Lecture 25:

Regression

Prediction

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What's the "best" guess about Y's value?

By "best" we mean minimizes mean squared error.

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$$\alpha = \mathbb{E}\,Y.$$

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the minimum mean squared error is 

Proof: $\mathbb{E}[(Y-\alpha)^2] = \mathbb{E}[Y^2] - 2\alpha\mathbb{E}[Y] + \alpha^2$

This is a parabola in α $a\alpha^2 + b\alpha + c$

with minimal value at $\alpha = \frac{-b}{2a} = \frac{2\mathbb{E}Y}{2} = \mathbb{E}Y.$

Prediction

Suppose X, Y are some r.v.

Suppose we learned X's value.

What's the best guess for Y's value?

Recap

Multiple Random Variables

Joint Distribution: If X and Y are two r.v.s over the same probability space then their joint distribution is defined as

$$\{(a, b, Pr[X=a, Y=b]) : a \in range(X), b \in range(Y)\}$$

Marginal Distributions

Marginal for X: $Pr[X=a] = \sum_{b \in range(Y)} Pr[X=a, Y=b]$

Marginal for Y: $Pr[Y=b] = \sum_{a \in range(X)} Pr[X=a, Y=b]$

Recap

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Joint Distribution:

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Marginal for X:

$$Pr[X=a] = \sum_{b \in range(Y)} Pr[X=a, Y=b]$$

Marginal for Y:

$$Pr[Y=b] = \sum_{a \in range(X)} Pr[X=a, Y=b]$$

Example:

X \ Y	1	2	3
1	0	0.1	0.2
2	0.3	0	0
3	0.1	0.2	0.1

$Pr[X=1] =$

$Pr[Y=3] =$

$Pr[X=1 \mid Y=3] =$

Conditional Expectation

Defn: Let X and Y be r.v.s over Ω.

The conditional expectation of Y given X is defined as

$$\mathbb{E}[Y|X] = g(X)$$

where

$$g(x) = \mathbb{E}[Y|X=x] = \sum_y y \cdot \Pr[Y=y \mid X=x].$$

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Note: $\mathbb{E}[Y|X]$ is a r.v. that is a func. of X.

$\forall x$: $\mathbb{E}[Y|X=x]$ is a number.

Properties of Conditional Expectation

$$\mathbb{E}[Y|X=x] = \sum_y y \cdot \Pr[Y=y|X=x]$$

1. If X, Y indep. $\Rightarrow$ $\mathbb{E}[Y|X] = \mathbb{E}[Y]$.
2. $\mathbb{E}[aY+b|X] = a\,\mathbb{E}[Y|X] + b$
3. $\forall$ fnc $h(\cdot)$ $\quad \mathbb{E}[h(X)Y|X] = h(X)\cdot\mathbb{E}[Y|X]$.
4. $\mathbb{E}[\mathbb{E}[Y|X]] = \mathbb{E}[Y]$
5. $\forall$ fnc $h(\cdot)$ $\quad \mathbb{E}[h(x)\,\mathbb{E}[Y|X]] = \mathbb{E}[h(x)\cdot Y]$.

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4. $\mathbb{E}[\mathbb{E}[Y|X]] = \mathbb{E}[Y]$
5. $\forall$ fnc $h(\cdot)$ $\quad \mathbb{E}[h(X)\mathbb{E}[Y|X]] = \mathbb{E}[h(X)\cdot Y]$

Proof: (1) true, by definition. (2) true, by linearity of expectation.

(3) For any x, $\mathbb{E}[h(x)\cdot Y|X=x] = h(x)\cdot\mathbb{E}[Y|X=x]$.

(4) $$\mathop{\mathbb{E}}_{X}\left[\mathop{\mathbb{E}}_{Y}[Y|X]\right] = \sum_x \Pr[X=x]\cdot\sum_y y\cdot\Pr[Y=y|X=x]$$

$$= \sum_y y\cdot\underbrace{\sum_x \Pr[X=x]\cdot\Pr[Y=y|X=x]}_{\Pr[Y=y]} = \mathbb{E}[Y].$$

5. For any $h(\cdot)$ $\quad \mathop{\mathbb{E}}_{X}[h(x) \mathop{\mathbb{E}}_{Y}[Y|x]] = \mathop{\mathbb{E}}_{X,Y}[h(x)Y]$.

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Proof:

$$\mathop{\mathbb{E}}_{X}[h(X)\cdot\mathop{\mathbb{E}}_{Y}[Y|X]] =$$

$$= \sum_{x} Pr[X=x]\cdot h(x)\cdot\sum_{y} Pr[Y=y|X=x]\cdot y.$$

$$= \sum_{x,y} h(x)\cdot y\cdot Pr[X=x, Y=y]$$

$$= \mathop{\mathbb{E}}_{X,Y}[h(X)\cdot Y].$$

Corollary: For all $h(\cdot)$ $\quad \mathbb{E}[(Y - \mathbb{E}[Y|X]) \cdot h(X)] = 0$

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Proof:

$$\mathbb{E}[(Y - \mathbb{E}(Y|X))h(X)] =$$

$$= \mathbb{E}[Y \cdot h(X)] - \mathbb{E}[\mathbb{E}[Y|X]\, h(X)]$$

$$= \mathbb{E}[Y \cdot h(X)] - \mathbb{E}[Y \cdot h(X)].$$

Theorem: Let X, Y be two r.v.s over Ω.

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Proof: Let $h(X)$ be any function of X.

$$\mathbb{E}[(Y-h(X))^2] = \mathbb{E}[(Y-g(x)+g(x)-h(x))^2]$$

$$= \mathbb{E}[(Y-g(x))^2] + 2\mathbb{E}[(Y-g(x))\cdot(g(x)-h(x))] + \mathbb{E}[(g(x)-h(x))^2]$$

$$\geq \mathbb{E}[(Y-g(x))^2]$$

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Alternative Proof: For any $x \in \text{range}(X)$, given $X=x$ the best predictor of Y is $\mathbb{E}[Y|X=x]$ from earlier.

Linear Regression

So far, we've seen:

- If we want to guess Y without knowing anything else

  best guess is $\mathbb{E}Y$.

- If we make some observation X related to Y:

  best guess is $g(x) = \mathbb{E}[Y|X]$.

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So far, we've seen:

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- If we make some observation X related to Y:

  best guess is $g(x) = \mathbb{E}[Y|X]$.

The latter is optimal but can be complicated.

What if we want a simpler fnc of X explaining Y.

For example: a linear function.

Motivation: Statistics

In real-life applications, we don't necessarily know the joint dist. of X, Y.

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To estimate $\mathbb{E}[Y|X=x]$ we need samples such that $X=x$, but typically we'll have few or no such examples.

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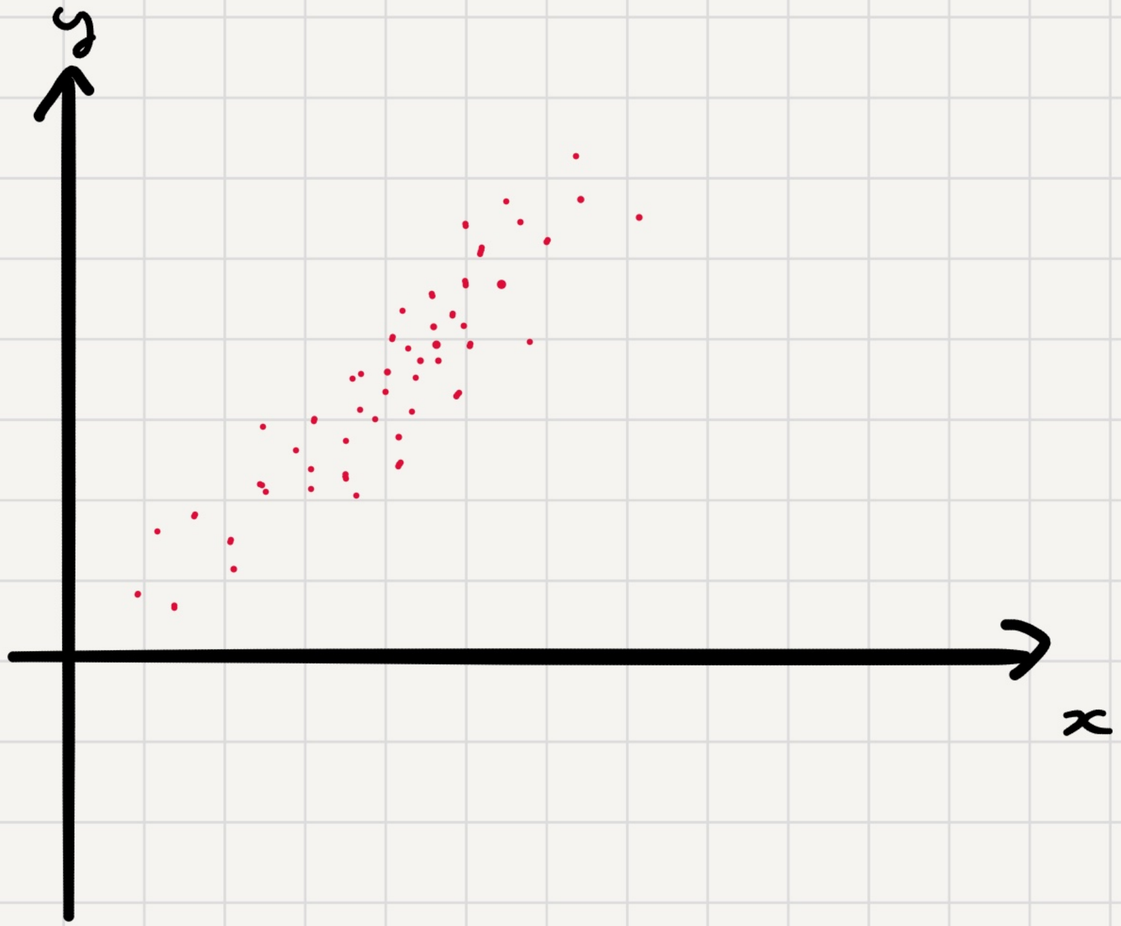
To estimate $\pi[\cdot,\cdot]$

samples such --, but typically we'll have few or no such examples.

For a simpler model, $\alpha X+\beta$, we can use all the samples to get a good estimate of the two parameters: α, β.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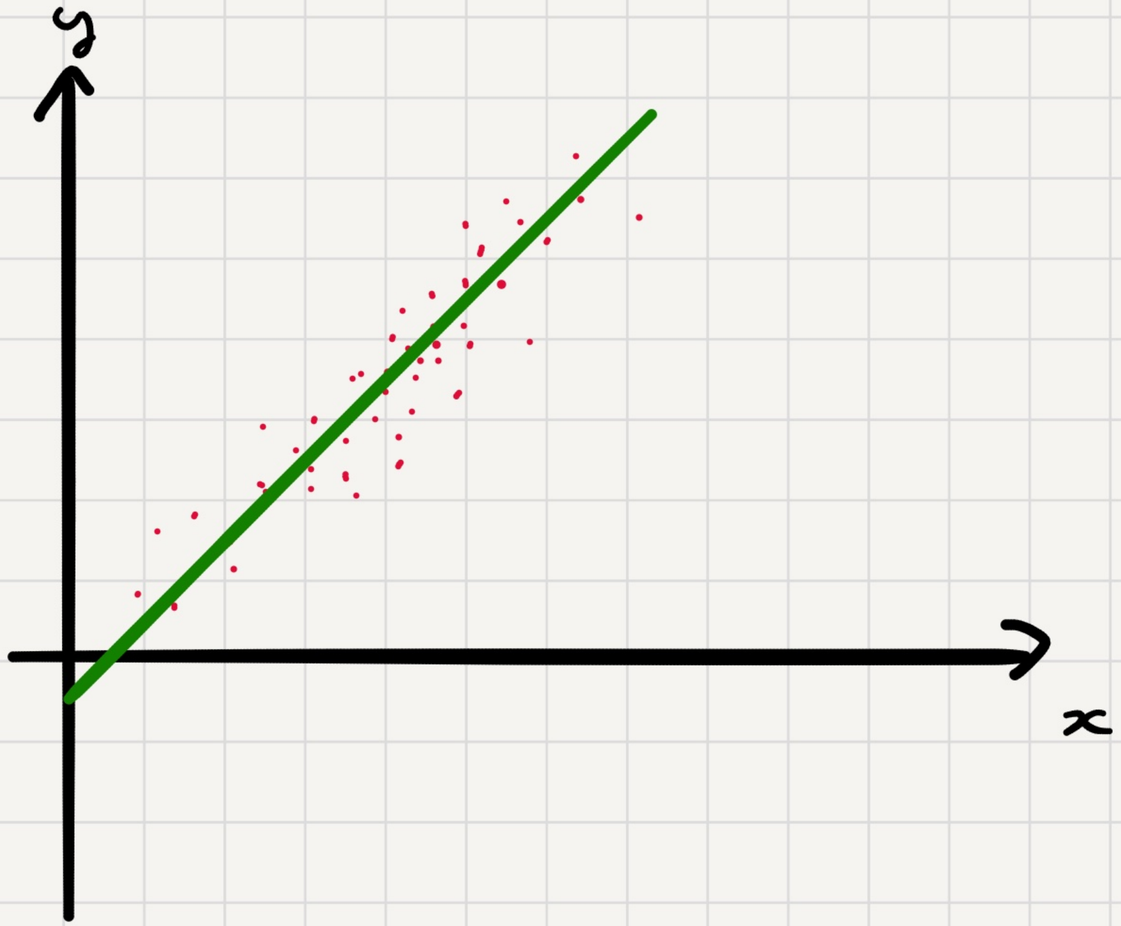
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x

Theorem: The best linear predictor of Y as a function of X is $\mathbb{E}[Y] + \frac{\text{cov}(X,Y)}{\text{var}(X)} \cdot (X - \mathbb{E}X)$.

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$$\min_{\alpha,\beta} \mathbb{E}[(\hat{Y} - (\alpha\hat{X} + \beta))^2] =$$

$$= \min_{\alpha,\beta} \mathbb{E}[\hat{Y}^2] - 2\mathbb{E}[\hat{Y}(\alpha\hat{X}+\beta)] + \mathbb{E}[(\alpha\hat{X}+\beta)^2]$$

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Solution: $\beta = 0$, $\alpha = \frac{\mathbb{E}[\hat{X}\cdot\hat{Y}]}{\mathbb{E}[\hat{X}^2]} = \frac{\text{cov}(X,Y)}{\text{var}(X)}$

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Solution: $\beta = 0$, $\alpha = \frac{\mathbb{E}[\hat{X}\cdot\hat{Y}]}{\mathbb{E}[\hat{X}^2]} = \frac{\text{cov}(X,Y)}{\text{var}(X)}$

$\Rightarrow$ Best linear predictor for $Y - \mathbb{E}Y$ is $\alpha \cdot (X - \mathbb{E}X)$

$\Rightarrow$ " " " " Y is $\mathbb{E}[Y] + \alpha \cdot (X - \mathbb{E}X)$

Theorem: The best linear predictor of Y as a function of X is $l(x) = \mathbb{E}[Y] + \frac{cov(X,Y)}{var(X)} \cdot (X - \mathbb{E}X)$.

Corollary: The minimum $\mathbb{E}[(Y - l(X))^2] = Var(Y) \cdot (1 - Corr(X,Y)^2)$.

Theorem: The best linear predictor of Y as a function of X is

$$\mathbb{E}Y + (X - \mathbb{E}X) \cdot \frac{\mathrm{cov}(X,Y)}{\mathrm{Var}(X)}.$$

Corollary: The minimum $\mathbb{E}[(Y - \ell(X))^2] = \mathrm{Var}(Y) \cdot (1 - \mathrm{Corr}(X,Y)^2)$.

Proof: By the theorem $\ell(X) = \mathbb{E}Y + (X - \mathbb{E}X)\frac{\mathrm{cov}(X,Y)}{\mathrm{Var}(X)}$

$$\mathbb{E}[(Y - \ell(X))^2] = \mathbb{E}\left[\left((Y - \mathbb{E}Y) - (X - \mathbb{E}X)\frac{\mathrm{cov}(X,Y)}{\mathrm{Var}(X)}\right)^2\right]$$

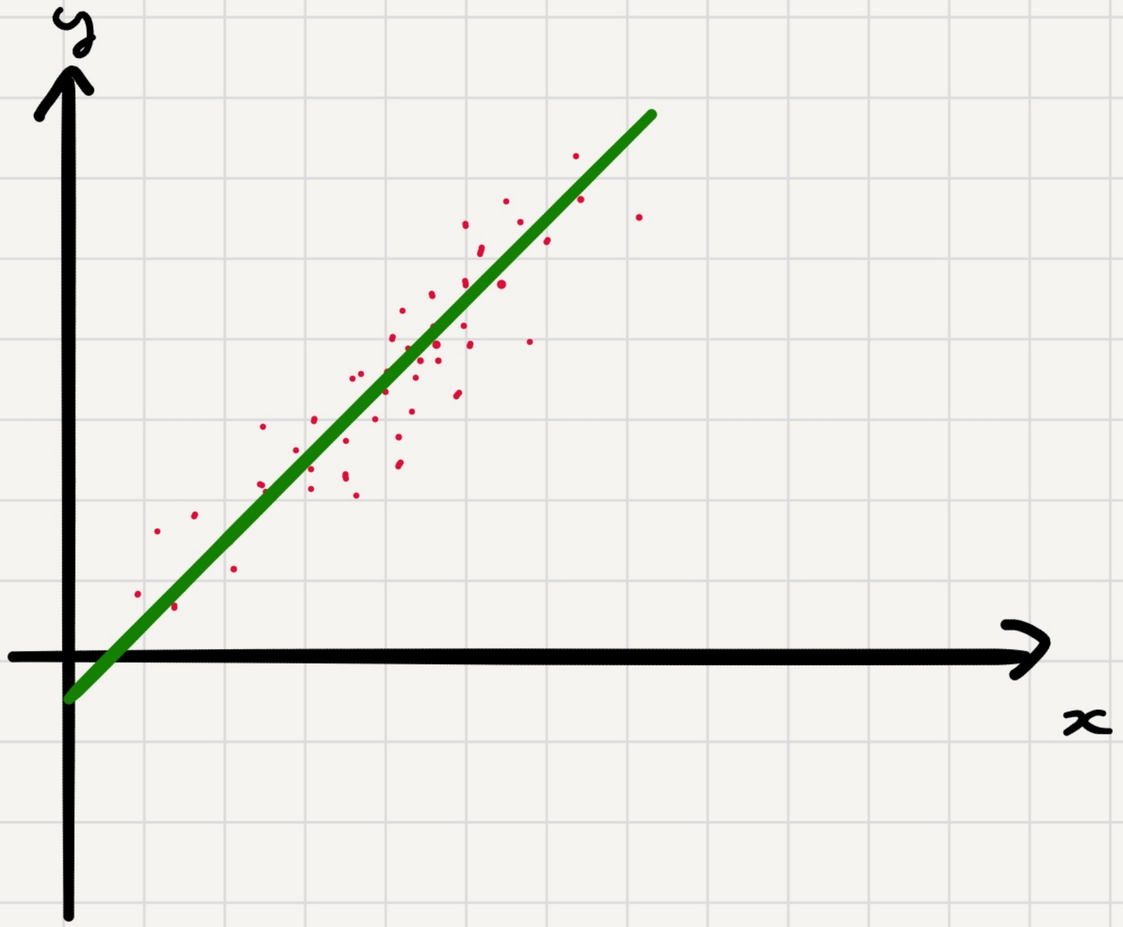
$$= \mathbb{E}[(Y - \mathbb{E}Y)^2] - 2\frac{\mathrm{cov}(X,Y)}{\mathrm{Var}(X)}\,\mathbb{E}[(Y - \mathbb{E}Y)(X - \mathbb{E}X)]$$

$$+ \left(\frac{\mathrm{cov}(X,Y)}{\mathrm{Var}(X)}\right)^2 \cdot \mathbb{E}[(X - \mathbb{E}X)^2]$$

$$= \mathrm{Var}(Y) - \frac{\mathrm{cov}(X,Y)^2}{\mathrm{Var}(X)}$$

$$= \mathrm{Var}(Y) - \mathrm{Var}(Y) \cdot \frac{\mathrm{cov}(X,Y)^2}{\mathrm{Var}(X)\mathrm{Var}(Y)} = \mathrm{Var}(Y) \cdot (1 - \mathrm{Corr}(X,Y)^2).$$

$$\ell(x) = \mathbb{E}Y + \frac{\mathrm{Cov}(x,Y)}{\mathrm{Var}(x)}(x - \mathbb{E}x)$$



The line goes through $(\mathbb{E}x, \mathbb{E}Y)$

The slope of the line is $\frac{\mathrm{cov}(x,Y)}{\mathrm{var}(x)}$.

Theorem: The best linear predictor of Y as a function of X is

$$\mathbb{E}Y + (X - \mathbb{E}X) \cdot \frac{\mathrm{cov}(X,Y)}{\mathrm{Var}(X)}.$$

Corollary: The minimum $\mathbb{E}[(Y - l(X))^2] = \mathrm{Var}(Y) \cdot (1 - \mathrm{Corr}(X,Y)^2)$.

This is what we mean by

"X explains 80% of the variance of Y"

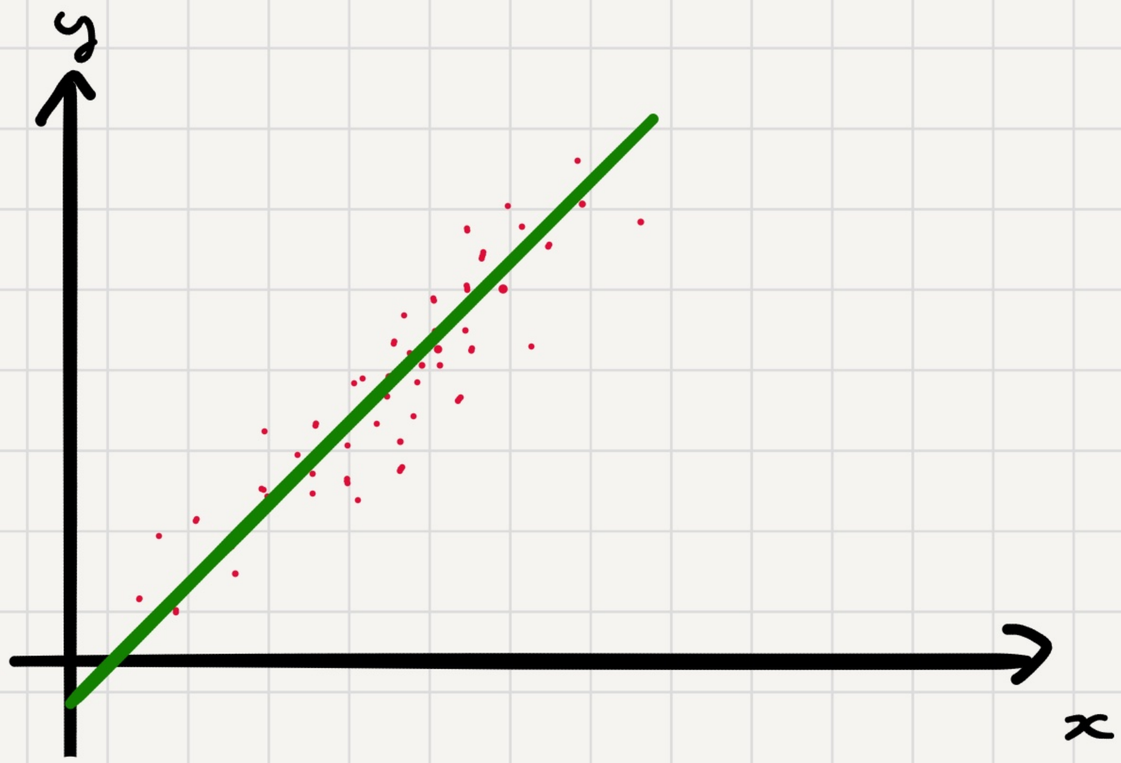
$$\updownarrow$$

$$\mathrm{corr}(X,Y)^2 = 0.8.$$

Minimizing Given Data

Suppose you get samples $(x_1, y_1), \ldots, (x_n, y_n)$ from the joint distribution, and you want to minimize

$$\sum_{i=1}^{n} (y_i - \alpha x_i + \beta)^2$$



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$$\sum_{i=1}^{n} (y_i - \alpha x_i + \beta)^2$$

You'll get:

$$\overline{x} = \frac{1}{n} \cdot \sum_{i=1}^{n} x_i, \quad \overline{y} = \frac{1}{n} \cdot \sum_{i=1}^{n} y_i$$

$$\alpha = \frac{\frac{1}{n}\sum_{i=1}^{n} x_i y_i - \overline{x} \cdot \overline{y}}{\frac{1}{n}\sum_{i=1}^{n} (x_i - \overline{x})^2}$$

(estimate to $\frac{\mathrm{Cov}(X,Y)}{\mathrm{Var}(X)}$)

$$\beta = \overline{y} - \alpha \cdot \overline{x}$$

(estimate to $\mathbb{E}Y - \alpha \mathbb{E}X$)