MINIMUM ENERGY SOLUTIONS TO ILL–CONDITIONED SYSTEMS

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1 Definitions

Notations. Given a vector $x \in \mathbb{C}^N$, we denote

$$\|x\| = \sqrt{x^* x}.$$

The symbol * denotes conjugate transposition. Therefore, for a complex matrix A, A^* is its adjoint (conjugate transposed).

The problem. Solve a square linear system

$$Ax_0 = b$$

where the conditioning of A is very large.

Minimum energy solutions. Given $\delta > 0$ (which we will call discrepancy),

$$\|x\| = \min!, \qquad \|Ax - b\| \leq \delta$$

Notice that

$$x = 0 \qquad \Longleftrightarrow \qquad \|b\| \leq \delta.$$

Proposition *The minimun energy solution exists and is unique.*

Proof. Its an elementary convexity argument. □

Tikhonov[1] regularization. Given $\alpha > 0$

$$\alpha \|x_\alpha\|^2 + \|Ax_\alpha - b\|^2 = \min!, \qquad x \in \mathbb{C}^N.$$

- as $\alpha \to 0$, then $x_\alpha \to x_0$
- as $\alpha \to \infty$, then $x_\alpha \to 0$.

To calculate the Tikhonov regularized solution of parameter α, we have solve the system

$$(\alpha I + A^* A) x_\alpha = A^* b.$$

[1] for Spanish speakers, Tijonov is the right form

Proposition *Given δ and α, let x_α be the Tikhonov reularized solution to the system. If*

$$\|Ax_\alpha - b\| = \delta,$$

then x_α is the minimun energy solution.

Proof. Let x be such that $\|Ax - b\| \leq \delta$. Then

$$\begin{aligned} \alpha\|x_\alpha\|^2 &= \alpha\|x_\alpha\|^2 + \|Ax_\alpha - b\|^2 \\ &\leq \alpha\|x^2\| + \|Ax - b\|^2 \\ &\leq \alpha\|x\|^2 + \delta^2 \end{aligned}$$

and therefore $\|x_\alpha\| \leq \|x\|$. □

Consequence. If $\delta < \|b\|$, to find the minimun energy solution, find a root of

$$G(\alpha) := \|Ax_\alpha - b\|^2 - \delta^2 = \|A(\alpha I + A^*A)^{-1}A^*b - b\|^2 - \delta^2.$$

The hypothesis means that the discrepancy level is smaller than data.

2 Two views on the problem

Lagrange multipliers. When solving the problem

$$\|x\|^2 = \min!, \qquad \|Ax - b\|^2 \leq \delta^2.$$

one faces two possibilities:

- The minimun is reached in the interior. The only local extremal point is $x = 0$. Therefore, this possibility holds if and only if

  $$\|b\| < \delta.$$

  Ii is the absolute minimun.

- The minimum is attained in the boundary, and we are the solving

  $$\|x\|^2 = \min!, \qquad \|Ax - b\|^2 - \delta^2 = 0.$$

  The associated Lagrangian is

  $$\mathcal{L}(x, \lambda) := \|x\|^2 + \lambda\left[\|Ax - b\|^2 - \delta^2\right]$$

  and the extrema are the solutions of the system in $\mathbb{R}^N \times \mathbb{R}$

  $$\begin{aligned} x + \lambda(A^*Ax - A^*b) &= 0 \\ \|Ax - b\|^2 &= \delta^2 \end{aligned}$$

  Each solution (x, λ) satisfies that $x = x_{1/\lambda}$ and therefore the Tikhonov regularization parameter matching the condition is the inverse of the Lagrange multiplier.

The singular value decomposition view. We recall the SVD of a square invertible matrix

$$A = P\Sigma Q^*, \qquad \Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix}$$

being P and Q unitary matrices, and $\sigma_j > 0$ for all j (σ_j are the singular values). Then the inverse of A is $Q\Sigma^{-1}P^*$ and

$$A^*A = Q\Sigma^2 Q^*.$$

Hence the equations $(\alpha I + A^*A)x_\alpha = A^*b$ are equivalent to

$$Q(\alpha I + \Sigma^2)Q^* x_\alpha = Q\Sigma P^* b$$

which implies that

$$x_\alpha = Q \underbrace{(\alpha I + \Sigma^2)^{-1}\Sigma}_{=:\,\Sigma_\alpha} P^* b, \qquad \Sigma_\alpha = \begin{bmatrix} \dfrac{\sigma_1}{\alpha + \sigma_1^2} & & \\ & \ddots & \\ & & \dfrac{\sigma_n}{\alpha + \sigma_n^2} \end{bmatrix}$$

(compare Σ_α with Σ^{-1}). If

$$P^* b = f = (f_1, \ldots, f_n)^\top, \qquad \sum_j |f_j|^2 = \|b\|^2$$

$$\begin{aligned} \|Ax_\alpha - b\|^2 &= \|P\Sigma Q^* Q \Sigma_\alpha P^* b - PP^* b\|^2 \\ &= \|P(\Sigma\,\Sigma_\alpha - I)P^* b\|^2 \\ &= \|(\Sigma\,\Sigma_\alpha - I)f\|^2 \\ &= \sum_j \left[\frac{\sigma_j^2}{\alpha + \sigma_j^2} - 1\right]^2 f_j^2 \\ &= \sum_j \frac{\alpha^2}{(\alpha + \sigma_j^2)^2} f_j^2, \end{aligned}$$

and therefore we solve

$$G(\alpha) = \sum_j \frac{\alpha^2}{(\alpha + \sigma_j^2)^2} f_j^2 - \delta^2 = 0$$

We remark that

- the singular values of A are σ_j
- those of A^{-1} are $1/\sigma_j$
- the regularized singular values are $\sigma_j/(\alpha + \sigma_j^2)$

Ill–conditioning means that the quantity

$$\frac{\max_j \sigma_j}{\min_j \sigma_j}$$

is large. Regularization flattens this ratio by clumping singular values.

3 Computation: Newton's method

The function G.

$$G(\alpha) := \|Ax_\alpha - b\|^2 - \delta^2 = \|A(\alpha I + A^*A)^{-1}A^*b - b\|^2 - \delta^2.$$

Basic algorithm. Starting with some α_0 we iterate

$$\alpha_{n+1} = \alpha_n - \frac{G(\alpha_n)}{G'(\alpha_n)}$$

stopping when

$$\frac{|\alpha_n - \alpha_{n+1}|}{|\alpha_n|} << 1.$$

Proposition *If $\delta < \|b\|$, then*

$$G(0) = -\delta^2 < 0 < \|b\|^2 - \delta^2 = \lim_{\alpha\to\infty} G(\alpha).$$

Moreover, G is strictly increasing.

Proof. From the definition of x_α

$$(\alpha I + A^*A)x_\alpha = A^*b$$

we deduce

$$x'_\alpha = -(\alpha I + A^*A)^{-1}x_\alpha, \qquad A^*(Ax_\alpha - b) = -\alpha x_\alpha$$

Then the derivative of G is

$$\begin{aligned} G'(\alpha) &= \frac{d}{d\alpha}\Big((Ax_\alpha - b)^*(Ax_\alpha - b)\Big) \\ &= 2\,\mathrm{Re}\Big((Ax_\alpha - b)^*Ax'_\alpha\Big) \\ &= 2\alpha\,\mathrm{Re}\, x^*_\alpha(\alpha I + A^*A)^{-1}x_\alpha \\ &= 2\alpha x^*_\alpha(\alpha I + A^*A)^{-1}x_\alpha \end{aligned}$$

and is positive for $\alpha > 0$. $\square$

Evaluation of G'. It can be done in three steps:

> **solve** $(\alpha I + A^*A)x_\alpha = A^*b$
> **solve** $(\alpha I + A^*A)y_\alpha = x_\alpha$
> $G'(\alpha) = 2\alpha x^*_\alpha y_\alpha$

Notice that we have the following closed form for G'

$$G'(\alpha) = 2\alpha b^*A(\alpha I + A^*A)^{-3}A^*b.$$

Proposition *The second derivative of G admits all the following expressions*

$$\begin{aligned} G''(\alpha) &= b^*A(A^*A-2\alpha I)(\alpha I+A^*A)^{-4}b \\ &= 2y_\alpha^*(A^*A-2\alpha I)y_\alpha \\ &= 2x_\alpha^*y_\alpha - 6\alpha y_\alpha^* y_\alpha, \end{aligned}$$

being $y_\alpha = (\alpha I + A^*A)^{-1}x_\alpha = -x'_\alpha$.

Proof. From the last expression of G' we derive

$$\begin{aligned} G''(\alpha) &= 2b^*A(\alpha I+A^*A)^{-3}A^*b - 6\alpha A(\alpha I+A^*A)^{-4}A^*b \\ &= 2b^*A[I-3\alpha(\alpha I+A^*A)^{-1}](\alpha I+A^*A)^{-3}A^*b \\ &= 2b^*A(A^*A-2\alpha I)(\alpha I+A^*A)^{-4}A^*b \end{aligned}$$

since $I - 3\alpha(\alpha I+B)^{-1} = (\alpha I+B)^{-1}(B-2\alpha I)$. Notice that matrices $(\lambda I+B)^{-1}$ and $(\mu I+B)$ commute and that

$$y_\alpha = (\alpha I + A^*A)^{-2}A^*b,$$

which gives the second expression. To obtain the third one, one simply has to notice that

$$A^*Ay_\alpha = x_\alpha - \alpha y_\alpha.$$

$\square$

Algorithm (Newton). Starting at an adequete value of α

```
B := A*A
c := A*b
for it = 1 : itmax
    M := B + αI
    x := solve(M, c)
    y := solve(M, x)
    r := Ax − b              % residual
    g := r*r − δ^2           % function
    gp := 2αx*y              % derivative
    β := α − g/gp            % Newton iteration
    if |β − α|/|α| < tol
        congergence reached at x
        stop
    end if
    α = β                    % actualization
end for
```

by F.–J. Sayas
Mathematics, Ho!, 2001