CS 450: Numerical Anlaysis[1]

Initial Value Problems for Ordinary Differential Equations

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[1] *These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book "Scientific Computing: An Introductory Survey" by Michael T. Heath (slides).*

Ordinary Differential Equations

- An *ordinary differential equation (ODE)* usually describes time-varying system by a function $\boldsymbol{y}(t)$ that satisfies a set of equations in its derivatives. *The general implicit form is*

$$\boldsymbol{g}(t, \boldsymbol{y}, \boldsymbol{y}', \boldsymbol{y}'', \ldots, \boldsymbol{y}^{(k)}) = \boldsymbol{0},$$

  but we restrict focus on the explicit form, $\boldsymbol{y}^{(k)} = \boldsymbol{f}(t, \boldsymbol{y}, \boldsymbol{y}', \boldsymbol{y}'', \ldots, \boldsymbol{y}^{(k-1)})$.

- An ODE of any *order* k can be transformed into a first-order ODE,

$$\boldsymbol{u}' = \begin{bmatrix} \boldsymbol{u}_1' \\ \vdots \\ \boldsymbol{u}_{k-1}' \\ \boldsymbol{u}_k' \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_2 \\ \vdots \\ \boldsymbol{u}_k \\ \boldsymbol{f}(t, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_k) \end{bmatrix} \quad \textit{where} \quad \boldsymbol{u}_i(t) = \boldsymbol{y}^{(i-1)}(t).$$

  Consequently, we restrict our focus to systems of first-order ODEs. Linear ODEs have the form $\boldsymbol{y}'(t) = \boldsymbol{A}(t)\boldsymbol{y}(t) + \boldsymbol{b}(t)$, *whose coefficients are said to be constant if* $\boldsymbol{A}(t) = \boldsymbol{A}$ *for all* t, *and is homogeneous if* $\boldsymbol{b}(t) = \boldsymbol{0}$.

Example: Newton's Second Law

- Consider, $F = ma$ for a given force F, which is a second order ODE,

  $$\begin{aligned} F &= my''(t), \\ y''(t) &= F/m. \end{aligned}$$

  The solution is $y(t) = \frac{1}{2}(F/m)t^2 + c_1 t + c_2$*, where* c_1 *and* c_2 *depend on initial conditions, i.e., values of* $y(0)$*,* $y'(0)$*.*
- We can transform it into a first order ODE in two variables:

  $$\boldsymbol{u} = \begin{bmatrix} y(t) \\ y'(t) \end{bmatrix},$$

  $$\begin{bmatrix} u_1' \\ u_2' \end{bmatrix} = \boldsymbol{u}' = \boldsymbol{f}(t, \boldsymbol{u}) = \begin{bmatrix} u_2 \\ F/m \end{bmatrix}.$$

Initial Value Problems

- Generally, a first order ODE specifies only the derivative, so the solutions are non-unique. An *initial condition* addresses this:

  $$\boldsymbol{y}(t_0) = \boldsymbol{y}_0$$

  This condition yields an initial value problem (IVP), which is the simplest example of a boundary condition.

- Given an initial condition, an ODE must satisfy an integral equation for any given point t:

  $$\boldsymbol{y}(t) = \boldsymbol{y}_0 + \int_{t_0}^{t} \boldsymbol{f}(s, \boldsymbol{y}(s))ds,$$

  If it is the case that $\boldsymbol{f}(t, \boldsymbol{y}(t))$ is not dependent on $\boldsymbol{y}(t)$, the integral can be computed directly by numerical quadrature to solve the ODE.

Existence and Uniqueness of Solutions

- For an ODE to have a unique solution, it must be defined on a closed domain D and be *Lipschitz continuous*:

  $$\forall \boldsymbol{y}, \hat{\boldsymbol{y}} \in D, \quad \|\boldsymbol{f}(t, \hat{\boldsymbol{y}}) - \boldsymbol{f}(t, \boldsymbol{y})\|_2 \le L\|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2,$$

  i.e. the rate of change of the ODE solution should itself change continuously. Any differentiable function $\boldsymbol{f}$ is Lipschitz continuous with

  $$L = \max_{(t,\boldsymbol{y}) \in D} \|\boldsymbol{J}_{\boldsymbol{f}}(t, \boldsymbol{y})\|_2,$$

  where $\boldsymbol{J}_{\boldsymbol{f}}$ is Jacobian of $\boldsymbol{f}$ with respect to $\boldsymbol{y}$. For an IVP, this continuity condition is also sufficient for existence and uniqueness of a solution.
- The solutions of an ODE can be stable, unstable, or asymptotically stable:

  Perturbation to the input causes a perturbation to the solution that
  - *has bounded growth for a stable ODE,*
  - *unbounded growth for an unstable ODE, and*
  - *shrinks for an asymptotically stable ODE.*

Stability of 1D ODEs

- The solution to the scalar ODE $y' = \lambda y$ is $y(t) = y_0 e^{\lambda t}$, with stability dependent on λ:

$$\lim_{t\to\infty} y(t) = \begin{cases} \infty & : \lambda > 0 \text{ \textit{(unstable)}} \\ y_0 & : \lambda = 0 \text{ \textit{(stable)}} \\ 0 & : \lambda < 0 \text{ \textit{(asymptotically stable)}} \end{cases}$$

- A constant-coefficient linear ODE has the form $\boldsymbol{y}' = \boldsymbol{A}\boldsymbol{y}$, with stability dependent on the real parts of the eigenvalues of $\boldsymbol{A}$:
  - *At a point $(t, \boldsymbol{y})$, any ODE can be approximated by a linear ODE of the form $\boldsymbol{z}' = \boldsymbol{J_f}(t, \boldsymbol{y})\boldsymbol{z}$.*
  - *For general ODEs, stability can be ascertained locally by considering the eigenvalues of $\boldsymbol{J_f}(t, \boldsymbol{y})$.*

Numerical Solutions to ODEs

***Demo:** Forward Euler stability*

- Methods for numerical ODEs seek to approximate $\boldsymbol{y}(t)$ at $\{t_k\}_{k=1}^m$.

  Compute $\boldsymbol{y}_k$ for $k \in \{1, \dots, m\}$ so as to approximate $\boldsymbol{y}(t_k) \approx \boldsymbol{y}_k$. For an IVP, typically form $\boldsymbol{y}_{k+1}$ using $\boldsymbol{y}_k$ or additionally (for multistep methods) $\boldsymbol{y}_{k-1}, \dots$

- Euler's method provides the simplest method (attempt) for obtaining a numerical solution:

  Approximation solution to ODE at $t_k + h$ by linear segment from $(t_k, \boldsymbol{y}_k)$ with slope $\boldsymbol{f}(t_k, \boldsymbol{y}_k)$,

  $$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + h_k \boldsymbol{f}(t_k, \boldsymbol{y}_k).$$

  This approximation is the first order form of various models (Taylor series, finite differences, interpolation, quadrature, undetermined coefficients).

Error in Numerical Methods for ODEs

- Truncation error is typically the main quantity of interest, which can be defined *globally* or *locally*:
  - *Global error is measured at all points*

    $$\boldsymbol{e}_k = \boldsymbol{y}_k - \boldsymbol{y}(t_k).$$

  - *Local error measures the deviation from the exact solution $\boldsymbol{u}_{k-1}(t)$ passing through the previous point $(t_{k-1}, \boldsymbol{y}_{k-1})$,*

    $$\boldsymbol{l}_k = \boldsymbol{y}_k - \boldsymbol{u}_{k-1}(t_k).$$

- The *order of accuracy* of a given method is one less than than the order of the leading order term in the local error $\boldsymbol{l}_k$:
  - *Accuracy is of order p if $\boldsymbol{l}_k = O(h_k^{p+1})$, for forward Euler $p = 1$ since*

    $$\boldsymbol{y}(t_{k+1}) = \boldsymbol{y}(t_k) + h_k \boldsymbol{f}(t_k, \boldsymbol{y}(t_k)) + O(h_k^2),$$

    so $\boldsymbol{l}_k = O(h_k^2)$.

Accuracy and Taylor Series Methods

- By taking a degree-r Taylor expansion of the ODE in t, at each consecutive $(t_k, \boldsymbol{y}_k)$, we achieve rth order accuracy.

  We can bound the local approximation error as the error in the Taylor expansion,

  $$\boldsymbol{y}(t_k + h) = \boldsymbol{y}(t_k) + \boldsymbol{y}'(t_k)h + \cdots + \boldsymbol{y}^{(r)}(t_k)h^r/r!$$

  which is $O(h^{r+1})$, leading to $O(h^r)$ accuracy in the approximation to $\boldsymbol{f}(t, \boldsymbol{y})$. Euler's method is a first-order Taylor series method.

- Taylor series methods require high-order derivatives at each step:
  - *Analytic differentiation is expensive, so seek to approximate.*
  - *Can perform a finite-differencing approximation by evaluating at points near $(t_k, \boldsymbol{y}_k)$ (multi-stage methods) or simply using previous points, e.g. $(t_{k-1}, \boldsymbol{y}_{k-1})$ (multi-step methods).*

Demo: *Stability regions*

Growth Factors and Stability Regions

- Stability of an ODE method discerns whether local errors are amplified, deamplified, or stay constant:
  - *A method is stable if the growth factor of the error is less than or equal to one.*
  - *The stability region for a method describes stablie step-sizes via*
    - *the step size h (assuming its constant) and*
    - *eigenvalues λ, usually as a function of $h\lambda$.*
- Basic stability properties follow from analysis of linear scalar ODE, which serves as a local approximation to more complex ODEs.
  - *Consider forward Euler for the ODE $y' = \lambda y$, where*

$$y_{k+1} = y_k + h\lambda y_k = \underbrace{(1 + h\lambda)}_{\text{growth factor}} y_k.$$

  - *Euler's method requires $|1 + h\lambda| \leq 1$ to be stable, which implies $-2 \leq h\lambda \leq 0$*
  - *Relative to the local errors $l_1, \ldots, l_k$, the global error e_k satisfies*

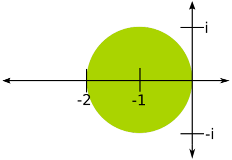
$$e_k = l_k + (1 + h\lambda)e_{k-1} = \sum_{i=1}^{k} (1 + h\lambda)^{k-i} l_i.$$

Stability Region for Forward Euler

- The stability region of a general ODE constrains the eigenvalues of $h\boldsymbol{J_f}$
  - *Given propogated error* $\boldsymbol{e}_k = \boldsymbol{y}_k - \boldsymbol{y}(t_k)$*, Forward Euler gives*

$$\begin{aligned}\boldsymbol{e}_{k+1} &= \boldsymbol{y}_k + h\boldsymbol{f}(t, \boldsymbol{y}_k) - \boldsymbol{y}(t_{k+1}) \\ &= \boldsymbol{y}_k + h\boldsymbol{f}(t, \boldsymbol{y}_k) - (\boldsymbol{y}(t_k) + \boldsymbol{f}(t_k, \boldsymbol{y}(t_k))h - \hat{l}_k) \\ &= \boldsymbol{e}_k + h\boldsymbol{J}_f(t_k, \boldsymbol{y}_k)\boldsymbol{e}_k + \hat{l}_k + O(\|\boldsymbol{e}_k\|^2)\end{aligned}$$

  - *Consequently the growth factor for Forward Euler is* $\boldsymbol{I} + h_k\boldsymbol{J_f}(t_k, \boldsymbol{y_k})$.
  - *Forward Euler is asymptotically stable if the spectral radius of the growth factor is less than one, so the eigenvalues of* $h_k\boldsymbol{J_f}(t_k, \boldsymbol{y}_k)$ *must always lie within a stability region that is a circle on the complex plane centered at* -1 *of radius* 1.



Demo: *Backward Euler stability*

Backward Euler Method

- Implicit methods for ODEs form a sequence of solutions that satisfy conditions on a local approximation to the solution:

  The most basic implicit method is the backward Euler method

  $$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \boldsymbol{h}_k \boldsymbol{f}(t_{k+1}, \boldsymbol{y}_{k+1}),$$

  which solves for $\boldsymbol{y}_{k+1}$ so that a linear approximation of the solution at t_{k+1} passes through the point $(t_k, \boldsymbol{y}_k)$. Just like forward Euler, first-order accuracy is achieved by the linear approximation.

- The stability region of the backward Euler method is the left half of the complex plane:

  Such a method is called unconditionally stable. Note that the growth factor can be derived via

  $$y_{k+1} = y_k + h\lambda y_{k+1} = \frac{1}{1 - h\lambda} y_k,$$

  and satisfies $|1/(1 - h\lambda)| \leq 1$ so long as $h\lambda \leq 0$.

Demo: *Stiffness*

Stiffness

- *Stiff* ODEs are ones that contain components that vary at disparate time-scales:
  - *These are challenging since they require both high accuracy and stability*
  - *A linear ODE is stiff if the eigenvalues of $\boldsymbol{A}$ are disparate in magnitude*
  - *Explicit methods must use small step size h to ensure stability*
  - *Implicit methods are stable with any step size and hence effective for stiff ODEs*

Trapezoid Method

- A second-order accurate implicit method is the *trapezoid method*

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \boldsymbol{h}_k(\boldsymbol{f}(t_k, \boldsymbol{y}_k) + \boldsymbol{f}(t_{k+1}, \boldsymbol{y}_{k+1}))/2,$$

  - *This method takes the average of the backward and forward Euler steps.*
  - *Its growth factor is* $\frac{1+h\lambda/2}{1-h\lambda/2}$.
  - *Since* $\left|\frac{1+h\lambda/2}{1-h\lambda/2}\right| \leq 1$ *for any* $\lambda < 0$, *the method is unconditionally stable.*
- Generally, methods can be derived from quadrature rules:
  - *Evaluate or approximate* $\boldsymbol{f}$ *at a set of points near* $(t_k, \boldsymbol{y}_k)$.
  - *Use weights from a given quadrature rule to approximate solution to local integral equation.*
  - *Finding appropriate quadrature nodes is hard, implicit methods in effect solve for them.*

Multi-Stage Methods

- *Multi-stage methods* construct $\boldsymbol{y}_{k+1}$ by approximating $\boldsymbol{y}$ between t_k and t_{k+1}:
  - *Runge-Kutta methods are the most well-known family of these, simple example is Heun's method,*

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + h\left[\underbrace{\boldsymbol{f}(t_k, \boldsymbol{y}_k)}_{\boldsymbol{v}_1}/2 + \boldsymbol{f}\Big(t_k + h, \boldsymbol{y}_k + h\underbrace{\boldsymbol{f}(t_k, \boldsymbol{y}_k)}_{\boldsymbol{v}_1}\Big)/2\right].$$

  - *We can think of the above method as employing the trapezoid quadrature rule.*
  - *The difference between Heun's method and the (implicit) trapezoid method is that we evaluate at $\boldsymbol{f}(t_k + h, \boldsymbol{y}_k + h\boldsymbol{v}_1)$ rather than working with the implicit value of $\boldsymbol{f}(t_k + h, \boldsymbol{y}_{k+1})$.*
- The 4th order Runge-Kutta scheme is particularly popular:

  This scheme uses Simpson's rule,

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + (h/6)(\boldsymbol{v}_1 + 2\boldsymbol{v}_2 + 2\boldsymbol{v}_3 + \boldsymbol{v}_4)$$

$$\boldsymbol{v}_1 = \boldsymbol{f}(t_k, \boldsymbol{y}_k), \qquad \boldsymbol{v}_2 = \boldsymbol{f}(t_k + h/2, \boldsymbol{y}_k + (h/2)\boldsymbol{v}_1),$$

$$\boldsymbol{v}_3 = \boldsymbol{f}(t_k + h/2, \boldsymbol{y}_k + (h/2)\boldsymbol{v}_2), \qquad \boldsymbol{v}_4 = \boldsymbol{f}(t_k + h, \boldsymbol{y}_k + h\boldsymbol{v}_3).$$

***Demo:** Dissipation in Runge-Kutta Methods*

Runge-Kutta Methods

- Runge-Kutta methods evaluate $\boldsymbol{f}$ at $t_k + c_i h$ for $c_0, \dots, c_r \in [0, 1]$,

$$\boldsymbol{u}_k(t_{k+1}) = \boldsymbol{y}_k + \int_{t_k}^{t_k+h} \boldsymbol{f}(s, \boldsymbol{y}(s))ds \quad \approx \quad \boldsymbol{y}_k + h \sum_{i=0}^{r-1} w_i \boldsymbol{f}(t_k + c_i h, \hat{\boldsymbol{y}}_{ki}),$$

  where $\{(c_i, w_i)\}_{i=0}^{r}$ are quadrature (node, weight) pairs.

- A general family of Runge Kutta methods can be defined by

$$\hat{\boldsymbol{y}}_{ki} = \boldsymbol{y}_k + h \sum_{j} a_{ij} \boldsymbol{f}(t_k + c_i h, \hat{\boldsymbol{y}}_{kj}).$$

  Runge Kutta methods can then be represented by a Butcher tableau,

$$\begin{array}{c|c} \boldsymbol{c} & \boldsymbol{A} \\ \hline & \boldsymbol{w}^T \end{array}$$

  e.g. for RK4 $\boldsymbol{A}$ has a single subdiagonal,

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$

  If $\boldsymbol{A}$ is strictly lower triangular ($a_{ij} = 0$ for $j \geq i$), the scheme is explicit, if $\boldsymbol{A}$ is lower-triangular then it is diagonally implicit, and otherwise implicit.

Multistep Methods

- *Multistep methods* employ $\{\boldsymbol{y}_i\}_{i=0}^{k}$ to compute $\boldsymbol{y}_{k+1}$:

  Linear multistep methods have the form,

  $$\boldsymbol{y}_{k+1} = \sum_{i=1}^{m} \alpha_i \boldsymbol{y}_{k+1-i} + h \sum_{i=0}^{m} \beta_i \boldsymbol{f}(t_{k+1-i}, \boldsymbol{y}_{k+1-i}).$$

  Interpolation is used to determine each α_i and β_i, method is explicit if $\beta_0 = 0$.
- Multistep methods are not self-starting, but have practical advantages:
  - *Can be initiated by Runge-Kutta methods.*
  - *They require few function evaluations.*
  - *Generalize to non-uniformly-spaced points (multivalue methods).*