Quadrature - Special Difficulties

We will consider 2 types of difficult problems and how they can be solved.
Infinite range problems (improper integrals):
The infinite integration, $\int_0^\infty f(x)dx$ is well-defined only if $\lim_{R\to\infty} \int_0^R f(x)dx$ exists. Some possible approaches for approximating $I(f) = \int_0^\infty f(x)dx$ when it exists:

- For $0 = R_0 < R_1 < \cdots R_j < \cdots$, define A_i as the approximation to $\int_{R_{i-1}}^{R_i} f(x)dx$ associated with a standard quadrature rule. We then have that,

$$S_j \equiv \sum_{i=1}^{j} A_i,$$

can be used as an approximation to $I(f)$ if $R_i \to \infty$. This process can halt (at a fixed value of j) when $|A_j| < TOL$.

Infinite Range Approaches

- If $f(x) = \omega(x)g(x)$ with $\omega(x)$ positive, then one can apply a generalized Gaussian rule. For example, if $\omega(x) = e^{-x}$ we obtain Gauss Laquerre rules. In this case we have,

$$\int_0^\infty \omega(x)g(x)dx \approx \sum_{i=0}^{n} \omega_i g(x_i),$$

  where the x_i's are the zeros of polynomials orthogonal on $[0, \infty)$ with respect to $\omega(x)$.

- Special transformation of variable. Let $x = \rho(t)$ for some differentiable function $\rho(t)$. We then have,

$$I(f) = \int_0^\infty f(x)dx = \int_{\rho^{-1}(0)}^{\rho^{-1}(\infty)} f(\rho(t))\rho^{'}(t)dt.$$

  For example, if $x = -\ln(t), \Rightarrow t = e^{-x}$ and we have $I(f) = \int_0^1 f(-\ln(t))/tdt$.

Singular Integrands

Consider the approximation of $I(f) = \int_a^b f(x)dx$ where $f(a)$ or $f(b)$ is undefined. For example,

$$I = \int_0^1 \frac{1}{x^{1/2} + x^{1/3}} dx.$$

For such problems we can attempt to 'remove' the singularity (at $t^* = a$ or $t^* = b$) as a 2-step process:

1. Determine the 'type' of the singularity at $t = t^*$, choose $s(x)$ where $\int_a^b s(x)dx$ can be computed analytically and where $(f(x) - s(x))$ is not singular at t^*.
2. Replace $\int f(x)dx$ by $\int (f(x) - s(x))dx + \int s(x)dx$ where standard methods can be used to approximate the first integral and the analytic formula used for the second.

Singular Integrands

For the above example, with $f(x) = \frac{1}{x^{1/2}+x^{1/3}}$ consider what happens as $x \to 0$,

$$\frac{1}{x^{1/2}+x^{1/3}} = \frac{1}{x^{1/3}(x^{1/6}+1)} = \frac{1}{1+x^{1/6}} - \frac{x^{1/6}-1}{x^{1/3}}.$$

We therefore have,

$$\int_0^1 \frac{1}{x^{1/2}+x^{1/3}} dx = \int_0^1 \frac{1}{1+x^{1/6}} dx + \int_0^1 \frac{1-x^{1/6}}{x^{1/3}} dx.$$

The first integral can then be approximated by standard methods while the second is equal to $3/10$.

For the general case the key step is to perform an expansion of the integrand about the point of singularity ($t^* = a$ or $t^* = b$) to allow one to 'remove' it.

2D Quadrature

- Consider the problem of approximating integrals in two dimensions,

$$I(f) = \int \int_D f(x, y) dx dy,$$

  This problem is more complicated than the one dimensional case since D can take many forms.

- One can develop the analogs of Gaussian rules or interpolatory rules but the weights and nodes will depend on the region D. Such rules can be determined and tabulated for simple regions such as rectangles, triangles and circles.

- An arbitrary region must then be transformed onto one of these simple regions before the rule can be used. Such a transformation will generally be nonlinear and may introduce an approximation error as well.

2D Quadrature (cont)

- An alternative approach is to apply a ‘product rule’, where one reduces the $2D$-integral to a sequence of two $1D$-integrals:

$$\int_a^b \int_{\alpha(y)}^{\beta(y)} f(x,y)dxdy = \int_a^b g(y)dy,$$

  where

$$g(y) \equiv \int_{\alpha(y)}^{\beta(y)} f(x,y)dx.$$

- Note that $g(y)$ is a $1D$-integral with upper and lower bounds depending on y.
- In this case $g(y)$ is approximated, for a fixed value of y, by a standard method (for example, $\approx \sum_{j=0}^{M} \omega_j f(x_j, y)$), and $\int_a^b g(y)dy$ is also approximated by a standard method.

2D Quadrature (cont)

That is,

$$\int_a^b \int_{\alpha(y)}^{\beta(y)} f(x,y)dxdy = \int_a^b g(y)dy \approx \sum_{r=0}^{M'} \hat{\omega}_r g(y_r),$$

$$\approx \sum_{r=0}^{M'} \hat{\omega}_r \left(\sum_{j=0}^{M} \omega_j f(x_j, y_r) \right),$$

$$= \sum_{r=0}^{M'} \sum_{j=0}^{M} (\hat{\omega}_r \omega_j) f(x_j, y_r).$$

Note that error estimates for product rules are not easy to develop since the function $g(y) \approx \sum_{j=0}^{M} \omega_j f(x_j, y)$ will not be a 'smooth' function of y unless M and the x_j's are fixed (which is unlikely since $\alpha(y)$ and $\beta(y)$ are not fixed). In particular this 'inner rule' cannot be adaptive.

Numerical ODEs

- Definition: A first-order ordinary differential equation is specified by:

$$y' = f(x, y), \quad \text{over a finite interval} \quad x \in [a, b].$$

- Note that a solution of this ODE, $y(x)$, is a function of one variable. When the solution depends on more than one variable (ie a multivariate function) it is called a partial differential equation – PDE. The term first-order refers to the highest derivative that appears in the equation.
- For ODEs the variable x is called the independent variable while y (which depends on x) is called the dependent variable. 'Solving' the ODE is interpreted as determining a technique for expressing y as a function of x in some explicit way.

ODEs-Mathematical Preliminaries

- A function $\Phi(x)$ is a solution of this ODE if $\Phi(x) \in C^1[a,b]$ and $\forall x \in [a,b]$ we have $\Phi^{'}(x) = f(x, \Phi(x))$. (Note that this condition is often easy to check or verify).
- For example the ODE,

$$y' = \lambda y,$$

has solutions $\Phi(x) = c\, e^{\lambda x}$ for any constant c since,

$$[c\, e^{\lambda x}]^{'} = \lambda c e^{\lambda x} = \lambda \Phi(x).$$

In particular this ODE does not have a unique solution but rather a whole family of solutions (characterized by the parameter c).

ODEs-Mathematical Preliminaries

- To determine a unique mathematical solution we must add an additional constraint. The most common way to do this is to prescribe the value of the solution at the initial point of the interval. That is we specify,

  $$y(a) = y_0.$$

  –Definition: An ODE together with the initial conditions specifies an initial value problem for an ordinary differential equation (IVP for an ODE).

- Before we can attempt to approximate a solution to an IVP we must consider some essential mathematical questions:
  - Does a solution exist?
  - If a solution exists, is it unique?
  - Can the problem be solved analytically (ie. in closed form)?

IVPs - Existence/Uniqueness

- Definition: The function $f(x,y)$ satisfies a Lipschitz condition in y (ie, wrt its second argument) if $\exists L > 0$ such that $\forall x \in [a,b]$ and $\forall\ u, v$ we have

$$|f(x,u) - f(x,v)| \le L|u-v|.$$

In particular, if $f(x,y)$ has a continuous partial derivative with respect to y and this derivative is bounded for all y, then f satisfies a Lipschitz condition in y since,

$$|f(x,u) - f(x,v)| = |\frac{\partial f}{\partial y}(x,\eta)|\ |u-v|,$$

for some η between u and v.

IVPs - Existence/Uniqueness

- A typical Theorem:
  Let $f(x, y)$ be continuous for $x \in [a, b]$ and $\forall y$ and satisfy a Lipschitz condition in y, then for any initial condition y_0 the IVP,

$$y' = f(x, y), \quad y(a) = y_0, \quad \text{over } [a, b],$$

  has a unique solution, $y(x)$ defined for all $x \in [a, b]$.

Systems of ODEs

- Often one must deal with a system of n 'unknown' dependent variables of the form:

$$
\begin{aligned}
y_1' &= f_1(x, y_1, y_2, \cdots y_n), \\
y_2' &= f_2(x, y_1, y_2, \cdots y_n), \\
\vdots &\quad \vdots \quad \vdots \\
y_n' &= f_n(x, y_1, y_2, \cdots y_n),
\end{aligned}
$$

with initial conditions all specified at the same point,

$$
\begin{aligned}
y_1(a) &= c_1, \\
y_2(a) &= c_2, \\
\vdots &\quad \vdots \quad \vdots \\
y_n(a) &= c_n,
\end{aligned}
$$

Systems of ODEs (cont)

In vector notation, this system of IVPs can be written

$$Y' = F(x, Y), \quad Y(a) = Y_0,$$

where $Y(x) = [y_1(x), y_2(x), \cdots y_n(x)]^T, \; Y_0 = [c_1, c_2, \cdots c_n]^T$ and $F(x, Y)$ is a vector-valued function,

$$F(x, Y) = \begin{bmatrix} f_1(x, Y) \\ f_2(x, Y) \\ \vdots \\ f_n(x, Y) \end{bmatrix}.$$

The theory and the investigation of numerical methods that we present will be the same for systems as for scalar IVPs. In particular, the Theorem quoted above holds for systems.

Some Examples

- From Biology:

  A predator-prey relationship can be modeled by the IVP:

$$y_1' = y_1 - 0.1 y_1 y_2 + 0.02x$$

$$y_2' = -y_2 + 0.02 y_1 y_2 + 0.008x$$

  with

$$y_1(0) = 30, \;\; y_2(0) = 20.$$

  Here $y_1(x)$ represents the 'prey' population at time x and $y_2(x)$ represents the 'predator' population at time x. The solution can then be visualized as a standard x/y solution plot or by a 'phase plane' plot. Figure 1 illustrates the solution to this system. We know that for different initial conditions solutions to this problem exhibit oscillatory behaviour as x increases.

Solution to PP problem

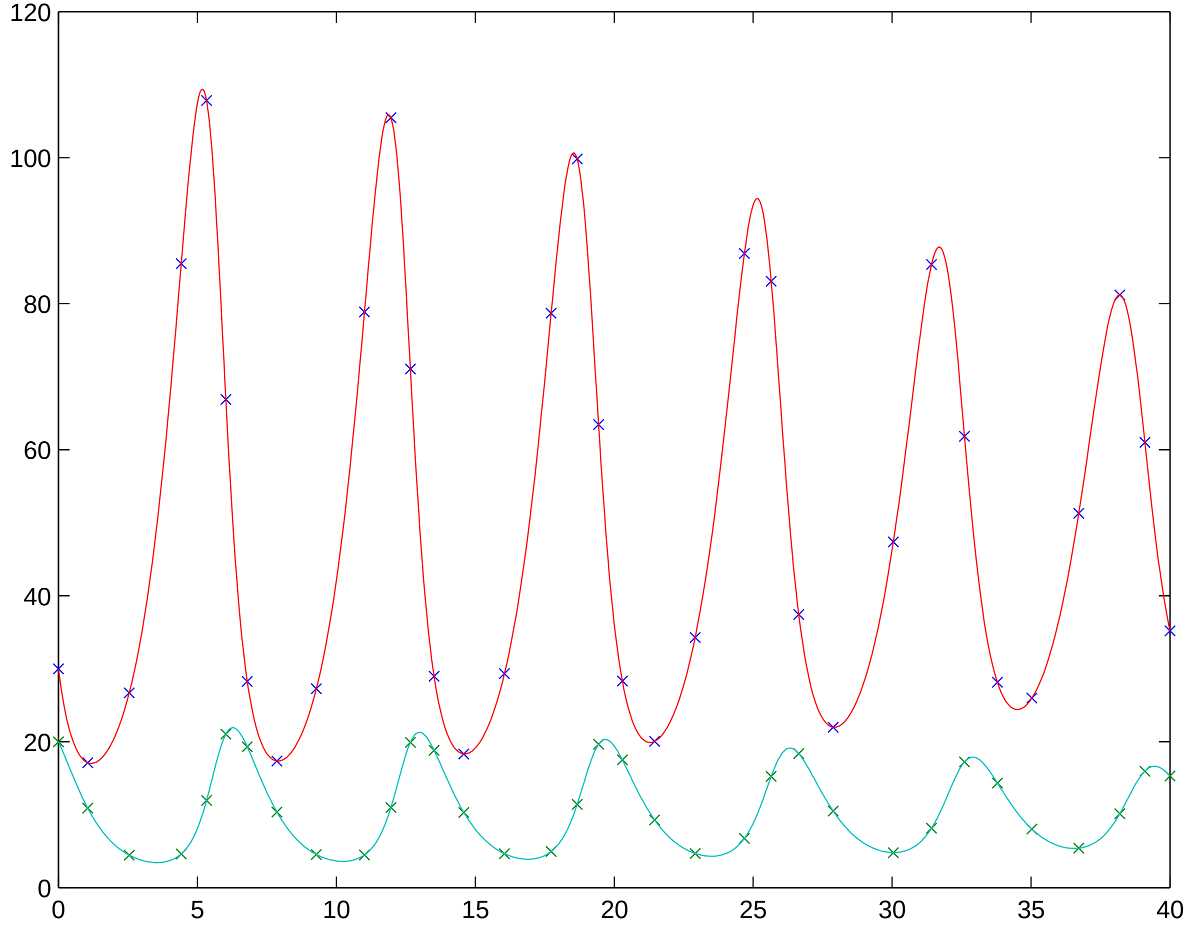

Figure 1. Solution plot for the Predator-Prey Problem.

Solution to PP problem

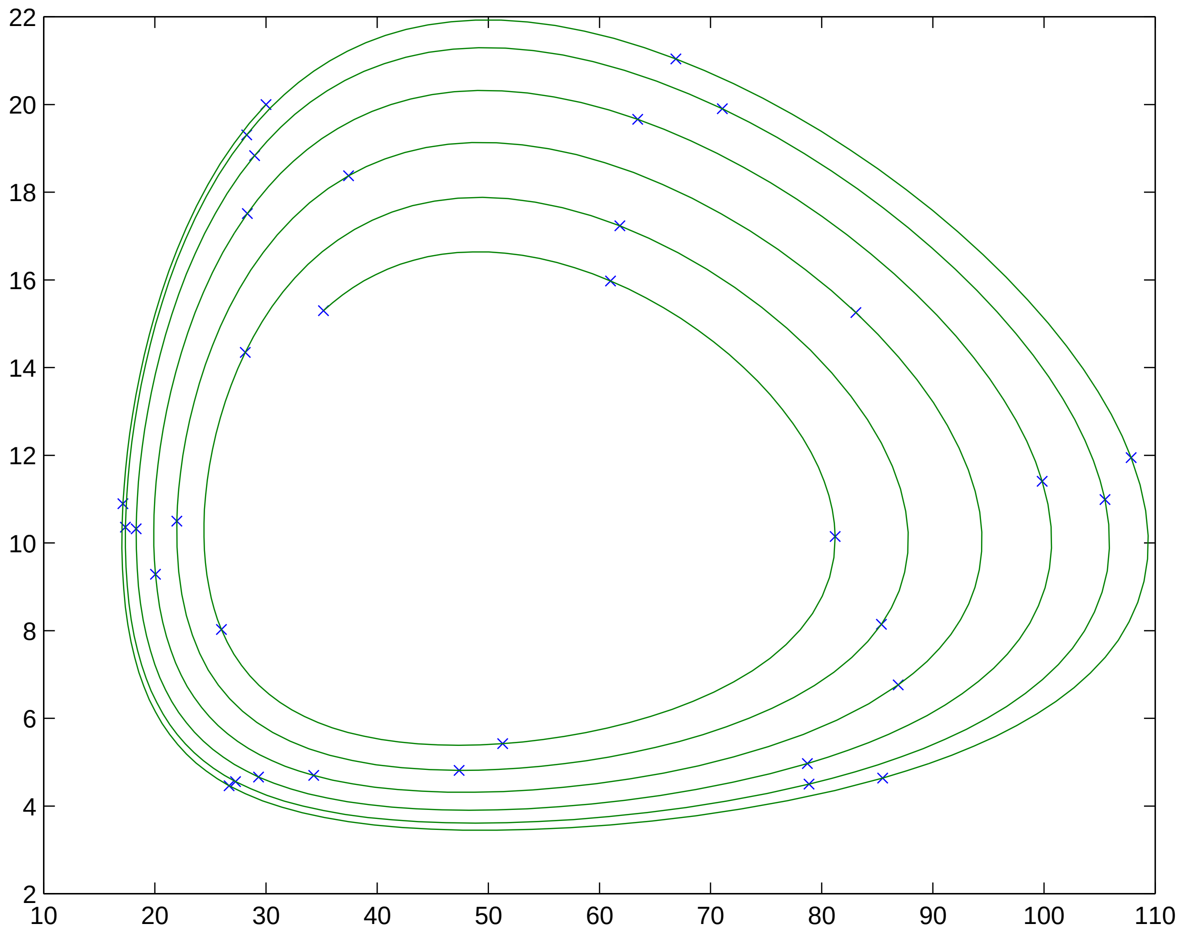

Figure 2. Phase Plane Plot for Predator-Prey Problem.