 0$ as well, consider it as a polynomial in λ_s. It has degree $s-2$, so it suffices to show $LS = 0$ for $\lambda_s = \lambda_1, \ldots, \lambda_{s-1}$. Let $\lambda_s = \lambda_n$, $\lambda_n = \lambda_1, \ldots, \lambda_{s-1}$. Then the product in LS is zero unless $j = n$ or $j = s$. Now, using (436) in (445) gives

$$\begin{aligned} LS &= (-1)^{s-1} \left((-1)^n \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq n}} (\lambda_i - \lambda_m) + (-1)^{s-1} \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq s}} (\lambda_i - \lambda_m) \right) \\ &= (-1)^s \left((-1)^n (-1)^{s-n-1} \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq s}} (\lambda_i - \lambda_m) + (-1)^s \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq s}} (\lambda_i - \lambda_m) \right) \\ &= 0 \\ &= RS. \end{aligned}$$

If $k = s-1$ then $s = 1$, and the products in LS and RS are both empty. Thus, $LS = -1 = RS$. This establishes the base case, $k = 0$.

Now consider the general case, $s \geq 2$, $k \geq 1$. We first derive a recurrence for $\theta_{kj}^{(s)}$ for $k \geq 1$ from (434).

$$\begin{aligned} \theta_{kj}^{(s)} &= (-1)^{s-1-k} \sum_{\substack{1 \leq i_1 < \cdots < i_k \leq s \\ i_1, \ldots, i_k \neq j}} \lambda_{i_1} \cdots \lambda_{i_k} \\ &= (-1)^{s-1-k} \left(\sum_{1 \leq i_1 < \cdots < i_k \leq s} \lambda_{i_1} \cdots \lambda_{i_k} - \sum_{\substack{1 \leq i_1 < \cdots < i_k \leq s \\ some\ i_l = j}} \lambda_{i_1} \cdots \lambda_{i_k} \right) \\ &= (-1)^{s-1-k} \left(\sum_{1 \leq i_1 < \cdots < i_k \leq s} \lambda_{i_1} \cdots \lambda_{i_k} - \lambda_j \sum_{\substack{1 \leq i_1 < \cdots < i_{k-1} \leq s \\ i_1, \ldots, i_{k-1} \neq j}} \lambda_{i_1} \cdots \lambda_{i_{k-1}} \right) \\ &= (-1)^{s-1-k} \left[(-1)^{s-k} \theta_k^{(s)} - \lambda_j (-1)^{s-1-(k-1)} \theta_{k-1,j}^{(s)} \right] \end{aligned}$$

$$= -\theta_k^{(s)} + \lambda_j \theta_{k-1,j}^{(s)}, \tag{446}$$

where

$$\theta_k^{(s)} \text{ is the coefficient of } x^k \text{ in } p(x) = \textstyle\prod_{j=1}^{s}(\lambda_j x - 1),\ k \geq 1.$$

Using this in (443) gives

$$\begin{aligned} LS &= \sum_{j=1}^{s} \theta_{kj}^{(s)} (-1)^j \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq j}} (\lambda_i - \lambda_m) \\ &= \sum_{j=1}^{s} \left(-\theta_k^{(s)} + \lambda_j \theta_{k-1,j}^{(s)} \right) (-1)^j \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq j}} (\lambda_i - \lambda_m) \\ &= -(-1)^j \theta_k^{(s)} \sum_{j=1}^{s} \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq j}} (\lambda_i - \lambda_m) \qquad (447) \\ &+ \sum_{j=1}^{s} (-1)^j \lambda_j \theta_{k-1,j}^{(s)} \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq j}} (\lambda_i - \lambda_m). \qquad (448) \end{aligned}$$

Now (447)=0 by the base case, (445)=0, and hence (443)=(448). Therefore we must show that

$$(448) = (444). \tag{449}$$

We use induction on s. Recall that $s \geq 2$ and $k \geq 1$, so the base case ($s = 2$) is

$$\begin{aligned} LS &= -\lambda_1 \theta_{k-1,1}^{(2)} + \lambda_2 \theta_{k-1,2}^{(2)}, \\ RS &= \begin{cases} 0, & k \geq 2, \\ \lambda_1 - \lambda_2, & k = 1. \end{cases} \end{aligned}$$

From (434), $\theta_{k-1,1}^{(2)} = \theta_{k-1,2}^{(2)} = -1$ when $k = 1$ and 0 for all $k > 1$. For $k = 1$ then, $LS = \lambda_1 - \lambda_2 = RS$, while for $k > 1$, $LS = 0 = RS$. We now handle the general case, $s > 2$. In (448), the $j = s$ term of the sum is zero because $\lambda_s = 0$. Also, by (439), $\theta_{k-1,j}^{(s)} = -\theta_{k-1,j}^{(s-1)}$, $j \neq s$. Thus,

$$\begin{aligned} (448) &= -\sum_{j=1}^{s-1} (-1)^j \lambda_j \theta_{k-1,j}^{(s-1)} \prod_{\substack{1 \leq i < m \leq s \\ i,m \neq j}} (\lambda_i - \lambda_m) \\ &= -\sum_{j=1}^{s-1} (-1)^j \lambda_j \theta_{k-1,j}^{(s-1)} \prod_{\substack{1 \leq i < m \leq s-1 \\ i,m \neq j}} (\lambda_i - \lambda_m) \prod_{\substack{1 \leq i < m = s \\ i,m \neq j}} \lambda_i \end{aligned}$$

$$
\begin{aligned}
&= -\left(\prod_{i=1}^{s-1}\lambda_i\right)\sum_{j=1}^{s-1}(-1)^j\lambda_j\theta_{k-1,j}^{(s-1)}\prod_{\substack{1\le i<m\le s-1\\ i,m\neq j}}(\lambda_i-\lambda_m)\\
&= -\left(\prod_{i=1}^{s-1}\lambda_i\right)\left\{\begin{array}{ll} 0, & k-1\neq s-2,\\ (-1)^{s-1}\prod_{1\le i<j\le s-1}(\lambda_i-\lambda_j), & k-1=s-2,\end{array}\right\}\ \text{by induction on (449)}\\
&= \left\{\begin{array}{ll} 0, & k\neq s-1\\ (-1)^s\prod_{1\le i<j\le s}(\lambda_i-\lambda_j), & k=s-1\end{array}\right.\\
&= (444),
\end{aligned}
$$

since $\lambda_s = 0$. This completes the proof of the Lemma. □

E Combinatorial Identities

The following combinatorial identities are taken from [14]. (The numbers given in brackets at the left are the original equation numbers from [14]).

(1.13)

$$\sum_{k=0}^{n}(-1)^k\left(\begin{array}{c} n\\ k\end{array}\right)k^j = \left\{\begin{array}{ll} 0, & 0\le j<n,\\ (-1)^n n!, & j=n.\end{array}\right. \tag{450}$$

(1.24)

$$\sum_{k=0}^{n}\left(\begin{array}{c} n\\ k\end{array}\right) = 2^n \tag{451}$$

(1.25)

$$\sum_{k=0}^{n}(-1)^k\left(\begin{array}{c} n\\ k\end{array}\right) = \left\{\begin{array}{ll} 0, & n\neq 0,\\ 1, & n=0.\end{array}\right. \tag{452}$$

(3.1)

$$\sum_{k=0}^{n}\left(\begin{array}{c} x\\ k\end{array}\right)\left(\begin{array}{c} y\\ n-k\end{array}\right) = \left(\begin{array}{c} x+y\\ n\end{array}\right) \tag{453}$$

(3.4)

$$\sum_{k=0}^{n}\left(\begin{array}{c} n\\ k\end{array}\right)\left(\begin{array}{c} x+y-n\\ x-k\end{array}\right) = \left(\begin{array}{c} x+y\\ x\end{array}\right) \tag{454}$$

(3.20)

$$\sum_{k=0}^{n}\left(\begin{array}{c} n\\ k\end{array}\right)\left(\begin{array}{c} x\\ k+r\end{array}\right) = \left(\begin{array}{c} n+x\\ n+r\end{array}\right) \tag{455}$$

(3.47)

$$\sum_{k=0}^{n}(-1)^k\left(\begin{array}{c} n\\ k\end{array}\right)\left(\begin{array}{c} x+k\\ r\end{array}\right) = (-1)^n\left(\begin{array}{c} x\\ r-n\end{array}\right) \tag{456}$$

(3.48)

$$\sum_{k=0}^{n}(-1)^k \left(\begin{array}{c} n \\ k \end{array} \right) \left(\begin{array}{c} x+k \\ r+k \end{array} \right) = (-1)^n \left(\begin{array}{c} x \\ n+r \end{array} \right) \tag{457}$$

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