

Does a solution even exist? How sensitive are they?

General case is harder than root finding, and we couldn't say much there.

→ Only consider linear BVP

$$(*) \begin{cases} \mathbf{y}'(x) = A(x)\mathbf{y}(x) + \mathbf{b}(x) \\ B_a\mathbf{y}(a) + B_b\mathbf{y}(b) = \mathbf{c} \end{cases}$$

$$\begin{aligned} y'' &= f \dots \\ y(a) &= \\ y(b) &= 0 \end{aligned}$$

To solve that, consider *homogeneous IVP*

$$\mathbf{y}'_i(x) = A(x)\mathbf{y}_i(x)$$

with initial condition

$$\mathbf{y}_i(a) = \mathbf{e}_i.$$

Note: $\mathbf{y} \neq \mathbf{y}_i$. \mathbf{e}_i is the i th unit vector. With that, build the **fundamental solution matrix**

$$Y(x) = \begin{bmatrix} | & & | \\ \mathbf{y}_1 & \cdots & \mathbf{y}_n \\ | & & | \end{bmatrix}$$

ODE Systems: Existence

Let

$$Q := B_a Y(a) + B_b Y(b)$$

Then (*) has a unique solution if and only if Q is invertible. Solve to find coefficients:

$$Q\alpha = c$$

Then $Y(x)\alpha$ solves (*) with $\mathbf{b}(x) = 0$.

Define $\Phi(x) := Y(x)Q^{-1}$. So $\Phi(x)c$ solves (*) with $\mathbf{b}(x) = 0$.

Define *Green's function*

$$G(x, y) := \begin{cases} \Phi(x)B_a\Phi(a)\Phi^{-1}(y) & y \leq x, \\ -\Phi(x)B_b\Phi(b)\Phi^{-1}(y) & y > x. \end{cases}$$

Then

$$\mathbf{y}(x) = \Phi(x)c + \int_a^b G(x, y)\mathbf{b}(y)dy.$$

$$y_i = \sum_{j=1}^n G_{ij} b_j$$

Can verify that this solves (*) by plug'n'chug.

ODE Systems: Conditioning

For perturbed problem with $\mathbf{b}(x) + \Delta\mathbf{b}(x)$ and $\mathbf{c} + \Delta\mathbf{c}$:

$$\|\Delta\mathbf{y}\|_{\infty} \leq \max(\|\Phi\|_{\infty}, \|G\|_{\infty}) \left(\|\Delta\mathbf{c}\|_1 + \int \|\Delta\mathbf{b}(y)\|_1 dy \right).$$

- ▶ Conditioning bound implies uniqueness.
- ▶ Also get continuous dependence on data.

Shooting Method

Idea: Want to make use of the fact that we can already solve IVPs.

Problem: Don't know *all* left BCs.

Demo: Shooting method [cleared]

What about systems?

$$y'' = f(y, y')$$
$$\Rightarrow y(a) = \dots$$
$$\cancel{y(b) = \dots} \quad \text{sh} \rightarrow y_s(b)$$
$$\Rightarrow y'(a) = s$$

Cannons aim in more than 1D.

What are some downsides of this method?

- Can Fail
- Can be unstable even if the ODE is stable

What's an alternative approach?

Write a big linear (-ized) system

Finite Difference Method

Idea: Replace u' and u'' with finite differences.

For example: second-order centered

$$u'(x) = \frac{u(x+h) - u(x-h)}{2h} + O(h^2)$$
$$\rightarrow u''(x) = \frac{u(x+h) - 2u(x) + u(x-h))}{h^2} + O(h^2)$$

Demo: Finite differences [cleared]

What happens for a nonlinear ODE?

Lineare, Newton

Demo: Sparse matrices [cleared]

Collocation Method

$$(*) \begin{cases} y'(x) = f(y(x)), \\ g(y(a), y(b)) = 0. \end{cases}$$

1. Pick a basis (for example: Chebyshev polynomials)

$$\hat{y}(x) = \sum_{i=1}^n \alpha_i T_i(x) \quad \# \text{DoF} = n$$

Want \hat{y} to be close to solution y . So: plug into $(*)$.

Problem: \hat{y} won't satisfy the ODE at all points at least.
We do not have enough unknowns for that.

2. **Idea:** Pick n points where we would like $(*)$ to be satisfied.
→ Get a big (non-)linear system
3. Solve that (LU/Newton) → done.

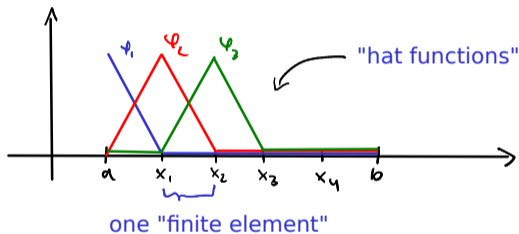
Galerkin/Finite Element Method

$$u''(x) - f(x) := r(x)$$

$$u''(x) = f(x), \quad u(a) = u(b) = 0.$$

Problem with collocation: Big dense matrix.

Idea: Use piecewise basis. Maybe it'll be sparse.



What's the problem with that?

u' does not exist

$u'' \sim \delta \delta \delta$

Weak solutions/Weighted Residual Method

Idea: Enforce a 'weaker' version of the ODE.

= moments $\int_a^b u''(x) \psi(x) dx = - \int_a^b u'(x) \psi'(x) dx + [u'(x) \psi(x)]_a^b$

Solve: $\int_a^b u''(x) \psi(x) dx = \int_a^b f(x) \psi(x) dx$

$$\int_a^b [u''(x) - f(x)] \cdot \underline{\underline{\psi(x)}} dx = 0$$

$$\sum r(x_i) \underline{\underline{\psi(x_i)}} W_i = 0$$

= weighted residual methods' collocation: $\psi_i(x) = \delta(x - x_j)$

Galerkin: Choices in Weak Solutions



Make some choices:

- ▶ Solve for $u \in \text{span} \{\text{hat functions } \varphi_i\}$
- ▶ Choose $\psi \in W = \text{span} \{\text{hat functions } \varphi_i\}$ with $\psi(a) = \psi(b) = 0$.
→ Kills boundary term $[u'(x)\psi(x)]_a^b$.

These choices are called the **Galerkin method**. Also works with other bases.

Discrete Galerkin

Assemble a matrix for the Galerkin method.

$$-\int_a^b \underline{u'(x)} \psi'(x) dx = \int_a^b f(x) \psi(x) dx, \quad \psi(x) \in \{\varphi_j(x)\}$$

$$-\int_a^b \sum_{j=1}^n \alpha_j \varphi_j'(x) \psi'(x) dx = \dots, \quad \text{let } \psi(x) = \varphi_i(x)$$

$$-\sum_{j=1}^n \left[\underbrace{\int_a^b \varphi_j'(x) \varphi_i'(x) dx}_{S_{ij}} \right] \alpha_j = \underbrace{\int_a^b f(x) \varphi_i(x) dx}_{r_i}$$

S_{ij}

$$S \vec{\alpha} = \vec{r}$$

sparse.

Outline

Introduction to Scientific Computing

Systems of Linear Equations

Linear Least Squares

Eigenvalue Problems

Nonlinear Equations

Optimization

Interpolation

Numerical Integration and Differentiation

Initial Value Problems for ODEs

Boundary Value Problems for ODEs

Partial Differential Equations and Sparse Linear Algebra

Sparse Linear Algebra
PDEs

Fast Fourier Transform

Additional Topics

Solving Sparse Linear Systems

Solving $A\mathbf{x} = \mathbf{b}$ has been our bread and butter.

Typical approach: Use factorization (like LU or Cholesky)

Why is this problematic?

Idea: Don't factorize, iterate.

Demo: Sparse Matrix Factorizations and "Fill-In" [cleared]

'Stationary' Iterative Methods

Idea: Invert only part of the matrix in each iteration. Split

$$A = M - N,$$

$$\boxed{A} x = b$$

where M is the part that we are actually inverting. Convergence?

$$\begin{aligned} Ax &= b \\ Mx &= Nx + b \\ Mx_{k+1} &= Nx_k + b \\ x_{k+1} &= M^{-1}(Nx_k + b) \end{aligned}$$

- ▶ These methods are called *stationary* because they do the same thing in every iteration.
- ▶ They carry out fixed point iteration.
→ Converge if contractive, i.e. $\rho(M^{-1}N) < 1$.
- ▶ Choose M so that it's easy to invert.

Choices in Stationary Iterative Methods

What could we choose for M (so that it's easy to invert)?

Name	M	N
Jacobi	D	$-(L + U)$
Gauss-Seidel	$D + L$	$-U$
SOR	$\frac{1}{\omega}D + L$	$(\frac{1}{\omega} - 1)D - U$

where L is the below-diagonal part of A , and U the above-diagonal.

[Demo: Stationary Methods \[cleared\]](#)