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

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Lecture 16, March 2, 2006
AvH 10
Outline

1. Chapter 4: Rank Deficiency and Ill-Conditioning
   - Discrete Ill-Posed Problems

2. Chapter 5: Tikhonov Regularization
   - Tikhonov Regularization and Implementation via SVD
   - 5.2: SVD Implementation of Tikhonov Regularization
What Are They?

These problems arise due to ill-conditioning of $G$, as opposed to a rank deficiency problem. Theoretically, they are not ill-posed, like the Hilbert matrix. But practically speaking, they behave like ill-posed problems. Authors present a hierarchy of sorts for a problem with system $Gm = d$. These order expressions are valid as $j \to \infty$.

- $O \left( \frac{1}{j^\alpha} \right)$ with $0 < \alpha \leq 1$, the problem is mildly ill-posed.
- $O \left( \frac{1}{j^\alpha} \right)$ with $\alpha > 1$, the problem is moderately ill-posed.
- $O \left( e^{-\alpha j} \right)$ with $0 < \alpha$, the problem is severely ill-posed.
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The Shaw Problem:

An optics experiment is performed by dividing a circle using a vertical transversal with a slit in the middle. A variable intensity light source is placed around the left half of the circle and rays pass through the slit, where they are measured at points on the right half of the circle.

- Measure angles counterclockwise from the $x$-axis, using $-\pi/2 \leq \theta \leq \pi/2$ for the source intensity $m(\theta)$, and $-\pi/2 \leq s \leq \pi/2$ for destination intensity $d(s)$.
- The model for this problem comes from diffraction theory:

$$d(s) = \int_{-\pi/2}^{\pi/2} (\cos(s) + \cos(\theta))^2 \left( \frac{\sin(\pi \sin(s) + \sin(\theta))}{\pi \sin(s) + \sin(\theta)} \right)^2 m(\theta) \, d\theta.$$
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- The forward problem: given source intensity $m(\theta)$, compute the destination intensity $d(s)$.
- The inverse problem: given destination intensity $d(s)$, compute the source intensity $m(\theta)$.
- It can be shown that the inverse problem is severely ill-posed.
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The Shaw Problem

How To Discretize The Problem:

- Discretize the parameter domain $-\pi/2 \leq \theta \leq \pi/2$ and the data domain $-\pi/2 \leq s \leq \pi/2$ into $n$ subintervals of equal size
  
  $\Delta s = \Delta \theta = \pi/n$.

- Therefore, and let $s_i$, $\theta_i$ be the midpoints of the $i$-th subintervals:
  
  $s_i = \theta_i = -\frac{\pi}{2} + \frac{(i - 0.5) \pi}{n}, \quad i = 1, 2, \ldots, n$.

- Define
  
  \[ G_{i,j} = (\cos(s_i) + \cos(\theta_j))^2 \left( \frac{\sin(\pi (\sin(s_i) + \sin(\theta_j)))}{\pi (\sin(s_i) + \sin(\theta_j))} \right)^2 \Delta \theta \]

- Thus if $m_j \approx m(\theta_j)$, $d_i \approx d(s_i)$, $m = (m_1, m_2, \ldots, m_n)$ and $d = (d_1, d_2, \ldots, d_n)$, then discretization and the midpoint rule give $Gm = d$, as in Chapter 3.
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Now we can examine the example files on the text CD for this problem. This file lives in 'MatlabTools/Examples/chap4/examp1'. First add the correctd path, then open the example file examp.m for editing. However, here’s an easy way to build the matrix $G$ without loops. Basically, these tools were designed to help with 3-D plotting.

```matlab
> n = 20
> ds = pi/n
> s = linspace(ds/2, pi - ds/2,n)
> theta = s;
> [S, Theta] = meshgrid(s,theta);
>G = (cos(S) + cos(Theta)).^2 .* (sin(pi*(sin(S) + ...
sin(Theta))))./(pi*(sin(S) + sin(Theta))).^2*ds;
> % want to see $G(s,\theta)$?
> mesh(S,Theta,G)
> cond(G)
> svd(G)
> rank(G)
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Regularization:

This means “turn an ill-posed problem into a well-posed ’near by’ problem”. Most common method is Tikhonov regularization, which is motivated in context of our possibly ill-posed $Gm = d$, i.e., minimize $\|Gm - d\|_2$, problem by:

- Problem: minimize $\|m\|_2$ subject to $\|Gm - d\|_2 \leq \delta$
- Problem: minimize $\|Gm - d\|_2$ subject to $\|m\|_2 \leq \epsilon$
- Problem: (damped least squares) minimize $\|Gm - d\|_2^2 + \alpha^2 \|m\|_2^2$. This is the Tikhonov regularization of the original problem.
- Problem: find minima of $f(x)$ subject to constraint $g(x) \leq c$.e function $L = f(x) + \lambda g(x)$, for some $\lambda \geq 0$. 
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All of the above problems are equivalent under mild restrictions thanks to the principle of Lagrange multipliers:

- Minima of \( f(x) \) occur at **stationary points** of \( f(x) \) \( (\nabla f = 0.) \)
- Minima of \( f(x) \) subject to constraint \( g(x) \leq c \) must occur at stationary points of function \( L = f(x) + \lambda g(x) \), for some \( \lambda \geq 0 \) (we can write \( \lambda = \alpha^2 \) to emphasize non-negativity.)
- We can see why this is true in the case of a two dimensional \( x \) by examining contour curves.
- Square the terms in the first two problems and we see that the associated Lagrangians are related if we take reciprocals of \( \alpha \).
- Various values of \( \alpha \) give a trade-off between the instability of the unmodified least squares problem and loss of accuracy of the smoothed problem. This can be understood by tracking the value of the minimized function in the form of a path depending on \( \delta, \epsilon \) or \( \alpha \).
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To solve the Tikhonov regularized problem, first recall:

\[ \nabla \left( \| Gm - d \|^2_2 + \alpha^2 \| m \|^2_2 \right) = (G^T Gm - G^T d) + \alpha^2 m \]

- Equate to zero and these are the normal equations for the system

\[ \begin{bmatrix} G \\ \alpha I \end{bmatrix} m = \begin{bmatrix} d \\ 0 \end{bmatrix}, \text{ or } (G^T G + \alpha^2 I) m = G^T d \]

- To solve, calculate \( (G^T G + \alpha^2 I)^{-1} G^T = \)

\[ U^T \begin{bmatrix} \frac{\sigma_1}{\sigma_1^2 + \alpha^2} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ \frac{\sigma_p}{\sigma_p^2 + \alpha^2} & \cdots & 0 \end{bmatrix} V \]
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SVD Implementation

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\[ V \begin{bmatrix} \frac{\sigma_1}{\sigma_1^2 + \alpha^2} \\ \cdots \\ \frac{\sigma_p}{\sigma_p^2 + \alpha^2} \\ 0 \cdots \end{bmatrix} U^T \]
From the previous equation we obtain that the Moore-Penrose inverse and solution to the regularized problem are given by

\[ G^\dagger = \sum_{j=1}^{p} \frac{\sigma_j}{\sigma_j^2 + \alpha^2} V_j U_j^T \]

\[ m_\alpha = G^\dagger d = \sum_{j=1}^{p} \frac{\sigma_j \left(U_j^T d\right)}{\sigma_j^2 + \alpha^2} V_j \]

which specializes to the generalized inverse solution we have seen in the case that \( G \) is full column rank and \( \alpha = 0 \). (Remember \( d = U h \) so that \( h = U^T d \).)
The Filter Idea

**About Filtering:**

The idea is simply to “filter” the singular values of our problem so that (hopefully) only “good” ones are used.

- We replace the $\sigma_i$ by $f(\sigma_i)$. The function $f$ is called a filter.
- $f(\sigma) = \sigma$ simply uses the original singular values.
- $f(\sigma) = \frac{\sigma}{\sigma^2 + \alpha^2}$ is the Tikhonov filter we have just developed.
- $f(\sigma) = \max\{\text{sgn}(\sigma - \epsilon)\sigma, 0\}$ is the TSVD filter with singular values smaller than $\epsilon$ truncated to zero.
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- $f(\sigma) = \max \{\text{sgn}(\sigma - \epsilon) \sigma, 0\}$ is the TSVD filter with singular values smaller than $\epsilon$ truncated to zero.
The Filter Idea

About Filtering:

The idea is simply to “filter” the singular values of our problem so that (hopefully) only “good” ones are used.

- We replace the $\sigma_i$ by $f(\sigma_i)$. The function $f$ is called a filter.
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- Make a plot of the curve $(\|m_\alpha\|_2, \|Gm_\alpha - d\|_2)$
- Typically, this curve looks to be asymptotic to the axes.
- Choose the value of $\alpha$ closest to the corner.
- Caution: L-curves are NOT guaranteed to work as a regularization strategy.
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Historical Notes

Tikhonov’s original interest was in operator equations

\[ d(s) = \int_a^b k(s, t) m(t) \, dt \]

or \( d = Km \) where \( K \) is a compact (bounded = continuous) linear operator from one Hilbert space \( H_1 \) into another \( H_2 \). In this situation:

- Such an operator \( K : H_1 \to H_2 \) has an adjoint operator \( K^* : H_2 \to H_1 \) (analogous to transpose of matrix operator.)
- Least squares solutions to \( \min ||Km - d|| \) are just solutions to the normal equation \( K^*Km = K^*d \) (and exist.)
- There is a Moore-Penrose inverse operator \( K^\dagger \) such that \( m = K^\dagger d \) is the least squares solution of least 2-norm. But this operator is generally unbounded (not continuous.)
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- The operator \((K^*K + \alpha I)\) is bounded with bounded inverse and the regularized problem \((K^*K + \alpha I) m = K^*d\) has a unique solution \(m_\alpha\).

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- Morozov’s discrepancy principle is a regular algorithm.

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