

Fast Algorithms and Integral Equation Methods

CS598 APK

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Fall 2019

Today:

- Sales pitch

Outline

Introduction

Notes

Notes (unfilled, with empty boxes)

Dense Matrices and Computation

Tools for Low-Rank Linear Algebra

Rank and Smoothness

Near and Far: Separating out High-Rank Interactions

Outlook: Building a Fast PDE Solver

Going Infinite: Integral Operators and Functional Analysis

Singular Integrals and Potential Theory

Boundary Value Problems

Back from Infinity: Discretization

Computing Integrals: Approaches to Quadrature

Going General: More PDEs

What's the point of this class?

- ▶ Starting point: Large-scale scientific computing
- ▶ Many popular numerical algorithms: $O(n^\alpha)$ for $\alpha > 1$
(Think Matvec, Matmat, Gaussian Elimination, LU, ...)
- ▶ Build a set of tools that lets you cheat: Keep α small
(Generally: probably not—Special purpose: possible!)
- ▶ Final goal: Extend this technology to yield PDE solvers
- ▶ But: Technology applies in many other situations
 - ▶ Many-body simulation
 - ▶ Stochastic Modeling
 - ▶ Image Processing
 - ▶ 'Data Science' (e.g. Graph Problems)
- ▶ This is class is about an even mix of math and computation

Survey

- ▶ Home dept
- ▶ Degree pursued
- ▶ Longest program ever written
 - ▶ in Python?
- ▶ Research area
- ▶ Interest in PDE solvers

Class web page

<https://bit.ly/fastalg-f19>

contains:

- ▶ Class outline
- ▶ Assignments
- ▶ Piazza
- ▶ Grading
- ▶ Video

← Interactive demos!

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?

$$(e^{i\alpha x})' = i\alpha e^{i\alpha x} \rightarrow$$

$$\kappa_2(A) = \|A\|_2 \|A^{-1}\|$$

$$\begin{array}{c} | \dots | \\ h \\ e^{inx} \end{array}$$

derivatives have a nullspace

derivatives give rise to unbounded operators

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.



Q: Are these problems real?



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

$$i \left(\begin{array}{c} \xrightarrow{\quad} \\ \psi_j(x_i) \end{array} \right) \left(\begin{array}{c} \\ \\ \end{array} \right)$$

$$\left(\begin{array}{c} \psi_j'(x_i) \\ \\ \end{array} \right)$$

1	2
1	2

Sketch: How do IEs work? $\Delta u = 0$ $\int u = g$

fundamental solution $\Delta G = \alpha_j \delta(x - y_j)$
 $\Delta u = \rho \rightarrow G'$

$$E = -\nabla u \quad \text{div } E = \rho$$

$$u_n(x) = \sum_{i=1}^n G(x - y_i) \alpha_i$$

$$u(x) = \int_{\Gamma} G(x-y) \alpha(y) dy$$

layer potentials

~ and what's wrong with them?



Problems:

- Singular quadrature \rightarrow Yuck!

\hookrightarrow Near

- Dense matrices?

- Ill-conditioned \leftarrow

$\hookrightarrow \frac{1}{2} I + D$

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Bonus Advertising Goodie

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



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