How good are Krylov methods for nonsymmetric discrete ill-posed problems?

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Discrete ill-posed problems

Often are problems of the form:

$$g(s) = \int k(s,t)f(t)dt, \qquad k \quad \text{smooth},$$

discretized to yield a linear algebraic system of equations:

$$b = Ax$$

$A \in \mathbf{R}^{n \times n}$, $x, b \in \mathbf{R}^n$. The matrix A is usually severely ill-conditioned and of ill-defined numerical rank.

Today we are interested in square matrices that may be nonsymmetric. n can be huge in many real-world problems.

Discrete ill-posed problems

The right hand side b may be contaminated by errors that we may know little about:

$$\tilde{b} = b + d, \qquad d \in \mathbf{R}^n.$$

Unfortunately,

$$\begin{aligned} \tilde{x} = A^{-1}\tilde{b} &= A^{-1}b + A^{-1}d \\ &= x + A^{-1}d \end{aligned}$$

is usually a very poor approximation of x.

Regularization

Replace the problem $Ax = \tilde{b}$ with a different, but related problem that reduces the influence of the noise on the solution.

We focus on regularization methods that constrain the solution to live in subspaces in which projections of A are much better-conditioned than A.

SVD and Truncated SVD

Express A using the singular value decomposition:

$$A = \sum_{j=1}^{n} \sigma_j u_j v_j^T, \qquad v_j^T v_k = u_j^T u_k = \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{o.w.,} \end{cases}$$

$u_j \in \mathbf{R}^n$, $v_j \in \mathbf{R}^n$, $j = 1, 2, \ldots, n$, and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$.

Truncated SVD methods constrain their solutions:

$$x_m^{TSVD} \in \text{span}\{v_1, v_2, \ldots, v_m\}, \quad m = 1, 2, \ldots, n.$$

Krylov subspaces

Let $A \in \mathbf{R}^{n\times n}$.

$$\mathcal{K}_m(A,b) = \mathrm{span}\{b, Ab, \ldots, A^{m-1}b\}, \;\; m = 1,2,3,\ldots,n\,.$$

Krylov methods constrain their solutions x_m to lie in $\mathcal{K}_m(A,b)$.

How “good” are these subspaces for discrete ill-posed problems?

That is, how good a choice is a subspace in which to seek a solution to a discrete ill-posed problem?

We can compare the relative error norm,

$$\|x - \mathcal{P}x\| / \|x\|,$$

of the exact solution and its orthogonal projection $\mathcal{P}x$ in the subspace for some famous test problems from Per Christian Hansen’s Regularization Toolbox.

Inverse Laplace transform example

Let $s, t \in [0, \infty)$. Let

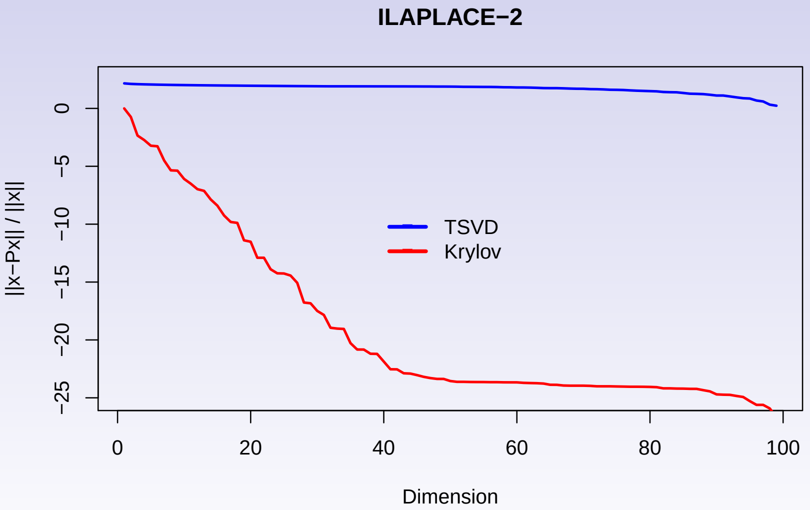
$$g(s) = \int \exp(-st) f(t) dt, \quad \text{where,}$$

ILAPLACE-2: $\quad g(s) = 1/(s+0.5), \qquad f(t) = \exp(-t/2).$

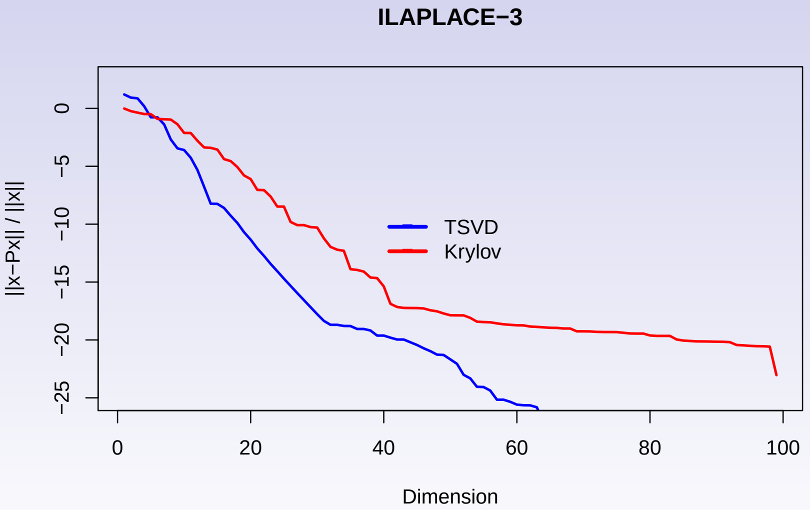
ILAPLACE-3: $\quad g(s) = 2/(s+0.5)^3, \qquad f(t) = t^2 \exp(-t/2).$

We discretize to form the 100×100 system $b = Ax$ and let $\tilde{b} = b + 0.01\|b\|d$, where d is a vector of normally distributed entries of zero mean and uniform variance scaled such that $\|d\| = 1$.

Inverse Laplace transform example



Inverse Laplace transform example



Other Toolbox examples (not all nonsymmetric)

Problem	Krylov subspaces	TSVD subspaces
baart	wins	
ilaplace-1		wins
ilaplace-2	wins	
ilaplace-3		wins
ilaplace-4	wins	
phillips	wins	
deriv2-1	wins	
heat		wins
shaw	tie	tie
foxgood	tie	tie

Solution methods

We usually solve a projected ordinary least-squares problem in the subspaces.

Krylov subspaces (the GMRES method):

$$\min_{x \in \mathcal{K}_m(A,b)} \|b - Ax\|,$$

or, for truncated SVD:

$$\min_{x \in \mathrm{span}\{v_1, v_2, \ldots, v_m\}} \|b - Ax\|.$$

The GMRES method

The GMRES method uses the Arnoldi process to efficiently compute projected ordinary least squares solutions in Krylov subspaces.

Assume that the dimension of $\mathcal{K}_m(A, \tilde{b}) = m$.

1. Let $\beta = \|\tilde{b}\|$.
2. Let $w_1 = \beta^{-1}\tilde{b}$.
3. Construct an ONB $\{w_1, w_2, \ldots, w_m\}$ of $\mathcal{K}_m(A, \tilde{b})$ such that
   3.1 $AW_m = W_{m+1}\bar{H}_m$, where
   3.2 $W_m = [w_1, w_2, \ldots, w_m]$ (an $n \times m$ matrix), $\bar{H}_m$ is upper-Hessenberg.

The GMRES method

Then,

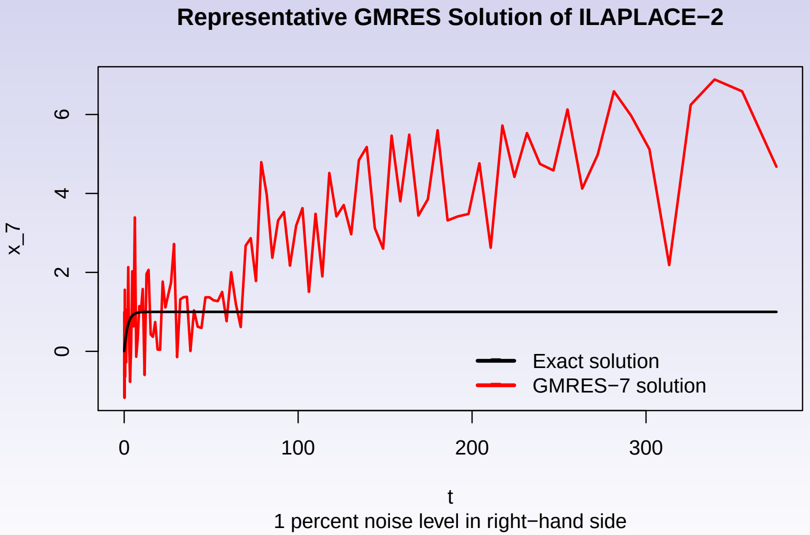
$$
\begin{aligned}
\min_{x \in \mathcal{K}_m(A,\tilde{b})} \|Ax - \tilde{b}\|^2 &= \min_{y \in \mathbf{R}^m} \|AW_m y - \tilde{b}\|^2 \\
&= \min_{y \in \mathbf{R}^m} \|W_{m+1} \bar{H}_m y - \beta W_{m+1} e_1\|^2 \\
&= \min_{y \in \mathbf{R}^m} \|\bar{H}_m y - \beta e_1\|^2. \qquad (1)
\end{aligned}
$$

Let y_m be the minimizer of (1). Then

$$x_m = W_m y_m$$

is the GMRES solution.

But GMRES solutions are not necessarily good!



Alternate solution methods

We see that Krylov subspaces are often good spaces to search for solutions, but projected OLS can be lousy.

Many hybrid, or "inner regularization" methods have been proposed:

- Penalized projected least-squares (projected Tikhonov). e.g., replace:

$$\min_{y \in \mathbf{R}^m} \|\bar{H}_m y - \beta e_1\|^2$$

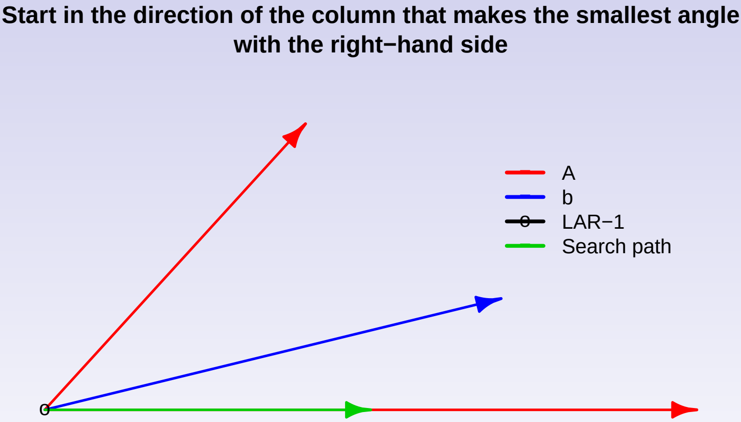
  with:

$$\min_{y \in \mathbf{R}^m} \left\{ \|\bar{H}_m y - \beta e_1\|^2 + \mu^{-2} \|y\|^2 \right\}.$$

- Truncated total least-squares
- ...

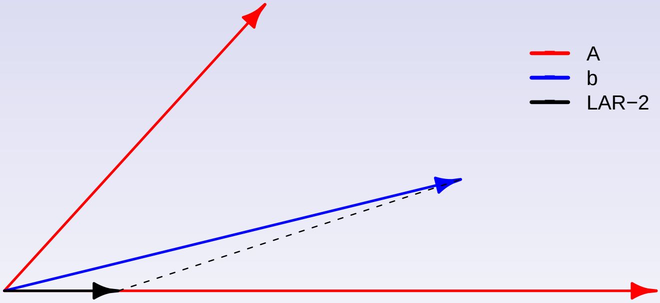
We propose a new method, projected LAR: compute the least-angle regression solution in the Krylov subspaces.

Least-angle regression (LAR)



Least-angle regression (LAR)

Proceed until one or more additional columns makes the same angle as the current search path with the current residual...



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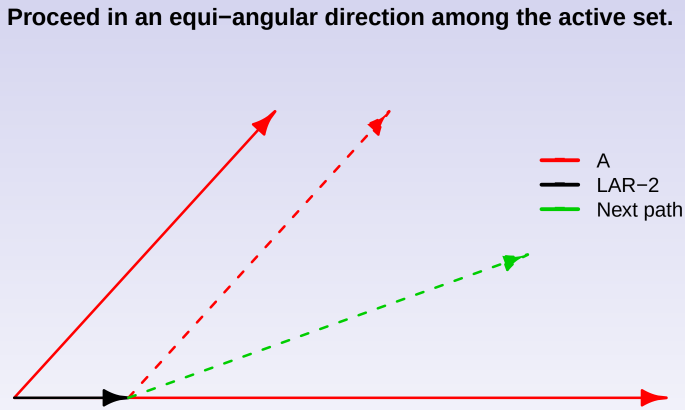

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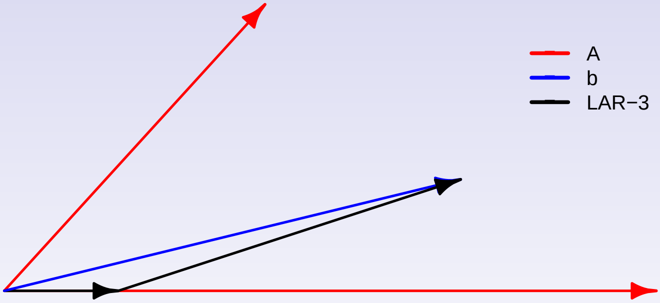
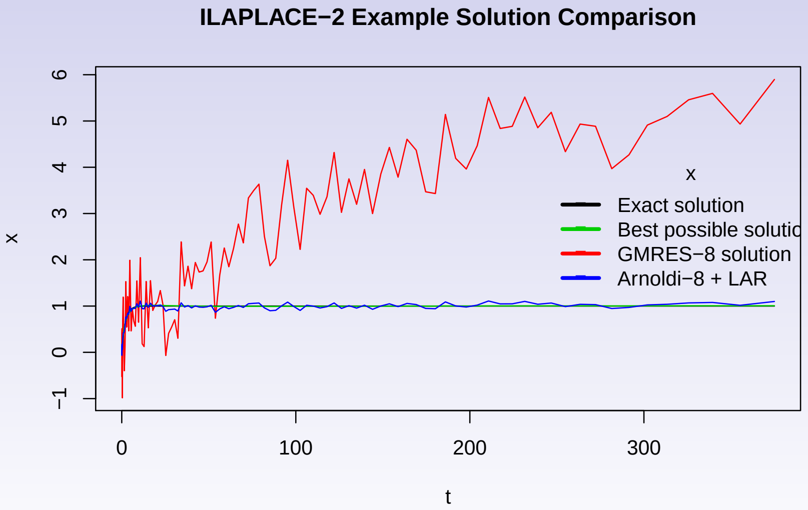


ILAPLACE-2: Arnoldi + Projected LAR example



Why LAR?

1. It's simple, computationally cheap, and computes the OLS solution anyway.
2. It only depends on angles and is easily orthogonally projected into Krylov subspaces.
3. Can outperform Tikhonov-corrected and other inner-regularized solutions.
4. It's very flexible; simple modifications produce projected L1-penalized solutions (the LASSO).

Parameter choice methods require further investigation for projected LAR (as, indeed for most solution methods!).

Summary

- Krylov subspaces are often good spaces in which to seek solutions to discrete ill-posed problems.
- Projecting ordinary least-squares into Krylov subspaces can produce lousy solutions.
- New solution methods and corresponding parameter choice methods, possibly related to LAR, are needed to find better solutions to discrete ill-posed problems in Krylov subspaces.