On the discretization of integral equations for elliptic PDEs with internal layers

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Here are a few references for the material in this talk:


We consider the following equation:

$$\nabla \cdot (\epsilon \nabla \varphi) = f \text{ in } \Omega,$$

with Dirichlet boundary conditions \( \varphi = g \) on \( \partial \Omega \).

Features of this equation

- Type: divergence-form elliptic differential equation
- The function \( \epsilon \) depends on \( x \) ("variable coefficient").
- The function \( \epsilon \) is positive and may have internal layers.

This equation appears, for example, in semiconductor device simulation.
Some notation: let $\psi = V_g(\nu)$ be the function (volume integral) which satisfies

$$\Delta \psi = \nu \text{ in } \Omega,$$

with $\psi = g$ on $\partial \Omega$. We then represent our solution $\varphi$ as $\varphi = V_g(\sigma)$ for an unknown density $\sigma$.

Plugging this representation of $\varphi$ into the differential equation results in the following integral equation for $\sigma$:

$$\sigma + \frac{\nabla \epsilon}{\epsilon} \cdot \nabla V_g(\sigma) = \frac{f}{\epsilon}.$$
The integral equation

$$\sigma + \frac{\nabla \epsilon}{\epsilon} \cdot \nabla V_g(\sigma) = \frac{f}{\epsilon}$$

is second-kind; however, in the presence of ever steeper internal layers in $\epsilon$, the **condition number** of the resulting discrete system can be arbitrarily large if traditional Nyström discretization is used. A large condition number can be detrimental when using an iterative solution scheme.
The Discontinuous Case

The poor conditioning described in the previous slide is especially strange because the case where \( \epsilon \) is piecewise constant (but discontinuous) can be handled in a well conditioned way by using boundary integrals to correct for the discontinuity.

Why would smoother \( \epsilon \) give rise to a more poorly conditioned problem?
For a continuous $\epsilon$, we use a volume integral to represent the solution so our density is a volume charge; however, in the limit as $\epsilon$ approaches a discontinuous function, this volume integral is trying to accomplish what is done by a boundary integral. These boundary integrals have densities which are like a point charge in 1-D, a line charge in 2-D, and a surface charge in 3-D — in particular, they are singular when viewed as volume charges.
“Physical” Intuition

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- How can we make the discretized system for the continuous case behave like the one for the discontinuous case?
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The fact that our density will approximate a $\delta$ function for steep $\epsilon$ is undesirable numerically. We are lead to the following questions:

- How can we make the discretized system for the continuous case behave like the one for the discontinuous case?
- How to formalize this?
Talk Outline

The rest of the talk will follow this brief outline:

- Description of a numerical analysis tool (1D).
- Some analytical results and their consequences (1D).
- Numerical results (1D and 2D).
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In order to analyze the condition number of discretized integral equations, it is convenient to introduce the following definition.

**Definition**

A mapping $\Phi : V \subset L^p[a, b] \rightarrow \mathbb{C}^n$ is said to be *p-norm-preserving* if

$$\|\Phi(g)\|_p = \|g\|_{L^p[a,b]}$$

for all $g \in V$. 
Some Definitions

Let $A$ be an invertible, bounded integral operator mapping $V \subset L^p$ to $U \subset L^p$.

**Definition**

A matrix $A_h$ is a norm-preserving discretization of $A$ on $V$ if there exist norm-preserving mappings $\Phi$ and $\Psi$ such that the diagram

$$
\begin{array}{ccc}
V \subset L^p[a, b] & \xrightarrow{A} & U \subset L^p[a, b] \\
\downarrow \Psi & & \downarrow \Phi \\
\mathbb{C}^n & \xrightarrow{A_h} & \mathbb{C}^n
\end{array}
$$

commutes.
Let $B|_W$ denote the restriction of an operator $B$ to the subspace $W$. If $A : V \subset L^p \to U \subset L^p$ is invertible and bounded, then we have the following mini result for condition numbers in $\ell^p$ and $L^p$.

**Theorem (1)**

If $A_h$ is a norm preserving discretization of $A$, then

$$\text{cond}_{\ell^p}(A_h|_{\Phi(V)}) = \text{cond}_{L^p}(A|_V).$$

**Proof.**

This is an immediate consequence of the definitions.

Note: In [Bremmer 2012], it was shown that for the case $p = 2$, the discretized operator actually has approximately the same singular values as the continuous operator if you choose an inner-product preserving discretization.
Consider a Nyström integration rule:

$$\int f(x) \, dx \approx \sum_i f(x_i)w_i.$$ 

Following [Bremmer 2012], an \textbf{approximately} $p$-norm preserving discretization is easily obtained from such a rule by setting $f_i = \Phi(f)_i = f(x_i)w_i^{1/p}$ because

$$\|\vec{f}\|_{\ell^p}^p = \sum_i |f(x_i)|^p w_i \approx \int |f(x)|^p \, dx = \|f\|_{L^p}^p.$$ 

We note that traditional Nyström discretization ($f_i = f(x_i)$) with a fine enough mesh is approximately $\infty$-norm preserving for continuous functions.
Let $A = I + K$, where $Kg(x) = \int K(x, y)g(y)$, be our integral operator and suppose we are solving the integral equation $A\sigma = f$. If we discretize $\sigma$ and $f$ as in the previous slide, the following discretization of $A$ is induced:

$$\sigma_i + w_i^{1/p} \sum_j K(x_i, x_j)\sigma_j w_j^{1-1/p} = f_i$$

where $\sigma_i = w_i^{1/p}\sigma(x_i)$, and likewise for $f$. Due to Theorem (1), we expect that the $\ell^p$ condition number of the corresponding matrix $A_h$ will be approximately the $L^p$ condition number of $A$. 
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*Discretization of integral equations*
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\[ [A_h]_{ij} = \delta_{ij} + K(x_i, x_j)w_i^{1/p}w_j^{1-1/p}. \]

If the \( w_i \) are all equal (corresponding to a uniform discretization), the matrix \( A_h \) is the same for every choice of \( p \).
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- While condition numbers are equivalent on finite dimensional spaces, the bounds relating them depend on the system size. E.g.

\[
\text{cond}_2(A_h) \leq n \cdot \text{cond}_1(A_h)
\]

where \(n\) is the system size. Adaptive quadrature will keep the system size \(n\) small.
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A Question

Using a norm preserving discretization allows us to construct a system matrix whose $\ell^p$ condition number is roughly that of the continuous operator acting on $L^p$ for a $p$ of our choice.

What do we know about the $L^p$ condition number of the integral operator for the divergence form elliptic problem for various $p$?
As a reminder, the integral equation we are concerned with is

$$\sigma + \frac{\nabla \epsilon}{\epsilon} \cdot \nabla V_g(\sigma) = \frac{f}{\epsilon},$$

where $V_g$ is a volume integral. To simplify the analysis, we consider the problem in 1D (say on the interval $[0, 1]$), with Dirichlet data $g \equiv 0$. In this case, $V_g(\sigma)$ is given by

$$V_g(\sigma)(x) = \int_0^1 G(x, y)\sigma(y) \, dy$$

where

$$G(x, y) = \begin{cases} 
  x(y - 1) & \text{if } x < y \\
  (x - 1)y & \text{if } x \geq y
\end{cases}$$

is the Green’s function for homogeneous Dirichlet data on $[0, 1]$. 

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Integral Operator Condition Numbers

Let $A(\epsilon)$ be the operator applied to $\sigma$ on the left-hand side of

$$\sigma + \frac{\epsilon x}{\epsilon} \int G_x(x, y) \sigma(y) \, dy = \frac{f}{\epsilon}.$$  

We have the following analytical result for the condition number of $A(\epsilon)$ acting on any $L^p$ space $1 \leq p < \infty$ and $L^\infty \cap C[0, 1]$. 

Theorem (2) Let $E \subset C^1[0, 1]$ be a family of functions with uniform upper and lower bounds given by $M$ and $m$. Then there exist $C_1$ and $C_2$ such that

$$C_1 \| \epsilon x \|_p \leq \text{cond}_p (A(\epsilon)) \leq C_2 \| \epsilon x \|_p + 1$$  

for any $\epsilon \in E$. The constants depend only on $M$ and $m$.

If you consider a coefficient $\epsilon$ with internal layers, you see that $A(\epsilon)$ will have a mild condition number in $L^1$ (essentially given by the total variation in $\epsilon$) and a very large condition number in $L^\infty$. 

Askham, Greengard Discretization of integral equations
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Let $\mathcal{E} \subset C^1[0, 1]$ be a family of functions with uniform upper and lower bounds given by $M$ and $m$. Then there exist $C_1$ and $C_2$ such that

$$C_1 \left( \left\| \frac{\epsilon_x}{\epsilon} \right\|_p^2 \right) \leq \text{cond}_p(A(\epsilon)) \leq C_2 \left( \left\| \frac{\epsilon_x}{\epsilon} \right\|_p^2 \right) + 1$$

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- Use a 1-norm-preserving discretization so that the $\ell^1$ condition number of our system matrix is small.
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- Work in $L^1$ because the condition number is much smaller for the continuous operator on this space.
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- Use adaptive quadrature so that the system size is small.
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- Then, the $\ell^2$ condition number of the matrix will be small.
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- Work in $L^1$ because the condition number is much smaller for the continuous operator on this space.
- Use a 1-norm-preserving discretization so that the $\ell^1$ condition number of our system matrix is small.
- Use adaptive quadrature so that the system size is small.
- Then, the $\ell^2$ condition number of the matrix will be small.
- A small $\ell^2$ condition number will improve the performance/stability of the iterative solution scheme GMRES.
We note that with a 1-norm-preserving scheme, the unknown is $\sigma_i = w_i \sigma(x_i)$. If $\sigma$ is nearly a point charge (a $\delta$ mass) at $x_i$, the unknown $w_i \sigma(x_i)$ will be like the strength of the charge at that point. The weight in the discretization will “integrate out” the singularity.
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\[ \epsilon_\delta(x) = 2 + \tanh(\delta(x - x_0)) \]

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\[ \| \frac{(\epsilon_\delta)_{x}}{\epsilon_\delta} \|_p = \Theta(\delta^{1-1/p}) \].
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\[ \left\| \frac{(\epsilon_\delta)_x}{\epsilon_\delta} \right\|_p = \Theta(\delta^{1-1/p}). \]

From Theorem 2, we expect that the \(p\) condition number of \(A(\epsilon_\delta)\) should be \(\Theta(1)\) for \(p = 1\), \(\Theta(\delta)\) for \(p = 2\), and \(\Theta(\delta^2)\) for \(p = \infty\).
We formed \( p \)-norm preserving discretizations of \( A(\epsilon_\delta) \) for a range of \( \delta \) values and for \( p = 1, 2, \) and \( \infty \). The condition numbers of the resulting matrices were calculated by brute force.
Results – Condition Number Experiment

We formed $p$-norm preserving discretizations of $A(\epsilon_\delta)$ for a range of $\delta$ values and for $p = 1, 2, \text{ and } \infty$. The condition numbers of the resulting matrices were calculated by brute force. The growth of the condition numbers below agrees with the analytical results.

**Figure:** The $\ell^p$ condition numbers of $A_h(\epsilon_\delta)$ over a range of $\delta$ values, for $p = 1$ (left), $p = 2$ (center), and $p = \infty$ (right).
We have run numerical tests in 1-D to observe the effect of using norm-preserving discretization (for $L_1$, $L_2$, and $L_\infty$ weighting). To solve our linear system, we used an iterative solver (GMRES).

A plot of the variable coefficient $\epsilon(x)$ used for this example.

A plot of the relative residual error versus the steps of GMRES taken, for $L_1$, $L_2$, and $L_\infty$ weighting.
We have also run numerical tests in 2-D to observe the effect of using norm-preserving discretization (for $L_1$, $L_2$, and $L_{\infty}$ weighting). To solve our linear system, we used an iterative solver (GMRES).

![A plot of the variable coefficient $e(x)$ used for this example.](image1)

![A plot of the relative residual error versus the steps of GMRES taken, for $L_1$, $L_2$, and $L_{\infty}$ weighting.](image2)
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Conclusion

- Thinking in terms of norm preservation results in discrete systems with predictable behavior.
- For the divergence form problem:
  - $L^1$ is good and corresponds with physical intuition as the coefficient $\epsilon$ approaches a discontinuous function.
  - Adaptivity is essential.
Thank you for having me.