Chapter 5

Least Squares Problems

Here we solve linear systems $Ax = b$ that do not have a solution. If b is not in the column space of A, there is no x such that $Ax = b$. The best we can do is to find a vector y that brings left and right hand side of the linear system as close as possible, in other words y is chosen to make the distance between Ay and b as small as possible. That is, we want to minimize the distance $\|Ax - b\|_2$ over all x, and distance will again be measured in the twonorm.

Definition 5.1 (Least Squares Problem). *Let $A \in \mathbb{C}^{m\times n}$ and $b \in \mathbb{C}^m$. The* least squares problem (LS) *consists of finding a vector $y \in \mathbb{C}^n$ so that*

$$\min_x \|Ax - b\|_2 = \|Ay - b\|_2.$$

The vector $Ay - b$ is called the least squares residual.

The name comes about as follows

$$\min_x \|Ax - b\|_2^2 = \underbrace{\min_x}_{\text{least}} \sum_i \underbrace{|(Ax - b)_i|^2}_{\text{squares}}.$$

5.1 Solutions of Least Squares Problems

We express the solutions of least squares problems in terms of the SVD.

Let $A \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A) = r$ and a SVD

$$A = U \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} V^*, \qquad U = \begin{pmatrix} \overset{r}{U_r} & \overset{m-r}{U_{m-r}} \end{pmatrix}, \qquad V = \begin{pmatrix} \overset{r}{V_r} & \overset{n-r}{V_{n-r}} \end{pmatrix},$$

where $U \in \mathbb{C}^{m\times m}$ and $V \in \mathbb{C}^{n\times n}$ are unitary, and Σ_r is a diagonal matrix with diagonal elements $\sigma_1 \geq \ldots \geq \sigma_r > 0$, i.e. Σ_r is nonsingular.

Fact 5.2 (All Least Squares Solutions) Let $A \in \mathbb{C}^{m\times n}$ and $b \in \mathbb{C}^m$. The solutions of $\min_x \|Ax-b\|_2$ are of the form $y = V_r\Sigma_r^{-1}U_r^*b + V_{n-r}z$ for any $z \in \mathbb{C}^{n-r}$.

Proof. Let y be a solution of the least squares problem, and partition

$$V^*y = \begin{pmatrix} V_r^*y \\ V_{n-r}^*y \end{pmatrix} = \begin{pmatrix} w \\ z \end{pmatrix},$$

and substitute the SVD of A into the residual,

$$Ay - b = U\begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} V^*y - b = U\begin{pmatrix} \Sigma_r w - U_r^*b \\ -U_{m-r}^*b \end{pmatrix}.$$

Two norms are invariant under multiplication by unitary matrices, so that

$$\|Ay-b\|_2^2 = \|\Sigma_r w - U_r^*b\|_2^2 + \|U_{m-r}^*b\|_2^2.$$

Since the second summand is constant and independent of w and z, the residual is minimized if the first summand is zero, that is, if $w = \Sigma_r^{-1}U_r^*b$. Therefore the solution of the least squares problem equals

$$y = V\begin{pmatrix} w \\ z \end{pmatrix} = V_r w + V_{n-r}z = V_r\Sigma_r^{-1}U_r^*b + V_{n-r}z.$$

Fact 4.20 implies that $V_{n-r}z \in \operatorname{Ker}(A)$ for any vector z. Hence $V_{n-r}z$ does not have any effect on the least squares residual, so that and z can assume any value. $\square$

Fact 5.1 shows that if A has rank $r < n$ then the least squares problem has infinitely many solutions. The first term in a least squares solution contains the matrix

$$V_r\Sigma_r^{-1}U_r^* = V\begin{pmatrix} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{pmatrix} U^*$$

which is obtained by inverting only the nonsingular parts of a SVD. This matrix is almost an inverse, but not quite.

Definition 5.3 (Moore-Penrose Inverse). *If* $A \in \mathbb{C}^{m\times n}$ *and* $\operatorname{rank}(A) = r \geq 1$, *let* $A = U\begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} V^*$ *be a SVD where* Σ_r *is nonsingular. The* $n \times m$ *matrix*

$$A^\dagger = V\begin{pmatrix} \Sigma_r^{-1} & 0 \\ 0 & 0 \end{pmatrix} U^*$$

is called Moore-Penrose inverse *of* A. *If* $A = 0_{m\times n}$ *then* $A^\dagger = 0_{n\times m}$.

The Moore-Penrose inverse of a full rank matrix can be expressed in terms of the matrix itself.

Remark 5.4 (Moore-Penrose Inverses of Full Rank Matrices). *Let* $A \in \mathbb{C}^{m\times n}$.

- *If A is nonsingular then $A^\dagger = A^{-1}$.*
- *If $A \in \mathbb{C}^{m\times n}$ and $\mathrm{rank}(A) = n$ then $A^\dagger = (A^*A)^{-1}A^*$.*
  This means $A^\dagger A = I_n$, so that $A^\dagger$ is left inverse of A.
- *If $A \in \mathbb{C}^{m\times n}$ and $\mathrm{rank}(A) = m$ then $A^\dagger = A^*(AA^*)^{-1}$.*
  This means $AA^\dagger = I_m$, so that $A^\dagger$ is a right inverse of A.

Now we can express the least squares solutions in terms of the Moore Penrose inverse, without reference to the SVD.

Corollary 5.5 (All Least Squares Solutions). *Let $A \in \mathbb{C}^{m\times n}$ and $b \in \mathbb{C}^{m\times n}$. The solutions of $\min_x \|Ax - b\|_2$ are of the form $y = A^\dagger b + q$, where $q \in \mathrm{Ker}(A)$.*

Proof. This follows from setting $q = V_{n-r}z \in \mathrm{Ker}(A)$ in Fact 4.20. □

Although a least squares problem can have infinitely many solutions, all solutions have the part $A^\dagger b$ in common, and they differ only in the part that belongs to $\mathrm{Ker}(A)$. As a result, all least squares solutions have not just residuals of the same norm, but they have the same residual.

Fact 5.6 (Uniqueness of the Least Squares Residual) Let $A \in \mathbb{C}^{m\times n}$, $b \in \mathbb{C}^m$. All solutions y of $\min_x \|Ax - b\|_2$ have the same residual $b - Ay = (I - AA^\dagger)b$.

Proof. Let y_1 and y_2 be solutions to $\min_x \|Ax - b\|_2$. Corollary 5.5 implies $y_1 = A^\dagger b + q_1$ and $y_2 = A^\dagger b + q_2$, where $q_1, q_2 \in \mathrm{Ker}(A)$. Hence $Ay_1 = AA^\dagger b = Ay_2$, and both solutions have the same residual, $b - Ay_1 = b - Ay_2 = (I - AA^\dagger)b$. □

Besides being unique, the least squares residual has another important property: It is orthogonal to the column space of the matrix.

Fact 5.7 (Residual is Orthogonal to Column Space) Let $A \in \mathbb{C}^{m\times n}$, $b \in \mathbb{C}^m$, and y a solution of $\min_x \|Ax - b\|_2$ with residual $r = b - Ay$. Then $A^*r = 0$.

Proof. Fact 5.6 implies that the unique residual is $r = (I - AA^\dagger)b$. Let A have a SVD

$$A = U \begin{pmatrix} \Sigma_r & 0 \\ 0 & 0 \end{pmatrix} V^*,$$

where U and V are unitary, and Σ_r is a diagonal matrix with positive diagonal elements. From Definition 5.3 of the Moore-Penrose we obtain

$$AA^\dagger = U \begin{pmatrix} I_r & 0 \\ 0 & 0_{(m-r)\times(m-r)} \end{pmatrix} U^*, \qquad I - AA^\dagger = U \begin{pmatrix} 0_{r\times r} & 0 \\ 0 & I_{m-r} \end{pmatrix} U^*.$$

Hence $A^*(I - AA^\dagger) = 0_{n\times m}$ and $A^*r = 0$. □

The part of the least squares problem solution $y = A^\dagger b + q$ that is responsible for lack of uniqueness is the term $q \in \mathrm{Ker}(A)$. We can force the least squares problem to have a unique solution if we add the constraint $q = 0$. It turns out that the resulting solution $A^\dagger b$ has minimal norm among all least squares solutions.

Fact 5.8 (Minimal Norm Least Squares Solution) Let $A \in \mathbb{C}^{m\times n}$ and $b \in \mathbb{C}^m$. Among all solutions of $\min_x \|Ax - b\|_2$ the one with minimal twonorm is $y = A^\dagger b$.

Proof. From the proof of Fact 5.2 follows that any least squares solution has the form

$$y = V \begin{pmatrix} \Sigma_r^{-1} U_r^* b \\ z \end{pmatrix}.$$

Hence

$$\|y\|_2^2 = \|\Sigma_r^{-1} U_r^* b\|_2^2 + \|z\|_2^2 \geq \|\Sigma_r^{-1} U_r^* b\|_2^2 = \|V_r \Sigma_r^{-1} U_r^* b\|_2^2 = \|A^\dagger b\|_2^2.$$

Thus, any least squares solution y satisfies $\|y\|_2 \geq \|A^\dagger b\|_2$. This means $y = A^\dagger b$ is the least squares solution with minimal twonorm. □

The most pleasant least squares problems are those where the matrix A has full column rank because then $\mathrm{Ker}(A) = \{0\}$ and the least squares solution is unique.

Fact 5.9 (Full Column Rank Least Squares) Let $A \in \mathbb{C}^{m\times n}$ and $b \in \mathbb{C}^m$. If $\mathrm{rank}(A) = n$ then $\min_x \|Ax - b\|_2$ has the unique solution $y = (A^*A)^{-1}A^*b$.

Proof. From Fact 4.22 we know that $\mathrm{rank}(A) = n$ implies $\mathrm{Ker}(A) = \{0\}$. Hence $q = 0$ in Corollary 5.5. The expression for $A^\dagger$ follows from Remark 5.4. □

In particular, when A is nonsingular then the Moore-Penrose inverse reduces to the ordinary inverse. This means, if we solve a least squares problem $\min_x \|Ax - b\|_2$ with a nonsingular matrix A we obtain the solution $y = A^{-1}b$ of the linear system $Ax = b$.

Exercises

(i) What is the Moore-Penrose inverse of a nonzero column vector, and of a nonzero row vector?

(ii) Let $u \in \mathbb{C}^{m\times n}$ and $v \in \mathbb{C}^n$ with $v \neq 0$. Show that $\|uv^\dagger\|_2 = \|u\|_2/\|v\|_2$.

(iii) Let $A \in \mathbb{C}^{m\times n}$. Show that the following matrices are idempotent:

$$AA^\dagger, \qquad A^\dagger A, \qquad I_m - AA^\dagger, \qquad I_n - A^\dagger A.$$

(iv) Let $A \in \mathbb{C}^{m\times n}$. Show: If $A \neq 0$ then $\|AA^\dagger\|_2 = \|A^\dagger A\|_2 = 1$.

(v) Let $A \in \mathbb{C}^{m\times n}$. Show:

$$(I_m - AA^\dagger)A = 0_{m\times n}, \qquad A(I_n - A^\dagger A) = 0_{m\times n}.$$

(vi) Let $A \in \mathbb{C}^{m\times n}$. Show: $\mathcal{R}(A^\dagger) = \mathcal{R}(A^*)$ and $\mathrm{Ker}(A^\dagger) = \mathrm{Ker}(A^*)$.

(vii) Let $A \in \mathbb{C}^{m\times n}$ have $\text{rank}(A) = r$. Show that $\|A^\dagger\|_2 = 1/\sigma_r$.

(viii) Let $A \in \mathbb{C}^{m\times n}$ have $\text{rank}(A) = n$. Show $\|(A^*A)^{-1}\|_2 = \|A^\dagger\|_2^2$.

(ix) Let $A = BC$ where $B \in \mathbb{C}^{m\times n}$ has $\text{rank}(B) = n$ and $C \in \mathbb{C}^{n\times n}$ is nonsingular. Show that $A^\dagger = C^{-1}B^\dagger$.

(x) Let $A \in \mathbb{C}^{m\times n}$ with $\text{rank}(A) = n$ and thin QR factorization $A = QR$, where $Q^*Q = I_n$ and R is upper triangular. Show that $A^\dagger = R^{-1}Q^*$.

(xi) Show: If A has orthonormal columns then $A^\dagger = A^*$.

(xii) Partial Isometry.
A matrix $A \in \mathbb{C}^{m\times n}$ is called a partial isometry if $A^\dagger = A^*$. Show: A is a partial isometry if and only if all its singular values are 0 or 1.

(xiii) What is the minimal norm solution to $\min_x \|Ax - b\|_2$ when $A = 0$?

(xiv) If y is the minimal norm solution to $\min_x \|Ax - b\|_2$ and $A^*b = 0$, then what can you say about y?

(xv) Given an *approximate* solution z to a linear system $Ax = b$, this problem shows how to construct a linear system $(A + E)x = b$ for which z is the *exact* solution.
Let $A \in \mathbb{C}^{m\times n}$ and $b \in \mathbb{C}^m$. Let $z \in \mathbb{C}^n$ with $z \neq 0$ and residual $r = b - Az$. Show: If $E = rz^\dagger$ then $(A + E)z = b$.

1. What is the minimal norm solution to $\min_x \|Ax - b\|_2$ when $A = uv^*$, where u and v are column vectors?
2. Let $A \in \mathbb{C}^{m\times n}$. Show that the singular values of $\begin{pmatrix} I_n \\ A \end{pmatrix}^\dagger$ are equal to $1/\sqrt{1+\sigma_j^2}$, $1 \le j \le n$.
3. Let $A \in \mathbb{C}^{m\times n}$ have $\text{rank}(A) = n$. Show that $\|I - AA^\dagger\|_2 = \min\{1, m - n\}$.
4. Let $A \in \mathbb{C}^{m\times n}$. Show: $A^\dagger$ is the Moore-Penrose inverse of A if and only if $A^\dagger$ satisfies

   MP1: $AA^\dagger A = A$, $A^\dagger AA^\dagger = A^\dagger$

   MP2: $AA^\dagger$ and $A^\dagger A$ are Hermitian.

5. Partitioned Moore-Penrose Inverse.
   Let $A \in \mathbb{C}^{m\times n}$ have $\text{rank}(A) = n$, and be partitioned as $A = \begin{pmatrix} A_1 & A_2 \end{pmatrix}$. Show:

   (a)
   $$A^\dagger = \begin{pmatrix} B_1^\dagger \\ B_2^\dagger \end{pmatrix}, \qquad \text{where} \quad B_1 = (I - A_2A_2^\dagger)A_1, \quad B_2 = (I - A_1A_1^\dagger)A_2.$$

   (b) $\|B_1\|_2 = \min_Z \|A_1 - A_2Z\|_2$ and $\|B_2\|_2 = \min_Z \|A_2 - A_1Z\|_2$.

   (c) Let $1 \le k \le n$, and V_{11} the leading $k\times k$ principal submatrix of V. Show: If V_{11} is nonsingular then $\|A_1^\dagger\|_2 \le \|V_{11}^{-1}\|_2/\sigma_k$.

5.2 Conditioning of Least Squares Problems

Least squares problems are much more sensitive to perturbations than linear systems. A least squares problems whose matrix is deficient in column rank is so sensitive that we cannot even define a condition number. The example below illustrates this.

Example 5.10 (Rank Deficient Least Squares Problems are Ill-Posed) Consider the least squares problem $\min_x \|Ax-b\|_2$ with

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = A^\dagger, \qquad b = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad y = A^\dagger b = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

The matrix A is rank deficient, and y is the minimal norm solution. Let us perturb the matrix so that

$$A + E = \begin{pmatrix} 1 & 0 \\ 0 & \epsilon \end{pmatrix}, \qquad \text{where} \qquad 0 < \epsilon \ll 1.$$

The matrix $A+E$ has full column rank and $\min_x \|(A+E)x-b\|_2$ has the unique solution z where

$$z = (A+E)^\dagger b = (A+E)^{-1} b = \begin{pmatrix} 1 \\ 1/\epsilon \end{pmatrix}.$$

Comparing the two minimal norm solutions shows that the second element of z grows as the $(2,2)$ element of $A+E$ decreases, i.e., $z_2 = 1/\epsilon \to \infty$ as $\epsilon \to 0$. But at $\epsilon = 0$ we have $z_2 = 0$. Therefore the least squares solution does not depend continuously on the $(2,2)$ element of the matrix. This is an *ill-posed* problem.

In an ill-posed problem the solution is not a continuous function of the inputs. The ill-posedness of a rank deficient least squares problem comes about because a small perturbation can increase the rank of the matrix. ∎

To avoid ill-posedness we restrict ourselves to least squares problems where the exact and perturbed matrices have full column rank. Below we determine the sensitivity of the least squares solution to changes in the righthand side.

Fact 5.11 (Righthand Side Perturbation) Let $A \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A) = n$, let y be the solution to $\min_x \|Ax-b\|_2$, and z the solution to $\min_x \|Ax-(b+f)\|_2$. If $y \neq 0$ then

$$\frac{\|z-y\|_2}{\|y\|_2} \le \kappa_2(A) \frac{\|f\|_2}{\|A\|_2 \|y\|_2},$$

and, if $z \neq 0$ then

$$\frac{\|z-y\|_2}{\|z\|_2} \le \kappa_2(A) \frac{\|f\|_2}{\|A\|_2 \|z\|_2},$$

where $\kappa_2(A) = \|A\|_2 \|A^\dagger\|_2$.

Proof. Fact 5.9 implies that $y = A^\dagger b$ and $z = A^\dagger(b+f)$ are the unique solutions to the respective least squares problems. From $y = A^\dagger b = (A^*A)^{-1}A^*b$, see Remark

5.4, and the assumption $A^*b \neq 0$ follows $y \neq 0$. Applying the bound for matrix multiplication in Fact 2.22 yields

$$\frac{\|z-y\|_2}{\|y\|_2} \leq \frac{\|A^\dagger\|_2\|b\|_2}{\|A^\dagger b\|_2}\,\frac{\|f\|_2}{\|b\|_2} = \|A^\dagger\|_2\frac{\|f\|_2}{\|y\|_2}.$$

Now multiply and divide by $\|A\|_2$ on the right. □

In Fact 5.11 we have extended the two-norm condition number with respect to inversion from nonsingular matrices to matrices with full column rank.

Definition 5.12. *Let $A \in \mathbb{C}^{m\times n}$ with $\operatorname{rank}(A) = n$. Then $\kappa_2(A) = \|A\|_2\|A^\dagger\|_2$ is the two-norm condition number of A with regard to left inversion.*

Fact 5.11 implies that $\kappa_2(A)$ is the normwise relative condition number of the least squares solution to changes in the righthand side. If the columns of A are close to being linearly dependent, then A is close to being rank deficient and the least squares solution is sensitive to changes in the righthand side.

With regard to changes in the matrix, though, the situation is much bleaker. It turns out that least squares problems are much more sensitive to changes in the matrix than linear systems.

Example 5.13 (Large Residual Norm) Let

$$A = \begin{pmatrix} 1 & 0 \\ 0 & \alpha \\ 0 & 0 \end{pmatrix}, \qquad b = \begin{pmatrix} \beta_1 \\ 0 \\ \beta_3 \end{pmatrix}, \qquad \text{where} \quad 0 < \alpha \leq 1, \quad 0 < \beta_1, \beta_3.$$

The element β_3 represents the part of b outside $\mathcal{R}(A)$. The matrix A has full column rank, and the least squares problem $\min_x \|Ax-b\|_2$ has the unique solution y where

$$A^\dagger = (A^*A)^{-1}A^* = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/\alpha & 0 \end{pmatrix}, \qquad y = A^\dagger b = \begin{pmatrix} \beta_1 \\ 0 \end{pmatrix}.$$

The residual norm is $\min_x \|Ax-b\|_2 = \|Ay-b\|_2 = \beta_3$.

Let us perturb the matrix and change its column space so that

$$A+E = \begin{pmatrix} 1 & 0 \\ 0 & \alpha \\ 0 & \epsilon \end{pmatrix}, \qquad \text{where} \quad 0 < \epsilon \ll 1.$$

Note that $\mathcal{R}(A+E) \neq \mathcal{R}(A)$. The matrix $A+E$ has full column rank and Moore-Penrose inverse

$$(A+E)^\dagger = \left[(A+E)^*(A+E)\right]^{-1}(A+E)^* = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{\alpha}{\alpha^2+\epsilon^2} & \frac{\epsilon}{\alpha^2+\epsilon^2} \end{pmatrix}.$$

The perturbed problem $\min_x \|(A+E)x-b\|_2$ has the unique solution z, where

$$z = (A+E)^\dagger b = \begin{pmatrix} \beta_1 \\ \epsilon\beta_3/(\alpha^2+\epsilon^2) \end{pmatrix}.$$

Since $\|y\|_2 = \beta_1$, the normwise relative error is

$$\frac{\|z-y\|_2}{\|y\|_2} = \frac{\beta_3 \epsilon}{\beta_1(\alpha^2+\epsilon^2)} \leq \frac{\beta_3}{\alpha^2\,\beta_1}\,\epsilon.$$

If $\beta_3 \geq \beta_1$ then $\beta_3/(\alpha^2\beta_1) \geq 1/\alpha^2$. This means, if more of b is outside $\mathcal{R}(A)$ then inside $\mathcal{R}(A)$, then the perturbation is amplified by at least $1/\alpha^2$.

In other words, since $\|E\| = \epsilon$, $\|A^\dagger\|_2 = 1/\alpha$, and $\beta_3/\beta_1 = \|Ay-b\|_2/\|y\|_2$, we can write

$$\frac{\|z-y\|_2}{\|y\|_2} \leq \|A^\dagger\|_2^2\,\frac{\|Ay-b\|_2}{\|y\|_2}\,\|E\|_2 = [\kappa_2(A)]^2\,\frac{\|r\|_2}{\|A\|_2\|y\|_2}\,\frac{\|E\|_2}{\|A\|_2},$$

where $r = Ay-b$ is the residual. This means, if the righthand side is far away from the column space then the condition number with respect to changes in the matrix is $[\kappa_2(A)]^2$ – rather than just $\kappa_2(A)$.

We can give a geometric interpretation for the relative residual norm. If we bound

$$\frac{\|r\|_2}{\|A\|_2\|y\|_2} \leq \frac{\|r\|_2}{\|Ay\|_2}$$

then we can exploit the relation between $\|r\|_2$ and $\|Ay\|_2$ from Exercise (iii) below. There it is shown that $\|b\|_2^2 = \|r\|_2^2 + \|Ay\|_2^2$, hence

$$1 = \left(\frac{\|r\|_2}{\|b\|_2}\right)^2 + \left(\frac{\|Ay\|_2}{\|b\|_2}\right)^2.$$

It follows that $\|r\|_2/\|b\|_2$ and $\|Ay\|_2/\|b\|_2$ behave like sine and cosine. Thus there is θ so that

$$1 = \sin\theta^2 + \cos\theta^2, \qquad \text{where} \quad \sin\theta = \frac{\|r\|_2}{\|b\|_2}, \quad \cos\theta = \frac{\|Ay\|_2}{\|b\|_2},$$

and θ can be interpreted as the angle between b and $\mathcal{R}(A)$. This allows us to bound the relative residual norm by

$$\frac{\|r\|_2}{\|A\|_2\|y\|_2} \leq \frac{\|r\|_2}{\|Ay\|_2} = \frac{\sin\theta}{\cos\theta} = \tan\theta.$$

This means, if the angle between righthand side and column space is large enough then the least squares solution is sensitive to perturbations in the matrix, and this sensitivity is represented by $[\kappa_2(A)]^2$. ■

The matrix in Example 5.13 is representative of the situation in general. Least squares solutions are more sensitive to changes in the matrix when the righthand side is too far from the column space. Below we present a bound for the relative error with regard to the perturbed solution z, because it is much easier to derive than a bound for the relative error with regard to the exact solution y.

Fact 5.14 (Matrix and Righthand Side Perturbation) Let $A, A+E \in \mathbb{C}^{m\times n}$ with $\text{rank}(A) = \text{rank}(A+E) = n$, let y be the solution to $\min_x \|Ax - b\|_2$, and let $z \neq 0$ be the solution to $\min_x \|(A+E)x - (b+f)\|_2$. Then

$$\frac{\|z-y\|_2}{\|z\|_2} \leq \kappa_2(A)\ (\epsilon_A + \epsilon_f) + [\kappa_2(A)]^2\, \frac{\|s\|_2}{\|A\|_2\|z\|_2}\, \epsilon_A,$$

where

$$s = (A+E)z - (b+f), \qquad \epsilon_A = \frac{\|E\|_2}{\|A\|_2}, \qquad \epsilon_f = \frac{\|f\|_2}{\|A\|_2\|z\|_2}.$$

Proof. From Fact 5.9 follows that $y = A^\dagger b$ and $z = (A+E)^\dagger(b+f)$ are the unique solutions to the respective least squares problems. Applying Fact 5.7 to the perturbed least squares problem gives $(A+E)^* s = 0$, hence $A^* s = -E^* s$. Multiplying by $(A^*A)^{-1}$ and using $A^\dagger = (A^*A)^{-1}A^*$ from Remark 5.4 gives

$$-(A^*A)^{-1}E^*s = A^\dagger s = A^\dagger\left((A+E)z - (b+f)\right) = z - y + A^\dagger(Ez - f).$$

Solving for $z-y$ yields $z - y = -A^\dagger(Ez-f) - (A^*A)^{-1}E^*s$. Now take norms, and use the fact that $\|(A^*A)^{-1}\|_2 = \|A^\dagger\|_2^2$, see Exercise (viii) in Section 5.1, to obtain

$$\|z-y\|_2 \leq \|A^\dagger\|_2\ (\|E\|_2\|z\|_2 + \|f\|_2) + \|A^\dagger\|_2^2\ \|E\|_2\|s\|_2.$$

At last divide both sides of the inequality by $\|z\|_2$, and multiply and divide the right side by $\|A\|_2^2$. □

Remark 5.15.

- *If $E = 0$ then the bound in Fact 5.14 is identical to that in Fact 5.11. Therefore the least squares solution is more sensitive to changes in the matrix than to changes in the right-hand side.*
- *The first term $\kappa_2(A)(\epsilon_A+\epsilon_f)$ in the above bound is the same as the perturbation bound for linear systems in Fact 3.8. It is because of the second term in Fact 5.14 that least squares problems are more sensitive than linear systems to perturbations in the matrix.*
- *We can interpret $\|s\|_2/(\|A\|_2\|z\|_2)$ as an approximation to the distance between perturbed right hand side and perturbed matrix. From Exercise (ii) and Example 5.13 follows*

$$\frac{\|s\|_2}{\|A\|_2\|z\|_2} \leq \frac{\|s\|_2}{\|A+E\|_2\|z\|_2}(1+\epsilon_A) \leq \tan\tilde{\theta}\,(1+\epsilon_A),$$

  where $\tilde{\theta}$ is the angle between $b+f$ and $\mathcal{R}(A+E)$.
- *If most of the righthand side lies in the column space then the condition number of the least squares problem is $\kappa_2(A)$.*
  In particular, if $\frac{\|s\|_2}{\|A\|_2\|z\|_2} \approx \epsilon_A$ then the second term in the bound in Fact 5.14 is about $[\kappa_2(A)]^2\epsilon_A^2$, and negligible for small enough ϵ_A.

- *If the righthand side is far away from the column space then condition number of the least squares problem is* $[\kappa_2(A)]^2$.
- *Therefore, the solution of the least squares is ill-conditioned in the normwise relative sense, if* A *is close to being rank deficient, i.e.* $\kappa_2(A) \gg 1$, *or if the relative residual norm is large, i.e.* $\|(A+E)z - (b+f)\|_2/(\|A\|_2\|z\|_2) \gg 0$.
- *If the perturbation does not change the column space so that* $\mathcal{R}(A+E) = \mathcal{R}(A)$ *then the least squares problem is no more sensitive than a linear system, see Exercise 1 below.*

Exercises

(i) Let $A \in \mathbb{C}^{m\times n}$ have orthonormal columns. Show that $\kappa_2(A) = 1$.

(ii) Under the assumptions of Fact 5.14 show that

$$\frac{\|s\|_2}{\|A+E\|_2\|z\|_2}(1-\epsilon_A) \le \frac{\|s\|_2}{\|A\|_2\|z\|_2} \le \frac{\|s\|_2}{\|A+E\|_2\|z\|_2}(1+\epsilon_A).$$

(iii) Let $A \in \mathbb{C}^{m\times n}$, and y be a solution to the least squares problem $\min_x \|Ay - b\|_2$. Show that

$$\|b\|_2^2 = \|Ay - b\|_2^2 + \|Ay\|_2^2.$$

(iv) Let $A \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A) = n$. Show that the solution y of the least squares problem $\min_x \|Ax - b\|_2$ and the residual $r = b - Ay$ can be viewed as solutions to the linear system

$$\begin{pmatrix} I & A \\ A^* & 0 \end{pmatrix}\begin{pmatrix} r \\ y \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix},$$

and that

$$\begin{pmatrix} I & A \\ A^* & 0 \end{pmatrix}^{-1} = \begin{pmatrix} I - AA^\dagger & (A^\dagger)^* \\ A^\dagger & -(A^*A)^{-1} \end{pmatrix}.$$

(v) In addition to the assumptions of the previous Exercise (ii), let $A+E \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A+E) = n$, and let z be the solution of the least squares problem $\min_x \|(A+E)x - (b+f)\|_2$ with residual $s = b + f - (A+E)z$. Show that

$$\begin{pmatrix} s - r \\ z - y \end{pmatrix} = \begin{pmatrix} I - AA^\dagger & (A^\dagger)^* \\ A^\dagger & -(A^*A)^{-1} \end{pmatrix}\begin{pmatrix} f - Ez \\ -E^*s \end{pmatrix}.$$

(vi) Let $A, A+E \in \mathbb{C}^{m\times n}$ and $\operatorname{rank}(A) = n$. Show: If $\|E\|_2\,\|A^\dagger\|_2 < 1$ then $\operatorname{rank}(A+E) = n$.

1. Matrices with the Same Column Space.
   When the perturbed matrix has the same column space as the original matrix then the least squares solution is less sensitive, and the error bound is the same as the one for linear systems in Fact 3.9.

Let $A, A+E \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A) = \operatorname{rank}(A+E) = n$. Let y be the solution to $\min_x \|Ax-b\|_2$, and $z \neq 0$ the solution to $\min_x \|(A+E)x-(b+f)\|_2$. Show: If $\mathcal{R}(A) = \mathcal{R}(A+E)$ then

$$\frac{\|z-y\|_2}{\|z\|_2} \leq \kappa_2(A)\left(\epsilon_A + \epsilon_f\right), \qquad \text{where} \quad \epsilon_A = \frac{\|E\|_2}{\|A\|_2}, \quad \epsilon_f = \frac{\|f\|}{\|A\|_2\|z\|_2}.$$

2. Conditioning of the Least Squares Residual.
This bound shows that the least squares residual is insensitive to changes in the righthand side.
Let $A \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A) = n$. Let y be the solution to $\min_x \|Ax-b\|_2$ with residual $r = Ay - b$, and let z be the solution to $\min_x \|Az-(b+f)\|_2$ with residual $s = Az-(b+f)$. Show that

$$\|s-r\|_2 \leq \|f\|_2.$$

3. Conditioning of the Least Squares Residual Norm.
The following bound gives an indication of how sensitive the norm of the least squares residual may be to changes in the matrix and righthand side.
Let $A, A+E \in \mathbb{C}^{m\times n}$ so that $\operatorname{rank}(A) = \operatorname{rank}(A+E) = n$. Let y be the solution to $\min_x \|Ax-b\|_2$ with residual $r = Ay-b$, and z be the solution to $\min_x \|(A+E)x-(b+f)\|_2$ with residual $s = (A+E)z-(b+f)$. Show: If $b \neq 0$ then

$$\frac{\|s\|_2}{\|b\|_2} \leq \frac{\|r\|_2}{\|b\|_2} + \kappa_2(A)\,\epsilon_A + \epsilon_b, \qquad \text{where} \quad \epsilon_A = \frac{\|E\|_2}{\|A\|_2}, \quad \epsilon_b = \frac{\|f\|_2}{\|b\|_2}.$$

4. This bound suggests that the error in the least squares solution depends on the error in the least squares residual.
Under the conditions of Fact 5.14 show that

$$\frac{\|z-y\|_2}{\|z\|_2} \leq \kappa_2(A)\left[\frac{\|r-s\|_2}{\|A\|_2\|z\|_2} + \epsilon_A + \epsilon_f\right].$$

5. Given an approximate least squares solution z, this problem shows how to construct a least squares problem for which z is the exact solution.
Let $z \neq 0$ be an approximate solution of the least squares problem $\min_x \|Ax-b\|_2$. Let $r_c = b - Az$ be the computable residual, h an arbitrary vector, and $F = -hh^\dagger A + (I - hh^\dagger)r_c z^\dagger$. Show that z is a least squares solution of $\min_x \|(A+F)x-b\|_2$.

5.3 Computation of Full Rank Least Squares Problems

We present two algorithms for computing the solution to a least squares problem with full column rank.

Let $A \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A) = n$ and a SVD

$$A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^*, \qquad U = \begin{array}{cc} n & m-n \\ \big(U_n & U_{m-n}\big) \end{array}$$

where $U \in \mathbb{C}^{m\times m}$ and $V \in \mathbb{C}^{n\times n}$ are unitary, and $\Sigma \in \mathbb{C}^{n\times n}$ is a diagonal matrix with diagonal elements $\sigma_1 \geq \ldots \geq \sigma_n > 0$.

Fact 5.16 (Least Squares via SVD) Let $A \in \mathbb{C}^{m\times n}$ with $\operatorname{rank}(A) = n$, $b \in \mathbb{C}^m$ and y the solution to $\min_x \|Ax - b\|_2$. Then

$$y = V\Sigma^{-1}U_n^* b, \qquad \min_x \|Ax - b\|_2 = \|U_{m-n}^* b\|_2.$$

Proof. The expression for y follows from Fact 5.9. With regard to the residual

$$Ay - b = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^* V \Sigma^{-1} U_n^* b - b = U \left[\begin{pmatrix} U_n^* b \\ 0 \end{pmatrix} - \begin{pmatrix} U_n^* b \\ U_{m-n}^* b \end{pmatrix} \right] = U \begin{pmatrix} 0 \\ -U_{m-n}^* b \end{pmatrix}.$$

Therefore $\min_x \|Ax - b\|_2 = \|Ay - b\|_2 = \|U_{m-n}^* b\|_2$. □

Algorithm 5.1. Least Squares Solution via SVD.

Input: Matrix $A \in \mathbb{C}^{m\times n}$ with $\operatorname{rank}(A) = n$, vector $b \in \mathbb{C}^m$
Output: Solution y of $\min_x \|Ax - b\|_2$, residual norm $\rho = \|Ay - b\|_2$

1. Compute a SVD $A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^*$ where $U \in \mathbb{C}^{m\times m}$ and $V \in \mathbb{C}^{n\times n}$ are unitary, and Σ is diagonal.
2. Partition $U = \begin{pmatrix} U_n & U_{m-n} \end{pmatrix}$, where U_n has n columns
3. Multiply $y \equiv V\Sigma^{-1}U_n^* b$
4. Set $\rho \equiv \|U_{m-n}^* b\|_2$.

The least squares solution can also be computed from a QR factorization which may be cheaper than a SVD. Let $A \in \mathbb{C}^{m\times n}$ have $\operatorname{rank}(A) = n$ and a QR factorization

$$A = Q \begin{pmatrix} R \\ 0 \end{pmatrix}, \qquad Q = \begin{array}{cc} n & m-n \\ \big(Q_n & Q_{m-n}\big) \end{array}$$

where $Q \in \mathbb{C}^{m\times m}$ is unitary and $R \in \mathbb{C}^{n\times n}$ is upper triangular with positive diagonal elements.

Fact 5.17 (Least Squares Solution via QR) Let $A \in \mathbb{C}^{m\times n}$ with $\operatorname{rank}(A) = n$, $b \in \mathbb{C}^m$ and y the solution to $\min_x \|Ax - b\|_2$. Then

$$y = R^{-1}Q_n^* b, \qquad \min_x \|Ax - b\|_2 = \|Q_{m-n}^* b\|_2.$$

Proof. Fact 5.9 and Remark 5.4 imply for the solution

$$y = A^\dagger b = (A^*A)^{-1}A^*b = \begin{pmatrix} R^{-1} & 0 \end{pmatrix} Q^*b = \begin{pmatrix} R^{-1} & 0 \end{pmatrix} \begin{pmatrix} Q_n^*b \\ Q_{m-n}^*b \end{pmatrix} = R^{-1}Q_n^*b.$$

With regard to the residual

$$Ay - b = Q\begin{pmatrix} R \\ 0 \end{pmatrix} R^{-1}Q_n^*b - b = Q\left[\begin{pmatrix} Q_n^*b \\ 0 \end{pmatrix} - \begin{pmatrix} Q_n^*b \\ Q_{m-n}^*b \end{pmatrix}\right] = Q\begin{pmatrix} 0 \\ -Q_{m-n}^*b \end{pmatrix}.$$

Therefore $\min_x \|Ax - b\|_2 = \|Ay - b\|_2 = \|Q_{m-n}^*b\|_2$. □

Algorithm 5.2. Least Squares via QR.

Input: Matrix $A \in \mathbb{C}^{m\times n}$ with $\operatorname{rank}(A) = n$, vector $b \in \mathbb{C}^m$
Output: Solution y of $\min_x \|Ax - b\|_2$, residual norm $\rho = \|Ay - b\|_2$

1. Factor $A = Q\begin{pmatrix} R \\ 0 \end{pmatrix}$ where $Q \in \mathbb{C}^{m\times m}$ is unitary and $R \in \mathbb{C}^{n\times n}$ is triangular
2. Partition $Q = \begin{pmatrix} Q_n & Q_{m-n} \end{pmatrix}$, where Q_n has n columns
3. Solve the triangular system $Ry = Q_n^*b$
4. Set $\rho \equiv \|Q_{m-n}^*b\|_2$

Exercises

1. Normal Equations.
   Let $A \in \mathbb{C}^{m\times n}$ and $b \in \mathbb{C}^m$. Show: y is a solution of $\min_x \|Ax - b\|_2$ if and only if y is a solution of $A^*Ax = A^*b$.
2. Numerical Instability of Normal Equations.
   Show that the normal equations can be a numerically unstable method for solving the least squares problem.
   Let $A \in \mathbb{C}^{m\times n}$ with $\operatorname{rank}(A) = n$, and $A^*Ay = A^*b$ with $A^*b \neq 0$. Let z be a perturbed solution with $A^*Az = A^*b + f$. Show:

   $$\frac{\|z - y\|_2}{\|y\|_2} \leq [\kappa_2(A)]^2 \, \frac{\|f\|_2}{\|A^*A\|_2\|y\|_2}.$$

   That is, the numerical stability of the normal equations is always determined by $[\kappa_2(A)]^2$, even if the least squares residual is small.