Fast Algorithms and Integral Equation Methods

CS598 APK

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Outline

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What's the point of this class?

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

Survey

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

Class web page

https://bit.ly/fastalg-f19

contains:

- Class outline
- Assignments
- Piazza
- Grading
- Video

Why study this at all?

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

FD/FEM: Issues

Idea of these methods:

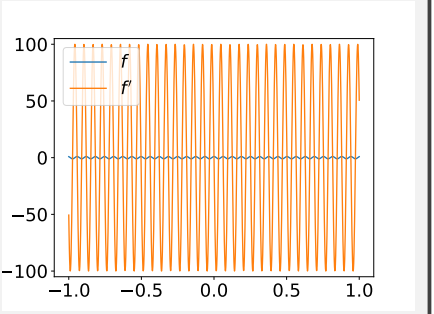
1. Take differential equations
2. Discretize derivatives
3. Make linear system
4. Solve

So what's wrong with doing that?

Discretizing Derivatives: Issues?

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?

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

Discretizing Derivatives: Issues?

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

Demo: Conditioning of Derivative Matrices

To be fair: Multigrid works around that (by judiciously using fewer points!)

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

> Inherent tradeoff: FP accuracy $\leftrightarrow$ Truncation error
>
> **Demo:** Floating point vs Finite Differences

Q: Are these problems real?

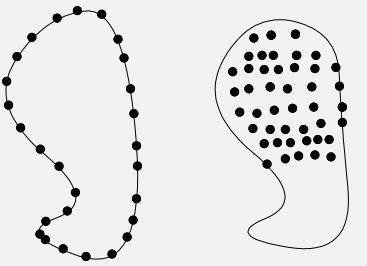
> $\rightarrow$ Try solving 3D Poisson with just FEM+CG.

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:



The number N is different! (And it's smaller for IEs.)
(Truth in advertising: Only for homogeneous problems.)

Outline

Matvec: A Slow Algorithm

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

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

Assume A dense.

Matrices and Point Interactions

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

Does that actually change anything?

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

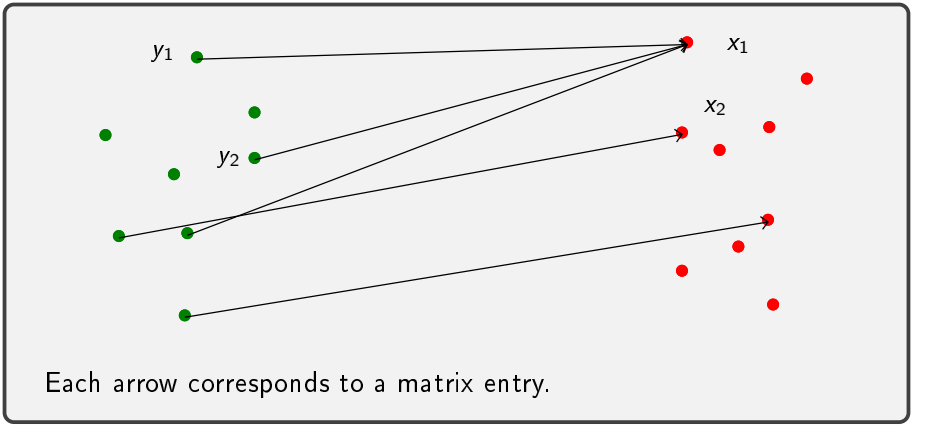
Technically: no difference.
Can translate back and forth between both views.
But: Gain terminology and intuition:

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

Matrices and Point Interactions

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

Graphically, too:



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 (I)

- (Lagrange) Interpolation: $\psi(x) = \sum_{j=1}^{N} \ell_j(x)\varphi(y_j)$
  - $(G(x, y_j) = \ell_j(x))$
  - Also: Interpolation Error!
- 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

Point Interaction Matrices: Examples (II)

- Potential Evaluation: Potential of an electron at the origin in 3D?

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

Potential of an electron at y in 3D? $U_y(x) = C \cdot \frac{1}{|x-y|}$

Potential of a number of electrons at a $y_1, \ldots, y_N$?

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

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

Point Interaction Matrices: Examples (III)

- 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, $O(n \log n)$ FFTs help
- Idea 3: If the matrix has low rank

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 (II)

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

Does this generalize? What is K here?

- $k = \operatorname{rank} A$
- Sure does generalize. Cost: $O(NK)$
- What if matrix has 'full' rank? Cost back to $O(N^2)$

Low-Rank Point Interaction Matrices

Usable with low-rank complexity reduction?

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

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

- *Separation of variables*
- Q: Did any of our examples look like this? Nope.
  $\rightarrow$ Check computationally.

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

- So it looks like the rank does decay, approximately
- Echelon form: good idea?

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

Theorem (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

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

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.

Representation (in context)

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 $\mathbb{R}^3$)

Outline

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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: $A \approx QQ^TA$, i.e. A being approximated by an orthogonal projection of its columns.
(Q has orthogonal columns, i.e. $Q^TQ = I$, and fewer 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 $C = Q^TA$.

Using LRA bases

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

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: $k^2 N$
- Step 3: $k^2 N$

Can we hope to do better overall? (#entries?)

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 construct 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

Tweaking the Range Finder (I)

Can we accelerate convergence?

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:

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

Tweaking the Range Finder (II)

What is one possible issue with the power method?

- Overflow/FP problems
- Normalization, orthogonalization
- If FP is a concern, apply QR after every application of A or A^T.

Even Faster Matvecs for Range Finding

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.

Outline

Errors in Random Approximations

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

Theorem

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 $|E|_2$.

Adaptive Range Finding: Algorithm

- 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

Outline

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

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

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 bottom half of R (and the corresponding bits of Q)
- Π is an $n \times n$ (column) permutation matrix

Using RRQR for LRA

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 developing: Find an orthogonal basis of the range.
- But: an $O(N^3)$ factorization.

Interpolative Decomposition (ID): Definition

Would be helpful to know *columns of A* that contribute 'the most' to the rank.
(orthogonal transformation like in QR 'muddies the waters')

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.

ID: Computation

How do we construct this (from RRQR): (short/fat case)

$A\Pi = Q \begin{bmatrix} R_{11} & R_{12} \end{bmatrix}$ Set $B = QR_{11} = (A\Pi)_{(:,J)}$.

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

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

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

ID Q vs ID A

What does row selection mean for the LRA?

Starting point: At end of stage 1, have LRA $A \approx QQ^T A$.
Run an ID on the *rows* (i.e. a *transpose ID*) of Q: $Q \approx PQ_{(J,:)}$
(Recall: Q is tall and skinny. $Q_{(J,:)}$ is a square subset.)

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

Now consider: $A_{(J,:)} \approx \underbrace{P_{(J,:)}}_{\text{Id}} Q_{(J,:)}Q^T A$

So $PA_{(J,:)} \approx PQ_{(J,:)}Q^T A \approx A$.
I.e. P for Q and A are essentially interchangeable!

[Martinsson, Rokhlin, Tygert '06]

ID: Remarks

Slight tradeoff here: what?

> Accuracy (two $\approx$ on previous slide) vs. expense

How would we use the ID in the context of the range finder?

- Can simply use ID on the sample matrix Y
- Because of (essentially) the same argument, P made from Y should transfer to A.

Demo: Interpolative Decomposition

What does the ID buy us?

Name a property that the ID has over other factorizations.

> It preserves (a subset of) matrix entries exactly.
> Copmosition with other transforms without (expensive!) matmats.

All our randomized tools have two stages:

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

Complexity?

> First step of this: $C = Q^T A \rightarrow O(N^2 k)$.
> For now, both stages are $O(N^2 k)$.

What is the impact of the ID?

- We avoid the need to form/work with $C = Q^T A$.
- Row subset $A_{(J,:)}$ assumes role of $Q^T A$

Leveraging the ID for SVD (I)

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:

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

Leveraging the ID for SVD (II)

In what way does this give us an SVD of A?

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

Leveraging the ID for SVD (III)

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 and do useful work (using SVD as a proxy for "useful work") in $O(N \cdot K^{\alpha})$ time (assuming availability of a cheap matvec).

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

Outline

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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.
Types 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!)

Smoothing Operators

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

1D Taylor: $f(c+h) \approx \sum_{p=0}^{k} \frac{f^{(p)}(c)}{p!} h^p$

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 and Error (I)

How can we estimate the error in a Taylor expansion?

Back to 1D: (nD is analogous)

$$\left| f(c+h) - \sum_{p=0}^{k} \frac{f^{(p)}(c)}{p!} h^p \right|$$

$$= \left| \sum_{p=k+1}^{\infty} \frac{f^{(p)}(c)}{p!} h^p \right|,$$

assuming that the function is identical to its infinite Taylor expansion.

Taylor and Error (II)

Now suppose that we had an estimate that $\left|\frac{f^{(p)}(c)}{p!}h^p\right| \leqslant \alpha^p$.

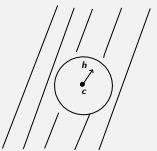
$$\begin{aligned}
&\left|\sum_{p=k+1}^{\infty}\frac{f^{(p)}(c)}{p!}h^p\right| \\
\leqslant &\sum_{p=k+1}^{\infty}\left|\frac{f^{(p)}(c)}{p!}h^p\right| \\
\leqslant &\sum_{p=k+1}^{\infty}\alpha^p = \frac{1}{1-\alpha}\cdot\alpha^{k+1}
\end{aligned}$$

If $\alpha < 1$, then this gives a viable bound.

- Slightly different technique from 'textbook' calculus technique.
- 'Textbook' like mean value theorem: not what we'll use.

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, then *low rank*!

Taylor on Potentials (I)

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, $\mathbf{c} = \mathbf{0}$. $\psi(\mathbf{h}) \approx \sum_{|p| \leq k} \frac{D^p \psi(\mathbf{0})}{p!} \mathbf{h}^p$

Taylor on Potentials (Ia)

Why is it interesting to consider Taylor expansions of Laplace point potentials?

- Fairly non-smooth (singular)
  - What works for them will also work for smoother functions
- Important application in its own right
  - N-body simulation
  - Integral equation solvers

Taylor on Potentials (II)

```
Maxima 5.42.1 http://maxima.sourceforge.net
(%i1) phi0: log(sqrt(y1**2 + y2**2));
                                        2     2
                                   log(y2  + y1 )
(%o1)                              --------------
                                         2
(%i2) diff(phi0, y1);
                                        y1
(%o2)                               ---------
                                      2     2
                                     y2  + y1
(%i3) diff(phi0, y1, 5);
                                            3               5
                      120 y1         480 y1          384 y1
(%o3)              ------------ - ------------ + ------------
                     2     2 3      2     2 4      2     2 5
                   (y2  + y1 )    (y2  + y1 )    (y2  + y1 )
(%i4)
```

Taylor on Potentials (III)

Which of these is the most dangerous (largest) term?
$\rightarrow$ Hard to say. They all contain the same number of powers of components of $\mathbf{y}$.

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

$$\left| \frac{5040 y_1}{(y_2^2 + y_1^2)^4} \right| \leqslant C \left| \frac{y_1}{R^8} \right| \leqslant C \frac{1}{R^7}.$$

'Generalize' this bound:

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

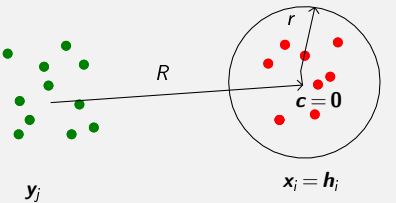
Appears true at least from the few p we tried. (Actually is true.)
C_p is a 'generic constant'–its value could change from one time it's written to the next.

Taylor on Potentials (IV)

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.)

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



Taylor on Potentials (V)

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.

Taylor on Potentials (VI)

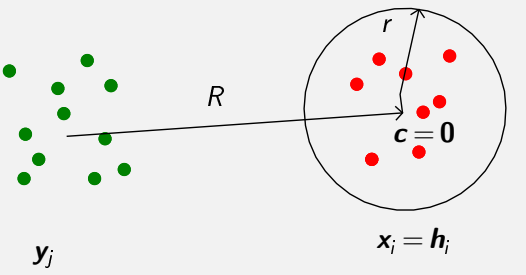
A few remarks:

- 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

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

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.

Outline

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*.

Multipole Expansions (I)

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

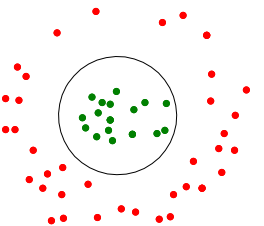
$$(*) \leqslant C_p \left(\frac{\max_j \|\mathbf{y}_i - \mathbf{c}\|_2}{\min_i \|\mathbf{x}_i - \mathbf{c}\|_2} \right)^p.$$

Multipole Expansions (II)

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

- it converges on the exterior 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

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



The multipole expansion converges everywhere outside the circle!
(Possibly: slowly, if the targets are too close–but it does!)

Multipole Expansions (III)

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

Outline

Taylor on Potentials: Low Rank?

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 (#terms in Taylor series) 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.

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?

Taylor and PDEs

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 $H_\ell^{(1)}(\kappa r)$
- 3D: Spherical harmonics, ...

Expansions for Helmholtz

How do expansions for other PDEs arise?

- 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':

$$H_0^{(1)}\left(\kappa \left\|x-y\right\|_2\right) = \sum_{\ell=-\infty}^{\infty} \underbrace{H_\ell^{(1)}\left(\kappa \left\|y-c\right\|_2\right) e^{i\ell\theta'}}_{\text{singular}} \underbrace{J_\ell\left(\kappa \left\|x-c\right\|_2\right) e^{-i\ell\theta}}_{\text{nonsingular}}$$

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

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

Outline

Making Multipole/Local Expansions using Linear Algebra

Actual expansions 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?

The Proxy Trick

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
- SVD-based linear algebra should match or beat that
- Proxy-based linear algebra... may or may not?

Investigation 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.
  ('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 already believe it.)

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

Where are we now? (I)

Summarize what we know about interaction ranks.

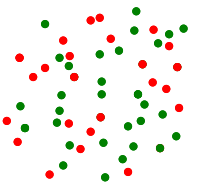
- We know that far interactions with a smooth kernel have low rank. (Because: short Taylor expansion suffices)
- If

$$\psi(\mathbf{x}) = \sum_j G(\mathbf{x}, \mathbf{y}_j)\varphi(\mathbf{y}_j)$$

  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.

Where are we now? (II)

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.



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.)

Outline

Outline

Preliminaries: Convolution

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

- Convolution with shifted δ is the same as shifting the function;

$$[f * (\xi \mapsto \delta(\xi - a))](x) = f(x - a)$$

- Convolution is linear (in both arguments) and commutative.

Preliminaries: Fourier Transform

$$\mathcal{F}(f)(\omega) = \int_{\mathbb{R}} f(x) e^{-2\pi i \omega x} dx$$

- Convolution turns into multiplication: $\mathcal{F}\{f * g\} = \mathcal{F}f \cdot \mathcal{F}g$,
- A single δ turns into: $\mathcal{F}\{\delta(x-a)\}(\omega) = e^{-ia\omega}$
- And a "train" of δs turns into:

$$\mathcal{F}\left\{\sum_{\ell \in \mathbb{Z}} \delta(x-\ell)\right\}(\omega) = \sum_{k \in \mathbb{Z}} \delta(\omega - 2\pi k).$$

What is $\mathcal{F}\{f(x-a)\}$?

$$\mathcal{F}\{x \mapsto f(x-a)\} = \mathcal{F}\{f\}\mathcal{F}\{\delta(x-a)\} = \mathcal{F}\{f\}e^{-ia\omega}$$

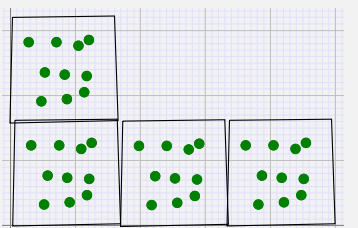
See e.g. [Décoret '04].

Simple and Periodic: Ewald Summation

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

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

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



Clear: Expressible as a convolution.

Lattice Sums: Convergence

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:

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

where d is space dimension. Have:

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

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

Ewald Summation: Dealing with Smoothness

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

Clear: a discrete convolution. Would like to make use of the fact that the Fourier transform turns convolutions into products. How?

- G is nonsmooth, it will have a Fourier transform with a long tail, hard to compute.
- Idea: separate near (singular) and far part in such a way that far kernel is smooth enough for Fourier, and near is close enough to allow for direct summation.

Ewald Summation: Screens

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, suppose

- 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)

Ewald Summation: Field Splitting

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)

Ewald Summation: Summation (1D for simplicity)

Interesting bit: How to sum G_{LR}.

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

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

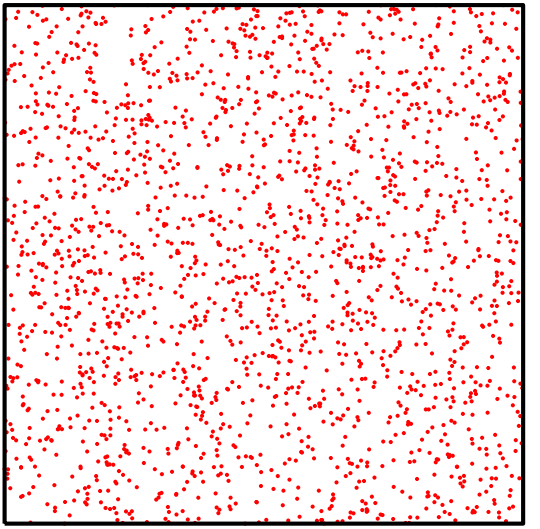
Ewald Summation: Remarks

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')

Outline

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson)

Barnes-Hut: The Task At Hand

Want: All-pairs interaction.

Caution:

- In these (stolen) figures: targets sources
- Here: targets and sources

Specifically, want

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

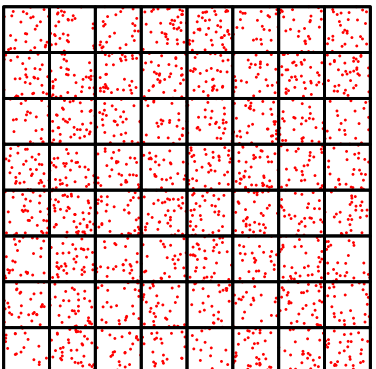
where

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

Idea: We have all this multipole technology, but no way to use it: No targets are cleanly separated from other sources.

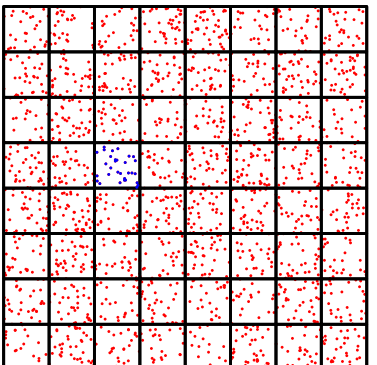
Lesson from PME: If you can't compute the entire interaction, compute parts of it. To help do so, put down a grid.

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson)

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson)

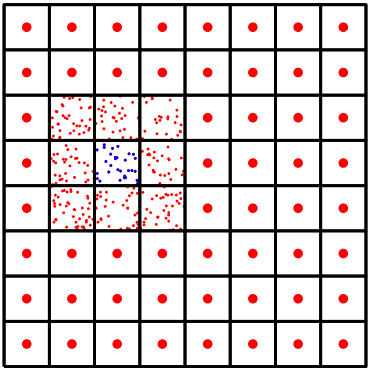
Barnes-Hut: Box Targets

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 (via the expansion order)!

Barnes-Hut: Putting Multipole Expansions to Work



(Figure credit: G. Martinsson)

Barnes-Hut: Accuracy

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.

What	How often	Cost	Total
Compute mpoles	N/m boxes	Km	KN
Evaluate mpoles	N tgts $\cdot$ N/m src boxes	K	N^2K/m
9 close boxes	$9\cdot(N/m$ boxes$)$	m^2	Nm

- Assume $m \sim \sqrt{N}$ or $N \sim m^2$.
  Q: Where does this assumption come from?

Barnes-Hut Single Level Cost: Observations

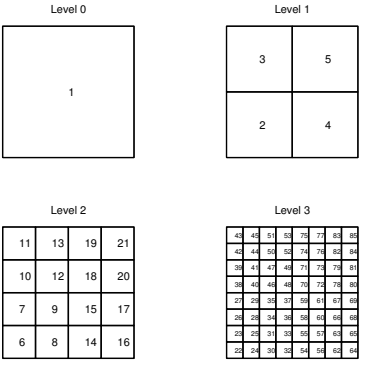
Forget K (small, constant). Only mpole eval matters:

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

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*.

Box Splitting



(Figure credit: G. Martinsson)

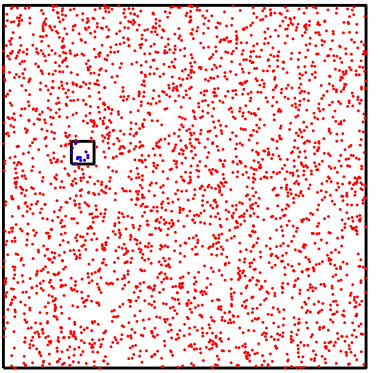
Level Count

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

Box Sizes

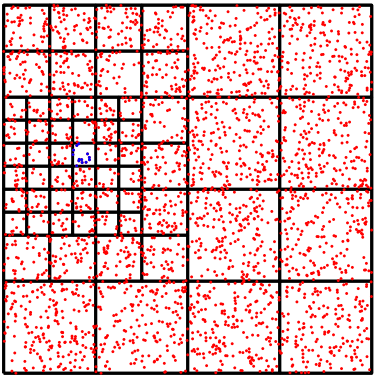


(Figure credit: G. Martinsson)

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?

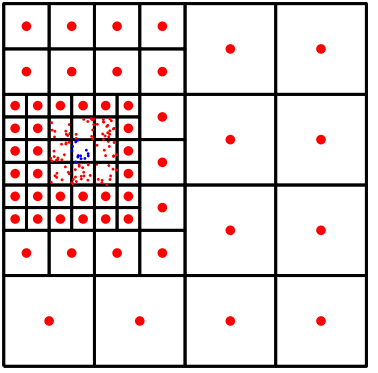
Multipole Sources



(Figure credit: G. Martinsson)

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)

Barnes-Hut: Box Properties



(Figure credit: G. Martinsson)

What properties do these boxes have?
Simple observation: The further, the bigger.

Barnes-Hut: Box Properties

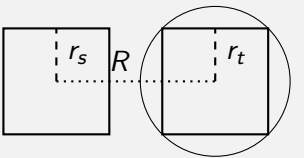
More complete: We can put a uniform bound on the error in the (function) expansion at the target:

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)

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

Barnes-Hut: Well-separated-ness

Which boxes in the tree should be allowed to contribute via multipole?



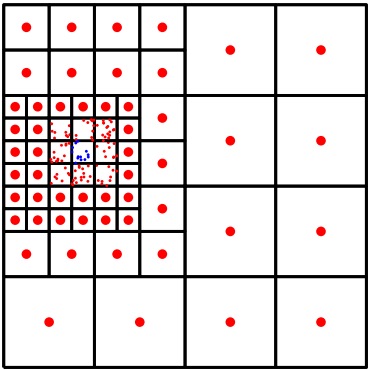
Convergent iff $r_s\sqrt{2} < R - r_t$. $\quad (*)$
Convergent *if* (picture) $R \geqslant 3 \cdot \max(r_t, r_s)$ $\quad (**)$
because $(*) \Leftrightarrow \left(r_t + \sqrt{2}r_s\right) < R$.

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')

Barnes-Hut: Revised Cost Estimate

Which of these boxes are well-separated from one another?



(Figure credit: G. Martinsson)

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

Barnes-Hut: Revised Cost Estimate

- L be the number of levels
- N be #particles
- K be #terms in expansion
- m be #particles/box. Assume bounded (say, $m \leqslant 100$)
- Then $L \sim \log(N)$

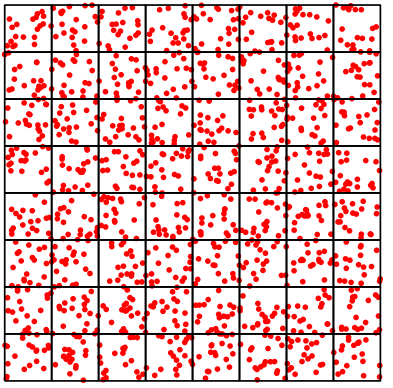
What do we need to do?

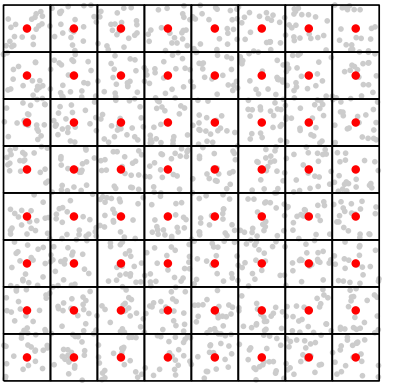
- 9 boxes of direct evaluation (self and touching neighbors)
  $\rightarrow O(m) = O(1)$
- L levels of multipoles, each of which contains:
  - $\leqslant 27$ source boxes (!) (in 2D)

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

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: Next Revised Cost Estimate





(Figure credit: G. Martinsson)

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

Barnes-Hut: Next Revised Cost Estimate

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

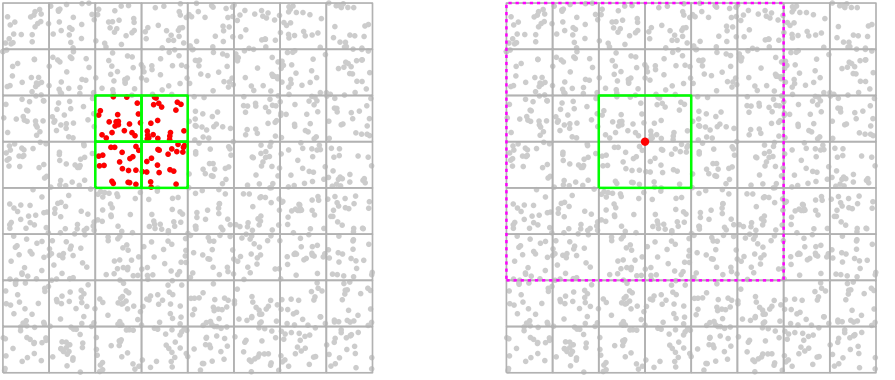
	How often	Cost	Total cost
Compute mpoles	N srcs	LK	$KN \log N$
Evaluate mpoles	N tgts $\cdot$ $27L$ src boxes	K	$NK \log N$
9 close boxes	$9 \cdot (N/m$ boxes)	m^2	N/m

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



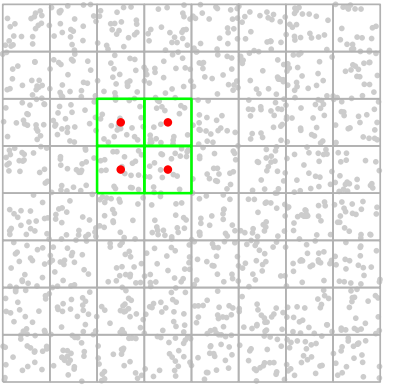
(Figure credit: G. Martinsson)

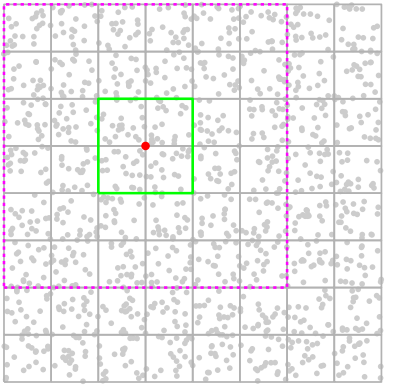
How could this process be sped up?

Barnes-Hut: Clumps of Boxes?

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)

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

Barnes-Hut: Translations

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

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

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

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

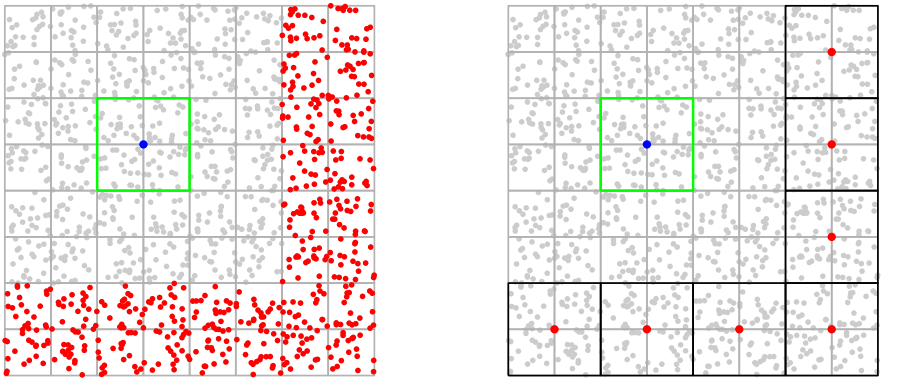
Cost of Multi-Level Barnes-Hut: Observations

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.

Outline

Using Multipole-to-Local



(Figure credit: G. Martinsson)

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

Using Multipole-to-Local

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

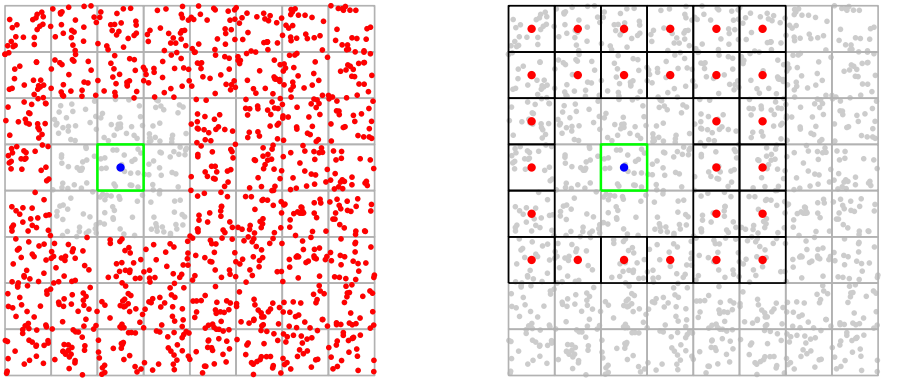
1. Form multipoles
2. Translate multipole to local
3. Evaluate local

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: Next Level



(Figure credit: G. Martinsson)

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

Using Multipole-to-Local: Next Level

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 $\ell = L-1, \ldots, 2$:
   - 4.1 Compute multipoles at level ℓ by mp $\to$ mp

Downward pass

1. Loop over levels $\ell = 2, 3, \ldots, L-1$:
   - 1.1 Loop over boxes b on level ℓ :
     - 1.1.1 Add contrib from I_b to local expansion by mp $\to$ loc
     - 1.1.2 Add contrib from parent to local exp by loc $\to$ 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?

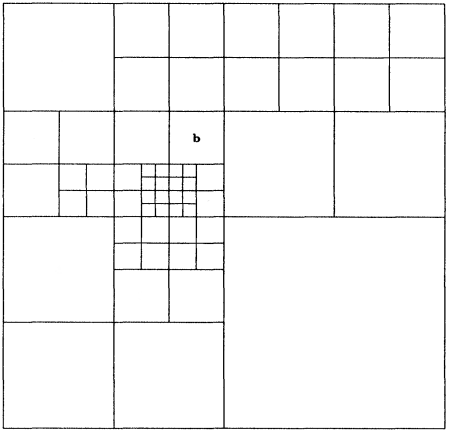


Figure credit: Carrier et al. ('88)

What about adaptivity?

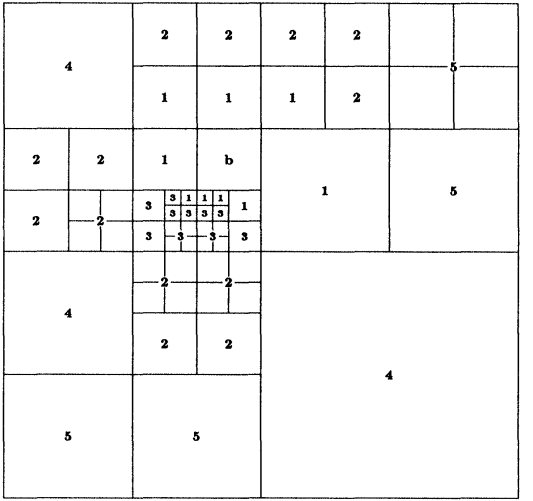


Figure credit: Carrier et al. ('88)

Adaptivity: what changes?

- Boxes interacting with a target box b can be at many levels
- Both higher and lower

FMM: List of Interaction Lists

Make a list of cases:

1. Near/touching neighbor: direct
2. Well-separated, same level: mp $\to$ loc
3. Well-separated, lower level: mp $\to$ tgt
4. Not well-separated, higher level: src $\to$ 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', ...

Outline

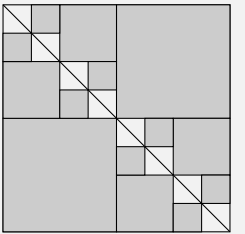
What about solving?

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?

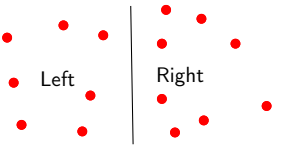


where shaded blocks have low rank.

Remarks about this matrix form:

- This structure is obviously dependent on ordering.
  Realize that finding tree boxes constitutes an ordering.

(Recursive) Coordinate Bisection (RCB)



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

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

The off-diagonal blocks have low-ish rank.

Block-separable matrices

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

where A_{ij} has low rank: How to capture 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:

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

Proxy Recap

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?

Rank and Proxies

Unlike FMMs, partitions here do not include "buffer" zones of near elements. What are the consequences?

- IDs will be built using proxies
- If near-neighbor particles inside the proxy circle, simply include them as 'additional proxies' to enlarge the space enough to get accuracy for those interactions
- Will have higher rank as a result
- It's possible to use buffering in the sovler, but the math gets more involved

Block-Separable Matrices

A *block-separable matrix* looks like this:

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

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?

Block-Separable Matrix: Questions

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.

BSS Solve (I)

Use the following notation:

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

and

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

Then $A = D + B\Pi$ and

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

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

BSS Solve (II)

Q: What are the matrix sizes? The vector lengths of $\mathbf{x}$ and $\widetilde{\mathbf{x}}$?

(Π : small $\times$ large)

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

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

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

BSS Solve (III)

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

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

Define a diagonal entry:

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

The nomenclature makes (some) sense, because $\widetilde{A}_{ii}$ is a 'downsampled' version of D_i (with two inverses thrown in for good measure).

BSS Solve (IV)

Next, left-multiply $(\mathrm{Id} + \Pi D^{-1} B)$ by $\mathrm{diag}(\tilde{A}_{ii})$:

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

Summary: Need to solve

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

BSS Solve: Summary

What have we achieved?

- Instead of solving a linear system of size

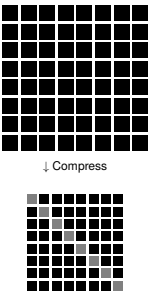
$$(N_{L0\,\text{boxes}} \cdot m) \times (N_{L0\,\text{boxes}} \cdot m)$$

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)

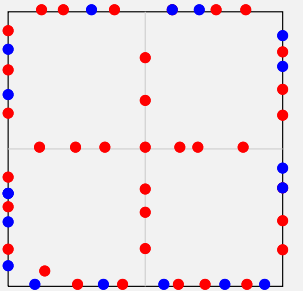
Hierarchically Block-Separable

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

- group skeletons
- eliminate more variables.

Where does this process start?

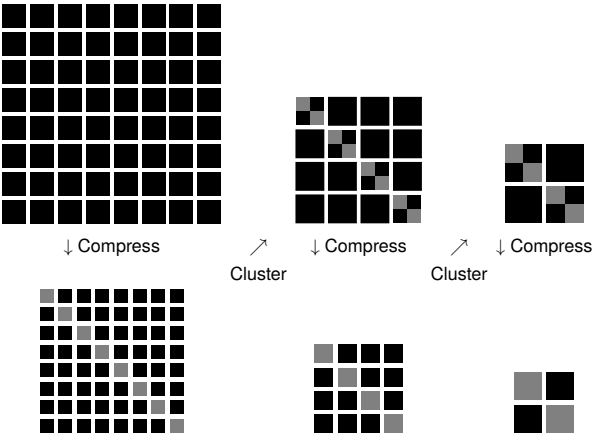
Start from the 'most refined' level:



Coarser level skeletons · Finest skeletons

Hierarchically Block-Separable

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

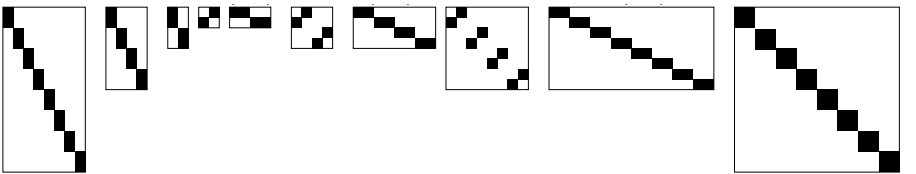


(Figure credit: G. Martinsson)

Hierarchically Block-Separable

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

Telescoping Factorization



(Figure credit: G. Martinsson)

- 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!

Outline

Recap: Fast Fourier Transform

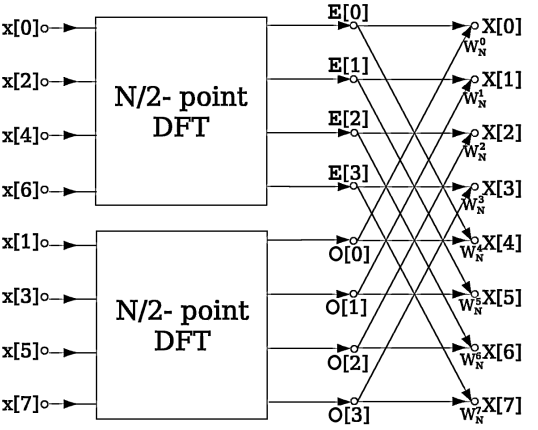
The *Discrete Fourier Transform (DFT)* is given by:

$$X_k = \sum_{n=0}^{N-1} x_n e^{-\frac{2\pi i}{N} nk} \quad (k = 0, \ldots, N-1)$$

The foundation of the *Fast Fourier Transform (FFT)* is the factorization:

$$X_k = \underbrace{\sum_{m=0}^{N/2-1} x_{2m} e^{-\frac{2\pi i}{N/2} mk}}_{\text{DFT of even-indexed part of } x_n} + e^{-\frac{2\pi i}{N} k} \underbrace{\sum_{m=0}^{N/2-1} x_{2m+1} e^{-\frac{2\pi i}{N/2} mk}}_{\text{DFT of odd-indexed part of } x_n} .$$

FFT: Data Flow



Perhaps a little bit like a butterfly?

Fourier Transforms: A Different View

Claim:

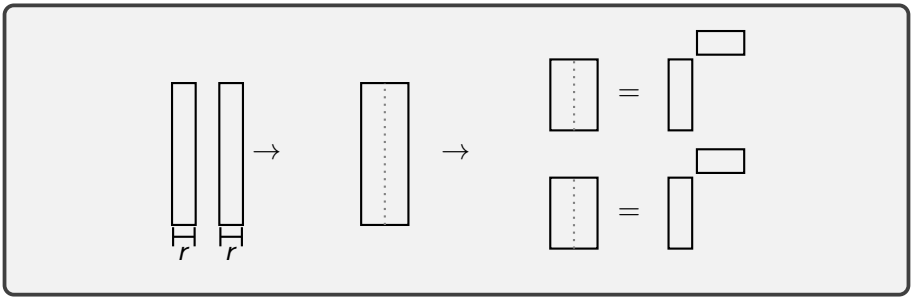
> *The [numerical] rank of the normalized Fourier transform with kernel $e^{i\gamma xt}$ is bounded by a constant times γ, at any fixed precision ϵ.*

(i.e. rank is bounded by the area of the rectangle swept out by x and t)
[O'Neil et al. '10]

Demo: Butterfly Factorization (Part I)

Recompression: Making use of Area-Bounded Rank

How do rectangular submatrices get expressed so as to reveal their constant rank?



Observations

Demo: Butterfly Factorization (Part II)

For which types of matrices is the Butterfly factorization guaranteed accurate?

> All of them.

For which types of $n \times n$ matrices does the butterfly lead to a reduction in cost?

> "Matrices for which $p \times q$ subblocks have rank proportional to pq/n." [O'Neil et al. '10]

Explore the limit cases of the characterization.

> Reducing p to 1 leads to a rank of one, which doesn't make sense. Instead, the claim needs to be viewed as $n \to \infty$.

Observations: Cost

What is the cost (in the reduced-cost case) of the matvec?

- Level 0: $P_{0,k}$ have size $r \times n/2^L$
- Level ℓ: $P_{\ell,i,j}$ have size $r \times 2r$
- Postprocess: $B_{L,j}$ have size $n/(2^L) \times r$

Comments?

In the typical case, even Level 0 will not be so oversampled that the cost of applying is substantially less than $O(n^2)$.

Outline

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:

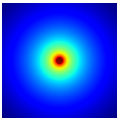
$$\partial_t^2 \tilde{u} = \triangle \tilde{u}$$

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

Fundamental Solutions

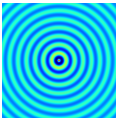
Laplace

$-\triangle u = \delta$



Helmholtz

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



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.

Green's Functions

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.

Green's Functions (II)

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

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

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

Layer Potentials (I)

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

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

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

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

- 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)

Layer Potentials (II)

- 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

IE BVP Solve: Observations (I)

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?

IE BVP Solve: Observations (II)

- 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 $D\sigma(x)\ldots$
  Q: How?

$\rightarrow$ Need some theory

Outline

Outline

Norms

Definition

(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 (Convergent sequence)

$x_n \to x :\Leftrightarrow \|x_n - x\| \to 0$ "convergence in norm"

Definition (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 (Complete/"Banach" space)

Cauchy $\Rightarrow$ Convergent

Q: Counterexample?

Operators

X, Y: Banach spaces, $A : X \to Y$ linear operator

Definition (Operator norm)

$\|A\| := \sup\{\|Ax\| : x \in X, \|x\| = 1\}$

Theorem

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

Other facts?

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

- 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 Equations: 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 (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 $|\alpha| < 1$!

Attempt 1: The Neumann series (II)

Theorem

$A : X \to X$ *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?

Outline

Compact Sets

Definition (Precompact/Relatively compact)

$M \subseteq X$ precompact:$\Leftrightarrow$ all sequences $(x_k) \subset M$ contain a subsequence converging in X

Definition (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!)

Compact Sets (II)

Counterexample to 'precompact $\Leftrightarrow$ bounded'? (∞ dim)

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 (Compact operator)

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

Theorem

- 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 (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 $|f(x) - f(y)| < \epsilon$.

Arzelà-Ascoli: Proof Sketch

- Pick a dense seuqence in G
- Use a diagonal argument to find pointwise convergent subsequence
- Use equicontinuity to show uniform convergence

Arzelà-Ascoli (II)

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.

(Note: Kress LIE 2nd ed. defines 'uniform equicontinuity' in one go.)

Outline

Integral Operators are Compact

Theorem (Continuous kernel $\Rightarrow$ compact [Kress LIE 2nd ed. Thm. 2.20])

$G \subset \mathbb{R}^m$ 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: K *uniformly* continuous on $G \times G$ because $G \times G$ compact.

Weakly singular

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

Definition (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 (Weakly singular kernel $\Rightarrow$ compact [Kress LIE 2nd ed. Thm. 2.22])

K weakly singular. Then

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

is compact on $C(G)$, where $\mathrm{cl}(G^\circ) = G$.

Weakly singular: Proof Outline

Outline the proof of 'Weakly singular kernel $\Rightarrow$ compact'.

- $$\int |x-y|^{\alpha-n} \leq \omega_n \int_0^d \rho^{\alpha-n} \rho^{n-1} d\rho = d^\alpha / \alpha \omega_n$$
- 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, $\partial\Omega$ is C^1 (what does that mean?)

Definition (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 (Weakly singular kernel $\Rightarrow$ compact [Kress LIE 2nd ed. Thm. 2.23])

K weakly singular on $\partial\Omega$. Then $(A\phi)(x) := \int_{\partial\Omega} K(x,y)\phi(y)dy$ is compact on $C(\partial\Omega)$.

Q: Has this estimate gotten worse or better?

Outline

Riesz Theory (I)

Still trying to solve

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

with A compact.

Theorem (First Riesz Theorem [Kress, Thm. 3.1])

$N(L)$ is finite-dimensional.

Questions:

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

Riesz First Theorem: Proof Outline

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 (II)

Theorem (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:

Sol. $(I - A)\varphi = 0$ unique $(\varphi = 0) \Rightarrow (I - A)\varphi = f$ unique sol.
A real existence result!

Key shortcoming?

Gives out completely if there happens to be a nullspace.

Riesz Theory: Boundedness Proof Outline

Assuming $(I - A)$ is bijective, show that $(I - A)^{-1}$ is bounded.

- Assume L^{-1} unbounded, so there exists a sequence (f_n) with $\|f_n\| = 1$ and $\left\|L^{-1} f_n\right\| \geq n$.
- Define $g_n = f_n / \left\|L^{-1} f_n\right\| \to 1$ and $\phi_n = L^{-1} f_n / \left\|L^{-1} f_n\right\|$
- $\phi_n - A\phi_n = g_n$
- Pick a convergent subsequence out of $(A\phi_n)$, let $A\phi_n \to \phi$
- $A\phi = \phi$, so $\phi \in N(L)$.

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

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

Continuous and Square-Integrable

Can we carry over $C^0(G)$ boundedness/compactness results to $L^2(G)$?

X, Y normed spaces with a scalar product so that $|(\phi, \psi)| \leq \|\phi\| \, \|\psi\|$ for $\phi, \psi \in X$.

Theorem (Lax dual system [Kress LIE 3rd ed. Thm. 4.13])

Let $U \subseteq X$ be a subspace and let $A : X \to Y$ and $B : Y \to X$ be bounded linear operators with

$$A\phi, \psi) = (\phi, B\psi) \qquad (\phi \in U, \psi \in Y).$$

Then $A : U \to Y$ is bounded with respect to $\|\cdot\|_s$ induced by the scalar product and $\|A\|_s^2 \leq \|A\| \, \|B\|$.

Based on this, it is also possible to carry over compactness results.

Adjoint Operators

Definition (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

Adjoint Operator: Observations?

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 (Fredholm Alternative [Kress LIE 2nd ed. Thm. 4.14])

$A : X \to X$ compact. Then either:

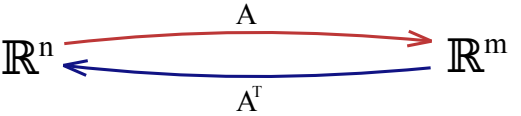
- *$I - A$ and $I - A^*$ are bijective*

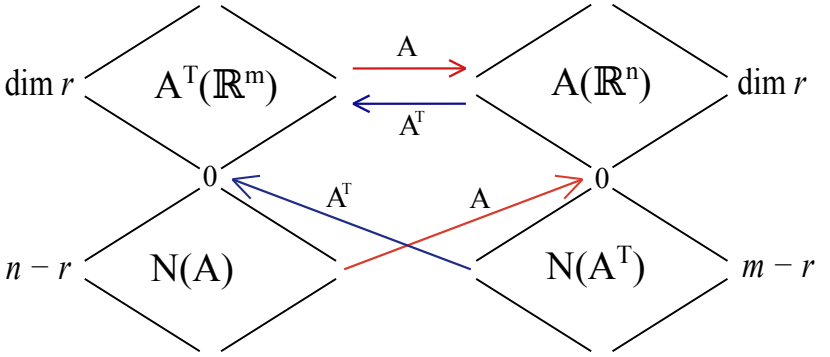
  or:
- $\dim N(I - A) = \dim N(I - A^*)$
- $(I - A)(X) = N(I - A^*)^\perp$
- $(I - A^*)(X) = N(I - A)^\perp$

Seen these statements before?

Fundamental thm of linear algebra $\to$ next slide

Fundamental Theorem of Linear Algebra





Fredholm Alternative in IE terms

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 $(I - A)\varphi = 0$.

Fredholm Alternative: Further Thoughts

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

$A = A^*$.

Where to get uniqueness?

Will work on that.

Outline

Spectral Theory: Terminology

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

Definition (Eigenvalue)

There exists an element $\phi \in X$, $\phi \neq 0$ with $A\phi = \lambda\phi$.

Definition (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.

Resolvent Set and Spectrum

Definition (Resolvent set)

$\rho(A) := \{\lambda \text{ is regular}\}$

Definition (Spectrum)

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

Spectral Theory of Compact Operators

Theorem

$A : X \to X$ 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*

Spectral Theory of Compact Operators: Proofs

Show the first part.

If $0 \notin \sigma(A)$, 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.

Spectral Theory of Compact Operators: Implications

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 $\dim N(I - A)$

Outline

Outline

Recap: Layer potentials

$$(S\sigma)(x) := \int_\Gamma G(x-y)\sigma(y)ds_y$$

$$(S'\sigma)(x) := PV\ \hat{n}\cdot\nabla_x \int_\Gamma G(x-y)\sigma(y)ds_y$$

$$(D\sigma)(x) := PV \int_\Gamma \hat{n}\cdot\nabla_y G(x-y)\sigma(y)ds_y$$

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

Definition (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:

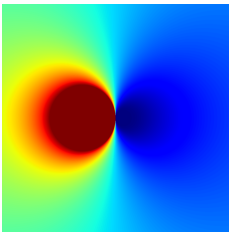
Definition (Weakly singular kernel)

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

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

Actual Singularity in the Double Layer

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



- 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 well-defined

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

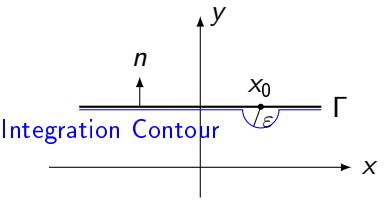
Not defined really.

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

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: *hypersingular*
- CPV integrals: *singular*

Recap: Layer potentials

$$(S\sigma)(x) := \int_\Gamma G(x-y)\sigma(y)ds_y$$

$$(S'\sigma)(x) := \text{PV}\ \hat{n}\cdot\nabla_x \int_\Gamma G(x-y)\sigma(y)ds_y$$

$$(D\sigma)(x) := \text{PV} \int_\Gamma \hat{n}\cdot\nabla_y G(x-y)\sigma(y)ds_y$$

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

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

Outline

Green's Theorem

Ω bounded

Theorem (Green's Theorem [Kress LIE 2nd ed. Thm 6.3])

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

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

If $\triangle v = 0$ and $u = 1$, then

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

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

Green's Formula

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

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

Can you write that more briefly?

$$(S(\hat{n} \cdot \nabla u) - Du)(x) = u(x)$$

Green's Formula (Full Version)

Ω bounded

Theorem (Green's Formula [Kress LIE 2nd ed. Thm 6.5])

If $\triangle u = 0$, *then*

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

Green's Formula and Cauchy Data

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

Compute u anywhere.

What if Ω is an exterior domain?

No longer holds

What if $u = 1$? Do you see any practical uses of this?

S term disappears, $-D1$ is an indicator function for the domain D. Indicator functions can be useful, for example to set representations to zero where they're invalid.

Mean Value Theorem

Theorem (Mean Value Theorem [Kress LIE 2nd ed. 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 $\overline{\int}$?

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

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

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

Maximum Principle

Theorem (Maximum Principle [Kress LIE 2nd ed. 6.9])

If $\triangle u = 0$ on compact set $\bar{\Omega}$:
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 (layer potentials) do there?

Good question $\rightarrow$ next slide.

Green's Formula at Infinity: Statement

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

Theorem (Green's Formula in the exterior [Kress LIE 3rd ed. Thm 6.11])

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

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

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

Realize the power of this statement:

Every bounded harmonic function is representable as...

Green's Formula at Infinity: Proof (1/4)

We will focus on $\mathbb{R}^3$. WLOG assume $0 \in \Omega$. Let $M = \|u\|_{L^\infty(\mathbb{R}^n \setminus \bar{\Omega})}$. First, show $\|\nabla u\| \leq 6M/\|x\|$ for $x \geq R_0$.

Choose R_0 so that $B(0, R_0/2)^c \cap \Omega = \emptyset$ and assume $\|x\| \geq R_0$. Since $\partial_i u$ is also harmonic, we may apply the mean value theorem and Gauss's theorem:

$$\nabla u(x) = \frac{1}{(4/3)\pi r^3} \int_{B(x,r)} \nabla u(y) dy = -\frac{3}{4\pi r^3} \int_{\partial B(x,r)} \hat{n}(y) u(y) dy,$$

where $\hat{n}(y)$ is the unit normal to $\partial B(x, r)$ towards the interior of the ball (hence the sign flip). The second equality follows from Gauss's theorem by applying it to $\vec{v} := \vec{e}_i u$, where $\vec{e}_i$ is the ith unit vector. Choosing $r = \|x\|/2$ yields that

$$\|\nabla u(x)\| \leq \frac{3M}{r} = \frac{6M}{\|x\|}.$$

Green's Formula at Infinity: Proof (2/4)

Let $x \in \mathbb{R}^3 \setminus \bar{\Omega}$. Let r be such that $\bar{\Omega} \subset B(x,r)$. Apply Green's formula on *bounded* domains to $B(x,r) \setminus \bar{\Omega}$:

$$(S_{\partial\Omega}(\partial_n u) - D_{\partial\Omega} u)(x) + (S_{\partial B(x,r)}(\partial_n u) - D_{\partial B(x,r)} u)(x) = u(x).$$

Show $S_{\partial B(x,r)}(\partial_n u) \to 0$ as $r \to \infty$:

Consider

$$0 = \int_{\partial(B(x,r)\cap\bar{\Omega}^c)} (\partial_n u)(y) = \int_{\partial B(x,r)} (\partial_n u)(y) - \int_{\partial\Omega} (\partial_n u)(y).$$

(The minus sign in the last term comes from the sign flip in the normal.) So

$$S_{\partial B(x,r)}(\partial_n u) = \frac{1}{4\pi r} \int_{\partial B(x,r)} (\partial_n u)(y) = \frac{1}{4\pi r} \int_{\partial\Omega} (\partial_n u)(y) \to 0.$$

Green's Formula at Infinity: Proof (3/4)

It remains to bound the term

$$D_{\partial B(x,r)}u)(x) = \frac{4\pi}{r^2}\int_{\partial B(x,r)} u(y)dS_y.$$

Can we transplant that ball to the origin in some sense?

$$u(x+y) - u(y) = \nabla u((1-\theta)y + \theta x)\cdot x$$

for some $\theta \in [0,1]$, so that if y is sufficiently large,

$$|u(x+y) - u(y)| \leq \frac{6M\,\|x\|}{\|y\| - \|x\|}.$$

So

$$\left|\frac{4\pi}{r^2}\int_{\partial B(x,r)} u(y)dS_y - \frac{4\pi}{r^2}\int_{\partial B(0,r)} u(y)dS_y\right| \leq \frac{C}{r}.$$

Green's Formula at Infinity: Proof (4/4)

Observe

$$\left| \frac{4\pi}{r^2} \int_{\partial B(0,r)} u(y) dS_y \right| \leq 4\pi M.$$

Consider the sequence

$$\mu_n := \frac{4\pi}{r_n^2} \int_{\partial B(0,r_n)} u(y) dS_y.$$

Because of its boundedness and sequential compactness of the bounding interval, out of a sequence of radii r_n, we can pick a subsequence so that $(\mu_{n(k)})$ converges. Call the limit u_∞.

Green's Formula at Infinity: Impact

Can we use this to bound u as $x \to \infty$?
Consider the behavior of the kernel as $r \to \infty$. Focus on 3D for simplicity. (But 2D holds also.)

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

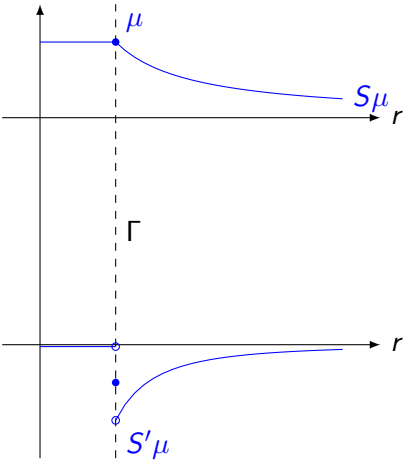
(2D uses mean-0 property of $\partial_n u$.)

How about u's derivatives?

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

Outline

Jump relations:



Jump Relations: Mathematical Statement

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

Theorem (Jump Relations [Kress LIE 2nd ed. Thm. 6.14, 6.17,6.18])

$$[S\sigma] = 0$$

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

$$\lim_{x \to x_0 \pm} (D\sigma) = \left(D \pm \frac{1}{2} I \right)(\sigma)(x_0) \quad \Rightarrow \quad [D\sigma] = \sigma$$

$$[D'\sigma] = 0$$

Truth in advertising: Assumptions on Γ?

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

Jump Relations: Proof Sketch for SLP

Sketch the proof for the single layer.

- Use same cut-off function approach as in proof for weakly singular $\Rightarrow$ compact
- Single layer potential is uniform limit of continuous functions.

Jump Relations: Proof Sketch for DLP

Sketch proof for the double layer.

- Represent tgt point x near boundary as

$$x = z + h\hat{n}(z)$$

  where $z \in \Gamma$.
- DLP becomes

$$D\sigma(x) = \sigma(z)D1(x) + D[\sigma - \sigma(z)].$$

- Argument of $D[\sigma - \sigma(z)]$ disappears as $h \to 0$; exists as improper integral. Remains to mop up limit behavior.

Outline

Outline

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 $f(x) = o(1)$?)

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

Uniqueness Proofs

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:

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

Uniqueness: Remaining Points

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 (Nullspaces [Kress LIE 2nd ed. Thm 6.20])

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

IE Uniqueness: Proofs (1/3)

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

IE Uniqueness: Proofs (2/3)

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

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

IE Uniqueness: Proofs (3/3)

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 $\partial\Omega$.
- "$\supseteq$": Can use Green's thm to show that D1+1/2=0.

What conditions on the RHS do we get for int. Neumann and ext. Dirichlet?

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

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

Patching up Exterior Dirichlet

Problem: $N(I/2 + S') = \{\psi\}\ldots$ do not know ψ. Use different kernel:

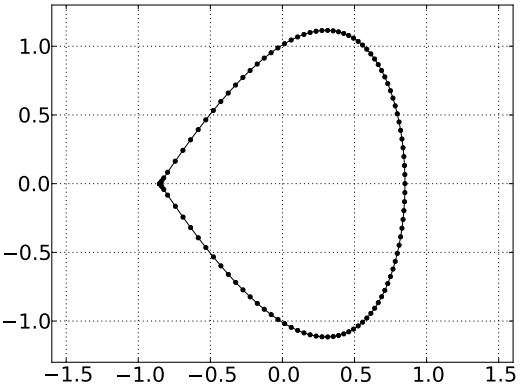
$$\hat{n} \cdot \nabla_y G(x,y) \qquad \rightarrow \qquad \hat{n} \cdot \nabla_y G(x,y) + \frac{1}{|x|^{n-2}}$$

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.
  - Consider $\partial_n G = O(1/r^{n-1})$.
- $|x|^{n-2} u(x) =?$ as $|x| \to \infty$?
- 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.

Domains with Corners



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

Domains with Corners (II)

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? How do we fix this mess?

- Continuous functions
- I + Bounded (Neumann) + Compact (Fredholm)
- Use L^2 theory
  (point behavior "invisible")

Numerically: Needs consideration, can drive up cost through refinement.

Outline

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?

(c: Sound speed) 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*.

Helmholtz vs. Yukawa

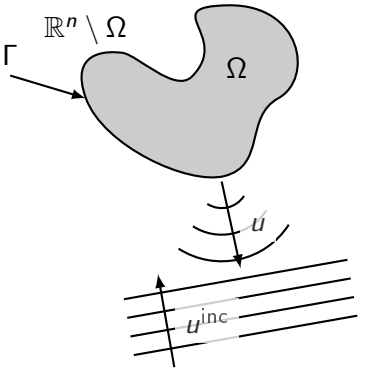
Helmholtz Equation

- $\triangle u + k^2 u(x) = 0$
- Indefinite operator
- Oscillatory solution
- Difficult to solve, especially for large k

Yukawa Equation

- $-\triangle u + k^2 u(x) = 0$
- Positive definite operator
- Smooth solutions
- 'Screened Coulomb' interaction
- Generally quite simple to solve

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

Interfaces between media: What's continuous?

> Normal velocity, pressure.

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

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

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

Unchanged from Laplace

Theorem (Green's Formula [Colton/Kress IAEST Thm 2.1])

If $\triangle u + k^2 u = 0$, *then*

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

$$[Su] = 0$$

$$\lim_{x \to x_0 \pm} (S'u) = \left(S' \mp \frac{1}{2} I \right)(u)(x_0) \quad \Rightarrow \quad [S'u] = -u$$

$$\lim_{x \to x_0 \pm} (Du) = \left(D \pm \frac{1}{2} I \right)(u)(x_0) \quad \Rightarrow \quad [Du] = u$$

$$[D'u] = 0$$

Unchanged from Laplace

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

$e^{ikr} = 1 + O(r)$ as $r \to 0$

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.	$\lim_{x \to \partial D-} u(x) = g$ 0 unique ($-$resonances)	$\lim_{x \to \partial D-} \hat{n} \cdot \nabla u(x) = g$ 0 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* or *combined field integral equation*)

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

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

Patching up resonances: CFIE (1/3)

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 $\varphi = 0$.

Patching up resonances: CFIE (2/3)

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

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

Patching up resonances: CFIE (3/3)

Equating right the right hand sides, we get

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

Green's first theorem $\int u\triangle v + \nabla u\cdot\nabla v = \int_\partial u\partial_n v$ yields

$$\underbrace{\int_\Omega -k^2|u|^2 + |\nabla u|^2}_{\in\mathbb{R}} = \int_\Omega u\triangle\bar{u} + |\nabla u|^2 = \int_{\partial\Omega} u^-\overline{(\hat{n}\cdot\nabla u)^-}\mathrm{d}s$$

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

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.

Helmholtz Uniqueness

Uniqueness for remaining IEs similar:

- 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.

Outline

A word about D'

Show that D' is self-adjoint. [Kress LIE 3rd ed. Sec 7.6]

- 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:

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

Towards Calderón

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

Let $w := S\phi$ and $v = D\psi$.

$$(S\phi, D'\psi) = (w, \partial_n v) = (\partial_n w, v) = ((S' + I/2)\varphi, (D - I/2)\psi).$$

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

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

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*

Outline

Outline

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* or *DoFs*) $\leftrightarrow$ Functions

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 $\rightarrow$?

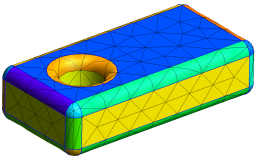
Complete the table.

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?
- What is a 'reference element'?

Demo: CAD software

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?	Examples?
▶ Piecewise Polynomials	▶ Global Fourier
	▶ Global Orth. Polynomials

What assumptions are buried in each of these?

Smoothness: Piecewise vs. Global

Fixed-order vs Spectral

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.
→ Use point values to compute those. (*Pseudospectral methods*)

Vandermonde Matrices

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

Generalized Vandermonde Matrices

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

Generalized Vandermonde Matrices

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

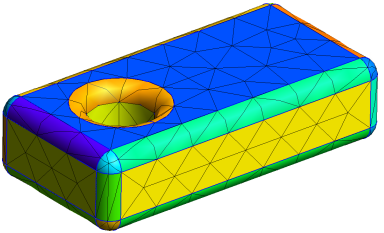
- Node placement? **Demo:** Interpolation node placement
- Vandermonde conditioning? **Demo:** Vandermonde conditioning
- What about multiple dimensions?
  - **Demo:** Visualizing the 2D PKDO Basis
  - **Demo:** 2D Interpolation Nodes

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?

Demo: Working with Unstructured Meshes

Outline

Integral Equation Discretizations: Overview

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

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

Projection/Galerkin

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

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–the integrals need to be computed *exactly*.

Outline

Nyström Discretizations (1/4)

Nyström consists of two distinct steps:

1. Approximate integral by quadrature:

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

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

$$\varphi_j^{(n)} - \sum_{k=1}^{n} \omega_k K(x_j, y_k)\varphi_k^{(n)} = f(x_j) \tag{2}$$

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

Is version (1) solvable?

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

Nyström Discretizations (2/4)

What's special about (2)?

> 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.

Nyström Discretizations (3/4)

Does (1) $\Rightarrow$ (2) hold?

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

Does (2) $\Rightarrow$ (1) hold?

Actually–it must! $\varphi_k^{(n)}$ are point values of the density (since we satisfied (2)!), and so the 'approximate' $\tilde{\varphi}$ was not so approximate after all–it must be the function that solves (1).

Nyström Discretizations (4/4)

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 (1) and the IE (than (2) 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 (1/2)

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)

Convergence for Nyström (2/2)

Will we get norm convergence $\|A_n - A\|_\infty \to 0$ for Nyström? {[Kress LIE 2nd ed. Thm. 12.8]}

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 (Not-quite-norm convergence [Kress LIE 2nd ed. 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!

Collective Compactness

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

Definition (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.)

Collective Compactness: Questions (1/2)

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

Yes.

Is collective compactness the same as "every operator in $\mathcal{A}$ is compact"?

No.

Collective Compactness: Questions (2/2)

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 (Post-compact convergence [Kress LIE 2nd ed. Cor 10.8])

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

Anselone's Theorem

$(I - A)^{-1}$ exists, with $A : X \to X$ compact, $(A_n) : X \to X$ collectively compact and $A_n \to A$ functionwise.

Theorem (Nyström error estimate [Kress LIE 3nd ed. Thm 10.12])

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?)

Anselone's Theorem: Proof (I)

Define approximate inverse $B_n = I + (I - A)^{-1} A_n$.

How good of an inverse is it?

$$
\begin{aligned}
\mathrm{Id} \quad \approx^{?} \quad & B_n(I - A_n) \\
= \quad & (I + (I - A)^{-1} A_n)(I - A_n) \\
= \quad & [I + (I - A)^{-1} A_n] - [A_n + (I - A)^{-1} A_n A_n] \\
= \quad & [I + (I - A)^{-1} A_n] - [(I - A)^{-1}(I - A) A_n + (I - A)^{-1} A_n A_n] \\
= \quad & [I + (I - A)^{-1} A_n] - [(I - A)^{-1} I A_n - (I - A)^{-1} A A_n + (I - A)^{-1} A_n A_n] \\
= \quad & I + (I - A)^{-1} \mathrm{A}\mathrm{A}_n - (I - A)^{-1} A_n A_n \\
= \quad & I + \underbrace{(I - A)^{-1}(A - A_n) A_n}_{-S_n} = I - S_n
\end{aligned}
$$

Anselone's Theorem: Proof (II)

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:

$$(I - A_n)^{-1} = (I - S_n)^{-1} B_n,$$

Anselone's Theorem: Proof (III)

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.

Anselone: A Question

Nyström: *specific to I + compact.* Why?

> Used identity to fish out density more than once.

Nyström: Collective Compactness

We *assumed* collective compactness. Do we have that? Assume

$$\sum |\text{quad. weights for } n \text{ points}| \leq C \qquad \text{(independent of } n\text{)} \qquad (3)$$

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

$$\begin{aligned} & |(A_n\varphi)(x_1) - (A_n\varphi)(x_2)| \\ = & \left| \sum_{i=1}^{n} \omega_i (K(x_1, y_i)\varphi(y_i) - K(x_2, y_i)\varphi(y_i)) \right| \\ \leqslant & \sum_{i=1}^{n} |\omega_i| \underbrace{(K(x_1, y_i) - K(x_2, y_i))}_{(*)} \|\varphi\|_\infty . \end{aligned}$$

$(*)$ bounded because K lives on a compact domain.

Nyström: Collective Compactness

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 (3) is important to make all this work!

Outline

Projection Method

X Banach space, $U \subset X$ nontrivial subspace, $A : X \to Y$ injective, $X_n \subset X$, $Y_n \subset Y$, $\dim X_n = n$, $\dim Y_n = n$, $P_n :? \to ?$

- P is a projection $\Leftrightarrow P|_U = \mathrm{Id} \Leftrightarrow P^2 = P$
- $\|P\| \geq 1$
- Orthogonal projectors: $\|P\| = 1$
- Interpolators ("collocation projection"): Also projections
- Projection method: $P_n A \phi_n = P_n f$ $(\#)$

Define convergence:

Convergent if there exists $n_0 \in \mathbb{N}_0$ so that for $n \geq n_0$

- for each $f \in A(X)$ $(\#)$ has a unique solution ϕ_n
- $\phi_n \to \phi$, where $A\phi = f$.

I.e. functionwise convergence.

Assumptions on the Approximation Spaces

What's needed of X_n so that it can even approximate the solution?

Denseness

$$\inf_{\psi \in X_n} \|\psi - \phi\| \to 0 \quad (n \to \infty)$$

Norm Convergence of Inverses

X, Y Banach spaces, $A : X \to Y$ bounded, A^{-1} bounded

Theorem (Norm Convergence of Inverses [Kress LIE 3rd ed. Thm. 10.1])

If $\|A_n - A\| \to 0$ as $n \to \infty$. Then for sufficiently large n, A_n^{-1} exists and is bounded by

$$\left\|A_n^{-1}\right\| \leqslant \frac{\left\|A^{-1}\right\|}{1 - \|A^{-1}(A_n - A)\|}.$$

For $A\varphi = f$ and $A_n\varphi_n = f_n$, we have the estimate

$$\|\varphi_n - \varphi\| \leqslant \frac{\left\|A^{-1}\right\|}{1 - \|A^{-1}(A_n - A)\|} \left[\|(A_n - A)\varphi\| + \|f_n - f\|\right].$$

Norm Convergence of Inverses: Proof

Prove the result:

Note: $I - A^{-1}(A_n - A) = A^{-1}A_n$.

Neumann series: If $\left\|A^{-1}(A_n - A)\right\| < 1$, then $[I - A^{-1}(A_n - A)]^{-1}$ exists and

$$\left\|[I - A^{-1}(A_n - A)]^{-1}\right\| \leqslant \frac{1}{1 - \|A^{-1}(A_n - A)\|}.$$

But $[I - A^{-1}(A_n - A)]^{-1}A^{-1} = A_n$, hence the bound.

For the error estimate, consider $A_n(\varphi_n - \varphi) = f_n - f + (A - A_n)\varphi$.

Projection Methods for Second Kind

Write out the projected version of the second-kind equation $\varphi - A\varphi = f$:

$$P_n\varphi_n - P_nA\varphi_n = P_nf$$

Valid, but necessarily non-unique. Better (but distinct!):

$$\varphi_n - P_nA\varphi_n = P_nf.$$

Each solution $\varphi_n \in X$ of this equation is automatically in X_n

$\rightarrow$ better chance of uniqueness.

(Error estimate connecting the two below!)

Error Estimate for Second Kind Projection

X Banach, $A : X \to X$ compact, $I - A$ injective

Theorem (Second Kind Projection Estimate [Kress LIE 3rd ed. Thm. 13.10]**)**

Assume $\|P_n A - A\| \to 0$ $(n \to \infty)$. *Then for sufficiently large* n,

$$\varphi_n - P_n A \varphi_n = P_n f$$

is uniquely solvable for all $f \in X$, *and we have* $\|\varphi_n - \varphi\| \leqslant M \|P_n \varphi - \varphi\|$ *for* M *a constant depending on* A.

Error Estimate for Second Kind Projection: Proof

Prove the result:

Riesz' theorem: $(I - A)$ invertible.

Norm convergence of inverses: $(I - P_n A)^{-1}$ exists and uniformly bounded (if n large enough).

Consider P_n applied to the continuous IE:

$$\begin{aligned} P_n(\varphi - A\varphi) &= P_n f \\ \Leftrightarrow \quad \varphi - P_n A\varphi &= P_n f + \varphi - P_n \varphi \end{aligned}$$

Subtract the latter from the projection method:

$$(I - P_n A)(\varphi_n - \varphi) = P_n \varphi - \varphi.$$

That and the uniform boundedness gives the error estimate.

Perturbations of Projection Methods for Second Kind

In actual numerical use, we're not solving

$$\varphi_n - P_n A \varphi_n = P_n f$$

but

$$\tilde{\varphi}_n - P_n A_n \tilde{\varphi}_n = P_n f_n,$$

where

- A_n approximates A,
- f_n approximates f.

Perturbations of Projection Methods for Second Kind: Estimate

X Banach, $A : X \to X$ compact, $I - A$ injective

Theorem (SK Projection Perturbation [Kress LIE 3rd ed. Cor. 13.11])

Assume that functionwise $P_n A_n - P_n A \to 0$ and $\|P_n A_n - P_n A\| \to 0$ $(n \to \infty)$. Then for sufficiently large n $\tilde{\varphi}_n - P_n A_n \tilde{\varphi}_n = P_n f_n$ is uniquely solvable and for some positive constant M,

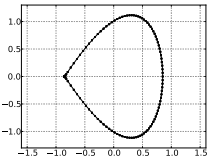
$$\|\tilde{\varphi}_n - \varphi\| \leqslant M \left(\|P_n \varphi - \varphi\| + \|(P_n A_n - P_n A)\varphi_n\| + \|P_n(f_n - f)\| \right).$$

Norm convergence of inverses: Existence and uniform boundedness of $(I - P_n A_n)^{-1}$ (from $(I - P_n A)^{-1}$).
Error estimate from there:

$$\|\tilde{\varphi}_n - \varphi_n\| \leqslant C \left(\|(P_n A_n - P_n A)\varphi_n\| + \|P_n(f_n - f)\| \right).$$

Use earlier estimate and uniform boundedness principle.

Iterative Methods and Corners [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:

$$\overline{\sigma}_h := \begin{bmatrix} \sqrt{\omega_1}\sigma(x_1) \\ \vdots \\ \sqrt{\omega_n}\sigma(x_n) \end{bmatrix} = \sqrt{\omega}\sigma_h$$

So $\overline{\sigma}_h \cdot \overline{\sigma}_h =$?
Also fixes system conditioning! Why?

Outline

Outline

'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:

$$\left| \int f - \sum f(x_i)\omega_i \right| \leqslant C \left\| f^{(p)} \right\| h^p$$

$\left\| f^{(p)} \right\|$ blows up!

Singular and Near-Singular Quadrature

Numerically distinct scenarios:

- Near-Singular quadrature
  - Integrand nonsingular
  - But may locally require lots of
  - Adaptive quadrature works, but...
- Singular quadrature
  - Integrand singular
  - Conventional quadrature fails

Kussmaul-Martensen quadrature

Theorem (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

$$\int \int_{\partial\Omega} K(\mathbf{x},\mathbf{y})\phi(y)ds_y$$

$$=$$

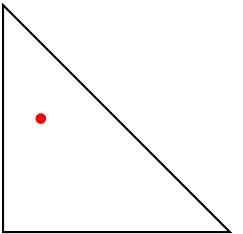
$$\int_0^R \int_{\mathbf{x}+\mathbf{r}\in\partial\Omega\cap\partial B(\mathbf{x},r)} K(\mathbf{x},\mathbf{x}+\mathbf{r})\phi(\mathbf{x}+\mathbf{r})d\langle\text{angles}\rangle\, r\, dr$$

$$=$$

$$\int_0^R \int_{\mathbf{x}+\mathbf{r}\in\partial\Omega\cap\partial B(\mathbf{x},r)} \frac{K_{\text{less singular}}(\mathbf{x},\mathbf{x}+\mathbf{r})}{r}\phi(\mathbf{x}+\mathbf{r})d\langle\text{angles}\rangle\, r\, dr$$

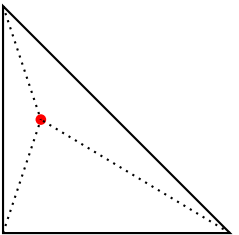
where $K_{\text{less singular}} = K \cdot r$.

Quadrature on Triangles



Problem: Singularity can sit *anywhere* in triangle
$\rightarrow$ need *lots* of quadrature rules (one per target)

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!*

$$\frac{\dots}{\sqrt{(x-y)^2}} \quad \rightarrow \quad \frac{\dots}{\sqrt{(x-y)^2+\epsilon^2}}$$

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]

Acceleration and Quadature

How can singular quadrature and FMM acceleration be made compatible?

- FMM is a point-to-point algorithm: requires point discretization
  - Kussmaul-Martensen and FMM?
- If singular quadrature applies to all targets:
  - Simply feed $\sigma(x_j) \cdot w_j$ to FMM as 'charges'
- If singular quadrature applies only near singularity:
  - Exclude 'near sources' from FMM processing for each target
  - Inconvenient when 'near sources' have no relationship to FMM
  - Desperate: Carry out full FMM, subtract 'near source' contributions

FMMs and other Layer Potentials

How does an FMM evaluate a double layer?

Expand double layer kernel into 'regular' expansions.

How does an FMM evaluate S'?

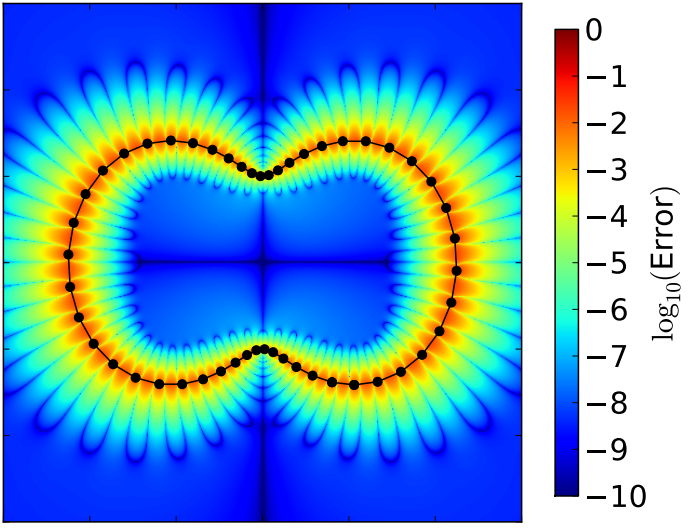
Take derivatives ∂_x and ∂_y of the local expansion at the end.

What effect does this have on accuracy?

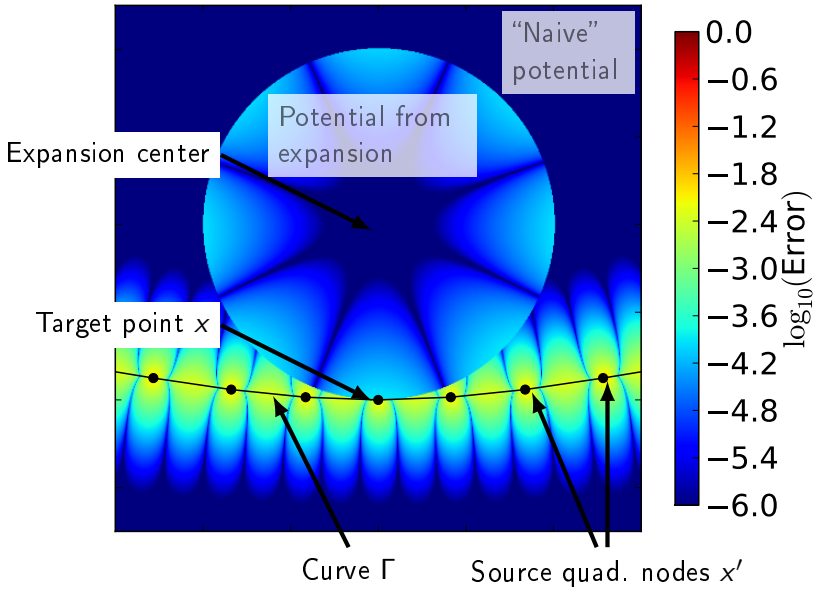
Loses an FMM order.

Outline

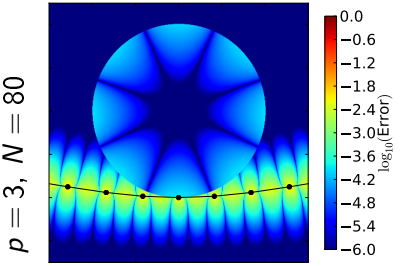
Layer Potential Evaluation: Some Intuition



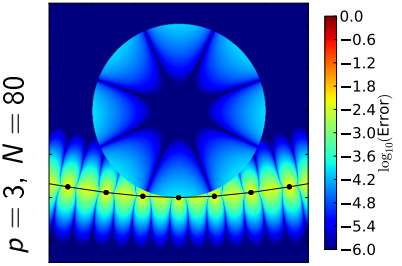
QBX: Idea

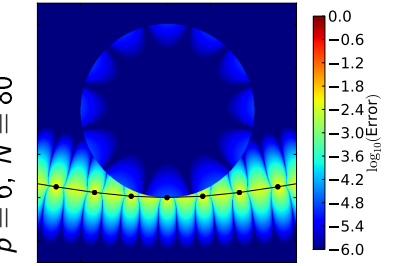

"Naive" potential
Potential from expansion
Expansion center
Target point x
Curve Γ
Source quad. nodes x'
0.0
−0.6
−1.2
−1.8
−2.4
−3.0
−3.6
−4.2
−4.8
−5.4
−6.0
$\log_{10}$(Error)

QBX: An Experiment

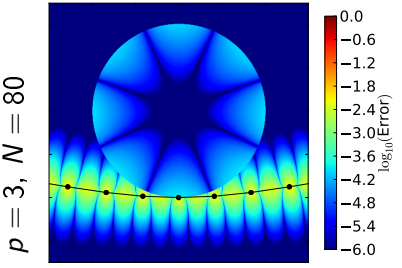


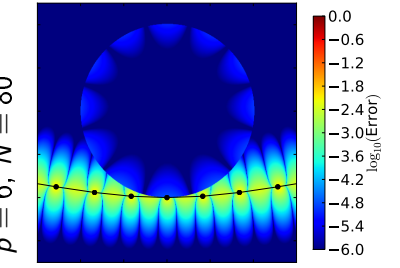
QBX: An Experiment

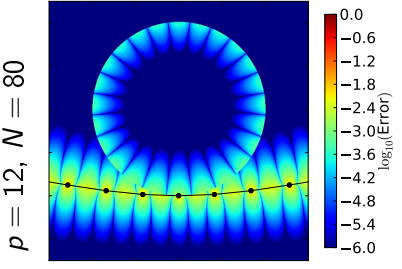




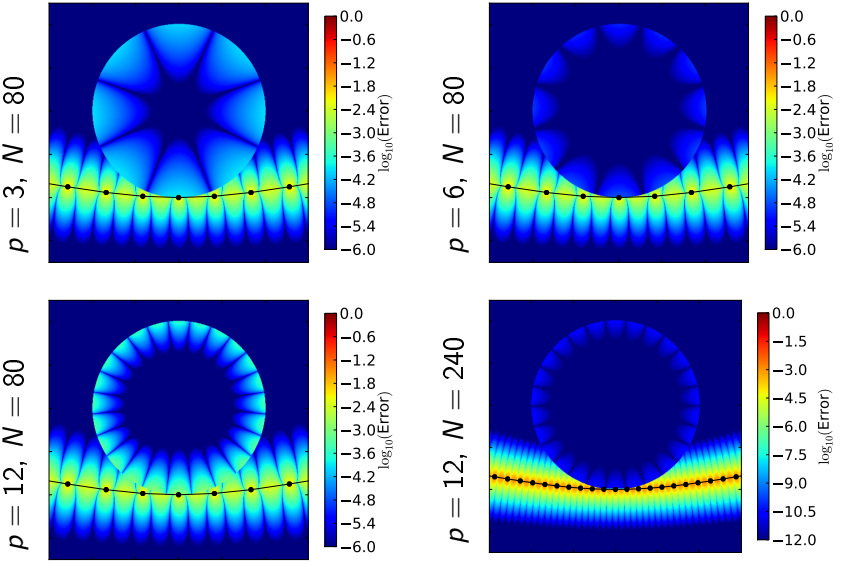
QBX: An Experiment





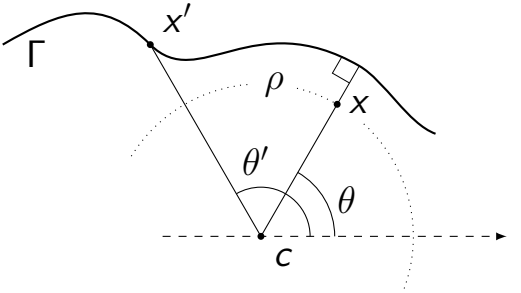


QBX: An Experiment



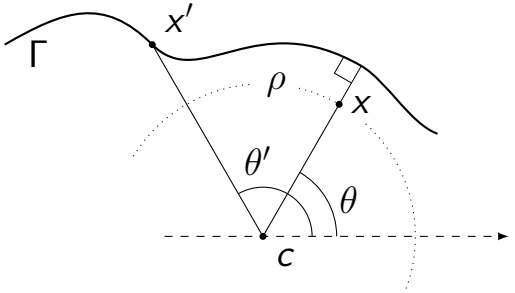
QBX: Notation, Basics

Graf's addition theorem



Graf's ad

Requires: $|x - c| < |x' - c|$ ("local expansion")



$$H_0^{(1)}(k|x - x'|) = \sum_{l=-\infty}^{\infty} H_l^{(1)}(k|x' - c|)e^{il\theta'} J_l(k|x - c|)e^{-il\theta}$$

QBX: Formulation, Discretization

Compute layer potential on the disk as

$$S_k\sigma(x) = \sum_{l=-\infty}^{\infty} \alpha_l J_l(k\rho) e^{-il\theta}$$

with

$$\alpha_l = \frac{i}{4} \int_\Gamma H_l^{(1)}(k|x' - c|) e^{il\theta'} \sigma(x') \, \mathrm{d}x' \quad (l = -\infty, \ldots, \infty)$$

$S\sigma$ is a smooth function *up to* Γ.

QBX: Formulation, Discretization

Compute layer potential on the disk as

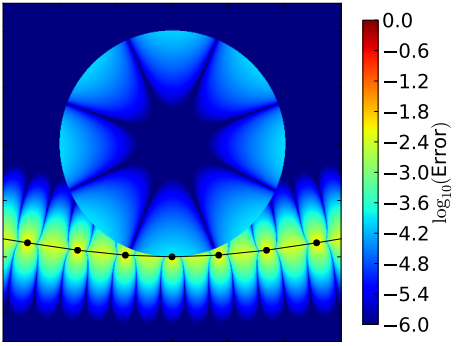
$$S_k\sigma(x) = \sum_{l=-p}^{p} \alpha_l J_l(k\rho) e^{-il\theta}$$

with

$$\alpha_l = \frac{i}{4}\, T_N\left(\int_\Gamma H_l^{(1)}(k|x' - c|) e^{il\theta'} \sigma(x')\, \mathrm{d}x' \right) \quad (l = -\infty, \ldots, \infty)$$

$S\sigma$ is a smooth function *up to* Γ.

Quadrature by Expansion (QBX)



$$\text{Error} \leq \left(C \underbrace{r^{p+1}}_{\text{Truncation error}} + C \underbrace{\left(\frac{h}{r}\right)^{q}}_{\text{Quadrature error}} \right) \|\sigma\|$$

[K, Barnett, Greengard, O'Neil JCP '13]

Achieving high order

$$\text{Error} \leq \left(C \underbrace{r^{p+1}}_{\text{Truncation error}} + C \underbrace{\left(\frac{h}{r}\right)^{q}}_{\text{Quadrature error}} \right) \|\sigma\|$$

Two approaches:

- *Asymptotically convergent*: $r = \sqrt{h}$
  - ⊕ Error $\to 0$ as $h \to 0$
  - ⊖ Low order: $h^{(p+1)/2}$
- *Convergent with controlled precision*: $r = 5h$
  - ⊖ Error $\not\to 0$ as $h \to 0$
  - ⊕ High order: h^{p+1} to controlled precision $\epsilon := (1/5)^q$

Other layer potentials

Can't just do single-layer potentials:

$$\alpha_l^D = \frac{i}{4} \int_\Gamma \frac{\partial}{\partial \hat{n}_{x'}} H_l^{(1)}(k|x' - c|) e^{il\theta'} \mu(x') \, \mathrm{d}x'.$$

Even easier for target derivatives (S' et al.): Take derivative of local expansion.
Analysis says: Will lose an order.
Slight issue: QBX computes one-sided limits.
Fortunately: Jump relations are known–e.g.

$$(PV) D^* \mu(x)|_\Gamma = \lim_{x^\pm \to x} D\mu(x^\pm) \mp \frac{1}{2}\mu(x).$$

Alternative: Two-sided average $\rightarrow$ Preferred because of conditioning

Understanding Truncation Behavior

Let $\Gamma = \partial\Omega^-$ be piecewise C^2 with no inward facing cusps. Let Ψ be the exterior Riemann map that maps the exterior Ω^+ onto the exterior of the unit disk.

Theorem (A basis of QBX-exact densities)

A function on the interior $f : \Omega^- \to \mathbb{R}$ is a harmonic polynomial of degree n if and only if f has the representation $f = D\varphi$ and the associated double-layer density function φ takes the form

$$\varphi(z) = \sum_{k=0}^{n} \lambda_k \cos(k\theta(z) + \mu_k), \quad z \in \Gamma$$

for some set of real coefficients λ_k, μ_k, where $\theta(w) = \arg \Psi(w)$ is the boundary correspondence.

[Wala, K '18]

QBX and Conformal Mapping

Require: A smooth Jordan boundary Γ, with 0 in the interior.
Require: A boundary sign s: $+1$ for exterior, -1 for interior.
Ensure: Computes the boundary correspondence θ.

Stage 1

Solve the following integral equation for the density σ, for all $\zeta \in \Gamma$:

$$\begin{cases} \zeta = \left(\mathcal{D} - \frac{1}{2}\right)\sigma(\zeta) & \text{if } s = +1 \\ \overline{\zeta^{-1}} = \left(\mathcal{D} + \int + \frac{1}{2}\right)\sigma(\zeta) & \text{if } s = -1. \end{cases}$$

Stage 2

Let $\tilde{\sigma}(\zeta) = \sigma(\zeta) + \frac{s}{2\pi i}\int_\Gamma \frac{\sigma(y)}{y}\,dy$ $(\zeta \in \Gamma)$.

Stage 3

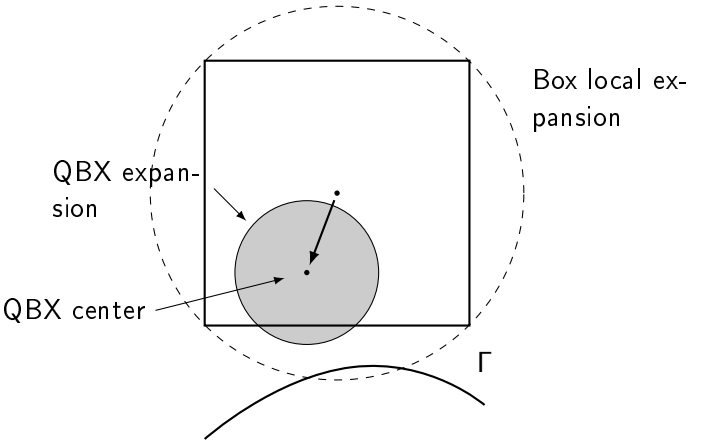
Let $\theta(\zeta) = \arg\left(-s\frac{\tilde{\sigma}(\zeta)}{|\tilde{\sigma}(\zeta)|}\right)$ $(\zeta \in \Gamma)$.

Outline

Local QBX: Viewing QBX as a Local Correction

What happens if one attempts to use QBX quadrature as a 'local correction'?

QBX + FMM : A straightforward coupling

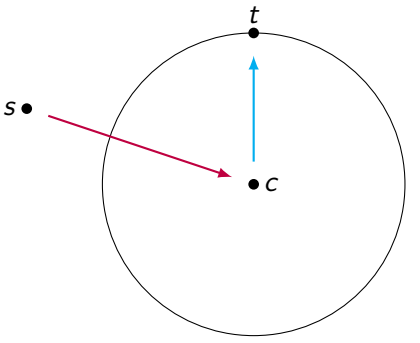


Accuracy vs FMM/QBX orders: Straightforward (2D)

$(1/2)^{p_{\text{FMM}}+1}$	p_{FMM}	$p_{\text{QBX}} = 3$	$p_{\text{QBX}} = 5$	$p_{\text{QBX}} = 7$	$p_{\text{QBX}} = 9$
0	(direct)	4.35e−6	6.21e−7	1.05e−7	5.71e−8
6e−2	3	2.55e−2	2.96e−2	4.07e−2	5.77e−2
2e−2	5	6.94e−3	1.61e−2	2.29e−2	3.10e−2
5e−4	10	4.95e−4	1.75e−3	5.80e−3	9.48e−3
2e−5	15	1.58e−5	1.85e−4	6.40e−4	3.17e−3
5e−7	20	4.35e−6	1.31e−5	8.99e−5	5.01e−4

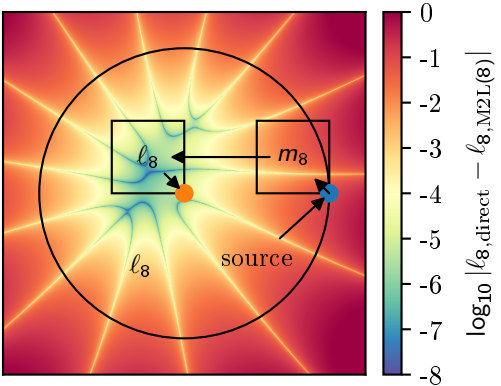
ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u) - \mathcal{D}(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 65-armed starfish γ_{65}, using the conventional QBX FMM algorithm. 3250 Gauss-Legendre panels, with 33 nodes per panel.

Recap: Local Expansions of Potentials



$$\text{Truncation Error} \sim \left(\frac{\text{furthest target}}{\text{closest source}} \right)^{p+1}$$

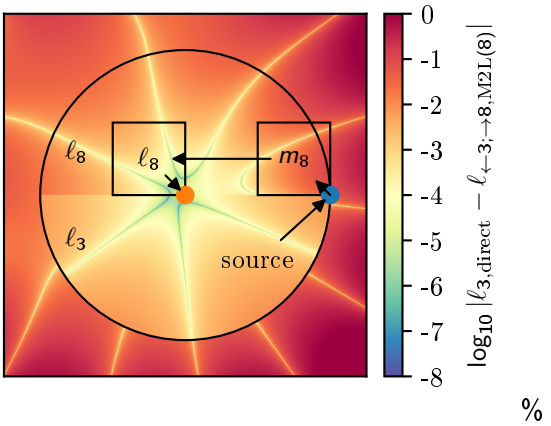
QBX + FMM: Sources of Inaccuracy



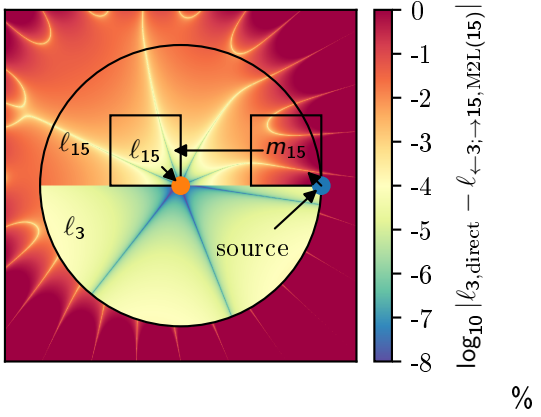
Possible Expansion Sequences

- Source $\to$ Multipole(p) $\to$ QBX-Local(q)
- Source $\to$ Local(p) $\to$ QBX-Local(q)
- Source $\to$ Multipole(p) $\to$ Local(p) $\to$ QBX-Local(q)

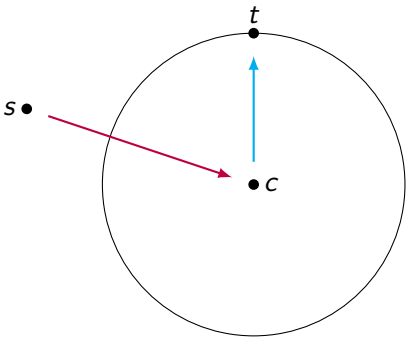
Translation chains for QBX



Translation chains for QBX



Expansions of Expansions?



$$\text{Truncation Error} \sim \left(\frac{\text{furthest target}}{\text{closest source}} \right)^{p+1}$$

This holds for point evaluations of a single expansion.

Question: Can we generalize it to hold when forming *expansions of expansions*?

Example: Local(p) $\rightarrow$ Local(q) Truncation Error (2D Lap.)

Lemma

Let $c, r > 0$. Suppose that a single unit strength charge is placed at z_0, with $|z_0| \geq (c+1)r$. Suppose that $y, z \in \overline{B}(0, r)$. If $|z| < r$ and $|y - z| \leq r - |z|$, the potential ϕ due to the charge is described by a power series $\phi(y) = \sum_{l=0}^{\infty} \beta_l (y-z)^l$. Fix the intermediate local order $p \geq 0$. For $n \geq 0$, let

$$\tilde{\beta}_n = \frac{1}{n!} \frac{d^n}{dz^n} \left(\sum_{k=0}^{p} \frac{\phi^{(k)}(0)}{k!} z^k \right).$$

Fix the local expansion order $q \geq 0$. Define $\alpha = 1/(1+c)$. Then

$$\left| \sum_{k=0}^{q} \beta_k (y-z)^k - \sum_{k=0}^{q} \tilde{\beta}_k (y-z)^k \right| \leq \left(\frac{q+1}{p+1} \right) \left(\frac{\alpha^{p+1}}{1-\alpha} \right).$$

[Wala, K '18a – arxiv:1801.04070]

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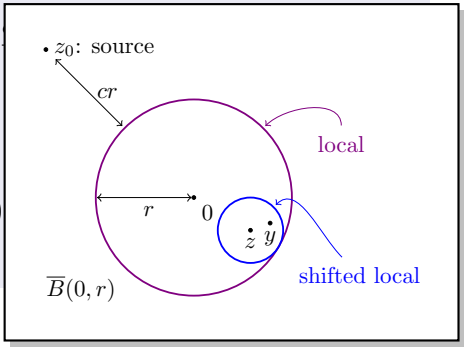
$$\tilde{\beta}_n = \frac{1}{n!} \frac{d^n}{dz^n} \left(\sum_{k=0}^{p}$$

Fix the local expansion order $q \geq 0$. Define

$$\left| \sum_{k=0}^{q} \beta_k (y-z)^k - \sum_{k=0}^{q} \tilde{\beta}_k (y-z)$$



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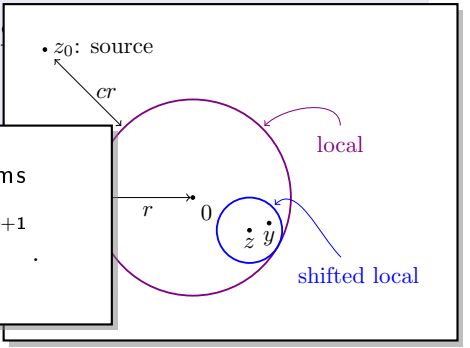
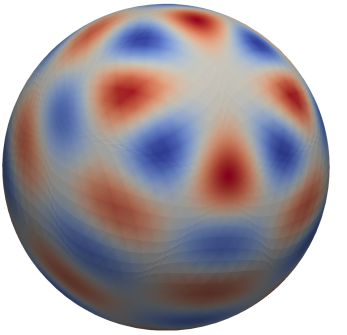


Slightly more subtle, but essentially confirms

$$\text{Truncation Error} \sim \left(\frac{\text{furthest target}}{\text{closest source}} \right)^{p+1}.$$

A Glimpse of Expansion Technology

- M/L expansions typically work by separation of variables
  - In angular + radial coordinates
- Basis for capturing the angular dependency in 3D?
- Known: Expanded potential solves PDE
- So: Expansion fully specified if known on surface of sphere
  - (Interior Dirichlet BVP, e.g.)
  - Radial dependency: find ODE, straightforward to evaluate



Expansions on the Surface of a Sphere

- Generalizing to n dimensions: (we care about $d = 2, 3$)
  $\mathbb{S}^{d-1} = \{\boldsymbol{x} \in \mathbb{R}^d : \|\boldsymbol{x}\| = 1\}$
- A polynomial $p : \mathbb{R}^d \to \mathbb{C}$ is *homogeneous* of degree k if p if p satisfies $p(r\boldsymbol{x}) = r^k p(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^d$.
- Space of spherical harmonics $\mathbb{Y}_n^d$: restrictions to the unit sphere $\mathbb{S}^{d-1}$ of the harmonic ($\triangle p = 0$), homogeneous polynomials of degree n.
- Fourier-Laplace series:

$$\mathcal{F}_p f(\boldsymbol{\xi}) = \sum_{n=0}^{p} \mathcal{P}_n f(\boldsymbol{\xi}), \quad \boldsymbol{\xi} \in \mathbb{S}^{d-1},$$

where $\mathcal{P}_n[\cdot]$ is an orthogonal projection onto $\mathbb{Y}_n^d$.

Convergence of Fourier-Laplace Series

Proposition (Norm of the Fourier-Laplace partial sum)

Let $f \in C(\mathbb{S}^{d-1})$. Then a constant $\Lambda_{n,d} > 0$ exists such that

$$\|\mathcal{F}_p f\|_\infty \leq \Lambda_{p,d} \|f\|_\infty ,$$

where, in dimensions $d = 2$ and $d = 3$,

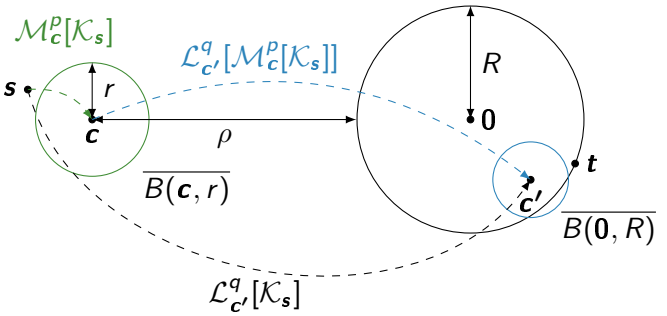
$$\Lambda_{p,2} = \frac{4}{\pi^2} \log p + O(1),$$

$$\Lambda_{p,3} = 2\sqrt{\frac{2p}{\pi}} + o(\sqrt{p}),$$

asymptotically as $p \to \infty$.

[Rivlin '69], [Gronwall 1911]

Expansions of Expansions: M2QBXL



Analyzing M2QBXL

Lemma (Source → Multipole(p) → Local(q))

Let $R > 0$ and $\rho > r > 0$. Consider a closed ball of radius r centered at $\boldsymbol{c}$, with $\|\boldsymbol{c}\| = R + \rho$, containing a unit-strength source $\boldsymbol{s}$. Also, let a ball of radius R centered at the origin contain points t and $\boldsymbol{c'}$ satisfying $\|\boldsymbol{c}\| \leq R$ and $\|\boldsymbol{t} - \boldsymbol{c'}\| \leq R - \|\boldsymbol{c'}\|$.

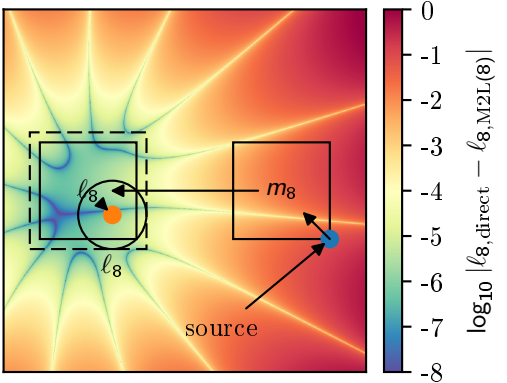
Then, in the situation of the previous slide:

$$\left|\mathcal{L}^q_{\boldsymbol{c'}}[\mathcal{K}_{\boldsymbol{s}}](\boldsymbol{t}) - \mathcal{L}^q_{\boldsymbol{c'}}[\mathcal{M}^p_{\boldsymbol{c}}[\mathcal{K}_{\boldsymbol{s}}]](\boldsymbol{t})\right| \leq \Lambda_{q,d} \left\| (\mathcal{K}_{\boldsymbol{s}} - \mathcal{M}^p_{\boldsymbol{c}}[\mathcal{K}_{\boldsymbol{s}}])|_{\overline{B(\boldsymbol{0},R)}} \right\|_\infty .$$

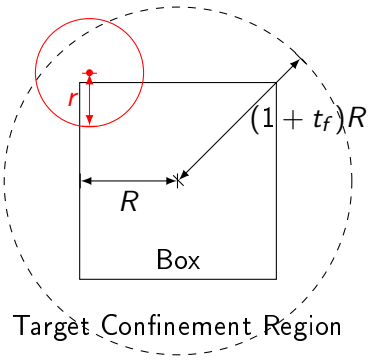
[Wala-K '19—in prep.]

Translation Chains for QBX

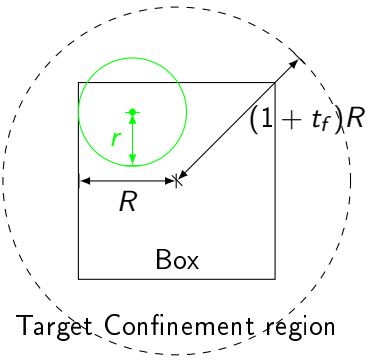
Rigorous truncation error bounds for local expansions for scenarios QBX locals *near* box locals:



Targets with Extent: Target Confinement Regions

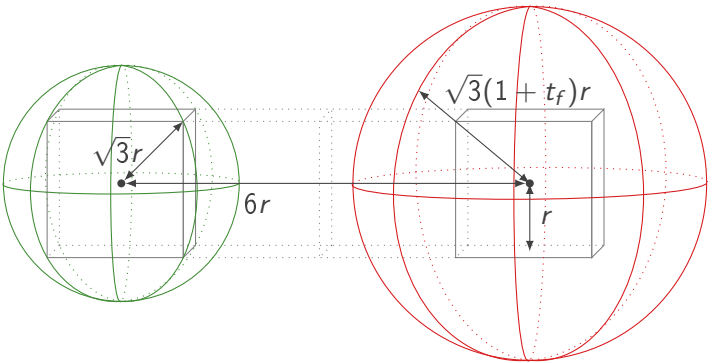


QBX center '*not in*' box



QBX center '*in*' box

M2L Convergence Factor with 2-Away, TCF (3D)



3D, $t_f = 0.9$: Conv. factor ≈ 0.77

GIGAQBX Fast Algorithm: End-to-End Accuracy (2D/3D)

Theorem (GIGAQBX FMM for Laplace (2D/3D))

Let the center $\boldsymbol{c}$ *be owned by the box* b *and let* $\boldsymbol{t}$ *be a target associated with the center* $\boldsymbol{c}$*. Assuming that* $0 \leq t_f \leq 6/\sqrt{d} - 2$*, and defining the constants*

$$\omega = \frac{\sqrt{d}(1+t_f)}{6-\sqrt{d}}, \quad A = \sum_{i=1}^{N_S} |w_i|,$$

and letting D *be the minimum box width in the tree, the (absolute) acceleration error in the GIGAQBX FMM is bounded as follows:*

$$\|\mathcal{L}_c^q[\phi](\boldsymbol{t}) - G_c^{p,q}[\phi](\boldsymbol{t})\| \leq \begin{cases} A\Lambda_{q,2} \max\left(\frac{1}{1-\frac{\sqrt{2}}{3}}\left(\frac{\sqrt{2}}{3}\right)^{p+1}, \frac{1+\Lambda_{p,2}}{1-\omega}\omega^{p+1}\right), & d=2, \\ \frac{A\Lambda_{q,3}}{D} \max\left(\frac{1}{3-\sqrt{3}}\left(\frac{\sqrt{3}}{3}\right)^{p+1}, \frac{1+\Lambda_{p,3}}{6-2\sqrt{3}-\sqrt{3}t_f}\omega^{p+1}\right), & d=3. \end{cases}$$

[Wala-K '19—in prep.]

GIGAQBX Fast Algorithm: End-to-End Accuracy (2D/3D)

Theorem (GIGAQBX FMM for Laplace (2D/3D))

Let the center $\boldsymbol{c}$ *be owned by the box b and let* $\boldsymbol{t}$ *be a target associated with the center* $\boldsymbol{c}$*. Assuming that* $0 \leq t_f \leq 6/\sqrt{d} - 2$*, and defining the constants*

$$\omega = \frac{\sqrt{d}(1 +$$
$$6 - \sqrt{d}$$

and letting D be the minimum box
acceleration error in the GIGAQBX

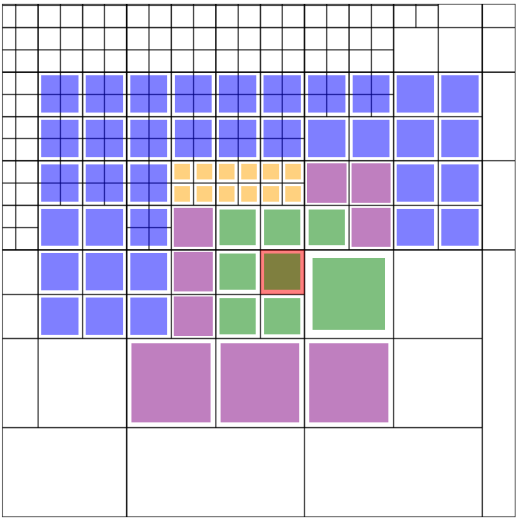
$$\|\mathcal{L}_{\boldsymbol{c}}^{q}[\phi](\boldsymbol{t}) - G_{\boldsymbol{c}}^{P,q}[\phi](\boldsymbol{t})\| \leq \begin{cases} A\Lambda_{q,\mathbf{2}} \max\left(\\ \frac{A\Lambda_{q,\mathbf{3}}}{D} \max\left(\end{cases}$$

"GIGAQBX":

- Consider **sized targets** (QBX expansions)
- Introduce a **Target Confinement Rule**
- Some M2P and P2L must be direct
- **Targets in Non-Leaf Boxes**
- **Two-Box Separation**

[Wala-K '19—in prep.]

Interaction Lists



Complexity (3D, Point-and-Shoot)

Modeled Operation Count	What
NL	Build tree
$N_S {p_{\text{FMM}}}^2 + N_B {p_{\text{FMM}}}^3$	Form M, Upward pass
$(27(N_C + N_S) n_{\max} + N_C M_C) {p_{\text{QBX}}}^2$	List 1: P2QBXL
$875 N_B {p_{\text{FMM}}}^3$	List 2: M2L
$N_C M_C q^2 + 124 L N_S n_{\max} {p_{\text{QBX}}}^2$	List 3: P2QBXL+M2QBXL
$375 N_B n_{\max} {p_{\text{FMM}}}^2 + 250 N_C n_{\max} {p_{\text{QBX}}}^2$	List 4: P2QBXL+P2L
$8 N_B {p_{\text{FMM}}}^3$	Downward
$N_C {p_{\text{FMM}}}^3$	L2QBXL
$N_T {p_{\text{QBX}}}^2$	QBXL2P

Complexity (3D)

Theorem

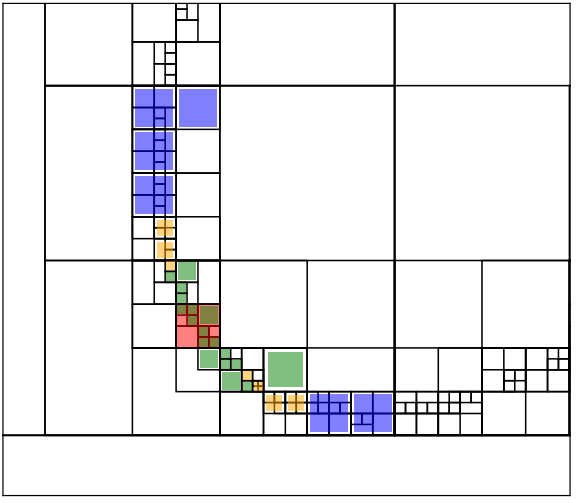
Assume that $p_{FMM} = O(|\log \epsilon|)$, and that $p_{QBX} \leq p_{FMM}$. For a fixed value of n_{max}, using a level-restricted octree and with $t_f < \sqrt{3} - 1$, the cost in modeled flops of the evaluation stage of the GIGAQBX FMM is

$$O((N_C + N_S + N_B)|\log \epsilon|^3 + N_C M_C |\log \epsilon|^2 + N_T |\log \epsilon|^2).$$

Assuming that the particle distribution satisfies $N_B = O(N)$ and $M_C = O(1)$, the worst-case modeled cost using a level-restricted octree and $t_f < \sqrt{3} - 1$ is linear in N.

[Wala-K '18]

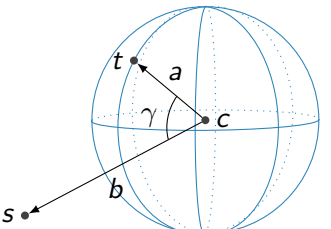
Curve Interaction Lists



Outline

Spherical Harmonic Expansions: Notation

- s: source point
- t: target point
- c: expansion center
- $a = t - c$
- $b = s - c$
- γ: angle between a and b
- p: expansion order



Spherical Harmonic Expansions: Notation

Expansion of Laplace potential in 3D:

$$\frac{(4\pi)^{-1}}{\|a-b\|} = \sum_{n=0}^{\infty} \frac{1}{2n+1} \frac{\|a\|^n}{\|b\|^{n+1}} \sum_{m=-n}^{n} Y_n^m(\theta_a, \phi_a) Y_n^{-m}(\theta_b, \phi_b)$$

Valid for $|a| < |b|$.

Total cost: $O((p+1)^2(N+M))$ (for M targets, N sources)

Spherical Harmonic Expansions: An Identity

By *Legendre addition theorem*

$$P_n(\cos\gamma) = \frac{1}{2n+1} \sum_{m=-n}^{n} Y_n^m(\theta_a, \phi_a) Y_n^{-m}(\theta_b, \phi_b)$$

P_n are Legendre polynomials
Results in line expansion (or 'target-specific expansion'):

$$\frac{(4\pi)^{-1}}{\|a-b\|} = \sum_{n=0}^{\infty} \frac{\|a\|^n}{\|b\|^{n+1}} P_n(\cos\gamma)$$

Total cost: $O((p+1)NM)$

First use in 'local' QBX: [Siegel, Tornberg '17]
Downside: Sources/targets no longer separated.

Details

- QBX [K et al '13]: Unifies toolset for quad. and accel.
- QBX FMM [Rachh et al '16]: Geometry proc., first fast alg.
- Truncation Result [Wala, K '18]: Exact density basis
- GIGAQBX 2D [Wala, K '18]: Guaranteed-Accuracy Accel.
- GIGAQBX 3D [Wala, K '18]: ℓ^2 TC, improved geom. proc.
- GIGAQBX-TS [Wala, K '19]: Reduce accel. cost
- Fourier-Laplace bounds [Wala, K '19–in prep.]:
  2D/3D analysis

Outline

Layer Potentials: Accuracy (2D GIGAQBX)

$(1/2)^{p_{\text{FMM}}+1}$	p_{FMM}	$p_{\text{QBX}} = 3$	$p_{\text{QBX}} = 5$	$p_{\text{QBX}} = 7$	$p_{\text{QBX}} = 9$
0	(direct)	4.35e−6	6.21e−7	1.05e−7	5.71e−8
6e−2	3	5.16e−3	6.35e−3	6.33e−3	6.34e−3
2e−2	5	3.83e−4	5.95e−4	5.95e−4	5.93e−4
5e−4	10	4.35e−6	4.82e−6	6.94e−6	9.30e−6
2e−5	15	4.35e−6	6.21e−7	1.05e−7	1.76e−7
5e−7	20	4.35e−6	6.21e−7	1.05e−7	5.71e−8

ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u) - \mathcal{D}(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 65-armed starfish γ_{65}, using the GIGAQBX FMM algorithm.
3250 Gauss-Legendre panels, with 33 nodes per panel.

Layer Potentials: Accuracy (2D Straightforward)

$(1/2)^{p_{\text{FMM}}+1}$	p_{FMM}	$p_{\text{QBX}} = 3$	$p_{\text{QBX}} = 5$	$p_{\text{QBX}} = 7$	$p_{\text{QBX}} = 9$
0	(direct)	4.35e−6	6.21e−7	1.05e−7	5.71e−8
6e−2	3	2.55e−2	2.96e−2	4.07e−2	5.77e−2
2e−2	5	6.94e−3	1.61e−2	2.29e−2	3.10e−2
5e−4	10	4.95e−4	1.75e−3	5.80e−3	9.48e−3
2e−5	15	1.58e−5	1.85e−4	6.40e−4	3.17e−3
5e−7	20	4.35e−6	1.31e−5	8.99e−5	5.01e−4

ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u) - \mathcal{D}(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 65-armed starfish γ_{65}, using the conventional QBX FMM algorithm. 3250 Gauss-Legendre panels, with 33 nodes per panel.

Layer Potentials: Accuracy in 3D

$(3/4)^{p_{\mathrm{FMM}}+1}$	p_{FMM}	$p_{\mathrm{QBX}} = 3$	$p_{\mathrm{QBX}} = 5$	$p_{\mathrm{QBX}} = 7$	$p_{\mathrm{QBX}} = 9$
3.16e−1	3	8.29e−3	9.68e−3	9.15e−3	9.18e−3
1.78e−1	5	1.43e−3	2.67e−3	2.85e−3	2.78e−3
4.22e−2	10	6.08e−5	6.44e−5	1.27e−4	1.47e−4
1.00e−2	15	6.08e−5	6.38e−6	3.24e−6	7.07e−6
2.38e−3	20	6.08e−5	6.38e−6	1.41e−6	2.51e−7

ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u) - \mathcal{D}(u) = u/2$, scaled by $1/\|u\|_\infty$, for the 8-armed 'urchin' geometry γ_8.
Stage 1: 48500 triangles, stage 2: 277712 triangles, with 295 nodes per triangle.

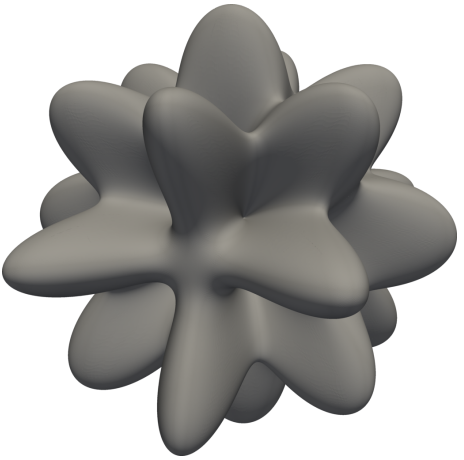
Layer Potentials: Accuracy in 3D

$(3/4)^{p_{\mathrm{FMM}}+1}$	p_{FMM}	$p_{\mathrm{QBX}} = 3$
3.16e−1	3	8.29e−3
1.78e−1	5	1.43e−3
4.22e−2	10	6.08e−5
1.00e−2	15	6.08e−5
2.38e−3	20	6.08e−5

ℓ^∞ error in Green's formula $\mathcal{S}(\partial_n u)$

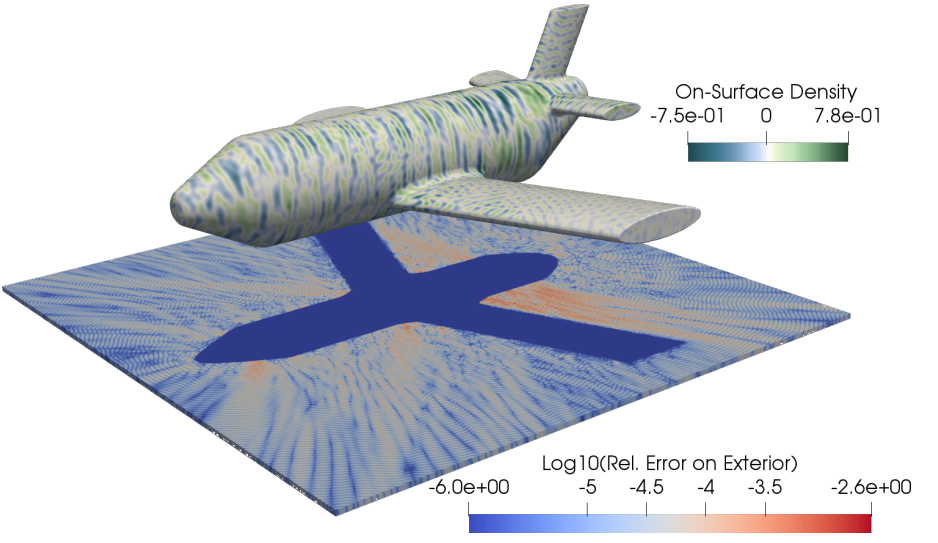
8-armed 'ur

Stage 1: 48500 triangles, stage 2: 27

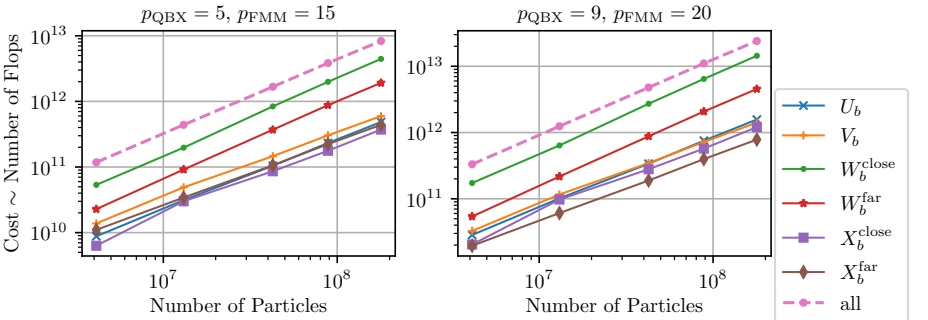


'Urchin' geometry γ_8, based on 8th order spherical harmonics

Layer Potentials: (Somewhat) Complex Geometry

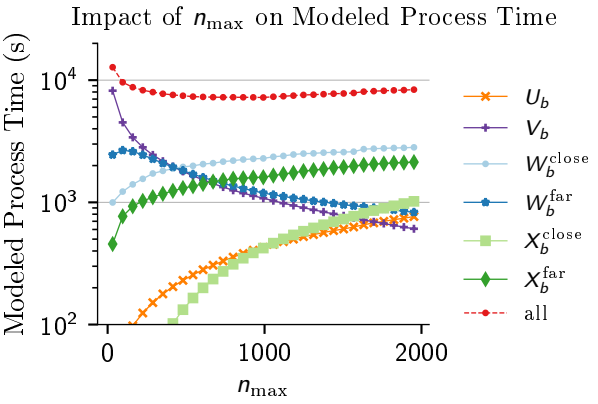


Cost Scaling: 3D GIGAQBX FMM



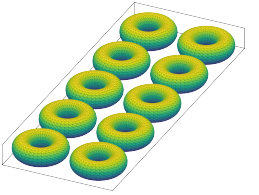
Modeled operation counts for the GIGAQBX FMM for $S\mu$.
$n_{\mathsf{max}} = 512$ and $t_f = 0.9$. Geometries: $\gamma_2, \gamma_4, \ldots, \gamma_{10}$.

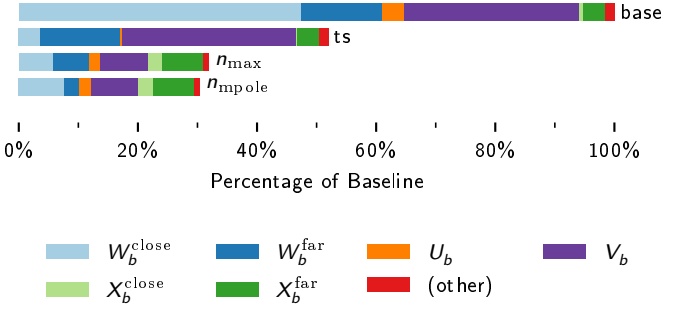
"Balancing" an FMM



Line/Target-Specific Expansions: Cost Impact

- Operator: Single layer
- Orders: QBX: 9, FMM: 20 (9~digits)
- Points: 19M $\rightarrow$ 2.1M





Line/Target-Specific Expansions: Cost Impact

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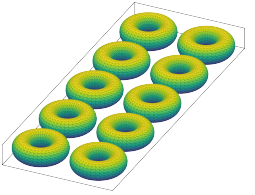
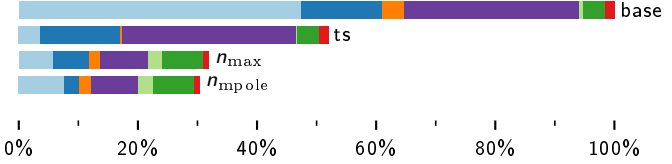




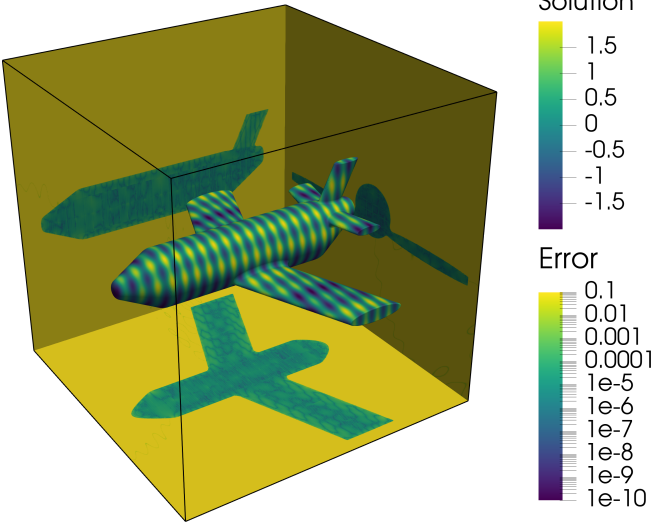
W_b^{close}

X_b^{close}

$n_{\max}$: 96 $\rightarrow$ 928, n_{mpole}: 40 $\rightarrow$ 380
Speedup: 3.3$\times$ [Wala-K '19]

Outline

Poisson: 3D, CAD Geometry



Volume degree: 7 · Boundary degree: 6 · QBX order: 3

Outline

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 $\vec{J}_s$ (physically) amounts to a surface *current density*.

Maxwell's: Towards the MFIE

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 project presentation)