1. The least squares fitting using non-orthogonal basis

We have learned how to find the least squares approximation of a function \( f \) using an orthogonal basis. For example, \( f \) can be approximated by a truncated trigonometric Fourier series or by a truncated series based on orthogonal polynomials. Such series converge fast if \( f(x) \) is smooth.

Now we switch to the case where \( f(x) \) is not necessarily smooth or its values are available only at the given set of points \( x_1, \ldots, x_n \).

Let a function \( f(x) \) is given by the set of values \( \{ f_j, x_j \}_{j=0}^{m-1} \). The values of \( f \) contain noise which makes interpolation not appropriate for finding \( f \) at intermediate points. We want to (i) smooth \( f \) and (ii) be able to find its values in the intermediate points.

Let \( \{ \phi_i \}_{i=0}^{n-1} \) be a set of basis functions. In order to represent \( f \) as their linear combination \( f(x) \approx \sum_{i=0}^{n-1} c_i \phi_i(x) \) we need to solve the following \( m \times n \) system of linear equations

\[
\begin{bmatrix}
\phi_0(x_0) & \phi_1(x_0) & \ldots & \phi_{n-1}(x_0) \\
\phi_0(x_1) & \phi_1(x_1) & \ldots & \phi_{n-1}(x_1) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_0(x_{m-1}) & \phi_1(x_{m-1}) & \ldots & \phi_{n-1}(x_{m-1})
\end{bmatrix}
\begin{bmatrix}
c_0 \\
c_1 \\
\vdots \\
c_{n-1}
\end{bmatrix}
= \begin{bmatrix}
f_0 \\
f_1 \\
\vdots \\
f_{m-1}
\end{bmatrix}.
\]

In the typical case there are many data points and a few basis functions, i.e., \( m \gg n \).

The first question is what is a good set of basis functions? In order to answer this question we need to recall the basic linear algebra concepts.

**Definition 1.** A norm of a matrix is associated with the vector norm \( \| \cdot \| \) is defined as

\[
\| A \| = \max_{x \neq 0} \frac{\| Ax \|}{\| x \|}.
\]

**Exercise** Show that if \( A \) is a symmetric square \( n \times n \) matrix then

\[
\| A \| = \rho(A) = \max_i |\lambda_i|,
\]

where \( \lambda_i \)'s, \( i = 1, \ldots, n \) are its eigenvalues.

**Exercise** Show that if \( A \) is an \( m \times n \) matrix, \( m \geq n \), then

\[
\| A \| = \sqrt{\rho(A^T A)}.
\]

The condition number of a square matrix \( A \) is defined as

\[
\kappa(A) = \| A \| \| A^{-1} \|.
\]
The condition number allows to bound the relative error of the solution \( x \) in terms of the relative error in the data \( b \). Let \( A \) be a square matrix and let \( b \) be the right-hand side. Let \( x \) and \( x + \delta x \) be the solutions of 

\[
Ax = b \quad \text{and} \quad A(x + \delta x) = b + \delta b
\]

respectively, where \( \delta b \) be the perturbation of the right-hand side. Then

\[
\delta x = A^{-1}\delta b, \quad \text{hence} \quad \|\delta x\| \leq \|A^{-1}\|\|\delta b\|.
\]

On the other hand, since \( Ax = b \), we have

\[
\|A\|\|x\| \geq \|b\|. \quad \text{Hence} \quad \|x\| \geq \frac{\|b\|}{\|A\|}.
\]

Therefore,

\[
\frac{\|\delta x\|}{\|x\|} \leq \|A\|\|A^{-1}\|\|\delta b\|/\|b\| \equiv \kappa(A)\|\delta b\|/\|b\|.
\]

Hence, for a good set of basis functions the condition number of the matrix in Eq. (1) is not large. For example, \( \phi_i = x^i \) is a bad set of basis functions. Do not use it unless \( n \) is really small!

Exercise Calculate the condition numbers for the matrix defined in Eq. (1) for \( \phi_i = x^i \) and \( x_j = j/m \). Set \( m = n \) and plot the graph of \( \kappa(A) \) versus \( n \). The matlab function that computed the condition number is \( \text{cond}(A) \).

Since we are going to deal with overdetermined systems of linear equations whose matrices are \( m \times n \) with \( m > n \), we need to define the condition number for a rectangular matrix. A very useful concept in the matrix theory is the singular value decomposition (SVD). We are going to consider it in details.

1.1. Singular Value Decomposition.

**Theorem 1.** Let \( a \) be an arbitrary \( m \times n \) matrix with \( m \geq n \). Then we can write

\[
A = U\Sigma V^T,
\]

where

\[
U \text{ is } m \times n \text{ and } U^TU = I_{n \times n},
\]

\[
\Sigma = \text{diag}\{\sigma_1, \ldots, \sigma_n\}, \quad \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0,
\]

and \( V \) is \( n \times n \) and \( V^TV = I_{n \times n} \).

The columns of \( U, u_1, \ldots, u_n \), are called left singular vectors. The columns of \( V, v_1, \ldots, v_n \), are called right singular vectors. The numbers \( \sigma_1, \ldots, \sigma_n \), are called singular values. If \( m < n \), the SVD is defined for \( A^T \).

The geometric sense of this theorem is the following. Let us view the matrix \( A \) as a map from \( \mathbb{R}^n \) into \( \mathbb{R}^m \):

\[
A : \mathbb{R}^n \to \mathbb{R}^m, \quad x \mapsto Ax.
\]
Then one can find orthogonal bases in $\mathbb{R}^n$, $v_1, \ldots, v_n$, and in $\mathbb{R}^m$, $u_1, \ldots, u_m$ and numbers $\sigma_1, \ldots, \sigma_n$, such that

$$v_j \mapsto \sigma_j u_j, \ j = 1, \ldots, n.$$ 

Then for any $x \in \mathbb{R}^n$ we have:

$$\text{if } x = \sum_{j=1}^n x_j v_j \text{ then } Ax = \sum_{j=1}^n x_j \sigma_j u_j.$$ 

For a rectangular matrix $A$ the condition number is

$$\kappa(A) = \frac{\sigma_{\max}}{\sigma_{\min}},$$

where $\sigma_{\max}$ and $\sigma_{\min}$ are the largest and the smallest singular values of $A$.

**Proof.** We use induction in $m$ and $n$. We assume that the SVD exists for $(m-1) \times (n-1)$ matrices and prove it for $m \times n$. We assume $A \neq 0$; otherwise we take $\Sigma = 0$ and $U$ and $V$ are arbitrary orthogonal matrices.

The basic step occurs when $n = 1$ (since $m > n$). We write

$$A = U \Sigma V^T \text{ with } U = \frac{A}{\|A\|}, \ \Sigma = \|A\|, \ V = 1,$$

where $\|\cdot\|$ is the 2-norm.

For the induction step, choose $v$ so that

$$\|v\| = 1 \text{ and } \|A\| = \|Av\| > 0.$$ 

Let

$$u = \frac{Av}{\|Av\|},$$

which is a unit vector. Choose $\tilde{U}$ and $\tilde{V}$ so that $U = [u, \tilde{U}]$ and $V = [v, \tilde{V}]$ are $m \times n$ and $n \times n$ orthogonal matrices respectively. Now write

$$U^T AV = \begin{bmatrix} u^T \\ \tilde{U}^T \end{bmatrix} \cdot A \cdot \begin{bmatrix} v \\ \tilde{V} \end{bmatrix} = \begin{bmatrix} u^T Av & u^T \tilde{A} \\ \tilde{U}^T Av & \tilde{U}^T \tilde{A} \end{bmatrix}.$$

Then

$$u^T Av = \frac{(Av)^T (Av)}{\|Av\|} = \|Av\| := \sigma$$

and

$$\tilde{U}^T Av = 0 = \tilde{A}^T u \|Av\| = 0.$$ 

We claim that $u^T \tilde{A} \tilde{V} = 0$ too because otherwise

$$\sigma = \|A\| = \|U^T AV\| \geq \|[1, 0, \ldots, 0] U^T AV \sigma u^T \tilde{A} \tilde{V}\| > \sigma,$$

a contradiction. Therefore,

$$U^T AV = \begin{bmatrix} \sigma & 0 \\ 0 & \tilde{U}^T \tilde{A} \end{bmatrix} = \begin{bmatrix} u^T Av & 0 \\ 0 & \tilde{A} \end{bmatrix}.$$
Now we apply the induction hypothesis that
\[ \tilde{A} = U_1 \Sigma_1 V_1^T. \]
Hence,
\[ U^T A V = \begin{bmatrix} \sigma & 0 \\ 0 & U_1 \Sigma_1 V_1^T \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & U_1 \end{bmatrix} \begin{bmatrix} \sigma & 0 \\ 0 & \Sigma_1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & V_1 \end{bmatrix} \]
or
\[ A = \left( U \begin{bmatrix} 1 & 0 \\ 0 & U_1 \end{bmatrix} \right) \begin{bmatrix} \sigma & 0 \\ 0 & \Sigma_1 \end{bmatrix} \left( V \begin{bmatrix} 1 & 0 \\ 0 & V_1 \end{bmatrix} \right)^T, \]
which is our desired decomposition. □

The SVD has a large number of important algebraic and geometric properties, the most important of which are summarized in the following theorem.

**Theorem 2.** Let \( A = U \Sigma V^T \) be the SVD of the \( m \times n \) matrix \( A \), \( m \geq n \).

1. Suppose \( A \) is symmetric and \( A = U \Lambda U^T \) be an eigendecomposition of \( A \). Then the SVD of \( A \) is \( U \Sigma V^T \) where \( \sigma_i = |\lambda_i| \) and \( v_i = u_i \text{sign}(\lambda_i) \), where \( \text{sign}(0) = 1 \).
2. The eigenvalues of the symmetric matrix \( A^T A \) are \( \sigma_i^2 \). The right singular vectors \( v_i \) are the corresponding orthonormal eigenvectors.
3. The eigenvectors of the symmetric matrix \( AA^T \) are \( \sigma_i^2 \) and \( m - n \) zeroes. The left singular vectors \( u_i \) are the corresponding orthonormal eigenvectors for the eigenvalues \( \sigma_i^2 \). One can take any \( m - n \) orthogonal vectors as eigenvectors for the eigenvalue 0.
4. If \( A \) has full rank, the solution of
\[ \min_x \|Ax - b\| \] is \( x = V \Sigma^{-1} U^T b \).
5. \( \|A\| = \sigma_1 \).
   If \( A \) is square and nonsingular, then
   \( \|A^{-1}\| = \frac{1}{\sigma_n} \)
   and
   \[ \kappa(A) = \|A\|\|A^{-1}\| = \frac{\sigma_1}{\sigma_n} \]
6. Suppose \( \sigma_1 \geq \ldots \geq \sigma_r > \sigma_{r+1} = \ldots = \sigma_n = 0 \).
   Then
   \[ \text{rank}(A) = r, \]
   \[ \text{null}(A) = \{ x \in \mathbb{R}^n : Ax = 0 \in \mathbb{R}^m \} = \text{span}(v_{r+1}, \ldots, v_n), \]
   \[ \text{range}(A) = \text{span}(u_1, \ldots, u_r). \]
\( A = U \Sigma V^T = \sum_{i=1}^{n} \sigma_i u_i v_i^T, \)

i.e., \( A \) is a sum of rank 1 matrices. Then a matrix of rank \( k < n \) closest to \( A \) is

\[ A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T, \quad \text{and} \quad \| A - A_k \| = \sigma_{k+1}. \]

**Example** This example illustrates the low rank approximation of a large matrix. The original image is shown in Fig. 1(a). The rank 3, 10, and 20 approximations are shown in Figs. 1 (b), (c), and (d) respectively. The sequence of matlab commands to create an approximation of rank \( m \) for a given image is the following.

![Figures](image1.png)

**Figure 1.** Low rank approximations of image. (a): original; (b): rank 3; (c) rank 10; (d) rank 20.
>> clear all
>> im=imread('IMG_1413.jpg');
>> [m n k]=size(im)
m = 1600
n = 1200
k = 3
>> mimi=zeros(m,n);
>> mimi=sum(im,3);
>> fig=figure;
>> imagesc(mimi)
>> colormap gray
>> set(gca,'DataAspectRatio',[1 1 1])
>> [U S V]=svd(mimi);
>> size(U)
ans = 1600 1600
>> size(V)
ans = 1200 1200
>> size(S)
ans = 1600 1200
>> fig=figure;
>> m=10;
>> rm=U(:,1:m)*S(1:m,1:m)*V(:,1:m)';
>> colormap gray
>> set(gca,'DataAspectRatio',[1 1 1])

1.2. The QR decomposition.

1.2.1. Normal equations. Consider the overdetermined system of linear equations

\[ Ax = b, \quad A_{m \times n}, \quad m \geq n. \]

Definition 2. We say that \( x^* \) is the least squares solution of \( Ax = b \), \( A \) is \( m \times n \), \( m \geq n \), if

\[ x^* = \arg \min_{x \in \mathbb{R}^n} \| Ax - b \|. \]

Now we will show that \( x^* \) is given by the formula

(3) \[ x^* = (A^T A)^{-1} A^T b. \]

Note that \( x^* \) is the solution of the so called normal equation that is obtained from \( Ax = b \) by multiplication by \( A^T \) from the left. If the matrix \( A \) has full rank, i.e., \( \text{rank}(A) = n \), the matrix \( A^T A \) is symmetric positive definite. Write \( x = x^* + e \) and consider \( \| Ax - b \|^2 \). We
want to show that it is minimal if and only if $e = 0$, i.e., $x = x^*$.

$$\|Ax - b\|^2 = (Ax - b)(Ax - b) = (Ax^* + Ae - b)^T(Ax^* + Ae - b) =$$

$$\|Ax\|^2 + \|Ax^* - b\|^2 + 2(Ae)^T(Ax^* - b) =$$

$$\|Ax\|^2 + \|Ax^* - b\|^2 + 2e^T(A^T Ax^* - A^T b) =$$

$$\|Ax\|^2 + \|Ax^* - b\|^2 \geq \|Ax^* - b\|^2$$

The equality occurs if and only if $e = 0$, i.e., the norm $\|Ax - b\|$ is minimal if and only if $x = x^*$ given by Eq. (3).

The geometric sense of the least squares solution is the following: the residual $r := Ax - b$ is orthogonal to the space spanned by the columns of the matrix $A$, i.e., $r$ dotted with any column of $A$ is zero, or

$$A^T r = 0.$$

### 1.2.2. Gram-Schmidt Algorithm.

**Theorem 3.** Let $A$ be $m \times n$, $m \geq n$. Suppose that $A$ has full column rank. Then there exist a unique $m \times n$ orthogonal matrix $Q$, i.e., $Q^T Q = I_{n \times n}$, and a unique $n \times n$ upper-triangular matrix $R$ with positive diagonals $r_{ii} > 0$ such that $A = QR$.

**Proof.** The proof of this theorem is given by the Gram-Schmidt orthogonalization process.

**Algorithm 1:** Gram-Schmidt orthogonalization

<table>
<thead>
<tr>
<th>Input</th>
<th>matrix $A$, $m \times n$, rank($A$) = $n$.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Output</td>
<td>orthogonal matrix $Q$ $m \times n$, $Q^T Q = I_{n \times n}$, and upper-triangular $n \times n$ matrix $R$ with $r_{ii} &gt; 0$.</td>
</tr>
</tbody>
</table>

for $i = 1, \ldots, N$ do

$q_i = a_i$;

for $j = 1, \ldots, i - 1$ do

$$\begin{cases} r_{ji} = q_j^T a_i & \text{CGS} \\ r_{ji} = q_j^T q_i & \text{MGS} \end{cases};$$

$q_i = q_i - r_{ji} q_j$;

end

$r_{ii} = \|q_i\|;$

$q_i = q_i / r_{ii};$

end

Here CGS and MGS stand for the Classic Gram-Schmidt and the Modified Gram-Schmidt respectively.

Unfortunately the Classic Gram-Schmidt algorithm is numerically unstable when the columns of $A$ are nearly linearly dependent. The Modified Gram-Schmidt is better but
still can result in $Q$ that is far from orthogonal (i.e., $\|Q^T - I\|$ is much larger than the machine $\epsilon$) when $A$ is ill-conditioned.

**Exercise** Show that the least squares solution of $Ax = b$ is given by

$$x^* = R^{-1}Q^Tb,$$

where $A = QR$ is the QR decomposition of $A$.

1.2.3. **Householder reflections.** A numerically stable way to perform the QR decomposition is via using the Householder transformations or reflections.

**Definition 3.** A Householder transformation (or reflection) is a matrix of the form $P = I - 2uu^T$ where $\|u\| = 1$.

**Exercise** Show that $P$ is both symmetric and orthogonal, i.e., $P = P^T$ and $PP^T = I$.

The Householder transformation is called reflection because it $Px$ is the reflection of $x$ with respect to the plane normal to $u$.

Given a vector $x$ we can find $u$ such that $P = I - 2uu^T$ zeros out all entries of $x$ except the first one, i.e.,

$$Px = [c, 0, \ldots, 0]^T = ce_1.$$

We do it as follows. Write

$$Px = x - 2u(u^Tx) = ce_1.$$

Hence

$$u = \frac{x - ce_1}{2u^Tx},$$

i.e., $u$ is a linear combination of $x$ and $e_1$. Since

$$\|x\| = \|Px\| = |c|,$$

$u$ is parallel to $\tilde{u} = x \pm \|x\|e_1$. Hence

$$u = \frac{\tilde{u}}{\|\tilde{u}\|}.$$

One can verify that either choice of sign yields a $u$ satisfying $Px = ce_1$ as long as $\tilde{u} \neq 0$. We will stick with $\tilde{u} = x + \text{sign}(x_1)\|x\|e_1$. In summary we have

$$\tilde{u} = \begin{bmatrix} x_1 + \text{sign}(x_1)\|x\| \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \text{with} \quad u = \frac{\tilde{u}}{\|\tilde{u}\|}.$$  

**Example** We will show how to compute the QR decomposition of a 5 x 4 matrix $A$ using the Householder reflections. $x$ denotes a generic nonzero entry of $A$.

(1) Choose $P_1$ so that $A_1 := P_1A = \begin{bmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \\ 0 & x & x & x \end{bmatrix}$.
(2) Choose $P_2 = \begin{bmatrix} 1 & 0_{1\times4} & 0_{1\times4} \\ 0_{4\times1} & P'_2 \\ \end{bmatrix}$ so that $A_2 := P_2A_1 = \begin{bmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & x & x \\ \end{bmatrix}$.

(3) Choose $P_3 = \begin{bmatrix} 1 & 0 & 0_{2\times3} \\ 0 & 1 & P'_3 \\ 0_{3\times2} & P'_3 \\ \end{bmatrix}$ so that $A_3 := P_3A_2 = \begin{bmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & 0 & x \\ \end{bmatrix}$.

(4) Choose $P_4 = \begin{bmatrix} 1 & 0 & 0_{3\times2} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0_{2\times3} & P'_4 \\ \end{bmatrix}$ so that $A_4 := P_4A_3 = \begin{bmatrix} x & x & x & x \\ 0 & x & x & x \\ 0 & 0 & x & x \\ 0 & 0 & 0 & x \\ \end{bmatrix}$.

Now we need to understand how to extract the matrices $Q$ and $R$. Then

$$A_4 = P_4P_3P_2P_1A.$$ 

Therefore

$$A = (P_4P_3P_2P_1)^{-1}A_4 = P_1^{-1}P_2^{-1}P_3^{-1}P_4^{-1}A_4.$$ 

Since $P_j$’s $j = 1, 2, 3, 4$ are symmetric and orthogonal,

$$A = P_1^{-1}P_2^{-1}P_3^{-1}P_4^{-1}A_4 = P_1^TP_2^TP_3^TP_4^TA_4 = P_1P_2P_3P_4A_4.$$ 

On the other hand,

$$A = QR.$$ 

Hence $R$ is the first 4 rows of $A_4$ and $Q$ is the first 4 columns of $P_1^TP_2^TP_3^TP_4^T = P_1P_2P_3P_4$.

In Matlab, the least squares solution of $Ax = b$ is found by $A\backslash b$. The QR decomposition per se can be obtained by $[Q,R]=qr(A)$.

**References**