## Lecture 26

Math 22 Summer 2017
August 16, 2017

## Just for today

- §6.4 Finish up
- §6.5 Least-squares problems


## §6.4 Gram-Schmidt Review

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\mathbf{v}_{k}=\mathbf{x}_{k}-\left(\sum_{i=1}^{k-1} \frac{\mathbf{x}_{k} \cdot \mathbf{v}_{i}}{\mathbf{v}_{i} \cdot \mathbf{v}_{i}} \mathbf{v}_{i}\right) .
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Moreover, $\operatorname{Span}\left\{\mathbf{v}_{1}, \ldots, \mathbf{v}_{k}\right\}=\operatorname{Span}\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{k}\right\}$ for every $k \in\{1, \ldots, p\}$.

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$$
\mathbf{x}_{k}=r_{1 k} \mathbf{u}_{1}+\cdots+r_{k k} \mathbf{u}_{k}+0 \mathbf{u}_{k+1}+\cdots+0 \mathbf{u}_{n}=Q \mathbf{r}_{k}, \quad \mathbf{r}_{k}=\left[\begin{array}{c}
r_{k k} \\
0 \\
\vdots \\
0
\end{array}\right]
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Then $R:=\left[\mathbf{r}_{1} \cdots \mathbf{r}_{n}\right]$ is upper triangular and $A=\left[\begin{array}{lll}\mathbf{x}_{1} & \cdots & \mathbf{x}_{n}\end{array}\right]=\left[\begin{array}{lll}Q \mathbf{r}_{1} & \cdots & Q \mathbf{r}_{n}\end{array}\right]=Q R$. How do we guarantee that the diagonal of $R$ is nonnegative?

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Let's see how the details work.

## §6.5 Example

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Let $A=\left[\begin{array}{ll}\mathbf{a}_{1} & \mathbf{a}_{2}\end{array}\right]=\left[\begin{array}{ll}2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 8 & 1\end{array}\right]$, and $\mathbf{b}=\left[\begin{array}{l}1 \\ 2 \\ 3 \\ 3\end{array}\right]$.


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\text { Let } A=\left[\mathbf{a}_{1} \mathbf{a}_{2}\right]=\left[\begin{array}{ll}
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\end{array}\right] \text {, and } \mathbf{b}=\left[\begin{array}{l}
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No!

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$$
\mathbf{v}_{2}=\mathbf{a}_{2}-\frac{\mathbf{a}_{2} \cdot \mathbf{v}_{1}}{\mathbf{v}_{1} \cdot \mathbf{v}_{1}} \mathbf{v}_{1}=\left[\begin{array}{r}
49 / 71 \\
16 / 71 \\
-6 / 71 \\
-17 / 71
\end{array}\right]
$$

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So $W$ has orthogonal basis $\left\{\mathbf{v}_{1}, \mathbf{v}_{2}\right\}$.

## §6.5 Example continued

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We can now compute

$$
\hat{\mathbf{b}}=\frac{\mathbf{b} \cdot \mathbf{v}_{1}}{\mathbf{v}_{1} \cdot \mathbf{v}_{1}} \mathbf{v}_{1}+\frac{\mathbf{b} \cdot \mathbf{v}_{2}}{\mathbf{v}_{2} \cdot \mathbf{v}_{2}} \mathbf{v}_{2}=\left[\begin{array}{r}
1 \\
29 / 14 \\
39 / 14 \\
22 / 7
\end{array}\right] .
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[A \hat{\mathbf{b}}] \sim\left[\begin{array}{rrr}
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0 & 1 & 2 / 7 \\
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## §6.5 Example continued

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to get that $\hat{\mathbf{x}}=\left[\begin{array}{r}5 / 14 \\ 2 / 7\end{array}\right]$ is a least-squares solutions to $A \mathbf{x}=\mathbf{b}$.

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## §6.5 Example continued

Alternatively, we can use the $Q R$ factorization of $A$ to compute $\hat{\mathbf{b}}$. Let $\mathbf{u}_{i}=\mathbf{v}_{i} /\left\|\mathbf{v}_{i}\right\|$ for $i=1,2$. Then

$$
Q=\left[\begin{array}{ll}
\mathbf{u}_{1} & \mathbf{u}_{2}
\end{array}\right]=\left[\begin{array}{ll}
2 / \sqrt{142} & (49 / 71) / \sqrt{42 / 71} \\
5 / \sqrt{142} & (16 / 71) / \sqrt{42 / 71} \\
7 / \sqrt{142} & (-6 / 71) / \sqrt{42 / 71} \\
8 / \sqrt{142} & (-17 / 71) / \sqrt{42 / 71}
\end{array}\right]
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## §6.5 Example continued

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$$

and

$$
R=Q^{T} A=\left[\begin{array}{rr}
\sqrt{142} & (11 / 71) \sqrt{142} \\
0 & \sqrt{42 / 71}
\end{array}\right]
$$

## §6.5 Example continued

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and

$$
Q Q^{T}=\left[\begin{array}{rrrr}
5 / 6 & 1 / 3 & 0 & -1 / 6 \\
1 / 3 & 11 / 42 & 3 / 14 & 4 / 21 \\
0 & 3 / 14 & 5 / 14 & 3 / 7 \\
-1 / 6 & 4 / 21 & 3 / 7 & 23 / 42
\end{array}\right] .
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## §6.5 Example continued

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What is $\hat{\mathbf{b}}$ ?

## §6.5 Example continued

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What is $\hat{\mathbf{b}}$ ? $\hat{\mathbf{b}}=Q Q^{\top} \mathbf{b}$.

## §6.5 Example continued

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\end{array}\right] .
$$

What is $\hat{\mathbf{b}}$ ? $\hat{\mathbf{b}}=Q Q^{T} \mathbf{b}$. We then find $\hat{\mathbf{x}}=[5 / 142 / 7]^{T}$ as before.

## §6.5 Theorem 13

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In the previous example, most of the work was in computing the projection $\hat{\mathbf{b}}$.

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## Theorem

The set of least-squares solutions of $A \mathbf{x}=\mathbf{b}$ is precisely the solutions of $A^{T} A \mathbf{x}=A^{T} \mathbf{b}$.

## §6.5 Theorem 13

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## Theorem

The set of least-squares solutions of $A \mathbf{x}=\mathbf{b}$ is precisely the solutions of $A^{T} A \mathbf{x}=A^{T} \mathbf{b}$. The linear system represented by the boxed equation represents a system of linear equations called the normal equations for $A \mathbf{x}=\mathbf{b}$.

## §6.5 Proof of Theorem 13

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Proof.

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Let $A=\left[\begin{array}{lll}\mathbf{a}_{1} & \ldots & \mathbf{a}_{n}\end{array}\right]$. Let $W=\operatorname{Col} A$.

## §6.5 Proof of Theorem 13

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## §6.5 Proof of Theorem 13

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## §6.5 Proof of Theorem 13

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Suppose $A \hat{\mathbf{x}}=\hat{\mathbf{b}}$. Then $\mathbf{b}-\hat{\mathbf{b}}=\mathbf{b}-A \hat{\mathbf{x}}$ is in $W^{\perp}$.

## §6.5 Proof of Theorem 13

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Let $A=\left[\begin{array}{lll}\mathbf{a}_{1} & \ldots & \mathbf{a}_{n}\end{array}\right]$. Let $W=\operatorname{Col} A$.
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Suppose $A \hat{\mathbf{x}}=\hat{\mathbf{b}}$. Then $\mathbf{b}-\hat{\mathbf{b}}=\mathbf{b}-A \hat{\mathbf{x}}$ is in $W^{\perp}$. This means that $\mathbf{b}-A \hat{\mathbf{x}}$ is orthogonal to every column of $A$

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Suppose $A \hat{\mathbf{x}}=\hat{\mathbf{b}}$. Then $\mathbf{b}-\hat{\mathbf{b}}=\mathbf{b}-A \hat{\mathbf{x}}$ is in $W^{\perp}$. This means that $\mathbf{b}-A \hat{\mathbf{x}}$ is orthogonal to every column of $A$ (every row of $A^{T}$ ).

## §6.5 Proof of Theorem 13

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(き)

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Conversely, suppose $A^{T} A \hat{\mathbf{x}}=A^{T} \mathbf{b}$.

## §6.5 Proof of Theorem 13

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Let $A=\left[\begin{array}{lll}\mathbf{a}_{1} & \ldots & \mathbf{a}_{n}\end{array}\right]$. Let $W=\operatorname{Col} A$.
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Suppose $A \hat{\mathbf{x}}=\hat{\mathbf{b}}$. Then $\mathbf{b}-\hat{\mathbf{b}}=\mathbf{b}-A \hat{\mathbf{x}}$ is in $W^{\perp}$. This means that $\mathbf{b}-A \hat{\mathbf{x}}$ is orthogonal to every column of $A$ (every row of $A^{T}$ ). But this means that $A^{T}(\mathbf{b}-A \hat{\mathbf{x}})=\mathbf{0}$ so that $A^{T} A \hat{\mathbf{x}}=A^{T} \mathbf{b}$.
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## §6.5 Proof of Theorem 13

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## §6.5 Proof of Theorem 13

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Let $A=\left[\begin{array}{lll}\mathbf{a}_{1} & \ldots & \mathbf{a}_{n}\end{array}\right]$. Let $W=\operatorname{Col} A$.
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Conversely, suppose $A^{T} A \hat{\mathbf{x}}=A^{T} \mathbf{b}$. Then $A^{T}(\mathbf{b}-A \hat{\mathbf{x}})=\mathbf{0}$ so that $\mathbf{b}-A \hat{\mathbf{x}}$ is orthogonal to the rows of $A^{T}$ (columns of $A$ ). Thus $\mathbf{b}-A \hat{\mathbf{x}} \in W^{\perp}$.

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Let $A=\left[\begin{array}{lll}\mathbf{a}_{1} & \ldots & \mathbf{a}_{n}\end{array}\right]$. Let $W=\operatorname{Col} A$.
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$\mathbf{b}-A \hat{\mathbf{x}} \in W^{\perp}$. Moreover, we have

$$
\mathbf{b}=\underbrace{A \hat{\mathbf{x}}}_{\in W}+\underbrace{\mathbf{b}-A \hat{\mathbf{x}}}_{\in W^{\perp}}
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Proof.
Let $A=\left[\begin{array}{lll}\mathbf{a}_{1} & \ldots & \mathbf{a}_{n}\end{array}\right]$. Let $W=\operatorname{Col} A$.
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Suppose $A \hat{\mathbf{x}}=\hat{\mathbf{b}}$. Then $\mathbf{b}-\hat{\mathbf{b}}=\mathbf{b}-A \hat{\mathbf{x}}$ is in $W^{\perp}$. This means that $\mathbf{b}-A \hat{\mathbf{x}}$ is orthogonal to every column of $A$ (every row of $A^{T}$ ). But this means that $A^{T}(\mathbf{b}-A \hat{\mathbf{x}})=\mathbf{0}$ so that $A^{T} A \hat{\mathbf{x}}=A^{T} \mathbf{b}$.
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\mathbf{b}=\underbrace{A \hat{\mathbf{x}}}_{\in W}+\underbrace{\mathbf{b}-A \hat{\mathbf{x}}}_{\in W^{\perp}}
$$

By the uniqueness of orthogonal decompositions, $A \hat{\mathbf{x}}$ must be the projection of $\mathbf{b}$ onto $W$.

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Proof.
Let $A=\left[\begin{array}{lll}\mathbf{a}_{1} & \ldots & \mathbf{a}_{n}\end{array}\right]$. Let $W=\operatorname{Col} A$.
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Suppose $A \hat{\mathbf{x}}=\hat{\mathbf{b}}$. Then $\mathbf{b}-\hat{\mathbf{b}}=\mathbf{b}-A \hat{\mathbf{x}}$ is in $W^{\perp}$. This means that $\mathbf{b}-A \hat{\mathbf{x}}$ is orthogonal to every column of $A$ (every row of $A^{T}$ ). But this means that $A^{T}(\mathbf{b}-A \hat{\mathbf{x}})=\mathbf{0}$ so that $A^{T} A \hat{\mathbf{x}}=A^{T} \mathbf{b}$.
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Conversely, suppose $A^{T} A \hat{\mathbf{x}}=A^{T} \mathbf{b}$. Then $A^{T}(\mathbf{b}-A \hat{\mathbf{x}})=\mathbf{0}$ so that $\mathbf{b}-A \hat{\mathbf{x}}$ is orthogonal to the rows of $A^{T}$ (columns of $A$ ). Thus $\mathbf{b}-A \hat{\mathbf{x}} \in W^{\perp}$. Moreover, we have

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## §6.5 Example continued

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Let's revisit our example using the previous theorem.

## §6.5 Example continued

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## §6.5 Example sontinued

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$$
A^{T} A=\left[\begin{array}{llll}
2 & 5 & 7 & 8 \\
1 & 1 & 1 & 1
\end{array}\right]\left[\begin{array}{ll}
2 & 1 \\
5 & 1 \\
7 & 1 \\
8 & 1
\end{array}\right]=\left[\begin{array}{rr}
142 & 22 \\
22 & 4
\end{array}\right]
$$

## §6.5 Example continued

Let's revisit our example using the previous theorem. We are given $A$ and $\mathbf{b}$. We compute

$$
\begin{gathered}
A^{T} A=\left[\begin{array}{llll}
2 & 5 & 7 & 8 \\
1 & 1 & 1 & 1
\end{array}\right]\left[\begin{array}{ll}
2 & 1 \\
5 & 1 \\
7 & 1 \\
8 & 1
\end{array}\right]=\left[\begin{array}{rr}
142 & 22 \\
22 & 4
\end{array}\right] \\
A^{T} \mathbf{b}=\left[\begin{array}{llll}
2 & 5 & 7 & 8 \\
1 & 1 & 1 & 1
\end{array}\right]\left[\begin{array}{l}
1 \\
2 \\
3 \\
3
\end{array}\right]=\left[\begin{array}{r}
57 \\
9
\end{array}\right]
\end{gathered}
$$

## §6.5 Example continued

Let's revisit our example using the previous theorem. We are given $A$ and $\mathbf{b}$. We compute

$$
\begin{gathered}
A^{T} A=\left[\begin{array}{llll}
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8 & 1
\end{array}\right]=\left[\begin{array}{rr}
142 & 22 \\
22 & 4
\end{array}\right] \\
A^{T} \mathbf{b}=\left[\begin{array}{llll}
2 & 5 & 7 & 8 \\
1 & 1 & 1 & 1
\end{array}\right]\left[\begin{array}{l}
1 \\
2 \\
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3
\end{array}\right]=\left[\begin{array}{r}
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\end{array}\right]
\end{gathered}
$$

How do we find $\hat{x}$ ?

## §6.5 Example continued

Let's revisit our example using the previous theorem. We are given $A$ and $\mathbf{b}$. We compute

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A^{T} A=\left[\begin{array}{llll}
2 & 5 & 7 & 8 \\
1 & 1 & 1 & 1
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2 & 1 \\
5 & 1 \\
7 & 1 \\
8 & 1
\end{array}\right]=\left[\begin{array}{rr}
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22 & 4
\end{array}\right] \\
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2 & 5 & 7 & 8 \\
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\end{array}\right]\left[\begin{array}{l}
1 \\
2 \\
3 \\
3
\end{array}\right]=\left[\begin{array}{r}
57 \\
9
\end{array}\right]
\end{gathered}
$$

How do we find $\hat{x}$ ?

$$
\left[\begin{array}{rrr}
142 & 22 & 57 \\
22 & 4 & 9
\end{array}\right] \sim\left[\begin{array}{rrr}
1 & 0 & 5 / 14 \\
0 & 1 & 2 / 7
\end{array}\right]
$$

## §6.5 Example «

## §6.5 Example 』

Are least-squares solutions always unique?

## §6.5 Example «

Are least-squares solutions always unique? No!

## §6.5 Example 』

Are least-squares solutions always unique? No!

$$
\text { Let } A=\left[\begin{array}{llll}
1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 \\
1 & 0 & 0 & 1
\end{array}\right], \quad \mathbf{b}=\left[\begin{array}{r}
-3 \\
-1 \\
0 \\
2 \\
5 \\
1
\end{array}\right]
$$

## §6.5 Example ©

Are least-squares solutions always unique? No!
Let $A=\left[\begin{array}{llll}1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1\end{array}\right], \quad \mathbf{b}=\left[\begin{array}{r}-3 \\ -1 \\ 0 \\ 2 \\ 5 \\ 1\end{array}\right]$. Then

$$
A^{T} A=\left[\begin{array}{llll}
6 & 2 & 2 & 2 \\
2 & 2 & 0 & 0 \\
2 & 0 & 2 & 0 \\
2 & 0 & 0 & 2
\end{array}\right], \quad A^{T} \mathbf{b}=\left[\begin{array}{r}
4 \\
-4 \\
2 \\
6
\end{array}\right]
$$

## §6.5 Example ©

Are least-squares solutions always unique? No!
Let $A=\left[\begin{array}{llll}1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1\end{array}\right], \quad \mathbf{b}=\left[\begin{array}{r}-3 \\ -1 \\ 0 \\ 2 \\ 5 \\ 1\end{array}\right]$. Then

$$
A^{T} A=\left[\begin{array}{llll}
6 & 2 & 2 & 2 \\
2 & 2 & 0 & 0 \\
2 & 0 & 2 & 0 \\
2 & 0 & 0 & 2
\end{array}\right], \quad A^{T} \mathbf{b}=\left[\begin{array}{r}
4 \\
-4 \\
2 \\
6
\end{array}\right]
$$

and

$$
\left[A^{T} A A^{T} \mathbf{b}\right] \sim\left[\begin{array}{rrrrr}
1 & 0 & 0 & 1 & 3 \\
0 & 1 & 0 & -1 & -5 \\
0 & 0 & 1 & -1 & -2 \\
0 & 0 & 0 & 0 & 0
\end{array}\right]
$$

## §6.5 Theorem 14

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$$
\begin{aligned}
\hat{\mathbf{x}} & =\left(A^{T} A\right)^{-1} A^{T} \mathbf{b} \\
& =\left[\begin{array}{rr}
1 / 21 & -11 / 42 \\
-11 / 42 & 71 / 42
\end{array}\right] A^{T} \mathbf{b} \\
& =\left[\begin{array}{rrr}
-1 / 6 & -1 / 42 & 1 / 14 \\
7 / 6 & 5 / 21 & -1 / 7 \\
\hline
\end{array}\right]\left[\begin{array}{l}
1 \\
2 \\
3 \\
3
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$$
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A \hat{\mathbf{x}} & =Q R \hat{\mathbf{x}} \\
& =Q R R^{-1} Q^{T} \mathbf{b} \\
& =Q Q^{T} \mathbf{b}=\hat{\mathbf{b}}
\end{aligned}
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7 / 6 & 8 / 21 & -1 / 7 \\
-17 / 42
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Note that this also shows the unilluminating fact that $\left(A^{T} A\right)^{-1} A^{T}=R^{-1} Q^{T}$ when defined.

## §6.5 Example concluded

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Consider the quantitative data $(2,1),(5,2),(7,3),(8,3)$ in the $(t, y)$-plane.

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Consider the quantitative data $(2,1),(5,2),(7,3),(8,3)$ in the $(t, y)$-plane. How do we find a line $y=c t+d$ that "best fits" this data?

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Consider the quantitative data $(2,1),(5,2),(7,3),(8,3)$ in the $(t, y)$-plane. How do we find a line $y=c t+d$ that "best fits" this data? Well, to do this we need a notion of error.

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\sum_{i=1}^{4}\left(y_{i}-c t_{i}-d\right)^{2}=(1-2 c-d)^{2}+(2-5 c-d)^{2}+(3-7 c-d)^{2}+(3-8 c-3)^{2}
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If we let $A=\left[\begin{array}{ll}2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 8 & 1\end{array}\right], \quad \mathbf{b}=\left[\begin{array}{l}1 \\ 2 \\ 3 \\ 3\end{array}\right], \quad \mathbf{x}=\left[\begin{array}{l}c \\ d\end{array}\right]$,

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error for a given $\mathbf{x}$ is precisely $\|\mathbf{b}-A \mathbf{x}\|^{2}$. This quantity is minimized precisely when you guessed it $\mathbf{x}$ is a least-squares solution to $A \mathbf{x}=\mathbf{b} . \hat{\mathbf{x}}=[5 / 142 / 7]^{T}$.

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