MATH 393C: Fast Methods in Scientific Computing

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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

$$f = A q$$

$$m \times 1 \quad m \times n \quad n \times 1$$

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

\[\text{\textbf{Source locations \{y\}_j^{n}}\]

\[\text{\textbf{Target locations \{x\}_i^{m}}}\]
$A$ 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

$$\left| \log |x - y| - \sum_{p=0}^{k} B_p(x) C_p(y) \right| \lesssim (\sqrt{2}/3)^{k/2}.$$
\( \mathbf{A} \) is the \( m \times n \) matrix with entries
\[
A(i,j) = \log |x_i - y_j|.
\]
We seek to evaluate
\[
\mathbf{q} \mapsto \mathbf{f} = \mathbf{Aq}.
\]

**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
\[
\log |\mathbf{x} - \mathbf{y}| \approx \sum_{p=1}^{k} B_p(\mathbf{x}) C_p(\mathbf{y}).
\]
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 \( k \sim \log(1/\varepsilon) \).
Suppose \( \mathbf{A} \) is a given \( m \times n \) matrix.

**Question:** What is the theoretically “best” factorization of \( \mathbf{A} \) for any given \( \varepsilon \)?

**Answer:** Consider the **singular value decomposition (SVD)** of \( \mathbf{A} \):

\[
\mathbf{A} \approx \mathbf{U} \mathbf{D} \mathbf{V}^*.
\]

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

\[
\mathbf{U} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_r] \quad \text{is a matrix holding the “left singular vectors” } \mathbf{u}_i,
\]

\[
\mathbf{V} = [\mathbf{v}_1 \ \mathbf{v}_2 \ \cdots \ \mathbf{v}_r] \quad \text{is a matrix holding the “right singular vectors” } \mathbf{v}_i,
\]

\[
\mathbf{D} = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r) \quad \text{is a diagonal matrix holding the “singular values” } \sigma_i.
\]

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

\[
e_k = \min\{\| \mathbf{A} - \mathbf{A}_k \| : \mathbf{A}_k \text{ has rank } k \}.
\]

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

\[
e_k = \sigma_{k+1}, \quad \text{when the spectral norm is used}
\]

\[
e_k = \sqrt{\sigma_{k+1}^2 + \sigma_{k+2}^2 + \cdots + \sigma_r^2}, \quad \text{when the Frobenius norm is used}
\]

and the minimal error is attained for the SVD truncated to the first \( k \) terms

\[
e_k = \| \mathbf{A} - \sum_{j=1}^{k} \mathbf{u}_j \sigma_j \mathbf{v}_j^* \| = \| \mathbf{A} - \mathbf{U}_k \mathbf{D}_k \mathbf{V}_k^* \|.\]
**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

$$A \approx B \ C$$

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

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
\[
A = A^{(\text{skel})} V^*,
\]
\[
m \times n = m \times k \quad k \times n
\]
where
1. \( A^{(\text{skel})} = A(:, \tilde{i}) \) 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
  \[
  A(:, l) = Q [R_{11} \quad R_{12}] = \underbrace{QR_{11}}_{= A^{(\text{skel})}} \underbrace{[I \quad R_{11}^{-1} R_{12}]}_{= V^*}.
  \]
- If \( A \) does not have exact rank \( k \), but its singular values decay rapidly, then the ID resulting from Gram-Schmidt satisfies
  \[
  \| A - A^{(\text{skel})} V^* \| \approx \sigma_{k+1}.
  \]
\( \mathbf{A} \) is the \( m \times n \) matrix with entries
\[
\mathbf{A}(i,j) = \log |x_i - y_j|.
\]
We seek to evaluate
\[
\mathbf{q} \rightarrow \mathbf{f} = \mathbf{A}\mathbf{q}.
\]

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

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
\[
\mathbf{A} \approx \mathbf{U} \mathbf{A}^{(\text{skel})} \mathbf{V}^* \\
\hspace{2cm} m \times n \quad m \times k \quad k \times k \quad k \times n
\]
where \( \mathbf{A}^{(\text{skel})} = \mathbf{A}(\tilde{I}_t, \tilde{I}_s) \) is a \( k \times k \) sub-matrix of \( \mathbf{A} \).
Approximation errors as a function of the rank $k$.

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

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

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 *continuum operator* $A$:

$$f(x) = [Aq](x) = \int_{\Omega_s} \log |x - y| q(y) \, dy,$$

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.

Errors.
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 \( A^{\text{skel}} \) 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 $H_0^{(1)}(|x|) = J_0(|x|) + iY_0(|x|)$. 

Real part $J_0$

Negative imaginary part $-Y_0$
Plots of the fundamental solution $H^{(1)}_0(|x|) = J_0(|x|) + i Y_0(|x|)$.

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 $-\Delta u - \kappa^2 u = g$

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

Skeleton points: $\varepsilon=1.0\times10^{-12}$, $k=49$, 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: eps=1.0e−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 not be sufficient.

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

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

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