Large-Scale Tikhonov Regularization via Reduction by Orthogonal Projection

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Outline

1. Problem definition
2. Approaches in the literature
3. Iterative projection method
4. Numerical Example
Abstract

Problem definition

Approaches in the literature

Iterative projection method

Numerical Example
Problem

\[ \min_{x \in \mathbb{R}^n} \| Ax - b \| \]  

(1)

where \( A \in \mathbb{R}^{m \times n} \), \( m \geq n \), is severely ill-conditioned (not necessarily of full rank).

b \in \mathbb{R}^m \) represents observations and is assumed to be contaminated by an error \( e \in \mathbb{R}^m \), i.e. \( b = b_{\text{true}} + e \).

The linear system of equations \( Ax = b_{\text{true}} \) associated with the least-squares problem (1) is assumed to be consistent.

We would like to determine an approximation of its solution of minimal pseudo-norm by computing a suitable approximate solution of (1).
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Problem

Due to the ill-conditioning of $A$ and the error $e$ in $b$, straightforward solution of (1) often does not yield a meaningful approximation of $x_{\text{true}}$. 

To stabilize the computations apply Tykhonov regularization, i.e. replace (1) by

$$\min_{x \in \mathbb{R}^n} \{ \|Ax - b\|^2_2 + \mu^{-1} \|Lx\|^2_2 \}. \quad (2)$$

The scalar $\mu \in (0, \infty)$ is referred to as the regularization parameter and $L \in \mathbb{R}^{p \times n}$, $p \leq n$, as the regularization matrix.

The normal equations associated with (2) are given by

$$ \left( A^T A + \mu^{-1} L^T L \right) x = A^T b. \quad (3)$$

They have the unique solution

$$ x_{\mu} = \left( A^T A + \mu^{-1} L^T L \right)^{-1} A^T b. \quad (4)$$

for any $\mu > 0$ when $\text{rank} \begin{bmatrix} A & L \end{bmatrix} = n$. \quad (5)

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Approaches in the literature

TUHH Heinrich Voss Tikhonov Regularization via Reduction ICIAM, July 2011
Approaches in the literature

Small dimension

When $A$ and $L$ are small, solutions $x_\mu$ of (2) can be determined easily for many values of $\mu > 0$ by first computing the generalized singular value decomposition (GSVD) of the matrix pair \{A, L\} (Van Loan (1976), Varah (1979)).
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For large-scale problems and a fixed $\mu > 0$, an approximation of $x_\mu$ can be determined by applying an iterative method, such as LSQR, to (3). However, generally, a suitable value of the parameter $\mu$ is not known a priori and has to be determined during the solution process.
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Many approaches to determining an appropriate value of $\mu$, including the L-curve criterion, the discrepancy principle, generalized cross validation, and information criteria, require the normal equations (3) to be solved repeatedly for many different values of the parameter $\mu$. This can make application of LSQR costly.
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The computed approximation, $x_\ell^\mu$, lives in the Krylov subspace

$$K_\ell(A^T A, A^T b) = \text{span}\{A^T b, (A^T A)A^T b, \ldots, (A^T A)^{\ell-1} A^T b\} \quad (6)$$

for some $\ell \geq 1$. 
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Due to the shift invariance of Krylov subspaces, i.e., the property that

$$K_\ell(A^T A, A^T b) = K_\ell(A^T A + \mu^{-1} I, A^T b), \quad \mu > 0,$$

the spaces (6) can be used for all values of $\mu > 0$. 
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the spaces (6) can be used for all values of $\mu > 0$.

This makes it possible to first project the problem (3) onto a Krylov subspace (6) and then regularize the projected problem by Tikhonov’s method.
A-weighted pseudoinverse

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This transformation is carried out with the aid of the substitutions $y = Lx$ and $x = L_A^\dagger y$, where the matrix

$$L_A^\dagger := (I - (A(I - L^\dagger L)^\dagger A)L^\dagger)$$

is referred to as the \textit{A-weighted pseudoinverse of L} (Eldén (1982)).
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When $L$ is banded with small bandwidth and has a known null space, transformation of (2) to standard form is attractive. Other situations when transformation to standard form is feasible are discussed in Reichel & Ye (2009).
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However, when (2) is the discretization of an integral equation of the first kind in two or more space-dimensions, the regularization matrix $L$ often is chosen to be a sum of Kronecker products. The expression for $L_A^\dagger$ then is complicated and unattractive to use.
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An attractive property of this method is that the computed approximate partial GSVD is independent of \( \mu \).

However, the inner-outer iteration scheme may be expensive, due to the possibly fairly large number of required matrix-vector product evaluations with \( A \) and its transpose \( A^T \).
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The regularization parameter $\mu = \mu(\varepsilon)$ is determined by the discrepancy principle, i.e. so that the computed approximation $\tilde{x}_\mu$ of the solution $x_\mu$ of (2) satisfies

$$\| A\tilde{x}_\mu - b \| = \eta \varepsilon =: \delta,$$  (7)

where $\eta > 1$ is a user-specified constant, whose size depends on the accuracy of the estimate $\varepsilon$ of $\| e \|$. 

The function $\phi(\mu) := \| Ax_\mu - b \|_2$. We are looking for $\mu$ with $\phi(\mu) = \delta^2$. The function $\phi(\mu)$ is convex and monotone such that finding $\mu$ is an easy task, but note that for large $A$ the evaluation of $\phi(\mu)$ is expensive. A numerical method for inexpensively computing upper and lower bounds for $\bar{\mu}$ when $L=I$ is described in Calvetti & Reichel (2003).
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Iterative projection method

**Setting**

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Introduce a subspace $\mathcal{V} \subset \mathbb{R}^n$ of small dimension $k \ll n$, and approximate $\phi(\mu)$ by the function

$$\phi(\mu, \mathcal{V}) := \|Ax^k_\mu - b\|^2$$

where $x^k_\mu$ is obtained by solving the Tikhonov problem restricted to $\mathcal{V}$. 

If a given accuracy is not met then expand the search space $\mathcal{V}$. This yields the following type of iterative projection method.
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This yields the following type of iterative projection method.
Algorithm 1 Iterative Projection Tikhonov Method

Require: Initial basis $V_0$ of $\mathcal{V}$, $V_0^T V_0 = I$
1: for $i = 0, 1, \ldots$ until convergence do
2: Find the root $\mu_i$ of $f(\mu; V_i) := \phi(\mu, V) - \delta^2 = 0$
3: Solve $(V_i^T (A^T A + \mu_i^{-1} L^T L)V_i)y_{\mu_i} = V_i^T A^T b$
4: Compute $r_{\mu_i} := (A^T A + \mu_i^{-1} L^T L)V_iy_{\mu_i} - A^T b$
5: Reorthogonalize (optional) $\tilde{r}_{\mu_i} = (I - V_i V_i^T)r_{\mu_i}$
6: Normalize $v_{\text{new}} = \tilde{r}_{\mu_i} / \|\tilde{r}_{\mu_i}\|
7: Enlarge search space $V_{i+1} = [V_i, v_{\text{new}}]$
8: end for
9: Determine approximate Tikhonov solution $x_{\mu_i} = V_i y_{\mu_i}$
Iterative projection method

Algorithm 2 Iterative Projection Tikhonov Method

Require: Initial basis $V_0$ of $V$, $V_0^T V_0 = I$

1: for $i = 0, 1, \ldots$ until convergence do
2: \hspace{1em} Find the root $\mu_i$ of $f(\mu; V_i) := \phi(\mu, V) - \delta^2 = 0$
3: \hspace{1em} Solve $(V_i^T (A^T A + \mu_i^{-1} L^T L) V_i) y_{\mu_i} = V_i^T A^T b$
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In every iteration step have to

- determine $\mu_i$
- expand search space with $v_{\text{new}}$
\[ y_\mu = (V^T(A^T A + \mu^{-1}L^T L)V)^{-1} V^T A^T b \]

solves the projected least squares problem

\[ \| \begin{bmatrix} AV \\ \mu^{-1/2}LV \end{bmatrix} y_\mu - \begin{bmatrix} b \\ 0 \end{bmatrix} \|^2 = \text{min!} \]
Solving projected problem

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i.e. with QR-factorizations \( AV = Q_A R_A \) and \( LV = Q_L R_L \)

\[ \left\| \begin{bmatrix} R_A \\ \mu^{-1/2} R_L \end{bmatrix} y_\mu - \begin{bmatrix} Q_A^T b \\ 0 \end{bmatrix} \right\|^2 = \min! \]
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i.e. with QR-factorizations \( AV = Q_AR_A \) and \( LV = Q_LR_L \)

\[ \| [R_A_{\mu^{-1/2}}R_L] y_\mu - [Q_A^T b \ 0] \|^2 = \text{min!} \]

Hence \( \phi(\mu; V) = \|AVy_\mu - b\|_2^2 \) can be evaluated by solving a least squares problem with a \( 2k \times k \) system matrix consisting of two stacked triangular matrices.
Solving projected problem

\[ \phi'(\mu; V) = 2 \left( (R_A y_\mu)^T R_A y'_\mu - \mu^{-2} (R_L y_\mu)^T (R_L y_\mu) \right), \]
Iterative projection method

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where \( y'_\mu \) solves the least squares problem

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\| \begin{bmatrix} R_A \\ \mu^{-1/2} R_L \end{bmatrix} y'_\mu - \begin{bmatrix} 0 \\ \mu^{-3/2} R_L y_\mu \end{bmatrix} \| = \min!
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Notice that the system matrix is the same as in the last problem. Hence, reusing its QR factorization \( \phi'(\mu; V) \) can be evaluated very cheaply.
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Notice that the system matrix is the same as in the last problem. Hence, reusing its QR factorization \( \phi'(\mu; V) \) can be evaluated very cheaply.

Due to the monotonicity and convexity of \( f(\cdot; V) \) its root \( \bar{\mu} \) can be determined safely with Newton’s method with initial approximation \( \mu_0 = 0 \). However, this will be very time consuming.
Typical behavior of $f(\mu) = \phi(\mu; V) - \delta^2$. Figure: Plot of a typical function $f(\mu; V_0)$ for problem shaw(2000).
Iterative projection method

Zero-finder based on rational inverse iteration

Consider a rational model for the inverse of $f$,

$$f^{-1} \approx h(f) := \frac{p(f)}{f - f_\infty}, \quad p(f) = \sum_{j=0}^{3} a_j f^j,$$

where

$$f_\infty = \lim_{\mu \to \infty} f(\mu; V) = \|b\|^2 - b^T Q_A (R_A R_A^\dagger) Q_A^T b - \delta^2.$$
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For

$$0 < \mu_1 < \mu_2 \quad \text{such that} \quad f(\mu_1) > 0 > f(\mu_2)$$

we determine $p$ such that $h(f(\mu_j)) = \mu_j$ and $h'(f(\mu_j)) = 1/f'(\mu_j)$ for $j = 1, 2$, and $\mu_{\text{new}} := h(0)$, and replace the value $\mu_1$ or $\mu_2$ which is on the same side of the root as $\mu_{\text{new}}$.
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Consider a rational model for the inverse of $f$,

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For

$$0 < \mu_1 < \mu_2 \quad \text{such that} \quad f(\mu_1) > 0 > f(\mu_2)$$

we determine $p$ such that $h(f(\mu_j)) = \mu_j$ and $h'(f(\mu_j)) = 1/f'(\mu_j)$ for $j = 1, 2$, and $\mu_{new} := h(0)$, and replace the value $\mu_1$ or $\mu_2$ which is on the same side of the root as $\mu_{new}$

Typically, one requires approximately 5 to 10 iteration steps to find an initial interval, and in the following iterations 2 (or even 1) iterations suffice.
Consider the restoration of a grey-scale image which is represented by an array of $256 \times 256$ pixels. The pixels are stored column-wise in a vector in $\mathbb{R}^{65536}$. 

The picture is blurred using the function $\text{blur}$ with parameters $\text{band} = 5$ and $\text{sigma} = 1.0$ and Gaussian noise corresponding to the noise level $\sigma = 10^{-2}$ is added.

To restore the picture we apply the iterative projection method with $\eta = 1.05$ and regularization matrix $L = [L_1 \otimes I_{256} \ I_{256} \otimes L_1]$ where $L_1 \in \mathbb{R}^{255 \times 256}$ is the discrete first order derivative in one space dimension.
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Original image
Blurred image
Convergence history of Tikhonov parameter

Value of $\mu_i$ vs. Dimension of the search space
Convergence history of residual norm

Convergence history of the Residualnorm

\[ \frac{\| T(\mu_i) x(\mu_i) - A^T b \|}{\| A^T b \|} \]
restored picture
Numerical Example

Four pictures

Original picture

Blurred and noisy picture

Restored with $L=I$

Restored with $L=L_{1,2D}$
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Conclusions

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Computed examples indicate that search spaces of fairly small dimension suffice.