Parameter Selection Tool for Solution to Ill-Posed Problems

Brianna R. Cash\textsuperscript{1} \quad Advisor: Dianne O’Leary\textsuperscript{2}

\textsuperscript{1}Applied Math Scientific Computing (AMSC)
University of Maryland, College Park

\textsuperscript{2}Department of Computer Science
University of Maryland, College Park

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The problem:

![Tomography image of a mastectomy specimen](image.png)

**Figure**: Tomography image of a mastectomy specimen. Stevens G M et al. Radiology 2003;228:569-575

- In application images can be expensive to produce.
- Used for making decisions
- Images can be distorted and/or noisy.
  - physics of the measurement
  - non-homogeneous material
The discrete model: \( Ax + \epsilon = b, \epsilon \sim \mathbf{N}(0, S^2) \) where

- \( A \) is a known \( m \times n \) matrix where \( m \geq n \) (Blurring matrix)
- \( x \) is unknown \( n \times 1 \) vector (true image) where \( n = n_h \times n_v \)
- \( \epsilon \) is a \( m \times 1 \) vector (noise)
- \( S^2 \) is known \( m \times m \) (variance matrix for \( \epsilon \))
- \( b \) is a known \( m \times 1 \) vector (blurred and noisy image) where \( m = m_h \times m_v \)

Inherent to image deblurring and seismic tomographic problems, \( A \) is ill-conditioned.
Formulation of regularization problem:
\[ \min \frac{1}{2} \| A x - b \|_2^2 + \gamma R(x) \]

Where \( R(x) \) is a penalty function and \( \gamma \) is the regularization parameter.

**Tikhonov:** \( R(x) = \| x \|_2^2 \).

**Total Variation:** \( R(x) = TV(x) \) where \( TV(x) = \| \nabla x \|_1 \).
Selecting a method and good regularization parameter is problem dependent and subject to bias:

*Figure:* Images courtesy of Dianne O’Leary

But what is unexpected is often what we are interested in!
Selecting a method and good regularization parameter is problem dependent and subject to bias:

Figure: Images courtesy of Dianne O’Leary

But what is unexpected is often what we are interested in!
Outline

1. Motivation
2. Tool for Method and Parameter Selection
   - Methods
     - Initial Parameter Selection
     - Diagnostics
3. Implementation of Tool
   - Software Package
4. Results and Testing
   - Testing
   - Results
5. Validation
   - Software
   - Usefulness
6. Deliverables
Singular Value Decomposition (SVD) based methods: SVD of \( \mathbf{A} \) is give by
\[
\mathbf{A} = \mathbf{USV}^T = \sum_{i=1}^{n} \mathbf{u}_i \sigma_i \mathbf{v}_i^T.
\]
where \( \mathbf{U} = (\mathbf{u}_1, \ldots, \mathbf{u}_n) \) is a \( m \times n \) matrix and \( \mathbf{V} = (\mathbf{v}_1, \ldots, \mathbf{v}_n) \) is a \( n \times n \) matrix both with orthonormal columns, and \( \mathbf{S} = \text{diag}(\sigma_1, \ldots, \sigma_n) \) is a matrix of the non-negative singular values that appear in decreasing order.

The Tikhonov regularization solution is given by
\[
\mathbf{x}_{tik} = \sum_{i=1}^{n} \frac{\sigma_i \mathbf{u}_i \mathbf{v}_i^T \mathbf{b}}{\sigma_i^2 + \gamma}.
\]
And Truncated SVD regularization solution is given by
\[
\mathbf{x}_{TSVD} = \sum_{i=1}^{n} \phi_i \frac{\mathbf{u}_i \mathbf{v}_i^T \mathbf{b}}{\sigma_i} \quad \text{where} \quad \phi_i = 1 \text{ for } i = 1, \ldots, k \quad \text{and} \quad \phi_i = 0 \text{ for } i = k + 1, \ldots, n.
\]
Total variation based regularization method:

\[
\min_x \frac{1}{2} \|Ax - b\|_2^2 + \gamma TV(x).
\]

\[
TV(x) = \sum_{i=1}^n \|D_i^T x\|_2 \quad \text{where } D_i^T x = [x_{i+n_v} - x_i, x_{i+1} - x_i]^T.
\]

First order condition:

\[
g(x) = A^T (Ax - b) + \gamma \sum_{i=1}^n \frac{D_iD_i^T x}{\|D_i^T x\|_2} = 0
\]

replace \(\|D_i^T x\|_2\) with \(\sqrt{\|D_i^T x\|_2^2 + \beta}\) where \(\beta > 0\) and small.
Motivation for an improved implementation [Chan1996]:

Consider $g(x)$ (ignoring $\beta$ for simplicity):

$$g(x) = A^T(Ax - b) + \gamma \sum_{i=1}^{n} \frac{D_i D_i^T x}{\|D_i^T x\|_2}$$

Introduce a new variable:

$$y_i = \frac{D_i^T x}{\|D_i^T x\|_2}$$

where $y_i$ is $2 \times 1$.

Then the first order condition becomes:

$$g(y, x) = A^T(Ax - b) + \gamma \sum_{i=1}^{n} D_i y_i = 0,$$

$$h(y, x) = \|D_i^T x\|_2 y_i - D_i^T x = 0 \forall i,$$

and $\|y_i\| \leq 1$.

Primal-Dual Newton’s Method [Chan1996]
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Primal-Dual Newton’s Method [Chan1996]
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Initial parameter selection ($\gamma$):

- **Generalized Cross Validation (GCV):**
  
  Minimize $G(\gamma) = \sum_{k=1}^{m} [b_k - (A\tilde{x}^{(k)})_k]^2$
  
  where the $\tilde{x}^{(k)}$ minimizes
  
  \[
  \frac{1}{2}\|Ax - b\|_2^2 + \gamma R(x)
  \]
  
  when the $k^{th}$ measurement of $b$ is omitted.
  
  - Simple implementation for Tikhonov and TSVD regularization
  - Too expensive to use directly for TV method.

- **Discrepancy Principle:**
  
  Choose $\gamma$ such that $\|Ax_\gamma - b\|_2 = \nu E[\|\epsilon\|_2]$ where $\nu = 2$ is a safety factor.
  
  - Requires prior knowledge of the distribution of $\epsilon$ which we have assumed we know. -> good alternative for TV method.
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Motivation for statistical based diagnostics.

\[ b = Ax + \epsilon \]

Assumptions: The noise $\epsilon$ where $\epsilon \sim N(0, I_m)$

$x^*$ is the estimate of $x$ the the residual vector is

\[ r = b - Ax^* \]

Where we expect $r \sim N(0, I_m)$

This characteristic of the residual inspired three diagnostics [RustOleary2008]
Motivation for statistical based diagnostics.

\[ \mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{\epsilon} \]

Assumptions: The noise \( \mathbf{\epsilon} \) where \( \mathbf{\epsilon} \sim N(\mathbf{0}, \mathbf{I}_m) \)

\( \mathbf{x}^* \) is the estimate of \( \mathbf{x} \) the residual vector is

\[ \mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}^* \]

Where we expect \( \mathbf{r} \sim N(\mathbf{0}, \mathbf{I}_m) \)

This characteristic of the residual inspired three diagnostics [RustOleary2008]
Diagnostic 1: The residual norm squared should be within two standard deviations of the expected value of $\|\epsilon\|_2^2$ of $\|r\|_2^2 \in [m - 2\sqrt{2}m, m + 2\sqrt{2}m]$ where $m = E[\|\epsilon\|_2^2]$. 
Diagnostic 2: Goodness of fit of the normal curve to the histogram of the elements of the residual vector $r$.

Figure: checkperiod.m by Dianne O’Leary
Diagnostic 3: Consider the elements $r$ as time series with index $j = 1, \ldots, m$. Find the cumulative periodogram of the residual time-series and check if it is within 95% confidence band of the cumulative periodogram of the time series of white noise.

The cumulative periodogram is the partial sum of the periodogram where the periodogram is the sum of the square of the real and imaginary parts of the discrete Fourier transform.
Diagnostic 3:

Figure: checkperiod.m by Dianne O’Leary
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Software package

**Frontend**
- Graphical User Interface (GUI) built using Matlab’s GUI toolbox

**Backend**
- Regularization method
  - Tikhonov and Truncated SVD methods from *RestoreTool* [Nagy2002]
  - Total Variation regularization method [Cash 2012]
- Method for initial parameter selection
  - Generalized Cross-Validation (GCV) in *RestoreTool* for regularization methods included.
  - Discrepancy Principle [Cash 2012]
- Validate candidate solutions using statistical diagnostics
  - Adapt existing code for statistical diagnostics from Dianne O’Leary [Cash 2012]
GUI Demonstration in Matlab
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Effect of SNR on statistical diagnostics

$$SNR = 10 \log_{10}(\frac{||b||^2}{||\epsilon||^2}).$$

**Figure:** Length of interval of parameter satisfying Diagnostic 1 for Tikhohnov Method on a $16 \times 16$ segment of the image “cell.tif”.
Effects of $\gamma$ on computation time

**Figure:** The difference in $\log_{10}$ of the computational time for the TV regularization method for parameters between $\gamma = 1$ and $\gamma = 10^{-9}$

Computation time of the TV regularization method is dependent on the number of CG iterations, preconditioners were explored but included.
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Results for larger images

Figure: 256 × 256 image of Satellite with PSF provided in *RestoreTool* with zero boundary conditions and SNR=9
Results for larger images

Figure: $129 \times 129$ image of “cell.tif” with Gaussian blur and zero boundary conditions with SNR of 60
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Validation of software

- Modularly developed
- Modules validated independently with small examples that could be confirmed by hand or by comparing to existing code or functions
  - CG code was both validated by solving a known test problem as well as the code and results could be compared to matlabs `pcg.m`.
  - search direction on dual variable was first verified that solution met the constraints as well results were compared to the Vogel’s code implementation independently.
- Results found using implementations of the Primal-Dual Newton’s method implemented by Curtis Vogel
Primal-Dual Newton’s method

Figure: Results of the TV regularization method for my implementation and code by Curtis Vogel.

Relative error of my implementation was 0.9% compared to 1.02% for the given example.
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Validation of software usefulness

- Presented as part of AMSC 663/664
- Presented and distributed to undergraduate students in Deblurring Digital Images (CMSC/AMSC 498D) as an educational tool
- Presented to the AMSC student seminar
- Proof of concept for tool for picking regularization method and parameter
Project Deliverables:
Parameter Selection Tool for Solution to Ill-Posed Problems

- Graphical user interface that could be used by a researcher/student
- All the necessary code for computing the regularization solution, selecting an initial parameter, validating solutions with the diagnostics.


References II

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