Linear Regression

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Outline

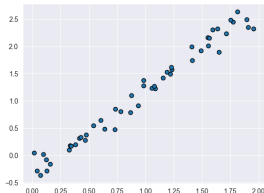Overview of linear regression

The procedure

Implementing the procedure

Examples

- Setting: have points in the plane, P of them. Say the points are $(x_1, y_1), (x_2, y_2), \ldots, (x_P, y_P)$.
- **Goal:** *Model* them as "approximately" coming from a line (or, being "noisy" samples from line), finding "best fit" line. This line is also called the **least squares regression** (LSR) line.

The goal

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- **Goal:** *Model* them as "approximately" coming from a line (or, being "noisy" samples from line), finding "best fit" line. This line is also called the **least squares regression** (LSR) line.

- **Running example:** A simulated data set, `'Example1.csv'`, with $P = 50$ points, is available here; these points are displayed in the plot below.

Outline

Finding the LSR line

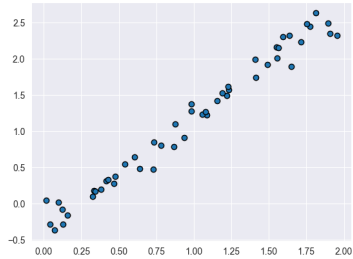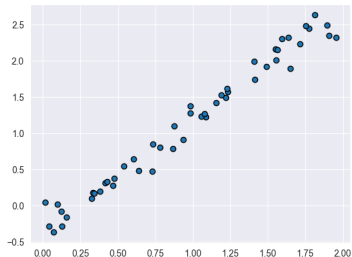**Figure 1:** Our running example

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How do we find the LSR line?

NumPy will do this: if x, y are the arrays containing the *x*- and *y*-coordinates, the slope and intercept for LSR line are given by:

```
np.polyfit(x,y,1)
```

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- If a slope w and intercept b existed so that $(x_1, y_1), \ldots, (x_{50}, y_{50})$ *were* points on $y = wx + b$, then

$$y_i = wx_i + b$$

would hold for all $1 \leq i \leq 50$.

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1. Write those 50 equations as a matrix equation. Setting:

$$A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_{50} \end{bmatrix} ; \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{50} \end{bmatrix},$$

and writing[1] $\tilde{\mathbf{w}} = \begin{bmatrix} b \\ w \end{bmatrix}$, the matrix equation is $A\tilde{\mathbf{w}} = \mathbf{y}$.

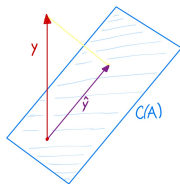[1] Will use $\tilde{\mathbf{w}}$ for this vector, for the rest of these slides.

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- Find a $\hat{\mathbf{y}}$ *as close to* $\mathbf{y}$ *as possible* so that $A\tilde{\mathbf{w}} = \hat{\mathbf{y}}$ has a solution. For each i, making a (hopefully small) change $y_i \rightsquigarrow \hat{y}_i$ to get $\hat{\mathbf{y}}$.

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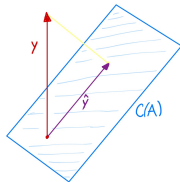**Considering points as approx. on a line:** (*noise in y-coordinate direction*)

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2. Done by solving
   $A^T A\tilde{\mathbf{w}} = A^T\mathbf{y}$ (normal equations).
   If solution is $\tilde{\mathbf{w}}^\star = \begin{bmatrix} b^\star \\ w^\star \end{bmatrix}$, then
   $\hat{\mathbf{y}} = A\tilde{\mathbf{w}}^\star$.

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Related to orthogonal vectors in $\mathbb{R}^P$ (in the example, $\mathbb{R}^{50}$).

- $\mathbf{y} = \mathbf{z}_1 + \mathbf{z}_2$, for some $\mathbf{z}_1$ in null space of A^T, $\mathbf{z}_2$ in column space of A.
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- $\mathbf{z}_2$ is closest to $\mathbf{y}$ (in col. space), since $\mathbf{z}_1$ is orthogonal to column space: $\mathbf{z}_2 = \hat{\mathbf{y}}$.
- As $\mathbf{z}_2$ in column space, $\exists \tilde{\mathbf{w}}^\star$ so that $A\tilde{\mathbf{w}}^\star = \mathbf{z}_2 = \hat{\mathbf{y}}$. But then,

$$A^T(A\tilde{\mathbf{w}}^\star) = A^T \mathbf{z}_2 = A^T(\mathbf{y} - \mathbf{z}_1) = A^T \mathbf{y}.$$

So the $\tilde{\mathbf{w}}^\star$ that you want must be a solution to the normal equations.

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So, three steps:

1. Write the P equations in matrix form. (get matrix A, vector $\mathbf{y}$)
2. Get matrix $A^T A$ and vector $A^T \mathbf{y}$ for normal equations.
3. Use a method to solve normal equations for $\tilde{\mathbf{w}}$.

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Solving normal equation, in pseudocode

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Given $(x_1, y_1), (x_2, y_2), \ldots, (x_P, y_P)$, as a NumPy array (call it D, with shape (P, 2)):

```
A ← [ [x1, 1], ..., [xP, 1] ] # 2-column matrix
y ← y-coordinate array
# next, get 2x2 matrix and 2-vector
Compute A.T times A; compute A.T times y
Solve normal eq'ns (e.g., using inverse)
return solution
```

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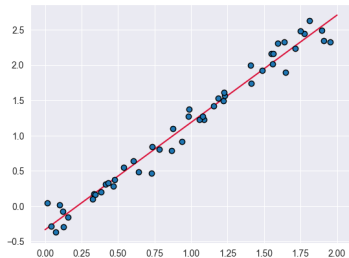
($b^\star = -0.33458$ and $w^\star = 1.520275$)

A plot of the line (in red), alongside the points, looks as follows.

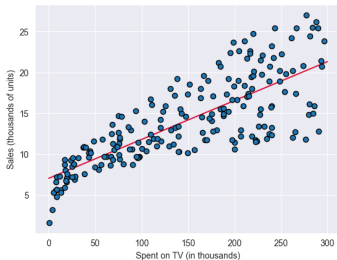## Another example, Advertising data

In the DataSets folder, the `'Advertising.csv'` file contains data on amounts spent (in thousands of dollars) on TV, Radio, and Newspaper advertising in 200 different markets, as well as the amounts sold in each market (in thousands of units).
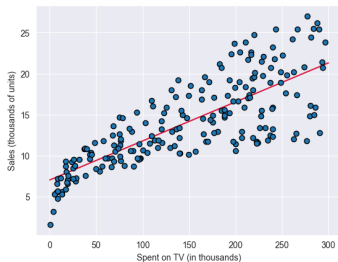
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We will look more at this data later. For now, plotted here are the columns (`'TV'`, `'Sales'`).
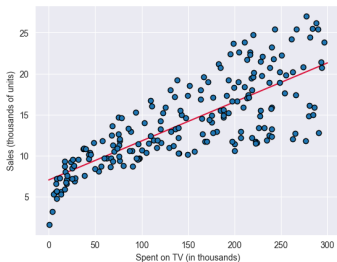
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The LSR line for the data is then **not** the same line, if you switch the roles of TV and Sales in the algorithm to get $\tilde{\mathbf{w}}^\star$. (Use domain knowledge.)