

# Matrix Computations

## Lecture 2: Least-squares Problems & QR Decomposition

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# Main content

- Least-squares Problems and Applications
- QR Decomposition

# Least-squares Problem and Its Solution

**LS Problem:** Given  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and  $\mathbf{y} \in \mathbb{R}^m$ , solve

$$\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 \quad (\text{LS})$$

## Theorem (LS Optimality Condition)

$\mathbf{x}_{\text{LS}} \in \mathbb{R}^n$  is an optimal solution to the LS problem  $\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2$  if and only if it satisfies the following *normal equation*:

$$\mathbf{A}^T \mathbf{A} \mathbf{x}_{\text{LS}} = \mathbf{A}^T \mathbf{y}. \quad (*)$$

- When  $\mathbf{A}$  has full-column rank, the *unique* solution to  $(*)$  is

$$\mathbf{x}_{\text{LS}} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{y}$$

## Application 1: Polynomial approximation

**Aim:** Given a set of input-output data pairs  $(t_i, y_i) \in \mathbb{R} \times \mathbb{R}$ ,  $i = 1, \dots, N$ , find a polynomial  $p(t) = a_0 + a_1 t + a_2 t^2 + \dots + a_p t^p$  that approximates the data by minimizing the residual  $\sum_{i=1}^N (y_i - p(t_i))^2$ , where  $p \leq N$ .

$$\underbrace{\begin{bmatrix} y_1 \\ \vdots \\ y_t \\ \vdots \\ y_N \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} 1 & t_1 & \cdots & t_1^p \\ 1 & t_2 & \cdots & t_2^p \\ \vdots & & & \vdots \\ 1 & t_N & \cdots & t_N^p \end{bmatrix}}_{=\mathbf{A} \text{ (full rank for distinct } t_i)} \underbrace{\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_p \end{bmatrix}}_{=\mathbf{x}}$$

The polynomial approximation problem can be viewed as

$$\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{y} - \mathbf{Ax}\|_2^2 \longrightarrow \mathbf{x} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{y}$$

## Exercise: Linear prediction

**Aim:** Predict future values of a time-series based on linear prediction. Suppose  $y_t$  is determined by  $y_{t-1}, \dots, y_{t-m}$  at time  $t$ , i.e.,

$$y_t = a_1 y_{t-1} + a_2 y_{t-2} + \dots + a_m y_{t-m}, \quad t = 1, 2, \dots$$

Now given  $y_0, y_1, \dots, y_{99}$  ( $n \geq m$ ), predict  $y_{100}, y_{101}, \dots, y_{199}$  with predictor coefficients  $a_1, a_2, a_3, a_4$ .

*hint: model the linear prediction as a least-square problem*

## Application 2: System identification

**System identification:** Given an input signal block  $\{x_t\}_{t=0}^{T-1}$  and an output signal block  $\{y_t\}_{t=0}^{T-1}$ , find the system impulse response  $\{h_t\}_{t=0}^p$

- Applications: channel estimation in communications, identification of acoustic impulse responses, etc.

$$\underbrace{\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_p \\ \vdots \\ \vdots \\ y_{T-1} \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} x_0 & & & & \\ x_1 & x_0 & & & \\ \vdots & & \ddots & & \\ x_p & \dots & x_1 & x_0 & \\ \vdots & & & \vdots & \\ \vdots & & & \vdots & \\ x_{T-1} & \dots & x_{T-p} & x_{T-1-p} & \end{bmatrix}}_{=\mathbf{X}} \underbrace{\begin{bmatrix} h_0 \\ h_1 \\ \vdots \\ h_p \end{bmatrix}}_{=\mathbf{h}}$$

The system impulse response  $\mathbf{h}$  can be estimated by

$$\min_{\mathbf{h} \in \mathbb{R}^n} \|\mathbf{y} - \mathbf{X}\mathbf{h}\|_2^2 \longrightarrow \mathbf{h} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

## Application 3: Smoothing

**Aim:** Find a smooth signal  $\mathbf{x}$  that approximates a noisy signal  $\mathbf{y}$ .

**Method:** One approach to smooth a noisy signal is based on least squares weighted regularization.

$$\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{y} - \mathbf{x}\|_2^2 + \lambda \|\mathbf{D}\mathbf{x}\|^2 \quad (1)$$

- $\lambda > 0$  a parameter for tuning smoothness. Larger  $\lambda$ , more smooth signal  $\mathbf{x}$ .

- $\mathbf{D} = \begin{bmatrix} 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & & \ddots & \\ & & & 1 & -2 & 1 \end{bmatrix}$ ,  $\mathbf{D}\mathbf{x}$  is a discrete form of the

second-order derivative of  $\mathbf{x}$ , which measures the smoothness of a signal. the signal  $x(n)$ .

- The solution of (1) is  $\mathbf{x} = (\mathbf{I} + \lambda \mathbf{D}^\top \mathbf{D})^{-1} \mathbf{y}$  (setting the derivative to zero ).

## Exercise: Deconvolution

**Deconvolution:** Given an output signal block  $\{y_t\}_{t=0}^{T-1}$  and the system impulse response  $\{h_t\}_{t=0}^p$ , estimate the input signal block  $\{x_t\}_{t=0}^{T-1}$

$$\underbrace{\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_p \\ \vdots \\ \vdots \\ y_{T-1} \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} h_0 & & & & \\ h_1 & h_0 & & & \\ \vdots & & \ddots & & \\ h_p & \dots & h_1 & h_0 & \\ & \ddots & & \ddots & \\ & & \ddots & & \ddots & \\ & & & h_p & \dots & h_1 & h_0 \end{bmatrix}}_{=\mathbf{A} \in \mathbb{R}^{T \times T}} \underbrace{\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_p \\ \vdots \\ \vdots \\ x_{T-1} \end{bmatrix}}_{=\mathbf{x}}$$

- Since  $\mathbf{A}$  is often singular, instead of solving  $\mathbf{y} = \mathbf{A}\mathbf{x}$ , we solve the problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 + \lambda \|\mathbf{x}\|^2 \quad (2)$$

**Aim:** Using the given data, plot the input signal  $\mathbf{x}$  under different  $\lambda$ .



## QR decomposition

# Thin QR Decomposition for Full Column-Rank Matrices

Suppose  $\mathbf{A} \in \mathbb{R}^{m \times n}$  has full column rank. Then,  $\mathbf{A}$  admits a decomposition

$$\mathbf{A} = \mathbf{Q}_1 \mathbf{R}_1 \quad (\text{Thin QR Decomposition})$$

- $\mathbf{Q}_1 \in \mathbb{R}^{m \times n}$  is semi-orthogonal
- $\mathbf{R}_1 \in \mathbb{R}^{n \times n}$  is nonsingular and upper triangular

## Gram-Schmidt Procedure (cont'd)

**Algorithm:** Gram-Schmidt

**input:** a collection of linearly independent vectors  $\mathbf{a}_1, \dots, \mathbf{a}_n$

$\tilde{\mathbf{q}}_1 = \mathbf{a}_1$ ,  $\mathbf{q}_1 = \tilde{\mathbf{q}}_1 / \|\tilde{\mathbf{q}}_1\|_2$

for  $i = 2, \dots, n$

$\tilde{\mathbf{q}}_i = \mathbf{a}_i - \sum_{j=1}^{i-1} (\mathbf{q}_j^T \mathbf{a}_i) \mathbf{q}_j$

$\mathbf{q}_i = \tilde{\mathbf{q}}_i / \|\tilde{\mathbf{q}}_i\|_2$

end

**output:**  $\mathbf{q}_1, \dots, \mathbf{q}_n$

- Complexity:  $O(mn^2)$
- $\text{span}\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n\} = \text{span}\{\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n\}$
- $[\mathbf{q}_1 \quad \mathbf{q}_2 \quad \dots \quad \mathbf{q}_n]$  is a semi-orthogonal matrix

# Thin QR Decomposition via Gram-Schmidt

From Gram-Schmidt,

$$\mathbf{a}_i = \sum_{j=1}^i r_{ji} \mathbf{q}_j, \quad i = 1, \dots, n$$

where

$$r_{ii} = \|\tilde{\mathbf{q}}_i\|_2, \quad r_{ji} = \mathbf{q}_j^T \mathbf{a}_i, \quad j = 1, \dots, i-1$$

Equivalently,

$$\mathbf{A} = [\mathbf{a}_1 \quad \mathbf{a}_2 \quad \cdots \quad \mathbf{a}_n] = \mathbf{Q}_1 \mathbf{R}_1$$

where

- $\mathbf{Q}_1 = [\mathbf{q}_1 \quad \mathbf{q}_2 \quad \cdots \quad \mathbf{q}_n]$  semi-orthogonal
- $\mathbf{R}_1$  is nonsingular, upper triangular with  $[\mathbf{R}_1]_{ij} = r_{ij}$  for  $i \leq j$

## Example & Exercise

- **Example 1:** Use the Gram-Schmidt to decompose

$$\mathbf{A} = \begin{bmatrix} 0 & -20 & -14 \\ 3 & 27 & -4 \\ 4 & 11 & -2 \end{bmatrix}$$

- **Exercise 1:** Use the Gram-Schmidt to decompose

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & -1 \\ 1 & 2 & 1 \\ 1 & 3 & -1 \\ 0 & 1 & 1 \end{bmatrix}$$

- see Chapter 5.2.7 of **[Golub-van-Loan'13]** for the Gram-Schmidt Algorithm

# Numerical Error Issue of Gram-Schmidt

Gram-Schmidt is numerically unstable due to propagation of numerical errors

**Example:** Given

$\mathbf{a}_1 = [1 \ \epsilon \ 0 \ 0]^T$ ,  $\mathbf{a}_2 = [1 \ 0 \ \epsilon \ 0]^T$ ,  $\mathbf{a}_3 = [1 \ 0 \ 0 \ \epsilon]^T$  with tiny  $\epsilon$  so that the approximation  $1 + \epsilon^2 \approx 1$  can be made

Applying Gram-Schmidt with the above approximation yields

- $\mathbf{q}_1 = \frac{\mathbf{a}_1}{\|\mathbf{a}_1\|_2} = [1 \ \epsilon \ 0 \ 0]^T$
- $\tilde{\mathbf{q}}_2 = \mathbf{a}_2 - \mathbf{q}_1^T \mathbf{a}_2 \mathbf{q}_1 = [0 \ -\epsilon \ \epsilon \ 0]^T$   
 $\mathbf{q}_2 = \frac{\tilde{\mathbf{q}}_2}{\|\tilde{\mathbf{q}}_2\|_2} = \frac{1}{\sqrt{2}} [0 \ -1 \ 1 \ 0]^T$
- $\tilde{\mathbf{q}}_3 = \mathbf{a}_3 - \mathbf{q}_1^T \mathbf{a}_3 \mathbf{q}_1 - \mathbf{q}_2^T \mathbf{a}_3 \mathbf{q}_2 = [0 \ -\epsilon \ 0 \ \epsilon]^T$   
 $\mathbf{q}_3 = \frac{\tilde{\mathbf{q}}_3}{\|\tilde{\mathbf{q}}_3\|_2} = \frac{1}{\sqrt{2}} [0 \ -1 \ 0 \ 1]^T$

**Orthogonality is lost!**

## Modified Gram-Schmidt

Instead of computing  $\tilde{\mathbf{q}}_i = \mathbf{a}_i - (\mathbf{q}_1^T \mathbf{a}_i)\mathbf{q}_1 - (\mathbf{q}_2^T \mathbf{a}_i)\mathbf{q}_2 - \cdots - (\mathbf{q}_{i-1}^T \mathbf{a}_i)\mathbf{q}_{i-1}$  in Gram-Schmidt (full column rank case), compute

$$\tilde{\mathbf{q}}_i^{(1)} = \mathbf{a}_i - (\mathbf{q}_1^T \mathbf{a}_i)\mathbf{q}_1$$

$$\tilde{\mathbf{q}}_i^{(2)} = \tilde{\mathbf{q}}_i^{(1)} - (\mathbf{q}_2^T \tilde{\mathbf{q}}_i^{(1)})\mathbf{q}_2$$

$$\vdots$$

$$\tilde{\mathbf{q}}_i^{(j)} = \tilde{\mathbf{q}}_i^{(j-1)} - (\mathbf{q}_j^T \tilde{\mathbf{q}}_i^{(j-1)})\mathbf{q}_j$$

$$\vdots$$

$$\tilde{\mathbf{q}}_i = \tilde{\mathbf{q}}_i^{(i-1)} = \tilde{\mathbf{q}}_i^{(i-2)} - (\mathbf{q}_{i-1}^T \tilde{\mathbf{q}}_i^{(i-2)})\mathbf{q}_{i-1}$$

## Modified Gram-Schmidt (cont'd)

**Example** (revisit): Given

$\mathbf{a}_1 = [1 \ \epsilon \ 0 \ 0]^T$ ,  $\mathbf{a}_2 = [1 \ 0 \ \epsilon \ 0]^T$ ,  $\mathbf{a}_3 = [1 \ 0 \ 0 \ \epsilon]^T$  with tiny  $\epsilon$   
so that the approximation  $1 + \epsilon^2 \approx 1$  can be made

Applying modified Gram-Schmidt with the above approximation yields

- $\tilde{\mathbf{q}}_1 = [1 \ \epsilon \ 0 \ 0]^T$   
 $\mathbf{q}_1 = [1 \ \epsilon \ 0 \ 0]^T$
- $\tilde{\mathbf{q}}_2 = \mathbf{a}_2 - \mathbf{q}_1^T \mathbf{a}_2 \mathbf{q}_1 = [0 \ -\epsilon \ \epsilon \ 0]^T$   
 $\mathbf{q}_2 = \frac{1}{\sqrt{2}} [0 \ -1 \ 1 \ 0]^T$
- $\tilde{\mathbf{q}}_3^{(1)} = \mathbf{a}_3 - \mathbf{q}_1^T \mathbf{a}_3 \mathbf{q}_1 = [0 \ -\epsilon \ 0 \ \epsilon]^T$   
 $\tilde{\mathbf{q}}_3 = \tilde{\mathbf{q}}_3^{(2)} = \tilde{\mathbf{q}}_3^{(1)} - \mathbf{q}_2^T \tilde{\mathbf{q}}_3^{(1)} \mathbf{q}_2 = [0 \ -\frac{\epsilon}{2} \ -\frac{\epsilon}{2} \ \epsilon]^T$   
 $\mathbf{q}_3 = \frac{1}{\sqrt{6}} [0 \ -1 \ -1 \ 2]^T$

**Orthogonality is preserved approximately**



## Example & Exercise

- **Example 2:** Use the modified Gram-Schmidt to decompose

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 \\ 0.001 & 0.001 & 0 \\ 0.001 & 0 & 0.001 \end{bmatrix}$$

- **Exercise 2:** Use the modified Gram-Schmidt to decompose

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 \\ 0.001 & 0 & 0 \\ 0 & 0.001 & 0 \\ 0 & 0 & 0.001 \end{bmatrix}$$

- see Chapter 5.2.8 of **[Golub-van-Loan'13]** for the modified Gram-Schmidt Algorithm

# Householder Reflections

Householder reflection: Given  $\mathbf{x} \in \mathbb{R}^m$ , let

$$\mathbf{v} = \mathbf{x} \mp \|\mathbf{x}\|_2 \mathbf{e}_1 \quad \mathbf{H} = \mathbf{I} - \frac{2}{\|\mathbf{v}\|_2^2} \mathbf{v} \mathbf{v}^T$$

$$\Rightarrow \quad \mathbf{H} \mathbf{x} = \pm \begin{bmatrix} \|\mathbf{x}\|_2 \\ \mathbf{0} \end{bmatrix} = \|\mathbf{x}\|_2 \mathbf{e}_1$$

- $\mathbf{H} \in \mathbb{R}^{m \times m}$  is orthogonal
- The sign in the expression of  $\mathbf{v}$  may be determined to be the one that maximizes  $\|\mathbf{v}\|_2$  for the sake of numerical stability

# Householder QR

1. Let  $\mathbf{H}_1 \in \mathbb{R}^{m \times m}$  be the Householder reflection w.r.t.  $\mathbf{a}_1$ . Transform  $\mathbf{A}$  as

$$\mathbf{A}^{(1)} = \mathbf{H}_1 \mathbf{A} = \begin{bmatrix} \times & \times & \dots & \times \\ 0 & \color{red}{\times} & \dots & \times \\ \vdots & \vdots & & \vdots \\ 0 & \color{red}{\times} & \dots & \times \end{bmatrix}$$

2. Let  $\tilde{\mathbf{H}}_2 \in \mathbb{R}^{(m-1) \times (m-1)}$  be the Householder reflection w.r.t.  $\mathbf{A}^{(1)}(2:m, 2)$  (marked red above). Transform  $\mathbf{A}^{(1)}$  as

$$\mathbf{A}^{(2)} = \underbrace{\begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{H}}_2 \end{bmatrix}}_{=\mathbf{H}_2} \mathbf{A}^{(1)} = \begin{bmatrix} \times & \times & \dots & \times \\ 0 & \tilde{\mathbf{H}}_2 \mathbf{A}^{(1)}(2:m, 2:n) \end{bmatrix} = \begin{bmatrix} \times & \times & \times & \dots & \times \\ 0 & \times & \times & \dots & \times \\ \vdots & 0 & \times & \dots & \times \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & \times & \dots & \times \end{bmatrix}$$

- $\mathbf{A}^{(n-1)} = \mathbf{H}_{n-1} \dots \mathbf{H}_2 \mathbf{H}_1 \mathbf{A}$ ,  $\mathbf{A}^{(n-1)}$  is upper triangular
- $\mathbf{R} = \mathbf{A}^{(n-1)}$  and  $\mathbf{Q} = (\mathbf{H}_{n-1} \dots \mathbf{H}_2 \mathbf{H}_1)^T$

## Example & Exercise

- **Example 3:** Use the Householder reflection to decompose

$$\mathbf{A} = \begin{bmatrix} 1 & 19 & -34 \\ -2 & -5 & 20 \\ 2 & 8 & 37 \end{bmatrix}$$

- **Exercise 3:** Use the Householder reflection to decompose

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & -1 \\ 1 & 2 & 1 \\ 1 & 1 & -3 \\ 0 & 1 & 1 \end{bmatrix}$$

- see Algorithm 5.2.1 in **[Golub-van-Loan'13]** for the Householder QR Algorithm

# Givens Rotations

**Example:** Let

$$\mathbf{J} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix}$$

where  $c = \cos(\theta)$ ,  $s = \sin(\theta)$  for some  $\theta$

$$\mathbf{y} = \mathbf{J}\mathbf{x} \iff \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} cx_1 + sx_2 \\ -sx_1 + cx_2 \end{bmatrix}$$

Observe that

- $\mathbf{J}$  is orthogonal
- $y_2 = 0$  if  $\theta = \tan^{-1}(x_2/x_1)$ , or if

$$c = \frac{x_1}{\sqrt{x_1^2 + x_2^2}}, \quad s = \frac{x_2}{\sqrt{x_1^2 + x_2^2}}$$

# Givens QR

**Example:** Consider a  $4 \times 3$  matrix.

$$\begin{aligned}
 \mathbf{A} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} &\xrightarrow{\mathbf{J}_{1,2}} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \xrightarrow{\mathbf{J}_{1,3}} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ \times & \times & \times \end{bmatrix} \xrightarrow{\mathbf{J}_{1,4}} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix} \\
 &\xrightarrow{\mathbf{J}_{2,3}} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & \times & \times \end{bmatrix} \xrightarrow{\mathbf{J}_{2,4}} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{bmatrix} \xrightarrow{\mathbf{J}_{3,4}} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{bmatrix} = \mathbf{R}
 \end{aligned}$$

- $\mathbf{B} \xrightarrow{\mathbf{J}} \mathbf{C}$  means  $\mathbf{C} = \mathbf{JB}$
- **Givens QR** ( $m \geq n$ ): Perform a sequence of Givens rotations to annihilate the lower triangular parts of  $\mathbf{A}$

$$\underbrace{(\mathbf{J}_{n,m} \dots \mathbf{J}_{n,n+2} \mathbf{J}_{n,n+1}) \dots (\mathbf{J}_{2m} \dots \mathbf{J}_{24} \mathbf{J}_{23})(\mathbf{J}_{1m} \dots \mathbf{J}_{13} \mathbf{J}_{12})}_{=\mathbf{Q}^T} \mathbf{A} = \mathbf{R}$$

where  $\mathbf{R}$  is upper triangular and  $\mathbf{Q}$  is orthogonal

## Example & Exercise

- **Example 4:** Use the Givens rotations to decompose

$$\mathbf{A} = \begin{bmatrix} 1 & 19 & -34 \\ -2 & -5 & 20 \\ 2 & 8 & 37 \end{bmatrix}$$

- **Exercise 3:** Use the Givens rotations to decompose

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & -1 \\ 1 & 2 & 1 \\ 1 & 1 & -3 \\ 0 & 1 & 1 \end{bmatrix}$$

- see Algorithm 5.2.4 in **[Golub-van-Loan'13]** for the Givens QR Algorithm

# References

**[Golub-van-Loan'13]** G. H. Golub and C. F. Van Loan, *Matrix Computations*, 4rd edition, JHU Press, 2013.