Fast Algorithms

and
Integral Equation Methods

CS 598 APK - Fall 2017

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

`bit.ly/fastalg-f15`

contains:

- Class outline
- Assignments
- Virtual Machine Image
- Piazza
- Grading
- Video

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

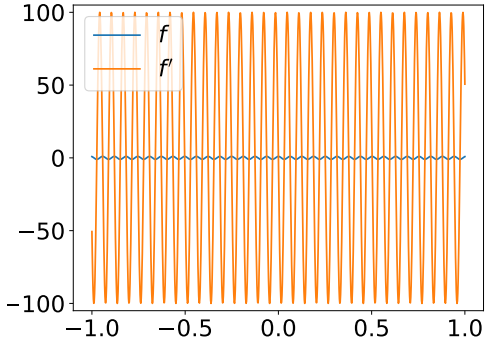
Idea of these methods:

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

So what's wrong with doing that?

- Differentiation is 'unbounded'. Example:

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



So a 'small' function can become an arbitrarily big function.

Does that matter?

- $\kappa(A) => A >> A^{-1} >$, and this increases $> A >$.
- Also, $> A^{-1} >$ doesn't exist for derivatives.

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

To be fair: Multigrid works around that

(by judiciously using *fewer* points!)

But there's another issue that's not fixable.

- Inherent tradeoff: FP accuracy $\leftrightarrow$ Truncation error

  Demo: Floating point vs Finite Differences

Q: Are these problems real?

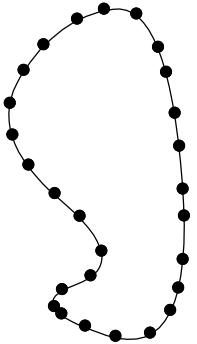
$\rightarrow$ Try solving 3D Poisson with just FEM+CG.

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

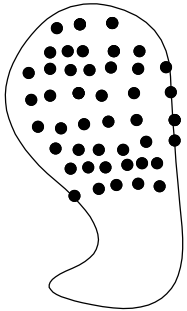
Bonus Advertising Goodie

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

But:



IE DOFs



FD/FEM DOFs

The number N is different! (And it's smaller for IEs.)

(Truth in advertising: Only for homogeneous problems.)

1 Dense Matrices and Computation

Matvec: A slow algorithm

Matrix-vector multiplication: our first 'slow' algorithm.

$O(N^2)$ complexity.

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

Assume A dense.

Matrices and Point Interactions

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

Does that actually change anything?

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

Technically: **no difference**.

Can **translate back and forth** between both views.

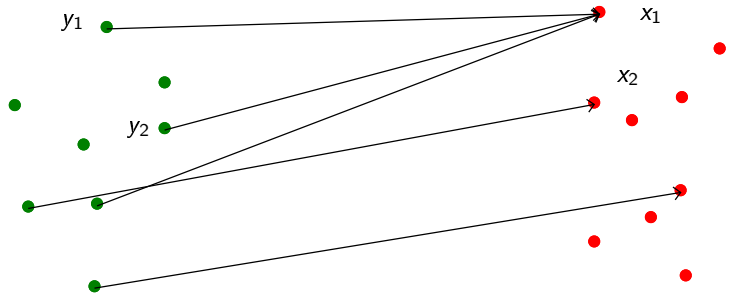
But: Gain **terminology** and **intuition**:

- x_i: "Targets"
- y_i: "Sources"
- G: "Kernel"

Matrices and Point Interactions

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

Graphically, too:



Each arrow corresponds to a matrix entry.

Matrices and point interactions

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

This *feels* different.

It's supposed to!

$G(x, y)$ defined for all $x \in \mathbb{R}^3$? **Possibly!** (Maybe also all $y \in \mathbb{R}^3$?)

In former case: ψ defined everywhere. ("Matrix infinitely tall")

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

Point interaction matrices: Examples

What kind of matrices, then?

- (Lagrange) Interpolation:

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

  Here: $G(x, y_j) = \ell_j(x)$

- Numerical Differentiation:

$$\psi(x) = \sum_{j=1}^{N} \ell_j'(x)\varphi(y_j)$$

- Numerical Integration:

$$\psi(x) = \sum_{j=1}^{N} \int_{a}^{x} \ell_j(\xi) d\xi \varphi(y_j)$$

- Equivalents of the above for other bases: e.g. Fourier
- Potential Evaluation:

Sidetrack: What is the potential of a single electron at the origin in 3D space?

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

(where q_{el} is the charge of the electron)

Sidetrack 2: What is the potential of a single electron at location y in 3D space?

$$U_y(x) = C \cdot \frac{1}{|x - y|}$$

So what's the potential of a number of electrons at a bunch of locations $y_1, \ldots, y_N$?

$$U(x) = \sum_{j=1}^{N} \frac{1}{|x - y_j|} \varphi(y_j)$$

You might feel like that sum wants to be an integral, to make things 'fair' between sources and targets. Hold on to that feeling.

- Convolutions:

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

Quiz: What do these do, visually?

Notice: Potential evaluation is actually an *example* of convolution.

Once again, infinitely many sources is a possibility–just make the sum an integral. So yes, there are indeed lots of these things.

Integral 'Operators'

Why did we go through the trouble of rephrasing matvecs as

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

- We're headed towards *Integral Operators* (or 'Integral Transforms') that look like this:

$$\psi(x) = \int_{\Omega} G(x, y)\varphi(y)\,\mathrm{d}y$$

- We'll rely on ψ being defined everywhere to derive some important properties that we can't 'see' if there are only finitely many targets.

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?

- **Idea 1:** Make sure G evaluates to mostly zeros.

  (i.e. make it sparse) $\rightarrow$ FEM/FD approach

  How? Limit 'domain of influence' of each source, e.g. by using piecewise interpolation.

  This is *not* the approach in this class though.

- **Idea 2:** If the matrix is very special (e.g. Toeplitz/circulant) or a DFT matrix, special cheaper techniques may exist (such as $O(n \log n)$ FFTs)
- **Idea 3:** If the matrix has low rank, the matvec can be made cheaper.

Fast Dense Matvecs

Consider

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

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

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

$$A = \mathbf{u}\mathbf{v}^T, \text{so}$$
$$A\mathbf{x} = (\mathbf{u}\mathbf{v}^T)\mathbf{x} = \mathbf{u}(\mathbf{v}^T\mathbf{x})$$

Cost: $O(N)$.

Q: What is the *row rank* of A? (# of lin.indep. rows)

Q: What is the *column rank* of A? (# of lin.indep. columns)

Remark: Row and column rank are always equal, not just here.

Fast Dense Matvecs

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

Does this generalize?

Q: What is K here? Rank.

Sure does generalize. Cost: $O(NK)$

What if matrix has 'full' rank? Cost back to $O(N^2)$

Low-Rank Point Interaction Matrices

What would this:

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

look like for a low-rank matrix?

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

Q: Did any of our examples look like this? Nope.

So let's check computationally.

Demo: Rank of a Potential Evaluation Matrix (Attempt 1)

So it looks like the rank *does* decay, at least to a good approximation.

Is echelon form the right way of capturing that?

Numerical Rank

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

First, what does *exact* rank mean?

$$A = UV,$$

with $U \in \mathbb{R}^{m \times k}$, $V \in \mathbb{R}^{k \times n}$.

Idea: Let's loosen that definition to a precision ε.

If $A \in \mathbb{R}^{m \times n}$:

$$\text{numrank}(A, \varepsilon) = \min\{k : \exists U \in \mathbb{R}^{m \times k}, V \in \mathbb{R}^{k \times n} : |A - UV|_2 \leqslant \varepsilon\}.$$

Q: That's great, but how do we find those matrices?

Eckart-Young-Mirsky Theorem

Oddly enough, with the help of the SVD:

Theorem 1 *(Eckart-Young-Mirsky) SVD $A = U\Sigma V^T$. If $k < r = \text{rank}(A)$ and*

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

then

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

Bonus 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.

Suppose we wanted to use this to make the matvec cheaper.

That wouldn't quite work:

We would need to build the entire matrix ($O(N^2)$), factorize it ($O(N^3)$), and then apply the low-rank-approximation ($O(N)$).

So we would need to make the *factorization* cheaper as well.

Big Q: Possible?

Representation

What does all this have to do with (right-)preconditioning?

Idea behind Right Preconditioning: Instead of

$$Ax = b$$

solve

$$AMy = b,$$

then find $x = My$.

What this does is change the *meaning* of the degrees of freedom in the linear system.

You could say: We change how we *represent* the solution.

Connection with what we've been doing:

- Assume $Ax = b$ is a big, bad problem
- Assume we can apply M cheaply

  (with the help of low-rank machinery)
- Or, even better, apply all of AM cheaply
- Assume M is tall and skinny
- Then solving $AMy = b$ is as good as solving $Ax = b$, but (ideally) lots cheaper
- These 'point interaction' matrices we've been discussing are the prototypes of such M matrices

  (Go from few points to all of $\mathbb{R}^3$)

2 Tools for Low-Rank Linear Algebra

Rephrasing Low-Rank Approximations

SVD answers low-rank-approximation ('LRA') question. But: too expensive.

First, rephrase the LRA problem:

Instead of the *factorization form*,

$$A \approx BC^T$$

we will ask for the *projection form* of LRA:

$$A \approx QQ^T A,$$

i.e. A being approximated by an orthogonal projection of its columns.

(Q has orthogonal columns, i.e. $Q^T Q = I$, and fewer of them than A)

Call the columns of Q the *LRA basis*.

If we have the projection form, can we find the factorization form?

Sure: Set $B = Q$ and $C = Q^T A$.

Using LRA bases

If we have an LRA basis Q, can we compute an SVD?

Sure:

1. $B = Q^T A$
2. Compute an SVD of B: $B = \bar{U}\Sigma V^T$
3. Set $U = Q\bar{U}$

Then:

$$A \approx QQ^T A = Q\bar{U}\Sigma V^T = U\Sigma V^T.$$

Cost:

- Assume A is $N \times N$, Q has k columns.
- Step 1: kN^2
- Step 2: kN^2
- Step 3: kN^2

Can we hope to do better overall?

Finding an LRA basis

How would we *find* an LRA basis?

Goal: Find Q columns so that

$$|A - QQ^T A|_2 \leqslant \varepsilon.$$

Question: Do we know the number of columns k of Q ahead of time?

- Yes: *'Fixed-rank approximation'*
- No: *'Adaptive LRA'*

Idea 1: SVD $\rightarrow$ First k columns of U in $A = U\Sigma V^T$ provide the *optimal answer*.

$\rightarrow$ You've got to be joking.

$\rightarrow$ Give up optimality, allow 'slack' in accuracy and column count.

Idea 2: Use a randomized algorithm, based on the same intuition as the power method.

Giving up optimality

What problem should we actually solve then?

Instead of

$$|A - QQ^T A|_2 = \min_{\text{rank}(X) \leqslant k} |A - X|_2 = \sigma_{k+1}$$

with Q having k columns,

we'll only go for

$$|A - QQ^T A|_2 \approx \min_{\text{rank}(X) \leqslant k} |A - X|_2$$

with Q having $k + p$ columns.

Recap: The Power Method

How did the power method work again?

A square, eigenvalues

$$|\lambda_1| \geqslant |\lambda_2| \geqslant \cdots \geqslant |\lambda_n| \geqslant 0.$$

with eigenvectors $\mathbf{v}_i$.

Goal: Find eigenvector to largest (by-magnitude) eigenvalue.

Start with random vector $\mathbf{x}$:

$$\mathbf{x} = \alpha_1 \mathbf{v}_1 + \cdots + \alpha_n \mathbf{v}_n.$$

Then

$$A\mathbf{x} = \alpha_1 \lambda_1 \mathbf{v}_1 + \cdots + \alpha_n \lambda_n \mathbf{v}_n.$$

Important observation: Matvecs with random vectors 'kill' the 'unimportant' bits of the range.

How do we cosntruct the LRA basis?

Put randomness to work:

Design a *randomized range finder*:

1. Draw an $n \times \ell$ *Gaussian* (iid) random matrix Ω
2. $Y = A\Omega$
3. Orthogonalize columns of Y, e.g. by QR factorization:

$$Y = \mathrm{QR}$$

$\rightarrow$ Q has ℓ orthogonal columns

Possible tweak: Kill the unimportant bits of the range faster, by inserting a few iterations of the power method into Step 2:

$$Y = (AA^T)^q A\Omega.$$

Q: Why multiply by (AA^T) and not just A?

$\rightarrow$Retains singular vectors!

$$AA^TA = (U\Sigma V^T)(V\Sigma U^T)(U\Sigma V^T).$$

But: singular values decay much faster:

$$\sigma_i(AA^TA) = \sigma_i(A)^3!$$

Q: What is one possible issue with the power method?

$\rightarrow$ Overflow/FP problems

Q: How are those problems usually controlled?

$\rightarrow$ Normalization, orthogonalization

$\rightarrow$ If FP is a concern, apply QR after every application of A or A^T.

Another neat idea:

Assumptions on Ω are pretty weak–can use more or less anything we want. $\rightarrow$ Make it so that we can apply the matvec $A\Omega$ in $O(n \log \ell)$ time. How? Pick Ω as a carefully-chosen subsampling of the Fourier transform.

Q: How well does this have a right to work?

Errors in Random Approximations

If we use the randomized range finder, how close do we get to the optimal answer?

Theorem 2 *For an $m \times n$ matrix A, a target rank $k \geqslant 2$ and an oversampling parameter $p \geqslant 2$ with $k + p \leqslant \min(m, n)$, with probability $1 - 6 \cdot p^{-p}$,*

$$\left| A - QQ^T A \right|_2 \leqslant \left(1 + 11\sqrt{k+p}\sqrt{\min(m,n)} \right) \sigma_{k+1}.$$

(given a few more very mild assumptions on p)

[Halko/Tropp/Martinsson '10, 10.3]

Message: We can *probably* (!) get away with oversampling parameters as small as $p = 5$.

A-posteriori and Adaptivity

The result on the previous slide was *a-priori*. Once we're done, can we find out 'how well it turned out'?

Sure: Just consider the error:

$$A - QQ^T A$$

Realize that what this does is instead of projecting onto the columns of Q, it projects onto their orthogonal complement:

$$E = (I - QQ^T)A$$

Idea: Use a randomized technique as well.

- We are interested in $|E|_2 = \sigma_1(E)$
- If the previous techniques work,

  $|E\omega|_2$ for a randomly drawn Gaussian vector ω should give us a pretty good idea of $|E|_2$.

Realize that that's all we need to make the fixed-rank algorithm adaptive:

- Compute small-ish fixed rank LRA
- Check error
- Too big? Throw in a few more vectors, repeat

Next, realize that the error estimator relies on the same thing as the range finder, multiplication by random vector: Not hard to modify algorithm to make both use the same data!

Demo: Randomized SVD

Rank-revealing/pivoted QR

Sometimes the SVD is too *good* (aka expensive)–we may need less accuracy/weaker promises, for a significant decrease in cost.

This is where *RRQR* or *pivoted QR* comes in.

For $A \in \mathbb{R}^{m \times n}$,

$$A\Pi = \mathrm{QR} = Q \begin{pmatrix} R_{11} & R_{12} \\ & R_{22} \end{pmatrix},$$

where

- $R_{11} \in \mathbb{R}^{k \times k}$,
- $|R_{22}|_2$ is (hopefully) 'small'.
- $Q \in \mathbb{R}^{m \times n}$ with $Q^T Q = I$
- It is possible to skip computing the right half of R

  (and the corresponding bits of Q)

- Π is an $n \times n$ permutation matrix

Given a RRQR factorization, we know

- $\sigma_{k+1} \leqslant |R_{22}|_2$ (i.e. it can't do better than an SVD)
- To precision $|R_{22}|_2$, A has *at most* numerical rank k.

(see e.g. Golub and Van Loan, ch. 5)

Demo: Rank-revealing QR

Stop and think:

- RRQR delivers essentially the same service as what we've been devloping: Find an orthogonal basis of the range.
- But: an $O(N^3)$ factorization.

Interpolative Decomposition (ID)

Sometimes it would be helpful to know *which columns of A* contribute the most to the rank.
(rather than have the waters muddied by an orthogonal transformation like in QR)

For a rank-k matrix A, the *Interpolative Decomposition* provides this:

$$A_{m\times n} = A_{(:,J)} P_{k\times n},$$

where

- J is an index set of length k representing column selection,
- k columns of P contain only a single entry of 1, and
- P is well-conditioned.

  In particular, the magnitude of its entries is bounded by 2.

How do we construct this (starting from RRQR):

$$A\Pi = Q \begin{pmatrix} R_{11} & R_{12} \end{pmatrix}$$

Set $B = QR_{11}$.

Q: What is B, in terms of the RRQR?

Next, set

$$P = \begin{pmatrix} \mathrm{Id} & R_{11}^{-1} R_{12} \end{pmatrix} \Pi^T,$$

then

$$\begin{aligned} BP &= QR_{11} \begin{pmatrix} \mathrm{Id} & R_{11}^{-1} R_{12} \end{pmatrix} \Pi^T \\ &= Q \begin{pmatrix} R_{11} & R_{12} \end{pmatrix} \Pi^T \\ BP\Pi &= Q \begin{pmatrix} R_{11} & R_{12} \end{pmatrix} \\ A\Pi &= Q \begin{pmatrix} R_{11} & R_{12} \end{pmatrix}. \end{aligned}$$

Remarks:

- Earlier, we've used

  $$A \approx QQ^T A$$

  as our LRA. We can simplify that with the ID. Compute the row (i.e. transpose) ID of Q:

  $$Q = PQ_{(J,:)},$$

so

$$A_{(J,:)} \approx P Q_{(J,:)} Q^T A.$$

So

$$A \approx P A_{(J,:)}.$$

[Martinsson, Rokhlin, Tygert '06]

Demo: Interpolative Decomposition

What does the ID buy us?

Specifically: Name a property that the ID has that other factorizations do not have.

It preserves (a subset of) matrix entries exactly.

As a result, composing it with other transforms can often be done without having to perform (expensive!) matrix-matrix multiplications.

All our randomized tools have two stages:

1. Find ONB of approximate range
2. Do actual work only on approximate range

   First step of this: $C = Q^T A \to O(N^2 k)$.

For now, both stages are $O(N^2 k)$.

The ID helps squeeze stage 2 down to $O(Nk^2)$.

How?

- Approximate range still has N rows.
- Of which only k contribute to the rank.
- The rest of them are just 'along for the ride'.
- **So:** Use ID to pick subset of rows

  $\rightarrow$ and do actual work on

  - the rows that matter (k of them) of
  - the approximate range (k columns)

ID Q vs ID A

What does row selection mean for the LRA?

Starting point: At end of stage 1, have LRA

$$A \approx QQ^T A.$$

If we then run an ID on the *rows* (i.e. a *transpose ID* if you want) of Q:

$$Q \approx PQ_{(J,:)}$$

(Recall: Q is tall and skiny. $Q_{(J,:)}$ is a square subset.)

we get:

$$A \approx PQ_{(J,:)}Q^T A.$$

Consequence:

$$\begin{aligned} A_{(J,:)} &\approx \underbrace{P_{(J,:)}}_{\text{Id}} Q_{(J,:)}Q^T A \\ &= Q_{(J,:)}Q^T A \end{aligned}$$

Consider

$$\begin{aligned} & PA_{(J,:)} \\ = \; & PQ_{(J,:)}Q^T A \\ \approx \; & QQ^T A \\ \approx \; & A \end{aligned}$$

I.e.: Use the row extraction directly on A, forget about Q.

In practice: Run ID on sample matrix $Y = A\Omega$.

Remark: There is a (slight) trade-off here:

- Notice: Two '$\approx$' above!
- ID not as accurate as SVD
- BUT: *Much* faster

Leveraging the ID

Build a low-rank SVD with row extraction.

1. Obtain the row subset J and upsampler $\underset{N\times k}{P}$.

   (via Q or directly from Y)

2. Compute row QR of remaining rows:

$$\underset{N\times k}{(A_{(J,:)})^T} = \underset{N\times k}{\bar{Q}}\,\underset{k\times k}{\bar{R}}$$

3. Upsample the row coefficients $\bar{R}^T$:

$$\underset{N\times k}{Z} = \underset{N\times k}{P}\,\underset{k\times k}{\bar{R}^T}$$

4. SVD the result:

$$Z = U\Sigma\tilde{V}^T$$

5. Then

$$
\begin{aligned}
& \underset{N\times k}{U}\ \underset{k\times k}{\Sigma}\left(\underset{N\times k}{\bar{Q}}\ \underset{k\times k}{\tilde{V}}\right)^T \\
= \;& U\Sigma\tilde{V}^T\bar{Q}^T \\
= \;& Z\bar{Q}^T \\
= \;& P\bar{R}^T\bar{Q}^T \\
= \;& PA_{(J,:)} \\
\approx \;& A.
\end{aligned}
$$

Q: Why did we need to do the row QR?

Because otherwise we wouldn't have gotten a 'real' SVD:

$$
\begin{aligned}
A_{(J,:)} &= U\Sigma V^T \\
PA_{(J,:)} &= \underbrace{PU}_{\text{orth?}}\Sigma V^T
\end{aligned}
$$

$\rightarrow$ So 'hide' P in matrix being SVD'd–but: can't do full reconstruction. Use (small)R in QR as a proxy!

Cost: Finally $O(Nk^2)$!

Putting all this together in one code: $\rightarrow$ HW exercise :)

Where are we now?

- We have observed that we can make matvecs faster if the matrix has low-ish numerical rank
- In particular, it seems as though if a matrix has low rank, there is no end to the shenanigans we can play.
- We have observed that some matrices we are interested in (in some cases) have low numerical rank (cf. the point potential example)
- We have developed a toolset that lets us obtain LRAs without having to compute $O(N^3)$ factorizations (!)

Next stop: Get some insight into *why* these matrices have low rank in the first place, to perhaps help improve our machinery even further.

3 Rank and Smoothness

Punchline

What do (numerical) rank and smoothness have to do with each other?

If the result of a (continuous) operation is smooth, its result can be represented with a short expansion in a function basis.

What kind of basis?

- Polynomials (orthogonal, or monomials if you must),
- Sines/Cosines,
- Eigenfunctions of Sturm-Liouville operators, ...
- It mostly doesn't matter.

Even shorter punchline:

Smooth functions are boring.

(But useful!)

If the operations you are considering are *smoothing*, you can expect to get a lot of mileage out of low-rank machinery.

What types of operations are smoothing?

- Derivatives: nope. Make a function 'rougher'.
  (Consider the idea of a function 'having n derivatives' as a measure of how smooth it is, i.e. the C^n function spaces.)
- Integrals: yep.

This provides a good computational justification to try and use integral operators as a tool to construct numerical methods.

Now: Consider some examples of smoothness, with justification.

How do we judge smoothness? *Decay of Taylor remainders.*

Recap: Multivariate Taylor

How does Taylor's theorem get generalized to multiple dimensions?

1D Taylor:

$$f(c+h) \approx \sum_{p=1}^{k} \frac{f^{(p)}(x)}{p!} h^p$$

Notational tool: *Multi-Index* in n dimensions

$$\begin{aligned} p &= (p_1, p_2, \ldots, p_n), \quad (\text{all} \geqslant 0) \\ |p| &= p_1 + \cdots + p_n, \\ p! &= p_1! \cdot \cdots \cdot p_n!, \\ \mathbf{x}^p &= x_1^{p_1} \cdot \cdots \cdot x_n^{p_n} \\ D^p f &= \frac{\partial^{|p|} f}{\partial x_1^{p_1} \cdot \cdots \cdot \partial x_n^{p_n}}. \end{aligned}$$

With that: For f scalar,

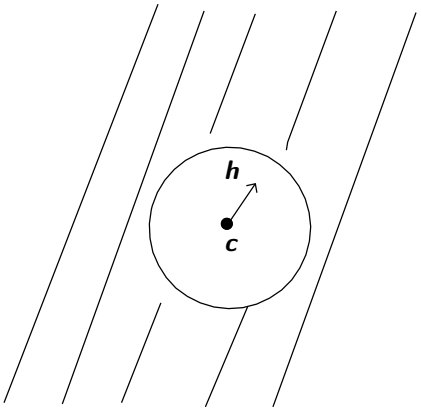
$$f(\mathbf{c}+\mathbf{h}) \approx \sum_{|p|\leqslant k} \frac{D^p f(\mathbf{c})}{p!}\mathbf{h}^p$$

(Taylor remainder: analogous to 1D)

Connect Taylor and Low Rank

Can Taylor help us establish low rank of an interaction?

Taylor makes a statement about evaluating a function in a vicinity:



$$\begin{aligned} f(\mathbf{x}) = f(\mathbf{c}+\mathbf{h}) &= \sum_{|p|\leqslant k} \frac{D^p f(\mathbf{c})}{p!}\mathbf{h}^p \\ &= \sum_{|p|\leqslant k} (\text{coeff}_p) G(\mathbf{x}, p) \end{aligned}$$

So if we can Taylor expand with a small remainder and a short expansion ($O(1)$ coefficients), then yes, we have every reason to expect low rank!

Taylor on Potentials

Compute a Taylor expansion of a 2D Laplace point potential.

$$\begin{aligned}\psi(x) &= \sum_{i=1}^{n} G(x, y_j)\varphi(y_j) \\ &= \sum_{i=1}^{n} \log\left(\|x - y\|_2\right)\varphi(y_j)\end{aligned}$$

Since this is a superposition anyway: Just consider a single source.

$$\psi(x) = \log\left(\|x - y\|_2\right)$$

Pick an expansion center $\mathbf{c}$. WLOG, $\mathbf{c} = \mathbf{0}$.

$$\psi(\mathbf{h}) \approx \sum_{|p| \leqslant k} \frac{D^p \psi(\mathbf{0})}{p!} \mathbf{h}^p$$

```
Maxima 5.36.1 http://maxima.sourceforge.net
(%i 2)  phi0:  log(sqrt(y1**2 + y2**2));
```

$$(\%o2)\quad \frac{\log(y2^2+y1^2)}{2}$$

```
(%i 4)  diff(phi0, y1);
```

$$(\%o4)\quad \frac{y1}{y2^2+y1^2}$$

```
(%i 5)  diff(phi0, y1, 5);
```

$$(\%o5)\quad \frac{120y1}{(y2^2+y1^2)^3}-\frac{480y1^3}{(y2^2+y1^2)^4}+\frac{384y1^5}{(y2^2+y1^2)^5}$$

```
(%i 6)  diff(phi0, y1, 7);
```

$$(\%o6)\quad -\frac{5040y1}{(y2^2+y1^2)^4}+\frac{40320y1^3}{(y2^2+y1^2)^5}-\frac{80640y1^5}{(y2^2+y1^2)^6}+\frac{46080y1^7}{(y2^2+y1^2)^7}$$

```
(%i 7)
```

Which of these is the most dangerous (largest) term?

$\rightarrow$ The first one.

What's a bound on it? Let $R = \sqrt{y_1^2 + y_2^2}$.

$$\left| \frac{5040\mathrm{y1}}{(\mathrm{y2}^2 + \mathrm{y1}^2)^4} \right| \leqslant C \left| \frac{y_1}{R^8} \right| \leqslant C \frac{1}{R^7}.$$

'Generalize' this bound:

$$|D^p \psi| \leqslant C_p \begin{cases} \log(R) & |p| = 0 \\ R^{-|p|} & |p| > 0 \end{cases}.$$

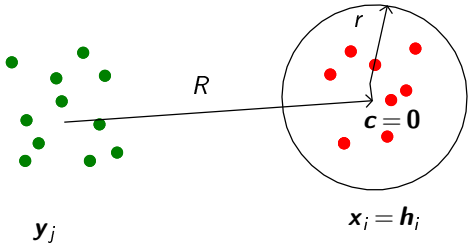
Appears true at least from the few p we tried. (Actually is true.)

C_p is a 'generic constant'–its value could change from one time it's written to the next.

What does this mean for the convergence of the Taylor series as a whole?

$\rightarrow$ Need to estimate each term. Recall that $\mathbf{h}$ is the vector from $\mathbf{c}$ to the target (aka point where we evaluate) $\mathbf{x}$. (Assume $|p| > 0$ to keep it simple.)

$$\left| \frac{D^p \psi(\mathbf{0})}{p!} \mathbf{h}^p \right|_2 \leqslant C_p |D^p \psi(\mathbf{0}) \mathbf{h}^p|_2 \leqslant C_p \left(\frac{|\mathbf{h}|}{R} \right)^p.$$



Lesson: As long as

$$\frac{\max_i |\mathbf{x}_i - \mathbf{c}|_2}{\min_j |\mathbf{y}_j - \mathbf{c}|_2} = \frac{r}{R} < 1,$$

the Taylor series converges.

A few remarks:

- We have just invented one specific example of what we will call a *local expansion* (of a potential ψ).
- The abstract idea of a *local expansion* is that:
  - it converges on the interior of a ball as long as the closest source is outside that ball,

– The error in approximating the potential by a truncated (at order k) local expansion is

$$C_p \left(\frac{r}{R}\right)^{k+1} = \left(\frac{\text{dist}(\mathbf{c}, \text{ furthest target})}{\text{dist}(\mathbf{c}, \text{ closest source})}\right)^{k+1}$$

- Connect this to the numerical rank observations:

> We have just shown that point→point potential interactions have low numerical rank!

Specifically, to precision

$$C_p \left(\frac{r}{R}\right)^{k+1}$$

the interaction from sources to targets has a numerical rank of at most

$$\text{(however many terms are in the Taylor sum)},$$

aka

$$\frac{(k+1)(k+2)}{2} = O(k^2)$$

in 2D, and

$$\frac{(k+1)(k+2)(k+3)}{2 \cdot 3} = O(k^3)$$

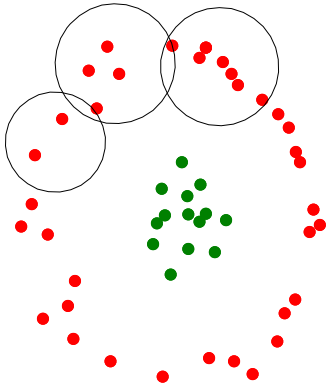
in 3D.

- Low numerical rank is no longer a numerically observed oddity, it's mathematical fact.

> Away from the sources, point potentials are smooth enough that their Taylor series ('local expansions') decay quickly. As a result, the potential is well-approximated by truncating those expansions, leading to low rank.

Local expansions as a Computational Tool

Low rank makes evaluating interactions cheap(er). Do local expansions help with that goal?



No, not really. In a roughly uniform target distribution with $O(N)$ targets, we need $O(N)$ local expansion $\rightarrow$ nothing saved really.

Taylor on Potentials, Again

Stare at that Taylor formula again.

$$\psi(\mathbf{x}-\mathbf{y}) \approx \sum_{|p|\leqslant k} \underbrace{\frac{D_{\mathbf{x}}^p \psi(\mathbf{x}-\mathbf{y})|_{\mathbf{x}=\mathbf{c}}}{p!}}_{\text{depends on src/ctr}} \underbrace{(\mathbf{x}-\mathbf{c})^p}_{\text{dep. on ctr/tgt}}$$

Recall:

- $\mathbf{x}$: targets
- $\mathbf{y}$: sources

At least formally, nothing goes wrong if I swap the roles of $\mathbf{x}$ and $\mathbf{y}$ in the Taylor expansion:

$$\psi(\mathbf{x}-\mathbf{y}) \approx \sum_{|p|\leqslant k} \underbrace{\frac{D_{\mathbf{y}}^p \psi(\mathbf{x}-\mathbf{y})|_{\mathbf{y}=\mathbf{c}}}{p!}}_{\text{depends on ctr/tgt}} \underbrace{(\mathbf{y}-\mathbf{c})^p}_{\text{dep. on src/ctr}} .$$

In comparison to the local expansion above, we will call this (and other expansions like it) a *multipole expansion*.

At first sight, it doesn't look like much happened, but mathematically/geometrically, this is a very different animal.

First Q: When does this expansion converge?

The analysis is the same as earlier:

$$(*) = \left| \frac{D_{\mathbf{y}}^p \psi(\mathbf{x}-\mathbf{y})|_{\mathbf{y}=\mathbf{c}}}{p!}(\mathbf{y}-\mathbf{c})^p \right| \leqslant C_p \frac{\|\mathbf{y}-\mathbf{c}\|_2^p}{\|\mathbf{x}-\mathbf{c}\|_2^p} = C_p \left(\frac{\|\mathbf{y}-\mathbf{c}\|_2}{\|\mathbf{x}-\mathbf{c}\|_2} \right)^p$$

(just with the roles of $\mathbf{x}$ and $\mathbf{y}$ reversed). If we admit multiple sources/targets, we get

$$(*) \leqslant C_p \left(\frac{\max_j \|\mathbf{y}_i - \mathbf{c}\|_2}{\min_i \|\mathbf{x}_i - \mathbf{c}\|_2} \right)^p.$$

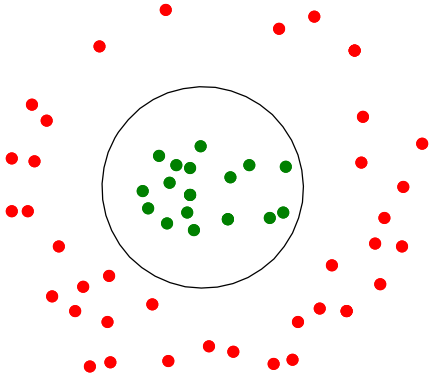
The abstract idea of a *multipole expansion* is that:

- it converges on the **ex**terior of a ball as long as the furthest source is closer to the center than the closest target,

- The error in approximating the potential by a truncated (at order k) local expansion is

$$\left(\frac{\text{dist}(\mathbf{c},\ \text{furthest source})}{\text{dist}(\mathbf{c},\ \text{closest target})} \right)^{k+1}.$$

Geometrically:



The multipole expansion converges everywhere outside the circle!

(Possibly: slowly, if the targets are too close–but it does!)

If our particle distribution is like in the figure, then a multipole expansion is a computa-

tionally useful thing. If we set

- $S = \#\text{sources}$,
- $T = \#\text{targets}$,
- $K = \#\text{terms in expansion}$,

then the cost *without* the expansion is $O(ST)$,

whereas the cost *with* the expansion is $O(SK + KT)$.

If $K \ll S, T$, then that's going from $O(N^2)$ to $O(N)$.

The rank (#terms) of the multipole expansion is the same as above for the local expansion.

Demo: Multipole/local expansions

On Rank Estimates

So how many terms do we need for a given precision ε?

$$\varepsilon \approx \left(\frac{\text{dist}(\mathbf{c}, \text{furthest target})}{\text{dist}(\mathbf{c}, \text{closest source})} \right)^{k+1} = \rho^{k+1}$$

Want to relate this to K (#terms = rank). Take (2D) $K \approx k^2$, i.e. $k \approx \sqrt{K}$, so $\varepsilon \approx \rho^{\sqrt{K}+1}$ or

$$\begin{aligned} \log \varepsilon &\approx \left(\sqrt{K} + 1\right) \log \rho \\ \sqrt{K} + 1 &\approx \frac{\log \varepsilon}{\log \rho} \\ K &\approx \left(\frac{\log \varepsilon}{\log \rho} - 1 \right)^2 . \end{aligned}$$

Demo: Checking rank estimates

Estimated vs Actual Rank

Our rank estimate was off by a power of $\log \varepsilon$. What gives?

Possible reasons:

- Maybe by some happy accident some of the Taylor coefficients are zero?

  $\rightarrow$ No, doesn't look like it.

- The Taylor basis uses $O(\log(\varepsilon)^2)$ terms.

  That's just an existence proof of an expansion with that error.

  Maybe a better basis exists?

Look at $\partial_x^2 G$ and $\partial_y^2 G$ in the multipole demo again. Notice anything?

How does that relate to $\Delta G = 0$?

- $\partial_x G = -\partial_y^2 G$ means that we can reduce from $O(p^2)$ to $O(p)$ *actually* distinct terms $\rightarrow$ problem solved: same value of expansion (i.e. same accuracy), many fewer terms

- Alternatively: be clever

Being Clever about Expansions

How could one be clever about expansions? (i.e. give examples)

- Realize that in 2D, harmonic functions ($\Delta u = 0$) map one-to-one to complex-analytic ones.

  Then, use complex-valued Taylor, reduces number of terms from $O(p^2)$ to $O(p)$

- Use DLMF:

  Example: Helmholtz kernel $(\Delta + \kappa^2)u = 0$

  Fundamental solutions:

  - Bessel functions $J_\ell(\kappa r)$
  - Hankel functions of the first kind $H_\ell^{(1)}(\kappa r)$

Aside: How do those come about?
- Transform Helmholtz PDE to polar coordinates
- Obtain the Bessel ODE (in r)
- Solve resulting 1D BVP (in r)

DLMF 10.23.6 shows 'Graf's addition theorem':

$$H_0^{(1)}\left(\kappa \left\|x-y\right\|_2\right) = \tag{1}$$

$$\sum_{\ell=-\infty}^{\infty} \underbrace{H_\ell^{(1)}\left(\kappa \left\|y-c\right\|_2\right) e^{i\ell\theta'}}_{\text{singular}} \underbrace{J_\ell\left(\kappa \left\|x-c\right\|_2\right) e^{-i\ell\theta}}_{\text{nonsingular}} \tag{2}$$

where $\theta = \angle(x-c)$ and $\theta' = \angle(x'-c)$.

Can apply same family of tricks as with Taylor to derive multipole/local expansions.

- 3D: Spherical harmonics, ...

Making Multipole/Local Expansions using Linear Algebra

Actual expansions seem vastly cheaper than LA approaches. Can this be fixed?

Compare costs for this situation:

- S sources
- T targets
- Actual interaction rank: $K \ll \min(S, T)$.

Cost for expansions:

- Compute expansion coefficients: $O(KS)$
- Evaluate expansion coefficients: $O(KT)$

Overall: $O(k(S + T))$: Cheap!

Cost for linear algebra:

- Build matrix: $O(ST)$

- ...

Oops. Can't be competitive, can it?

Idea: *Skeletonization using Proxies*

Demo: Skeletonization using Proxies

Q: What error do we expect from the proxy-based multipole/local 'expansions'?

- Function expansions give an indication of what is doable at a certain rank
- Linear algebra should match or beat that

Confirmation of this: $\rightarrow$ HW

Why Does the Proxy Trick Work?

> In particular, how general is this? Does this work for any kernel?

No. There are two (kernel-specific) miracles here:

- We can *represent* the far field of many sources in terms of the far field of a few–and that apparently regardless of what the targets are.

  (intuitively 'plausible', rigorously due to Green's formula $\rightarrow$ later)

- We only get a '*surface*' of sources because 'surface data' is enough to reconstruct '*volume*' data.

  This works because an (interior or exterior) Laplace potential is fully determined by its values on a boundary. (This is a fact that we will prove later, but if you believe that Laplace boundary value problems are solvable, you're already believing this.)

Remark: In both cases (Lin Alg and expansions), it's the PDE that provides the cost reduction from $O(k^d)$ ('volume') to $O(k^{d-1})$ ('surface')!

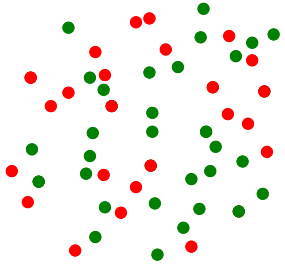
Where are we now?

- We know that far interactions with a smooth kernel have low rank. (Because: Short Taylor expansion suffices)
- If
$$\psi(\mathbf{x}) = \sum_j G(\mathbf{x}, \mathbf{y}_j)\varphi(\mathbf{y}_j)$$
satisfies a PDE (e.g. Laplace), i.e. if
$$G(\mathbf{x}, \mathbf{y}_j)$$
satisfies a PDE, then that low rank is *even* lower.
- Can construct interior ('local') and exterior ('multipole') expansions (using Taylor or other tools).
- Can lower the number of terms using the PDE.
- Can construct LinAlg-workalikes for interior ('local') and exterior ('multipole') expansions.

- Can make those cheap using proxy points.

So we can compute interactions where sources are distant from targets (i.e. where the interaction is low rank) quite quickly.

Problem: In general, that's not the situation that we're in.



(In general, it's more source-and-target soup.)

But: *Most* of the targets are far away from *most* of the sources.

($\Leftrightarrow$ Only a few sources are close to a chosen 'close-knit' group of targets.)

So maybe we can do business yet–we just need to split out the near interactions to get

a hold of the far ones (which (a) constitute the bulk of the work and (b) can be made cheap as we saw.)

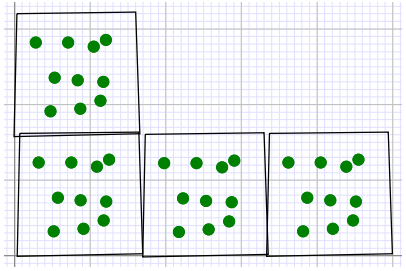
4 Near and Far: Separating out High-Rank Interactions

Simple and Periodic: Ewald Summation

Want to evaluate potential from an infinite periodic grid of sources:

$$\psi(\mathbf{x}) = \sum_{\mathbf{i} \in \mathbb{Z}^d} \sum_{j=1}^{N_{\text{src}}} G(\mathbf{x}, \mathbf{y}_j + \mathbf{i}) \varphi(\mathbf{y}_j)$$

'Potential' ψ is periodic as well ($\rightarrow$ just need values in one unit cell).



Q: When does this have a right to converge?

- $G = O(1)$ throghout obviously won't work

  $\rightarrow$ there must be some sort of fall-off

- $G = O\left(\|\mathbf{x}\|_2^{-p}\right)$. Now think in spherical shells:

$$\psi(\mathbf{0}) = \sum_{i=0}^{\infty} \sum_{\text{cells@}\ell^2 \text{ dist } [i,i+1) \text{ to } \mathbf{0}} \underbrace{O(i^{d-1})}_{\text{surface of shell}\sim\#\text{ cells}} \quad O(i^{-p})$$

  where d is space dimension. Have:

$$d - 1 - p < -1 \quad \Leftrightarrow \quad p > d.$$

  (because $\sum 1/n$ is diverges)

Ingredients:

- Use unit cells to separate near/far.

  But that's imperfect: Sources can still get arbitrarily close to targets.

- Use Fourier transform to compute far contribution.

  But that's also imperfect:

  - Fourier can only sum the *entire* (periodic) potential

    So: Cannot make exception for near-field

  - G non-smooth is the interesting case $\rightarrow$ Long Fourier series $\rightarrow$ expensive (if convergent at all)

Idea: Only operate on the smooth ('far') parts of G.

How? Split G into two parts with a *screen* σ that 'bleeps out' the singularity:

$$G(\mathbf{x}) = \sigma(\mathbf{x})G(\mathbf{x}) + (1 - \sigma(\mathbf{x}))G(\mathbf{x}).$$

How does that help? Consider $G = 1/r^4$.

$$G(\mathbf{x}) = \underbrace{\sigma(\mathbf{x})\frac{1}{\|\mathbf{x}\|_2^4}}_{G_{\text{LR}}} + \underbrace{(1 - \sigma(\mathbf{x}))\frac{1}{\|\mathbf{x}\|_2^4}}_{G_{\text{SR}}}$$

Then, if

- σ is smooth
- $\sigma(\mathbf{x}) = O\left(\|\mathbf{x}\|_2^4\right)$
- $1 - \sigma$ has bounded support (i.e. $\sigma(\mathbf{x}) = 1$ if $\|\mathbf{x}\|_2 > R$ for some R)

we can split the computation (from the perspective of a unit cell target) as follows:

	G_{SR}	G_{LR}
Close source	A: singular sum directly (few)	B: smooth use Fourier ($*$)
Far source	0	C: smooth use Fourier ($*$)

(where 'close' means 's $\rightarrow$ t distance $< R$' and 'far' the opposite)

The interesting part is now just how to obtain a sum G_{LR}. Let's consider that in 1D for simplicity.

Recall: Convolution

$$(f * g)(x) = \int_{\mathbb{R}} f(\xi) - g(x - \xi) d\xi.$$

The above sum then:

$$\psi = (x \mapsto G(x, 0)) * \left(x \mapsto \sum_{i \in \mathbb{Z}} \sum_{j=1}^{N_{\text{src}}} \delta(x - y_j - i) \right)$$

with the convention

$$f(x) = f * (\xi \mapsto \delta(\xi - x)).$$

Convolution is linear (in both arguments) and turns into multiplication under Fourier transforms:

$$\mathcal{F}\{f * g\} = \mathcal{F}f \cdot \mathcal{F}g,$$

possibly with a constant depending on normalization. Also:

$$\mathcal{F}\left\{\sum_{i\in\mathbb{Z}} \delta(x - i)\right\}(\omega) = \sum_{i\in\mathbb{Z}} \delta(\omega - i).$$

So

$$\begin{aligned}
&\mathcal{F}\{\psi\} - \mathcal{F}\{\psi_{\mathsf{SR}}\} = \mathcal{F}\{\psi_{\mathsf{LR}}\} \\
= \;& \mathcal{F}\{G_{\mathsf{LR}}\}\mathcal{F}\left\{ x \mapsto \sum_{i\in\mathbb{Z}} \sum_{j=1}^{N_{\mathsf{src}}} \delta(x - y_j - i) \right\} \\
= \;& \mathcal{F}\{G_{\mathsf{LR}}\}\left(\sum_{j=1}^{N_{\mathsf{src}}} e^{-2\pi i y_j \omega} \cdot \mathcal{F}\left\{ x \mapsto \sum_{i\in\mathbb{Z}} \delta(x - i) \right\} \right) \\
= \;& \mathcal{F}\{G_{\mathsf{LR}}\}\left(\sum_{j=1}^{N_{\mathsf{src}}} e^{-2\pi i y_j \omega} \cdot \left(\omega \mapsto \sum_{i\in\mathbb{Z}} \delta(\omega - i) \right) \right)
\end{aligned}$$

Now, since G_{LR} is smooth, $\mathcal{F}\{G_{\mathsf{LR}}\}(\omega)$ should fall off quickly as $|\omega|$ increases. $\rightarrow$ Well-approximated with finitely many terms of the sum over i. (Again: Smooth function leads to low rank!)

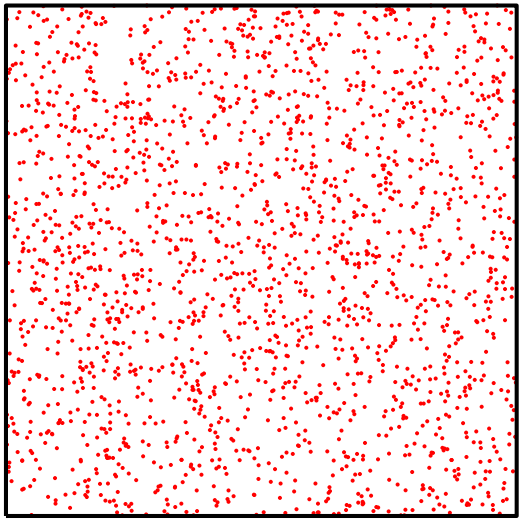
In practice: Fourier transforms carried out discretely, using FFT.

- Additional error contributions from interpolation

(small if screen smooth enough to be well-sampled by mesh)

- $O(N \log N)$ cost (from FFT)
- Need to choose evaluation grid ('mesh')
- Resulting method called Particle-Mesh-Ewald ('PME')

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

Want: All-pairs interaction.
Caution: In these (stolen) figures: targets sources.
Here: targets and sources.

Specifically, want

$$\mathbf{u} = A\mathbf{q}$$

where

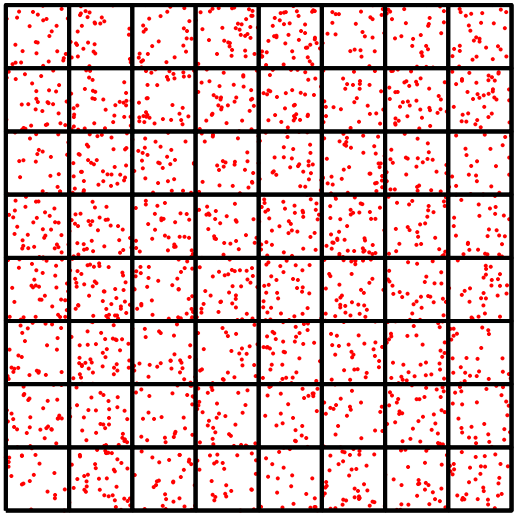
$$A_{ij} = \log(\mathbf{x_i} - \mathbf{x_j}).$$

Idea: We have all this multipole technology, but no way to use it:

No targets are cleanly separated from other sources.

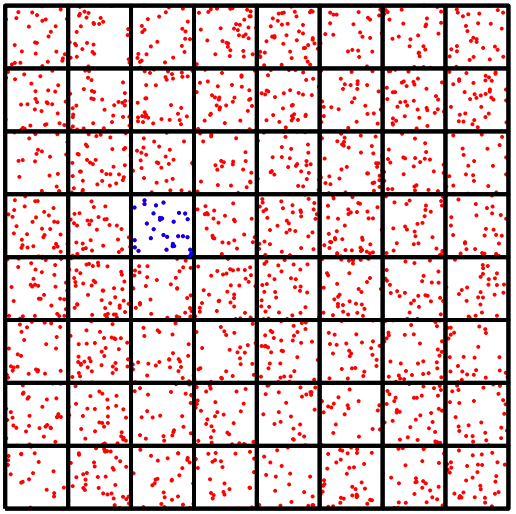
Lesson from PME: If you can't compute the entire interaction, compute parts of it. To help do so, put down a grid.

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

Barnes-Hut: Putting Multipole Expansions to Work



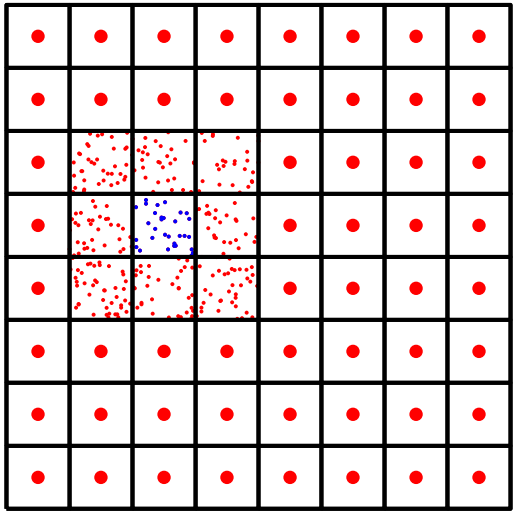
(Figure credit: G. Martinsson, Boulder)

For sake of discussion, choose one 'box' as targets.

Q: For which boxes can we then use multipole expansions?

A: Depends on the wanted accuracy!

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

With this computational outline, what's the accuracy?

$$\begin{aligned}
\varepsilon &\sim \left(\frac{d\left(\text{box ctr}, \text{furthest src}\right)}{d\left(\text{box ctr}, \text{closest tgt}\right)} \right)^{k+1} \\
&= \left(\frac{\text{box 'radius'} \cdot \sqrt{2}}{\text{box 'radius'} \cdot 3} \right)^{k+1} \\
&= \left(\frac{\sqrt{2}}{3} \right)^{k+1}
\end{aligned}$$

Observation: Dependent on space dimension!

Q: Does this get better or worse as dimension increases?

Barnes-Hut (single-level): Computational Cost

What's the cost of this algorithm?

Let:

- N be #particles
- K be #terms in expansion
- m be #particles/box.
- Assume $m \sim \sqrt{N}$ or $N \sim m^2$.

  Q: Where does this assumption come from?

	How often	**Individual cos**
Compute mpoles	N/m boxes	Km
Evaluate mpoles	N tgt particles $\cdot$ N/m src boxes	K
9 close boxes	$9\cdot(N/m$ boxes)	Km^2

Forget K (small, constant). Only mpole eval matters:

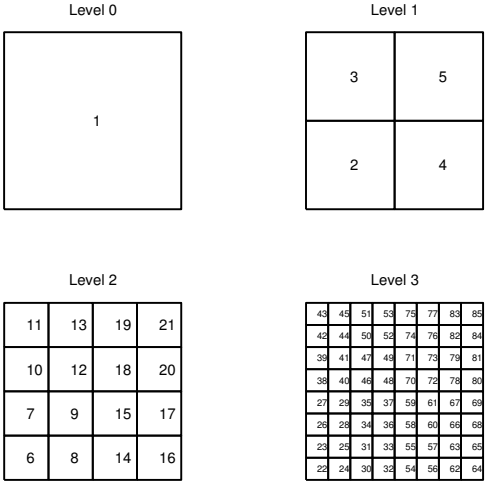
$$\text{cost} \sim \frac{N^2}{m} \sim N^{1.5}.$$

Observations: There are very many (very) far box-box interactions.

Idea: Summarize further $\rightarrow$ bigger boxes $\rightarrow$ 'larger' multipoles representing more sources.

Idea: To facilitate this 'clumping', don't use a *grid* of boxes, instead make a *tree*.

Barnes-Hut: Putting Multipole Expansions to Work



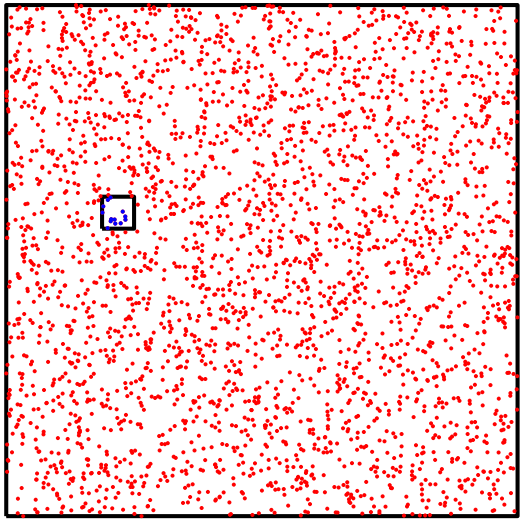
(Figure credit: G. Martinsson, Boulder)

How many levels?

Options:

- Keep refining until the number of sources in each leaf box is below a certain given constant
- *Obvious tweak:* Only do that for boxes that *actually* have too many sources ($\rightarrow$ '*adaptive*' tree, vs. the above *non-adaptive* strategy. *Downside of adaptive tree:* More bookkeeping)

Barnes-Hut: Putting Multipole Expansions to Work

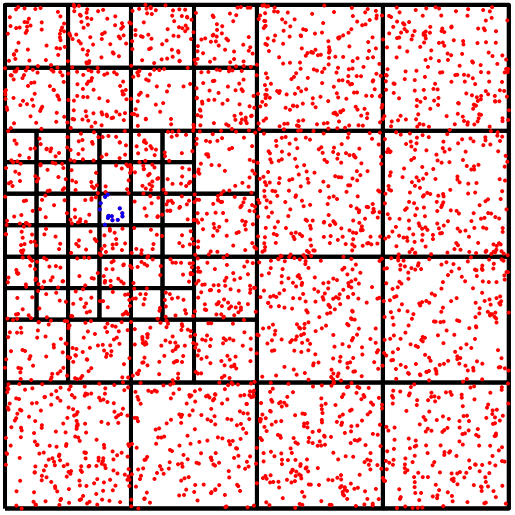


(Figure credit: G. Martinsson, Boulder)

Want to evaluate all the source interactions with the targets in the box.

Q: What would be good sizes for source boxes? What's the requirement?

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

Data from which of these boxes could we bring in using multipole expansions? Does that depend on the type of expansion? (Taylor/special function vs skeletons)

- Function expansions:
  - Near neighbors: $\rho = r/R > 1$: No convergence.
  - Non-near neighbors: Depends on the box size.
- Skeletons using proxy points:
  - Near neighbors: No convergence
  - Non-near neighbors: Depends on validity of proxy representation.
- Skeletons built directly:
  - Accurate, but at the cost of a higher rank
  - Non-near neighbors: Accurate, but expensive–better off using proxies.

Idea:

- Don't use multipoles from the near neighbors

  (Instead: Compute interactions directly)
- Do use multipoles from non-near neighbors

- I.e. have a *buffer* of non-multipole source boxes around each target box

Note: Whether or not to use buffering is a *choice*, with the following tradeoff:

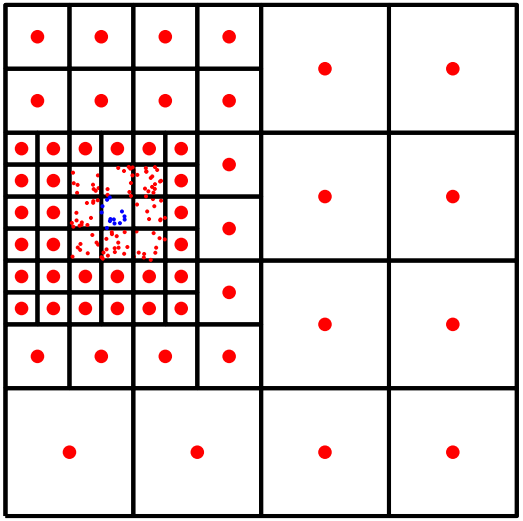
Pros:

- Simple, constant-rank interactions
- Works for all expansion types

Cons:

- Trickier bookkeeping

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

What properties do these boxes have?

Simple observation: The further, the bigger.

More complete: We can put a uniform bound on the error in the (function) expansion at the target:

r_s : Source box 'radius' (center to vertical/horizontal edge)

R: source center $\to$ target center distance

r_t : Target box 'radius' (center to vertical/horizontal edge)

$$\left(\frac{d\left(\text{src ctr, furthest src}\right)}{d\left(\text{src ctr, closest tgt}\right)}\right)^{k+1} = \left(\frac{r_s\sqrt{2}}{R - r_t}\right)^{k+1}$$

Convergent iff

$$r_s\sqrt{2} < R - r_t. \qquad (*)$$

Convergent *if* (picture)

$$R \geqslant 3 \cdot \max(r_t, r_s) \qquad (**)$$

because

$$(*) \;\Leftrightarrow\; 0 < R - \left(r_t + \sqrt{2}r_s\right).$$

We'll make a new word for that: A pair of boxes satisfying the condition $(**)$ is called *well-separated*.

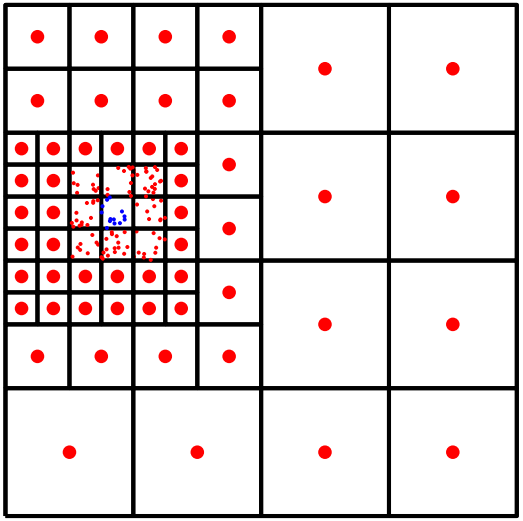
Observations:

- This is just *one* choice. (the one we'll use anyway)
- One can play games here, based on a target accuracy.

  $\rightarrow$ '*Multipole Acceptance Criterion*' ('MAC') or

  '*Admissibility Condition*'

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

What is the cost of evaluating the target potentials, assuming that we know the multipole expansions already?

Again, let:

- L be the number of levels
- N be #particles
- K be #terms in expansion
- m be #particles/box

  Assume m bounded by a fixed number (say, $\leqslant 100$)
- Then $L \sim \log(N)$

What do we need to do?

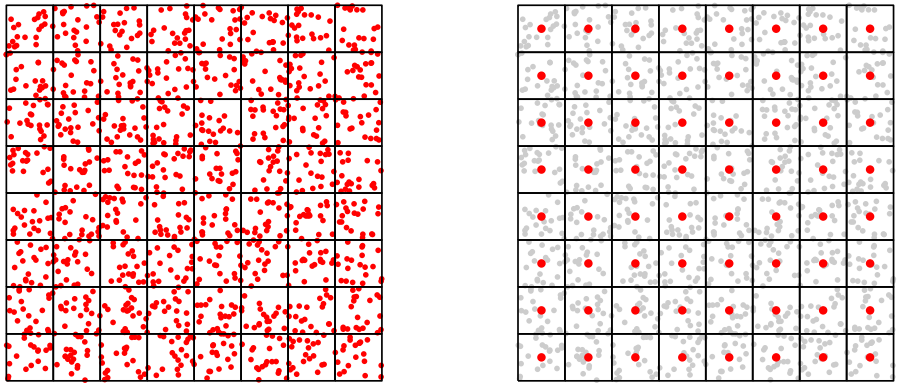
- 9 boxes of direct evaluation (self and touching neighbors)

  $\rightarrow O(m) = O(1)$
- L levels of multipoles, each of which contains:
  - $\leqslant 27$ source boxes (!) (in 2D)

  $\rightarrow O(LK) = O(\log N)$

There are $O(N)$ target boxes (because m is fixed), so we do the above $O(N)$ times $\rightarrow$ $O(N \log N)$ total work to evaluate.

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

Summarize the algorithm (so far) and the associated cost.

	How often	**Individual cos**
Compute mpoles	N src particles	LK
Evaluate mpoles	N tgt particles	K
	$\cdot\ 27L$ src boxes	
9 close boxes	$9\cdot(N/m$ boxes)	m^2

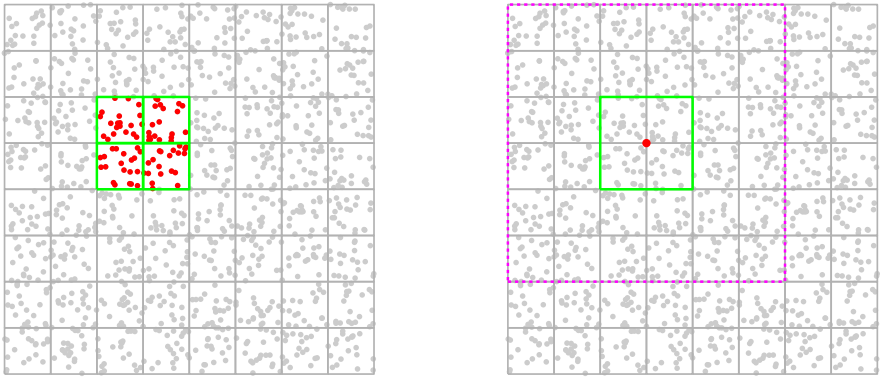
So even with the forming of the multipoles, the overall algorithm is

$$O(N \log N).$$

Also, if we wanted to get the whole thing down to $O(N)$, we would need to speed up both computing and evaluating the multipoles.

Let's start with the former.

Barnes-Hut: Putting Multipole Expansions to Work



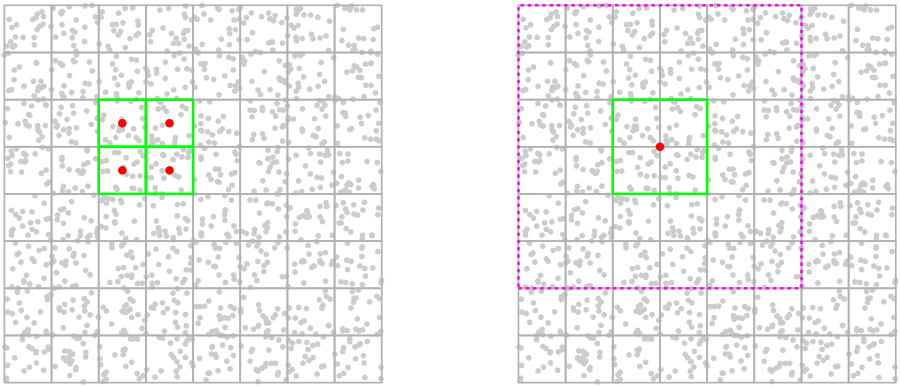
(Figure credit: G. Martinsson, Boulder)

How could this process be sped up?

Observation: The amount of work does not really decrease as we go up the tree: Fewer boxes, but more particles in each of them.

But we already compute multipoles to summarize lower-level boxes...

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson, Boulder)

To get a new 'big' multipole from a 'small' multipole, we need a new mathematical tool.

Nominally, all the tool needs to accomplish is to

- take in a multipole expansion at one center

- and 'translate it' so that it now serves as an expansion about a different center.

The transformation that accomplishes this is called a '*translation operator*', and this particular one is called *multipole-to-multipole translation*.

Questions:

- How do you do it?
- Where is the resulting expansion valid?

$\rightarrow$ HW

Cost of Multi-Level Barnes-Hut

Summarize the cost of the final algorithm (with upward translation)

Just the new construction phase:

Level	What	Cost	How many
L (lowest, leaves)	src $\to$ mpoles	mK	(N/m)
$L-1$	mpole $\to$ mpole	K^2	$(N/m)/4$
$L-2$	mpole $\to$ mpole	K^2	$(N/m)/16$
			$\vdots$

Altogether: $O(KN) + O(K^2N) \sim O(N)$

What	Total cost
Compute mpoles	$KN + K^2N$
Evaluate mpoles	$NK \log N$
9 close boxes	NK/m

Altogether: Still $O(N \log N)$, but the first stage is now $O(N)$.

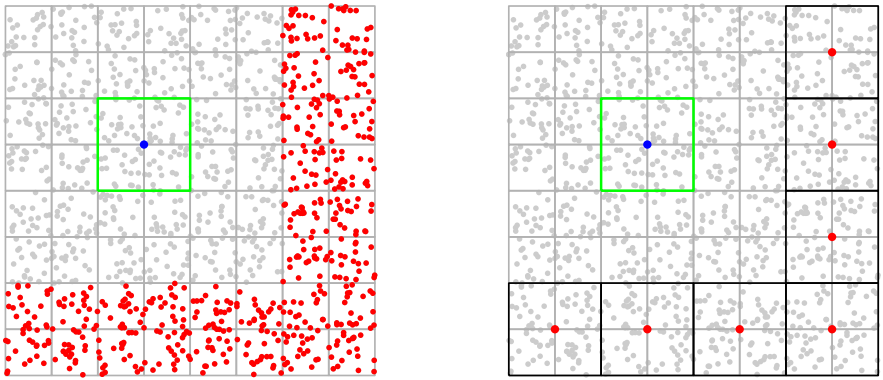
Observation: Multipole evaluation remains as the single most costly bit of this algorithm. *Fix?*

Idea: Exploit the tree structure also in performing this step.

If 'upward' translation of multipoles helped earlier,

maybe 'downward' translation of *local* expansions can help now.

Using Multipole-to-Local



(Figure credit: G. Martinsson, Boulder)

Come up with an algorithm that computes the interaction in the figure.

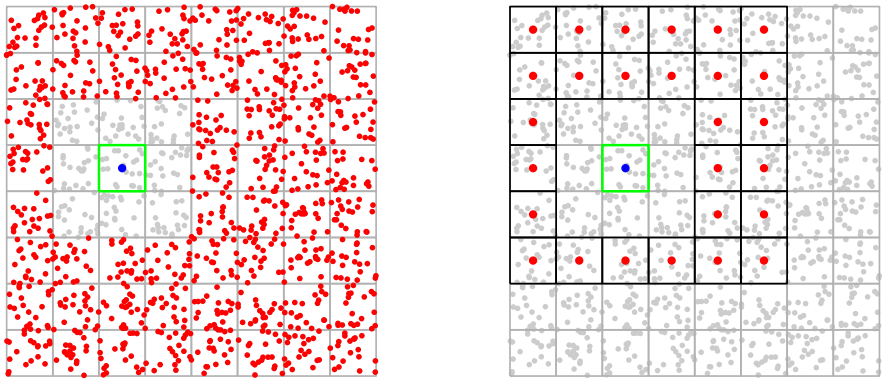
1. Form multipoles
2. Translate multipole to local
3. Evaluate local

But:

- Box has children. What about them?
- And there are a number of closer sources that we've neglected.

Let's consider the situation from the next level down.

Using Multipole-to-Local



(Figure credit: G. Martinsson, Boulder)

Assuming we retain information from the previous level, how can we obtain a valid local expansion on the target box?

1. Obtain contribution from well-separated boxes on previous level by local→local translation.
2. Obtain contribution from well-separated boxes on this level by

multipole→local translation. For our target box b, call this list of boxes the *interaction list* I_b.

3. Keep recursing until only touching boxes remain, compute interaction from those directly.

Define ‘Interaction List’

For a box b, the interaction list I_b consists of all boxes b' so that

- b and b' are on the same level,
- b and b' are well-separated, and
- the parents of b and b' touch.

The Fast Multipole Method ('FMM')

Upward pass

1. Build tree
2. Compute interaction lists
3. Compute lowest-level multipoles from sources
4. Loop over levels $\ell = L - 1, \ldots, 2$:
   (a) Compute multipoles at level ℓ by mp $\rightarrow$ mp

Downward pass

1. Loop over levels $\ell = 2, 3, \ldots, L - 1$:
   (a) Loop over boxes b on level ℓ :
      i. Add contrib from I_b to local expansion by mp $\rightarrow$ loc
      ii. Add contrib from parent to local exp by loc $\rightarrow$ loc
2. Evaluate local expansion and direct contrib from 9 neighbors.

Overall algorithm: Now $O(N)$ complexity.

Note: L levels, numbered $0, \ldots, L-1$. Loop indices above *inclusive.*

What about adaptivity?

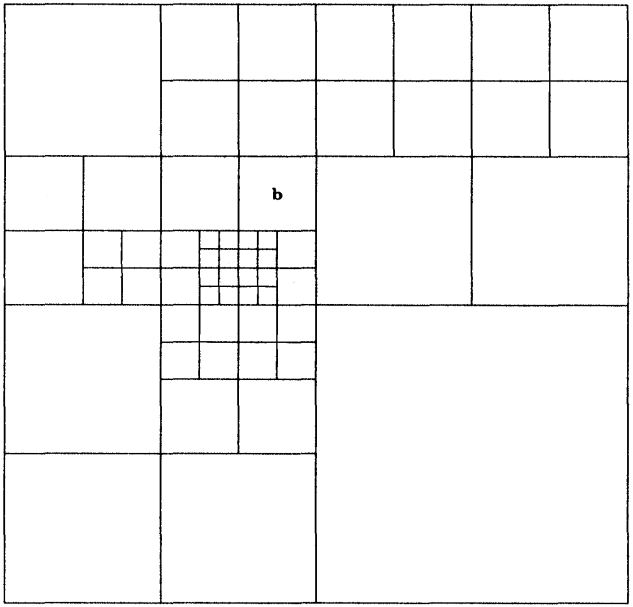


Figure credit: Carrier et al. ('88)

What changes?

- Boxes interacting with a target box b can be at many levels
- Both higher and lower
- Try to come up with a list of cases

  according to what computational method can be used

  (Solution on next slide)

What about adaptivity?

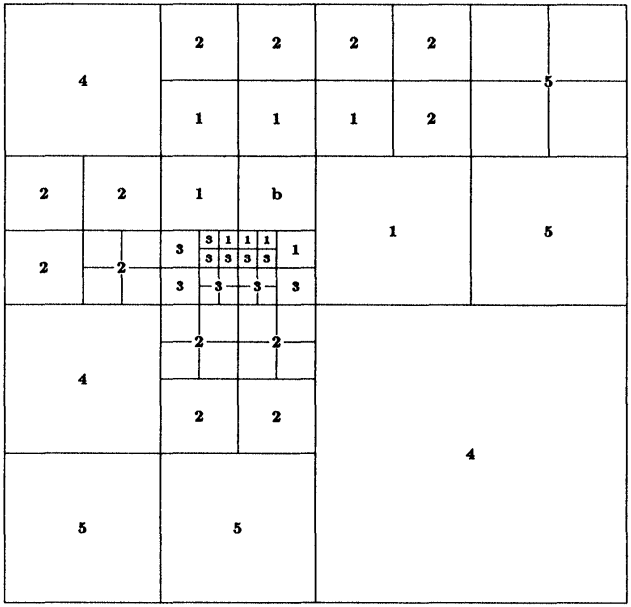


Figure credit: Carrier et al. ('88)

Make a list of cases:

1. Near/touching neighbor: direct
2. Well-separated, same level: mp $\rightarrow$ loc
3. Well-separated, lower level: mp $\rightarrow$ loc
4. Not well-separated, higher level: src $\rightarrow$ loc
5. Well-separated, higher level: nothing to do

In the FMM literature, the resulting interaction lists are 'insightfully' often called 'List 1', 'List 2', ... (with the case numbers above). Alternatively: 'List U', 'List V', ...

What about solving?

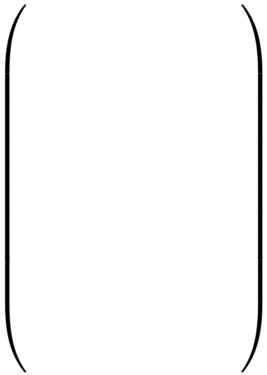
Likely computational goal: Solve a linear system $Ax = b$. How do our methods help with that?

- Barnes-Hut/FMM/Ewald provide a matvec.

  If iterative solvers (e.g. GMRES) work (i.e. converge quickly), we're done here.
- If not, how would we construct the equivalent of a direct solver (e.g. LU)?

A Matrix View of Low-Rank Interaction

Only *parts of the matrix are low-rank*! What does this look like from a matrix perspective?



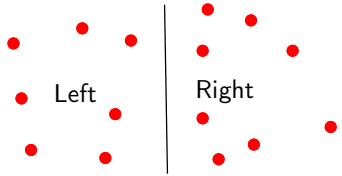
where shaded blocks have low rank.

Remarks about this matrix form:

- This structure is obviously dependent on ordering.

  Realize that finding tree boxes constitutes an ordering.

- The easiest way to see where a matrix like this would come from is to consider sources and targets sitting in a bisected 2D plane:



  Then, assuming the right ordering, the matrix captures the following interactions:

$$\begin{pmatrix} \text{Left} \to \text{Left} & \text{Right} \to \text{Left} \\ \text{Left} \to \text{Right} & \text{Right} \to \text{Right} \end{pmatrix}$$

  The off-diagonal blocks have low-ish rank.

- **Note:** *Some* close interactions are caught up in the off-diagonal blocks *if* they touch the diagonal.

  Note 2: FMMs and tree codes do extra bookkeeping to avoid those. (Recall definition of 'well-separated') For linear algebra: simply accept slightly increased

rank and move on. (I.e. don't do 'buffering')

Block-separable matrices

How do we represent the low-rank structure of a matrix like this?

$$A = \begin{pmatrix} D_1 & A_{12} & A_{13} & A_{14} \\ A_{21} & D_2 & A_{23} & A_{24} \\ A_{31} & A_{32} & D_3 & A_{34} \\ A_{41} & A_{42} & A_{43} & D_4 \end{pmatrix}$$

where A_{ij} has low-rank structure?

Recall column ID:

$$A_{ij} \approx (A_{ij})_{(:,J)} \Pi_{\text{col}}$$

Recall row ID:

$$A_{ij} \approx P_{\text{row}} (A_{ij})_{(I,:)}$$

Both together:

$$A_{ij} \approx P_{\text{row}} \underbrace{(A_{ij})_{(I,J)}}_{\tilde{A}_{ij}} \Pi_{\text{col}}.$$

Saw: If A comes from a kernel for which Green's formula holds, then the same skeleton will work for all of space, for a given set of sources/targets.

What would the resulting matrix look like?

Block-Separable Matrices

A *block-separable matrix* looks like this:

$$A = \begin{pmatrix} D_1 & P_1\tilde{A}_{12}\Pi_2 & P_1\tilde{A}_{13}\Pi_3 & P_1\tilde{A}_{14}\Pi_4 \\ P_2\tilde{A}_{21}\Pi_1 & D_2 & P_2\tilde{A}_{23}\Pi_3 & P_2\tilde{A}_{24}\Pi_4 \\ P_3\tilde{A}_{31}\Pi_1 & P_3\tilde{A}_{32}\Pi_2 & D_3 & P_3\tilde{A}_{34}\Pi_4 \\ P_4\tilde{A}_{41}\Pi_1 & P_4\tilde{A}_{42}\Pi_2 & P_4\tilde{A}_{43}\Pi_3 & D_4 \end{pmatrix}$$

Here:

- $\tilde{A}_{ij}$ smaller than A_{ij}
- D_i has full rank (not necessarily diagonal)
- P_i shared for entire row
- Π_i shared for entire column

Q: Why is it called that?

The word *separable* arises because what low-rank representations do is (effectively) apply 'separation of variables', i.e. $u(x, y) = v(x)w(y)$, just in the row/column indices.

Q: How expensive is a matvec?

A matvec with a block-separable matrix costs $O(N^{3/2})$ like the single-level Barnes-Hut scheme.

Q: How about a solve?

$\rightarrow$ To do a solve, we need some more technology.

Engineering a cheap solve

Use the following notation:

$$B = \begin{pmatrix} 0 & P_1\tilde{A}_{12} & P_1\tilde{A}_{13} & P_1\tilde{A}_{14} \\ P_2\tilde{A}_{21} & 0 & P_2\tilde{A}_{23} & P_2\tilde{A}_{24} \\ P_3\tilde{A}_{31} & P_3\tilde{A}_{32} & 0 & P_3\tilde{A}_{34} \\ P_4\tilde{A}_{41} & P_4\tilde{A}_{42} & P_4\tilde{A}_{43} & 0 \end{pmatrix}$$

and

$$D = \begin{pmatrix} D_1 & & & \\ & D_2 & & \\ & & D_3 & \\ & & & D_4 \end{pmatrix}, \quad \Pi = \begin{pmatrix} \Pi_1 & & & \\ & \Pi_2 & & \\ & & \Pi_3 & \\ & & & \Pi_4 \end{pmatrix}.$$

Then $A = D + B\Pi$ and

$$\begin{pmatrix} D & B \\ -\Pi & \mathrm{Id} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \widetilde{\mathbf{x}} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{0} \end{pmatrix}$$

is equivalent to $A\mathbf{x} = \mathbf{b}$.

Q: What are the matrix sizes? The vector lengths of $\mathbf{x}$ and $\tilde{\mathbf{x}}$?
(Π : small $\times$ large)

Now work towards doing *just* a 'coarse' solve on $\tilde{\mathbf{x}}$, using, effectively, the Schur complement. Multiply first row by ΠD^{-1}, add to second:

$$\begin{pmatrix} \Pi D^{-1} D & \Pi D^{-1} B \\ -\Pi & \mathrm{Id} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \widetilde{\mathbf{x}} \end{pmatrix} = \begin{pmatrix} \Pi D^{-1} \mathbf{b} \\ \mathbf{0} \end{pmatrix}$$

$$\begin{pmatrix} \Pi D^{-1} D & \Pi D^{-1} B \\ 0 & \mathrm{Id} + \Pi D^{-1} B \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \widetilde{\mathbf{x}} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \Pi D^{-1} \mathbf{b} \end{pmatrix}$$

Focus in on the second row:

$$(\mathrm{Id} + \Pi D^{-1} B)\widetilde{\mathbf{x}} = \Pi D^{-1} \mathbf{b}$$

Every non-zero entry in $\Pi D^{-1} B$ looks like

$$\Pi_i D_i^{-1} P_i \tilde{A}_{ij}.$$

So set

$$\tilde{A}_{ii} = (\Pi_i D_i^{-1} P_i)^{-1}$$

The nomenclature makes (some) sense, because $\widetilde{A}_{ii}$ is a 'downsampled' version of D_i

(with two inverses thrown in for good measure). Next,

$$\begin{pmatrix} \tilde{A}_{11} & & & \\ & \tilde{A}_{22} & & \\ & & \tilde{A}_{33} & \\ & & & \tilde{A}_{44} \end{pmatrix} (\mathrm{Id} + \Pi D^{-1} B) = \underbrace{\begin{pmatrix} \tilde{A}_{11} & \tilde{A}_{12} & \tilde{A}_{13} & \tilde{A}_{14} \\ \tilde{A}_{21} & \tilde{A}_{22} & \tilde{A}_{23} & \tilde{A}_{24} \\ \tilde{A}_{31} & \tilde{A}_{32} & \tilde{A}_{33} & \tilde{A}_{33} \\ \tilde{A}_{41} & \tilde{A}_{42} & \tilde{A}_{43} & \tilde{A}_{44} \end{pmatrix}}_{\tilde{A}}.$$

Summary: Need to solve

$$\tilde{A}\tilde{\mathbf{x}} = (\Pi_i D_i^{-1} P_i)^{-1} \Pi D^{-1} \mathbf{b}.$$

What have we achieved?

- Instead of solving a linear system of size

  $$(N_{L0\,\text{boxes}} \cdot m) \times (N_{L0\,\text{boxes}} \cdot m)$$

  we solve a linear system of size

  $$(N_{L0\,\text{boxes}} \cdot K) \times (N_{L0\,\text{boxes}} \cdot K),$$

  which is cheaper by a factor of $(K/m)^3$.

- We are now only solving on the skeletons:

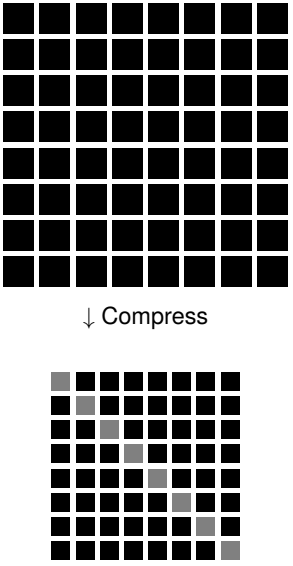


Figure credit: G. Martinsson, Boulder

Solving with Block-Separable Matrices

In order to get $O(N)$ complexity, could we apply this procedure recursively?

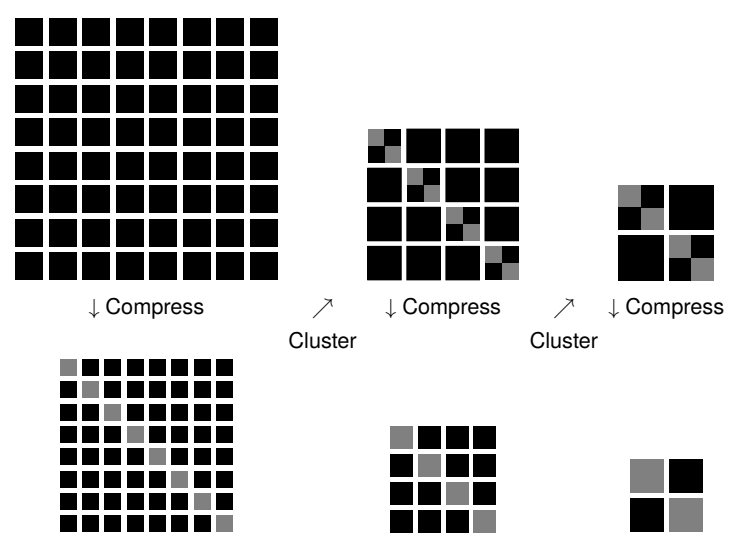
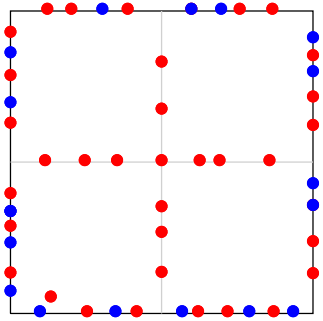


Figure credit: G. Martinsson, Boulder

- To get to $O(N)$, realize we can *recursively*

  - group skeletons
  - eliminate more variables.



Level 1 skeletons · Level 0 skeletons

- Using this hierarchical grouping gives us

  '*Hierarchically Block-Separable*' ('*HBS*') matrices.

- If you have heard the word '$\mathcal{H}$*-matrix*' and '$\mathcal{H}^2$*-matrix*', the ideas are very similar. Differences:
  - $\mathcal{H}$-family matrices don't typically use the ID

(instead often use ‘Adaptive Cross Approximation’–‘ACA’)

– $\mathcal{H}^2$ does target clustering (like FMM), $\mathcal{H}$ does not (like Barnes-Hut)

Telescoping Factorization

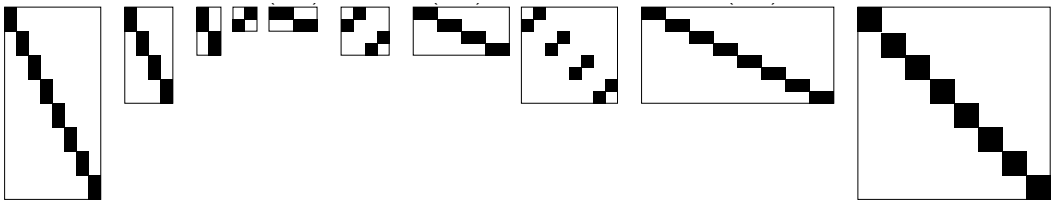


Figure credit: G. Martinsson, Boulder

Observations?

- The most decrease in 'volume' happens in the off-diagonal part of the matrix. $\rightarrow$ Rightfully so!
- All matrices are block-diagonal, except for the highest-level matrix–but that is small!

5 Outlook: Building a Fast PDE Solver

PDEs: Simple Ones First, More Complicated Ones Later

Laplace

$\triangle u = 0$

- Steady-state $\partial_t u = 0$ of wave propagation, heat conduction
- Electric potential u for applied voltage
- Minimal surfaces/"soap films"
- ∇u as velocity of incompressible flow

Helmholtz

$\triangle u + k^2 u = 0$

- Assume time-harmonic behavior $\tilde{u} = e^{\pm i\omega t} u(x)$ in time-domain wave equation:

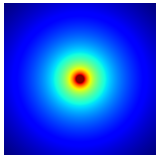
$$\partial_t^2 \tilde{u} = \triangle \tilde{u}$$

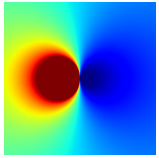
- Sign in $\tilde{u}$ determines direction of wave: Incoming/outgoing if free-space problem
- *Applications:* Propagation of sound, electromagnetic waves

Fundamental Solutions

Laplace

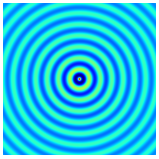
$-\triangle u = \delta$

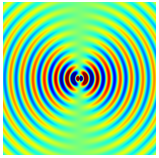


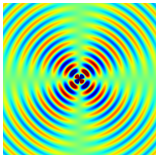


Helmholtz

$\triangle u + k^2 u = \delta$







Monopole

Dipole

Quadrupole

aka. *Free space Green's Functions*

How do you assign a precise meaning to the statement with the δ-function?

Multiply by a test function, integrate by parts.

Why care about Green's functions?

If you know them, they make solving the PDE simple:

$$\triangle G = \delta \quad \Rightarrow \quad \triangle(G * f) = (f * \delta) = f,$$

i.e. $G * f$ is the solution to free-space Poisson $\triangle u = f$.

What is a non-free-space Green's function? I.e. one for a specific domain?

One that satisfies $\Delta G = \delta$ *and* a boundary condition.

Why not just use domain Green's functions?

We don't know them! (for general domains)

What if we don't know a Green's function for our PDE... at all?

Use a known one that works for the highest-order derivative parts of the PDE.

Fundamental solutions

Laplace

$$G(x) = \begin{cases} \frac{1}{-2\pi} \log |x| & \text{2D} \\ \frac{1}{4\pi} \frac{1}{|x|} & \text{3D} \end{cases}$$

$$\frac{\partial}{\partial_x} G(x)$$

Helmholtz

Monopole

$$G(x) = \begin{cases} \frac{i}{4} H_0^1(k|x|) & \text{2D} \\ \frac{1}{4\pi} \frac{e^{ik|x|}}{|x|} & \text{3D} \end{cases}$$

Dipole

$$\frac{\partial}{\partial_x} G(x)$$

Layer Potentials

$$(S_k\sigma)(x) := \int_\Gamma G_k(x-y)\sigma(y)ds_y$$

$$(S'_k\sigma)(x) := n\cdot\nabla_x PV\int_\Gamma G_k(x-y)\sigma(y)ds_y$$

$$(D_k\sigma)(x) := PV\int_\Gamma n\cdot\nabla_y G_k(x-y)\sigma(y)ds_y$$

$$(D'_k\sigma)(x) := n\cdot\nabla_x f.p.\int_\Gamma n\cdot\nabla_y G_k(x-y)\sigma(y)ds_y$$

- G_k is the Helmholtz kernel ($k=0 \rightarrow$ Laplace)
- Operators–map function σ on Γ to...
  - ...function on $\mathbb{R}^n$
  - ...function on Γ (in particular)
- Alternate ("standard") nomenclature:

Ours	Theirs
S	V
D	K
S'	K'
D'	T

- S'' (and higher) analogously
- Called *layer potentials*:
  - S is called the *single-layer potential*
  - D is called the *double-layer potential*
- (Show pictures using `pytential/examples/layerpot.py`, observe continuity properties.)

How does this actually solve a PDE?

Solve a (interior Laplace Dirichlet) BVP, $\partial\Omega = \Gamma$

$$\triangle u = 0 \quad \text{in } \Omega, \qquad u|_\Gamma = f|_\Gamma.$$

1. Pick *representation*:
$$u(x) := (S\sigma)(x)$$
2. Take (interior) limit onto Γ:
$$u|_\Gamma = S\sigma$$
3. Enforce BC:
$$u|_\Gamma = f$$
4. Solve resulting linear system:
$$S\sigma = f$$
(quickly–using the methods we've developed: It is precisely of the form that suits our fast algorithms!)
5. Obtain PDE solution in Ω by evaluating representation

Observations:

- One can choose representations relatively freely. Only constraints:
  - Can I get to the solution with this representation?

    I.e. is the solution I'm looking for represented?
  - Is the resulting integral equation solvable?

  Q: How would we know?
- Some representations lead to better integral equations than others. The one above is actually terrible (both theoretically and practically).

  Fix above: Use $u(x) = D\sigma(x)$ instead of $u(x) = S\sigma(x)$.

  Q: How do you tell a good representation from a bad one?
- Need to actually *evaluate* $S\sigma(x)$ or $D\sigma(x)$...

  Q: How?

$\rightarrow$ Need some theory

6 Going Infinite: Integral Operators and Functional Analysis

6.1 Norms and Operators

Norms

Definition 1 *(Norm) A* norm $\|\cdot\|$ *maps an element of a* vector space *into* $[0, \infty)$. *It satisfies:*

- $\|x\| = 0 \Leftrightarrow x = 0$
- $\|\lambda x\| = |\lambda|\|x\|$
- $\|x + y\| \leq \|x\| + \|y\|$ *(triangle inequality)*

Can create norm from *inner product*: $\|x\| = \sqrt{\langle x, x \rangle}$

Function Spaces

Name some function spaces with their norms.

$C(\Omega)$	f continuous, $\|f\|_\infty := \sup_{x\in\Omega} \|f(x)\|$
$C^k(\Omega)$	f k-times continuously differentiable
$C^{0,\alpha}(\Omega)$	$\|f\|_\alpha := \|f\|_\infty + \sup_{x\neq y} \frac{\|f(x)-f(y)\|}{\|x-y\|^\alpha}$ $(\alpha \in (0,1))$
$C_L(\Omega)$	$\|f(x) - (y)\| \leq L\|x-y\|$
$L^p(\Omega)$	$\|f\|_p := \sqrt[p]{\int_D \|f(x)\|^p dx} < \infty$
	L^2 special because?

Convergence

Name some ways in which a sequence can 'converge'.

Definition 2 (Convergent sequence) $x_n \to x :\Leftrightarrow \|x_n - x\| \to 0$ *"convergence in norm"*

Definition 3 (Cauchy sequence) *For all* $\epsilon > 0$ *there exists an* n *for which* $\|x_\nu - x_\mu\| \leq \epsilon$ *for* $\mu, \nu \geq n$

(Convergence without known limit!)

Definition 4 (Complete/"Banach" space) *Cauchy* $\Rightarrow$ *Convergent*

Q: Counterexample?

Operators

X, Y: Banach spaces

$A : X \to Y$ linear operator

Definition 5 (Operator norm) $\|A\| := \sup\{\|Ax\| : x \in X, \|x\| = 1\}$

Theorem 3 $\|A\|$ *bounded* $\Leftrightarrow$ A *continuous*

- The set of bounded linear operators is itself a Banach space: $L(X, Y)$
- $\|Ax\| \leq \|A\|\|x\|$
- $\|BA\| \leq \|B\|\|A\|$

Questions:

- What does 'linear' mean here?
- Is there a notion of 'continuous at x' for linear operators?

Operators: Examples

Which of these is bounded as an operator on functions on the real line?

- Multiplication by a scalar
- "Left shift"
- Fourier transform
- Differentiation
- Integration
- Integral operators

Need to know spaces (norms really) to answer that!

Integral Operators: Zoology

Volterra	Fredholm
$\int_a^x k(x,y)f(y)dy = g(x)$	$\int_G k(x,y)f(y)dy = g(x)$
First kind	**Second kind**
$\int_G k(x,y)f(y)dy = g(x)$	$f(x) + \int_G k(x,y)f(y)dy = g(x)$

Questions:

- First row: First or second kind?
- Second row: Volterra or Fredholm?
- Matrix (i.e. finite-dimensional) analogs?
- What can happen in 2D/3D?
- Factor allowable in front of the identity?
- Why even talk about 'second-kind operators'?
  - Throw a $+\delta(x-y)$ into the kernel, back to looking like first kind. So?

– Is the identity in $(I + K)$ crucial?

Connections to Complex Variables

Complex analysis is *full* of integral operators:

- Cauchy's integral formula:

$$f(a) = \frac{1}{2\pi i} \oint_\gamma \frac{1}{z-a} f(z)\, dz$$

- Cauchy's differentiation formula:

$$f^{(n)}(a) = \frac{n!}{2\pi i} \oint_\gamma \frac{1}{(z-a)^{n+1}} f(z)\, dz$$

Integral Operators: Boundedness (=Continuity)

Theorem 4 (Continuous kernel $\Rightarrow$ bounded) *$G \subset \mathbb{R}^n$ closed, bounded ("compact"), $K \in C(G^2)$. Let*

$$(A\phi)(x) := \int_G K(x,y)\phi(y)dy.$$

Then

$$\|A\|_\infty = \max_{x\in G} \int_G |K(x,y)|dy.$$

Show '$\leqslant$'.

Solving Integral Equations

Given

$$(A\phi)(x) := \int_G K(x,y)\varphi(y)dy,$$

are we allowed to ask for a solution of

$$(\mathrm{Id} + A)\varphi = g?$$

Will see three attempts to answer that, in roughly historical order:

- Neumann
- Riesz
- Fredholm

Attempt 1: The Neumann series

Want to solve

$$\varphi - A\varphi = (I - A)\varphi = g.$$

Formally:

$$\varphi = (I - A)^{-1} g.$$

What does that remind you of?

$$\sum_{k=0}^{\infty} \alpha^k = \frac{1}{1-\alpha}$$

Only works if $|\alpha| < 1$!

Theorem 5 *$A : X \to X$ Banach, $\|A\| < 1$*

$$(I - A)^{-1} = \sum_{k=0}^{\infty} A^k$$

with $\|(I - A)^{-1}\| \leq 1/(1 - \|A\|)$.

- How does this rely on completeness/Banach-ness?
- There's an iterative procedure hidden in this.

  (Called '*Picard Iteration*'. Cf: Picard-Lindelöf theorem.)

  Hint: How would you compute $\sum_k A^k f$?
- **Q:** Why does this fall short?

  $\|A\| \leqslant 1$ is *way* to restrictive a condition.

  $\to$ We'll need better technology.

  Biggest Q: If Cauchy sequences are too weak a tool to deliver a limit, where else

are we going to get one?

6.2 Compactness

Compact sets

Definition 6 (Precompact/Relatively compact) $M \subseteq X$ *precompact*:$\Leftrightarrow$ *all sequences* $(x_k) \subset M$ *contain a subsequence converging in* X

Definition 7 (Compact/'Sequentially complete') $M \subseteq X$ *compact*:$\Leftrightarrow$ *all sequences* $(x_k) \subset M$ *contain a subsequence converging in* M

- Precompact $\Rightarrow$ bounded
- Precompact $\Leftrightarrow$ bounded (finite dim. only!)

Counterexample?

Looking for a bounded set where not every sequence contains a convergent subsequence.
$\rightarrow$ Make use of the fact that there are infinitely many 'directions' (dimensions).

Precompactness 'replaces' boundedness in ∞ dim (because boundedness is 'not strong enough')

Compact Operators

X, Y: Banach spaces

Definition 8 (Compact operator) $T : X \to Y$ *is* compact $:\Leftrightarrow$ T(*bounded set*) *is precompact.*

- T, S compact $\Rightarrow \alpha T + \beta S$ compact
- *One of* T, S compact $\Rightarrow S \circ T$ compact
- T_n all compact, $T_n \to T$ in operator norm $\Rightarrow$ T compact

Questions:

- Let $\dim T(X) < \infty$. Is T compact?
- Is the identity operator compact?

Intuition about Compact Operators

- Compact operator: As finite-dimensional as you're going to get in infinite dimensions.
- Not clear yet–but they are moral (∞-dim) equivalent of a matrix having *low numerical rank*.
- Are compact operators continuous (=bounded)?
- What do they do to high-frequency data?
- What do they do to low-frequency data?

Arzelà-Ascoli

Let $G \subset \mathbb{R}^n$ be compact.

Theorem 6 (Arzelà-Ascoli) *$U \subset C(G)$ is precompact iff it is bounded and* equicontinuous.

Equicontinuous means

For all $x, y \in G$

for all $\epsilon > 0$ there exists a $\delta > 0$ such that for all $f \in U$

if $|x - y| < \delta$, then $|f(x) - f(y)| < \epsilon$.

Continuous means:

For all $x, y \in G$

for all $\epsilon > 0$ there exists a $\delta > 0$ such that

if $|x - y| < \delta$, then $|f(x) - f(y)| < \epsilon$.

Intuition?

Equicontinuity prevents the functions from 'running away'.

"Uniformly continuous"?

One δ works for all x.

When does *uniform continuity* happen?

Continuous on a closed and bounded ('compact') set.

6.3 Integral Operators

Integral Operators are Compact

Theorem 7 (Continuous kernel $\Rightarrow$ compact [Kress LIE Thm. 2.21]) *$G \subset \mathbb{R}^m$ compact, $K \in C(G^2)$. Then*

$$(A\phi)(x) := \int_G K(x,y)\phi(y)dy.$$

is compact on $C(G)$.

Use A-A. (a statement about compact *sets*)

What is there to show?

Pick $U \subset C(G)$. $A(U)$ bounded?

Yes, because the operator is bounded.

$A(U)$ equicontinuous?

Yes, because K *uniformly* continuous on $G \times G$ because $G \times G$ compact.

Weakly singular

$G \subset \mathbb{R}^n$ compact

Definition 9 (Weakly singular kernel)

- *K defined, continuous everywhere except at $x = y$*
- *There exist $C > 0$, $\alpha \in (0, n]$ such that*

$$|K(x, y)| \leq C|x - y|^{\alpha - n} \qquad (x \neq y)$$

Theorem 8 (Weakly singular kernel $\Rightarrow$ compact [Kress LIE Thm. 2.22]**)** *K weakly singular. Then*

$$(A\phi)(x) := \int_G K(x, y)\phi(y)dy.$$

is compact on $C(G)$.

Outline the proof.

- Show boundedness/existence as improper integral.

  (polar coordinates)
- Bleep out the singularity with a C^0 PoU that shrinks with n: A_n
- Each A_n compact by previous thm.
- Shrink singularity with n. A_n converge uniformly (because of weak singularity).
- A is limit of compact operators.

Weakly singular (on surfaces)

$\Omega \subset \mathbb{R}^n$ bounded, open, C^1

Definition 10 (Weakly singular kernel (on a surface))
- *K defined, continuous everywhere except at $x = y$*
- *There exist $C > 0$, $\alpha \in (0, n-1]$ such that*

$$|K(x,y)| \leq C|x-y|^{\alpha-n+1} \qquad (x, y \in \partial\Omega,\ x \neq y)$$

Theorem 9 (Weakly singular kernel $\Rightarrow$ compact [Kress LIE Thm. 2.23]) *K weakly singular on $\partial\Omega$. Then*

$$(A\phi)(x) := \int_G K(x,y)\phi(y)dy.$$

is compact on $C(G)$.

Q: Has this estimate gotten worse or better?

6.4 Riesz and Fredholm

Riesz Theory (I)

Still trying to solve

$$L\phi := (I - A)\phi = \phi - A\phi = f$$

with A compact.

Theorem 10 (First Riesz Theorem [Kress, Thm. 3.1]) *$N(L)$ is finite-dimensional.*

Questions:

- What is $N(L)$ again?
- Why is this good news?
- Show it.

Good news because each dimension in $N(L)$ is an obstacle to invertibility. Now we know that there's only 'finitely many obstacles'.

Proof:

- $N(L)$ closed. (Why?)

- $L\phi = 0$ means what for A?
- When is the identity compact again?

Riesz Theory (Part II)

Theorem 11 (Riesz theory [Kress, Thm. 3.4]) *A compact.* **Then:**

- *$(I - A)$ injective $\Leftrightarrow$ $(I - A)$ surjective*
  - *It's either bijective or neither s nor i.*
- *If $(I - A)$ is bijective, $(I - A)^{-1}$ is bounded.*

Rephrase for solvability

If the solution to $(I - A)\varphi = 0$ is unique ($\varphi = 0$),then $(I - A)\varphi = f$ has a unique solution!

Main impact?

A real solvability result!

Key shortcoming?

Gives out completely if there happens to be a nullspace.

Hilbert spaces

Hilbert space: Banach space with a norm coming from an *inner product*:

$$(\alpha x + \beta y, z) = ?$$

$$(x, \alpha y + \beta z) = ?$$

$$(x, x)?$$

$$(y, x) = ?$$

Is $C^0(G)$ a Hilbert space?

No, no inner product generates $\|\cdot\|_\infty$.

Name a Hilbert space of functions.

$L^2(\Omega)$ with

$$(f, g) = \int_\Omega f \cdot g.$$

Is $C^0(G)$ "equivalent" to $L^2(G)$?

- **NO!**
- Won't be too bothered by this fact.
- Compactness results *do* transfer over. [Thm. 4.11, Pb. 4.5 in Kress LIE]

Why do compactness results transfer over nonetheless? Hint: What is

$$|(x, y)| \leq ?$$

(The *Cauchy-Schwarz inequality*.)

Adjoint Operators

Definition 11 (Adjoint oeprator) *A^* called adjoint to A if*

$$(Ax, y) = (x, A^* y)$$

for all x, y.

Facts:

- A^* unique
- A^* exists
- A^* linear
- A bounded $\Rightarrow$ A^* bounded
- A compact $\Rightarrow$ A^* compact

What is the adjoint operator in finite dimensions? (in matrix representation)

The transpose.

What do you expect to happen with integral operators?

Sources and targets swap roles.

Adjoint of the single-layer?

Itself. ('self-adjoint')

Adjoint of the double-layer?

S'

Fredholm Alternative

Theorem 12 (Fredholm Alternative [Kress LIE Thm. 4.14]) *$A : X \to X$ compact.* **Then either:**

- *$I - A$ and $I - A^*$ are bijective*

or:

- $\dim N(I - A) = \dim N(I - A^*)$
- $(I - A)(X) = N(I - A^*)^\perp$
- $(I - A^*)(X) = N(I - A)^\perp$

Seen these statements before?

Fundamental thm of linear algebra $\to$ next slide

Translate to language of integral equation solvability:

- **Either** $\varphi(x) - \int K(x, y)\varphi(y) = 0$ and $\psi(x) - \int K(y, x)\psi(y) = 0$ have only the trivial solution and their inhom counterparts are uniquely solvable,

- **or** the homogeneous and inhomogeneous int.eqs. have the same finite number of lin.indep. solutions. In particular, the inhom equations

$$\begin{aligned} \varphi(x) - \int K(x,y)\varphi(y) &= f(x) \\ \psi(x) - \int K(y,x)\psi(y) &= g(x) \end{aligned}$$

  are solvable iff

  - $f \perp \psi$ for all solutions ψ of $(I - A^*)\psi = 0$,
  - *or* $g \perp \varphi$ for all solutions φ of $(I - A)\varphi = 0$.

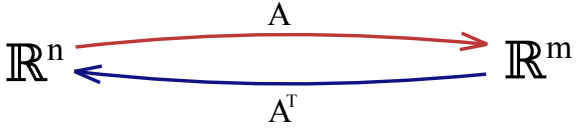
What about symmetric kernels ($K(x,y) = K(y,x)$)?

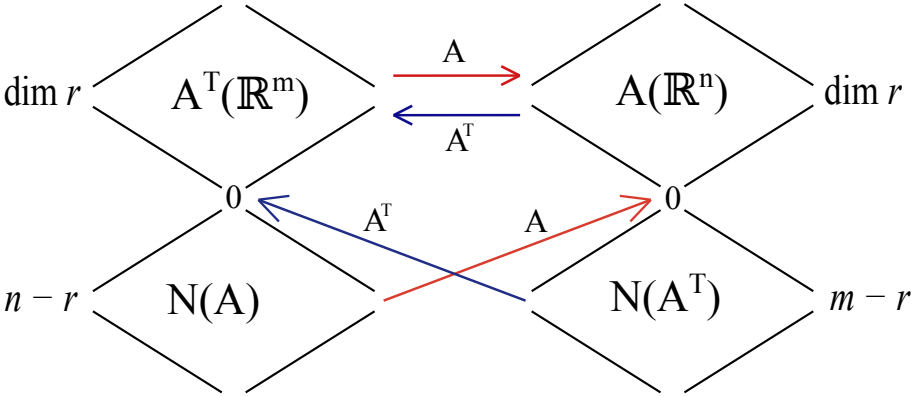
$A = A^*$.

Where to get uniqueness?

Will work on that.

Fundamental Theorem of Linear Algebra





6.5 A Tiny Bit of Spectral Theory

Spectral Theory: Terminology

$A : X \to X$ bounded, λ is a ____ value:

Definition 12 (Eigenvalue) *There exists an element $\phi \in X$, $\phi \neq 0$ with $A\phi = \lambda\phi$.*

Definition 13 (Regular value) *The "resolvent" $(\lambda I - A)^{-1}$ exists and is bounded.*

Can a value be regular and "eigen" at the same time?

No: eigen means that $(\lambda I - A)$ has a nullspace, so there isn't an inverse.

What's special about ∞-dim here?

Not all non-regular values are eigen.

Definition 14 (Resolvent set) $\rho(A) := \{\lambda \textit{is regular}\}$

Definition 15 (Spectrum) $\sigma(A) := \mathbb{C} \setminus \rho(A)$

Spectral Theory of Compact Operators

Theorem 13 *$A : X \to X$ compact linear operator, X ∞-dim.*
Then:

- $0 \in \sigma(A)$ *(show!)*
- $\sigma(A) \setminus \{0\}$ *consists* only *of eigenvalues*
- $\sigma(A) \setminus \{0\}$ *is at most countable*
- $\sigma(A)$ *has no accumulation point except for 0*

Show first part.

If $0 \not\in \sigma(A)$, then, A^{-1} exists and is bounded. Then $I = AA^{-1}$ is compact.

Show second part.

By Riesz, nullspaces and non-invertibility (of $\lambda I - A$) coincide.

Rephrase last two: how many eigenvalues with $|\cdot| \geq R$?

Finitely many

Recap: What do compact operators do to high-frequency data?

Dampen it.

Don't confuse $I - A$ with A itself!

(For example: $\dim N(A)$ vs $\dim N(I - A)$

7 Singular Integrals and Potential Theory

Recap: Layer potentials

$$
\begin{aligned}
(S\sigma)(x) &:= \int_\Gamma G(x-y)\sigma(y)ds_y \\
(S'\sigma)(x) &:= PV\ \hat{n}\cdot\nabla_x \int_\Gamma G(x-y)\sigma(y)ds_y \\
(D\sigma)(x) &:= PV \int_\Gamma \hat{n}\cdot\nabla_y G(x-y)\sigma(y)ds_y \\
(D'\sigma)(x) &:= f.p.\ \hat{n}\cdot\nabla_x \int_\Gamma \hat{n}\cdot\nabla_y G(x-y)\sigma(y)ds_y
\end{aligned}
$$

Definition 16 (Harmonic function) $\triangle u = 0$

Where are layer potentials harmonic?

Away from the boundary.

On the double layer again

Is the double layer *actually* weakly singular?

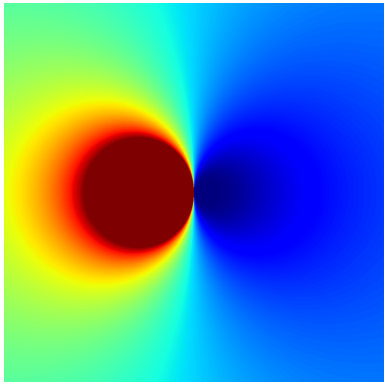
Recap:

Definition 17 (Weakly singular kernel)

- K *defined, continuous everywhere except at* $x = y$
- *There exist* $C > 0$, $\alpha \in (0, n-1]$ *such that*

$$|K(x,y)| \leq C|x-y|^{\alpha-n+1} \qquad (x, y \in \partial\Omega,\ x \neq y)$$

$$\frac{\partial}{\partial_x} \log(|0 - x|) = \frac{x}{x^2 + y^2}$$



- Singularity with approach on $y = 0$?
- Singularity with approach on $x = 0$?

So life is simultaneously worse and better than discussed.

How about 3D? $(-x/|x|^3)$

Would like an analytical tool that requires 'less' fanciness.

Cauchy Principal Value

But I don't **want** to integrate across a singularity!

$\rightarrow$ punch it out.

Problem: Make sure that what's left over is sensible

(in the sense of a mathematical definition)

$$\int_{-1}^{1} \frac{1}{x} dx?$$

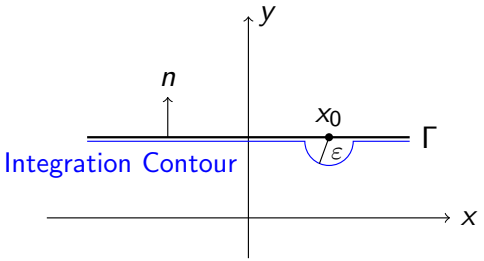
Not defined really.

$$PV \int_{-1}^{1} \frac{1}{x} dx := \lim_{\epsilon \to 0+} \left(\int_{-1}^{-\epsilon} \frac{1}{x} + \int_{\epsilon}^{1} \frac{1}{x} \right)$$

Q: Slight wrinkle–Symmetry matters!

$$\text{NOPE} : \int_{-1}^{-2\epsilon} \frac{1}{x} + \int_{\epsilon}^{1} \frac{1}{x}$$

Principal Value in n dimensions



Again: Symmetry matters!

Not an ellipse, not a potato, a circle. Sphere in 3D.

What about even worse singularities?

"Hadamard finite part"

- HFP integrals: "*hyper*singular"

- CPV integrals: “singular”

Recap: Layer potentials

$$
\begin{aligned}
(S\sigma)(x) &:= \int_\Gamma G(x-y)\sigma(y)ds_y \\
(S'\sigma)(x) &:= \mathrm{PV}\ \hat{n}\cdot\nabla_x \int_\Gamma G(x-y)\sigma(y)ds_y \\
(D\sigma)(x) &:= \mathrm{PV} \int_\Gamma \hat{n}\cdot\nabla_y G(x-y)\sigma(y)ds_y \\
(D'\sigma)(x) &:= f.p.\ \hat{n}\cdot\nabla_x \int_\Gamma \hat{n}\cdot\nabla_y G(x-y)\sigma(y)ds_y
\end{aligned}
$$

Important for us: Recover 'average' of interior and exterior limit without having to refer to off-surface values.

Green's Theorem

Theorem 14 (Green's Theorem [Kress LIE Thm 6.3])

$$\int_D u\triangle v + \nabla u \cdot \nabla v = \int_{\partial D} u(\hat{n}\cdot\nabla v)ds$$

$$\int_D u\triangle v - v\triangle u = \int_{\partial D} u(\hat{n}\cdot\nabla v) - v(\hat{n}\cdot\nabla u)ds$$

If $\triangle v = 0$, then

$$\int_{\partial D} \hat{n}\cdot\nabla v = ?$$

Pick $u = 1$.

$$\int_D 1\underbrace{\triangle v}_{0} - v\underbrace{\triangle 1}_{0} = \int_{\partial D} u1(\hat{n}\cdot\nabla v) - v(\underbrace{\hat{n}\cdot\nabla 1}_{0})ds$$

What if $\triangle v = 0$ and $u = G(|y - x|)$ in Green's second identity?

Can you write that more briefly?

Green's Formula

Theorem 15 (Green's Formula [Kress LIE Thm 6.5]) *If* $\triangle u = 0$, *then*

$$(S(\hat{n} \cdot \nabla u) - Du)(x) = \begin{cases} u(x) & x \in D \\ \frac{u(x)}{2} & x \in \partial D \\ 0 & x \notin D \end{cases}$$

Suppose I know 'Cauchy data' $(u|_{\partial D}, \hat{n} \cdot \nabla u|_{\partial D})$ of u. What can I do?

Compute u anywhere.

What if D is an exterior domain?

No longer holds

Things harmonic functions (don't) do

Theorem 16 (Mean Value Theorem [Kress LIE Thm 6.7]) *If* $\Delta u = 0$,

$$u(x) = \overline{\int_{B(x,r)}} u(y)dy = \overline{\int_{\partial B(x,r)}} u(y)dy$$

Define $\overline{\int}$?

$$|\Omega| := \int_\Omega 1dx, \qquad \overline{\int_\Omega} f(x)dx = \frac{1}{|\Omega|}\int_\Omega f(x)dx.$$

Trace back to Green's Formula (say, in 2D):

$$u(x) = (S(\hat{n} \cdot \nabla u) - Du)(x) = \frac{1}{2\pi} \log(r) \underbrace{\int_{\partial B} \hat{n} \cdot \nabla u}_{0} - \frac{1}{2\pi r} \int_{\partial B} u.$$

Theorem 17 (Maximum Principle [Kress LIE 6.9]) *If $\triangle u = 0$ on compact set $\bar{D}$: u attains its maximum on the boundary.*

Suppose it were to attain its maximum somewhere inside an open set...

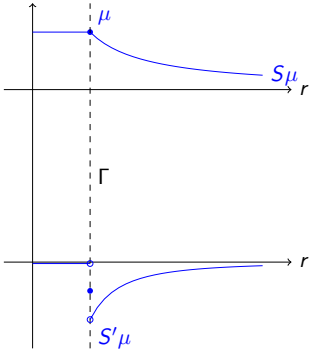
Then we'd be able to get the value there by averaging over a neighborhood. $\rightarrow$ some points there have to be as high or higher.

So boundaries are special.

What do our *constructed* harmonic functions (i.e. layer potentials) do there?

Good question $\rightarrow$ next slide.

Jump relations



Let $[X] = X_+ - X_-$. (Normal points towards "+"="exterior".)

[Kress LIE Thm. 6.14, 6.17,6.18]

$$
\begin{aligned}
& & & [S\sigma] = 0 \\
\lim_{x \to x_0 \pm} (S'\sigma) = \left(S' \mp \frac{1}{2} I \right) (\sigma)(x_0) & \quad \Rightarrow \quad & [S'\sigma] = -\sigma \\
\lim_{x \to x_0 \pm} (D\sigma) = \left(D \pm \frac{1}{2} I \right) (\sigma)(x_0) & \quad \Rightarrow \quad & [D\sigma] = \sigma \\
& & & [D'\sigma] = 0
\end{aligned}
$$

Truth in advertising: Assumptions on Γ?

Needs to be C^2, i.e. twice continuously differentiable.

Green's Formula at Infinity (skipped)

$\Omega \subseteq \mathbb{R}^n$ bounded, C^1, connected boundary, $\triangle u = 0$, u bounded

$$(S_{\partial\Omega}(\hat{n} \cdot \nabla u) - D_{\partial\Omega} u)(x) + (S_{\partial B_r}(\hat{n} \cdot \nabla u) - D_{\partial B_r} u)(x) = u(x)$$

for x between $\partial\Omega$ and B_r.

Now $r \to \infty$.

Behavior of individual terms?

Theorem 18 (Green's Formula in the exterior [Kress LIE Thm 6.10])

$$(S_{\partial\Omega}(\hat{n} \cdot \nabla u) - D_{\partial\Omega} u)(x) + \mathrm{PV} u_\infty = u(x)$$

for some constant u_∞. Only *for* $n = 2$,

$$u_\infty = \frac{1}{2\pi r} \int_{|y|=r} u(y) ds_y.$$

Theorem 19 (Green's Formula in the exterior [Kress LIE Thm 6.10])

$$(S_{\partial\Omega}(\hat{n} \cdot \nabla u) - D_{\partial\Omega} u)(x) + u_\infty = u(x)$$

Realize the power of this statement:

Every bounded harmonic function is representable as...

Behavior of the fundamental solution as $r \to \infty$?

$$u(x) = u_\infty + O\left(\frac{1}{|x|}\right)$$

How about its derivatives?

$$\nabla u(x) = O\left(\frac{1}{|x|^{n-1}}\right)$$

8 Boundary Value Problems

8.1 Laplace

Boundary Value Problems: Overview

	Dirichlet	**Neumann**
Int.	$\lim_{x\to\partial\Omega-} u(x) = g$ ⊕ unique	$\lim_{x\to\partial\Omega-} \hat{n}\cdot\nabla u(x) = g$ ⊖ may differ by constant
Ext.	$\lim_{x\to\partial\Omega+} u(x) = g$ $u(x) = \begin{cases} O(1) & 2D \\ o(1) & 3D \end{cases}$ as $\lvert x\rvert \to \infty$ ⊕ unique	$\lim_{x\to\partial\Omega+} \hat{n}\cdot\nabla u(x) = g$ $u(x) = o(1)$ as $\lvert x\rvert \to \infty$ ⊕ unique

with $g \in C(\partial\Omega)$.

What does $f(x) = O(1)$ mean? (and $f(x) = o(1)$?)

$$f(x) = O(g(x)) \Leftrightarrow \frac{f(x)}{g(x)} \leqslant C, \qquad f(x) = o(g(x)) \Leftrightarrow \frac{f(x)}{g(x)} \to 0.$$

Dirichlet uniqueness: why?

(Hint: Maximum principle)

Neumann uniqueness: why?

Suppose two solutions exist and difference $\tilde{u} = u_1 - u_2$ is not constant. Then $\nabla \tilde{u} \neq 0$ somewhere. Then:

$$\int_\Omega u \triangle u + \nabla u \cdot \nabla v = \int_{\partial\Omega} u(\hat{n} \cdot \nabla v) ds$$

gives:

$$0 < \int_\Omega |\nabla \tilde{u}|^2 = \int_{\partial\Omega} \tilde{u}(\underbrace{\hat{n} \cdot \nabla \tilde{u}}_{0}) ds = 0.$$

Truth in advertising: Missing assumptions on Ω?

Above works cleanly if boundary is C^2, i.e. twice continuously differentiable.

What's a DtN map?

Given Dirichlet data, find Neumann data. Possible!

Next mission: Find IE representations for each.

Uniqueness of Integral Equation Solutions

Theorem 20 (Nullspaces [Kress LIE Thm 6.20])

- $N(I/2+D) = \text{span}\{1\}$, $N(I/2+S') = \text{span}\{\psi\}$, *where* $\int \psi \neq 0$.
- $N(I/2-D) = N(I/2-S') = \{0\}$

Show $N(I/2 - D) = \{0\}$.

- Suppose $\varphi/2 - D\varphi = 0$. To show: $\varphi = 0$.
- $u(x) := D\varphi(x)$ is harmonic off $\partial\Omega$, $u^- = D\varphi - \varphi/2 = 0$.
- Because of interior Dirichlet uniqueness, $u|_\Omega = 0$.
- $(\partial_n u)^+ = 0$ by the jump relations.
- u has the right decay at ∞, so solves ext. Neumann problem (unique)

- $u = 0$ everywhere.
- $\varphi = u^+ - u^- = 0$.

Show $N(I/2 - S') = \{0\}$.

$I/2 - S' = I/2 - D^*$, Fredholm alternative.

Show $N(I/2 + D) = \text{span}\{1\}$.

- Suppose $\varphi/2 + D\varphi = 0$. To show: φ constant
- $u(x) := D\varphi(x)$ is harmonic off $\partial\Omega$, $u^+ = D\varphi + \varphi/2 = 0$.
- Has right decay, so exterior Dirichlet uniqueness says $u|_{\bar{\Omega}^c} = 0$.
- Jump relations for $\partial_n u$ yield $(\partial_n u)^- = 0$.
- Interior Neumann 'uniqueness' says $u = \text{const}$ in Ω.
- Jump relations say $\varphi = \text{const}$ on $\partial\Omega$.

- Can use Green's thm to show that D1+1/2=0.

What extra conditions on the RHS do we obtain?

$(I - A)(X) = N(I - A^*)^{\perp}$

$\rightarrow$ "Clean" Existence for 3 out of 4.

Patching up Exterior Dirichlet (skipped)

Problem: $N(I/2 + S') = \{\psi\}$...but we do not know ψ.

Use a different kernel:

$$\hat{n} \cdot \nabla_y G(x, y) \qquad \rightarrow \qquad \hat{n} \cdot \nabla_y G(x, y) + \frac{1}{|x|^{n-2}}$$

Note: Singularity only at origin! (assumed $\in \Omega$)

- 2D behavior? 3D behavior?
- Still a solution of the PDE?
- Compact?
- Jump condition? Exterior limit? Deduce $u = 0$ on exterior.
- $|x|^{n-2} u(x) =?$ on exterior
- Thus $\int \phi = 0$. Contribution of the second term?
- $\phi/2 + D\phi = 0$, i.e. $\phi \in N(I/2 + D) =?$

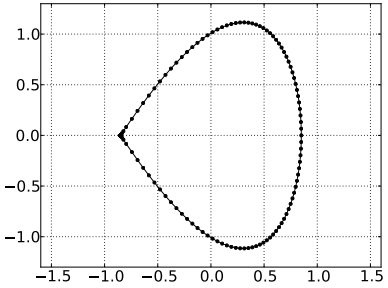
- Existence/uniqueness?

$\rightarrow$ Existence for 4 out of 4.

> Remaining key shortcoming of IE theory for BVPs?

Smooth domains only $\rightarrow$ next slide

Domains with Corners



What's the problem? *(Hint: Jump condition for constant density)*

At corner x_0: (2D)

$$\lim_{x \to x_0 \pm} = \int_{\partial\Omega} \hat{n} \cdot \nabla_y G(x, y) \phi(y) ds_y \pm \frac{1}{2} \frac{\langle \text{opening angle on } \pm \text{ side} \rangle}{\pi} \phi$$

$\rightarrow$ non-continuous behavior of potential on Γ at x_0

What space have we been living in?

Fixes:

- I + Bounded (Neumann) + Compact (Fredholm)

- Use L^2 theory

  (point behavior "invisible")

Numerically: Needs consideration, but ultimately easy to fix.

8.2 Helmholtz

Where does Helmholtz come from?

Derive the Helmholtz equation from the wave equation

$$\partial_t^2 U = c^2 \triangle U,$$

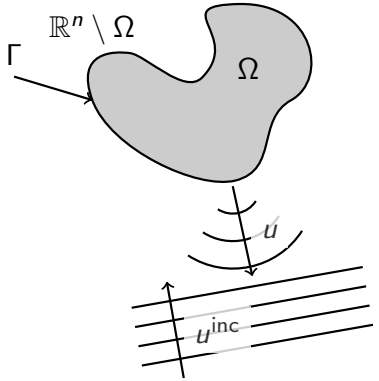
Q: What is c? "*Sound speed*"/Speed of propagation

Ansatz: $U(x,t) = u(x)e^{-i\omega t}$. Plug in:

$$\begin{aligned}
u(x)\partial_t^2[e^{-i\omega t}] &= c^2 e^{-i\omega t}\triangle u(x) \\
u(x)(-i\omega)^2 e^{-i\omega t} &= c^2 e^{-i\omega t}\triangle u(x) \\
-u(x)\omega^2 &= c^2 \triangle u(x) \\
0 &= c^2\triangle u(x) + \omega^2 u(x) \\
&= \triangle u(x) + \left(\frac{\omega}{c}\right)^2 u(x) \\
0 &= \triangle u(x) + k^2 u(x)
\end{aligned}$$

where $k = \omega/c$ is called the *wave number*.

The prototypical Helmholtz BVP: A Scattering Problem



Ansatz:

$$u^{\text{tot}} = u + u^{\text{inc}}$$

Solve for scattered field u.

Helmholtz: Some Physics

Physical quantities:

- Velocity potential: $U(x,t) = u(x)e^{-i\omega t}$

  (fix phase by e.g. taking real part)
- Velocity: $v = (1/\rho_0)\nabla U$
- Pressure: $p = -\partial_t U = i\omega u e^{-i\omega t}$
  - Equation of state: $p = f(\rho)$

What's ρ_0?

The wave equation is a linearization of (nonlinear) Euler, and ρ_0 is the 'equilibrium' density about which we've linearized.

What happens to a pressure BC as $\omega \to 0$?

It disappears!

Helmholtz: Boundary Conditions

- **Sound-soft**: Pressure remains constant
  - Scatterer "gives"
  - $u = f \rightarrow$ Dirichlet
- **Sound-hard**: Pressure same on both sides of interface
  - Scatterer "does not give"
  - $\hat{n} \cdot \nabla u = 0 \rightarrow$ Neumann
- **Impedance**: Some pressure translates into motion
  - Scatterer "resists"
  - $\hat{n} \cdot \nabla u + ik\lambda u = 0 \rightarrow$ Robin $(\lambda > 0)$
- **Sommerfeld** radiation condition: allow only outgoing waves

$$r^{\frac{n-1}{2}} \left(\frac{\partial}{\partial r} - ik \right) u(x) \rightarrow 0 \qquad (r \rightarrow \infty)$$

(where n is the number of space dimensions)

Many interesting BCs $\rightarrow$ many IEs! :)

Transmission between media: What's continuous?

Normal velocity, pressure.

Unchanged from Laplace

Theorem 21 (Green's Formula [Colton/Kress IAEST Thm 2.1]) *If* $\triangle u + k^2 u = 0$, *then*

$$(S(\hat{n} \cdot \nabla u) - Du)(x) = \begin{cases} u(x) & x \in D \\ \frac{u(x)}{2} & x \in \partial D \\ 0 & x \notin D \end{cases}$$

$$\begin{aligned} & & [Su] &= 0 \\ \lim_{x \to x_0 \pm} (S'u) = \left(S' \mp \frac{1}{2} I\right)(u)(x_0) \quad & \Rightarrow \quad & [S'u] = -u \\ \lim_{x \to x_0 \pm} (Du) = \left(D \pm \frac{1}{2} I\right)(u)(x_0) \quad & \Rightarrow \quad & [Du] = u \\ & & &= 0 \end{aligned}$$

Why is singular behavior (esp. jump conditions) unchanged?

$e^{ikr} = 1 + O(r)$

Why does Green's formula survive?
Remember Green's theorem:

$$\int_{\Omega} u \triangle v - v \triangle u = \int_{\partial\Omega} u(\hat{n} \cdot \nabla v) - v(\hat{n} \cdot \nabla u) ds$$

Resonances

$-\triangle$ on a bounded (interior) domain with homogeneous Dirichlet/Neumann BCs has countably many real, positive eigenvalues.

What does that have to with Helmholtz?

$$-\triangle u = \lambda u$$
$$\triangle u + k^2 u = 0$$

Why could it cause grief?

Non-uniqueness/nullspaces.

Helmholtz: Boundary Value Problems

Find $u \in C(\bar{D})$ with $\triangle u + k^2 = 0$ such that

	Dirichlet	**Neumann**
Int.	$\lim_{x \to \partial D-} u(x) = g$ unique ($-$resonances)	$\lim_{x \to \partial D-} \hat{n} \cdot \nabla u(x) = g$ unique ($-$resonances)
Ext.	$\lim_{x \to \partial D+} u(x) = g$ Sommerfeld unique	$\lim_{x \to \partial D+} \hat{n} \cdot \nabla u(x) = g$ Sommerfeld unique

with $g \in C(\partial D)$.

Find layer potential representations for each.

First idea: Same as Dirichlet. But: (see next slide).

Patching up resonances

Issue: Ext. IE inherits non-uniqueness from 'adjoint' int. BVP

Fix: Tweak representation [Brakhage/Werner '65, ...]

(also called the '*CFIE*'–'*combined field integral equation*')

$$u = D\phi - i\alpha S\phi$$

(α: tuning knob $\to 1$ is fine, $\sim k$ better for large k)

How does this help?

For simplicity, we'll choose the the scaling parameter $\alpha = 1$, so that

$$u = D\varphi + iS\varphi.$$

The exterior Dirichlet BC yields the integral equation (by way of the jump relations for S and D):

$$\frac{\varphi}{2} + D\varphi - iS\varphi = g.$$

Suppose $\varphi/2 + D\varphi - iS\varphi = 0$. We want to show $\varphi = 0$.

From the IE, we conclude that $\lim_+ u = 0$. Using exterior uniqueness, we conclude that $u = 0$ in the entire exterior, thus $\lim_+ \hat{n} \cdot \nabla u = 0$ also. The jump relations for the double and single layer then give us

$$\begin{aligned} 0 - (\hat{n} \cdot \nabla u)^- = [\hat{n} \cdot \nabla u] &= [\hat{n} \cdot \nabla (D\varphi - iS\varphi)] = -[iS'\varphi] = i\varphi \\ 0 - u^- = u^+ - u^- = [u] &= [D\varphi - iS\varphi] = [D\varphi] = \varphi \end{aligned}$$

Equating right the right hand sides, we get

$$-i(\hat{n} \cdot \nabla u)^- = u^-.$$

Green's first theorem then yields

$$\int_\Omega -k^2|u|^2 + |\nabla u \Big|^2 = \int_\Omega u \triangle \bar{u} + |\nabla u \Big|^2 = \int_{\partial\Omega} u^- \overline{(\hat{n} \cdot \nabla u)^-} \mathrm{d}s = -i \int_{\partial\Omega} |u^-|^2 \mathrm{d}s.$$

Taking the imaginary part yields

$$\int_{\partial\Omega} |u^-|^2 \mathrm{d}s = 0.$$

Using $u^+ = u^- = 0$ and the jump relation for the double layer, we obtain $\varphi = 0$ as desired.

Uniqueness for remaining IEs similar. (skipped)

- Set RHS of IE to 0.
- Use uniqueness to get zero limit on one side.
- Use jump condition to get zero limit on other side.
- Go to "other" jump condition to get zero limit on other side.
- Use jump condition to show density $= 0$.

$\Rightarrow$ Existence for all four BVPs.

8.3 Calderón identities

Show that D' is self adjoint.

- To show: $(D'\varphi, \psi) = (\varphi, D'\psi)$
- Introduce: $u = D\varphi, \quad v = D\psi$
- Green's second thm (here, in part thanks to Sommerfeld):

$$\int_{\partial\Omega} (\hat{n} \cdot \nabla u) v = \int_{\partial\Omega} u (\hat{n} \cdot \nabla v)$$

- Then:

$$\begin{aligned} & (D'\varphi, \psi) \\ = \; & (\hat{n} \cdot \nabla u, [v]) \\ = \; & (u^+, \hat{n} \cdot \nabla v^+) - (u^-, \hat{n} \cdot \nabla v^-) \\ = \; & (u^+ - u^-, \hat{n} \cdot \nabla v) \\ = \; & (\varphi, D'\psi) \end{aligned}$$

Show that $(S\varphi, D'\psi) = ((S' + I/2)\varphi, (D - I/2)\psi)$.

(Ideas similar as above, only use an interior limit since S and D' are continuous.)

$(\varphi, SD'\psi)$?

$$
\begin{aligned}
& (\varphi, SD'\psi) \\
= \; & (S\varphi, D'\psi) \\
= \; & ((S' + I/2)\varphi, (D - I/2)\psi) \\
= \; & (\varphi, (D + I/2)(D - I/2)\psi) \\
= \; & (\varphi, (D + I/2)(D - I/2)\psi) \\
= \; & (\varphi, (D^2 - I/4)\psi)
\end{aligned}
$$

Calderón Identities: Summary

- $SD' = D^2 - I/4$
- $D'S = S'^2 - I/4$

Also valid for Laplace (jump relation same after all!)

Why do we care?

$\rightarrow$ Exterior Neumann IE has D'. But: Hypersingular is yucky.

Right-precondition with a single layer.

$\rightarrow$ "*Calderón preconditioning*"

9 Back from Infinity: Discretization

9.1 Fundamentals: Meshes, Functions, and Approximation

Numerics: What do we need?

- Discretize curves and surfaces
  - Interpolation
  - Grid management
  - Adaptivity
- Discretize densities
- Discretize integral equations
  - Nyström, Collocation, Galerkin
- Compute integrals on them
  - "Smooth" quadrature
  - Singular quadrature
- Solve linear systems

Constructing Discrete Function Spaces

Floating point numbers (*Degrees of Freedom*/*DoFs*)	$\rightarrow$	Functions
	$\leftarrow$	

Discretization relies on three things:

- Base/reference domain
- Basis of functions
- Meaning of DoFs

Related finite element concept: *Ciarlet triple*

Discretization options for a curve?

- Equispaced
- Fourier modes (actually different from equispaced?)

- Piecewise polynomials

What do the DoFs mean?

Common DoF choices:

- Point values of function
- Point values of (directional?) derivatives
- Basis coefficients
- Moments

Often: useful to have both “modes”, “nodes”, jump back and forth

Why high order?

Order p: Error bounded as

$$|u_h - u| \leq Ch^p$$

Thought experiment:

First order	Fifth order
1,000 DoFs $\approx$ 1,000 triangles	1,000 DoFs $\approx$ 66 triangles
Error: 0.1	Error: 0.1
Error: 0.01 $\rightarrow$?	Error: 0.01 $\rightarrow$?

Complete the table.

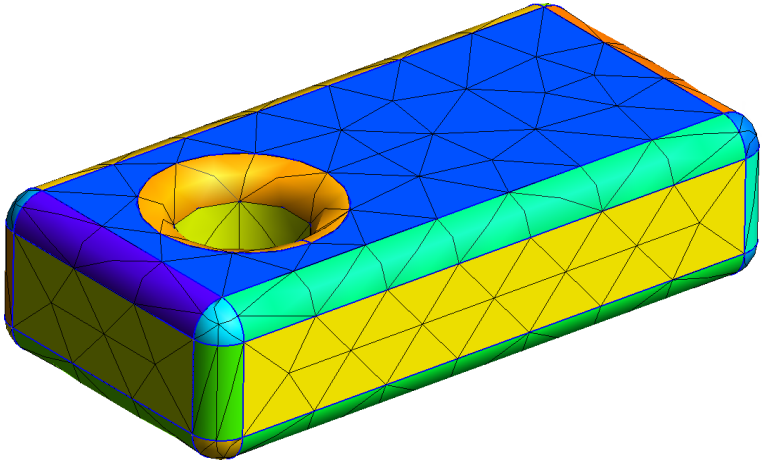
First	Fifth
@100,000 DoFs $\approx$ 100,000 triangles	@1,800 DoFs$\approx$ 120 triangles

Remarks:

- Want $p \geq 3$ available.

- **Assumption:** Solution sufficiently smooth
- Ideally: p chosen by user

What is an Unstructured Mesh?



Why have an unstructured mesh?

- Adaptable to many engineering problems
- Deal with topology
- Deal with solution non-smoothness

- Adaptivity in space
- Adaptivity in time

What is the trade-off in going unstructured?

- Complexity: Data structures, algorithms, generation
- Where do meshes come from?

  Demo: CAD software
- What is a ‘reference element’?

Fixed-order vs Spectral

Fixed-order	Spectral
Number of DoFs n	Number of DoFs n
$\sim$	$\sim$
Number of 'elements'	Number of modes resolved
$\text{Error} \sim \frac{1}{n^p}$	$\text{Error} \sim \frac{1}{C^n}$
Examples? • Piecewise Polynomials	Examples? • Global Fourier • Global Orth. Polynomials

What assumptions are buried in each of these?

Smoothness: Piecewise vs. Global

What should the DoFs be?

Natural DoF match:

- Fixed-order: point values
- Spectral: modal coefficients

What's the difficulty with purely modal discretizations?

Nonlinearities are hard to express.

$\rightarrow$ Use point values to compute those. ('*Pseudospectral methods*')

Vandermonde Matrices

$$\begin{pmatrix} x_0^0 & x_0^1 & \cdots & x_0^n \\ x_1^0 & x_1^1 & \cdots & x_1^n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^0 & x_n^1 & \cdots & x_n^n \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = ?$$

Generalized Vandermonde Matrices

$$\begin{pmatrix} \phi_0(x_0) & \phi_1(x_0) & \cdots & \phi_n(x_0) \\ \phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_n(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_n) & \phi_1(x_n) & \cdots & \phi_n(x_n) \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = ?$$

Generalized Vandermonde Matrices

$$\begin{pmatrix} \phi_0(x_0) & \phi_1(x_0) & \cdots & \phi_n(x_0) \\ \phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_n(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_n) & \phi_1(x_n) & \cdots & \phi_n(x_n) \end{pmatrix} \text{MODAL COEFFS} = \text{NODAL COEFFS}$$

Node placement?

Demo: Interpolation node placement

Vandermonde conditioning?

Demo: Vandermonde conditioning

What about multiple dimensions?

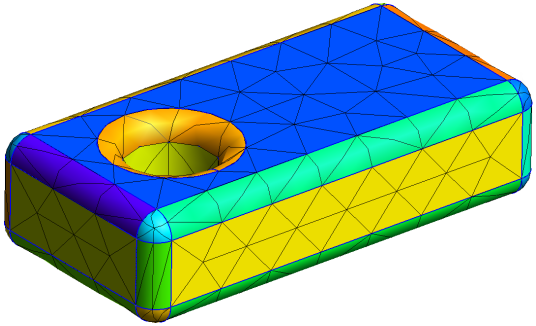
Demo: Visualizing the 2D PKDO Basis

Common Operations

(Generalized) Vandermonde matrices simplify common operations:

- Modal $\leftrightarrow$ Nodal ("Global interpolation")
  - Filtering
  - Up-/Oversampling
- Point interpolation (Hint: solve using V^T)
- Differentiation
- Indefinite Integration
- Inner product
- Definite integration

Unstructured Mesh



- Design a data structure to represent this
- Compute normal vectors
- Compute area
- Compute integral of a function
- How is the function represented?

9.2 Integral Equation Discretizations

Integral Equation Discretizations: Overview

$$\phi(x) - \int_\Gamma K(x,y)\phi(y)dy = f(y)$$

Nyström	Projection
• Approximate integral by quadrature: $\int_\Gamma f(y)dy \quad \to \quad \sum_{k=1}^n \omega_k f(y_k)$ • Evaluate quadrature'd IE at quadrature nodes, solve	• Consider residual: $R := \phi - A\phi - f$ • Pick projection P_n onto finite-dimensional subspace $P_n\phi := \sum_{k=1}^n \langle \phi, v_k \rangle w_k$ $\to$ DOFs $\langle \phi, v_k \rangle$ • Solve $P_n R = 0$

- Equivalent to projection: Test IE with test functions
- Important in projection methods: *sub*space (e.g. of $C(\Gamma)$)

Name some possible bases for projection?

Name some generic discrete projection bases.

- Galerkin: $v_k = w_k$

  Commonly: polynomials.
- Collocation:

  $v_k = \delta(x_k)$, $w_k(x_j) = \delta_{jk}$
- Petrov-Galerkin: $v_k \neq w_k$

  Commonly: polynomials

Collocation and Nyström: the same?

No–collocation demands that the integrals be computed *exactly*.

Are projection methods implementable?

No, not usually–because the integrals would need to be computed *exactly*.

Nyström discretizations

Nyström consists of two distinct steps:

1. Approximate integral by quadrature:

$$\varphi_n(x) - \sum_{k=1}^{n} \omega_k K(x, y_k)\varphi_n(y_k) = f(x) \tag{3}$$

2. Evaluate quadrature'd IE at quadrature nodes, solve discrete system

$$\varphi_j^{(n)} - \sum_{k=1}^{n} \omega_k K(x_j, y_k)\varphi_k^{(n)} = f(x_j) \tag{4}$$

with $x_j = y_j$ and $\varphi_j^{(n)} = \varphi_n(x_j) = \varphi_n(y_j)$

Is version (3) solvable?

No–still deals with functions in x. Infinitely many 'rows', but only n 'columns'.

What's special about (4)?

Density only known at point values

No continuous density

Solution density also only known at point values. But: can get approximate continuous density. How?

$$\tilde{\varphi}(x) = f(x) - \sum_{k=1}^{n} \omega_k K(x, y_k) \varphi_k^{(n)}.$$

Assuming the IE comes from a BVP. Do we also only get the BVP solution at discrete points?

No: Using the (now discrete) representation, we can still evaluate the BVP solution anywhere.

Does (3) $\Rightarrow$ (4) hold?

Sure–if it's true for a function φ, it should be true for point values of that function.

Does (4) $\Rightarrow$ (3) hold?

Actually–it must! $\varphi_k^{(n)}$ are point values of the density (since we satisfied (4)!), and so the 'approximate' $\tilde{\varphi}$ was not so approximate after all–it must be the function that solves (3).

What good does that do us?

Goal: say something about error

I.e.: does the method work at all?

Point: much easier to examine error between (3) and the IE

(than (4) and the IE)

Can stay in function space, no need to mess with varying dimensionality.

> Does Nyström work for first-kind IEs?

No. Specifically because backing out the density relies on second-kind.

Convergence for Nyström

Increase number of quadrature points n:

Get sequence (A_n)

Want $A_n \to A$ in some sense

What senses of convergence are there for sequences of functions f_n?

- pointwise
- uniform ('in the $\|\cdot\|_\infty$ norm')
- (and a few more)

What senses of convergence are there for sequences of operators A_n?

- functionwise (the analog to 'pointwise')
- uniform (in the operator norm)
- for sequences of operators (A_n)?

Will we get norm convergence $\|A_n - A\|_\infty \to 0$ for Nyström?

No: Pick $\psi_\epsilon = 1$ everywhere except in ϵ-nbh of quad nodes, 0 there.

Show:

- $\|A\phi\psi_\epsilon - A\phi\|_\infty \to 0$ $(\epsilon \to 0)$
- $\|A - A_n\|_\infty \geq \|A\|_\infty$

Is functionwise convergence good enough?

No, not at all. When we're solving $A\varphi = b$, we want all possible densities to be roughly 'equally far along' in convergence.

So neither notion of convergence really 'works' for Nyström.

$\to$ Compactness to the rescue.

Compactness-Based Convergence

X Banach space (think: of functions)

Theorem 22 (Not-quite-norm convergence [Kress LIE Cor 10.4]) $A_n : X \to X$ *bounded linear operators,*
functionwise convergent to $A : X \to X$
Then convergence is uniform on compact subsets $U \subset X$*, i.e.*

$$\sup_{\phi \in U} \|A_n \phi - A\phi\| \to 0 \qquad (n \to \infty)$$

How is this different from norm convergence?

Only on compact subsets of X*!*

Set $\mathcal{A}$ of operators $A : X \to X$

Definition 18 (Collectively compact) $\mathcal{A}$ *is called* collectively compact *if and only if*
for $U \subset X$ *bounded,* $\mathcal{A}(U)$ *is relatively compact.*

What was relative compactness (=precompactness)?

Has a convergent subsequence.

(that doesn't necessarily converge in the set.)

Is each operator in the set $\mathcal{A}$ compact?

Yes.

When is a sequence collectively compact?

The definition applies to sequences-viewed-as-sets as is.

Is the limit operator of such a sequence compact?

Yes.

How can we use the two together?

- We'll have a sequence of operators A_n that's collectively compact.
- Then we get norm convergence on the range of the operators A.

Making use of Collective Compactness

X Banach space, $A_n : X \to X$, (A_n) collectively compact, $A_n \to A$ functionwise.

Corollary 1 (Post-compact convergence [Kress LIE Cor 10.8])

- $\|(A_n - A)A\| \to 0$
- $\|(A_n - A)A_n\| \to 0$

$(n \to \infty)$

Anselone's Theorem

Assume:

$(I - A)^{-1}$ exists, with $A : X \to X$ compact, $(A_n) : X \to X$ collectively compact and $A_n \to A$ functionwise.

Theorem 23 (Nyström error estimate [Kress LIE Thm 10.9]) *For sufficiently large n, $(I - A_n)$ is invertible and*

$$\|\phi_n - \phi\| \leq C(\|(A_n - A)\phi\| + \|f_n - f\|)$$

$$C = \frac{1 + \|(I - A)^{-1}A_n\|}{1 - \|(I - A)^{-1}(A_n - A)A_n\|}$$

$I + (I - A)^{-1}A =?$

$(I - A)^{-1}$. (Idea: What would happen for fractions?)

Show the theorem.

Define approximate inverse $B_n = I + (I - A)^{-1}A_n$.

How good of an inverse is it?

$$
\begin{aligned}
\mathrm{Id} &\approx^{?} B_n(I - A_n) \\
&= (I + (I - A)^{-1}A_n)(I - A_n) \\
&= [I + (I - A)^{-1}A_n] - [A_n + (I - A)^{-1}A_nA_n] \\
&= [I + (I - A)^{-1}A_n] - [(I - A)^{-1}(I - A)A_n + (I - A)^{-1}A_nA_n] \\
&= [I + (I - A)^{-1}A_n] - [(I - A)^{-1}IA_n - (I - A)^{-1}AA_n + (I - A)^{-1}A_nA_n] \\
&= I + (I - A)^{-1}\,\mathrm{A}A_n - (I - A)^{-1}A_nA_n \\
&= I + \underbrace{(I - A)^{-1}(A - A_n)A_n}_{-S_n} = I - S_n
\end{aligned}
$$

Want $S_n \to 0$ somehow. Prior result gives us $\|(A - A_n)A_n\| \to 0$.

So $\|S_n\| \to 0$.

Using Neumann series:

$$\left\|(I - S_n)^{-1}\right\| \leqslant \frac{1}{1 - \|S_n\|}$$

if $\|S_n\| < 1$. In particular: The inverse exists!

Long story short from earlier:

$$B_n(I - A_n) = I - S_n,$$

So $I - A_n$ must also be invertible. Rearrange:

$$(I - A_n)^{-1} = (I - S_n)^{-1} B_n,$$

Let φ be the exact density that solves $(I - A)\varphi = f$ and φ_n the approximate density that solves $(I - A_n)\varphi_n = f_n$. Then consider

$$\begin{aligned}(I - A_n)(\varphi_n - \varphi) &= f_n - (I - A_n)\varphi \\ &= f_n - (I - A)\varphi + (A - A_n)\varphi \\ &= f_n - f + (A - A_n)\varphi\end{aligned}$$

Combining all this knowledge as

$$\begin{aligned} \|\varphi_n - \varphi\| &\leqslant \|(I - A_n)^{-1}\|(\|f_n - f\| + \|(A_n - A)\varphi\|) \\ &\leqslant \frac{\|B_n\|}{1 - \|S_n\|}(\|f_n - f\| + \|(A_n - A)\varphi\|) \end{aligned}$$

gives the desired estimate.

Nyström: *specific to I+compact.* Why?

Used identity to fish out density more than once.

Nyström: Collective Compactness

Assume

$$\sum |\text{quad. weights for } n \text{ points}| \leq C \qquad \text{(independent of } n\text{)} \tag{5}$$

We've *assumed* collective compactness. Do we have that?

To use Arzelà-Ascoli, we'll need to show uniform boundedness (easy!) and equicontinuity of the sequence $(A_n\varphi)$ for a given density φ. To show the latter, consider

$$\begin{aligned} & |(A_n\varphi)(x_1) - (A_n\varphi)(x_2)| \\ = & \left| \sum_{i=1}^{n} \omega_i (K(x_1, y_i)\varphi(y_i) - K(x_1, y_i)\varphi(y_i)) \right| \\ \leqslant & \sum_{i=1}^{n} |\omega_i| \underbrace{(K(x_1, y_i) - K(x_1, y_i))}_{(*)} > \varphi >_\infty . \end{aligned}$$

$(*)$ bounded because K lives on a compact domain.

And

$$\sum_{i=1}^{n} |\omega_i|,$$

is bounded because we assumed it is. Since the constant doesn't depend on n: Collectively compact.

Also assumed functionwise uniform convergence, i.e. $\|A_n\phi - A\phi\| \to 0$ for each ϕ.

Follows from equicontinuity of $(A_n\phi)$.

Assumption (5) is important to make all this work!

9.3 Integral Equation Discretizations: Projection

Error Estimates for Projection

X Banach spaces, $A : X \to X$ injective, $P_n : X \to X_n$

Theorem 24 (Céa's Lemma [Kress LIE Thm 13.6]) *Convergence of the projection method*
$\Leftrightarrow$ *There exist n_0 and M such that for $n \geq n_0$*
1. *$P_n A : X_n \to X_n$ are invertible,*
2. *$\|(P_n A)^{-1} P_n A\| \leq M$.*

In this case,

$$\|\phi_n - \phi\| \leq (1 + M) \inf_{\psi \in X_n} \|\phi - \psi\|$$

Proof? (skipped)

- Defining equation for ϕ_n? (Write RHS in terms of ϕ.)
- Solve for ϕ_n

- Components of the error? What if $\phi \in X_n$?
- Build error estimate.

Core message of the theorem?

Projection doesn't destroy invertibility.

What goes into P_n?

The projection onto the finite-dimensional space.

Note domain of invertibility for $P_n A$.

It's just X_n! Cannot be all of X, because the projection is not (assumed to be) injective.

Domain/range of $(P_n A)^{-1} P_n A$?

Domain: All of X.

Range: Reachable solutions for $P_n A\varphi = f$.

Relationship to conditioning?

$\|(P_n A)^{-1} P_n A\| \leqslant \left\|(P_n A)^{-1}\right\| \|P_n A\| = \kappa$

Relationship to second-kind?

$A = (I - B)$ where B is the actual compact operator.

Exact projection methods: hard. (Why?) What if we implement a perturbation? (i.e. apply quadature instead of computing exact integrals?)

Possible to still do theory, but things get shakier.

Decisions, Decisions: Nyström or Galerkin?

Quote Kress LIE, 2nd ed., p. 244 (Sec. 14.1):

> [...] the Nyström method is generically stable whereas the collocation and Galerkin methods may suffer from instabilities due to a poor choice of basis for the approximating subspace.

Quote Kress LIE, 2nd ed., p. 244 (Sec. 13.5):

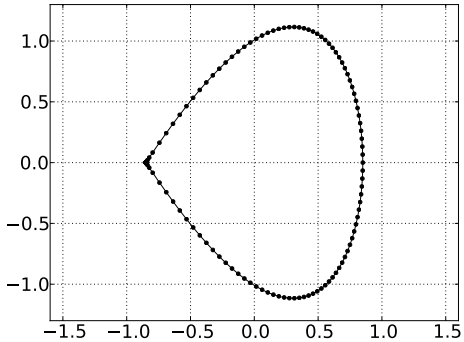
> In principle, for the Galerkin method for equations of the second kind the same remarks as for the collocation method apply. As long as numerical quadratures are available, in general, the Galerkin method cannot compete in efficiency with the Nyström method.
> Compared with the collocation method, it is less efficient, since its matrix elements require double integrations.

Need good quadratures to use Nyström.

Remaining advantage of Galerkin:

Can be made not to break for non-second-kind.

Galerkin without the Pain [Bremer et al. '11]



Problem: Singular behavior at corner points. Density may blow up.

Can the density be convergent in the $\|\cdot\|_\infty$ sense?

Conditioning of the discrete system?

GMRES will flail and break, because it sees $\ell^2 \sim l^\infty \sim L^\infty$ convergence.

Make GMRES 'see' L^2 convergence by redefining density DOFs:

$$\overline{\boldsymbol{\sigma}}_h := \begin{pmatrix} \sqrt{\omega_1}\sigma(x_1) \\ \vdots \\ \sqrt{\omega_n}\sigma(x_n) \end{pmatrix} = \sqrt{\boldsymbol{\omega}}\boldsymbol{\sigma}_h$$

So $\overline{\boldsymbol{\sigma}}_h \cdot \overline{\boldsymbol{\sigma}}_h =$?

Also fixes system conditioning! Why?

10 Computing Integrals: Approaches to Quadrature

‘Off-the-shelf’ ways to compute integrals

How do I compute an integral of a nasty singular kernel?

Symbolic integration

Good when it works.

Why not Gaussian?

Error estimate:

$$\left| \int f - \sum f(x_i)\omega_i \right| \leqslant \left\| f^{(p)} \right\| h^p$$

$\left\| f^{(p)} \right\|$ blows up!

Kussmaul-Martensen quadrature

Theorem 25 (A special integral [Kress LIE Lemma 8.21])

$$\frac{1}{2\pi}\int_0^{2\pi} \log\left(4\sin^2\frac{t}{2}\right) e^{imt}\,dt = \begin{cases} 0 & m = 0, \\ -\frac{1}{|m|} & m = \pm 1, \pm 2 \ldots . \end{cases}$$

Why is that exciting?

Demo: Kussmaul-Martensen quadrature

Singularity Subtraction

$$\int \langle \text{Thing } X \text{ you would like to integrate} \rangle$$
$$= \int \langle \text{Thing } Y \text{ you } \textit{can} \text{ integrate} \rangle$$
$$+ \int \langle \text{Difference } X - Y \text{ which is easy to integrate (numerically)} \rangle$$

Give a typical application.

Helmholtz: $H_0^{(1)}(x) = \log(x) + \text{smooth}$

Drawbacks?

Two integrals to compute.

High-Order Corrected Trapezoidal Quadrature

- Conditions for new nodes, weights

  ($\rightarrow$ linear algebraic system, dep. on n)

  to integrate

  $$\langle \text{smooth} \rangle \cdot \langle \text{singular} \rangle + \langle \text{smooth} \rangle$$

- Allowed singularities: $|x|^\lambda$ (for $|\lambda| < 1$), $\log |x|$
- Generic nodes and weights for log singularity
- Nodes and weights copy-and-pasteable from paper

[Kapur, Rokhlin '97]

Alpert '99 conceptually similar:

- Hybrid Gauss-Trapezoidal
- Positive weights

- Somewhat more accurate (empirically) than K-R
- Similar allowed singularities ($\lambda > -1$)
- Copy-paste weights

Generalized Gaussian

- "Gaussian":
  - Integrates $2n$ functions exactly with n nodes
  - Positive weights
- Clarify assumptions on system of functions ("Chebyshev system") for which Gaussian quadratures exist
- When do (left/right) singular vectors of integral operators give rise to Chebyshev systems?
  - In many practical cases!
- Find nodes/weights by Newton's method
  - With special starting point
- Very accurate
- Nodes and weights for download

[Yarvin/Rokhlin '98]

Singularity cancellation: Polar coordinate transform

$$\int \int_{\partial\Omega} K(\mathbf{x}, \mathbf{y})\phi(y) ds_y$$

$$=$$

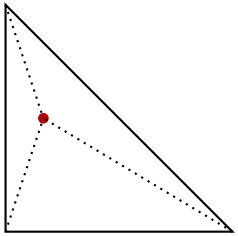
$$\int_0^R \int_{\mathbf{x}+\mathbf{r}\in\partial\Omega\cap\partial B(\mathbf{x},r)} K(\mathbf{x}, \mathbf{x}+\mathbf{r})\phi(\mathbf{x}+\mathbf{r}) d\langle \text{angles} \rangle \, r \, dr$$

$$=$$

$$\int_0^R \int_{\mathbf{x}+\mathbf{r}\in\partial\Omega\cap\partial B(\mathbf{x},r)} \frac{K_{\text{less singular}}(\mathbf{x}, \mathbf{x}+\mathbf{r})}{r} \phi(\mathbf{x}+\mathbf{r}) d\langle \text{angles} \rangle \, r \, dr$$

where $K_{\text{less singular}} = K \cdot r$.

Quadrature on triangles



Problem: Singularity can sit *anywhere* in triangle

$\rightarrow$ need *lots* of quadrature rules (one per target)

Kernel regularization

Singularity makes integration troublesome: *Get rid of it!*

$$\frac{\cdots}{\sqrt{(x-y)^2}} \quad \rightarrow \quad \frac{\cdots}{\sqrt{(x-y)^2+\epsilon^2}}$$

Use Richardson extrapolation to recover limit as $\epsilon \rightarrow 0$.

(May also use geometric motivation: limit along line towards singular point.)

Primary drawbacks:

- Low-order accurate
- Need to make ϵ smaller (i.e. kernel more singular) to get better accuracy

Can take many forms–for example:

- Convolve integrand to smooth it

  ($\rightarrow$ remove/weaken singularity)
- Extrapolate towards no smoothing

Related: [Beale/Lai '01]

10.1 Quadrature by expansion ('QBX')

(see the corresponding section of `http://bit.ly/1Msw0EQ`)

11 Going General: More PDEs

Inhomogeneous Problems

Example: Poisson

$$\triangle u = f, \qquad u = g \text{ on } \partial\Omega.$$

Steps:

1. Solve the PDE (without the boundary condition) using the free-space Green's function G:

   $$\tilde{u} = G * f,$$

   where '$*$' represents convolution.

2. Solve

   $$\triangle \hat{u} = 0, \qquad \hat{u} = g - \tilde{u} \text{ on } \partial\Omega$$

   using a boundary integral equation.

3. Add

   $$u = \tilde{u} + \hat{u},$$

   which solves the Poisson problem.

Eigenvalue Problems

Example: Solve

$$\triangle u = \lambda u.$$

Two options:

- Volume linear eigenvalue problem with Laplace kernel
- Surface nonlinear eigenvalue problem with Helmholtz kernel

Maxwell's equations

Example: Solve a scattering problem from a perfect electric conductor.

Use *Vector Potential* $\vec{A}$ to represent magnetic field:

$$\vec{H} = \vec{\nabla} \times \vec{A},$$

where

$$\triangle \vec{A} + k^2 \vec{A} = \vec{0}.$$

Since $\vec{A}$ solves vector Helmholtz, simply represent as

$$\vec{A}(x) = S_k \vec{J}_s,$$

where $\overrightarrow{J}_s$ (physically) amounts to a surface *current density*.

Then use

- the *continuity condition*

$$\vec{n} \times [\vec{H}_{\text{tot}}] = \vec{J}_s,$$

- the '*extinction theorem*' for perfect electrical conductors:

$$\vec{H}^{-}_{\text{tot}} = \vec{0}$$

  inside the scatterer.

- the jump conditions

together to obtain the *Magnetic Field Integral Equation* (*MFIE*):

$$\vec{n} \times \vec{H}^{+}_{\text{inc}} = \frac{J_s}{2} - \vec{n} \times (\text{PV}) \vec{\nabla} \times S_k \vec{J}_s.$$

Stokes flow

(see Nek's project presentation)