APPM 4720/5720 — week 13:

The Potential Evaluation Map

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The potential evaluation map

In this lecture, we will look more carefully at the map that given a source distribution \( q \) in a (“source”) domain \( \Omega_s \) evaluates the potential in a (“target”) domain \( \Omega_t \):

\[
[Aq](x) = \int_{\Omega_s} \phi(x - y) q(y) \, dA(y), \quad x \in \Omega_t.
\]

We will cover two cases in detail:

1. Laplace: \( \phi(x) = \log |x| \).
2. Helmholtz: \( \phi(x) = H_{0}^{(1)}(\kappa |x|) \).

The discussion will more generally apply to elasticity, Stokes, the equations of elasticity, time-harmonic Maxwell, etc.

Themes:

- The effective “rank of interaction”.
- Loss of information.
- Techniques for “compressing” the interaction.
Let us start with a Laplace problem (for me, it helps to think of it as electro-statics). Suppose we are given two “well-separated” domains $\Omega_s$ and $\Omega_t$. There are $m$ sources in $\Omega_s$ inducing $n$ potentials in $\Omega_t$.

Let $A$ denote the $m \times n$ matrix with entries

$$A(i,j) = \log |x_i - y_j|.$$ 

Given a vector $q \in \mathbb{R}^n$ of source strengths, we seek a vector of potentials $f \in \mathbb{R}^m$, where

$$f = Aq \quad m \times 1 \quad m \times n \quad n \times 1$$

Using direct evaluation, the cost is $O(mn)$. 

Source locations $\{y_j\}_{j=1}^n$  

Target locations $\{x_i\}_{i=1}^m$
A is the $m \times n$ matrix with entries

$$A(i, j) = \log |x_i - y_j|.$$ 

We seek to evaluate

$$q \mapsto f = Aq.$$
\( A \) is the \( m \times n \) matrix with entries
\[
A(i,j) = \log |x_i - y_j|.
\]
We seek to evaluate
\[
q \mapsto f = Aq.
\]

**Multipole Expansion:** We showed that we can separate variables in the kernel,
\[
\log |x - y| = \sum_{p=0}^{\infty} B_p(x) C_p(y).
\]

Using polar coordinates,
\[
x - c_s = r e^{i\theta}, \quad \text{and} \quad y - c_s = r' e^{i\theta'},
\]
the functions \( B_p \) and \( C_p \) can (for instance) be
\[
B_0(x) = \log r, \quad C_0(y) = 1
\]
\[
B_{2p-1}(x) = -\frac{\sin(p\theta)}{pr^p}, \quad C_{2p-1}(y) = (r')^p \sin(p\theta'),
\]
\[
B_{2p}(x) = -\frac{\cos(p\theta)}{pr^p}, \quad C_{2p}(y) = (r')^p \cos(p\theta').
\]

Upon truncation, we have
\[
\left| \log |x - y| - \sum_{p=0}^{k} B_p(x) C_p(y) \right| \lesssim (\sqrt{2}/3)^{k/2}.
\]
$A$ is the $m \times n$ matrix with entries

$$A(i,j) = \log |x_i - y_j|.$$  

We seek to evaluate

$$q \mapsto f = Aq.$$  

**Multipole Expansion:** The precise form of the factors is not directly relevant for the discussion at hand, so to keep the notation uncluttered, let us simply write the approximation as

$$\log |x - y| \approx \sum_{p=1}^{k} B_p(x) C_p(y).$$

Note that we truncated the expansion after $k$ terms, incurring an error $\approx (\sqrt{2}/3)^{k/2}$. (We changed the summation index to start at 1, too.)
A is the $m \times n$ matrix with entries
\[ A(i, j) = \log |x_i - y_j|. \]
We seek to evaluate
\[ q \mapsto f = Aq. \]

**Multipole Expansion:** Recall the $k$ term multipole expansion:

\[
\log |x - y| \approx \sum_{p=1}^{k} B_p(x) C_p(y).
\]

An approximation (1) is called a *separation of variables*, and directly leads to a low-rank factorization

\[
A \approx B C.
\]

where $B$ has entries $B(i, p) = B_p(x_i)$ and $C$ has entries $C(p, j) = C_p(y_j)$.

Reduction in cost: *From $mn$ flops to $2k(m + n)$ flops*, where $k \sim \log(1/\varepsilon)$. 

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Source locations $\{y_j\}_{j=1}^n$

Target locations $\{x_i\}_{i=1}^m$
Suppose $A$ is a given $m \times n$ matrix.

**Question:** What is the theoretically “best” factorization of $A$ for any given $\varepsilon$?

**Answer:** Consider the *singular value decomposition (SVD)* of $A$:

$$
A \approx U D V^*.
$$

where $r = \min(m, n)$ and where

- $U = [u_1 \ u_2 \ \cdots \ u_r]$ is a matrix holding the “left singular vectors” $u_i$,
- $V = [v_1 \ v_2 \ \cdots \ v_r]$ is a matrix holding the “right singular vectors” $v_i$,
- $D = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r)$ is a diagonal matrix holding the “singular values” $\sigma_i$.

Let $|| \cdot ||$ denote a matrix norm and let $e_k$ denote the minimal error in a rank-$k$ factorization

$$
e_k = \min\{||A - A_k|| : A_k \text{ has rank } k\}.
$$

**Theorem (Eckart-Young):** The minimal error is

$$
e_k = \begin{cases} 
\sigma_{k+1}, & \text{when the spectral norm is used} \\
\sqrt{\sigma_{k+1}^2 + \sigma_{k+2}^2 + \cdots + \sigma_r^2}, & \text{when the Frobenius norm is used}
\end{cases}
$$

and the minimal error is attained for the SVD truncated to the first $k$ terms

$$
e_k = ||A - \sum_{j=1}^{k} u_j \sigma_j v_j^*|| = ||A - U_k D_k V_k^*||.
A is the $m \times n$ matrix with entries

$$A(i, j) = \log |x_i - y_j|.$$ 

We seek to evaluate

$$q \mapsto f = Aq.$$ 

**Optimal factorization — SVD:** Compute the SVD of $A$, and pick $k$ such that $\sigma_{k+1} \leq \varepsilon$. Set $B = U_k$ and $C = D_k V_k^*$. Then

$$A \approx B C$$

$$m \times n \quad m \times k \quad k \times n$$

is the theoretically most economical factorization of $A$.

However, the SVD is not quite ideal:

- All factors are determined numerically — expensive!
- The factors $B$ and $C$ depend on the precise geometry.

You have to custom-build all translation operators.

We will next describe a factorization that is almost optimal, and is also easy and economical to work with.
The Interpolative Decomposition (ID):

Let $A$ be an $m \times n$ matrix of (precise) rank $k$. Then $A$ admits a factorization

$$A = A^{(skel)} V^*,$$

where

1. $A^{(skel)} = A(:, \tilde{I})$ consists of $k$ columns of $A$.
2. $V$ contains a $k \times k$ identity matrix.
3. No entry of $V$ has magnitude greater than 1 (so $V$ is reasonably well-conditioned).

How do you construct an ID in practice?

- Computing an ID that satisfies (3) is (in general) very hard.
- If we relax condition (3) slightly, and require only that, say, $\max_{ij} |V(i,j)| \leq 1.1$, then it can be done efficiently [1996, Gu & Eisenstat].
- In practice, simply performing Gram-Schmidt on the columns works great.
  After $k$ steps of column pivoted QR, we have

$$A(:, I) = Q [R_{11} \ R_{12}] = \underbrace{Q R_{11}}_{=A^{(skel)}} \underbrace{[I \ R_{11}^{-1} R_{12}]}_{=V^*}.$$

- If $A$ does not have exact rank $k$, but its singular values decay rapidly, then the ID resulting from Gram-Schmidt satisfies $||A - A^{(skel)} V^*|| \approx \sigma_{k+1}$.
$A$ is the $m \times n$ matrix with entries
\[ A(i,j) = \log |x_i - y_j|. \]
We seek to evaluate
\[ q \mapsto f = Aq. \]

**Interpolative decomposition (ID):** Performing G-S on the columns of $A$, we obtain
\[ A \approx A^{(\text{ske})} V^* \]
\[ m \times n \quad m \times k \quad k \times n \]
where $A^{(\text{ske})} = A(\cdot, \tilde{I})$ consists of $k$ columns of $A$.

The nodes marked in red above are the nodes marked by the index vector $\tilde{I}$.

*The interaction of $\Omega_s$ with the outside is through the original kernel function.*
\( \mathbf{A} \) is the \( m \times n \) matrix with entries

\[ A(i, j) = \log |x_i - y_j|. \]

We seek to evaluate

\[ q \mapsto f = \mathbf{A} q. \]

**Interpolative decomposition (ID):** Let’s do G-S on the rows of \( \mathbf{A} \) as well

\[
\mathbf{A} \approx U \mathbf{A}^{(\text{skel})} V^* \\
\text{where } \mathbf{A}^{(\text{skel})} = \mathbf{A}(\tilde{I}_t, \tilde{I}_s) \text{ is a } k \times k \text{ sub-matrix of } \mathbf{A}.
\]
Approximation errors as a function of the rank $k$.

Interaction potential is Laplace, $\mathbf{A}(i,j) = \log |\mathbf{x}_i - \mathbf{y}_j|$. 
The 20 skeleton points required for (relative) accuracy $\varepsilon = 10^{-12}$.

Interaction potential is Laplace, $A(i,j) = \log |x_i - y_j|$. 
Conclusions from experiments:

- The SVD and ID are comparable in effectiveness.
  (In our case! When the singular values decay slowly, this is not true.)
- The multipole expansion requires more terms.

But, the comparison is not quite fair — the multipole expansion is valid for any source point that is well-separated.

**Question:** Can we find skeleton points that “work” for any well-separated target point?
First observe that we do not need to consider “every” potential target point.

Let $u$ denote the potential caused by the source points: $u(x) = \sum_{j=1}^{n} q_j \log |x - y_j|$. 

Now suppose that we can accurately reconstruct $u$ on the green square shown:

Observe that $u$ is harmonic (i.e. $-\Delta u = 0$) outside the green square. Since the Laplace problem has a unique solution, we know that if we correctly reproduce $u$ on the green square, then it is correctly reproduced *everywhere* outside the square.
Let \( \{y_j\}_{j=1}^n \) be sources in the small red box.
Let \( \{x_i\}_{i=1}^m \) be targets on the large blue box.
Let \( A \) be the matrix with elements \( A(i, j) = \log |x_i - y_j| \).
Perform Gram-Schmidt on the columns of \( A \),
Let \( \{ y_j \}_{j=1}^n \) be sources in the small red box.
Let \( \{ x_i \}_{i=1}^m \) be targets on the large blue box.
Let \( A \) be the matrix with elements \( A(i,j) = \log |x_i - y_j| \).

Perform Gram-Schmidt on the columns of \( A \),

\[
A \approx A^{(\text{skeleton})} V^* \quad \text{where} \quad m \times n \quad m \times k \quad k \times n
\]

We know that (to within precision \( \varepsilon \)), this skeleton is valid at any well-separated point.
For \( \varepsilon = 10^{-12} \), we now have \( k = 45 \). It as \( k = 20 \) for the two-box geometry.
One concern remains: So far, we’ve looked at a given distribution of source locations. The skeleton points chosen are not “universal”.

To address this issue, we will henceforth investigate the \textit{continuum operator} $A$:

\[
f(x) = [A q](x) = \int_{\Omega_s} \log |x - y| q(y) \, dy, \quad x \in \Omega_t
\]

which maps a source distribution $q$ in a source domain $\Omega_s$ to a potential $f$ in a target domain $\Omega_t$.

Let \(\{x_i, v_i\}_{i=1}^m\) be a quadrature for the target domain, and let \(\{y_j, w_j\}_{j=1}^n\) be a quadrature for the source domain.

Let the vector $f$ have entries $f(i) = \sqrt{v_i} f(x_i)$ so that $\|f\|_{L^2(\Omega_t)} \approx \|f\|_{\ell^2}$.

Let the vector $q$ have entries $q(j) = \sqrt{w_j} q(y_j)$ so that $\|q\|_{L^2(\Omega_s)} \approx \|q\|_{\ell^2}$.

Finally, let $A$ be the $m \times n$ matrix with entries $A(i, j) = \sqrt{v_i} \log |x_i - y_j| \sqrt{w_j}$.

Then the singular values/vectors of $A$ are accurate approximations of the singular values/vectors of $A$.

Observe that when $\Omega_s$ and $\Omega_t$ are not “too close,” the kernel $\log |x - y|$ is smooth.
Example: Two concentric circles — ideal for multipole expansion.

Sources in a disc of radius 0.5, targets on a circle of radius 1.5.
Example: Two concentric circles — ideal for multipole expansion.

Sources in a disc of radius 0.5, targets on a circle of radius 1.5.

Skeleton to precision $\varepsilon = 10^{-12}$, which requires $k = 44$. 
Example: Two concentric circles — ideal for multipole expansion.

Errors. For this geometry, $E_{\text{mpole}} = E_{\text{svd}}$ exactly!
Example: Two concentric circles — now much tighter.

Sources in a disc of radius 0.5, targets on a circle of radius 0.75.
Example: Two concentric circles — now much tighter.

Sources in a disc of radius 0.5, targets on a circle of radius 1.5.

Skeleton to precision $\varepsilon = 10^{-12}$, which requires $k = 81$. 
Example: Two concentric circles — now much tighter.

Errors. For this geometry, $E_{\text{mpole}} = E_{\text{svd}}$ exactly!

(The weirdness at the end reflects the discretization error.)
Example: Two squares — realistic FMM geometry.

Sources in a box of side length 1, targets on a box of side length 3.
**Example:** Two squares — realistic FMM geometry.

Sources in a box of side length 1, targets on a box of side length 3.

*Skeleton to precision $\varepsilon = 10^{-12}$, which requires $k = 47$.***
Example: Two squares — realistic FMM geometry.
**Example:** Two squares — now tighter.

Sources in a box of side length 1, targets on a box of side length 1.6.
Example: Two squares — now tighter.

Sources in a box of side length 1, targets on a box of side length 1.6.  
Skeleton to precision $\varepsilon = 10^{-12}$, which requires $k = 108$.  

Example: Two squares — now tighter.

Sources in a box of side length 1, targets on a box of side length 1.6.
Example: Two squares — now even tighter.

Sources in a box of side length 1, targets on a box of side length 1.2.
Example: Two squares — now even tighter.

Sources in a box of side length 1, targets on a box of side length 1.2.

Skeleton to precision $\varepsilon = 10^{-12}$, which requires $k = 260$. 
Example: Two squares — now even tighter.

Sources in a box of side length 1, targets on a box of side length 1.2.
**Example:** A piece of a contour.
Example: A piece of a contour.

Skeleton to precision $\varepsilon = 10^{-12}$, which requires $k = 25$. 
Example: A piece of a contour.
Skeletonization can be performed for $\Omega_S$ and $\Omega_T$ of various shapes.

Rank = 29 at $\varepsilon = 10^{-10}$. 
Rank = 48 at $\varepsilon = 10^{-10}$. 
Adjacent boxes can be skeletonized.

Rank = 46 at $\varepsilon = 10^{-10}$. 
Benefits:

- The rank is typically very close to optimal.
- The projection and interpolation are well-conditioned.
- An inexpensive local computation (e.g. Gram-Schmidt) determines:
  - The $k$ skeleton points.
  - Matrices $U$ and $V$.
- The map $A^{\text{ske}}$ has the same kernel as $A$. (We loosely say that “the physics of the problem is preserved”.)
- The skeleton points can be determined either as generic points valid for any source distribution, or as a subset of a given set of points. In the latter case $U$ and $V$ contain $k \times k$ identity matrices.
- Interaction between adjacent boxes can be compressed (no buffering is required).
Before closing this topic, let us briefly consider the *Helmholtz problem.*

Recall that the Helmholtz equation is associated with the classical wave equation

$$-v^2 \Delta \phi = -\frac{\partial^2 \phi}{\partial t^2},$$

where $v$ is the wave-speed. Assume $\phi(x, t) = u(x) e^{i\omega t}$. Then (2) turns into

$$-v^2 \Delta u = \omega^2 u,$$

We define the “wave number” as $\kappa = \omega/v$, and can then write (3) as

$$-\Delta u - \kappa^2 u = 0.$$

A typical “free-space” problem for the Helmholtz equation could read

$$\begin{cases} 
-\Delta u(x) - \kappa^2 u(x) = q(x), & x \in \mathbb{R}^2 \\
\frac{\partial u(x)}{\partial |x|} - i\kappa u(x) = O \left( \frac{1}{|x|} \right) & |x| \to \infty,
\end{cases}$$

where the condition “at infinity” is called a “radiation condition.”

We typically consider $u$ to be a *complex valued* potential.

The fundamental solution is $H_0^{(1)}(\kappa|x|)$, so the solution to (5) is

$$u(x) = \int_{\mathbb{R}^2} H_0^{(1)}(\kappa|x - y|) q(y) \, dy.$$
Plots of the fundamental solution $H_0^{(1)}(|\mathbf{x}|) = J_0(|\mathbf{x}|) + i Y_0(|\mathbf{x}|)$.
Plots of the fundamental solution $H_0^{(1)}(|x|) = J_0(|x|) + i Y_0(|x|)$.

Now zoom in to the origin:

Real part $J_0$

Negative imaginary part $-Y_0$

Logarithmic singularity at the origin!
Example of solution of the Helmholtz equation $-\Delta u - \kappa^2 u = g$

Suppose we are given point charges $\{q_j\}_{j=1}^5$ in a “source domain” $\Omega_S$.

We are interested in the potential in a “target domain” $\Omega_t$.

The source domain $\Omega_S$ (red) and the target domain $\Omega_t$ (blue).
Example of solution of the Helmholtz equation $-\Delta u - \kappa^2 u = g$

Suppose we are given point charges $\{q_j\}_{j=1}^5$ in a “source domain” $\Omega_s$.

We are interested in the potential in a “target domain” $\Omega_t$.

Real part of field generated by the sources (truncated — the peaks go to infinity).
Example of solution of the Helmholtz equation $-\Delta u - \kappa^2 u = g$

Suppose we are given point charges $\{q_j\}_{j=1}^5$ in a “source domain” $\Omega_S$.

We are interested in the potential in a “target domain” $\Omega_t$.

Real part of field generated by the sources (truncated — the peaks go to infinity).
Example of solution of the Helmholtz equation \(-\Delta u - \kappa^2 u = g\)

Suppose we are given point charges \(\{q_j\}_{j=1}^5\) in a “source domain” \(\Omega_S\).

We are interested in the potential in a “target domain” \(\Omega_t\).

Real part of field generated by the sources (truncated — the peaks go to infinity).
Example of solution of the Helmholtz equation \(-\Delta u - \kappa^2 u = g\)

Suppose we are given point charges \(\{q_j\}_{j=1}^5\) in a “source domain” \(\Omega_s\).
We are interested in the potential in a “target domain” \(\Omega_t\). Now for larger \(\kappa\)!

Real part of field generated by the sources (truncated — the peaks go to infinity).
Example of solution of the Helmholtz equation $-\Delta u - \kappa^2 u = g$

Suppose we are given point charges $\{q_j\}_{j=1}^5$ in a “source domain” $\Omega_S$. We are interested in the potential in a “target domain” $\Omega_t$. Now for larger $\kappa$!

Real part of field generated by the sources (truncated — the peaks go to infinity).
Example of solution of the Helmholtz equation $-\Delta u - \kappa^2 u = g$

Suppose we are given point charges $\{q_j\}_{j=1}^5$ in a “source domain” $\Omega_S$. We are interested in the potential in a “target domain” $\Omega_T$. Now for larger $\kappa$!

Real part of field generated by the sources (truncated — the peaks go to infinity).
Example of solution of the Helmholtz equation

\[-\Delta u - \kappa^2 u = g\]

Suppose we are given point charges \(\{q_j\}_{j=1}^5\) in a “source domain” \(\Omega_S\).

We are interested in the potential in a “target domain” \(\Omega_t\). Now for larger \(\kappa\)!

Absolute value of field generated by the sources (truncated — the peaks go to infinity).
Example of solution of the Helmholtz equation $-\Delta u - \kappa^2 u = g$

Suppose we are given point charges $\{q_j\}_{j=1}^5$ in a “source domain” $\Omega_S$.

We are interested in the potential in a “target domain” $\Omega_t$. Now for larger $\kappa$!

Absolute value of field generated by the sources (truncated — the peaks go to infinity).
Superficially, almost everything we’ve discussed for the Laplace case carries right over to the Helmholtz case.

For instance, there is a “multipole expansion.” Set

\[ S_n(x) = H_n^{(1)}(\kappa r) e^{-in\theta} \]
\[ R_n(x) = J_n(\kappa r) e^{in\theta}. \]

Then

\[ H_0^{(1)}(\kappa|x-y|) = \sum_{n=-\infty}^{\infty} S_n(x) R_n(y), \quad \text{when } |x| > |y|. \]
Example: Two squares — Helmholtz — small wave number.

The geometry: Source region has side = 0.875 lambda

Sources in a box of side length 0.9\lambda, targets on a box of side length 2.6\lambda.
Example: Two squares — Helmholtz — small wave number.

Skeleton points: \( \varepsilon = 1.0 \times 10^{-12} \quad k = 49 \quad \text{side of source box} = 0.875 \lambda \)

Sources in a box of side length 0.9\( \lambda \), targets on a box of side length 2.6\( \lambda \).

Skeleton to precision \( \varepsilon = 10^{-12} \), which requires \( k = 49 \).
**Example:** Two squares — Helmholtz — small wave number.

*Sources in a box of side length $0.9\lambda$, targets on a box of side length $2.6\lambda$.***
Example: Two squares — Helmholtz — medium wave number.

The geometry: Source region has side = 8.117 lambda

Sources in a box of side length 8.1\lambda, targets on a box of side length 24.4\lambda.
Example: Two squares — Helmholtz — medium wave number.

Skeleton points: \( \varepsilon = 1.0 \times 10^{-12} \) \( k = 118 \) side of source box = 8.117 \( \lambda \)

Sources in a box of side length \( 8.1 \lambda \), targets on a box of side length \( 24.4 \lambda \).

Skeleton to precision \( \varepsilon = 10^{-12} \), which requires \( k = 118 \).

Observe how many points are now internal — they used to cluster along the boundary.
**Example:** Two squares — Helmholtz — medium wave number.

Sources in a box of side length $8.1\lambda$, targets on a box of side length $24.4\lambda$. 
Complications with the Helmholtz problem:

1. Decay of singular values starts happening only for *sub-wave-length scales*. For geometries that are “large” in terms of wave-lengths, rank considerations alone will be not be sufficient.

2. Resonances are possible. Consider for instance the Dirichlet boundary value problem:

\[
\begin{aligned}
-\Delta u(x) - \kappa^2 u(x) &= 0, \quad x \in \Omega, \\
 u(x) &= f(x), \quad x \in \partial \Omega,
\end{aligned}
\]

where $\Omega$ is a “simple” finite domain. There exist a sequence of wave-numbers $0 \leq \kappa_1 \leq \kappa_2 \leq \kappa_3 \leq \cdots$ for which the BVP is ill-posed. These are the numbers for which $\kappa_j^2$ is an eigenvalue of $-\Delta$. At these “resonant wave-numbers” there exist non-trivial solutions for $f = 0$.

This creates complications in setting up proxy charges (need *two* layers, or use both monopoles and dipoles, e.g.).

3. While the Laplace equation has a simple “maximum principle” (a harmonic function attains its max on the boundary), the Helmholtz equation is more complicated.

4. Etc.
Similar schemes have been proposed by many researchers:

1993 - C.R. Anderson
1995 - C.L. Berman
1996 - E. Michielssen, A. Boag
1999 - J. Makino
2004 - L. Ying, G. Biros, D. Zorin

A mathematical foundation:
1996 - M. Gu, S. Eisenstat