On the use of ‘arc length’ and ‘defect’ for mesh selection for differential equations *

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Abstract

In this note we will consider mesh selection techniques for ordinary differential equations (ODEs) and for partial differential equations (PDEs) based on arc length and defect. We assume we are trying to approximate $y(x)$ for $x \in [0,T]$ in the ODE case and $u(x,y)$ for $(x,y) \in \Omega$ in the PDE case. The two specific areas of application that we have in mind are the numerical solution of boundary value problems (BVPs) in ODEs and the numerical solution of PDEs when a method of lines (MOL) approach is employed. The approach we develop is applicable to a wider class of PDEs including mixed-order problems and 3D problems.

1 Introduction:

It is well known that in the numerical solution of differential equations one must use adaptive mesh refinement to obtain reliable and efficient performance, especially on nonlinear problems. Automatic mesh refinement (AMR) is therefore a key component of many methods for BVPs in ODEs and methods for PDEs that use a MOL approach. In these applications the overall performance of the method (especially on nonlinear problems or problems with boundary layers) can depend critically on the choice of an effective mesh selection scheme (see for example [5], [2], [7], [8] for a more detailed discussion of this issue).

Developing suitable automatic mesh refinement strategies for particular classes of problems and methods is a very active research area and very effective special purpose and general purpose strategies have recently been proposed and implemented. In recent investigations Russell and his colleagues (see for example [6], [2]) have presented and discussed some promising general purpose strategies and demonstrated their effectiveness on some model problems. As they note, it is often effective to introduce a simple change of variable from the

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'physical coordinate' system to a 'computational coordinate' system, where an appropriate mesh refinement strategy is easier to develop and justify. In this note we adopt the terminology and viewpoint they have used and propose some new approaches which can lead to new general purpose schemes for both ODEs and PDEs.

2 The ODE case:

We first consider the ODE case where we parametrize the physical variables with respect to arc length and represent the solution curve $(x, y(x))_{x=0}^{T}$ (in the physical coordinate system) by $(x(s), y(s))_{s=0}^{L}$ in the computational coordinate system, where L is the total length of the curve ($L =$ the value of s such that $x(s) = T$).

We assume that $y(x)$ satisfies an initial value problem (IVP) of the form,

$$y' = f(x, y), \quad y(0) = y_0 \ \text{ for } \ x \in [0, T], \tag{1}$$

although y_0 may not be known explicitly.

For the curve $(x, y(x))_{x=0}^{T}$, and s equal to arc length, we have as $\Delta s \to 0$,

$$(\Delta s)^2 = (\Delta x)^2 + (\Delta y)^2 \text{ and this implies } 1 = (\frac{dx}{ds})^2 + (\frac{dy}{ds})^2.$$

Now since $\frac{dx}{ds} > 0$ and $\frac{dy}{dx} = f(x, y(x))$, we have

$$(\frac{dy}{ds})^2 = (f\frac{dx}{ds})^2 = f^2(\frac{dx}{ds})^2 = f^2(1 - (\frac{dy}{ds})^2).$$

This implies

$$(\frac{dy}{ds})^2(1 + f^2) = f^2.$$

(Note that here, and in what follows, unless otherwise indicated, f will refer to $f(x(s), y(s))$.)

Therefore, with respect to the computational variables, we have an associated IVP,

$$\begin{aligned} \frac{dy}{ds} &= \left(\frac{f^2}{1+f^2}\right)^{1/2} \\ \frac{dx}{ds} &= [1 - (\frac{dy}{ds})^2]^{1/2} = \left(\frac{1}{1+f^2}\right)^{1/2} \\ x(0) = 0, &\qquad y(0) = y_0. \end{aligned} \tag{2}$$

2.1 Mesh generation for ODEs:

We assume that a reliable numerical method has generated a discrete approximation to the IVP (1) on a given mesh

$$[x_i, y_i]_{i=0}^{N}, \text{ with } y_i \approx y(x_i).$$

A new mesh and corresponding discrete approximation is determined by a mesh selection strategy which usually attempts to 'equidistribute' (across each subinterval) some measure of the error or uncertainty in the discrete solution. For a detailed and readable discussion of this task see [1]. We will consider some alternative strategies for this task that are based on measures of arc length of $y(x)$ or the defect of one of the above IVPs that are known to be satisfied by $y(x)$.

In each case we will assume that, at the time of re-meshing, in addition to having a current discrete approximation available (in the physical coordinate system), our underlying numerical method has generated a piecewise polynomial $S(x)$ (an accurate approximation to $y(x)$) associated with the underlying discrete mesh and satisfying

$$S(x_i) = y_i, \text{ for } i = 0, 1 \cdots N.$$

Note that this requirement is satisfied by most current ODE software, and if it isn't, one can usually compute such a piecewise polynomial at a relatively small cost. Furthermore we assume that a new mesh (and corresponding discrete approximation) is desired with $\bar{N}$ subintervals. (Often $\bar{N}$ will be equal to N.)

2.1.1 Mesh generation based on arc length:

1. Compute L by solving the associated IVP (2) with a Continuous Runge-Kutta (CRK) method (see for example, [4]). That is, solve the IVP saving the piecewise polynomials $[S_1(s), S_2(s)]$ which are defined for $s \in [0, L]$. (Recall L is the first value such that $S_1(L) = T$.)

2. Let $h = L/\bar{N}$ and then set the new mesh and corresponding discrete approximation to be
$$[S_1(ih), S_2(ih)]_{i=0}^{\bar{N}}.$$

Note that this approach extends to systems where the 'length of $y(x)$' can be interpreted as a norm of the vector of lengths of the individual components of $y(x)$. That is, if L_j is the 'length' of the j^{th} component of $y(x)$, then we equidistribute $\|L\|$ when determining the new mesh. Although the cost of this approach involves the solution of an IVP by a CRK method, this is a small part of the overall cost in the applications we are considering.

A related alternative, less expensive, scheme exploits the fact that $S^{'}(x)$ is an accurate approximation to $f(x, y(x))$. One could then replace the system of

IVPs (2) by the perturbed scalar IVP,

$$\frac{dx}{ds} = \left[\frac{1}{1 + (S'(x(s)))^2}\right]^{1/2}, \quad x(0) = 0. \tag{3}$$

Solving this IVP by a CRK method (as above) we would obtain a continuous approximation to $x(s)$, $\bar{S}(s)$. After determining the value L such that $\bar{S}(L) = T$ we set $h = L/\bar{N}$, and $\bar{x}_i = \bar{S}(ih)$, $\bar{y}_i = S(\bar{x}_i)$ for $i = 0, 1 \cdots \bar{N}$.

2.1.2 Mesh selection based on the defect of the physical variables

Now consider the case where we use the defect (rather than arc length) to determine the new mesh. With the defect or residual defined by,

$$\delta(x) \equiv S'(x) - f(x, S(x)),$$

let

$$\bar{\delta}_i \approx \int_{x_{i-1}}^{x_i} |\delta(t)| dt \text{ and } D = \sum_{i=1}^{N} \bar{\delta}_i. \tag{4}$$

A mesh selection scheme based on equidistribution of the $\bar{\delta}_i$'s aims at achieving a new mesh that satisfies,

$$\int_{\bar{x}_{i-1}}^{\bar{x}_i} |\delta(t)| dt \quad = D/\bar{N}.$$

This can be implemented in the usual fashion by approximating $\delta(t)$ by a piecewise constant function $DEL(t)$ defined by the $\bar{\delta}_i$ and setting $\bar{x}_0 = x_0$ and determining $\bar{x}_i$ for $i > 0$ by setting it to the value of $x > x_{i-1}$ such that

$$\int_{\bar{x}_{i-1}}^{x} DEL(t) dt \ = \ D/\bar{N}.$$

2.1.3 Mesh selection based on the defect of the computational variables

When solving the IVP (1) one can consider adopting error control and mesh selection strategies based on the defect of the ODE associated with the computational variables. One could approximate the solution of the IVP (2) using a CRK (that employs defect error control). The numerical solution would then be a vector of piecewise polynomials, $[S_1(s), S_2(s)]$ whose defect is bounded in magnitude by a small multiple of TOL on each step. That is, since the defect associated with the IVP (2) is,

$$\Delta(s) = \begin{bmatrix} S_1'(s) & - & \left(\frac{1}{1+f^2}\right)^{1/2} \\ S_2'(s) & - & \left(\frac{f^2}{1+f^2}\right)^{1/2} \end{bmatrix},$$

(where, in this case, $f \equiv f(S_1(s), S_2(s)))$ then the CRK will attempt to ensure that the maximum magnitude of $\Delta(s)$ is bounded by TOL on each step (from s_{i-1} to s_i) for $i = 1, 2 \cdots N$. The corresponding discrete approximation with respect to the physical variables can now be defined to be $(x_i, y_i) = (S_1(s_i), S_2(s_i))$ for $i = 0, 1 \cdots N$. If we let Del_i be the estimate of the maximum magnitude of $\Delta(s)$ on step i (of the numerical integration of IVP (2)) then we can determine a new mesh for the physical variables by using Del_i as the error measure and using the standard 'equidistribution' idea to define $(\bar{x}_i, \bar{y}_i), i = 1, 2 \cdots \bar{N}$.

In the case of static re-meshing with a MOL method for PDEs, it is important to cope effectively with moving 'fronts' or shocks that move across the space domain as time evolves. In this case one could enforce a constraint that the new mesh be 'quasi-uniform' or one could make the error measure associated with the i^{th} subinterval more sensitive to its neighbors. For example, in the defect mesh selection strategy one could modify the error measure given by equation (4) and use,

$$\bar{\delta}_i \approx \int_{x_{i-1}-C_1}^{x_i+C_2} |\delta(t)| dt \text{ and } D = \sum_{i=1}^{N} \bar{\delta}_i. \tag{5}$$

Similarly for mesh selection strategies based on arc length, where the error measure we are equidistributing is $Del_i = S_1(ih) - S_1((i-1)h) = L/\bar{N}$, we can modify this to be $Del_i = S_1(ih + C_1) - S_1((i-1)h - C_2) = \bar{L}/\bar{N}$ (where $\bar{L}$ is defined as the sum of the Del_is. These definitions would have to be adjusted near the boundaries (the first and last subintervals) and the best values for C_1 and C_2 would depend on the problem. (They would depend on the speed and direction of the moving fronts.)

3 The PDE case:

For PDEs in general (either the MOL approach with more than one space dimension or a general PDE) the notions of arc length and defect can be extended to develop error measures that would be natural and inexpensive to compute, and therefore be suitable for use in a mesh selection strategy based on equidistribution. We will identify specific measures that can be defined, but the difficult question of how to 'redistribute' based on these measures will be not be fully investigated as it is an active area of research in its own right.

We have recently shown ([3]) how the approach of developing continuous discrete ODE methods based on Runge-Kutta formulas can be extended to a wide class of PDE methods. If the underlying discrete PDE method produces accurate approximations to $u(x, y)$ and possibly its low order derivatives $u_x(x, y), u_y(x, y)$, on an unstructured mesh, we can effectively determine a bivariate piecewise polynomial, $U(x, y)$ that provides accurate off-mesh approximations to the solution $u(x, y)$ for all (x, y) in Ω, the domain of interest, and interpolates the underlying discrete values at the unstructured mesh points.

One can define the defect of the numerical solution, $U(x,y)$ in the obvious way and associate an error measure with each element of the underlying mesh based on the maximum magnitude of this defect. A mesh selection strategy, based on 'equidistributing' this measure by updating the current mesh could be effective.

Similarly the notion of arc length (in 1D) can be extended to higher dimensions. For example, for 2D problems we could parametrize with respect to 'surface area'. That is, the surface $(x, y, u(x, y))$, defined for all $(x, y) \in \Omega$ (the physical variables), can be defined in terms of the computational variables (s,t), where the surface is $(x(s,t), y(s,t), u(s,t))$. In this case an approximation to the value of the surface area associated with each mesh element could be used to determine an appropriate measure to be redistributed during mesh refinement. If $T_i, i = 1, 2 \cdots N$ are the mesh elements associated with the current discrete solution, and $S_{T_i}(x,y)$ is the bivariate polynomial approximation to $u(x,y)$ defined for $(x,y) \in T_i$, then the surface area associated with T_i is,

$$A_{T_i} \equiv \int\int_{T_i} \sqrt{1 + (\frac{\partial u}{\partial x})^2 + (\frac{\partial u}{\partial y})^2}\, dxdy.$$

Since $U(x,y) \approx u(x,y)$ is a piecewise polynomial defined for $(x,y) \in \Omega$, $U_x(x,y)$ and $U_y(x,y)$ are also bivariate piecewise polynomials which are approximations to $u_x(x,y)$ and $u_y(x,y)$ respectively. An obvious inexpensive measure that can be used as a basis for mesh refinement and which is analogous to arc length (for ODEs) is an approximation to A_{T_i}. That is, we redistribute the error measure, $\bar{A}_{T_i}$, where

$$\bar{A}_{T_i} \equiv \int\int_{T_i} \sqrt{1 + (\frac{\partial U}{\partial x})^2 + (\frac{\partial U}{\partial y})^2}\;\, dxdy.$$

and the objective would then be to determine a new mesh of $\bar{N}$ elements such that,

$$\bigcup_{i=1}^{\bar{N}} \bar{T}_i \;=\; \Omega, \;\; \text{with each } \; \bar{A}_{\bar{T}_i} \approx L/\bar{N} \text{ for } i = 1, 2 \cdots \bar{N},$$

and $L = \sum_{i=1}^{N} A_{T_i}$.

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