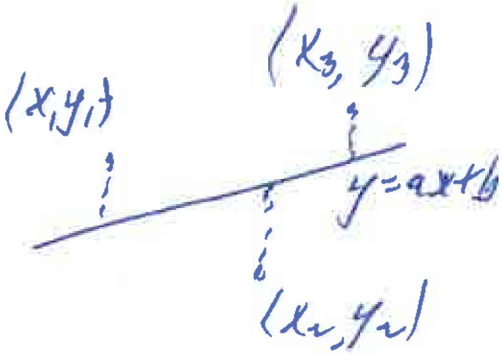
Line of best fit

Data set $D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$

Let
$$A = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_n \end{pmatrix}, \quad \vec{y} = \begin{pmatrix} y_1 \\ \vdots \\ \vdots \\ y_n \end{pmatrix}, \quad \vec{u} = \begin{pmatrix} a \\ b \end{pmatrix}$$

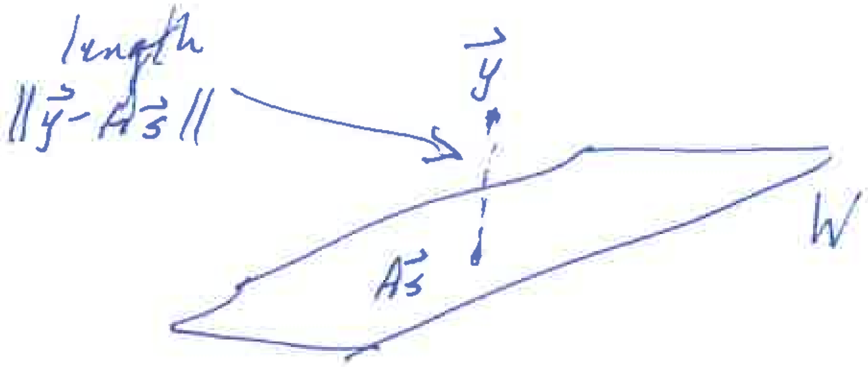
so that
$$\vec{y} - A\vec{u} = \begin{pmatrix} y_1 - (a + bx_1) \\ \vdots \\ y_n - (a + bx_n) \end{pmatrix}$$



Goal: Minimize $\|\vec{y} - A\vec{u}\|$.

Let
$$W = \{ A\vec{u} \mid \vec{u} = \begin{pmatrix} a \\ b \end{pmatrix} \in \mathbb{R}^2 \}$$

and
$$\vec{s} \in \mathbb{R}^2 \quad \text{such that} \quad A\vec{s} = \mathrm{proj}_W(\vec{y})$$



$\|\vec{y}-A\vec{s}\|$ will be minimal

if $\vec{y}-A\vec{s}$ is perpendicular to W.

So we want

if $\vec{u}\in\mathbb{R}^2$ then $\langle \vec{y}-A\vec{s}, A\vec{u}\rangle = 0$.

So we want

if $\vec{u}\in\mathbb{R}^2$ then $\vec{u}^tA^t(\vec{y}-A\vec{s}) = 0$.

So we want

$$A^t\vec{y}-A^tA\vec{s}=0$$

So we want

$$A^tA\vec{s}=A^t\vec{y}.$$

So we want $\vec{s}=(A^tA)^{-1}A^t\vec{y}$.

<u>Example 14</u>

Data set $D=\{(-1,1),(1,1),(2,3)\}$

$$A=\begin{pmatrix}1&-1\\1&1\\1&2\end{pmatrix} \quad\text{and}\quad \vec{y}=\begin{pmatrix}1\\1\\3\end{pmatrix}$$

Then

$$A^tA=\begin{pmatrix}1&1&1\\-1&1&2\end{pmatrix}\begin{pmatrix}1&-1\\1&1\\1&2\end{pmatrix}=\begin{pmatrix}3&2\\2&6\end{pmatrix}$$

$$A^t\vec{y} = \begin{pmatrix}1&1&1\\-1&1&2\end{pmatrix}\begin{pmatrix}1\\1\\3\end{pmatrix} = \begin{pmatrix}5\\6\end{pmatrix},$$

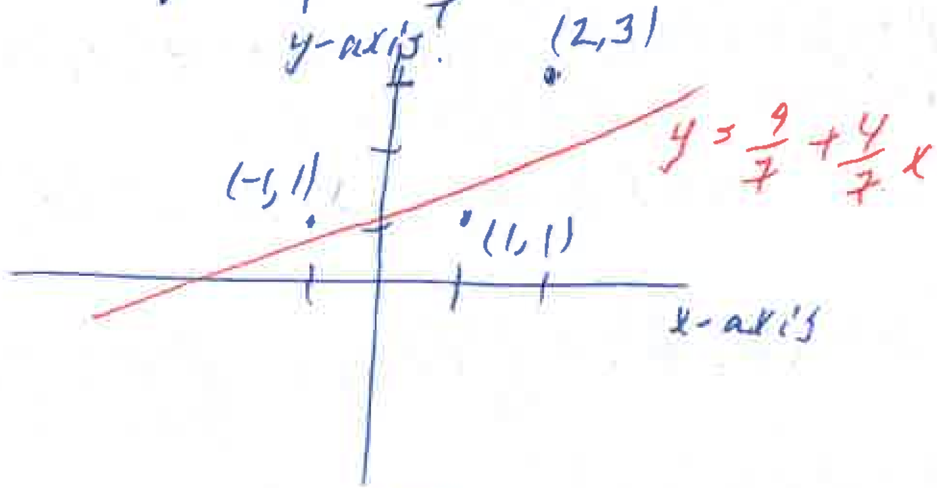
$$(A^tA)^{-1} = \frac{1}{14}\begin{pmatrix}6&-2\\-2&3\end{pmatrix}.$$

So

$$\vec{s} = \frac{1}{14}\begin{pmatrix}6&-2\\-2&3\end{pmatrix}\begin{pmatrix}5\\6\end{pmatrix} = \frac{1}{14}\begin{pmatrix}18\\8\end{pmatrix} = \begin{pmatrix}9/7\\4/7\end{pmatrix}.$$

So the line of best fit is

$$y = \frac{9}{7} + \frac{4}{7}x.$$



<u>Example 13</u> $V = \mathbb{R}^3$ with the standard inner product.

$S = \{\vec{v}_1, \vec{v}_2, \vec{v}_3\}$ with
$\vec{v}_1 = \langle 1,1,1\rangle$
$\vec{v}_2 = \langle 0,1,1\rangle$
$\vec{v}_3 = \langle 0,0,1\rangle$

Convert S into an orthonormal basis B.

<u>Step 1</u> Make $\vec{v}_1$ into a unit vector.

Let

$$\vec{b}_1 = \frac{1}{\|\vec{v}_1\|}\vec{v}_1 = \frac{1}{\sqrt{3}}\langle 1,1,1\rangle = \left\langle \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\rangle$$

and let $S_1 = \{\vec{b}_1, \vec{v}_2, \vec{v}_3\}$.

<u>Step 2</u> Make $\vec{u}_2$ orthogonal to $\vec{b}_1$.

Let

$$\vec{u}_2 = \vec{v}_2 - \langle \vec{v}_2, \vec{b}_1\rangle \vec{b}_1$$
$$= \langle 0,1,1\rangle - \frac{2}{\sqrt{3}}\left\langle \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\rangle$$
$$= \left\langle \frac{-2}{3}, \frac{1}{3}, \frac{1}{3}\right\rangle$$

and $S_2 = \{\vec{b}_1, \vec{u}_2, \vec{v}_3\}$.

<u>Step 3</u> Make $\vec{u}_2$ into a unit vector.

Let

$$\vec{b}_2 = \frac{1}{\|\vec{u}_2\|}\vec{u}_2 = \frac{1}{\frac{\sqrt{6}}{3}}\left\langle \frac{-2}{3}, \frac{1}{3}, \frac{1}{3}\right\rangle = \left\langle \frac{-2}{\sqrt{6}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{6}}\right\rangle$$

And $S_3 = \{\vec{b}_1, \vec{b}_2, \vec{v}_3\}$.

<u>Step 4</u> Make $\vec{v}_3$ orthogonal to $\vec{b}_1$ and $\vec{b}_2$.

Let

$$\vec{u}_3 = \vec{v}_3 - \langle \vec{v}_3, \vec{b}_1\rangle \vec{b}_1 - \langle \vec{v}_3, \vec{b}_2\rangle \vec{b}_2$$
$$= \langle 0,0,1\rangle - \frac{1}{\sqrt{3}}\left\langle \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\rangle - \frac{1}{\sqrt{6}}\left\langle \frac{-2}{\sqrt{6}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{6}}\right\rangle$$
$$= \left\langle -\frac{1}{3}+\frac{2}{6}, -\frac{1}{3}-\frac{1}{6}, 1-\frac{1}{3}-\frac{1}{6}\right\rangle = \left\langle 0, \frac{-1}{2}, \frac{1}{2}\right\rangle.$$

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<u>Step 5</u> Make $\vec{u}_3$ into a unit vector.

$$\vec{b}_3 = \frac{1}{\|\vec{u}_3\|}\vec{u}_3 = \frac{1}{\sqrt{\frac{2}{4}}}\left\langle 0, \frac{-1}{2}, \frac{1}{2}\right\rangle = \left\langle 0, \frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\rangle.$$

Let $B = \{\vec{b}_1, \vec{b}_2, \vec{b}_3\}$.

Then B is an orthonormal set.