Inverse Problems — Summary

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A *direct problem* is a problem where given an object or *cause*, we must determine the data or *effect*. In an *inverse problem*, we observe data and wish to recover the object.

A problem is called *well-posed* if a unique solution exists that depends continuously on the data. Most inverse problems are, unfortunately, ill-posed.

1 Generalised Solutions

Recap 1.1.

1. An operator $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ is called *bounded* if

$$\|A\|_{\mathcal{L}(\mathcal{X},\mathcal{Y})} \coloneqq \sup_{u \neq 0} \frac{\|Au\|_{\mathcal{Y}}}{\|u\|_{\mathcal{X}}} = \sup_{\|u\|_{\mathcal{X}} \leq 1} < \infty.$$

It is known that a linear operator between normed spaces is continuous if and only if it is bounded.

2. We let $\mathcal{D}(A)$, $\mathcal{N}(A)$ and $\mathcal{R}(A)$ denote the domain, null space, and range of A respectively.

3. We will assume $\mathcal{X}$ and $\mathcal{Y}$ are Hilbert spaces, so there is an inner product $\langle \cdot, \cdot \rangle$ and any bounded operator $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ has a unique adjoint $A^* \in \mathcal{L}(\mathcal{Y}, \mathcal{X})$ which satisfies

$$\langle Au, v \rangle_{\mathcal{Y}} = \langle u, A^* v \rangle_{\mathcal{X}} \quad \text{for all } u \in \mathcal{X},\ v \in \mathcal{Y}.$$

4. For any $\mathcal{X}' \subseteq \mathcal{X}$ we define the *orthogonal complement* of $\mathcal{X}'$ as

$$(\mathcal{X}')^\perp \coloneqq \{u \in \mathcal{X} \mid \langle u, v \rangle_{\mathcal{X}} = 0\ \forall v \in \mathcal{X}'\}.$$

It is known that $(\mathcal{X}')^\perp$ is a closed subspace of $\mathcal{X}$ and that $\mathcal{X}' \subseteq ((\mathcal{X}')^\perp)^\perp$, where equality holds if and only if $\mathcal{X}'$ is a closed subspace of $\mathcal{X}$. For a non-closed subspace $\mathcal{X}'$ we have $((\mathcal{X}')^\perp)^\perp = \overline{\mathcal{X}'}$.

5. If $\mathcal{X}'$ is a closed subspace of $\mathcal{X}$, then for any $u \in \mathcal{X}$ there exist unique $x_u \in \mathcal{X}'$, $x_u^\perp \in (\mathcal{X}')^\perp$ such that $u = x_u + x_u^\perp$. The map $u \mapsto x_u$ is denoted $P_{\mathcal{X}'}$ and is called the *orthogonal projection* on $\mathcal{X}'$. Properties are:

   (a) $P_{\mathcal{X}'}$ is bounded and self-adjoint with norm 1;

   (b) $P_{\mathcal{X}'} + P_{(\mathcal{X}')^\perp} = I$;

   (c) $P_{\mathcal{X}'}u$ minimises the distance from u to $\mathcal{X}'$;

   (d) $x = P_{\mathcal{X}'}u$ if and only if $x \in \mathcal{X}'$ and $u - x \in (\mathcal{X}')^\perp$.

6. For any $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ we have

$$\mathcal{R}(A)^\perp = \mathcal{N}(A^*) \quad \text{and} \quad \mathcal{N}(A)^\perp = \overline{\mathcal{R}(A^*)}.$$

Lemma 1.2. *For any $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ we have $\overline{\mathcal{R}(A^*A)} = \overline{\mathcal{R}(A^*)}$.*

Proof. It is trivial that $\overline{\mathcal{R}(A^*A)} \subseteq \overline{\mathcal{R}(A^*)}$.

Now, suppose $u \in \overline{\mathcal{R}(A^*)}$ and let $\varepsilon > 0$. Then there exists $v \in \mathcal{X}$ such that $\|A^*v - u\| < \varepsilon/2$. Writing $v = e + f$ with $e \in \mathcal{N}(A^*)$, $f \in \mathcal{N}(A^*)^\perp = \overline{\mathcal{R}(A)}$, we see that $\|A^*f - u\| < \varepsilon/2$.

Since $f \in \overline{\mathcal{R}(A)}$, there exists $x \in \mathcal{X}$ such that $\|Ax - f\| < \varepsilon/(2\|A\|)$. We now compute

$$\|A^*Ax - u\| \leq \|A^*Ax - A^*f\| + \|A^*f - u\| < \|A^*\| \frac{\varepsilon}{2\|A\|} + \frac{\varepsilon}{2} = \varepsilon,$$

and conclude that $u \in \overline{\mathcal{R}(A^*A)}$. This shows that $\overline{\mathcal{R}(A)} \subseteq \overline{\mathcal{R}(A^*A)}$. □

1.1 Generalised inverses

We consider the equation

$$Au = f, \tag{1}$$

$A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$, f is known, and we wish to find u.

Definition 1.3. An element $u \in \mathcal{X}$ is called a *least-squares solution* of eq. (1) if u is a minimiser of the function $v \mapsto \|Av - f\|_{\mathcal{Y}}$. It is called a *minimal-norm solution* of eq. (1) if it has minimal norm among all least-squares solutions.

Note that a least-squares solution may not exist. If a least-squares solution u exists, then the affine subspace of all least-squares solutions is given by $u + \mathcal{N}(A)$. By writing $u = u^\dagger + v$ for $u^\dagger \in \mathcal{N}(A)^\perp$, $v \in \mathcal{N}(A)$, we find that the space of least-squares solutions is given by $u^\dagger + \mathcal{N}(A)$, and it is now clear that $u^\dagger$ is the unique minimum-norm solution.

Theorem 1.4. *Let $f \in \mathcal{Y}$ and $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$. Then the following are equivalent:*

1. *$u \in \mathcal{X}$ satisfies $Au = P_{\overline{\mathcal{R}(A)}} f$;*
2. *u is a least-squares solution of eq. (1);*
3. *u solves the normal equation*

$$A^* f = A^* A u. \tag{2}$$

Proof. "(1) $\implies$ (2)": We have

$$\|Au - f\|_{\mathcal{Y}} = \left\| P_{\overline{\mathcal{R}(A)}} f - f \right\| = \inf_{g \in \overline{\mathcal{R}(A)}} \|g - f\| \leq \inf_{g \in \mathcal{R}(A)} \|g - f\| = \inf_{u \in \mathcal{X}} \|Au - f\|.$$

"(2) $\implies$ (3)": Let $u \in \mathcal{X}$ be a least-squares solution and $v \in \mathcal{X}$ arbitrary. Define the quadratic polynomial

$$\begin{aligned} F \colon \mathbb{R} \to \mathbb{R} \colon \lambda \mapsto & \|A(u + \lambda v) - f\|^2 \\ &= \langle Au + \lambda Av - f, Au + \lambda Av - f \rangle \\ &= \lambda^2 \|Av\|^2 - 2\lambda \langle Av, f - Au \rangle + \|f - Au\|^2. \end{aligned}$$

As u is a least-squares solution, we know that F attains a minimum in $\lambda = 0$ and therefore that

$$0 = F'(0) = 2\langle Av, f - Au \rangle = 2\langle v, A^*(f - Au) \rangle.$$

Since v is arbitrary, we must have $A^*(f - Au) = 0$, so u satisfies *eq.* (2).

"(3) $\implies$ (1)": From the normal equation we know that $A^*(f - Au) = 0$. For any $x \in \mathcal{X}$, we have

$$\langle Ax, f - Au \rangle = \langle x, A^*(f - Au) \rangle = \langle x, 0 \rangle = 0,$$

so $f - Au \in \mathcal{R}(A)^\perp$.

So we have $Au \in \overline{\mathcal{R}(A)}$ and $f - Au \in \mathcal{R}(A)^\perp = \overline{\mathcal{R}(A)}^\perp$, from which it follows that $Au = P_{\overline{\mathcal{R}(A)}} f$. □

The following lemma gives a precise condition for when a least-squares solution exists:

Lemma 1.5. *Equation (1) has a least-squares solution if and only if $f \in \mathcal{R}(A) \oplus \mathcal{R}(A)^\perp$.*

Proof. " $\implies$ " Suppose u is a least-squares solution. Then $f - Au \in \mathcal{R}(A)^\perp$, so $f = Au + (f - Au) \in \mathcal{R}(A) \oplus \mathcal{R}(A)^\perp$.

" $\impliedby$ " Suppose $f = Au + g$ for some $u \in \mathcal{X}$, $g \in \mathcal{R}(A)^\perp = \overline{\mathcal{R}(A)}^\perp$. Then by the previous theorem, $Au = P_{\overline{\mathcal{R}(A)}} f$, so u is a least-squares solution. □

Corollary 1.6. *If $\mathcal{R}(A)$ is closed, then eq. (1) always has a least-squares solution.*

In particular, this holds if $\mathcal{R}(A)$ is finite-dimensional. Therefore, if either $\mathcal{X}$ or $\mathcal{Y}$ is finite-dimensional, eq. (1) has a least-squares solution for any A.

We have already seen that if a least-squares solution u exists, then the affine subspace of all least-sqares solutions is $u + \mathcal{N}(A)$, and the unique minimum-norm solution is the projection of 0 onto this affine subspace, which is the unique element of $u + \mathcal{N}(A)$ that lies in $\mathcal{N}(A)^\perp$.

Definition 1.7. Let $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$, and define

$$\tilde{A} \coloneqq A\restriction_{\mathcal{N}(A)^\perp} \colon \mathcal{N}(A)^\perp \to \mathcal{R}(A).$$

Clearly $\tilde{A}$ is bijective and we define the *Moore-Penrose inverse*

$$A^\dagger \colon \mathcal{R}(A) \oplus \mathcal{R}(A)^\perp \to \mathcal{N}(A)^\perp \colon f \mapsto \tilde{A}^{-1} P_{\overline{\mathcal{R}(A)}} f.$$

Remark. Note that $\overline{\mathcal{R}(A) \oplus \mathcal{R}(A)^\perp} = \overline{\mathcal{R}(A)} \oplus \mathcal{R}(A)^\perp = \overline{\mathcal{R}(A)} \oplus \overline{\mathcal{R}(A)}^\perp = \mathcal{Y}$, and therefore the operator $\tilde{A}$ is *densely defined*, and it is defined on all of $\mathcal{Y}$ if and only if $\mathcal{R}(A)$ is closed.

We will not prove the following theorem, but it is interesting:

Theorem 1.8. *The Moore-Penrose inverse $A^\dagger$ is continuous if and only if $\mathcal{R}(A)$ is closed.*

The following characterises all important facts about the Moore-Penrose inverse:

Theorem 1.9 (Moore-Penrose equations)**.** *The operator $A^\dagger$ satisfies the following equations:*

(1) $A^\dagger A = P_{\mathcal{N}(A)^\perp}$;

(2) $A A^\dagger = P_{\overline{\mathcal{R}(A)}}\restriction_{\mathcal{D}(A^\dagger)}$;

(3) $A A^\dagger A = A$;

(4) $A^\dagger A A^\dagger = A^\dagger$.

Conversely, if any linear operator $B \colon \mathcal{Y} \to \mathcal{X}$ satisfies (1) and (2), then $B = A^\dagger$.

Proof. We will not prove (1) and (2). Point (3) and (4) follow immediately from (1) and (2) respectively. □

The Moore-Penrose inverse has the important property that it maps every f in its domain to the corresponding minimum-norm least-squares solution:

Theorem 1.10. *For every $f \in \mathcal{D}(A^\dagger)$, the minimum-norm solution $u^\dagger$ to eq. (1) is given by $u^\dagger = A^\dagger f$.*

Proof. Since $f \in \mathcal{R}(A) \oplus \mathcal{R}(A)^\perp$, we know that there exists a unique minimum-norm solution $u^\dagger \in \mathcal{N}(A)^\dagger$. We write

$$u^\dagger = P_{\mathcal{N}(A)^\perp}(u^\dagger) = A^\dagger A u^\dagger = A^\dagger P_{\overline{\mathcal{R}(A)}} f = A^\dagger A A^\dagger f = A^\dagger f.$$

□

Remark. We can also consider the normal equation $A^* f = A^* A u$ as a least-squares problem, whose minimum-norm solution is $(A^* A)^\dagger A^* f$. It is clear that this expression must equal the minimum-norm solution $u^\dagger$ from eq. (1).

1.2 Compact operators

Definition 1.11. Let $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$. Then A is called *compact* if for any bounded $B \subseteq \mathcal{X}$, the image $A(B)$ is precompact in $\mathcal{Y}$. The set of compact operators in $\mathcal{L}(\mathcal{X}, \mathcal{Y})$ is denoted $\mathcal{K}(\mathcal{X}, \mathcal{Y})$.

Lemma 1.12. *Let $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$. Then A is compact if and only if, for every bounded sequence $(x_n) \subseteq X$, the sequence $(Ax_n) \subseteq Y$ has a convergent subsequence.*

Theorem 1.13. *Let $A \in \mathcal{K}(\mathcal{X}, \mathcal{Y})$ with $\dim(\mathcal{R}(A)) = \infty$. Then $A^\dagger$ is discontinuous.*

Proof. If $\dim \mathcal{R}(A) = \infty$, then $\mathcal{X}$ and $\mathcal{N}(A)^\perp$ are infinite-dimensional as well. Chose an orthonormal sequence $(x_n) \subseteq \mathcal{N}(A)^\perp$, then after taking a subsequence if necessary, we can assume that $f_n := Ax_n$ converges. However, we have

$$\left\|A^\dagger(f_n - f_m)\right\|^2 = \left\|A^\dagger A(x_n - x_m)\right\|^2 = \left\|P_{\mathcal{N}(A)^\perp}(x_n - x_m)\right\|^2 = \|x_n - x_m\|^2 = 2,$$

and in particular the sequence $(A^\dagger f_n)$ does not converge. This shows that $A^\dagger$ is discontinuous. □

In particular, combining this with theorem 1.8 shows that the range of a compact operator is always open, and that not every element in $\mathcal{Y}$ has a least-squares solution.

We will need the following theorem, an infinite-dimensional analogue of the spectral theorem:

Theorem 1.14 (Eigenvalue decomposition of self-adjoint compact operators)**.** *Let $\mathcal{X}$ be a Hilbert space, and $A \in \mathcal{K}(\mathcal{X}, \mathcal{X})$ self-adjoint. Then there exists an orthonormal basis (x_j) of $\overline{\mathcal{R}(A)}$ and a sequence of eigenvalues $|\lambda_1| \geq |\lambda_2| \geq \cdots > 0$ such that for all $u \in \mathcal{X}$ we have*

$$Au = \sum_{j=1}^{\infty} \lambda_j \langle u, x_j \rangle x_j.$$

The sequence (λ_j) is either finite or converges to 0.

The previous theorem gives rise to an infinite-dimensional analogue of the SVD:

Theorem 1.15. *Let $A \in \mathcal{K}(\mathcal{X}, \mathcal{Y})$. Then there exists a (not necessarily infinite) sequence $\sigma_1 \geq \sigma_2 \geq \cdots > 0$ converging to 0, and orthonormal bases (x_j), (y_j) of $\mathcal{N}(A)^\perp$ and $\overline{\mathcal{R}(A)}$ respectively, such that*

$$Ax_j = \sigma_j y_j, \quad A^* y_j = \sigma_j x_j \quad \text{for all } j \in \mathbb{N},$$

and such that for all $u \in \mathcal{X}$ and $f \in \mathcal{Y}$ we have

$$Au = \sum_{j=1}^{\infty} \sigma_j \langle u, x_j \rangle y_j, \quad A^* f = \sum_{j=1}^{\infty} \sigma_j \langle f, y_j \rangle x_j.$$

The sequence $\{(\sigma_j, x_j, y_j)\}$ is called the singular value decomposition (SVD) of A.

Proof. Define $B := A^*A$ and $C := AA^*$, which are both compact, self-adjoint, and positive semi-definite operators. By the previous theorem, we can write

$$Cf = \sum_{j=1}^{\infty} \sigma_j^2 \langle f, y_j \rangle y_j,$$

where (y_j) is a basis of $\overline{\mathcal{R}(AA^*)} = \overline{\mathcal{R}(A)}$ and (σ_j) is a positive decreasing sequence converging to 0.

Note that

$$BA^* y_j = A^*AAy_j = A^*Cy_j = A^*\sigma^2 y_j = \sigma_j^2 A^* y_j,$$

so $A^* y_j$ is an eigenvector of B with eigenvector σ_j^2.

We show that $\left(\frac{A^*y_j}{\sigma_j}\right)$ is an orthonormal basis of $\mathcal{R}(A)^\perp$. is an orthonormal basis of $\mathcal{N}(A)^\perp$: their inner product is given by

$$\left\langle \frac{A^*y_j}{\sigma_j}, \frac{A^*y_k}{\sigma_k} \right\rangle = \frac{1}{\sigma_j\sigma_k}\langle y_j, Cy_k\rangle = \frac{\sigma_k}{\sigma_j}\langle y_j, y_k\rangle = 0,$$

and since the (y_j) are a basis of $\overline{\mathcal{R}(A)} = \mathcal{N}(A^*)^\perp$ it is clear that the span of (A^*y_j) is dense in $\overline{\mathcal{R}(A^*)} = \mathcal{N}(A)^\perp$.

If we choose $x_j = \frac{A^*y_j}{\sigma_j}$, we find by construction that $A^*y_j = \sigma_j x_j$ and

$$Ax_j = \frac{AA^*y_j}{\sigma_j} = \frac{Cy_j}{\sigma_j} = \sigma_j y_j.$$

Finally, we see that

$$Au = \sum_{j=1}^{\infty}\langle u, x_j\rangle Ax_j = \sum_{j=1}^{\infty}\sigma_j\langle u, x_j\rangle y_j \quad \text{and} \quad A^*f = \sum_{j=1}^{\infty}\langle f, y_j\rangle A^*y_j = \sum_{j=1}^{\infty}\sigma_j\langle f, y_j\rangle x_j.$$

$\square$

Theorem 1.16. *Let $A \in \mathcal{K}(\mathcal{X}, \mathcal{Y})$ with SVD $\{(\sigma_j, x_j, y_j)\}$ and let $f \in \mathcal{D}(A^\dagger)$. Then*

$$A^\dagger f = \sum_{j=1}^{\infty}\frac{1}{\sigma_j}\langle f, y_j\rangle x_j.$$

Remark. Note that this is comparable to $A^*f = \sum_{j=1}^{\infty}\sigma_j\langle f, y_j\rangle x_j$, except that A^* is a smoothing operator (since $\sigma_j \to 0$), while $A^\dagger$ does the opposite. Furthermore, $A^\dagger$ amplifies the right singular vectors corresponding to small singular values the most — intuitively, the corresponding left singular vectors are vectors where A doesn't "see much".

Proof. Define $Bf = \sum_{j=1}^{\infty}\frac{1}{\sigma_j}\langle f, y_j\rangle x_j$. Then by theorem 1.9, we must check that $BA = P_{\mathcal{N}(A)^\perp}$ and $AB = P_{\overline{\mathcal{R}(A)}}\restriction_{\mathcal{D}(A^\perp)}$.

For the first equation, we compute

$$BAu = \sum_{j=1}^{\infty}\frac{1}{\sigma_j}\left\langle \sum_{i=1}^{\infty}\sigma_i\langle u, x_i\rangle y_i, y_j\right\rangle x_j = \sum_{j=1}^{\infty}\sum_{i=1}^{\infty}\frac{\sigma_i}{\sigma_j}\langle u, x_i\rangle\langle y_i, y_j\rangle x_j = \sum_{j=1}^{\infty}\langle u, x_j\rangle x_j.$$

Since (x_j) is a basis of $\mathcal{N}(A)^\perp$, this proves that $BA = P_{\mathcal{N}(A)^\perp}$.

For the second equation, an analogous computation gives $ABf = \sum_{i=1}^{\infty}\langle f, y_i\rangle y_i$, and since (y_i) is a basis of $\overline{\mathcal{R}(A)}$, this proves that $AB = P_{\overline{\mathcal{R}(A)}}\restriction_{\mathcal{D}(A^\dagger)}$. $\square$

Definition 1.17. Let $A \in \mathcal{K}(\mathcal{X}, \mathcal{Y})$ have SVD $\{(\sigma_j, x_j, y_j)\}$. We say that $f \in \mathcal{Y}$ satisfies the *Picard criterion* if

$$\sum_j \frac{|\langle f, y_j\rangle|^2}{\sigma_j^2} < \infty.$$

Note that the expression on the left corresponds to $\left\|A^\dagger f\right\|^2$ if $f \in \mathcal{D}(A^\dagger)$.

Theorem 1.18. *Let $f \in \overline{\mathcal{R}(A)}$. Then $f \in \mathcal{R}(A)$ if and only if f satisfies the Picard criterion.*

Proof. ‘ $\Longrightarrow$ ’ Write $f = Au$, then

$$\sum_j \frac{|\langle f, y_j\rangle|^2}{\sigma_j^2} = \sum_j \frac{|\langle Au, y_j\rangle|^2}{\sigma_j^2} = \sum_j \frac{|\langle u, A^* y_j\rangle|^2}{\sigma_j^2} = \sum_j |\langle u, x_j\rangle|^2 < \infty.$$

‘ $\Longleftarrow$ ’ Define $u \coloneqq \sum_{j=1}^{\infty} \frac{1}{\sigma_j}\langle f, y_j\rangle x_j$ (note that by assumption this sum converges). Then

$$Au = A\sum_{j=1}^{\infty} \frac{1}{\sigma_j}\langle f, y_j\rangle x_j = \sum_{j=1}^{\infty} \frac{1}{\sigma_j}\langle f, y_j\rangle A x_j = \sum_{j=1}^{\infty}\langle f, y_j\rangle y_j = P_{\overline{\mathcal{R}(A)}} f = f,$$

so $Au = f$ which implies $f \in \mathcal{R}(A)$. ☐

We have seen that the stability of $A^\dagger$ depends on the speed of decay of the singular values (σ_j). We formalise this:

Definition 1.19. Let $A \in \mathcal{K}(\mathcal{X}, \mathcal{Y})$ have singular values (σ_j). Then the ill-posed inverse problem $Au = f$ is called *mildly ill-posed* if the σ_j decay polynomially (i.e., $\frac{1}{\sigma_n} \leq Cn^\gamma$ for some C, γ) and *severely ill-posed* otherwise.

Example 1.20. Consider the heat equation with initial conditions and boundary values:

$$\begin{cases} v_t - v_{xx} = 0 & (x,t) \in (0,\pi) \times \mathbb{R}_{>0}, \\ v(0,t) = v(\pi,t) = 0 & t \geq 0, \\ v(x,0) = u(x) & x \in (0,\pi), \\ v(x,T) = f(x) & x \in (0,\pi). \end{cases}$$

Then the forward problem is to determine f given u, while the inverse problem is to determine u given f. The solution for the foward problem is given by

$$f = Au \coloneqq \sum_{j=1}^{\infty} e^{-j^2 T}\langle u, \sin(jx)\rangle \sin(jx),$$

and the eigenvalues are therefore $\sigma_j = e^{-j^2 T}$. Since these clearly decay exponentially, this problem is severely ill-posed.

2 Classical regularisation theory

Definition 2.1. Let $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ and