1. First kind Fredholm integral equation provides a linear model for inverse problem analysis.

2. The SVE provides a means to analyse stability and existence of solutions.

3. Picard condition is necessary for existence of solution which is square integrable.

4. Right hand side \( g \) must be sufficiently smooth as measured by its SVE coefficients.

5. For more general inverse problems, e.g. Laplace transform, the operator is not compact, but a similar analysis for continuum of singular values can be applied.

6. Most cases we cannot calculate the SVE.
Solution with the SVD - defined as for the SVE
Discretizing the Integral
Using the SVD for the SVE
Spectral Filtering
Errors Rosemary Renaut
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Consider general overdetermined discrete problem

\[ Ax = b, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^{m}, \quad x \in \mathbb{R}^{n}, \quad m \geq n. \]

Thin singular value decomposition (SVD) of rectangular \( A \) is

\[ A = U \Sigma V^T = \sum_{i=1}^{n} u_i \sigma_i v_i^T, \quad \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n). \]

\( U \) of size \( m \times n \), \( V \) and \( \Sigma \) square of size \( n \):

\[ U = [u_1, \ldots, u_n], \quad V = [v_1, \ldots, v_n], \quad \sigma_1 \geq \sigma_2 \geq \sigma_n \geq 0 \]

Orthonormal columns in \( U \) and \( V \), left and right singular vectors for \( A \)

\[ u_i^T u_j = v_i^T v_j = \delta(i - j) \rightarrow U^T U = V^T V = V V^T = I_n. \]

If \( A \) has full column rank \( \sigma_n > 0 \)

\[ A^\dagger = V \Sigma^{-1} U^T = A^{-1}, \quad m = n. \]
Moore Penrose Generalized Inverse

1. \( AA^\dagger A = A \)
2. \( A^\dagger AA^\dagger = A^\dagger \)
3. \( (AA^\dagger)^* = AA^\dagger \)
4. \( (A^\dagger A)^* = A^\dagger A \)
Deriving the Solution: Similarly to SVE

1. We can write \( \mathbf{x} = \mathbf{V} \mathbf{V}^T \mathbf{x} = \sum_{i=1}^{n} (\mathbf{v}_i^T \mathbf{x}) \mathbf{v}_i \) and

   \[ \mathbf{A} \mathbf{x} = \sum_{i=1}^{n} (\mathbf{v}_i^T \mathbf{x}) \mathbf{A} \mathbf{v}_i \]

2. But \( \mathbf{A} \mathbf{v}_i = \mathbf{U} \Sigma \mathbf{V}^T \mathbf{v}_i = \mathbf{U} \Sigma \mathbf{e}_i = \sigma_i \mathbf{u}_i \). Thus

   \[ \mathbf{A} \mathbf{x} = \sum_{i=1}^{n} \sigma_i (\mathbf{v}_i^T \mathbf{x}) \mathbf{u}_i \]

3. Similarly, for \( m = n \), \( \mathbf{b} = \sum_{i=1}^{n} (\mathbf{u}_i^T \mathbf{b}) \mathbf{u}_i \).

4. Immediately compare coefficients and obtain

   \( \sigma_i (\mathbf{v}_i^T \mathbf{x}) = \mathbf{u}_i^T \mathbf{b}, \ i = 1, \ldots, n \) and

   \[ \mathbf{x} = \sum_{i=1}^{n} \frac{(\mathbf{u}_i^T \mathbf{b})}{\sigma_i} \mathbf{v}_i \]

5. Sensitivity of solutions depends on \( \text{cond}(\mathbf{A}) = \sigma_1 / \sigma_n \)
Let $U = [U_1, U_2]$ be square of size $m$, $\Sigma$ rectangular of size $m \times n$:

$$A = U \Sigma V^T = [U_1, U_2] \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^T$$

The inverse is replaced by the pseudo inverse: if $A$ has rank $r$

$$A^\dagger = \sum_{i=1}^{r} \frac{1}{\sigma_i} v_i u_i^T$$

Solution of the LS problem is given by

$$x = \sum_{i=1}^{r} \frac{(u_i^T b)}{\sigma_i} v_i$$

Sensitivity of solution depends on the condition as measured by $\sigma_1/\sigma_r$.

Recall singular values relation to eigenvalues $\lambda_i$ of $A^T A$, $\sigma_i^2 = \lambda_i$
Quadrature - how do we obtain $A$

Need to understand how we go from integral to matrix.

Integral Equation \[ < h, f > = g \]
Discrete Form \[ A\mathbf{x} = \mathbf{b} \]

Quadrature to evaluate the integral (finite range $[a, b] \rightarrow [0, 1]$)

\[
\int_{0}^{1} p(t)dt = \sum_{j=1}^{n} \omega_j p(t_j) + E_n(p)
\]

- $E_n$ is the error which depends on $n$ and the function $p$.
- $t_j$ are the abscissae, $\omega_j$ are weights for the rule.

For $< h, f > = g$, $p(t) = h(s, t)f(t)$. Thus

\[
\sum_{j=1}^{n} \omega_j h(s_i, t_j)f(t_j) = g(s_i) + E_n(s_i), \quad i = 1 \ldots m.
\]

Notice error depends also on the collocation point $s_i$. 
Neglecting $E$ and setting $\tilde{x}$ as the approximation to $x$ we obtain

$$\sum_{j=1}^{n} \omega_j h(s_i, t_j)\tilde{x}_j = g(s_i), \quad i = 1 \ldots m.$$ 

Thus defining $A = HD$, where

- $D$ is a diagonal matrix $d_{jj} = \omega_j$
- $H_{ij} = h(s_i, t_j)$

$$A\tilde{x} = b$$

We could solve for scaled $x$ say $\tilde{x} = D^{-1}\bar{x}$.

Given $b^{(m)}$ i.e. of length $m$ we obtain $x^{(n)}$ of length $n$.

What do we use for the weights $\omega_j$ and abscissae $t_j$?

Trapezium rule etc. are collocation based methods. Give values of $f$ at discrete $t_j$.

Expansion methods provide an expression for $f(t)$.
Galerkin Approach

SVE expands $f$ and $g$ in terms of basis functions and coefficients $g_i, f_j$.

\[ g^{(m)} \in \text{span}\{\psi_1(s), \psi_2(s), \ldots, \psi_m(s)\} \quad f^{(n)} \in \text{span}\{\phi_1(s), \phi_2(s), \ldots, \phi_n(s)\} \]

\[ g^{(m)}(s) = \sum_{i=1}^{m} g_i \psi_i(s), \quad f^{(n)}(t) = \sum_{j=1}^{n} f_j \phi_j(t) \quad \text{integrate} \]

\[ g(s) = \int_0^1 h(s, t)f(t)dt \approx \int_0^1 h(s, t)\sum_{j=1}^{n} f_j \phi_j(t)dt := \theta(s) \]

$g(s) - \theta(s)$ is the residual. Galerkin approach require $\theta(s) - g(s)$ orthogonal to span\{\psi_1(s), \ldots, \psi_m(s)\}

\[ <\psi_i(s), \theta(s) - g(s)> = 0 \quad i = 1 \ldots m \]

Hence $<\psi_i, \theta> = <\psi_i, g>$ \quad $i = 1 \ldots m$ gives

\[ <\psi_i, g> = <\psi_i, \theta> = \sum_{j=1}^{n} f_j <\psi_i(s), \int_0^1 h(s, t)\phi_j(t)dt > \]

\[ = \sum_{j=1}^{n} \left( \int_0^1 \int_0^1 h(s, t)\psi_i(s)\phi_j(t)dsdt \right) f_j \]
The integration defines $A$ and right hand side $b$ by

$$A_{ij} = \int_0^1 \int_0^1 h(s, t) \psi_i(s) \phi_j(t) ds dt, \quad b_i = <\psi_i, g>$$

Requires numerical quadrature for

$$\int_0^1 \int_0^1 h(s, t) \psi_i(s) \phi_j(t) ds dt \; \forall (i, j), \quad b_i = \int_0^1 \psi_i(s) g(s) ds, \; \forall i$$

If $h(s, t)$ is symmetric $h(s, t) = h(t, s)$; use $\phi_i(s) = \psi_i(s)$. Then $A$ is symmetric.

Consider the case $\phi_i = \psi_i = \rho_i$ where $\rho_i$ is the top hat

$$\rho_i(t) = \begin{cases} \frac{1}{\sqrt{h}} & t \in [(i - 1)h, ih] \\ 0 & \text{otherwise} \end{cases}$$

$$A_{ij} = \frac{1}{h} \int_{(i-1)h}^{ih} \int_{(j-1)h}^{jh} h(s, t) ds dt \quad b_i = \frac{1}{\sqrt{h}} \int_{(i-1)h}^{ih} g(s) ds$$
Sampling

$g$ is sampled at $s_i$, thus

$$g(s_i) = \int_0^1 \delta(s - s_i) g(s) \, ds$$

suggests $\psi_i(s) = \delta(s - s_i)$ and

$$A_{ij} = \int_0^1 \int_0^1 h(s, t) \delta(s - s_i) \phi_j(t) \, ds \, dt = \int_0^1 h(s_i, t) \phi_j(t) \, dt$$

so that the quadrature is reduced to one dimensional.

Sampling can also be implemented with the top hat and then

$$A_{ij} = \frac{1}{\sqrt{h}} \int_0^1 \phi_j(t) \left( \int_{(i-1)h}^{ih} h(s, t) \, ds \right) \, dt, \quad b_i = \sqrt{h}g(s_i)$$
Idea: calculate an approximate SVE numerically via the SVD. Given the SVD how are the relevant components $u_j, v_j$ (columns of $U$ and $V$) and $\sigma_j$ related to SVE basis functions $u_i(s), v_i(t)$, singular values $\mu_i$.

Discrete matrix $A$ depends on $\psi_i, i = 1, \ldots m$ and $\phi_j, j = 1 \ldots n$.

Continuous kernel $h$ depends on $\psi_i, \phi_j, (i, j) = 1 \ldots \infty$.

Consider the approximate kernel $\tilde{h}$ which is obtained by using the discrete set $\psi_i, i = 1 \ldots n$ and $\phi_j, j = 1 \ldots n$.

The result relates SVD of $A$ to SVE of $\tilde{h}$.
Suppose that matrix $A$ is calculated using the expansion method with functions $\psi_i, \phi_j, i, j = 1, \ldots n$. Calculate its SVD: $\Sigma = \text{diag}(\sigma_i), U = (u_{ij}), V = (v_{ij})$

Let $\tilde{u}_j^{(n)}(s) := \sum_{i=1}^{n} u_{ij} \psi_i(s), \tilde{v}_j^{(n)}(t) := \sum_{i=1}^{n} v_{ij} \phi_i(t), j = 1 : n$.

**Theorem** $\sigma_j^{(n)}, \tilde{u}_j^{(n)}, \tilde{v}_j^{(n)}$ are exact singular values and functions of degenerate kernel $h(s, t) := \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \psi_i(s) \phi_j(t)$

i.e. we have SVE for an approximate kernel - how does that relate to the exact kernel?

$$h(s, t) = \sum_{i} \mu_i u_i(s) v_i(t)$$
Limits with $n$, $\sigma_j^{(n)}$

SVD of $A^{(n)} = U^{(n)} \Sigma^{(n)} (V^{(n)})^T$

Error of the kernel: $\delta_n^2 := \|h - \tilde{h}\|^2 = \|h\|^2 - \|A\|^2_F$

Note $\| \cdot \|_F^2$ is the Frobenious norm $\|A\|^2_F = \sum_{i,j=1}^n a_{ij}^2$

Singular values converge $\sigma_i^{(n)} \leq \sigma_i^{(n+1)} \leq \mu_i$, $i = 1, \ldots, n$.

Errors are bounded $0 \leq \mu_i - \sigma_i^{(n)} \leq \delta_n$, $i = 1, \ldots, n$.

Hence if $\delta_n \to 0$ with $n$ increasing, approximate singular values converge uniformly to true singular values.

$$\text{SSE} \sum_{i=1}^n [\mu_i - \sigma_i^{(n)}]^2 \leq \delta_n^2.$$  

Estimation of $\delta_n$ from $\|h\|^2$

Orthonormality $\tilde{u}_i^{(n)}$, $\tilde{v}_i^{(n)}$ are orthonormal. Convergence

$$\max\{\|u_i - \tilde{u}_i^{(n)}\|, \|v_i - \tilde{v}_i^{(n)}\|\} \leq \left(\frac{2\delta_n}{\mu_i - \mu_{i+1}}\right)^{1/2}$$

Practically observe that approximate singular values are more accurate than approximate singular functions.
Significance of the Result

\[ \langle \tilde{u}_j^{(n)}, g^{(n)} \rangle \] is important in the Picard condition.

\[
\langle \tilde{u}_j^{(n)}, g^{(n)} \rangle = \int_0^1 \left( \sum_{i=1}^n u_{ij}^{(n)} \psi_i(s) \right) \left( \sum_{k=1}^n b_k \psi_k(s) \right) ds \\
= \sum_{i,k} u_{ij}^{(n)} b_k \langle \psi_i, \psi_k \rangle = \sum_i u_{ij}^{(n)} b_i = u_j^T b
\]

SVD and approximate inner products are related.
i.e. the exact inner products \( \langle u_j, g \rangle, i = 1, \ldots, \) are approximated by \( \langle u_j^{(n)}, g^{(n)} \rangle \) which is immediately obtained from the SVD for \( A \).

Discrete Picard Condition

Let \( \tau \) denote the level such that

\[ \forall j > r, \sigma_j \approx O(\tau), \] due to noise and rounding. The discrete Picard condition is satisfied if for \( j \leq r \) the coefficients \( |(u_j^{(n)})^T b| \) decay faster than \( \sigma_j \).

Picard condition applies only for \( \sigma_j > O(\tau) \). It is a condition on the size of the inner products \( (u_j^{(n)})^T b \) for \( j \leq r \).
Discrete Solution approximates Continuous Solution

\begin{align*}
\text{SVE Solution} & \quad \text{SVD Solution} \\
\quad f(t) = \sum_j \frac{\langle u_j, g \rangle}{\mu_j} v_j(t) & \quad \tilde{x} = \sum_{j=1}^n \frac{\langle u_j^{(n)}, b \rangle}{\sigma_j} v_j^{(n)}
\end{align*}

But \( \langle u_j^{(n)}, b \rangle = \langle \tilde{u}_j^{(n)}, g^{(n)} \rangle \) where \( \tilde{u}_j^{(n)} \) tends to \( u_j \) with increasing \( n \), while \( \sigma_j^{(n)} \) converges to \( \mu_j \) with \( n \).

Equivalently, if the discretization with increasing \( n \) is sufficiently good, the approximate solution obtained from the SVD is essentially independent of the discretization.

For solving the first kind Fredholm integral equation numerically, the coefficients \((u_j^{(n)})^T b\) and singular values \(\sigma_j\) reveal important information about the true quantities \(\langle u_j, g \rangle\) and \(\mu_j\).
Summary Approach - see Hansen for more details/examples

For increasing $n$ until converged
1. Choose the orthonormal basis functions $\psi_i(s)$ and $\phi_i(t)$.
2. Calculate matrix $A$ with entries $a_{ij} = \langle \psi_i, h\phi_j \rangle$,
   $i, j = 1, \ldots, n$.
3. Compute SVD of $A$
4. Estimate the singular functions $\tilde{u}_j(s)$ and $\tilde{v}_j(t)$

Test Convergence of set of singular values.

End For
Is square integrable required for the theory?

Consider solving for $f$ from the Laplace transform

$$g(s) = \int_0^\infty e^{-st} f(t) \, dt$$

Kernel $e^{-st}$ is not square integrable:

$$\int_0^a (e^{-st})^2 \, ds = \int_0^a e^{-2st} \, ds = \frac{1 - e^{-2ta}}{2t} \to \frac{1}{2t} \text{ for } a \to \infty$$

But $\int_0^\infty t^{-1}$ is infinite, $\int_0^\infty \int_0^\infty (e^{-st})^2 \, ds \, dt$ is infinite. No SVE

Now $f(t)$ bounded for $t \to \infty$ implies $g(s)$ is bounded $\forall s \geq 0$.

Truncation for large $a$ in Laplace transform introduces small error in $g$, and $g$ decays with $s$. We obtain integral equation

$$\int_0^a e^{-st} f(t) \, dt = g(s), \quad 0 \leq s \leq a.$$ 

Now the kernel is square integrable.

Pick $a$ and increase $n$, the SVD converges.

Pick $n$ and increase $a$, the SVD does not converge.

Demonstrates the lack of SVE for the Laplace Transform.
Solution for Noisy Data

- Denote noise by $e$ or $\text{array}(e) = E$.
- Spectral decomposition acts on the noise term in the same way it acts on the exact right hand side $b$. e.g.

$$x = \sum_{i=1}^{r} \left( \frac{u_i^T(b_{\text{exact}} + e)}{\sigma_i} \right) v_i = x_{\text{exact}} + \sum_{i=1}^{r} \left( \frac{u_i^T e}{\sigma_i} \right) v_i$$

- If $e$ is uniform, anticipate $|u_i^T e|$ of similar magnitude $\forall i$.
- Can only recover components that arise from $|u_i^T b|$ greater than the noise level.
- But anticipate $\sigma_i \rightarrow 0$. $\sigma_i$ small represents high frequency component in the sense that $u_i$, $v_i$ have more sign changes as $i$ increases.
- $\left( \frac{u_i^T e}{\sigma_i} \right)$ is the coefficient of $v_i$ in the error image.
- If $1/\sigma_i$ large the contribution of the high frequency error is magnified due to $\left( \frac{u_i^T e}{\sigma_i} \right)$. 
Truncating the SVD expansion

The SVD expansion shows the impact of the noise on the calculation of \( \mathbf{x} = \sum_{i=1}^{r} (\frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i}) \mathbf{v}_i \). Therefore it seems reasonable to consider the truncated solution

\[
\mathbf{x}_k = \sum_{i=1}^{k} (\frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i}) \mathbf{v}_i = A_k \mathbf{b}
\]

Here \( A_k \) is a rank \( k \) matrix.

- The use of the truncated expansion is feasible only if we can first calculate the SVD of \( A \) efficiently.
- The limit on the sum \( k \) is regarded as a regularization parameter. We can change \( k \) and obtain different solutions.
- Choice of \( k \) controls the degree of low pass filtering which is applied. i.e. controls the attenuation of the high frequency components.
- Look at the example: the image is over or under smoothed dependent on \( k \).
Example of Truncated SVD

Example from Hansen, Nagy and O’Leary, Fig 5.1
Notice under or over smoothing is dependent on choice of $k$ in the TSVD

Figure 5.1. Exact image (top left) and three TSVD solutions $x_k$ to the image deblurring problem, computed for three different values of the truncation parameter: $k = 658$ (top right), $k = 2813$ (bottom left), and $k = 7243$ (bottom right). The corresponding solutions range from oversmoothed to undersmoothed, as $k$ goes from small to large values.
Results suggest that we need information on SVD of $A$
Also need information on the spread of the singular values.
Ideally information on the noise level in the data is available.
Practically we need the \textbf{numerical} rank of $A$.
Practically it is not always viable to find the effective numerical rank
We turn to other methods to find acceptable solutions.
The Filtered SVD - more general than truncation

The truncated SVD is a special case of spectral filtering. Recall \( x = A^\dagger b = V\Sigma^\dagger U^T b \).

The filtered solution is given by

\[
\begin{align*}
x_{\text{filt}} &= \sum_{i=1}^{r} \gamma_i \left( \frac{u_i^T b}{\sigma_i} \right) v_i = V\Sigma_{\text{filt}}^\dagger U^T b, \\
\Sigma_{\text{filt}}^\dagger &= \text{diag}(\gamma_i \sigma_i, 0_{m-r})
\end{align*}
\]

i.e

\[
x = V\Gamma\Sigma^\dagger U^T b,
\]

where \( \Gamma \) is the diagonal matrix with entries \( \gamma_i \).

Notice again the relationship with the SVE - filter out the terms which are noise contaminated.

\( \gamma_i \approx 1 \) for large \( \sigma_i \), \( \gamma_i \approx 0 \) for small \( \sigma_i \)

Spectral filtering is used to filter the components in the spectral basis, such that noise in signal is damped.

How to chose filter factors \( \gamma_i \)?

Truncated SVD takes \( \gamma_i = 1 \), \( 1 \leq i \leq k \) and 0 otherwise to obtain solution \( x_k \).
Regularization by Spectral Filtering \( \mathbf{x}_{\text{filt}} = \sum_{i=1}^{r} \gamma_i \left( \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \right) \mathbf{v}_i \)

- **Tikhonov** \( \gamma_i = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2} \), \( i = 1 \ldots r \), \( \lambda \) is the regularization parameter, and solution is

\[
\mathbf{x}_\lambda = \arg \min_{\mathbf{x}} \{ \| \mathbf{b} - A\mathbf{x} \|^2 + \lambda^2 \| \mathbf{x} \|^2 \}
\]

- Regularized solution trades of \( \| \mathbf{x} \|^2 \) against \( \| \mathbf{b} - A\mathbf{x} \|^2 \).

- Notice

\[
\gamma_i = \begin{cases} 
1 - \left( \frac{\lambda}{\sigma_i} \right)^2 + O(|\frac{\lambda}{\sigma_i}|^4) & \sigma_i \gg \lambda \\
\left( \frac{\sigma_i}{\lambda} \right)^2 + O(|\frac{\sigma_i}{\lambda}|^4) & \sigma_i \ll \lambda
\end{cases}
\]

- If \( \lambda \in [\sigma_r, \sigma_1] \), \( \gamma_i \approx 1 \) for small \( i \), and \( \gamma \approx (\sigma_i/\lambda)^2 \) for large \( i \) (small \( \sigma_i \))

- **Conclude** Parameter \( \lambda \) controls the filtering. If \( \lambda \approx \gamma_k \), then filtered solution does not include components related to \( \sigma_{k+1} \ldots \sigma_r \).

- **Moreover** it is sensible to keep \( \lambda \in [\sigma_r, \sigma_1] \).
Again, now noting error in \( \mathbf{b} = \mathbf{b}_{\text{exact}} + \mathbf{e} \)

\[
\mathbf{x}_{\text{filt}} = V\Sigma_{\text{filt}}^\dagger U^T (\mathbf{b}_{\text{exact}} + \mathbf{e})
\]
\[
= V\Sigma_{\text{filt}}^\dagger U^T (U\Sigma V^T \mathbf{x}) + V\Sigma_{\text{filt}}^\dagger U^T \mathbf{e}
\]
\[
= V\Gamma V^T \mathbf{x} + V\Gamma\Sigma^\dagger U^T \mathbf{e}
\]

implies \( \mathbf{x} - \mathbf{x}_{\text{filt}} = (I_n - V\Gamma V^T)\mathbf{x} - V\Gamma\Sigma^\dagger U^T \mathbf{e} \)

\( = \) Regularization Perturbation

Error Error

**Regularization Error** due to using \( \Sigma_{\text{filt}} \) in place of \( \Sigma \).

**Perturbation Error** the inverted and filtered noise, consistently zero if \( \Gamma = 0 \).
Size of the Regularization Error

Notice

\[ \| (I_n - V\Gamma V^T)x \|_2^2 = \| (I_n - \Gamma)V^T x \|_2^2, \quad V \text{ orthogonal} \]
\[ = \| (I_n - \Gamma)\Sigma^\dagger U^T b \|_2^2 \]
\[ = \sum_{i=1}^{n} ((1 - \gamma_i) \frac{u_i^T b}{\sigma_i})^2 \]

- $|\frac{u_i^T b}{\sigma_i}|$ decays on average by Picard condition
- For small $i$ ($\sigma_i$ big) $\gamma_i \approx 1$, and $(1 - \gamma_i) \approx 0$. Little error from large $|\frac{u_i^T b}{\sigma_i}|$
- For large $i$ $(1 - \gamma_i) \approx 1$ provides little damping of smaller $|\frac{u_i^T b}{\sigma_i}|$
- Choice of $\Gamma$ controls size of regularization error.