Large-Scale Tikhonov Regularization via Reduction by Orthogonal Projection

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Outline

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$$\min_{x \in \mathbb{R}^n} \|Ax - b\| \tag{1}$$

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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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They have the unique solution

$$x_\mu = (A^T A + \mu^{-1} L^T L)^{-1} A^T b \tag{4}$$

for any $\mu > 0$ when

$$\text{rank} \begin{bmatrix} A \\ L \end{bmatrix} = n. \tag{5}$$

We assume this to be the case.

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Many approaches to determining an appropriate value of μ, 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 μ. This can make application of LSQR costly.

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$$\mathcal{K}_\ell(A^TA, A^Tb) = \text{span}\{A^Tb, (A^TA)A^Tb, \dots, (A^TA)^{\ell-1}A^Tb\} \tag{6}$$

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Due to the shift invariance of Krylov subspaces, i.e., the property that

$$\mathcal{K}_\ell(A^TA, A^Tb) = \mathcal{K}_\ell(A^TA + \mu^{-1}I, A^Tb), \qquad \mu > 0,$$

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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.

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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 μ.

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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$$\|A\widetilde{x}_\mu - b\| = \eta\varepsilon =: \delta, \tag{7}$$

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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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where x_μ^k is obtained by solving the Tikhonov problem restricted to $\mathcal{V}$.

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This yields the following type of iterative projection method.

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** $i = 0, 1, \dots$ until convergence **do**
2: Find the root μ_i of $f(\mu; V_i) := \phi(\mu, \mathcal{V}) - \delta^2 = 0$
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 $r_{\mu_i} := (A^T A + \mu_i^{-1} L^T L) V_i y_{\mu_i} - A^T b$
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 $x_{\mu_i} = V_i y_{\mu_i}$

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end for
Determine approximate Tikhonov solution $x_{\mu_i} = V_i y_{\mu_i}$

In every iteration step have to

- determine μ_i
- expand search space with v_{new}

Solving projected problem

$$y_\mu = (V^T(A^TA + \mu^{-1}L^TL)V)^{-1}V^TA^Tb$$

solves the projected lest squares problem

$$\left\| \begin{bmatrix} AV \\ \mu^{-1/2}LV \end{bmatrix} y_\mu - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|^2 = \text{min!}$$

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i.e. with QR-factorizations $AV = Q_A R_A$ and $LV = Q_L R_L$

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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.

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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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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 $f(\mu) = \phi(\mu; V) - \delta^2$

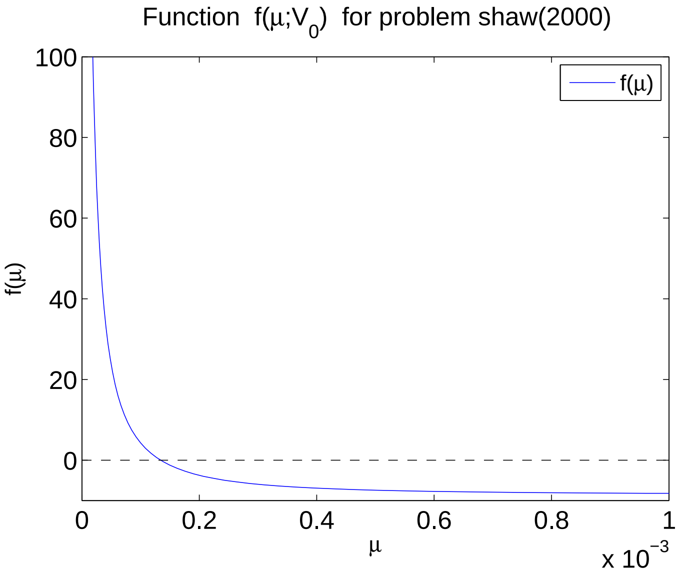

Figure: Plot of a typical function $f(\mu)$

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 $\mu_{new} := h(0)$, and replace the value μ_1 or μ_2 which is on the same side of the root as μ_{new}

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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.

Outline

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

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

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To restore the picture we apply the iterative projection method with $\eta = 1.05$ and regularization matrix

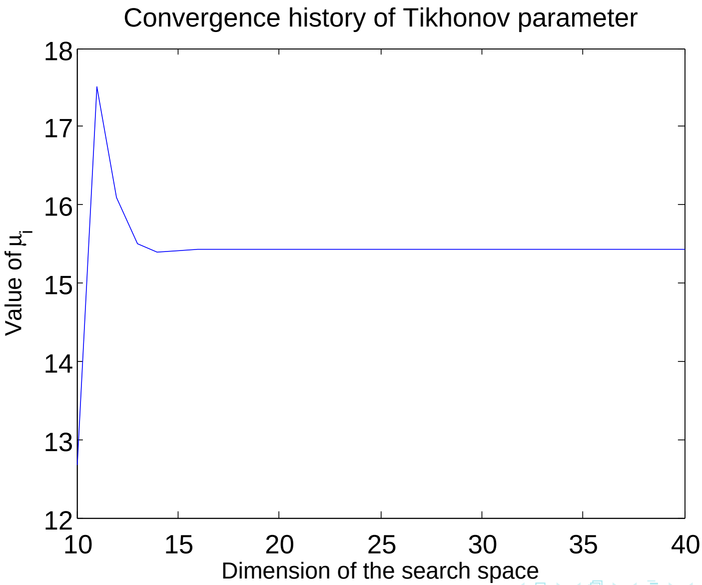
$$L = \begin{bmatrix} L_1 \otimes I_{256} \\ I_{256} \otimes L_1 \end{bmatrix}$$

where $L_1 \in \mathbb{R}^{255 \times 256}$ is the discrete first order derivative in one space dimension.

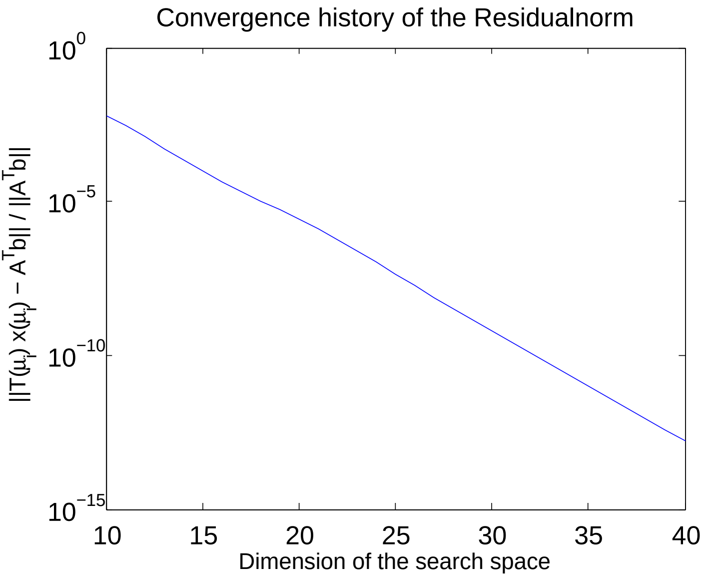
Original image

Blurred image

Convergence history of Tikhonov parameter

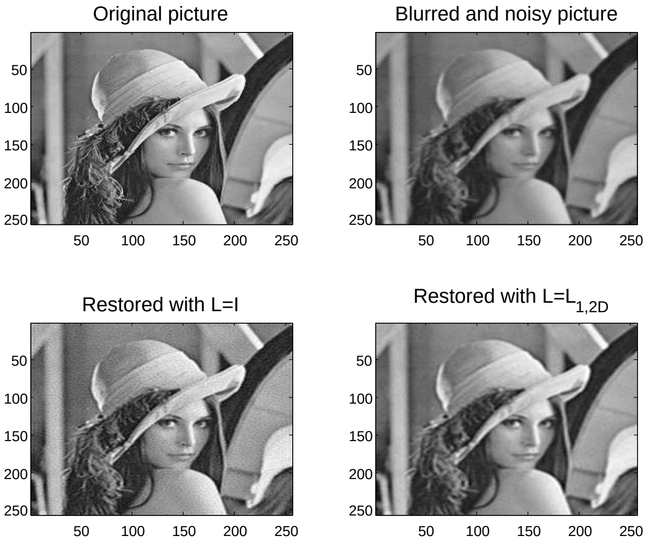


Convergence history of residual norm



restored picture

Four pictures



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An efficient zero-finder based on rational inverse interpolation is suggested.

Conclusions

A new iterative projection method for Tikhonov regularization for large problems with general regularization matrices is presented.

An efficient zero-finder based on rational inverse interpolation is suggested.

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