# Math 4/896: Seminar in Mathematics
# Topic: Inverse Theory

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AvH 10

# Outline

# A Motivating Example: Integral Equations

## Contaminant Transport

Let $C(x,t)$ be the concentration of a pollutant at point $x$ in a linear stream, time $t$, where $0 \le x < \infty$ and $0 \le t \le T$. The defining model

$$
\begin{aligned}
\frac{\partial C}{\partial t} &= D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} \\
C(0,t) &= C_{in}(t) \\
C(x,t) &\to 0,\ x \to \infty \\
C(x,0) &= C_0(x)
\end{aligned}
$$

# Solution

## Solution:

In the case that $C_0(x) \equiv 0$, the explicit solution is

$$C(x, T) = \int_0^T C_{in}(t) f(x, T - t)\, dt,$$

where

$$f(x, \tau) = \frac{x}{2\sqrt{\pi D \tau^3}} e^{-(x - v\tau)^2/(4D\tau)}$$

# The Inverse Problem

**Problem:**

Given simultaneous measurements at time $T$, to estimate the contaminant inflow history. That is, given data

$$d_i = C(x_i, T), \; i = 1, 2, \ldots, m,$$

to estimate

$$C_{in}(t), \; 0 \le t \le T.$$

More generally

**Problem:**

Given the IFK

$$d(s) = \int_a^b g(x,s)\, m(x)\, dx$$

and a finite sample of values $d(s_i)$, $i = 1, 2, \ldots, m$, to estimate parameter $m(x)$.

# Outline

# Quadrature

## Basic Ideas:

Approximate the integrals

$$d_i \approx d(s_i) = \int_a^b g(s_i, x)\, m(x)\; dx \equiv \int_a^b g_i(x)\, m(x)\; dx,\; i = 1, 2, \ldots, m$$

(where the representers or data kernels $g_i(x) = g_i(s_i, x)$) by

- Selecting a set of collocation points $x_j$, $j = 1, 2, \ldots, n$. (It might be wise to ensure $n < m$.)
- Select an integration approximation method based on the collocation points.
- Use the integration approximations to obtain a linear system $G\mathbf{m} = \mathbf{d}$ in terms of the unknowns $m_j \equiv m(x_j)$, $j = 1, 2, \ldots, n$.

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# Representers

Rather than focusing on the value of $m$ at individual points, take a global view that $m(x)$ lives in a function space which is spanned by the **representer** functions $g_1(x), g_2(x), \ldots, g_n(x), \ldots$

## Basic Ideas:

- Make a selection of the basis functions $g_1(x), g_2(x), \ldots, g_n(x)$ to approximate $m(x)$, say

$$m(x) \approx \sum_{j=1}^{n} \alpha_j g_j(x)$$

- Derive a system $\Gamma \mathbf{m} = \mathbf{d}$ with a Gramian coefficient matrix

$$\Gamma_{i,j} = \langle g_i, g_j \rangle = \int_a^b g_i(x) g_j(x)\, dx$$

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# Example

**The Most Famous Gramian of Them All:**

- Suppose the basis functions turn out to be $g_i(x) = x^{i-1}$, $i = 1, 2, \ldots, m$, on the interval $[0, 1]$.
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# Other Choices of Trial Functions

Take a still more global view that $m(x)$ lives in a function space spanned by a spanning set which may *not* be the representers!

## Basic Ideas:

- Make a selection of the basis functions $h_1(x), h_2(x), \ldots, h_n(x)$ with linear span $H_n$ (called "trial functions" in the weighted residual literature) to approximate $m(x)$, say

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## Orthogonal Idea:

An appealing choice of basis vectors is an orthonormal (o.n.) set of nonzero vectors. If we do so:

- $\|m(x)\| = \sum_{j=1}^{n} \alpha_j^2$
- $\mathrm{Proj}_{H_n}(g_i(x)) = \sum_{j=1}^{n} \langle g_i, h_j \rangle h_j(x)$, $i = 1, \ldots, m$.
- Meaning of $i$th equation: $\langle \mathrm{Proj}_{H_n}(g_i), m \rangle = d_i$

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# Backus-Gilbert Method

**Problem:** we want to estimate $m(x)$ at a single point $\widehat{x}$ using the available data, and do it well. How to proceed?

## Basic Ideas:

- Write $m(\widehat{x}) \approx \widehat{m} = \sum_{j=1}^{m} c_j d_j$ and $d_j = \int_a^b g_j(x)\, m(x)\, dx$.
- Reduce the integral conditions to $\widehat{m} = \int_a^b A(x)\, m(x)\, dx$ with $A(x) = \sum_{j=1}^{m} c_j g_j(x)$.
- Ideally $A(x) = \delta(x - \widehat{x})$. What's the next best thing?

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## Constraints on the averaging kernel $A(x)$:

- First, an area constraint: total area $\int_a^b A(x)\,dx = 1$. Set $q_j = \int_a^b g_j(x)\,dx$ and get $\mathbf{q}^T\mathbf{c} = 1$.
- Secondly, minimize second moment $\int_a^b A(x)^2 (x - \widehat{x})^2\,dx$.
- This becomes a quadratic programming problem: objective function quadratic and constraints linear.
- In fact, it is convex, i.e., objective function matrix is positive definite. We have a tool for solving this: `quad_prog.m`.
- One could constrain the variance of the estimate $\widehat{m}$, say $\sum_{i=1}^{m} c_i^2 \sigma_i^2 \leq \Delta$, where $\sigma_i$ is the known variance of $d_i$. This is a more complicated optimization problem.

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# A Case Study for the EPA

## The Problem:

A factory on a river bank has recently been polluting a previously unpolluted river with unaccepable levels of polychlorinated biphenyls (PCBs). We have discovered a plume of PCB and want to estimate its size to assess damage and fines, as well as confirm or deny claims about the amounts by the company owning the factory.

- We control measurements but have an upper bound on the number of samples we can handle, that is, at most 100.
- Measurements may be taken at different times, but at most 20 per time at different locales.
- How would we design a testing procedure that accounts for and reasonably estimates this pollution dumping using the contaminant transport equation as our model?

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# Basic Theory of SVD

## Theorem

*(Singular Value Decomposition) Let $G$ be an $m \times n$ real matrix. Then there exist $m \times m$ orthogonal matrix $U$, $n \times n$ orthogonal matrix $V$ and $m \times n$ diagonal matrix $S$ with diagonal entries $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_q$, with $q = \min\{m, n\}$, such that $U^T G V = S$. Moreover, numbers $\sigma_1, \sigma_2, \ldots, \sigma_q$ are uniquely determined by $G$.*

## Definition

With notation as in the SVD Theorem, and $U_p$, $V_p$ the matrices consisting of the first $p$ columns of $U$, $V$, respectively, and $S_p$ the first $p$ rows and columns of $S$, where $\sigma_p$ is the last nonzero singular value, then the **Moore-Penrose pseudoinverse** of $G$ is

$$G^\dagger = V_p S_p^{-1} U_p^T \equiv \sum_{j=1}^{p} \frac{1}{\sigma_j} \mathbf{V}_j \mathbf{U}_j^T.$$

# Matlab Knows It

Carry out these calculations in Matlab:

```
> n = 6
> G = hilb(n);
> svd(G)
>[U,S,V] = svd(G);
>U'*G*V - S
>[U,S,V] = svd(G,'econ');
> % try again with n=16 and then G=G(1:8)
> % what are the nonzero singular values of G?
```

# Applications of the SVD

Use notation above and recall that the null space and column space (range) of matrix $G$ are $N(G) = \{\mathbf{x} \in \mathbb{R}^n \mid G\mathbf{x} = \mathbf{0}\}$ and

$$R(G) = \{\mathbf{y} \in \mathbb{R}^m \mid \mathbf{y} = G\mathbf{x},\ \mathbf{x} \in \mathbb{R}^n\} = \operatorname{span}\{\mathbf{G}_1, \mathbf{G}_2, \ldots, \mathbf{G}_n\}$$

## Theorem

*(1)* $\operatorname{rank}(G) = p$ *and* $G = \sum_{j=1}^{p} \sigma_j \mathbf{U}_j \mathbf{V}_j^T$

*(2)* $N(G) = \operatorname{span}\{\mathbf{V}_{p+1}, \mathbf{V}_{p+2}, \ldots, \mathbf{V}_n\}$, $R(G) = \operatorname{span}\{\mathbf{V}_1, \mathbf{V}_2, \ldots, \mathbf{V}_p\}$

*(3)* $N\left(G^T\right) = \operatorname{span}\{\mathbf{U}_{p+1}, \mathbf{U}_{p+2}, \ldots, \mathbf{U}_m\}$, $R(G) = \operatorname{span}\{\mathbf{U}_1, \mathbf{U}_2, \ldots, \mathbf{U}_p\}$

*(4)* $\mathbf{m}_\dagger = G^\dagger \mathbf{d}$ *is a least squares solution to* $G\mathbf{m} = \mathbf{d}$ *of minimum 2-norm.*