Computational Methods

CMSC/AMSC/MAPL 460

Ordinary differential equations

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Nonlinearity

- In general the quantity on the right hand side, f, in the standard form can be a nonlinear function of t and y.
- Nonlinearity implies multiple solutions and "chaos"
- Also has a bearing on how well a numerical solver can integrate the ODE

Linearized Diff Eq.

- Standard form $$\frac{dy}{dt} = f\left(t, y\right) \qquad y\left(t_0\right) = y_0$$
- Local behavior of the solution to a differential equation near any point (t_c, y_c) can be analyzed by expanding $f(t,y)$ in a two-dimensional Taylor series.

$$f(t, y) = f(t_c,y_c) + \alpha(t - t_c) + J(y - yc) + \dots$$

- where $$\alpha = \partial f/\partial t \ (t_c,y_c)$$ $$J = \partial f/\partial y \ (t_c,y_c)$$
  - (We already used such expansions for deriving the RK method)
- These equations are linear and can consider the three terms on the rhs separately
- Behavior of differential equation governed by the structure of the Jacobian matrix J

Linearized differential equations

For a system of differential equations with n components,

$$\frac{d}{dt}\begin{bmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_n(t) \end{bmatrix} = \begin{bmatrix} f_1(t, y_1, \ldots, y_n) \\ f_2(t, y_1, \ldots, y_n) \\ \vdots \\ f_n(t, y_1, \ldots, y_n) \end{bmatrix}$$

the Jacobian is an n-by-n matrix of partial derivatives

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} & \cdots & \frac{\partial f_1}{\partial y_n} \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} & \cdots & \frac{\partial f_2}{\partial y_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial y_1} & \frac{\partial f_n}{\partial y_2} & \cdots & \frac{\partial f_n}{\partial y_n} \end{bmatrix}$$

Jacobian properties

- Interesting equation $$\frac{dy}{dt} = Jy$$
- In one dimension it can be integrated to obtain the local solution

$$y = C \exp(J\ t)$$

- Express solution similarly for a system.
- Use the eigendecomposition of the Jacobian matrix

$$J = V\Lambda V^{-1}$$

  - V matrix with columns as eigenvectors
  - Λ eigenvalues arranged as a diagonal matrix
- Why? It removes the coupling of terms in the right hand side by diagonalizing the matrix
- $y' = Jy$. So $V^{-1}y' = V^{-1}JVV^{-1}y$
- Let $V\,x = y$ *so* $x = V^{-1}y$
- transforms the local system of equations to
- $dx_k/dt = \lambda_k\, x_k$ $\quad x_k(t) = e^{\lambda_k (t-t_c)}\, x(t_c)$

- A single component $x_k(t)$ has the following behaviors according to $\lambda_k = \mu_k + i\ \nu_k$
- If μ_k is positive it grows
- It decays if μ_k is negative,
- and oscillates if ν_k is nonzero.
- Example: harmonic oscillator $d^2 y / d t^2 = -y$
- s a linear system. The Jacobian is simply the matrix
- J = [0 1]

  [-1 0]
- has purely imaginary eigenvalues

Eigenvalues of examples considered

Another example from the book

$$\ddot{u}(t) = -u(t)/r(t)^3$$
$$\ddot{v}(t) = -v(t)/r(t)^3$$

where

$$r(t) = \sqrt{u(t)^2 + v(t)^2}$$

$$J = \frac{1}{r^5}\begin{bmatrix} 0 & 0 & r^5 & 0 \\ 0 & 0 & 0 & r^5 \\ 2y_1^2 - y_2^2 & 3y_1y_2 & 0 & 0 \\ 3y_1y_2 & 2y_2^2 - y_1^2 & 0 & 0 \end{bmatrix}$$

- one eigenvalue is real and positive, so that component is growing.
- One eigenvalue is real and negative, corresponding to a decaying component.
- Two eigenvalues are purely imaginary, corresponding to oscillatory components.

The vector $y(t)$ has four components,

$$y(t) = \begin{bmatrix} u(t) \\ v(t) \\ \dot{u}(t) \\ \dot{v}(t) \end{bmatrix}$$

The differential equation is

$$\dot{y}(t) = \begin{bmatrix} \dot{u}(t) \\ \dot{v}(t) \\ -u(t)/r(t)^3 \\ -v(t)/r(t)^3 \end{bmatrix}$$

$$\lambda = \frac{1}{r^{3/2}}\begin{bmatrix} \sqrt{2} \\ i \\ -\sqrt{2} \\ -i \end{bmatrix}$$

Jacobian and ode behavior

- $J = \partial f / \partial y$
- Then a **single** ODE is
  - **stable** at a point (t_c, y_c) if $J(t_c, y_c) < 0$.
  - **unstable** at a point (t_c, y_c) if $J(t_c, y_c) > 0$.
  - **stiff** at a point (t_c, y_c) if $J(t_c, y_c) << 0$.
- A **system** of ODEs is
  - **stable** at a point (t_c, y_c) if the **real part** of all the **eigenvalues** of the matrix $J(t_c, y_c)$ are negative (converse if some are positive)
  - **stiff** at a point (t_c, y_c) if the **real parts** of more than one eigenvalue of $J(t_c, y_c)$ are negative and wildly different.

Stiffness

- Stiffness
  - *A problem is stiff if the solution being sought is varying slowly, but there are nearby solutions that vary rapidly, so the numerical method must take small steps to obtain satisfactory results.*
- Example problem: A match is lit and the fire grows as a ball of flame. until it reaches a critical size. It then remains at that size because the amount of oxygen being consumed by the combustion in the interior of the ball balances the amount available through the surface.
- Let $y(t)$ represent the ball radius. y^2 is proportional to the surface area while y^3 to the volume
  - $y' = y^2 - y^3$
  - $y(0) = \eta$
  - $0 \leq t \leq 2/\eta$

Solution using regular and stiff-solver

- choose η=0.01 and 0.0001
- Solve with RK45
- Observe
- Solve with ode23s
- Observe

```
help ode45; pause delta = 0.01;
F = inline('y^2 - y^3','t','y');
opts = odeset('RelTol',1.e-4);
ode45(F,[0 2/delta],delta,opts);
pause figure delta = 0.0001;
ode45(F,[0 2/delta],delta,opts);
opts = odeset('RelTol',1.e-6);
pause
figure
ode45(F,[0 2/delta],delta,opts);
pause
help ode23s
pause
figure
ode23s(F,[0 2/delta],delta,opts);
```

Error control

- Get estimate of the error at current step
  - change step size
  - change the order
- then use the difference in results to get an estimate of the error
- **Suppose error estimate is much too large:**
  - reduce the stepsize (usually by a factor of 2) and try again.
- **Suppose error estimate is much smaller than needed:**
  - Then we can increase the stepsize (usually doubling it) and save ourselves some work when we take the **next** step.

Chaos: The Lorenz attractor

- Expressed in standard form
- Seven of Nine coefficients are numerical
- Two are non-linear
- Solution keeps flipping between two basins of attraction

$$\dot{y} = Ay$$

$$y(t) = \begin{pmatrix} y_1(t) \\ y_2(t) \\ y_3(t) \end{pmatrix}$$

$$A = \begin{bmatrix} -\beta & 0 & y_2 \\ 0 & -\sigma & \sigma \\ -y_2 & \rho & -1 \end{bmatrix}$$