Inverse Problems
Classical regularisation theory

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February 13, 2020

Outline

Regularisation Theory

Spectral regularisation

More on parameter choice rules

Iterative regularisation

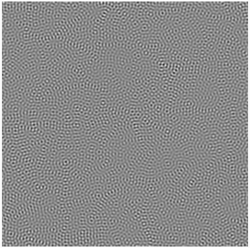
What is regularisation

We saw that $A^\dagger$ is generally unbounded and so, given noisy data f_δ such that $\|f_\delta - f\| \leqslant \delta$, we cannot expect $A^\dagger f_\delta \to A^\dagger f$ as $\delta \to 0$.

$f = Au = \kappa \star u$

$A^\dagger(f)$

$A^\dagger(f + \varepsilon)$



To achieve convergence, replace $A^\dagger$ with a family of well-posed (bounded) operators R_α with $\alpha = \alpha(\delta, f_\delta)$ such that

$$R_\alpha f_\delta \to A^\dagger f$$

for all $f \in \mathcal{D}(A^\dagger)$ and all $f_\delta \in \mathcal{V}$ such that $\|f - f_\delta\|_{\mathcal{V}} < \delta$ as $\delta \to 0$.

Definition 1 (Regularisation)

Let $A \in \mathcal{L}(\mathcal{U}, \mathcal{V})$. A family $\{R_\alpha\}_{\alpha>0}$ of continuous operators is called a regularisation of $A^\dagger$ if $R_\alpha f \to A^\dagger f = u^\dagger$ for all $f \in \mathcal{D}(A^\dagger)$ as $\alpha \to 0$.

$\alpha = 0.1$ $\alpha = 0.05$ $\alpha = 1\text{e-}4$ $\alpha = 1\text{e-}9$

We say that the family $\{R_\alpha\}_\alpha$ is a linear regularisation of $A^\dagger$ if they consist of linear operators.

No uniform boundedness of regularisers

We cannot expect to do better than this definition, i.e. in general, we cannot expect $R_\alpha f$ to converge for $f \notin \mathcal{D}(A^\dagger)$.

Assume: $A \in \mathcal{L}(\mathcal{U}, \mathcal{V})$ and let $\{R_\alpha\}_\alpha$ be a linear regularisation of $A^\dagger$.

Theorem 2

If $A^\dagger$ is not continuous, then $\{R_\alpha\}_\alpha$ cannot be uniformly bounded. In particular, there exists $f \in \mathcal{V}$ such that $\|R_\alpha f\| \to \infty$ as $\alpha \to 0$.

Theorem 3

If $\sup_{\alpha>0} \|AR_\alpha\|_{\mathcal{L}(\mathcal{V},\mathcal{V})} < \infty$, then $\|R_\alpha f\|_{\mathcal{V}} \to +\infty$ for all $f \notin \mathcal{D}(A^\dagger)$.

These results are consequences of the Banach Steinhaus theorem:

Theorem 4 (Banach Steinhaus)

Let $\mathcal{U}, \mathcal{V}$ be Hilbert spaces and let $\{A_j\}_{j\in\mathbb{N}} \subset \mathcal{L}(\mathcal{U}, \mathcal{V})$ be a family of pointwise bounded operators such that $\sup_{j\in\mathbb{N}} \left\|A_j u\right\|_{\mathcal{V}} \leqslant C(u)$ for all $u \in \mathcal{U}$. Then $\sup_{j\in\mathbb{N}} \left\|A_j\right\|_{\mathcal{L}(\mathcal{U},\mathcal{V})} < \infty$.

A corollary of this is that the following are equivalent

(a) There exists $A \in \mathcal{L}(\mathcal{U}, \mathcal{V})$ such that $Au = \lim_{j\to\infty} A_j u$ for all $u \in \mathcal{U}$.

(b) There is a dense subset $\mathcal{X} \subset \mathcal{U}$ such that $\lim_{j\to\infty} A_j u$ exists for all $u \in \mathcal{X}$ and $\sup_{j\in\mathbb{N}} \left\|A_j\right\|_{\mathcal{L}(\mathcal{U},\mathcal{V})} < \infty$.

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Suppose $\{R_\alpha\}$ are linear regularisers. If $A^\dagger$ is not continuous, then $\{R_\alpha\}_\alpha$ cannot be uniformly bounded. In particular, there exists $f \in \mathcal{V}$ such that $\|R_\alpha f\| \to \infty$ as $\alpha \to 0$.

Proof of Theorem 2.

- Suppose that $\{R_\alpha\}_\alpha$ is uniformly bounded, then since $\lim_{\alpha\to 0} R_\alpha(u) = A^\dagger u$ exists for all $u \in \mathcal{D}(A^\dagger)$ which is dense in $\mathcal{V}$, we have $A^\dagger \in \mathcal{L}(\mathcal{U}, \mathcal{V})$, which contradicts the discontinuity of $A^\dagger$.
- If there does not exist f such that $\|R_\alpha f\|$ is unbounded, then Banach Steinhaus says that $\{R_\alpha\}_\alpha$ is uniformly bounded in norm. Contradiction.

□

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Proof of Theorem 3.

By Banach Steinhaus, since $\sup_{\alpha>0} \|AR_\alpha\|_{\mathcal{L}(\mathcal{V},\mathcal{V})} < \infty$ and $\mathcal{D}(A^\dagger)$ is dense in $\mathcal{V}$, there exists $B \in \mathcal{L}(\mathcal{V},\mathcal{V})$ such that $Bg = \lim_{\alpha\to 0} AR_\alpha g$ for all $g \in \mathcal{V}$.

What can we say about B? For any $g \in \mathcal{D}(A^\dagger)$, $AR_\alpha g \to AA^\dagger g = P_{\overline{\mathcal{R}(A)}} g = Bg$. So, $B = P_{\overline{\mathcal{R}(A)}}$.

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- Since bounded sets in Hilbert spaces are weakly compact, there exists a weakly convergent subsequence $u_{\alpha_{k_n}}$ with weak limit $u \in \mathcal{U}$. Continuous linear operators are weakly continuous, so $Au_{\alpha_{k_n}} \rightharpoonup Au$.

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- By uniqueness of limits, $Bf = P_{\overline{\mathcal{R}(A)}} f = \lim_{n\to\infty} AR_{\alpha_{k_n}} f = Au$.
- Since $\mathcal{V} = \overline{\mathcal{R}(A)} \oplus (\overline{\mathcal{R}(A)})^\perp$, we can write $f = f_1 + f_2$ where $f_1 \in \overline{\mathcal{R}(A)}$ and $f_2 \in \overline{\mathcal{R}(A)}^\perp$. So, $Au = P_{\overline{\mathcal{R}(A)}} f = f_1 \in \mathcal{R}(A)$ and hence, $f \in \mathcal{D}(A^\dagger)$. Contradiction.

$\square$

Parameter choice

Want: as $\delta \to 0$, $R_\alpha(f_\delta) \to A^\dagger f$, for all $f \in \mathcal{D}(A^\dagger)$ and f_δ s.t. $\|f - f_\delta\| \leqslant \delta$.

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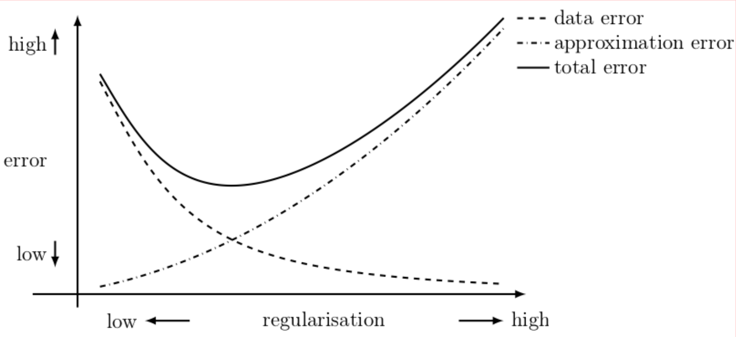
Let $u^\dagger = A^\dagger f$:

$$\left\| R_\alpha f_\delta - u^\dagger \right\|_{\mathcal{U}} \leqslant \| R_\alpha f_\delta - R_\alpha f \|_{\mathcal{U}} + \left\| R_\alpha f - u^\dagger \right\|_{\mathcal{U}} \leqslant \overbrace{\delta \, \| R_\alpha \|_{\mathcal{L}(\mathcal{V},\mathcal{U})}}^{\text{data error}} + \overbrace{\left\| R_\alpha f - A^\dagger f \right\|_{\mathcal{U}}}^{\text{approximation error}}$$



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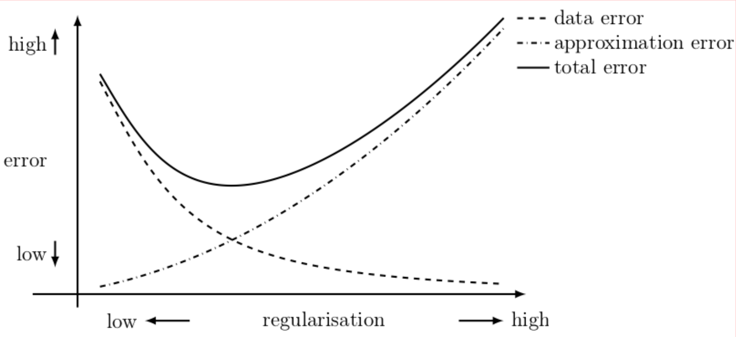

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The regularisation parameter need to be chosen to balance the two terms!

Definition 5

A function $\alpha : \mathbb{R}_{>0} \times \mathcal{V} \to \mathbb{R}_{>0}$, $(\delta, f_\delta) \to \alpha(\delta, f_\delta)$ is called a parameter choice rule. We distinguish between:

(a) a priori parameter choice rules which depend only on δ,

(b) a posteriori parameter choice rules which depend on both δ and f_δ.

(c) heuristic parameter choice rules which depend on f_δ only.

Let $\{R_\alpha\}_\alpha$ be a regularisation of $A^\dagger$. If for all $f \in \mathcal{D}(A^\dagger)$, α is a parameter choice rule such that

$$\lim_{\delta \to 0} \sup_{f_\delta : \|f - f_\delta\| \leqslant \delta} \left\| R_\alpha f_\delta - A^\dagger f \right\|_{\mathcal{U}} = 0 \quad \text{and} \quad \lim_{\delta \to 0} \sup_{f_\delta : \|f - f_\delta\| \leqslant \delta} \alpha(\delta, f_\delta) = 0,$$

then (R_α, α) is called a **convergent regularisation**.

A priori parameter choice rules for linear regularisers

Theorem 6

Let $\{R_\alpha\}_\alpha$ be a linear regularisation and α be an a priori parameter choice rule. Then, (R_α, α) is a convergent regularisation if and only if

(a) $\alpha(\delta) \to 0$ *as* $\delta \to 0$.

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Clearly, if (a) and (b) are satisfied, then for all $\|f_\delta - f\| \leqslant \delta$,
$\left\| R_{\alpha(\delta)} f_\delta - A^\dagger f \right\| \leqslant \delta \left\| R_{\alpha(\delta)} \right\| + \left\| R_{\alpha(\delta)} A - A^\dagger f \right\| \to 0$ as $\delta \to 0$.

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This means: taking a sequence $\delta_k \to 0$, for each δ_k, there exists $c > 0$ and f_{δ_k} with $\left\|f_{\delta_k} - f\right\| \leqslant \delta_k$ such that $\left\|R_{\alpha(\delta_k)}(f_{\delta_k} - f)\right\| \geqslant c$.

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So:

$$\left\| R_{\alpha(\delta_k)} f_{\delta_k} - A^\dagger f \right\| \geqslant \left\| R_{\alpha(\delta_k)} (f_{\delta_k} - f) \right\| - \left\| R_{\alpha(\delta_k)} - A^\dagger f \right\| \geqslant c - \left\| R_{\alpha(\delta_k)} - A^\dagger f \right\|.$$

Contradiction, since the LHS converges to 0, and the RHS converges to c.

Outline

Spectral regularisation

Recall that the spectral representation of $A^\dagger$:

$$A^\dagger f = \sum_{j\in\mathbb{N}} \frac{1}{\sigma_j}\langle f,\, v_j\rangle u_j$$

The source of ill-posedness of $A^\dagger$ is that the eigenvalues $1/\sigma_j$ explode as $j \to \infty$.

Spectral regularisation modifies the eigenvalues

$$R_\alpha f = \sum_{j\in\mathbb{N}} g_\alpha(\sigma_j)\langle f,\, v_j\rangle u_j$$

where $g_\alpha : (0,\infty) \to (0,\infty)$ such that

1. $\lim_{\alpha\to 0} g_\alpha(\sigma) = \frac{1}{\sigma}$
2. for all $\sigma > 0$, $g_\alpha(\sigma) \leqslant C_\alpha$.

Theorem 7 (Mild growth of g_α will ensures regularisation of $A^\dagger$)

Assume that $\sup_{\alpha,\sigma} \sigma g_\alpha(\sigma) \leqslant \gamma$ *for some* $\gamma > 0$.

- *Then,* $R_\alpha f \to A^\dagger f$ *as* $\alpha \to 0$ *for all* $f \in \mathcal{D}(A^\dagger)$.
- *If moreover,* $\alpha = \alpha(\delta)$ *is an a-priori parameter choice rule such that* $\lim_{\delta\to 0} \delta C_{\alpha(\delta)} = 0$, *then* $(R_{\alpha(\delta)}, \alpha(\delta))$ *is a convergent regularisation.*

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From the SVD of $A^\dagger$ and definition of R_α,

$$R_\alpha f - A^\dagger f = \sum_{j=1}^{\infty} \left(g_\alpha(\sigma_j) - \frac{1}{\sigma_j} \right) \langle f,\, v_j \rangle u_j = \sum_{j=1}^{\infty} \left(\sigma_j g_\alpha(\sigma_j) - 1 \right) \langle A^\dagger f,\, u_j \rangle u_j$$

By assumption, $\left|\sigma_j g_\alpha(\sigma_j) - 1\right| \leqslant 1 + \gamma$. So, $\left\|R_\alpha f - A^\dagger f\right\| \leqslant (1+\gamma) \left\|A^\dagger f\right\| < \infty$.

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By the reverse Fatou's lemma

$$\begin{aligned}
\limsup_{\alpha\to 0} \left\|R_\alpha f - A^\dagger f\right\|^2 &\leqslant \limsup_{\alpha\to 0} \sum_j \left(\sigma_j g_\alpha(\sigma_j) - 1\right)^2 \left|\langle A^\dagger f,\, u_j\rangle\right|^2 \\
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The claim on convergent regularisation is from Theorem 6 since $\left\| R_{\alpha(\delta)} \right\| \leqslant C_{\alpha(\delta)}$.

Truncated singular value decomposition

Truncated SVD: discard all singular values below threshold α:

$$g_\alpha(\sigma) = \begin{cases} \sigma^{-1} & \sigma \geqslant \alpha \\ 0 & \text{else.} \end{cases}$$

We then have

$$R_\alpha f = \sum_{\sigma_j \geqslant \alpha} \frac{1}{\sigma_j} \langle f,\, v_j \rangle u_j$$

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For all $\sigma > 0$, we naturally have $\lim_{\alpha \to 0} g_\alpha(\sigma) = \frac{1}{\sigma}$.
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Disadvantage: requires the knowledge of the singular vectors of A (only finitely many, but this number might be large).

Tikhonov regularisation

The idea is to shift the eigenvalues of A^*A by a constant factor: Let $g_\alpha(\sigma) = \frac{\sigma}{\sigma^2+\alpha}$ and the corresponding Tikhonov regularisation is

$$R_\alpha f = \sum_{j=1}^{\infty} \frac{\sigma_j}{\sigma_j^2 + \alpha} \langle f,\, v_j \rangle u_j.$$

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Is this a convergent regularisation of $A^\dagger$?
For all $\sigma > 0$, $\lim_{\alpha \to 0} g(\sigma) = \frac{1}{\sigma}$. We again have $\sup_{\alpha,\sigma} \sigma g_\alpha \leqslant 1$ and since $0 \leqslant (\sigma - \sqrt{\alpha})^2 = \sigma^2 - 2\sigma\sqrt{\alpha} + \alpha$, we get $\sigma^2 + \alpha \geqslant 2\sigma\sqrt{\alpha}$ which implies that

$$\frac{\sigma}{\sigma^2 + \alpha} \leqslant \frac{1}{2\sqrt{\alpha}}.$$

So, $g_\alpha(\sigma) \leqslant C_\alpha = \frac{1}{2\sqrt{\alpha}}$. We have a convergent regularisation if

$$\lim_{\delta \to 0} \delta/\sqrt{\alpha} = 0.$$

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$$R_\alpha f = \sum_{j=1}^{\infty} \frac{\sigma_j}{\sigma_j^2 + \alpha} \langle f,\, v_j \rangle u_j.$$

This is easy to compute:
Note that σ_j^2 are the eigenvalues of A^*A and $\sigma_j^2 + \alpha$ are the eigenvalues of $A^*A + \alpha \mathrm{Id}$. So, for $u_\alpha = R_\alpha f$, we have

$$(A^*A + \alpha \mathrm{Id}) u_\alpha = \sum_{j=1}^{\infty} \sigma_j \langle f,\, v_j \rangle u_j = A^* f.$$

So, we just need to invert this (well-posed) linear system. Knowledge of σ_j's not needed!

Convergence rates

Let's look at the error between $u_\alpha = R_\alpha f$ and $u_\alpha^\delta = R_\alpha f_\delta$, where $f \in \mathcal{D}(A^\dagger)$ and $f^\delta \in \mathcal{V}$ satisfies $\left\|f - f^\delta\right\| \leqslant \delta$ for some $\delta > 0$:

Theorem 8

Assume that $\sup_{\alpha,\sigma} \sigma g_\alpha(\sigma) \leqslant \gamma$. *Then*

$$\left\|Au_\alpha - Au_\alpha^\delta\right\|_{\mathcal{V}} \leqslant \gamma\delta \quad \textit{and} \quad \left\|u_\alpha - u_\alpha^\delta\right\|_{\mathcal{U}} \leqslant C_\alpha \delta.$$

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NB: the error on $\left\|Au_\alpha - Au_\alpha^\delta\right\|_{\mathcal{V}}$ is linear wrt δ, but since α depends on δ, the error on $\left\|u_\alpha - u_\alpha^\delta\right\|_{\mathcal{U}}$ will be slower than $\mathcal{O}(\delta)$.

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Proof:

$$Au_\alpha - Au_\alpha^\delta = \sum_j \sigma_j \langle u_\alpha - u_\alpha^\delta,\, u_j\rangle v_j = \sum_j \sigma_j g_\alpha(\sigma_j)\langle f - f_\delta,\, v_j\rangle v_j$$

So, $\left\|Au_\alpha - Au_\alpha^\delta\right\| \leqslant \sup_{\sigma,\alpha} \sigma g_\alpha(\sigma) \left\|f - f_\delta\right\| \leqslant \gamma\delta$.

Similarly, recall that $|g_\alpha(\sigma)| \leqslant C_\alpha$ for all $\sigma > 0$, so

$$u_\alpha - u_\alpha^\delta = \sum_j g_\alpha(\sigma_j)\langle f - f_\delta,\, v_j\rangle u_j$$

implies $\left\|u_\alpha - u_\alpha^\delta\right\| \leqslant C_\alpha \delta$.

Source condition

We have bounded the data error, but for the approximation error $\left\|u^\dagger - u_\alpha\right\|$ where $u_\alpha = R_\alpha f$ and $u^\dagger = A^\dagger f$, this depends on additional properties of $u^\dagger$:

The source condition: There exists $w \in \mathcal{U}$ and $\mu > 0$ such that $u^\dagger = (A^* A)^\mu w$. For arbitrary $\mu > 0$, this is interpreted as

$$(A^* A)^\mu w = \sum_{j=1}^{\infty} \sigma_j^{2\mu} \langle w,\, u_j \rangle u_j.$$

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Example (Differentiation): Let $(Au)(y) = \int_0^y u(x)\mathrm{d}x$. For $\mu = 1$, the source condition says that

$$u^\dagger(x) = \int_x^1 \int_0^y w(z)\mathrm{d}z\mathrm{d}y$$

i.e. $u^\dagger$ is twice differentiable.

Assume the source condition and $\sigma^{2\mu}\,|\sigma g_\alpha(\sigma) - 1| \leqslant \omega_\mu(\alpha)$ for all $\sigma > 0$.

Then since $\langle R_\alpha f,\, u_j\rangle = g_\alpha(\sigma_j)\langle f,\, v_j\rangle = g_\alpha(\sigma_j)\sigma_j\langle u^\dagger,\, u_j\rangle$,

$$\left\|R_\alpha f - A^\dagger f\right\|^2 \leqslant \sum_j \left|\sigma_j g_\alpha(\sigma_j) - 1\right|^2 \underbrace{\left|\langle u^\dagger,\, u_j\rangle\right|^2}_{\sigma_j^{4\mu}\left|\langle w,\, u_j\rangle\right|^2}$$

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So, $\left\| u_\alpha - u^\dagger \right\| \leqslant \omega_\mu(\alpha) \|w\|$ and

$$\left\| u_\alpha^\delta - u^\dagger \right\| \leqslant \omega_\mu(\alpha) \|w\| + C_\alpha \delta.$$

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Example of Truncated SVD.
Recall $C_\alpha = 1/\alpha$ and $g_\alpha(\sigma)=0$ for all $\sigma<\alpha$ and $g_\alpha(\sigma)=1/\sigma$ for $\sigma\geqslant\alpha$. So,

$$\sigma^{2\mu}\left|\sigma g_\alpha(\sigma)-1\right| \leqslant \alpha^{2\mu}.$$

Let $\omega_\mu(\alpha)=\alpha^{2\mu}$. To minimise $\alpha^{2\mu}\left\|w\right\| + \delta/\alpha$, choose $\alpha = \left(\frac{\delta}{2\mu\|w\|}\right)^{1/(2\mu+1)}$

This yields $\left\|u_\alpha^\delta - u^\dagger\right\| \leqslant \delta^{\frac{2\mu}{2\mu+1}}$.

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Whatever the choice of μ, the convergence rate is always slower than $\mathcal{O}(\delta)$. One can show that this rate is optimal.

Outline

A priori parameter choice rules

Theorem 9 (Existence of convergent a-priori parameter choice rules)

Let $\{R_\alpha\}_\alpha$ be a regularisation of $A^\dagger$, for $A \in \mathcal{L}(\mathcal{U}, \mathcal{V})$. Then, there exists an a-priori parameter choice rule $\alpha = \alpha(\delta)$ such that (R_α, α) is a convergent regularisation.

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Proof.

Need to show: $\forall \varepsilon > 0$, $\exists \delta$ such that $\left\| R_{\alpha(\delta)} f_\delta - A^\dagger f \right\|_{\mathcal{U}} \leqslant \varepsilon$ when $\|f_\delta - f\|_{\mathcal{V}} \leqslant \delta$.

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- For fixed ε, $R_{\gamma(\varepsilon)}$ is continuous. So, there exists $\rho(\varepsilon) > 0$ such that $\left\| R_{\gamma(\varepsilon)} f - R_{\gamma(\varepsilon)} g \right\| \leqslant \frac{\varepsilon}{2}$ for all $\| g - f \| \leqslant \rho(\varepsilon)$. WLOG, assume that ρ is a continuous strictly monotone increasing function with $\lim_{\varepsilon \to 0} \rho(\varepsilon) = 0$.

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- By the inverse function theorem, there exists ρ^{-1} which is also strictly monotone and continuous on the range of ρ such that $\lim_{\delta \to 0} \rho^{-1}(\delta) = 0$. Continuously extend ρ^{-1} to $(0, \infty)$ and define $\alpha(\delta) \stackrel{\text{def.}}{=} \gamma(\rho^{-1}(\delta))$. Then, $\lim_{\delta \to 0} \alpha(\delta) = 0$.

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- For all $\varepsilon > 0$, there exists $\delta \stackrel{\text{def.}}{=} \rho(\varepsilon)$ such that with $\alpha(\delta) = \gamma(\varepsilon)$,

$$\left\| R_{\alpha(\delta)} f_\delta - A^\dagger f \right\|_{\mathcal{U}} \leqslant \left\| R_{\alpha(\delta)} f_\delta - R_{\alpha(\delta)} f \right\| + \left\| R_{\gamma(\varepsilon)} f - A^\dagger f \right\|_{\mathcal{U}} \leqslant \varepsilon,$$

  for all f_δ with $\|f - f_\delta\| \leqslant \delta$.

□

We may want a parameter choice rule which takes the approximate data f_δ into account. One way of approaching this is via the Morozov's discrepancy principle:

Definition 10

Let $u_\alpha = R_\alpha f_\delta$ with $\alpha(\delta, f_\delta)$ chosen as follows:

$$\alpha(\delta, f_\delta) = \sup \left\{\alpha > 0 \,;\, \left\|A u_{\alpha(\delta, f_\delta)} - f_\delta\right\| \leqslant \eta\delta\right\}$$

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- Given $f \in \mathcal{D}(A^\dagger)$ and $f_\delta \in \mathcal{V}$ such that $\|f_\delta - f\| \leqslant \delta$, let $u^\dagger$ be the minimal norm solution to data f and define $\mu \stackrel{\text{def.}}{=} \left\|Au^\dagger - f\right\|$. Then,

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

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  It may be hard to estimate μ in practice, but if $\mathcal{R}(A)$ is dense in $\mathcal{V}$, then $\mu = 0$.
- In practice, pick a null sequence $\{\alpha_j\}_j$ and iteratively compute $u_{\alpha_j} \overset{\text{def.}}{=} R_{\alpha_j} f_\delta$ for $j = 1, \dots, j^*$, until $u_{\alpha_{j^*}}$ satisfies Morozov's discrepancy principle.

Heuristic parameter choice rules

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Heuristic rules yield convergent regularisation only for well-posed problems:

Theorem 11 (The Bakushinskii veto)

Let $A \in \mathcal{L}(\mathcal{U}, \mathcal{V})$ and $\{R_\alpha\}_\alpha$ be a regularisation for $A^\dagger$. Let $\alpha = \alpha(f_\delta)$ be such that (R_α, α) is a convergent regularisaton. Then, $A^\dagger$ is continuous from $\mathcal{V} \to \mathcal{U}$.

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If we have a convergent regularisation, then

$$\lim_{\delta \to 0} \sup \left\{ \left\| R_{\alpha(f_\delta)} f_\delta - A^\dagger f \right\| \; ; \; f \in \mathcal{D}(A^\dagger), \; \|f_\delta - f\| \leqslant \delta \right\} = 0$$

i.e. $R_{\alpha(f)} f = A^\dagger f$ for all $f \in \mathcal{D}(A^\dagger)$.

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i.e. $R_{\alpha(f)} f = A^\dagger f$ for all $f \in \mathcal{D}(A^\dagger)$.

Taking any sequence $f_j \in \mathcal{D}(A^\dagger)$ which converges to $f \in \mathcal{D}(A^\dagger)$, $\lim_{j \to \infty} A^\dagger f_j = \lim_{j \to \infty} R_{\alpha(f_j)} f_j = A^\dagger f$. Therefore, $A^\dagger$ is continuous on $\mathcal{D}(A^\dagger)$. Since $\mathcal{D}(A^\dagger)$ is dense in $\mathcal{V}$, there exists a continuous extension of $A^\dagger$ on $\mathcal{V}$.

Heuristic parameter choice rules

Despite this negative result of Bakushinskii, heuristic rules are still employed in practices because

- This only applies to infinite dimensional operators.
- This is an asymptotic and a worst-case result. For fixed noise levels or restricted noise values, heuristic rules can still give good performance.

Hanke-Raus rule

Hanke-Raus rule. Choose $\alpha(f^\delta)$ as

$$\alpha(f^\delta) \overset{\text{def.}}{=} \operatorname{argmin}_\alpha \frac{1}{\sqrt{\alpha}} \left\| A u_\alpha^\delta - f^\delta \right\|_{\mathcal{V}} .$$

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Recall that $\left\| Au_\alpha - Au_\alpha^\delta \right\| \leqslant \gamma\delta$ where $\gamma \geqslant \sup_{\alpha,\sigma} \sigma g_\alpha(\sigma)$. We also have

$$\left\| Au^\dagger - Au_\alpha \right\|^2 = \sum_j \left| g_\alpha(\sigma_j)\sigma_j - 1 \right|^2 \sigma_j^2 \left| \langle u^\dagger,\, u_j \rangle \right|^2 \leqslant \alpha^2 \left\| u^\dagger \right\|^2$$

for both truncated SVD and Tikhonov regularisation (check this!).

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for both truncated SVD and Tikhonov regularisation (check this!).

So,

$$\left\| Au^\dagger - Au_\alpha^\delta \right\| \lesssim \alpha + \delta \lesssim \delta$$

if we choose $\alpha \sim \delta$. Note that $\delta = \operatorname{argmin}_\alpha \frac{(\alpha+\delta)}{\sqrt{\alpha}}$.

The L-Curve

To motivate the L-Curve, recall our error bounds with $\gamma = \sup_{\alpha,\sigma} g_\alpha(\sigma)$.

- $\left\| A u_\alpha^\delta - A u^\dagger \right\| \leqslant \sqrt{\sum_j \left| g_\alpha(\sigma_j)\sigma_j - 1 \right|^2 \sigma_j^2 \left| \langle u^\dagger,\, u_j \rangle \right|^2} + \gamma\delta \leqslant \alpha \left\| u^\dagger \right\| + \gamma\delta$
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As we decrease α, the data error increases, so $\left\|u_\alpha^\delta\right\|$ grows, but $\left\|Au_\alpha^\delta - Au^\dagger\right\|$ remains roughly constant.

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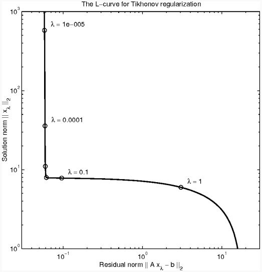

Plotting $\log \|Au_\alpha - f_\delta\|$ against $\log(\|u_\alpha\|)$ for varying α gives an L-curve.

L-Curve. Choose
$\alpha(f^\delta) = \operatorname{argmin}_{\alpha>0} \|u_\alpha\|_{\mathcal{U}} \left\|Au_\alpha - f^\delta\right\|_{\mathcal{V}}.$

Ordinary Cross Validation

Idea: withhold parts of f, and choose α such that we can predict this withheld data.

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Cross Validation: Let $A \in \mathbb{R}^{m \times n}$ and let $A^{(i)}$ be the matrix A with ith row removed, and $f^{(i)}$ be the vector with the ith entry removed. Let $u_\alpha^{(i)}$ be the regularised solution to $A^{(i)}u = f^{(i)}$.

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$$\alpha_* = \operatorname{argmin}_\alpha \frac{1}{m} \sum_{i=1}^{m} \left(A(i,:) u_\alpha^{(i)} - f_i \right)^2$$

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For Tikhonov regularisation, this is the same as

$$\alpha_* = \operatorname{argmin}_\alpha P(\alpha) \stackrel{\text{def.}}{=} \frac{1}{m}\sum_{i=1}^{m}\left(\frac{A(i,:)u_\alpha - f_i}{1-h_{ii}}\right)^2$$

where h_{ii} are diagonal elements of $A(A^\top A + \alpha \mathrm{Id})^{-1}A^\top$.

One of the problems with OCV is that it is not invariant to unitary transforms. In particular, if all entries of A are zero except for the diagonal entries A_{jj}, then one can show that $P(\alpha) = \sum_i f_i^2$ for all α, so there is no unique minimum.

Generalised Cross Validation: this is a rotationally invariant version of OCV, where we average the h_{ii}'s:

$\operatorname{tr}\left(A(A^\top A + \alpha \mathrm{Id})^{-1} A^\top\right) = \sum_{i=1}^n \sigma_i g_\alpha(\sigma_i)$ where $\sigma_i g_\alpha(\sigma_i) = \frac{\sigma_i^2}{\sigma_i^2+\alpha}$.

$$\alpha_* = \operatorname{argmin}_\alpha \frac{\|Au_\alpha - f\|^2}{\left(m - \sum_{i=1}^n \sigma_i g_\alpha(\sigma_i)\right)^2}$$

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In statistics, the term tr $\left(A(A^\top A + \alpha \mathrm{Id})^{-1} A^\top\right)$ is called the **effective number of parameters**.

In the case of Truncated SVD, $\sum_i \sigma_i g_\alpha(\sigma_i) = k_\alpha$ is the number of singular values retained, so

$$\alpha_* = \mathrm{argmin}_\alpha \frac{\|Au_\alpha - f\|^2}{(m - k_\alpha)^2}$$

Outline

Let us consider computing a least squares solution via gradient descent on

$$F(u) = \frac{1}{2} \|Au - f\|_{\mathcal{V}}^2 .$$

We have $\nabla F(u) = A^*(Au - f)$, and gradient descent on F is known as:

The Landweber iterations

$$\begin{aligned} u^{k+1} &= (\mathrm{Id} - \tau A^* A)u^k + \tau A^* f \\ u^0 &= 0 \end{aligned}$$

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$$u^{k+1} = (\mathrm{Id} - \tau A^* A)u^k + \tau A^* f$$
$$u^0 = 0$$

We don't want to compute $A^\dagger f$ if $f \notin \mathcal{D}(A^\dagger)$, we will see that k corresponds to a regularisation parameter and stopping early is a form of regularisation!

Lemma 4.1

Let $\tau \in (0, \frac{2}{\|A\|^2})$. *Then,* $\left\|Au^{k+1} - f\right\|_{\mathcal{V}} \leqslant \left\|Au^k - f\right\|_{\mathcal{V}}$, *with equality only if* $A^*(Au^k - f) = 0$.

Landweber iteration: Choosing the stepsize

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$$\begin{aligned}
\left\|Au^{k+1} - f\right\|^2 &= \left\|A(\mathrm{Id} - \tau A^* A)u^k + \tau AA^* f - f\right\|^2 \\
&= \left\|Au^k - f - \tau AA^* Au^k + \tau AA^* f\right\|^2 \\
&= \left\|Au^k - f\right\|^2 + \tau^2 \left\|AA^*(Au^k - f)\right\|^2 - 2\tau\langle A^*(Au^k - f), A^*(Au^k - f)\rangle \\
&\leqslant \left\|Au^k - f\right\|^2 + (\tau^2 \|A\|^2 - 2\tau) \left\|A^*(Au^k - f)\right\|^2
\end{aligned}$$

with equality only if $A^*(Au^k - f) = 0$ since $(\tau^2 \|A\|^2 - 2\tau)$ is negative by our choice of τ.

Landweber iteration is a form of spectral regularisation

By induction we have

$$u^k = \tau \sum_{\ell=0}^{k-1} (\mathrm{Id} - \tau A^* A)^\ell A^* f \stackrel{\text{def.}}{=} R_k f.$$

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Since $A^* f = \sum_{j=1}^\infty \sigma_j \langle f,\, v_j \rangle u_j$, we have

$$\begin{aligned} R_k f &= \tau \sum_{j=1}^\infty \sum_{\ell=0}^{k-1} \sigma_j \langle f,\, v_j \rangle (\mathrm{Id} - \tau A^* A)^\ell u_j \\ &= \tau \sum_{j=1}^\infty \sigma_j \langle f,\, v_j \rangle \sum_{\ell=0}^{k-1} (1 - \tau \sigma_j^2)^\ell u_j = \sum_{j=1}^\infty \frac{1 - (1 - \tau \sigma_j^2)^k}{\sigma_j} \langle f,\, v_j \rangle u_j. \end{aligned}$$

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Let $\tau \in (0, \frac{2}{\|A\|^2})$ and $g_k(\sigma) \stackrel{\text{def.}}{=} \frac{1-(1-\tau\sigma^2)^k}{\sigma}$. Then

$$R_k f = \sum_{j=1}^{\infty} g_k(\sigma_j) \langle f,\, v_j \rangle u_j.$$

Regularisation and convergence

Regularisation: Note that $\left|1 - \tau\sigma_j\right| < 1$ for $\tau \in (0, 2/\left\|A\right\|^2)$, so

$$g_k(\sigma) \stackrel{\text{def.}}{=} \frac{1 - (1 - \tau\sigma^2)^k}{\sigma} \to \frac{1}{\sigma}, \quad \text{as } k \to \infty.$$

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Note that R_k is a linear regulariser and

$$AR_k f = \sum_{j=1}^{\infty} \left(1 - (1 - \tau\sigma_j^2)^k\right) \langle f,\, v_j\rangle v_j \implies \|AR_k\|_{\mathcal{L}(\mathcal{V},\mathcal{V})} \leqslant 2,$$

so we have $\|R_k f\| \to +\infty$ for all $f \notin \mathcal{D}(A^\dagger)$.

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How to choose k to ensure convergence?
Recall that we need $g_k(\sigma) \leqslant C_k$ and $\lim_{\delta \to 0} \delta C_k = 0$. From applying $e^{-x} \geqslant 1 - x$ twice, we have

$$g_k(\sigma) \leqslant \frac{1 - e^{-\tau\sigma^2 k}}{\sigma} \leqslant \frac{\tau\sigma^2 k}{\sigma} = \tau k \sigma \leqslant \|A\| \, k\tau,$$

we need a stopping criteria of $k_*(\delta)$ such that $\lim_{\delta \to 0} k_*(\delta)\delta = 0$.

To summarise:

Lemma 4.2

Let $\tau \in (0, 2/\|A\|^2)$.

(i) *Let* $f \in \mathcal{D}(A^\dagger)$ *and* $u^\dagger = A^\dagger f$, *then* $\left\|u^k - u^\dagger\right\| \to 0$.

(ii) *If* $f \notin \mathcal{D}(A^\dagger)$, *then* $\left\|u^k\right\| \to \infty$.

(iii) *If* $\lim_{\delta \to 0} k_*(\delta)\delta = 0$, *then* $\left\|u^{k_*(\delta)} - u^\dagger\right\| \to 0$ *as* $\delta \to 0$, *when doing Landweber iteration on* f_δ *such that* $\|f_\delta - f\| \leqslant \delta$ *and* $f \in \mathcal{D}(A^\dagger)$.

Landweber iteration: error bounds

Interpret $\alpha \stackrel{\text{def.}}{=} 1/k$, then

$$u_\alpha = R_\alpha f = \sum_{j=1}^{\infty} \left(1 - (1 - \tau\sigma_j^2)^{1/\alpha}\right) \frac{1}{\sigma_j} \langle f,\, v_j \rangle u_j$$

Theorem 12

Let $\tau \in (0, 2/\|A\|^2)$. Assume that there exists $w \in \mathcal{V}$ such that $u^\dagger \stackrel{\text{def.}}{=} A^\dagger f = A^* w$. Then,

(i) *letting $f = Au^\dagger$,*

$$\left\| u^k - u^\dagger \right\|_{\mathcal{U}} = \mathcal{O}\left(\frac{1}{\sqrt{k}}\right) = \mathcal{O}(\sqrt{\alpha})$$

(ii) *letting $f = Au^\dagger$ and $f^\delta \in \mathcal{V}$ such that $\left\| f^\delta - f \right\| \leqslant \delta$,*

$$\left\| u_\delta^k - u^\dagger \right\|_{\mathcal{U}} \leqslant \sqrt{\tau k}\delta + \frac{\|w\|}{\sqrt{\tau(2k+1)}}$$

Note the trade-off between approximation and data error. We need to stop early!

Let $f = Au^\dagger$. Recall that

$$u^\dagger - u^k = u^\dagger - \tau \sum_{j=0}^{k-1} (\mathrm{Id} - \tau A^* A)^j A^* A u^\dagger.$$

One can check that $\sum_{j=0}^{k-1} (\mathrm{Id} - \tau A^* A)^j A^* A = A^* A \sum_{j=0}^{k-1} (\mathrm{Id} - \tau A^* A)^j$ and show by induction that

$$\mathrm{Id} - (\mathrm{Id} - \tau A^* A)^k = \tau A^* A \sum_{j=0}^{k-1} (\mathrm{Id} - \tau A^* A)^j$$

Therefore, $u^\dagger - u^k = (\mathrm{Id} - \tau A^* A)^k u^\dagger$.

Error bounds

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Therefore, $u^\dagger - u^k = (\mathrm{Id} - \tau A^* A)^k u^\dagger$.

For (i), using the source condition that $u^\dagger = A^* w$, we have

$$\langle u^\dagger - u^k, u_j \rangle = \langle A^* w, (1 - \tau \sigma_j^2)^k u_j \rangle = (1 - \tau \sigma_j^2)^k \sigma_j \langle w, v_j \rangle.$$

Therefore,

$$\left\| u^\dagger - u^k \right\| \leqslant \|w\| \max_\sigma (1 - \tau \sigma^2)^k \sigma \leqslant \|w\| \left((1 - \tau \sigma_*^2)^k \sigma_* \right) \leqslant \frac{\|w\|}{\sqrt{(2k+1)\tau}}$$

where the maximum is achieved at $\tau \sigma_*^2 = 1/(2k+1)$.

For (ii), recall that $u_k = R_k(f) \overset{\text{def.}}{=} \tau \sum_{j=0}^{k-1} (\mathrm{Id} - \tau A^*A)^j A^* f$ and $\mathrm{Id} - (\mathrm{Id} - \tau A^*A)^k = \tau A^*A \sum_{\ell=0}^{k-1} (\mathrm{Id} - \tau A^*A)^\ell$. So, $u_k - u_k^\delta = R_k(f - f_\delta)$. Now,

$$\begin{aligned} \|R_k\|^2 = \|R_k R_k^*\| &= \tau^2 \left\| \sum_{j=0}^{k-1} (\mathrm{Id} - \tau A^*A)^j A^*A \sum_{\ell=0}^{k-1} (\mathrm{Id} - \tau A^*A)^\ell \right\| \\ &= \tau \left\| \sum_{j=0}^{k-1} (\mathrm{Id} - \tau A^*A)^j \left(\mathrm{Id} - (\mathrm{Id} - \tau A^*A)^k \right) \right\| \\ &\leqslant \tau \left\| \sum_{j=0}^{k-1} (\mathrm{Id} - \tau A^*A)^j \right\| \leqslant k\tau. \end{aligned}$$

Therefore,

$$\left\| u_k - u_k^\delta \right\| \leqslant \sqrt{k\tau}\, \|f - f_\delta\| \leqslant \sqrt{k\tau}\,\delta.$$

Mozorov's discrepancy principle

Given noisy data $\|f - f_\delta\| \leqslant \delta$, consider Mozorov's discrepancy principle as a stopping criteria: Stop when

$$\left\| Au_\delta^k - f_\delta \right\| \leqslant \eta\delta, \quad \text{where} \quad \eta > 1.$$

Lemma 4.3

Let $\tau \in (0, \frac{2}{\|A\|})$. Then, for all $k \leqslant k^*$ and $f = Au^\dagger$ and $\left\| f^\delta - f \right\| \leqslant \delta$, we have

$$\left\| u_\delta^{k+1} - u^\dagger \right\| \leqslant \left\| u_\delta^k - u^\dagger \right\|_{\mathcal{U}}$$

where k^* is chosen in accordance to the discrepancy principle with $\eta = \frac{2}{2 - \tau\|K\|^2} > 1$. Equality is attained only for $A^*(Au_\delta^k - f_\delta) = 0$.

i.e. We move closer to $u^\dagger$ as long as the discrepancy principle is violated. One can in fact show that $\left\| u_\delta^{k^*} - u^\dagger \right\| = \mathcal{O}(\delta^{1/2})$ under the source condition of $u^\dagger = A^* w$.

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Assume that $\left\|Au_\delta^k - f_\delta\right\| > \eta\delta$.

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Assume that $\left\|Au_\delta^k - f_\delta\right\| > \eta\delta$.

Plug in the definition $u_\delta^{k+1} = u_\delta^k - \tau A^* A u_\delta^k + \tau A^* f_\delta$ and rearrange:

$$\begin{aligned}
\left\|u_\delta^{k+1} - u^\dagger\right\|^2 - \left\|u_\delta^k - u^\dagger\right\|^2 &= \left\|u_\delta^k - \tau A^* A u_\delta^k + \tau A^* f_\delta - u^\dagger\right\|^2 - \left\|u_\delta^k - u^\dagger\right\|^2 \\
&= \left\|-\tau A^* A u_\delta^k + \tau A^* f_\delta\right\|^2 + 2\langle -\tau A^* A u_\delta^k + \tau A^* f_\delta,\, u_\delta^k - u^\dagger\rangle \\
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\end{aligned}$$

Note that

- $\left\|-\tau A^* A u_\delta^k + \tau A^* f_\delta\right\|^2 \leqslant \tau^2 \left\|A\right\|^2 \left\|Au_\delta^k - f_\delta\right\|^2$
- $2\tau\langle -Au_\delta^k + f_\delta,\, Au_\delta^k - f\rangle = -2\tau\left\|Au_\delta^k + f_\delta\right\|^2 + 2\tau\langle -Au_\delta^k + f_\delta,\, f_\delta - f\rangle$

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Note that

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- $2\tau\langle -Au_\delta^k + f_\delta,\, Au_\delta^k - f\rangle = -2\tau\left\|Au_\delta^k + f_\delta\right\|^2 + 2\tau\langle -Au_\delta^k + f_\delta,\, f_\delta - f\rangle$

Therefore, unless $A^*(Au_\delta^k - A^* f_\delta) = 0$,

$$\begin{aligned}&\left\|u_\delta^{k+1} - u^\dagger\right\|^2 - \left\|u_\delta^k - u^\dagger\right\|^2 \\ &\qquad \leqslant \tau^2 \|A\|^2 \left\|Au_\delta^k - f_\delta\right\|^2 - 2\tau\left\|Au_\delta^k + f_\delta\right\|^2 + 2\tau\delta\left\|-Au_\delta^k + f_\delta\right\| \\ &\qquad = \tau\left\|Au_\delta^k - f_\delta\right\|\left((\tau\|A\|^2 - 2)\left\|Au_\delta^k - f_\delta\right\| + 2\delta\right) \\ &\qquad < \tau\left\|Au_\delta^k - f_\delta\right\|\left((\tau\|A\|^2 - 2)\eta\delta + 2\delta\right) < 0\end{aligned}$$

Summary

- We defined the notion of convergent regularisations: there is a trade-off between data error and approximation error, so parameters need to be chosen carefully.
- We looked at various forms of spectral (linear) regularisation
- Tikhonov and Landweber iteration are special forms of spectral regularisation which do not require explicit knowledge of the spectrum.
- Convergence rates were obtained under source conditions.