## Section 6.4-6.'s The Gram-Schmit Process, least-square problems, and applications to linear models

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Example

Ex. Let $x_{1}=\left[\begin{array}{l}1 \\ 1 \\ 1 \\ 1\end{array}\right], x_{2}=\left[\begin{array}{l}0 \\ 1 \\ 1 \\ 1\end{array}\right]$, and $x_{3}=\left[\begin{array}{l}0 \\ 0 \\ 1 \\ 1\end{array}\right], y=\left[\begin{array}{c}2 \\ -1 \\ 3 \\ 4\end{array}\right]$, and
$W=\operatorname{Span}\left\{x_{1}, x_{2}, x_{3}\right\}$. Find the projection of $y$ onto $W$.

$$
\operatorname{Proj} y=\frac{y \cdot x_{1}}{x_{1} \cdot x_{1}} x_{1}+\frac{y \cdot x_{2}}{x_{2} x_{2}} x_{2}+\frac{y \cdot x_{3}}{x_{3} \cdot x_{3}} x_{3}
$$

WRONG! not inthogmal sat

## Orthogonal basis

- Given a basis for a subspace $W$ of $\mathbf{R}^{n}$, how to find an orthogonal basis for $W$ ?
- Let $\left\{x_{1}, x_{2}, \ldots, x_{p}\right\}$ be a basis for $W$.
- The idea is as follows: let $v_{1}=x_{1}$ and take $W_{1}=\operatorname{Span}\left\{v_{1}\right\}$, then project $x_{2}$ to $W_{1}$ and let $v_{2}$ be the component of $x_{2}$ orthogonal to $W_{1}$; then let $W_{2}=\operatorname{Span}\left\{v_{1}, v_{2}\right\}$, and project $x_{3}$ to $W_{2}$ and let $v_{3}$ be the component of $x_{3}$ orthogonal to $W_{2}$. Then $\left\{v_{1}, v_{2}, v_{3}\right\}$ is an orthogonal basis for $W$; and so on.
- This is so-called Gram-Schmidt Process.


## The Gram-Schmidt Process

- Given a basis $\left\{x_{1}, x_{2}, \ldots, x_{p}\right\}$ for a nonzero subspace $W$ of $\mathbf{R}^{n}$, define

$$
\begin{aligned}
& v_{1}=x_{1} \\
& v_{2}=x_{2}-\frac{x_{2} \cdot v_{1}}{v_{1} \cdot v_{1}} v_{1}-X_{2}-P \cdot \hat{\jmath} x_{2} \\
& v_{3}=x_{3}-\frac{x_{3} \cdot v_{1}}{v_{1} \cdot v_{1}} v_{1}-\frac{x_{3} \cdot v_{2}}{v_{2} \cdot v_{2}} v_{2}=x_{3}-P \cdot{ }_{j} w_{2} \\
& \cdots \\
& v_{p}=x_{p}-\frac{x_{p} \cdot v_{1}}{v_{1} \cdot v_{1}} v_{1}-\frac{x_{p} \cdot v_{2}}{v_{2} \cdot v_{2}} v_{2}-\ldots-\frac{x_{p} \cdot v_{p-1}}{v_{p-1} \cdot v_{p-1}} v_{p-1}
\end{aligned}
$$

Then $\left\{v_{1}, v_{2}, \ldots, v_{p}\right\}$ is an orthogonal basis for $W$.

## Example

Ex. Let $W=\operatorname{span}\left\{x_{1}, x_{2}\right\}$, where $x_{1}=\left[\begin{array}{l}3 \\ 6 \\ 0\end{array}\right]$ and $x_{2}=\left[\begin{array}{l}1 \\ 2 \\ 2\end{array}\right]$. Construct an orthogonal basis $\left\{v_{1}, v_{2}\right\}$ for $W$.

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- So let $v_{1}=x_{1}$.
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v_{2}=x_{2}-p=x_{2}-\frac{x_{2} \cdot x_{1}}{x_{1} \cdot x_{1}} x_{1}=\left[\begin{array}{l}
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$V_{1}=X_{1}$.

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- $v_{2}=x_{2}-\operatorname{proj}_{1} x_{2}=x_{2}-\frac{x_{2} \cdot v_{1}}{v_{1} \cdot v_{1}} v_{1}=\left[\begin{array}{l}0 \\ 1 \\ 1 \\ 1\end{array}\right]-\frac{3}{4}\left[\begin{array}{l}1 \\ 1 \\ 1 \\ 1\end{array}\right]=\left[\begin{array}{c}-3 / 4 \\ 1 / 4 \\ 1 / 4 \\ 1 / 4\end{array}\right]$.
- $v_{3}=x_{3}-\operatorname{proj}_{2} x_{3}=x_{3}-\left(\frac{x_{3} \cdot v_{1}}{v_{1} \cdot v_{1}} v_{1}+\frac{x_{3} \cdot v_{2}}{v_{2} \cdot v_{2}} v_{2}\right)=\left[\begin{array}{c}-3 / 8 \\ -13 / 24 \\ 11 / 24 \\ 11 / 24\end{array}\right]$.


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- $\left\{v_{1}, v_{2}, v_{3}\right\}$ is an orthogonal basis for $W$.


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


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$$
\begin{array}{r}
u=\left[\begin{array}{l}
u_{1} \\
\vdots \\
u_{n}
\end{array}\right] \\
\|u\|=\sqrt{u_{1}^{2}+\ldots r u_{n}^{2}}
\end{array}
$$

The vector $\mathbf{b}$ is closer to $A \hat{\mathbf{x}}$ than to $A \mathbf{x}$ for other $\mathbf{x}$.

## Solution to the general least-squares problem

- Given $A$ and $b$, apply the Best Approximation Theorem to the subspace $\operatorname{Col} A$. Let $\hat{b}=\operatorname{proj}_{\mathrm{Col}} A b$.


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- Since $\hat{b}$ is the closest point in $\operatorname{Col} A$ to $b$, a vector $\hat{x}$ is a least-squares solution of $A x=b$ if and only if $\hat{x}$ satisfies $A \hat{x}=\hat{b}$.

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- Such an $\hat{x}$ in $\mathbf{R}^{n}$ is a list of weights that will build $\hat{b}$ 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 $\operatorname{Col} A$, so $b-A \hat{x}$ is orthogonal to each column of $A$.
- 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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- The matrix equation $A^{T} A x=A^{T} b$ represents a system of equations called the normal equations for $A x=b$.
- A solution to $A^{T} A x=A^{T} b$ is often denoted by $\hat{x}$.

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- By the uniqueness of the orthogonal decomposition, $A \hat{x}$ must be the orthogonal projection of $b$ onto $\operatorname{Col} A$.
- That is, $A \hat{x}=\hat{b}$ and $\hat{x}$ is a least-squares solution.


## Example

Ex. Find a least-squares solution of the inconsistent system $A x=b$ for

$$
A=\left[\begin{array}{ll}
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\end{array}\right], b=\left[\begin{array}{c}
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Sol. To use the normal equation, compute:

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- Solve it, we have $\hat{x}=\left[\begin{array}{l}1 \\ 2\end{array}\right]$.
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- When will we have a unique least-squares solution to $A x=b$ ?

THM Let $A$ be an $m \times n$ matrix. The following statements are logically equivalent:

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

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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.


## Alternative calculation

$A=$

- When the columns of $A\left[\begin{array}{llll}u_{1} & u_{2} & \ldots & u_{p}\end{array}\right]$ are orthogonal, we know exactly the orthogonal projection of $b$ on $\operatorname{Col} A$ :

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\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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- Such matrices often appear in linear regression problems.


## Example

Ex. Find a least-squares solution of $A x=b$ for

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A=\left[\begin{array}{cc}
1 & -6 \\
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1 & 1 \\
1 & 7
\end{array}\right], b=\left[\begin{array}{c}
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\end{array}\right]
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- We can also get the least-squares error: $\|b-A \hat{x}\|=\sqrt{\text { ? }}$.


## Applications to linear models

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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 $\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)$ that, when graphed, seem to lie close to



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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 $\left(x_{i}, y_{i}\right)$, there is a corresponding point $\left(x_{i}, \beta_{0}+\beta_{1} x_{i}\right)$ 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 want to determine $\beta_{0}$ and $\beta_{1}$ that make the line as "close" to the points as possible.
- Suppose that $\beta_{0}$ and $\beta_{1}$ are fixed, and consider the line $y=\beta_{0}+\beta_{1} x$.
- For each point $\left(x_{i}, y_{i}\right)$, there is a corresponding point $\left(x_{i}, \beta_{0}+\beta_{1} x_{i}\right)$ 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.
- 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.
- The $\beta_{0}$ and $\beta_{1}$ satisfy the following

$$
\begin{aligned}
& {\left[\begin{array}{cc}
1 & x_{1} \\
1 & x_{2} \\
\cdots & \\
1 & x_{n}
\end{array}\right]\left[\begin{array}{l}
\beta_{0} \\
\beta_{1}
\end{array}\right]=\left[\begin{array}{c}
y_{1} \\
y_{2} \\
\cdots \\
y_{n}
\end{array}\right]} \\
& \beta_{0}+\beta_{1} x_{1}=Y_{1} \\
& \beta_{0}+\beta_{1} x_{2}=y_{2} \\
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$$
y=\beta_{0}+\beta_{1} x_{1}+\beta_{2} x_{2}+\cdots+\beta_{k} x_{4}
$$

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- We can find the least-squares solution to $X \beta=y$ by solving the matrix equation $X^{\top} X \beta=X^{\top} y$.


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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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X=\left[\begin{array}{ll}
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- The equation can be written as

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\left[\begin{array}{cc}
4 & 22 \\
22 & 142
\end{array}\right]\left[\begin{array}{l}
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- The least-squares line is $y=2 / 7+5 / 14 x$.

