Class web page

Office hrs: ~~12:30~~ ~~-~~ 1:30pm (4318 Siebel)

today: in this room, right after class

https://bit.ly/fastalg-s24

contains:

- Class outline ✓
- Notes ✓
- Demos ✓
- Assignments ✓
- Discussion forum ✓
- Grading ✓
- Video ✓

$$\int k(x,y)\,\sigma(y)\,dy$$

Why study this at all?

- Finite difference/element methods are inherently
  - ill-conditioned
  - tricky to get high accuracy with
- Build up a toolset that does *not* have these flaws
- Plus: An interesting/different analytical and computational point of view
  - If you're not going to use it to solve PDEs, it (or the ideas behind it) will still help you gain insight.

FD/FEM: Issues

Idea of these methods:

1. Take differential equations
2. Discretize derivatives
3. Make linear system
4. Solve

So what's wrong with doing that?

Discretizing Derivatives: Issues?

- bad conditioning

$\kappa(A) = \|A\| \|A^{-1}\|$

$\|A\|_\infty = \sup_{f \in S} \frac{\|Af\|_\infty}{\|f\|_\infty}$

$A = \partial_x$

$(e^{i\alpha x})' = (i\alpha) e^{i\alpha x} \quad \alpha \in \mathbb{R}$

$\|e^{i\alpha x}\|_{L^\infty(0,2\pi)} = 1$

$\|i\alpha e^{i\alpha x}\|_\infty = |\alpha|$

$\|\partial_x f\|_\infty \le \underset{\|\partial_x\|_\infty}{?} \, \|f\|_\infty$

$\|\partial_x\|_\infty = \infty$

discrete ?

Discretizing Derivatives: Issues?

Result: The better we discretize (the more points we use), the worse the condition number gets.

Demo: Conditioning of Derivative Matrices

To be fair: Multigrid works around that (by judiciously using fewer points!)
But there's another issue that's not fixable.

As $h \to 0$

$$\frac{f(x+h) - f(x-h)}{2h}$$

cancellation

Q: Are these problems real?

Poisson $\Delta u = f$ ← need MG or other preconditioner

So this class is about starting fresh with methods that (rigorously!) don't have these flaws!

Bonus Advertising Goodie

Both multigrid and fast/IE schemes ultimately are $O(N)$ in the number of degrees of freedom N.

Open Source <3

These notes (and the accompanying demos) are open-source!

Bug reports and pull requests welcome:
https://github.com/inducer/fast-alg-ie-notes

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Outline

Matvec: A Slow Algorithm

Matrix-vector multiplication: our first 'slow' algorithm.
$O(N^2)$ complexity.

$$\beta_i = \sum_{j=1}^{N} A_{ij}\alpha_j$$

Assume A dense.

columns : sources
rows : targets

Matrices and Point Interactions

$$A_{ij} = G(x_i, y_j)$$

Does that actually change anything?

$$\psi(x_i) = \sum G(x_i, y_j)\,\varphi(y_j)$$

x_i y_j points ($\in \mathbb{R}^2$? $\in \mathbb{R}^3$?)

- x_i "targets" / "observation points"
- y_j "sources"
- G kernel

"where you look"

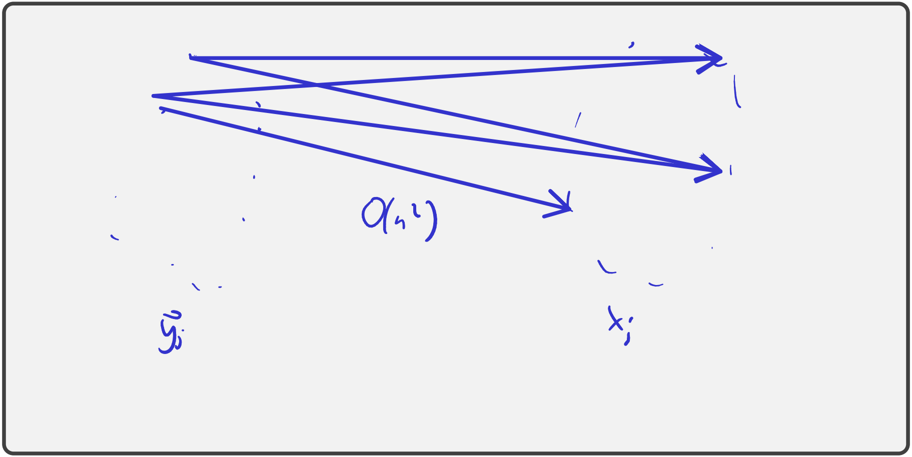
"electrons"

$$G(x,y) = \frac{1}{\|x-y\|_2}$$

Matrices and Point Interactions

$$A_{ij} = G(x_i, y_j)$$

Graphically, too:



Matrices and point Interactions

$$\psi(x_i) = \sum_{j=1}^{N} G(x_i, y_j)\varphi(y_j)$$

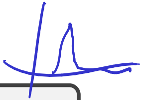
This *feels* different.

make x continuous: $\psi(x) = \sum_{j=1}^{N} G(x, y_j)\,\varphi(y_j)$ ← mat inf. tall

make y continuous: $\psi(x) = \int G(x,y)\,\varphi(y)\,dy$ ← mat. inf. wide

Q: Are there enough matrices that come from globally defined G to make this worth studying?

Point Interaction Matrices: Examples (I)



- Interpolation

$$\Psi(x) = \sum_{j=1}^{n} \underbrace{l_j(x)}\,\varphi(y_j) \qquad L$$

- Differentiation

$$\Psi(x) = \sum_{j=1}^{n} \underbrace{l_j'(x)}\,\varphi(y_j)$$

- Integration

$$\Psi(x) = \Psi(x) = \sum_{j=1}^{n} \int_0^x l_j(\xi)\,d\xi\,(y_j)$$

Point Interaction Matrices: Examples (II)

- Potential evaluation (3D)

$$U(x) = \frac{q_{el}}{4\pi} \cdot \frac{1}{|x|} \leftarrow \text{electrostatics}$$

$$u(x) = \sum_{j=1}^{N} \frac{q_{el}}{4\pi} \frac{1}{|x-y_j|} \varphi(y_j)$$

waves: $$U(x) = C \cdot \frac{e^{ik|x|}}{|x|}$$

Point Interaction Matrices: Examples (III)

- Convolutions

$$\psi(x) = \sum_{j=1}^{N} G(x - y_j)\, \varphi(y_j)$$

sub-$O(n^2)$ algorithm? FFT

↳ grid periodic equispaced

"Butterfly transform"

So yes, there are indeed lots of these things.

Integral Operators

Why did we go through the trouble of rephrasing matvecs as

$$\psi(x_i) = \sum_{j=1}^{N} G(x_i, y_j)\varphi(y_j)?$$

Cheaper Matvecs

$$\psi(x_i) = \sum_{j=1}^{N} G(x_i, y_j)\varphi(y_j)$$

So what can we do to make evaluating this cheaper?

- sparse (FD / FEM)
- special structure
  - Toeplitz
  - circulant

  } FFT-based trickery
- low rank

Fast Dense Matvecs

Consider

$$A_{ij} = u_i v_j,$$

outer product

$A = \vec{u}\vec{v}^T$

let $\mathrm{u} = (u_i)$ and $\mathrm{v} = (v_j)$.

Can we compute $A\mathrm{x}$ quickly? (for a vector x)

$$A\vec{x} = \vec{u}\vec{v}^T\vec{x}$$

$$= (\vec{u}\vec{v}^T)\vec{x} \quad ① \quad \leftarrow O(n^2)$$

$$= \vec{u}(\underbrace{\vec{v}^T\vec{x}}_{O(n)}) \quad ② \quad \leftarrow O(n) \checkmark$$

Fast Dense Matvecs (II)

$$A = \mathbf{u}_1 \mathbf{v}_1^T + \cdots + \mathbf{u}_K \mathbf{v}_K^T$$

$A \in \mathbb{R}^{N \times N}$

Does this generalize? What is K here?

$\operatorname{rank}(A) = K$

Cost: $O(NK)$

Low-Rank Point Interaction Matrices

Usable with low-rank complexity reduction?

$$\psi(x_i) = \sum_{j=1}^{N} G(x_i, y_j)\varphi(y_j)$$

$\vec{a}_1$ $\vec{a}_2$

$(\vec{a}_1 \ \vec{a}_2)$

$$\psi(x_i) = \sum_{j=1}^{N} \underbrace{G_1(x_i)\, G_2(y_j)}_{G(x_i, y_j)}\, \varphi(y_j)$$

"separation of variables"

$$G(x,y) = \frac{1}{\|x-y\|_2}$$ does not look like this.

rank hard to define numerically because of rounding

Numerical Rank

What would a *numerical* generalization of 'rank' look like?

Eckart-Young-Mirsky Theorem

Theorem (Eckart-Young-Mirsky)

SVD $A = U\Sigma V^T$. *If* $k < r = \operatorname{rank}(A)$ *and*

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T,$$

then

$$\min_{\operatorname{rank}(B)=k} |A - B|_2 = |A - A_k|_2 = \sigma_{k+1}.$$

Q: What's that error in the Frobenius norm?

So in principle that's good news:

- We can find the numerical rank.
- We can also find a factorization that reveals that rank (!)

Demo: Rank of a Potential Evaluation Matrix (Attempt 2)

Constructing a tool

There is still a slight downside, though.