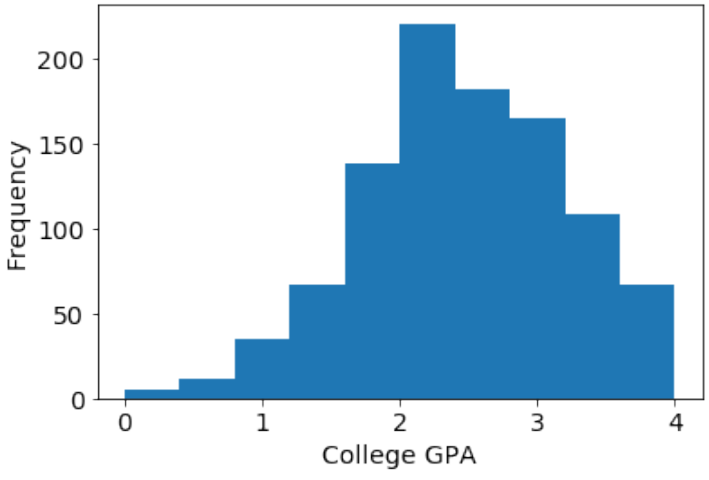
Linear regression

Linear regression

Fitting a line to a bunch of points.

Example: college GPAs

Distribution of GPAs of students at a certain Ivy League university.



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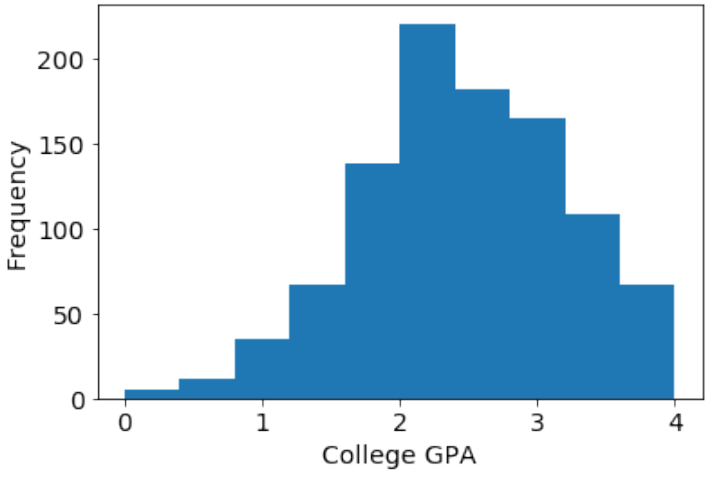

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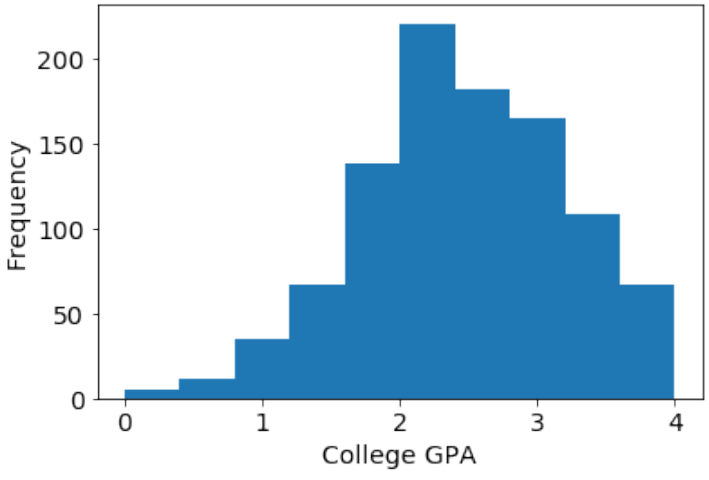

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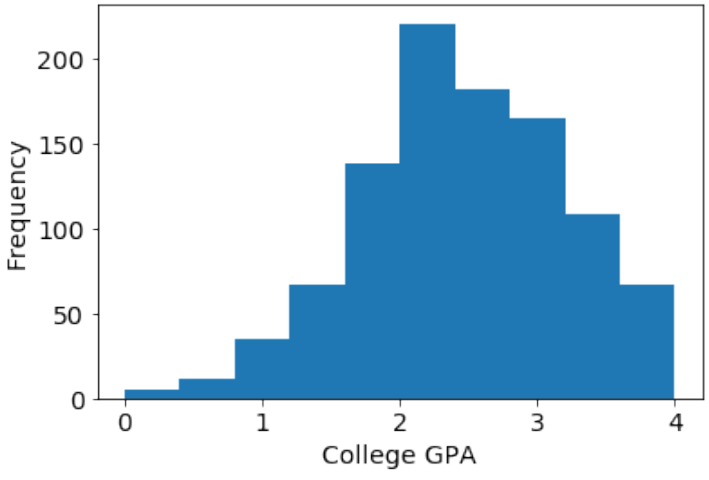

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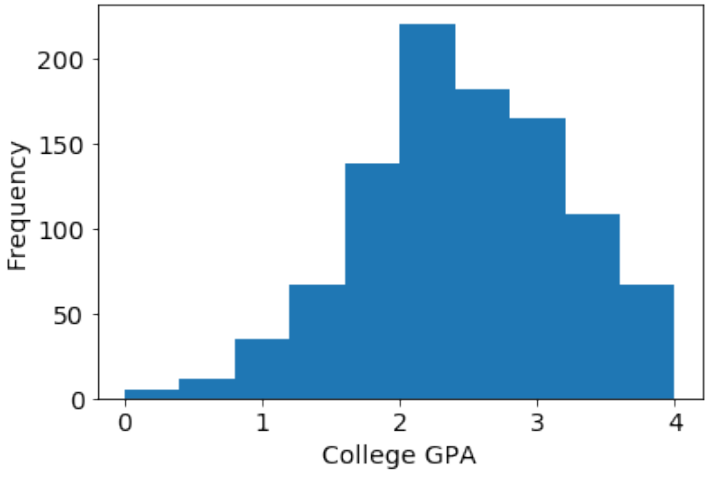

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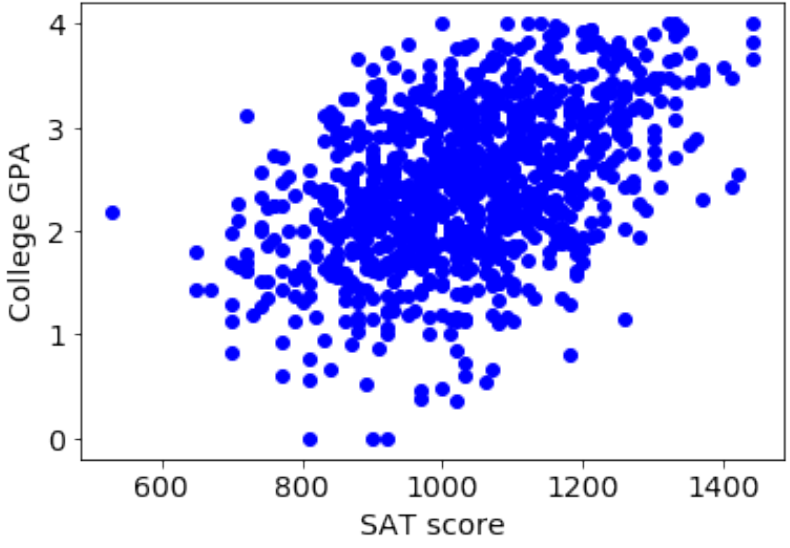
- What is the average squared error of this prediction? That is, $\mathbb{E}[((\text{student's GPA}) - (\text{predicted GPA}))^2]$? The **variance** of the distribution, 0.55.

Better predictions with more information

We also have SAT scores of all students.



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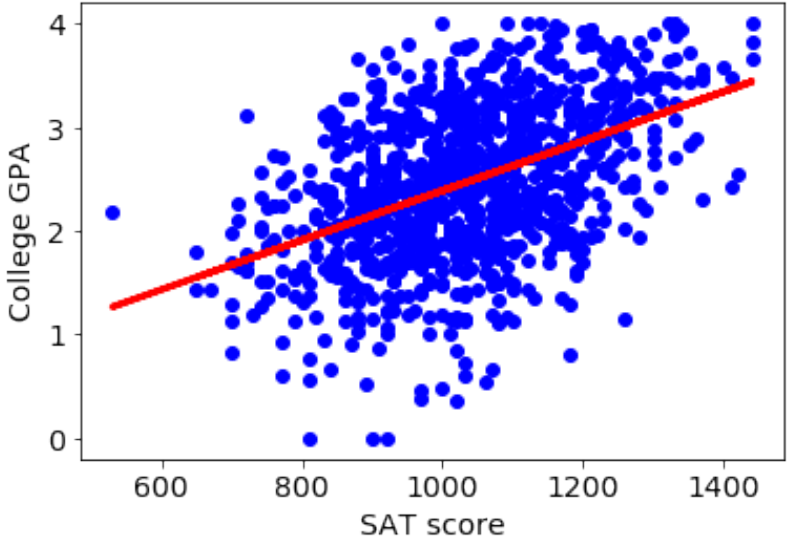

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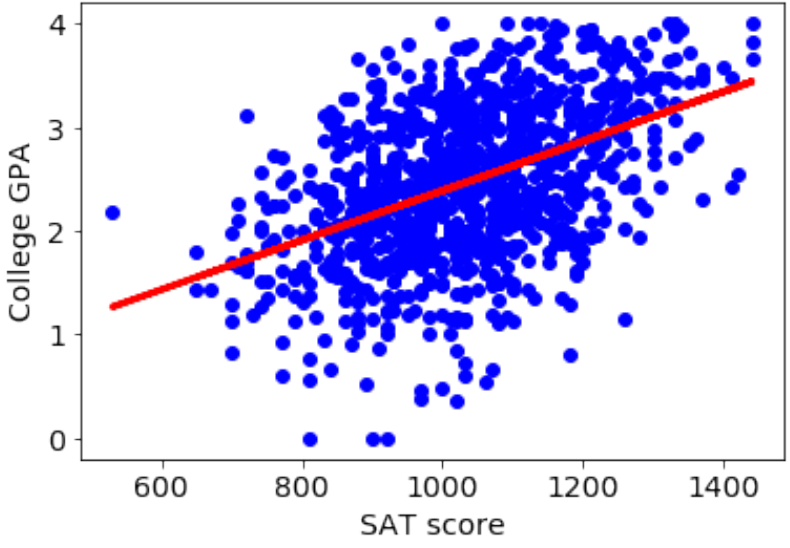

Mean squared error (MSE) drops to 0.43.

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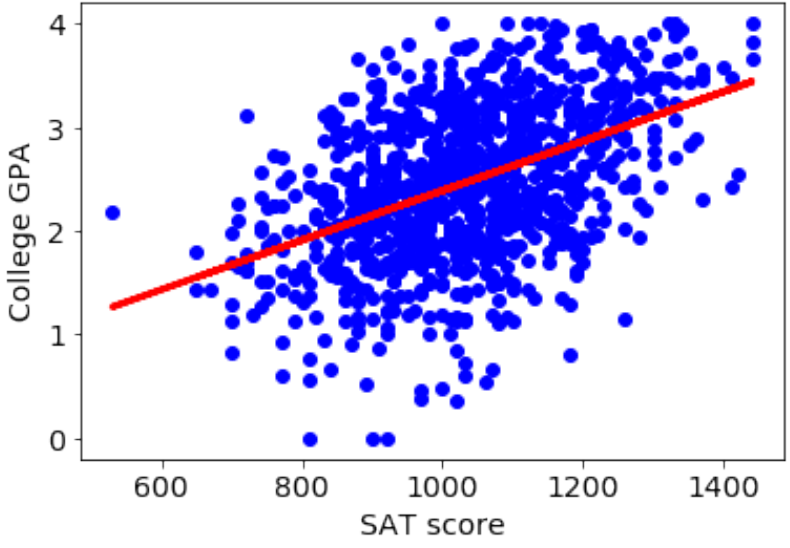

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This is a **regression** problem with:

- **Predictor variable**: SAT score
- **Response variable**: College GPA

Parametrizing a line

A line can be parameterized as $y = ax + b$ (a: slope, b: intercept).

The line fitting problem

Pick a line (a, b) based on $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R} \times \mathbb{R}$

- $x^{(i)}, y^{(i)}$ are predictor and response variables.
  E.g. SAT score, GPA of ith student.
- Minimize the mean squared error,

$$\text{MSE}(a, b) = \frac{1}{n} \sum_{i=1}^{n} (y^{(i)} - (ax^{(i)} + b))^2.$$

This is the **loss function**.

Minimizing the loss function

Given $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})$, minimize

$$L(a, b) = \sum_{i=1}^{n} (y^{(i)} - (ax^{(i)} + b))^2.$$

Multivariate regression: diabetes study

Data from $n = 442$ diabetes patients.

For each patient:

- 10 features $x = (x_1, \ldots, x_{10})$

  age, sex, body mass index, average blood pressure, and six blood serum measurements.

- A real value y: the progression of the disease a year later.

Regression problem:

- **response** $y \in \mathbb{R}$
- **predictor variables** $x \in \mathbb{R}^{10}$

Least-squares regression

Linear function of 10 variables: for $x \in \mathbb{R}^{10}$,

$$f(x) \;=\; w_1 x_1 + w_2 x_2 + \cdots + w_{10} x_{10} + b \;=\; w \cdot x + b$$

where $w = (w_1, w_2, \ldots, w_{10})$.

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Least-squares regression:

- *Given:* data $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^d \times \mathbb{R}$
- *Return:* linear function given by $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$
- *Goal:* minimize the **loss function**

$$L(w, b) = \sum_{i=1}^{n} (y^{(i)} - (w \cdot x^{(i)} + b))^2.$$

Back to the diabetes data

- No predictor variables: mean squared error (MSE) = 5930

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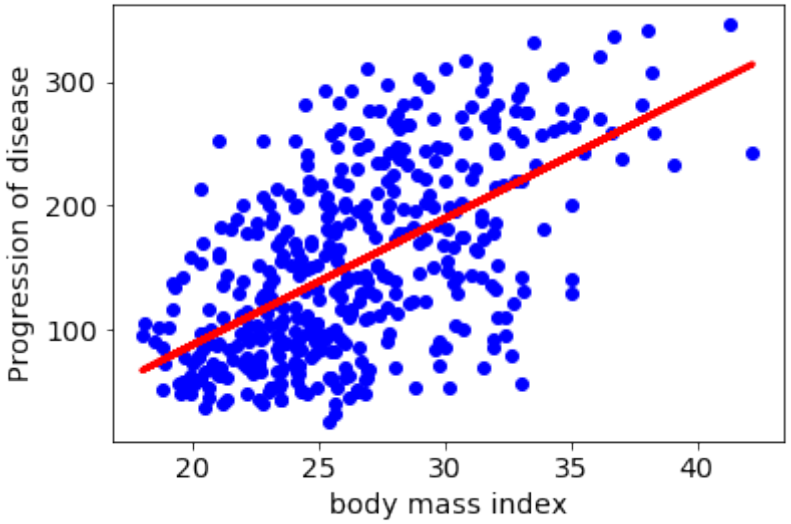

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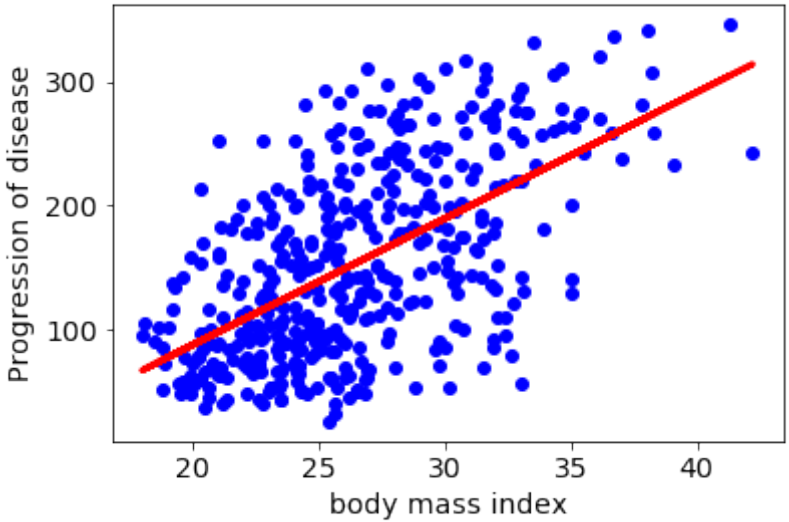

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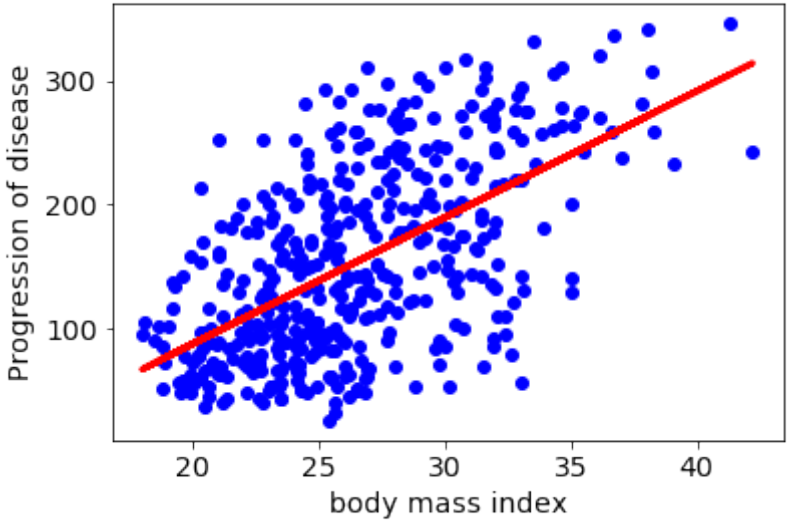

- Two predictors ('bmi', 'serum5'): MSE = 3205
- All ten predictors: MSE = 2860

Least-squares solution 1

Linear function of d variables given by $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$:

$$f(x) = w_1 x_1 + w_2 x_2 + \cdots + w_d x_d + b = w \cdot x + b$$

$$\begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix} \quad \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \rightarrow d \text{ dim}$$

$$\tilde{w} = \begin{bmatrix} b \\ w_1 \\ \vdots \\ w_d \end{bmatrix} \qquad \tilde{x} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}$$

$(d+1)$ - dim.

$$\langle \tilde{w}, \tilde{x} \rangle = \sum_{i=1}^{d+1} \tilde{w}_i \tilde{x}_i$$

$$= b + \sum_{i=1}^{d} w_i x_i$$

$$= b + \langle w, x \rangle$$

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Assimilate the intercept b into w:

- Add a new feature that is identically 1: let $\widetilde{x} = (1, x) \in \mathbb{R}^{d+1}$

$$\begin{pmatrix} 4 & 0 & 2 & \cdots & 3 \end{pmatrix} \Longrightarrow \begin{pmatrix} 1 & 4 & 0 & 2 & \cdots & 3 \end{pmatrix}$$

- Set $\widetilde{w} = (b, w) \in \mathbb{R}^{d+1}$
- Then $f(x) = w \cdot x + b = \widetilde{w} \cdot \widetilde{x}$

Goal: find $\widetilde{w} \in \mathbb{R}^{d+1}$ that minimizes

$$L(\widetilde{w}) = \sum_{i=1}^{n} \left(y^{(i)} - \widetilde{w} \cdot \widetilde{x}^{(i)} \right)^2$$

predicted value

actual response

Least-squares solution 2

Write

$$X = \begin{pmatrix} \longleftarrow & \widetilde{x}^{(1)} & \longrightarrow \\ \longleftarrow & \widetilde{x}^{(2)} & \longrightarrow \\ & \vdots & \\ \longleftarrow & \widetilde{x}^{(n)} & \longrightarrow \end{pmatrix}, \quad y = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{pmatrix}$$

X ↓ data matrix

$n \times (d+1)$

Then the loss function is

$$L(\widetilde{w}) = \sum_{i=1}^{n} (y^{(i)} - \widetilde{w} \cdot \widetilde{x}^{(i)})^2 = \|y - X\widetilde{w}\|^2$$

and it minimized at $\widetilde{w} = (X^T X)^{-1}(X^T y)$.

$(d+1) \times 1$.

$(d+1) \times (d+1)$ $(d+1) \times n$, $n \times 1$

$(d+1) \times 1$

Generalization behavior of least-squares regression

Given a **training set** $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^d \times \mathbb{R}$, find a linear function, given by $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$, that minimizes the squared loss

$$L(w, b) = \sum_{i=1}^{n} (y^{(i)} - (w \cdot x^{(i)} + b))^2.$$

Is training loss a good estimate of **future** performance?

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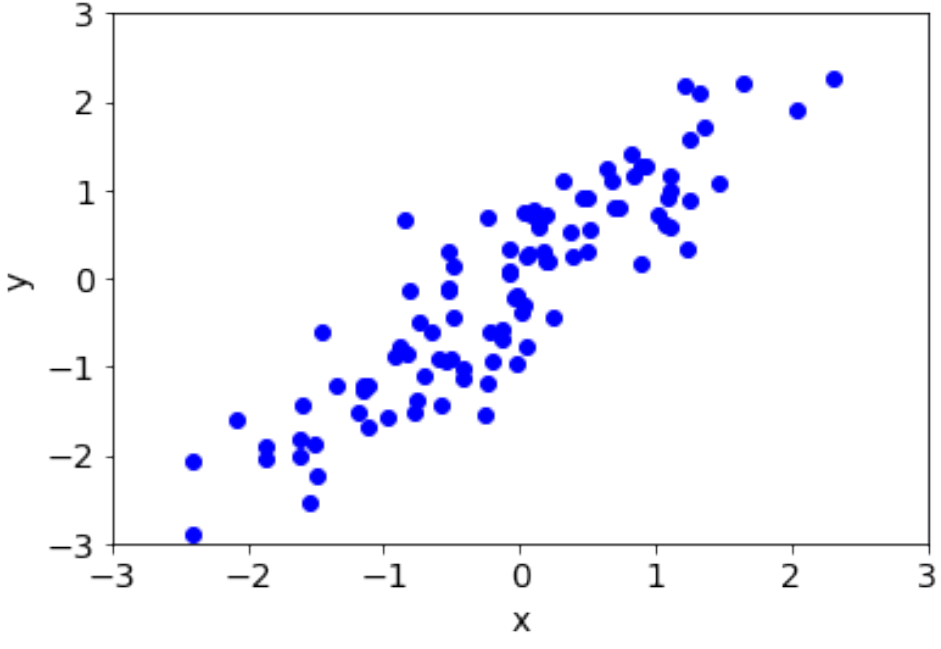
Is training loss a good estimate of **future** performance?

- If n is large enough: maybe.
- Otherwise: probably an underestimate.

Example



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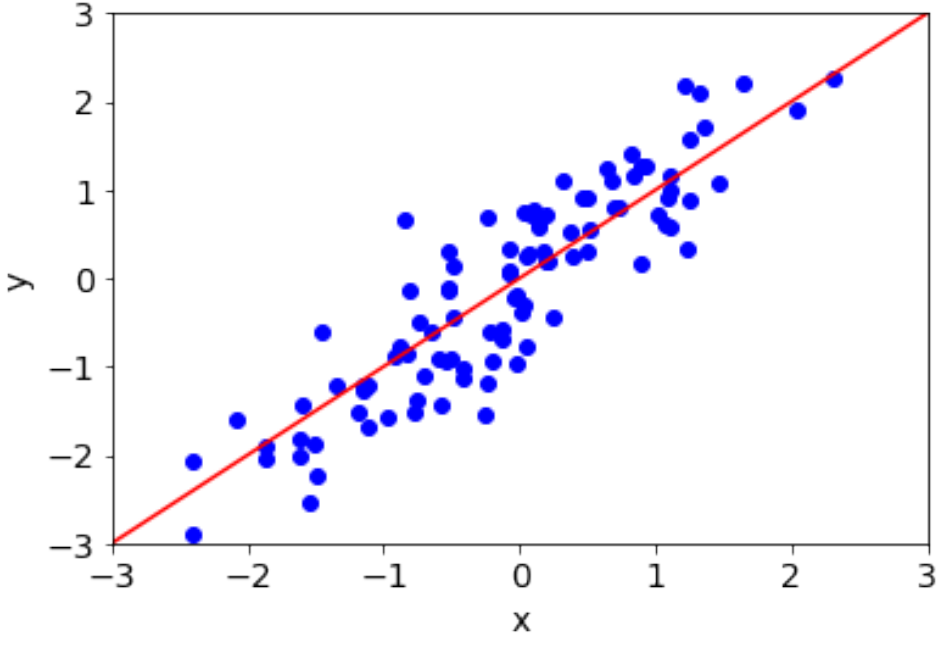

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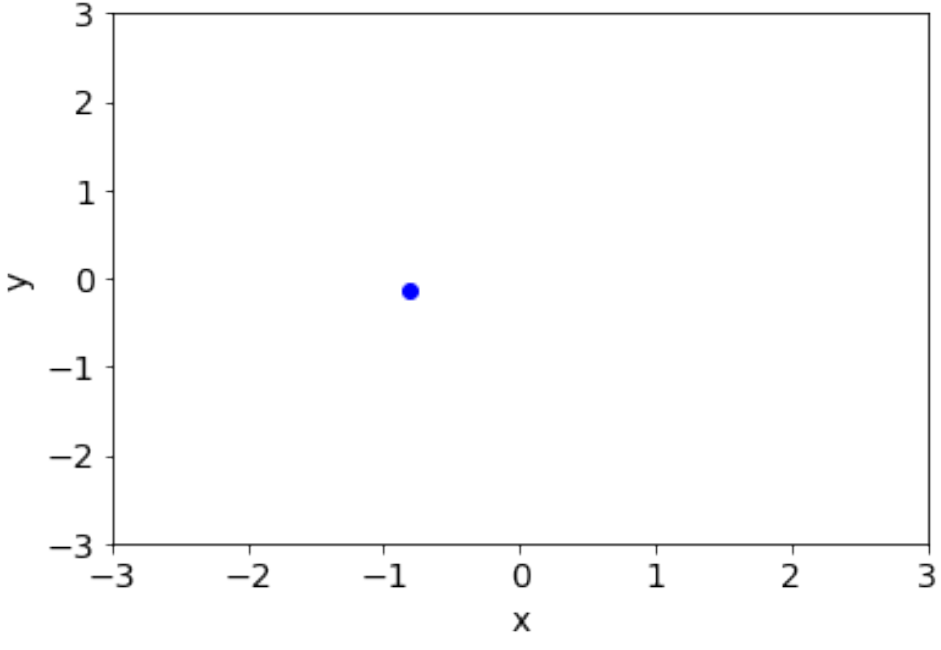


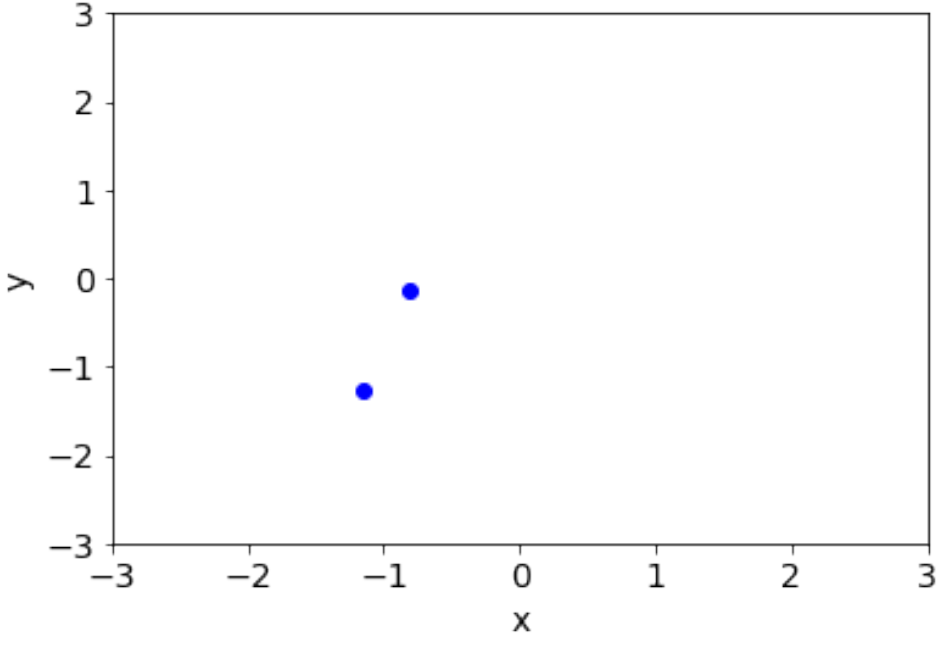
Example

$y^{(i)} = \langle w, x^{(i)} \rangle + b$

So $\text{Loss}(w, b) = \sum_i \left(y^{(i)} - (\langle w, x^{(i)} \rangle + b) \right)^2$

$y^{(i)} - (\langle w, x^{(i)} \rangle + b) = 0$

$= 0$



Better error estimates

Recall: k-**fold cross-validation**

- Divide the data set into k equal-sized groups $S_1, \ldots, S_k$
- For $i = 1$ to k:
  - Train a regressor on all data except S_i
  - Let E_i be its error on S_i
- Error estimate: average of $E_1, \ldots, E_k$

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A nagging question:
When n is small, should we be minimizing the squared loss?

$$L(w, b) = \sum_{i=1}^{n} (y^{(i)} - (w \cdot x^{(i)} + b))^2$$

Ridge regression

Minimize squared loss **plus** a term that penalizes "complex" w:

$$L(w, b) = \sum_{i=1}^{n} (y^{(i)} - (w \cdot x^{(i)} + b))^2 + \lambda \|w\|^2$$

Adding a penalty term like this is called **regularization**.

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Put predictor vectors in matrix X and responses in vector y:

$$w = (X^T X + \lambda I)^{-1} (X^T y)$$

Toy example

Training, test sets of 100 points

- $x \in \mathbb{R}^{100}$, each feature x_i is Gaussian $N(0, 1)$
- $y = x_1 + \cdots + x_{10} + N(0, 1)$

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λ	training MSE	test MSE
0.00001	0.00	585.81
0.0001	0.00	564.28
0.001	0.00	404.08
0.01	0.01	83.48
0.1	0.03	19.26
1.0	0.07	7.02
10.0	0.35	2.84
100.0	2.40	5.79
1000.0	8.19	10.97
10000.0	10.83	12.63

The lasso

Popular "shrinkage" estimators:

- **Ridge regression**

$$L(w, b) = \sum_{i=1}^{n} (y^{(i)} - (w \cdot x^{(i)} + b))^2 + \lambda \|w\|_2^2$$

- **Lasso**: tends to produce sparse w

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Toy example:
Lasso recovers 10 relevant features plus a few more.