10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green
Lecture #12: Ordinary Differential Equation Initial Value Problems (ODE-IVPs) and Numerical Integration.

From Last Lecture: Singular Value Decomposition

$$\begin{tikzcd} \underline{\underline{S}}_{observed}(\lambda_n,t_k) = \Sigma x_i(t_k)\underline{\underline{A}}_i(\lambda_n) + \text{noise} \arrow[d, "\text{SVD}"] \\ \Sigma\sigma_i\underline{\underline{U}}_i(t_k)\underline{\underline{V}}_i^T(\lambda_n) \end{tikzcd}$$

Fixed in time. Amplitude changes with wavelength

For a system where only one chemical absorbs light, expect one singular value to be bigger. The rest of the singular values relate to noise. Look in Beer's textbook for exact notation.

ODE-IVP: Numerical Integration

$d\underline{x}/dt = \underline{F}(\underline{x})$ ODE

$\underline{F} = m\underline{a}$

$d^2\underline{x}/dt^2 = \underline{F}(\underline{x}, d\underline{x}/dt)/m$

$d\underline{v}/dt = F/m$ $\quad$ $d\underline{x}/dt = \underline{v}$

$\frac{d}{dt}\begin{pmatrix} V \\ x \end{pmatrix} = \begin{pmatrix} F(\underline{x},\underline{v})/m \\ v \end{pmatrix}$ so setting $x_1=v$ and $x_2=x$ gives $\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} F(\underline{x})/m \\ x_1 \end{pmatrix} = \underline{F}(\underline{x})$

$\underline{g}(\underline{x}, {}^{d\underline{x}}/_{dt}) = 0$

DAE ➔ differential algebraic equations

Boundary Conditions: Initial Value Problems (IVPs)

$\underline{x}(t_0) = \underline{x}_0$

As you move away from $\underline{x}_0$, you are not sure whether you are correct. That is why the first step, if incorrect, can send you far away from the answer and errors can multiply.

Boundary Conditions: Boundary Value Problems (BVPs)

$\underline{x}(t_0) = x_{i0}$ $\quad$ $\underline{x}_j(t_f) = \underline{x}_{jf}$

→ $\underline{g}(\underline{x}_i(t_0), \underline{x}_j(t_f)) = 0$ $\qquad$ "a mess!!"

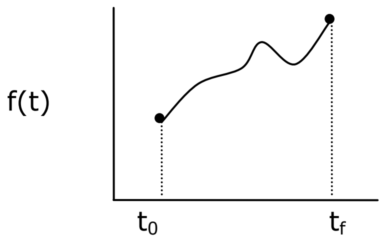
Integrals Can Be Rewritten as ODE-IVPs.

$I = \int_{t_0}^{t} f(t')dt'$ $\qquad \frac{dI}{dt} = f(t) \qquad I(t_0) = 0$

$\underline{x} = \begin{pmatrix} I \\ t \end{pmatrix} \qquad \frac{d\mathbf{x}}{dt} = \begin{pmatrix} dI/dt \\ 1 \end{pmatrix} = \begin{pmatrix} f(t) \\ 1 \end{pmatrix} = \begin{pmatrix} f(x_2) \\ 1 \end{pmatrix} = \underline{F}(\underline{x})$

$$x_1(t_f) = \int_{t_0}^{t_f} f(t')dt' \qquad x_0 = \begin{pmatrix} 0 \\ t_0 \end{pmatrix}$$

Numerical Integration



$\{t_i\}$ $\{f(t_i)\}$

$I \sim \Sigma f(t_i)\Delta t$

rectangle method (not very effective)

Figure 1. Graph of a function over a time interval.

Trapezoid Rule: in MatLAB: 'trapz'

Newton-Cotes Rules: polynomial interpolation between $\{f(t_i)\}$

Simpsons Rule (a.k.a. "Crafty Rule"): $f(t) \approx a_0 + a_1t + a_2t^2 + \ldots$ Error: $O(\Delta t^3)$

*area under parabolas. This technique involves 2 times more work but is many times more accurate.

1) High order methods have much faster convergence as $\Delta t \rightarrow$ small

If too high order, we are fitting the noise to f(t), but if too small Δt, we are adding big numbers and small numbers: $I_{new} = \underbrace{I_{old}}_{\text{big}} + \underbrace{f(t_i)}_{\substack{\text{very small if} \\ \Delta t \text{ is small}}} \Delta t$

2) Adaptive step sizing, adaptive meshing

With adaptive step sizing, or adaptive meshing, the time step sizes are smaller close to the steep peak and larger along the tail where the function is not changing as quickly.

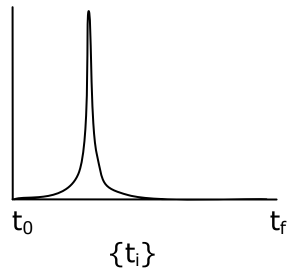


Figure 2. Graph of a function with a steep peak.

* ODE45 in MATLAB®

↳ 4th order polynomial and 5th order polynomial

* cut Δt until 4th and 5th order extrapolations agree within certain tolerance

Runge-Kutta 4-5 method

$\underline{x}(t_1) = \underline{x}(t_0) + \Delta t\{f(x_0)\} + O(\Delta t^N)$

$\underline{x}(t_2) = \underline{x}(t_1) + \Delta t\{f(x_1)\} + O(\Delta t^N)$

No way to guarantee global error

With ODE’s, the error in each step accumulates in a nonlinear way. In integration, the errors are present for each step separately, additive. Computing the integral incorrectly for a previous step does not affect the step at hand.