Example 49. (again) Determine the least squares line for the points $(2,1),(5,2),(7,3),(8,3)$.

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

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

```
>>> (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 earlier work):

```
>>> X.transpose()*X
```

$$\begin{pmatrix} 4 & 22 \\ 22 & 142 \end{pmatrix}$$

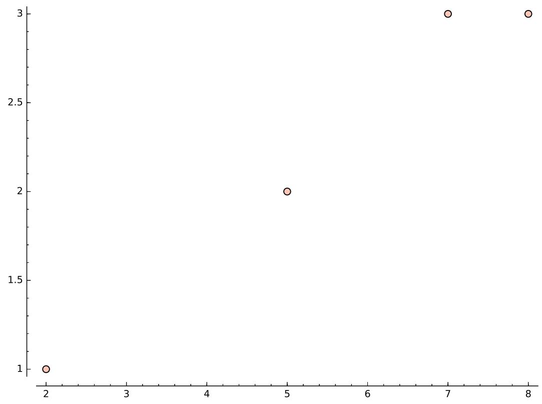
```
>>> X.transpose()*y
```

$$(9,\ 57)$$

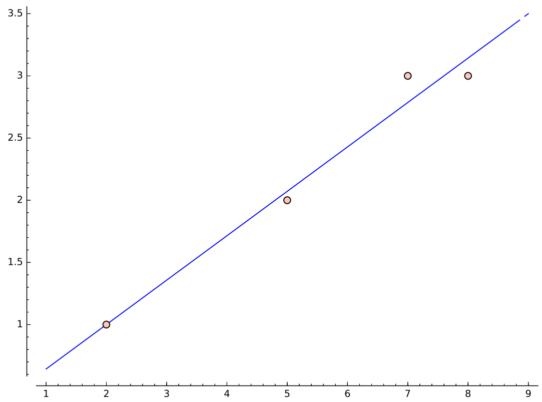
Let's plot the least squares line $y = \frac{2}{7} + \frac{5}{14}x$ in Sage to marvel at the good fit!

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

```
>>> scatter_plot(points)
```



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



Comment. As mentioned earlier, the least squares line minimizes the (sum of squares of the) vertical offsets:

http://mathworld.wolfram.com/LeastSquaresFitting.html

Comment. We get a (slightly) different "best fit" line if we change the role of x and y! Can you explain that?

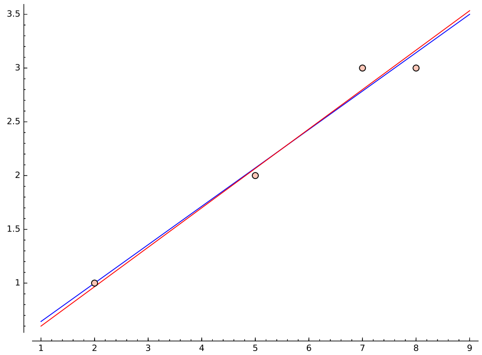
```
>>> X = matrix([[1,1],[1,2],[1,3],[1,3]]); y = vector([2,5,7,8])
```

```
>>> (X.transpose()*X).solve_right(X.transpose()*y)
```

$$\left(-\frac{7}{11}, \frac{30}{11}\right)$$

Note that $x = -\frac{7}{11} + \frac{30}{11}y$ is equivalent to $y = \frac{7}{30} + \frac{11}{30}x$.

```
>>> scatter_plot([[2,1],[5,2],[7,3],[8,3]]) + plot(2/7+5/14*x,1,9) + plot(7/30+11/30*x,1,
    9,color='red')
```



The explanation is that (see pictures at the beginning of this example) we are minimizing vertical offsets in one case and horizontal offsets in the other case.

In linear regression, the relationship between a dependent variable and one or more explanatory variables is modeled. If y is the dependent variable, with x the explanatory variable, then it is natural to minimize the error we make in "predicting y through x" (vertical offsets). See next example.

Example 50. A car rental company wants to predict the annual maintenance cost y (in 100USD/year) of a car using the age x (in years) of that car (as an explanatory variable). Based on the observations $(x, y) = (2, 1), (5, 2), (7, 3), (8, 3)$, predict the cost for a 4.5 year old car (using linear regression).

Solution. Once we compute the regression line $y = a + bx$ (we already did that: $y = \frac{2}{7} + \frac{5}{14}x$), our prediction is $\frac{2}{7} + \frac{5}{14} \cdot 4.5 = \frac{53}{28} \approx 1.89$, that is, 189 USD/year.

Application: multiple linear regression

> *In statistics,* ***linear regression*** *is an approach for modeling the relationship between a scalar dependent variable and one or more explanatory variables.*
>
> *The case of one explanatory variable is called simple linear regression.*
>
> *For more than one explanatory variable, the process is called multiple linear regression.*
>
> http://en.wikipedia.org/wiki/Linear_regression

The experimental data might be of the form (x_i, y_i, z_i), where now the dependent variable z_i depends on two explanatory variables x_i, y_i (instead of just x_i).

Example 51. Set up a linear system to find values for the parameters a, b, c such that $z = a + bx + cy$ best fits some given points $(x_1, y_1, z_1), (x_2, y_2, z_2), \ldots$

Solution. The equations $a + bx_i + cy_i = z_i$ translate into the system:

$$\underbrace{\begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \\ \vdots & \vdots & \vdots \end{bmatrix}}_{\text{design matrix } A} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \underbrace{\begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \end{bmatrix}}_{\substack{\text{observation} \\ \text{vector} \boldsymbol{z}}}$$

Of course, this is usually inconsistent. To find the best possible a, b, c we compute a least squares solution by solving $A^T A \begin{bmatrix} a \\ b \\ c \end{bmatrix} = A^T \boldsymbol{z}$.

Application: Fitting data to other curves

We can also fit the experimental data (x_i, y_i) using other curves.

Example 52. Set up a linear system to find values for the parameters a, b, c that result in the quadratic curve $y = a + bx + cx^2$ that best fits some given points $(x_1, y_1), (x_2, y_2), \ldots$

Solution. $y_i \approx a + bx_i + cx_i^2$ with parameters a, b, c.
The equations $y_i = a + bx_i + cx_i^2$ in matrix form:

$$\underbrace{\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ \vdots & \vdots & \vdots \end{bmatrix}}_{\text{design matrix} A} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{bmatrix}}_{\substack{\text{observation} \\ \text{vector } \boldsymbol{y}}}$$

Again, we determine values for a, b, c by computing a least squares solution to that system.

That is, we need to solve the system $A^T A \begin{bmatrix} a \\ b \\ c \end{bmatrix} = A^T \boldsymbol{y}$.

Example 53. (homework) Use Sage to find values for a, b, c that result in the quadratic curve $y = a + bx + cx^2$ that best fits the points $(0,1), (1,2), (2,3), (3,-4), (4,-7), (5,-12)$.

Solution. We first input the points:

```
>>> points = [[0,1],[1,2],[2,3],[3,-4],[4,-7],[5,-12]]
```

We set up the system described in the previous example, then determine a least-squares solution.

```
>>> X = matrix([[1,0,0],[1,1,1],[1,2,4],[1,3,9],[1,4,16],[1,5,25]])
```

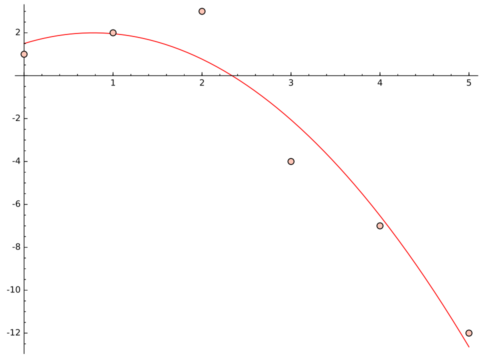
```
>>> y = vector([1,2,3,-4,-7,-12])
```

```
>>> (X.transpose()*X).solve_right(X.transpose()*y)
```

$$\left(\frac{3}{2}, \frac{179}{140}, -\frac{23}{28}\right)$$

Hence, the best fitting quadratic curve is $y = \frac{3}{2} + \frac{179}{140} - \frac{23}{28}x^2$. Here's a plot:

```
>>> scatter_plot(points) + plot(3/2+179/140*x-23/28*x^2,0,5,color='red')
```



Advanced comment. If you are comfortable with Python, you can avoid typing out X and $\boldsymbol{y}$:
[The plot command above now won't work anymore because we are overwriting x with numbers.]

```
>>> X = matrix([[1,x,x^2] for x,y in points])
```

```
>>> y = vector([y for x,y in points])
```