# Section 6.4-6.5 The Gram-Schmit Process, least-square problems, and applications to linear models

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- Given a basis for a subspace *W* of **R**<sup>*n*</sup>, how to find an orthogonal basis for *W*?
- Let  $\{x_1, x_2, \ldots, x_p\}$  be a basis for W.
- The idea is as follows: let  $v_1 = x_1$  and take  $W_1 = Span\{v_1\}$ , then project  $x_2$  to  $W_1$  and let  $v_2$  be the component of  $x_2$  orthogonal to  $W_1$ ; then let  $W_2 = Span\{v_1, v_2\}$ , and project  $x_3$  to  $W_2$  and let  $v_3$  be the component of  $x_3$  orthogonal to  $W_2$ . Then  $\{v_1, v_2, v_3\}$  is an orthogonal basis for W; and so on.
- This is so-called Gram-Schmidt Process.

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• Given a basis  $\{x_1, x_2, \dots, x_p\}$  for a nonzero subspace W of  $\mathbf{R}^n$ , define

$$v_{1} = x_{1}$$

$$v_{2} = x_{2} - \frac{x_{2} \cdot v_{1}}{v_{1} \cdot v_{1}}v_{1} - \frac{x_{2} \cdot v_{2}}{v_{2}}v_{2} = x_{3} - \frac{x_{3} \cdot v_{1}}{v_{1} \cdot v_{1}}v_{1} - \frac{x_{3} \cdot v_{2}}{v_{2} \cdot v_{2}}v_{2} = x_{3} - \frac{p(v)}{v_{4}}v_{4}$$

$$v_{p} = x_{p} - \frac{x_{p} \cdot v_{1}}{v_{1} \cdot v_{1}} v_{1} - \frac{x_{p} \cdot v_{2}}{v_{2} \cdot v_{2}} v_{2} - \dots - \frac{x_{p} \cdot v_{p-1}}{v_{p-1} \cdot v_{p-1}} v_{p-1}$$

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Ex. Let 
$$W = span\{x_1, x_2\}$$
, where  $x_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$  and  $x_2 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$ . Construct an orthogonal basis  $\{v_1, v_2\}$  for  $W$ .

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•  $v_3 = x_3 - proj_{W_2}x_3 = x_3 - (\frac{x_3 \cdot v_1}{v_1 \cdot v_1}v_1 + \frac{x_3 \cdot v_2}{v_2 \cdot v_2}v_2) = \begin{bmatrix} -3/8\\-13/24\\11/24\\11/24\end{bmatrix}$ .

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Least-square problems

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#### Least-squares problems

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- Note that no matter what x we select, the vector Ax will necessarily be in the column space of A, Col A.

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- Definition: If A is  $m \times n$  and b in  $\mathbb{R}^n$ , a least-squares solution of Ax = b is an  $\hat{x}$  in  $\mathbb{R}^n$  such that  $||b A\hat{x}|| \le ||b Ax||$  for all  $x \in \mathbb{R}^n$ .

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- Given A and b, apply the Best Approximation Theorem to the subspace Col A. Let  $\hat{b} = proj_{Col A}b$ .
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east-square solver to Ax=b  
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 s.t A $\hat{x}$  = Proj b  
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- Such an x̂ in R<sup>n</sup> is a list of weights that will build b̂ out of the columns of A.

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- Such an x̂ in R<sup>n</sup> is a list of weights that will build b̂ out of the columns of A.
- Suppose  $\hat{x}$  satisfies  $A\hat{x} = \hat{b}$ .
- By the Orthogonal Decomposition Theorem, the projection  $\hat{b}$  has the property that  $b \hat{b}$  is orthogonal to *Col A*, so  $b A\hat{x}$  is orthogonal to each column of *A*.

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• If  $a_j$  is any column of A, then  $a_j \cdot (b - A\hat{x}) = 0$ , and  $a_j^T (b - A\hat{x}) = 0$ .

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- Thus  $A^T b A^T A \hat{x} = 0$ , and  $A^T A \hat{x} = A^T b$ .

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- Thus  $A^T b A^T A \hat{x} = 0$ , and  $A^T A \hat{x} = A^T b$ .
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- These calculations show that each least-squares solution of Ax = b satisfies the equation  $A^T Ax = A^T b$ .
- The matrix equation  $A^T A x = A^T b$  represents a system of equations called the normal equations for A x = b.

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• A solution to 
$$A^T A x = A^T b$$
 is often denoted by  $\hat{x}$ .

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    - Hence the equation  $b = A\hat{x} + (b A\hat{x})$  is a decomposition of b into the sum of a vector in Col A and a vector orthogonal to Col A.

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    - Hence the equation  $b = A\hat{x} + (b A\hat{x})$  is a decomposition of b into the sum of a vector in Col A and a vector orthogonal to Col A.
    - By the uniqueness of the orthogonal decomposition,  $A\hat{x}$  must be the orthogonal projection of *b* onto *Col A*.

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- THM The set of least-squares solutions of Ax = b coincides with the nonempty set of solutions of the normal equation  $A^T Ax = A^T b$ .
  - PF. The set of least-squares solutions is nonempty and each least-squares solution  $\hat{x}$  satisfies the normal equations.
    - Conversely, suppose  $\hat{x}$  satisfies  $A^T A \hat{x} = A^T b$ .
    - Then  $\hat{x}$  satisfies  $A^T(b A\hat{x}) = 0$ , which shows that  $b A\hat{x}$  is orthogonal to the rows of  $A^T$ , and hence is orthogonal to the columns of A.
    - Since the columns of A span Col A, the vector  $b A\hat{x}$  is orthogonal to all of Col A.
    - Hence the equation  $b = A\hat{x} + (b A\hat{x})$  is a decomposition of b into the sum of a vector in Col A and a vector orthogonal to Col A.
    - By the uniqueness of the orthogonal decomposition,  $A\hat{x}$  must be the orthogonal projection of *b* onto *Col A*.
    - That is,  $A\hat{x} = \hat{b}$  and  $\hat{x}$  is a least-squares solution.

Ex. Find a least-squares solution of the inconsistent system Ax = b for

$$A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix}, b = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}.$$

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Sol. To use the normal equation, compute:

$$A^{\mathsf{T}}A = \begin{bmatrix} 17 & 1\\ 1 & 5 \end{bmatrix}, A^{\mathsf{T}}b = \begin{bmatrix} 19\\ 11 \end{bmatrix}$$

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• Solve it, we have  $\hat{x} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ .

• Note that the matrix equation  $A^T A x = A^T b$  may have infinite many solutions.

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  - The columns of A are linearly independent.
  - ► The matrix *A<sup>T</sup>A* is invertible.

When these statements are true, the least-squares solution  $\hat{x}$  is given by  $\hat{x} = (A^T A)^{-1} A^T b$ .  $\chi = (A^T A)^{-1} (A^T b)$ 

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• The distance from b to  $A\hat{x}$ ,  $||b - A\hat{x}||$ , is called the least-squares error of this approximation.

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## Alternative calculation

When the columns of A[u<sub>1</sub> u<sub>2</sub> ... u<sub>p</sub>] are orthogonal, we know exactly the orthogonal projection of b on Col A:

$$\hat{b} = \frac{b \cdot u_1}{u_1 \cdot u_1} u_1 + \ldots + \frac{b \cdot u_p}{u_p \cdot u_p} u_p$$

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• When the columns of  $A[u_1 \ u_2 \ \dots \ u_p]$  are orthogonal, we know exactly the orthogonal projection of *b* on *Col A*:

$$\mathbf{u}_{\mathbf{x}} + \mathbf{u}_{\mathbf{x}} + \cdots = \mathbf{A} \times \mathbf{f} \quad \hat{b} = \frac{b \cdot u_1}{u_1 \cdot u_1} u_1 + \cdots + \frac{b \cdot u_p}{u_p \cdot u_p} u_p$$

• Now to get the least-squares solution to  $A\hat{x} = \hat{b}$ , we just need to read:

$$x_1 = \frac{b \cdot u_1}{u_1 \cdot u_1}, x_2 = \frac{b \cdot u_2}{u_2 \cdot u_2}, \dots, x_p = \frac{b \cdot u_p}{u_p \cdot u_p}$$

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• Such matrices often appear in linear regression problems.

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Ex. Find a least-squares solution of Ax = b for

$$A = \begin{bmatrix} 1 & -6\\ 1 & -2\\ 1 & 1\\ 1 & 7 \end{bmatrix}, b = \begin{bmatrix} -1\\ 2\\ 1\\ 6 \end{bmatrix}$$

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Sol. We know that

$$\hat{b} = \frac{b \cdot u_1}{u_1 \cdot u_1} u_1 + \frac{b \cdot u_2}{u_2 \cdot u_2} u_2 = 2u_1 + 1/2u_2 = \begin{bmatrix} -1\\1\\5/2\\11/2 \end{bmatrix}$$

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• Now we solve 
$$A\hat{x} = \hat{b}$$
:  $\hat{x} = \begin{bmatrix} 2 \\ 1/2 \end{bmatrix}$ .  
• We can also get the least-squares error:  $||b - A\hat{x}|| = \sqrt{2}$ .

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• The simplest relation between two variables x and y is the linear equation  $y = \beta_0 + \beta_1 x$ . Experimental data often produce points  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$  that, when graphed, seem to lie close to a line.



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• For each point  $(x_i, y_i)$ , there is a corresponding point  $(x_i, \beta_0 + \beta_1 x_i)$ on the line.  $x_i \rightarrow y_i \quad \beta_i + \beta_i x_i$ 

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- Suppose that  $\beta_0$  and  $\beta_1$  are fixed, and consider the line  $y = \beta_0 + \beta_1 x$ .
- For each point (x<sub>i</sub>, y<sub>i</sub>), there is a corresponding point (x<sub>i</sub>, β<sub>0</sub> + β<sub>1</sub>x<sub>i</sub>) on the line.
- We call  $y_i$  the observed value of y and  $\beta_0 + \beta_1 x_i$  the predicted y-value. The difference of an observed y-value and the predicted y-value is called a residual.

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- We call  $y_i$  the observed value of y and  $\beta_0 + \beta_1 x_i$  the predicted y-value. The difference of an observed y-value and the predicted y-value is called a residual.
- The least-squares line, or the line of regression of y on x, is the line  $y = \beta_0 + \beta_1 x$  that minimizes the sum of the squares of the residuals.

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• The  $\beta_0$  and  $\beta_1$  satisfy the following

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \dots & \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix}$$

$$(\beta_{0} + (\beta_{1} \times_{1} = Y_{1} + \beta_{1} \times_{2} = Y_{2})$$
  
 $\vdots$   
 $\xi_{0} + (\beta_{1} \times_{2} = Y_{2})$ 

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• Or simply just  $X\beta = y$ .

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$$\gamma = (\beta_0 + (\beta_1 \times_1 + (\beta_2 \times_2 + \dots + (\beta_k \times_k))))$$

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• Or simply just  $X\beta = y$ .

 We can find the least-squares solution to Xβ = y by solving the matrix equation X<sup>T</sup>Xβ = X<sup>T</sup>y.

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• Find the equation  $y = \beta_0 + \beta_1 x$  of the least-squares line that best fits the data points (2, 1), (5, 2), (7, 3) and (8, 3).

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Sol. We solve the equation  $X^T X \beta = X^T y$ , where

$$X = \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix}, y = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}$$

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$$\begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$$

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- So the solution is  $[\beta_0 \ \beta_1] = [2/7 \ 5/14].$
- The least-squares line is y = 2/7 + 5/14x.