

# Inverse Problems

## Classical regularisation theory

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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  $f_\delta$  such that  $\|f_\delta - f\| \leq \delta$ , we cannot expect  $A^\dagger f_\delta \rightarrow A^\dagger f$  as  $\delta \rightarrow 0$ .

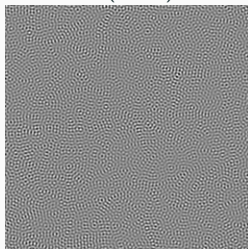
$$f = Au = \kappa \star u$$



$$A^\dagger(f)$$



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



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

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

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

## 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  $R_\alpha f \rightarrow A^\dagger f = u^\dagger$  for all  $f \in \mathcal{D}(A^\dagger)$  as  $\alpha \rightarrow 0$ .

$\alpha = 0.1$



$\alpha = 0.05$



$\alpha = 1e-4$



$\alpha = 1e-9$



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  $\|R_\alpha f\| \rightarrow \infty$  as  $\alpha \rightarrow 0$ .*

## Theorem 3

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

# The Banach Steinhaus Theorem

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  $\sup_{j \in \mathbb{N}} \|A_j u\|_{\mathcal{V}} \leq C(u)$  for all  $u \in \mathcal{U}$ . Then  $\sup_{j \in \mathbb{N}} \|A_j\|_{\mathcal{L}(\mathcal{U}, \mathcal{V})} < \infty$ .*

A corollary of this is that the following are equivalent

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

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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  $\|R_\alpha f\| \rightarrow \infty$  as  $\alpha \rightarrow 0$ .

## Proof of Theorem 2.

- Suppose that  $\{R_\alpha\}_\alpha$  is uniformly bounded, then since  $\lim_{\alpha \rightarrow 0} R_\alpha(u) = A^\dagger u$  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.

□

## No uniform boundedness of regularisers

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

### 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  $Bg = \lim_{\alpha \rightarrow 0} AR_\alpha g$  for all  $g \in \mathcal{V}$ .

What can we say about  $B$ ? For any  $g \in \mathcal{D}(A^\dagger)$ ,  $AR_\alpha g \rightarrow AA^\dagger g = P_{\overline{\mathcal{R}(A)}}g = Bg$ . 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,  $Bf = P_{\overline{\mathcal{R}(A)}} f = \lim_{n \rightarrow \infty} AR_{\alpha_{k_n}} f = Au$ .
- 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.

□

## Parameter choice

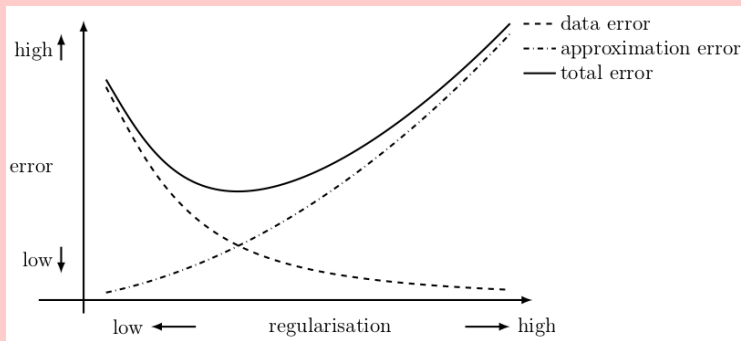
**Want:** as  $\delta \rightarrow 0$ ,  $R_\alpha(f_\delta) \rightarrow A^\dagger f$ , for all  $f \in \mathcal{D}(A^\dagger)$  and  $f_\delta$  s.t.  $\|f - f_\delta\| \leq \delta$ .

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

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



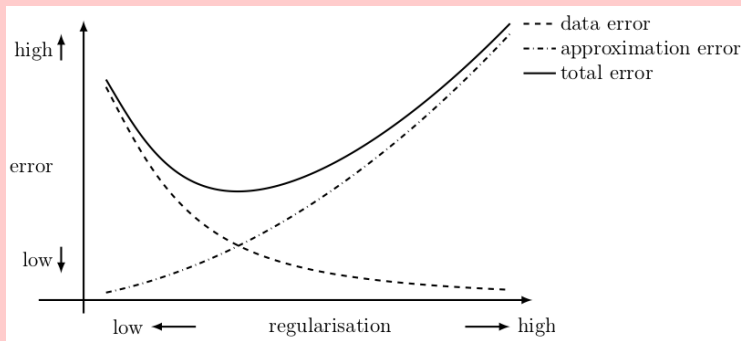
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The regularisation parameter need to be chosen to balance the two terms!

### Definition 5

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

- (a) a priori parameter choice rules which depend only on  $\delta$ ,
- (b) a posteriori parameter choice rules which depend on both  $\delta$  and  $f_\delta$ .
- (c) heuristic parameter choice rules which depend on  $f_\delta$  only.

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

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

then  $(R_\alpha, \alpha)$  is called a **convergent regularisation**.



### Theorem 6

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

- (a)  $\alpha(\delta) \rightarrow 0$  as  $\delta \rightarrow 0$ .
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Clearly, if (a) and (b) are satisfied, then for all  $\|f_\delta - f\| \leq \delta$ ,  
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This means: taking a sequence  $\delta_k \rightarrow 0$ , for each  $\delta_k$ , there exists  $c > 0$  and  $f_{\delta_k}$  with  $\|f_{\delta_k} - f\| \leq \delta_k$  such that  $\|R_{\alpha(\delta_k)}(f_{\delta_k} - f)\| \geq c$ .

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So:

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

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

Regularisation Theory

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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  $j \rightarrow \infty$ .

**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  $g_\alpha : (0, \infty) \rightarrow (0, \infty)$  such that

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

## Theorem 7 (Mild growth of $g_\alpha$ will ensures regularisation of $A^\dagger$ )

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

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



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

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

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

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By the reverse Fatou's lemma

$$\begin{aligned} \limsup_{\alpha \rightarrow 0} \|R_\alpha f - A^\dagger f\|^2 &\leq \limsup_{\alpha \rightarrow 0} \sum_j (\sigma_j g_\alpha(\sigma_j) - 1)^2 \left| \langle A^\dagger f, u_j \rangle \right|^2 \\ &\leq \sum_j \limsup_{\alpha \rightarrow 0} (\sigma_j g_\alpha(\sigma_j) - 1)^2 \left| \langle A^\dagger f, u_j \rangle \right|^2 = 0. \end{aligned}$$

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The claim on convergent regularisation is from Theorem 6 since  $\|R_{\alpha(\delta)}\| \leq C_{\alpha(\delta)}$ .

# Truncated singular value decomposition

**Truncated SVD:** discard all singular values below threshold  $\alpha$ :

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

We then have

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

This is always well-defined for compact operators (zero is the only accumulation point of singular values).

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

We then have

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

This is always well-defined for compact operators (zero is the only accumulation point of singular values).

**Is this a convergent regularisation of  $A^{\dagger}$ ?**

For all  $\sigma > 0$ , we naturally have  $\lim_{\alpha \rightarrow 0} g_{\alpha}(\sigma) = \frac{1}{\sigma}$ .

We have  $\sup_{\sigma, \alpha} \sigma g_{\alpha}(\sigma) = 1$  and  $C_{\alpha} = \alpha^{-1}$ .

So, the truncated SVD is a convergent regularisation if  $\lim_{\delta \rightarrow 0} \frac{\delta}{\alpha(\delta)} = 0$ .

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So, the truncated SVD is a convergent regularisation if  $\lim_{\delta \rightarrow 0} \frac{\delta}{\alpha(\delta)} = 0$ .

**Disadvantage:** requires the knowledge of the singular vectors of  $A$  (only finitely many, but this number might be large).

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  $\sigma > 0$ ,  $\lim_{\alpha \rightarrow 0} g(\sigma) = \frac{1}{\sigma}$ . We again have  $\sup_{\alpha, \sigma} \sigma g_\alpha \leq 1$  and since  $0 \leq (\sigma - \sqrt{\alpha})^2 = \sigma^2 - 2\sigma\sqrt{\alpha} + \alpha$ , we get  $\sigma^2 + \alpha \geq 2\sigma\sqrt{\alpha}$  which implies that

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

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

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



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## **This is easy to compute:**

Note that  $\sigma_j^2$  are the eigenvalues of  $A^*A$  and  $\sigma_j^2 + \alpha$  are the eigenvalues of  $A^*A + \alpha \text{Id}$ . So, for  $u_\alpha = R_\alpha f$ , we have

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

So, we just need to invert this (well-posed) linear system. Knowledge of  $\sigma_j$ '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  $\|f - f^\delta\| \leq \delta$  for some  $\delta > 0$ :

## Theorem 8

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

$$\|Au_\alpha - Au_\alpha^\delta\|_{\mathcal{V}} \leq \gamma\delta \quad \text{and} \quad \|u_\alpha - u_\alpha^\delta\|_{\mathcal{U}} \leq C_\alpha\delta.$$

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

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Proof:

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

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

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

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

$$\text{implies } \|u_\alpha - u_\alpha^\delta\| \leq C_\alpha\delta.$$

We have bounded the data error, but for the approximation error  $\|u^\dagger - u_\alpha\|$  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  $u^\dagger = (K^* K)^\mu w$ . 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  $(Au)(y) = \int_0^y u(x) dx$ . For  $\mu = 1$ , the source condition says that

$$u^\dagger(x) = \int_x^1 \int_0^y w(z) dx dy$$

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

## The source condition

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

Then

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

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

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



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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  $\sigma \geq \alpha$ . So,

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

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

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

Regularisation Theory

Spectral regularisation

More on parameter choice rules

Iterative regularisation

### 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  $(R_\alpha, \alpha)$  is a convergent regularisation.*

## A priori parameter choice rules

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### Proof.

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

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

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



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

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

for all  $f_\delta$  with  $\|f - f_\delta\| \leq \delta$ .

□

## A posteriori parameter choice rules

We may want a parameter choice rule which takes the approximate data  $f_\delta$  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:

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

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It may be hard to estimate  $\mu$  in practice, but if  $\mathcal{R}(A)$  is dense in  $\mathcal{V}$ , then  $\mu = 0$ .

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- In practice, pick a null sequence  $\{\alpha_j\}_j$  and iteratively compute  $u_{\alpha_j} \stackrel{\text{def.}}{=} R_{\alpha_j} f_\delta$  for  $j = 1, \dots, j^*$ , until  $u_{\alpha_{j^*}}$  satisfies Morozov's discrepancy principle.

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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  $(R_\alpha, \alpha)$  is a convergent regularisation. Then,  $A^\dagger$  is continuous from  $\mathcal{V} \rightarrow \mathcal{U}$ .*

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If we have a convergent regularisation, then

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

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



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Taking any sequence  $f_j \in \mathcal{D}(A^\dagger)$  which converges to  $f \in \mathcal{D}(A^\dagger)$ ,  
 $\lim_{j \rightarrow \infty} A^\dagger f_j = \lim_{j \rightarrow \infty} R_{\alpha(f_j)} f_j = A^\dagger f$ . 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.** Choose  $\alpha(f^\delta)$  as

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

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

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So,  $\|Au^\dagger - Au_\alpha^\delta\| \lesssim \alpha + \delta$ .

The optimal choice is  $\alpha \sim \delta$ . Note that  $\delta = \operatorname{argmin}_\alpha \frac{(\alpha + \delta)}{\sqrt{\alpha}}$ .

# The L-Curve

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

- $\|Au_{\alpha}^{\delta} - Au^{\dagger}\| \leq \sqrt{\sum_j |g_{\alpha}(\sigma_j)\sigma_j - 1|^2 \sigma_j^2 |\langle u^{\dagger}, u_j \rangle|^2} + \gamma\delta$
- $\|u_{\alpha}^{\delta} - u^{\dagger}\| \leq \sqrt{\sum_j |g_{\alpha}(\sigma_j)\sigma_j - 1|^2 |\langle u^{\dagger}, u_j \rangle|^2} + C_{\alpha}\delta.$

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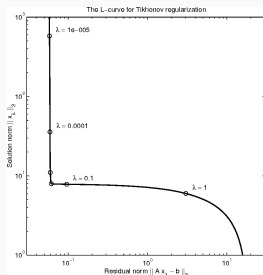
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Plotting  $\log \|Au_{\alpha} - f_{\delta}\|$  against  $\log(\|u_{\alpha}\|)$  for varying  $\alpha$  gives an L-curve.

**L-Curve.** Choose

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

## Generalized Cross Validation

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

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

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

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**Generalised Cross Validation:**  $h_{ii}$  depends on the way you order the rows of  $A$ . To remove this dependence, take the average of  $h_{ii}$ 's:

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

$$\alpha_* = \operatorname{argmin}_\alpha \frac{\|A u_\alpha - f\|^2}{(m - \sum_{i=1}^n \lambda_i)^2}$$

Regularisation Theory

Spectral regularisation

More on parameter choice rules

**Iterative regularisation**

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

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



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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,  $\|Au^{k+1} - f\|_{\mathcal{V}} \leq \|Au^k - f\|_{\mathcal{V}}$ , with equality only if  $A^*(Au^k - f) = 0$ .

## Landweber iteration: Choosing the stepsize

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

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

# Landweber iteration is a form of spectral regularisation

By induction we have

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

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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

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

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

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Note that  $R_k$  is a linear regulariser and

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

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



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## Regularisation and convergence

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

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Recall that we need  $g_k(\sigma) \leq C_k$  and  $\lim_{\delta \rightarrow 0} \delta C_k = 0$ . From applying  $e^{-x} \geq 1 - x$  twice, we have

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

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

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  $\|u^k - u^\dagger\| \rightarrow 0$ .
- (ii) If  $f \notin \mathcal{D}(A^\dagger)$ , then  $\|u^k\| \rightarrow \infty$ .
- (iii) If  $\lim_{\delta \rightarrow 0} k_*(\delta)\delta = 0$ , then  $\|u^{k_*(\delta)} - u^\dagger\| \rightarrow 0$  as  $\delta \rightarrow 0$ , when doing Landweber iteration on  $f_\delta$  such that  $\|f_\delta - f\| \leq \delta$  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  $f = Au^\dagger$ ,

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

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

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

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

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

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

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

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

## Error bounds

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

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,

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

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

For (ii), recall that  $u_k = R_k(f) \stackrel{\text{def.}}{=} \tau \sum_{j=0}^{k-1} (\text{Id} - \tau A^* A)^j A^* f$  and

$\text{Id} - (\text{Id} - \tau A^* A)^k = \tau A^* A \sum_{\ell=0}^{k-1} (\text{Id} - \tau A^* A)^\ell$ . So,  $u_k - u_k^\delta = R_k(f - f_\delta)$ . Now,

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

Therefore,

$$\|u_k - u_k^\delta\| \leq \sqrt{k\tau} \|f - f_\delta\| \leq \sqrt{k\tau} \delta.$$

# Mozorov's discrepancy principle

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

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

## Lemma 4.3

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

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

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

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



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

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

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

Note that

- $\|- \tau A^* Au_\delta^k + \tau A^* f_\delta\|^2 \leq \tau^2 \|A\|^2 \|Au_\delta^k - f_\delta\|^2$
- $2\tau \langle -Au_\delta^k + f_\delta, Au_\delta^k - f \rangle = -2\tau \|Au_\delta^k + f_\delta\|^2 + 2\tau \langle -Au_\delta^k + f_\delta, f_\delta - f \rangle$

# Mozorov's discrepancy principle

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

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

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

Note that

- $\|- \tau A^* Au_\delta^k + \tau A^* f_\delta\|^2 \leq \tau^2 \|A\|^2 \|Au_\delta^k - f_\delta\|^2$
- $2\tau \langle -Au_\delta^k + f_\delta, Au_\delta^k - f \rangle = -2\tau \|Au_\delta^k + f_\delta\|^2 + 2\tau \langle -Au_\delta^k + f_\delta, f_\delta - f \rangle$

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

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

- 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.