Inverse Problems — Summary

Lucas Riedstra

October 25, 2020

Contents

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 linear operator $A\colon \mathcal{X} \to \mathcal{Y}$ is called *bounded* if

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

   It is known that a linear operator between normed spaces is continuous if and only if it is bounded. The set of bounded linear operators from $\mathcal{X}$ to $\mathcal{Y}$ is denotes $\mathcal{B}(\mathcal{X},\mathcal{Y})$.

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 $A \in \mathcal{B}(\mathcal{X},\mathcal{Y})$ has a unique adjoint $A^* \in \mathcal{B}(\mathcal{Y},\mathcal{X})$ 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 $A \in \mathcal{B}(\mathcal{X},\mathcal{Y})$ 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 $A \in \mathcal{B}(\mathcal{X},\mathcal{Y})$ 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

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

where $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$ and f are 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 $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$. 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 $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$, 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 $B \colon \mathcal{R}(A) \oplus \mathcal{R}(A)^{\perp} \to \mathcal{N}(A)^{\perp}$ satisfies $BA = P_{\mathcal{N}(A)^{\perp}}$ and $AB = P_{\overline{\mathcal{R}(A)}}{\restriction_{\mathcal{D}(A^{\dagger})}}$ then $B = A^{\dagger}$.

Proof. We have

$$A^{\dagger} A u = \tilde{A}^{-1} A P_{\mathcal{N}(A)^{\perp}} u = P_{\mathcal{N}(A)^{\perp}} u,$$

which proves (1). Furthermore, we have

$$A A^{\dagger} f = A \tilde{A}^{-1} P_{\overline{\mathcal{R}(A)}} f = P_{\overline{\mathcal{R}(A)}} f,$$

which proves (2). Finally, (3) follows from (1) and (4) follows from (2).

Now, suppose B satisfies (1) and (2). First we show that $B{\restriction_{\mathcal{R}(A)}} = \tilde{A}^{-1}$, then we show that $B{\restriction_{\mathcal{R}(A)^{\perp}}} = 0$. This shows that $B = A^{\dagger}$. Let $f = Au \in \mathcal{R}(A)$ with $u \in \mathcal{N}(A)^{\perp}$, then

$$Bf = BAu = P_{\mathcal{N}(A)^{\perp}} u = u = \tilde{A}^{-1} f, \quad \text{so } B{\restriction_{\mathcal{R}(A)}} = \tilde{A}^{-1}.$$

Finally, let $f \in \mathcal{R}(A)^{\perp}$, then $ABf = P_{\overline{\mathcal{R}(A)}} f = 0$, and since $Bf \in \mathcal{N}(A)^{\perp}$ this implies $Bf = 0$. We conclude that $B{\restriction_{\mathcal{R}(A)^{\perp}}} = 0$, and this concludes the proof. □

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 $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$. 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 $\mathcal{B}(\mathcal{X}, \mathcal{Y})$ is denoted $\mathcal{K}(\mathcal{X}, \mathcal{Y})$.

Lemma 1.12. *Let $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$. 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 $f_n \coloneqq Ax_n$ 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 $B \coloneqq A^*A$ and $C \coloneqq AA^*$, 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

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

□

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 $AB = P_{\overline{\mathcal{R}(A)}} \restriction_{\mathcal{D}(A^\dagger)}$. □

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. '$\implies$' Write $f = Au$, then

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

'$\impliedby$' 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

Let $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$ such that $\mathcal{R}(A)$ is not closed (this happens for example when A is compact and does not have finite rank), and consider the inverse problem $Au = f$. Suppose we measure not f, but noisy data f_δ such that $\|f_\delta - f\| \leq \delta$. Then since $A^\dagger$ is discontinuous, we cannot expect that $A^\dagger f_\delta \to A^\dagger f$ as $\delta \to 0$. Therefore, we must replace $A^\dagger$ by operators that approximate it.

Definition 2.1. Let $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$. A family $(R_\alpha)_{\alpha>0}$ of continuous operators is called a *regularisation* of $A^\dagger$ if

$$\lim_{\alpha \to 0} R_\alpha f = A^\dagger f \quad \text{for all } f \in \mathcal{D}(A^\dagger).$$

If all R_α are linear (TODO: and bounded?), then we speak of a *linear regularisation* of $A^\dagger$.

Theorem 2.2 (Banach-Steinhaus)**.** *Let $\mathcal{X}, \mathcal{Y}$ be Hilbert spaces and $\{A_\alpha\} \subseteq \mathcal{B}(\mathcal{X}, \mathcal{Y})$ a family of pointwise bounded operators. Then $\{A_\alpha\}$ is bounded in norm.*

Corollary 2.3. *Let $\mathcal{X}, \mathcal{Y}$ be Hilbert spaces and $(A_j) \subseteq \mathcal{B}(\mathcal{X}, \mathcal{Y})$. Then (A_j) converges pointwise to some $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$ if and only if $\{A_j\}$ is norm-bounded and converges pointwise on some dense subset $\mathcal{X}' \subseteq \mathcal{X}$.*

Theorem 2.4. *Let $\mathcal{X}, \mathcal{Y}$ be Hilbert spaces, $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$ and $(R_\alpha)_{\alpha>0}$ a linear regularisation. If $A^\dagger$ is not continuous, (R_α) is not norm-bounded. In particular, there exists $f \in \mathcal{Y}$ with $\|R_\alpha f\| \to \infty$.*

Proof. Suppose (R_α) is norm-bounded. Let $\alpha_j \to 0$, then we know that $R_{\alpha_j} \to A^\dagger$ pointwise on $\mathcal{D}(A^\dagger)$. Since $\mathcal{D}(A^\dagger)$ is dense in $\mathcal{Y}$, corollary 2.3 then tells us that $A^\dagger$ is bounded and therefore continuous, a contradiction.

By the Banach-Steinhaus theorem, if (R_α) is not norm-bounded, it is not pointwise bounded, so there must exist $f \in \mathcal{Y}$ such that $\{\|R_\alpha f\|\}$ is not bounded. □

Recap 2.5. Recall that any bounded sequence in a Hilbert space has a weakly convergent subsequence.

Theorem 2.6. *Let $A \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$ and (R_α) a linear regularisation of $A^\dagger$. If $\{\|AR_\alpha\|\}_{\alpha>0}$ is bounded, then $\|R_\alpha f\| \to \infty$ as $\alpha \to 0$ for every $f \notin \mathcal{D}(A^\dagger)$.*

Proof. Define $u_\alpha := R_\alpha f$ for $f \notin \mathcal{D}(A^\dagger)$, and assume there exists a sequence $\alpha_k \to 0$ such that $\{\|u_{\alpha_k}\|\}$ is bounded. After taking a subsequence if necessary, we may assume that $u_{\alpha_k} \rightharpoonup u$ for some $u \in \mathcal{X}$, and therefore we also have $Au_{\alpha_k} \rightharpoonup Au$.

We also have $\lim_{\alpha \to 0} AR_\alpha f = AA^\dagger f = P_{\overline{\mathcal{R}(A)}} f$ for $f \in \mathcal{D}(A^\dagger)$, and since we assumed $\{AR_\alpha\}$ was norm-bounded, by corollary 2.3 we have $\lim_{\alpha \to 0} AR_\alpha f = P_{\overline{\mathcal{R}(A)}} f$ for all $f \in \mathcal{Y}$.

Since Au_{α_k} is convergent and has weak limit Au, it must also have limit Au, so we find $Au = P_{\overline{\mathcal{R}(A)}} f$ so $f \in \mathcal{D}(A^\dagger)$, a contradiction. □

We need some process to choose a parameter. To this end, note that we have

$$\left\|R_\alpha f_\delta - A^\dagger f\right\| \leq \|R_\alpha(f_\delta - f)\| + \left\|(R_\alpha - A^\dagger) f\right\| \leq \delta \|R_\alpha\| + \left\|(R_\alpha - A^\dagger) f\right\|. \tag{3}$$

The first term is called the *data error* and is unbounded for $\alpha \to 0$, and the second term is called the *approximation error* which does vanish for $\alpha \to 0$. Therefore, we want to choose α small enough to have a low approximation error, while keeping the data error at bay.

2.1 Parameter choice rules

Definition 2.7. A function $\alpha\colon \mathbb{R}_{>0} \times \mathcal{Y} \to \mathbb{R}_{>0}\colon (\delta, f_\delta) \mapsto \alpha(\delta, f_\delta)$ is called a *parameter choice rule* (PCR). We distinguish three types:

1. An *a priori* PCR depends only on δ;
2. An *a posteriori* PCR depends on both δ and f_δ;
3. A *heuristic* PCR depends only on f_δ.

Definition 2.8. Let $(R_\alpha)_{\alpha>0}$ be a regularisation of $A^\dagger$ and α a parameter choice rule. We call (R_α, α) a *convergent regularisation* if

$$\lim_{\delta\to 0} \sup_{f_\delta : \|f-f_\delta\|\le\delta} \left\| R_\alpha f_\delta - A^\dagger f \right\| = 0$$

and

$$\lim_{\delta\to 0} \sup_{f_\delta : \|f-f_\delta\|\le\delta} \alpha(\delta, f_\delta) = 0. \tag{4}$$

2.1.1 A priori parameter choice rules

We will not prove the following theorem, which guarantees the existence of a priori PCRs:

Theorem 2.9. *Let $(R_\alpha)_{\alpha>0}$ be a regularisation of $A^\dagger$. Then there exists an a priori PCR $\alpha = \alpha(\delta)$ such that (R_α, α) is convergent.*

We can characterise PCRs in the following way:

Theorem 2.10. *Let $(R_\alpha)_{\alpha>0}$ be a linear regularisation of $A^\dagger$, and $\alpha = \alpha(\delta)$ an a priori PCR. Then (R_α, α) is convergent if and only if*

$$\lim_{\delta\to 0} \delta \left\| R_{\alpha(\delta)} \right\| = 0 \quad \textit{and} \quad \lim_{\delta\to 0} \alpha(\delta) = 0.$$

Proof. " $\Longrightarrow$ " Suppose (R_α, α) is convergent. It is clear that $\lim_{\delta\to 0} \alpha(\delta) = 0$ by eq. (4). Suppose $\lim_{\delta\to 0} \delta \left\| R_{\alpha(\delta)} \right\| \neq 0$. Then there exists a sequence $(\delta_k) \to 0$ and a constant $C > 0$ such that $\delta_k \left\| R_{\alpha(\delta_k)} \right\| \geq C$ for all k. This implies we can find a sequence $(g_k) \subseteq \mathcal{Y}$ with $\|g_k\| = 1$ and $\delta_k \left\| R_{\alpha(\delta_k)} g_k \right\| \geq C$ for all k.

Now let $f \in \mathcal{D}(A^\dagger)$ and define $f_k \coloneqq f + \delta_k g_k$, then clearly we have $f_k \to f$, but also

$$C \leq \left\| R_{\alpha(\delta_k)}(\delta_k g_k) \right\| = \left\| R_{\alpha(\delta_k)}(f_{\delta_k} - f) \right\| \leq \left\| R_{\alpha(\delta_k)} f_{\delta_k} - A^\dagger f \right\| + \left\| (R_{\alpha(\delta_k)} - A^\dagger) f \right\|.$$

In particular we find that $\left\| (R_{\alpha(\delta_k)} - A^\dagger) f \right\| \geq C$, so clearly R_α is not convergent.

" $\Longleftarrow$ " This follows immediately from eq. (3). □

A problem with a priori PCRs is that they are scale-invariant: if $\alpha = \alpha(\delta)$ gives a convergent regularisation, then $\hat{\alpha} = \alpha(k\delta)$ also gives a convergent regularisation for any k. In practice, it is not always clear which scale should be chosen.

2.1.2 A posteriori parameter choice rules

Let $f \in \mathcal{D}(A^\dagger)$ and f_δ s.t. $\|f - f_\delta\| \leq \delta$. Letting $u^\dagger$ denote the minimum-norm solution of the problem $Au = f$, and defining $\mu \coloneqq \left\| Au^\dagger - f \right\| = \inf_{u\in\mathcal{X}} \|Au - f\|$, we see that

$$\left\| Au^\dagger - f_\delta \right\| \leq \left\| Au^\dagger - f \right\| + \|f - f_\delta\| \leq \mu + \delta.$$

Therefore, it is not useful to choose $\alpha(\delta, f_\delta)$ with $\|Au_\alpha - f_\delta\| < \mu + \delta$: if this is the case, we are most likely overfitting.

This motivates *Morozov's discrepancy principle*:

Definition 2.11. Let (R_α) be a (TODO: linear?) regularisation of $A^\dagger$ and assume $\mathcal{R}(A)$ is dense in $\mathcal{Y}$. Fix $\eta > 1$, and define

$$\alpha(\delta, f_\delta) = \sup\{\alpha > 0 : \|AR_\alpha f_\delta - f_\delta\| \le \eta\delta\}.$$

Then $\alpha(\delta, f_\delta)$ is said to satisfy *Morozov's discrepancy principle.*

It can be shown that the above α indeed gives a convergent regularisation.

2.1.3 Heuristic parameter choice rules

Heuristic parameter choice rules unfortunately only work if the original problem was well-posed:

Theorem 2.12 (Bakushinskii). *Let (R_α) be a regularisation of $A^\dagger$ and suppose there exists a heuristic parameter choice rule α such that (R_α, α) is convergent. Then $A^\dagger$ is continuous from $\mathcal{Y}$ to $\mathcal{X}$.*

2.2 Spectral regularisation

We will now start with specific examples of regularisations. Spectral regularisations are derived from the spectral decomposition

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

We construct a regularisation by replacing σ_j^{-1} by some function $g_\alpha(\sigma_j)$, i.e.,

$$R_\alpha f = \sum_{j=1}^{\infty} g_\alpha(\sigma_j) \langle f, y_j \rangle x_j. \tag{5}$$

Let us explore which conditions g_α must satisfy:

Theorem 2.13. *Let, for $\alpha > 0$, the function $g_\alpha \colon \mathbb{R}_{>0} \to \mathbb{R}_{>0}$ satisfy*

1. $\lim_{\alpha \to 0} g_\alpha(\sigma) = \frac{1}{\sigma}$ *for all* $\sigma > 0$*;*
2. $g_\alpha(\sigma) \le C_\alpha$ *for some* $C_\alpha > 0$*;*
3. $\sup_{\alpha,\sigma} \sigma g_\alpha(\sigma) \le \gamma$ *for some* $\gamma > 0$*.*

Then collection (R_α) defined by eq. (5) is a linear regularisation of $A^\dagger$, and in particular, we have $\|R_\alpha\| \le C_\alpha$.

Proof. From condition 2 it follows that all R_α are bounded. Since

$$\langle f, y_j \rangle = \langle P_{\overline{\mathcal{R}(A)}} f, y_j \rangle = \langle AA^\dagger f, y_j \rangle = \langle A^\dagger f, A^* y_j \rangle = \sigma_j \langle u^\dagger, x_j \rangle,$$

we compute

$$(R_\alpha - A^\dagger) f = \sum_j (g_\alpha(\sigma_j) - \sigma_j)^{-1} \langle f, y_j \rangle x_j = \sum_j (\sigma_j g_\alpha(\sigma_j) - 1) \langle u^\dagger, x_j \rangle x_j,$$

and since $\sigma g_\alpha(\sigma_j) \le \gamma$, we have $(\sigma_j g_\alpha(\sigma_j) - 1)^2 \le 1 + \gamma^2$, so that

$$\left\|(R_\alpha - A^\dagger) f\right\|^2 \le (1 + \gamma^2) \left\|u^\dagger\right\|^2 < \infty.$$

Since $\left\|(R_\alpha - A^\dagger) f\right\|$ is finite, we may apply the reverse Fatou lemma to the sum and obtain

$$\limsup_{\alpha \to 0} \left\|(R_\alpha - A^\dagger) f\right\|^2 \le \sum_j \left(\sigma_j \limsup_{\alpha \to 0} g_\alpha(\sigma_j) - 1\right)^2 \langle u^\dagger, x_j \rangle^2 = 0,$$

and therefore $R_\alpha f \to A^\dagger f$ as $\alpha \to 0$. $\square$

Example 2.14. The first, very simple example is the *truncated SVD*: we simply define

$$g_\alpha(\sigma) = \begin{cases} 1/\sigma & \sigma \geq \alpha, \\ 0 & \sigma < \alpha. \end{cases}$$

It is easy to check that g_α satisfies the conditions of theorem 2.13, and that all R_α are finite-rank operators with $\|R_\alpha\| \leq \frac{1}{\alpha}$. Therefore, if we choose $\alpha = \alpha(\delta)$ such that $\delta/\alpha(\delta) \to 0$, then we obtain a convergent regularisation.

This also highlights the problem with this method: as δ gets smaller, we need more and more singular vectors which are generally expensive to compute.

Example 2.15. The second example is *Tikhonov regularisation*. Here, we define $g_\alpha(\sigma) = \frac{\sigma}{\sigma^2+\alpha}$, and again it is easily checked that the conditions of theorem 2.13 are satisfied, noting that

$$\frac{\sigma}{\sigma^2 + \alpha} \leq \frac{\sigma}{2\sigma\sqrt{\alpha}} = \frac{1}{2\sqrt{\alpha}} =: C_\alpha.$$

Therefore, if $\delta/\sqrt{\alpha(\delta)} \to 0$, the regularisation is convergent.

This method does not require computing the SVD of A: it is easily shown that $u_\alpha \coloneqq R_\alpha f$ is the unique solution to the *regularised normal equation*

$$(A^*A + \alpha I)u_\alpha = A^*f.$$

While $A^*A + \alpha I$ is always invertible, computing the inverse is expensive, so we usually use some approximation of the inverse.

Finally, it can also be shown that

$$u_\alpha = \min_{u \in \mathcal{X}} \|Au - f\|^2 + \alpha\|u\|^2,$$

so we can also view u_α as the solution of an optimisation problem.