Example 40. Find the least squares solution to $A\boldsymbol{x} = \boldsymbol{b}$, where

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

Solution. First, $A^T A = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}$ and $A^T \boldsymbol{b} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$.

Hence, the normal equations $A^T A \hat{\boldsymbol{x}} = A^T \boldsymbol{b}$ take the form $\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix} \hat{\boldsymbol{x}} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$.
Solving, we immediately find $\hat{\boldsymbol{x}} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$.

Check. The error $A\hat{\boldsymbol{x}} - \boldsymbol{b} = \begin{bmatrix} 2 \\ 4 \\ -8 \end{bmatrix}$ is indeed orthogonal to $\operatorname{col}(A)$. Because $\begin{bmatrix} 2 \\ 4 \\ -8 \end{bmatrix} \cdot \begin{bmatrix} 4 \\ 0 \\ 1 \end{bmatrix} = 0$ and $\begin{bmatrix} 2 \\ 4 \\ -8 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix} = 0$.

Definition 41. The **(orthogonal) projection** $\hat{\boldsymbol{b}}$ of a vector $\boldsymbol{b}$ onto a subspace Y is the vector in Y closest to $\boldsymbol{b}$.

The (orthogonal) projection $\hat{\boldsymbol{b}}$ of $\boldsymbol{b}$ onto $\operatorname{col}(A)$ is $\hat{\boldsymbol{b}} = A\hat{\boldsymbol{x}}$.
Here, $\hat{\boldsymbol{x}}$ is a least squares solution to $A\boldsymbol{x} = \boldsymbol{b}$ (i.e. $\hat{\boldsymbol{x}}$ solves $A^T A \hat{\boldsymbol{x}} = A^T \boldsymbol{b}$).

Why? Why is $A\hat{\boldsymbol{x}}$ the projection of $\boldsymbol{b}$ onto $\operatorname{col}(A)$?
Because, for a least squares solution $\hat{\boldsymbol{x}}$, $A\hat{\boldsymbol{x}} - \boldsymbol{b}$ is as small as possible.

Note. This is a recipe for computing any orthogonal projection! That's because every subspace Y can be written as $\operatorname{col}(A)$ for some choice of the matrix A (take, for instance, A so that its columns are a basis for Y).

Example 42. What is the orthogonal projection of $\begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$ onto $\operatorname{span}\left\{ \begin{bmatrix} 4 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix} \right\}$?

Solution. This is the same question as: what is the projection of $\boldsymbol{b}$ onto $\operatorname{col}(A)$, with A and $\boldsymbol{b}$ as in the previous example.

The projection of $\boldsymbol{b}$ onto $\operatorname{Col}(A)$ is $A\hat{\boldsymbol{x}} = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 4 \\ 4 \\ 3 \end{bmatrix}$.

Example 43. (extra homework)

(a) What is the orthogonal projection of $\begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$ onto $\operatorname{span}\left\{ \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \right\}$?

(b) What is the orthogonal projection of $\begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$ onto $\operatorname{span}\left\{ \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \right\}$?

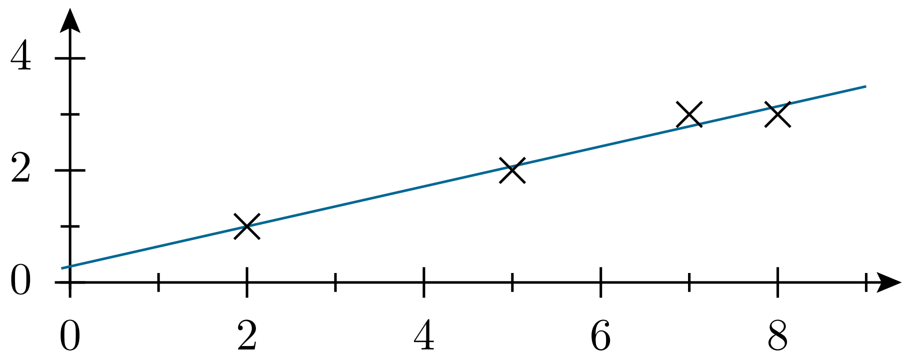
Solution. (final answer only) The projections are $\left(\frac{11}{6}, \frac{1}{3}, \frac{7}{6}\right)^T$ and $\left(\frac{3}{2}, 0, \frac{3}{2}\right)^T$.

Armin Straub
straub@southalabama.edu

Application: least squares lines

Experimental data: (x_i, y_i)

Wanted: parameters a, b such that $y_i \approx a + bx_i$ for all i



This approximation should be so that $\mathrm{SS}_{\mathrm{res}} = \underbrace{\sum_i [y_i - (a + bx_i)]^2}_{\text{residual sum of squares}}$ is as small as possible.

Example 44. Determine the line that best fits the data points $(2,1), (5,2), (7,3), (8,3)$.

Solution. We need to determine the values a, b for the best-fitting line $y = a + bx$.
If there was a line that fit the data perfectly, then:

$$\begin{aligned} a + 2b &= 1 \qquad (2,1) \\ a + 5b &= 2 \qquad (5,2) \\ a + 7b &= 3 \qquad (7,3) \\ a + 8b &= 3 \qquad (8,3) \end{aligned}$$

In matrix form, this is: $\underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ 1 & x_4 \end{bmatrix}}_{\text{design matrix } X} \begin{bmatrix} a \\ b \end{bmatrix} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}}_{\text{observation vector } \boldsymbol{y}}$ (writing the points as (x_i, y_i))

Using our points, these equations become $\begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}$. [This system is inconsistent (as expected).]

We compute a least squares solution.

$$X^T X = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} = \begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix}, \qquad X^T \boldsymbol{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}.$$

Solving the normal equations $\begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$, we find $\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 2/7 \\ 5/14 \end{bmatrix}$.

Hence, the least squares line is $y = \frac{2}{7} + \frac{5}{14}x$.

The plot above shows our points together with this line. It does look like a very good fit!

Armin Straub
straub@southalabama.edu

Let's repeat the computation we just did. This time, we let Sage do the actual work for us:

```
Sage] X = matrix([[1,2],[1,5],[1,7],[1,8]]); y = vector([1,2,3,3])
```

```
Sage] (X.transpose()*X).solve_right(X.transpose()*y)
```

$$\left(\frac{2}{7}, \frac{5}{14}\right)$$

Here are some intermediate steps to help see what's going on (and that it matches our work):

```
Sage] X.transpose()*X
```

$$\left[\begin{array}{rr} 4 & 22 \\ 22 & 142 \end{array}\right]$$

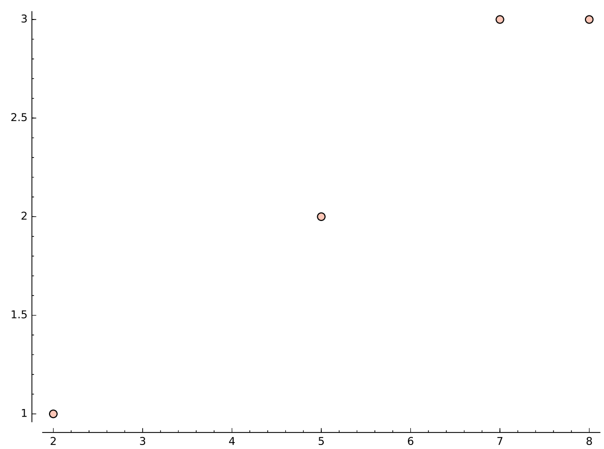
```
Sage] X.transpose()*y
```

$$(9, 57)$$

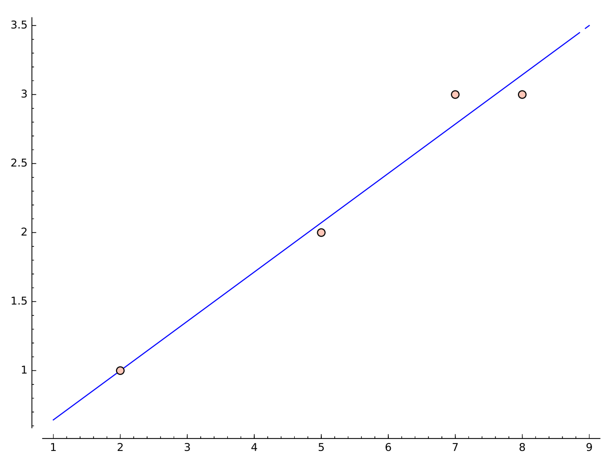
Let's plot the least squares line $y = \frac{2}{7} + \frac{5}{14}x$ in Sage to marvel at the good fit!

```
Sage] points = [[2,1],[5,2],[7,3],[8,3]]
```

```
Sage] scatter_plot(points)
```




```
Sage] scatter_plot(points) + plot(2/7+5/14*x,1,9)
```



Armin Straub
straub@southalabama.edu