Maximum Likelihood Estimation

Your first consulting job

- *Billionaire*: I have special coin, if I flip it, what's the probability it will be heads?
- *You*: Please flip it a few times:

HHTHHT

- *You*: The probability is: 3/5

- *Billionaire:* Why?

Coin – Binomial Distribution

- **Data**: sequence *D= (HHTHT…)*, **k heads** out of **n flips**
- **Hypothesis:** P(Heads) = θ, P(Tails) = 1-θ
  - Flips are i.i.d.:
    - Independent events
    - Identically distributed according to Binomial distribution

$P(T \mid HHTH, \theta) = P(T \mid \theta)$

$= (1-\theta)$

- $P(\mathcal{D}|\theta) =$ $P(HHTHT \mid \theta)$

$= P(T \mid HHTH, \theta)\, P(HHTH \mid \theta)$

$= (1-\theta)\, P(HHTH \mid \theta) = \theta^k (1-\theta)^{n-k}$

k=3 heads

n=5 flips

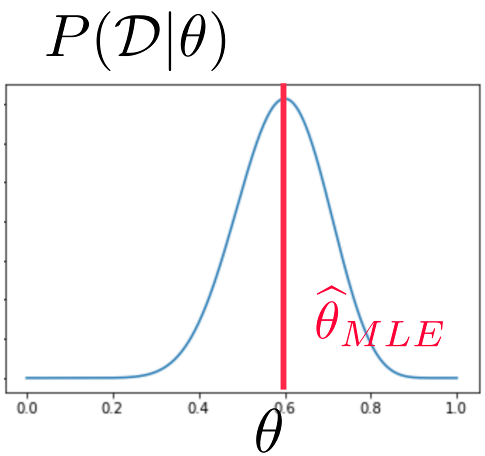
Maximum Likelihood Estimation

- **Data**: sequence *D= (HHTHT…),* **k heads** out of **n flips**
- **Hypothesis:** P(Heads) = θ, P(Tails) = 1-θ

$$P(\mathcal{D}|\theta) = \theta^k(1-\theta)^{n-k}$$

- Maximum likelihood estimation (MLE): Choose θ that maximizes the probability of observed data:

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} \; P(\mathcal{D}|\theta)$$
$$= \arg\max_{\theta} \; \log P(\mathcal{D}|\theta)$$



Your first learning algorithm

$p(\mathcal{D}|\theta) = \theta^{k}(1-\theta)^{n-k}$

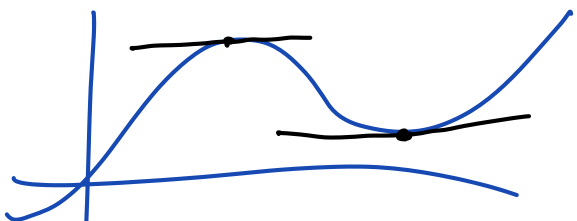
$\log(ab) = \log(a) + \log(b)$

$\log(x^y) = y\log(x)$

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} \; \log P(\mathcal{D}|\theta) =$$

$$= \arg\max_{\theta} \; \log \theta^k (1-\theta)^{n-k}$$

$$= \arg\max_{\theta} \; k\log(\theta) + (n-k)\log(1-\theta)$$



- Set derivative to zero: $\boxed{\frac{d}{d\theta} \log P(\mathcal{D}|\theta) = 0}$

$$\frac{d}{d\theta}\left[k\log(\theta) + (n-k)\log(1-\theta)\right] = \frac{k}{\theta} + \frac{n-k}{1-\theta}\cdot(-1) = 0$$

Multiply both sides by $\theta(1-\theta)$ and solve:

$$k(1-\theta) - (n-k)\theta = 0 \qquad k - n\theta = 0 \Rightarrow \hat{\theta}_{MLE} = \frac{k}{n}$$

Maximum Likelihood Estimation

Observe $X_1, X_2, \dots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Likelihood function $L_n(\theta) = \prod_{i=1}^{n} f(X_i;\theta)$

Log-Likelihood function $l_n(\theta) = \log(L_n(\theta)) = \sum_{i=1}^{n} \log(f(X_i;\theta))$

Maximum Likelihood Estimator (MLE) $\boxed{\widehat{\theta}_{MLE} = \arg\max_{\theta} L_n(\theta)}$

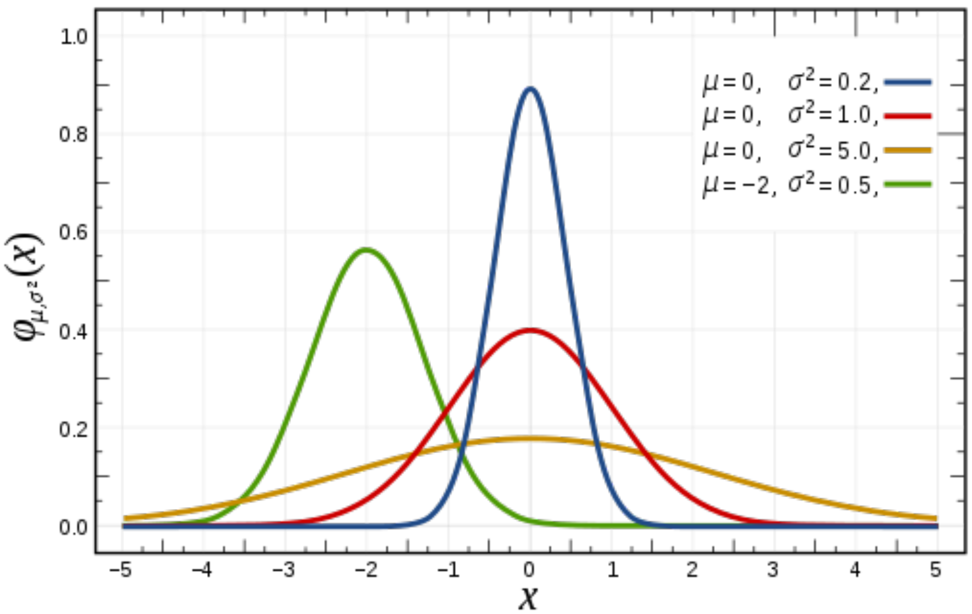
Recap

- Learning is…
  - Collect some data
    - E.g., coin flips
  - Choose a hypothesis class or model
    - E.g., binomial
  - Choose a loss function
    - E.g., data likelihood
  - Choose an optimization procedure
    - E.g., set derivative to zero to obtain MLE

What about continuous variables?

- *Billionaire*: What if I am measuring a **continuous variable**?
- ***You*: Let me tell you about Gaussians…**

$$\underbrace{P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}}$$



Some properties of Gaussians

- affine transformation (multiplying by scalar and adding a constant)
  - $X \sim N(\mu, \sigma^2)$ ← notation for X being Gaussian w/ mean μ var σ^2
  - $Y = aX + b \quad \rightarrow \quad Y \sim N(a\mu + b, a^2\sigma^2)$

- Sum of Gaussians
  - $X \sim N(\mu_X, \sigma^2_X)$
  - $Y \sim N(\mu_Y, \sigma^2_Y)$
  - $Z = X + Y \quad \rightarrow \quad Z \sim N(\mu_X + \mu_Y, \sigma^2_X + \sigma^2_Y)$

MLE for Gaussian

$\theta = (\mu, \sigma^2)$

- Prob. of i.i.d. samples $D=\{x_1,\ldots,x_n\}$ (e.g., temperature):

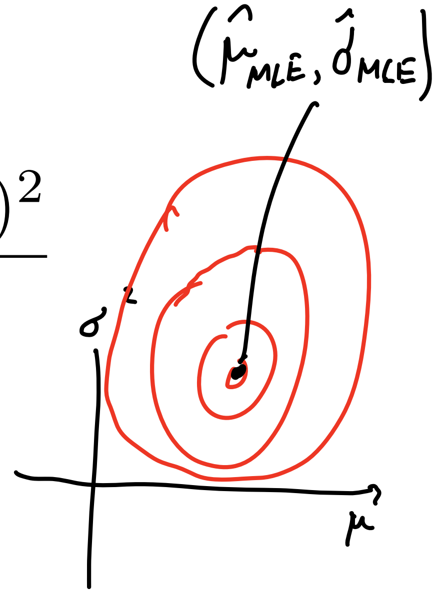
$$P(\mathcal{D}|\mu,\sigma) = P(x_1,\ldots,x_n|\mu,\sigma) = \prod_{i=1}^{n} P(x_i|\mu,\sigma)$$

$$= \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \prod_{i=1}^{n} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- Log-likelihood of data:

$$\log P(\mathcal{D}|\mu,\sigma) = -n\log(\sigma\sqrt{2\pi}) - \sum_{i=1}^{n}\frac{(x_i-\mu)^2}{2\sigma^2}$$

- What is $\widehat{\theta}_{MLE}$ for $\theta = (\mu, \sigma^2)$? Draw a picture!



Your second learning algorithm: MLE for mean of a Gaussian

- What's MLE for mean?

$$\frac{d}{d\mu}\log P(\mathcal{D}|\mu,\sigma) = \frac{d}{d\mu}\left[-n\log(\sigma\sqrt{2\pi}) - \sum_{i=1}^{n}\frac{(x_i-\mu)^2}{2\sigma^2}\right]$$

$$= -\sum_{i=1}^{n}\frac{\cancel{2}(x_i-\mu)}{\cancel{2}\sigma^2}\cdot(-1) = 0$$

multiply both sides by σ^2

$$\sum_{i=1}^{n}\frac{(x_i-\mu)}{\sigma^2} = 0$$

$$\sum_{i=1}^{n}(x_i-\mu) = 0$$

$$\left(\sum_{i=1}^{n}x_i\right) - \left(\sum_{i=1}^{n}\mu\right) = \left(\sum_{i=1}^{n}x_i\right) - n\mu = 0$$

$$\sum_{i=1}^{n}\frac{x_i}{\sigma^2} = \sum_{i=1}^{n}\frac{\mu}{\sigma^2} = \frac{n\mu}{\sigma^2}$$

$$\boxed{\hat{\mu}_{MLE} = \frac{1}{n}\sum_{i=1}^{n}x_i}$$

MLE for variance

- Again, set derivative to zero:

$$\frac{d}{d\sigma}\log P(\mathcal{D}|\hat{\mu}_{MLE},\sigma) = \frac{d}{d\sigma}\left[-n\log(\sigma\sqrt{2\pi}) - \sum_{i=1}^{n}\frac{(x_i-\hat{\mu}_{MLE})^2}{2\sigma^2}\right]$$

Learning Gaussian parameters

By assumption $x_i \stackrel{iid}{\sim} \mathcal{N}(\mu, \sigma^2)$

- MLE:

$$\widehat{\mu}_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\mathbb{E}[\widehat{\mu}_{MLE}] = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} x_i\right] = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}[x_i] = \mu$$

$$\widehat{\sigma^2}_{MLE} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \widehat{\mu}_{MLE})^2$$

- MLE for the variance of a Gaussian is **biased**

$$\mathbb{E}[\widehat{\sigma^2}_{MLE}] \neq \sigma^2$$

- Unbiased variance estimator:

$$\widehat{\sigma^2}_{unbiased} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \widehat{\mu}_{MLE})^2$$

Maximum Likelihood Estimation

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Maximum Likelihood Estimator (MLE) $\widehat{\theta}_{MLE} = \arg\max_{\theta} L_n(\theta)$

Under benign assumptions, as the number of observations $n \to \infty$ we have $\widehat{\theta}_{MLE} \to \theta_*$

The MLE is a "recipe" that begins with a *model* for data $f(x;\theta)$

Applications preview

Maximum Likelihood Estimation

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Why is it useful to recover the "true" parameters θ_* of a probabilistic model?

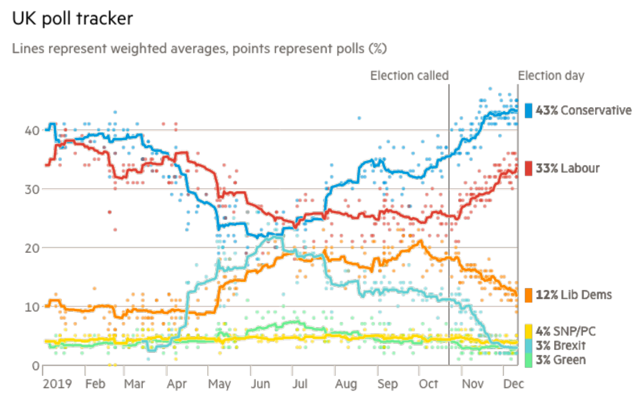
- **Estimation** of the parameters θ_* is the goal
- Help **interpret** or summarize large datasets
- Make **predictions** about future data
- **Generate** new data $X \sim f(\,\cdot\,;\widehat{\theta}_{MLE})$

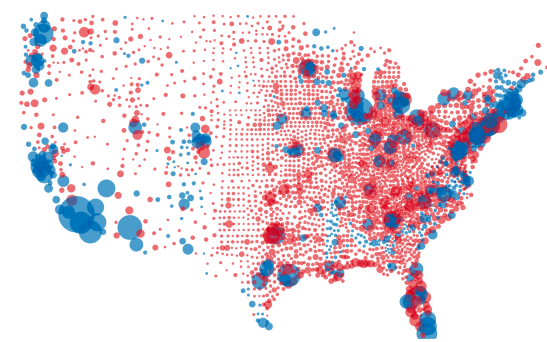
Estimation

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some “true” $\theta = \theta_*$

Opinion polls
How does the greater population feel about an issue? Correct for over-sampling?

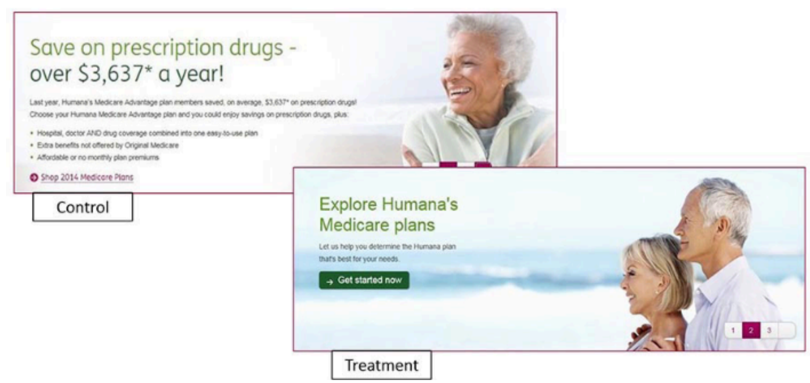
- θ_* is “true” average opinion
- $X_1, X_2, \ldots$ are sample calls





A/B testing
How do we figure out which ad results in more click-through?

- θ_* are the “true” average rates
- $X_1, X_2, \ldots$ are binary “clicks”

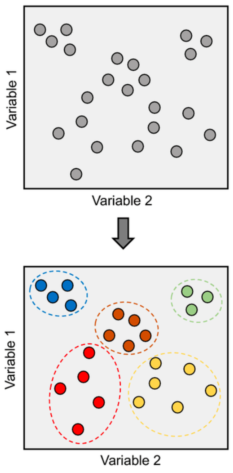


Interpret

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

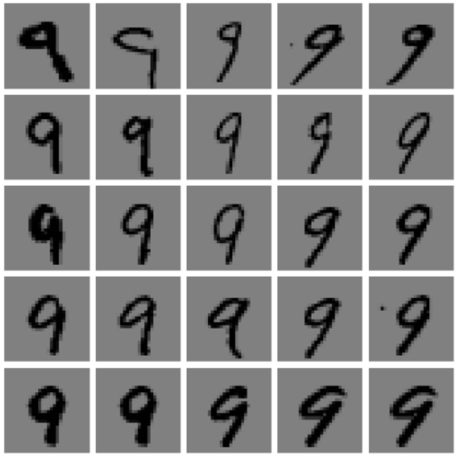
Customer segmentation / clustering
Can we identify distinct groups of customers by their behavior?

- θ_* describes "center" of distinct groups
- $X_1, X_2, \ldots$ are individual customers



Data exploration
What are the degrees of freedom of the dataset?

- θ_* describes the principle directions of variation
- $X_1, X_2, \ldots$ are the individual images



Predict

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Content recommendation
Can we predict how much someone will like a movie based on past ratings?

- θ_* describes user's preferences
- $X_1, X_2, \ldots$ are (movie, rating) pairs

Object recognition / classification
Identify a flower given just its picture?

- θ_* describes the characteristics of each kind of flower
- $X_1, X_2, \ldots$ are the (image, label) pairs

(a) (b) (c)

Figure 1.1: Three types of Iris flowers: Setosa, Versicolor and Virginica. Used with kind permission of Dennis Kramb and SIGNA.

index	sl	sw	pl	pw	label
0	5.1	3.5	1.4	0.2	Setosa
1	4.9	3.0	1.4	0.2	Setosa
	...				
50	7.0	3.2	4.7	1.4	Versicolor
	...				
149	5.9	3.0	5.1	1.8	Virginica

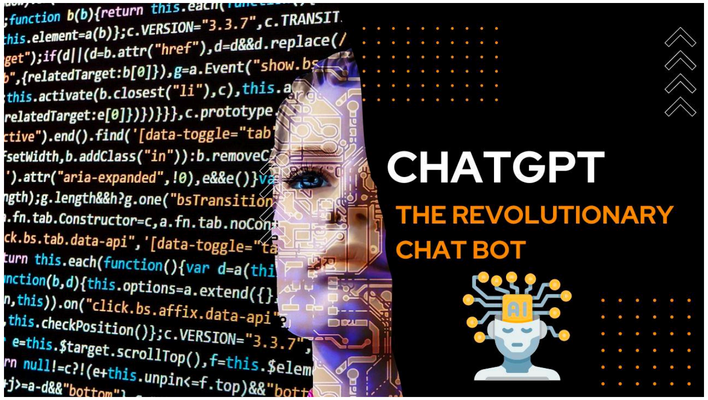
Generate

$$\textbf{Observe } X_1, X_2, \ldots, X_n \text{ drawn IID from } f(x;\theta) \text{ for some "true" } \theta = \theta_*$$

Text generation
Can AI generate text that could have been written like a human?

- θ_* describes language structure
- $X_1, X_2, \ldots$ are text snippets found online

"Kaia the dog wasn't a natural pick to go to mars. No one could have predicted she would…"



https://chat.openai.com/chat

Image to text generation
Can AI generate an image from a prompt?

- θ_* describes the coupled structure of images and text
- $X_1, X_2, \ldots$ are the (image, caption) pairs found online

"dog talking on cell phone under water, oil painting"

https://labs.openai.com/

Linear Regression

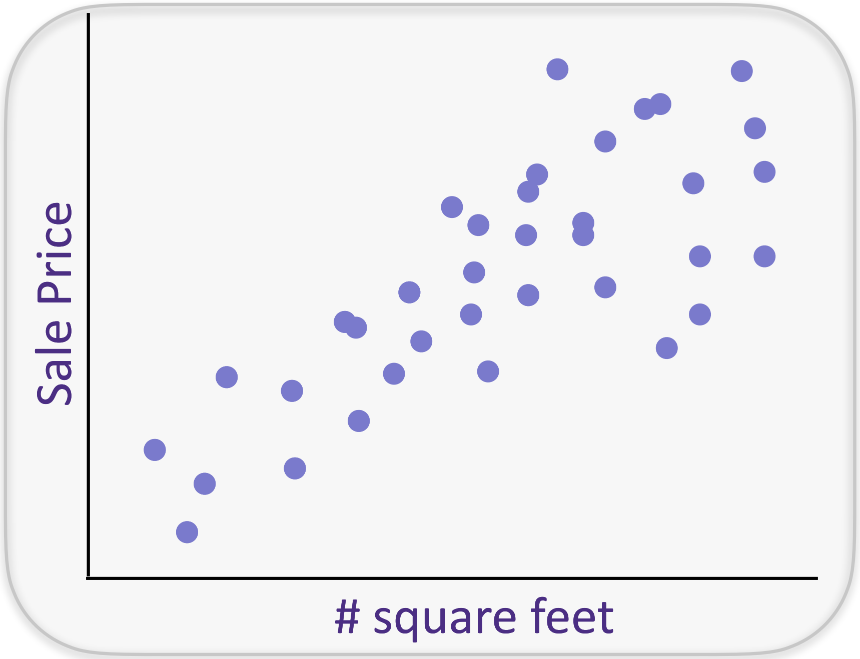
UNIVERSITY of WASHINGTON

The regression problem, 1-dimensional

Given past sales data on zillow.com, predict:

y = **House sale price** *from*

x = **{# sq. ft.}**



Training Data:

$$\{(x_i, y_i)\}_{i=1}^n$$

$$x_i \in \mathbb{R}$$
$$y_i \in \mathbb{R}$$

Fit a function to our data, 1-d

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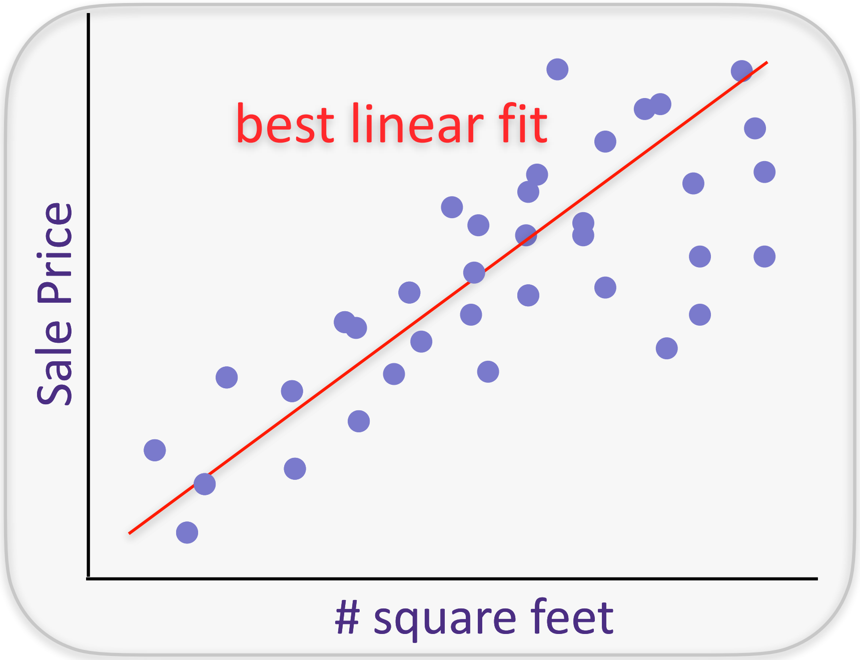

Training Data: $\{(x_i, y_i)\}_{i=1}^n$ $\quad x_i \in \mathbb{R}$ $\quad y_i \in \mathbb{R}$

Hypothesis/Model: linear

$$y_i = x_i w + \epsilon_i \qquad \epsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$$

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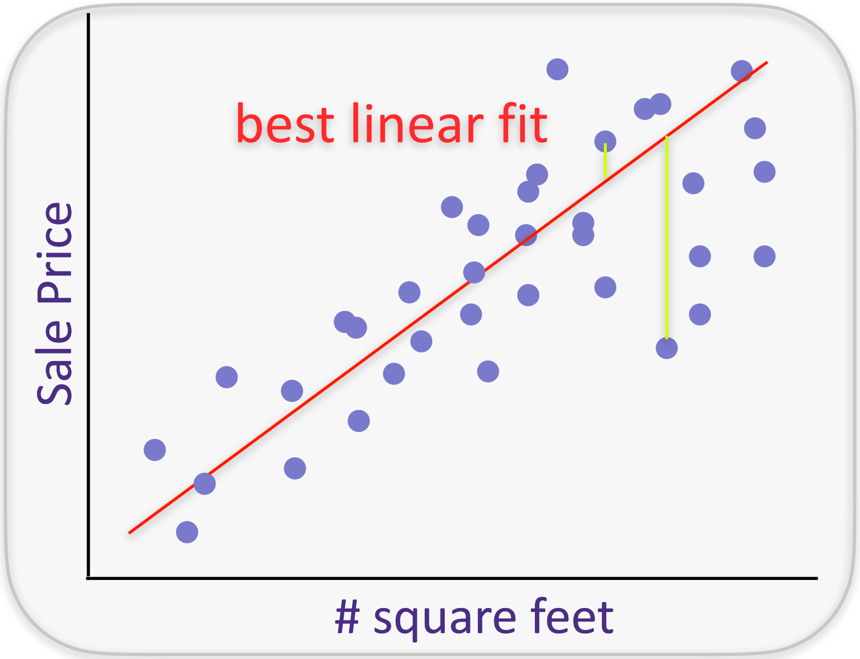

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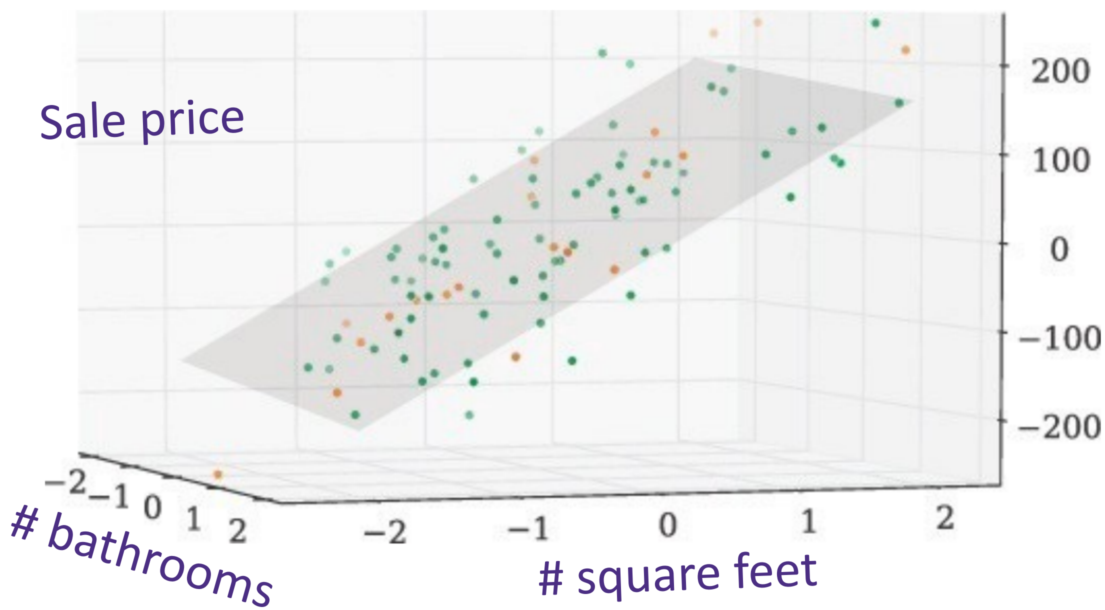

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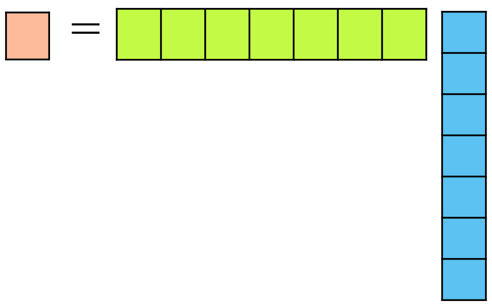

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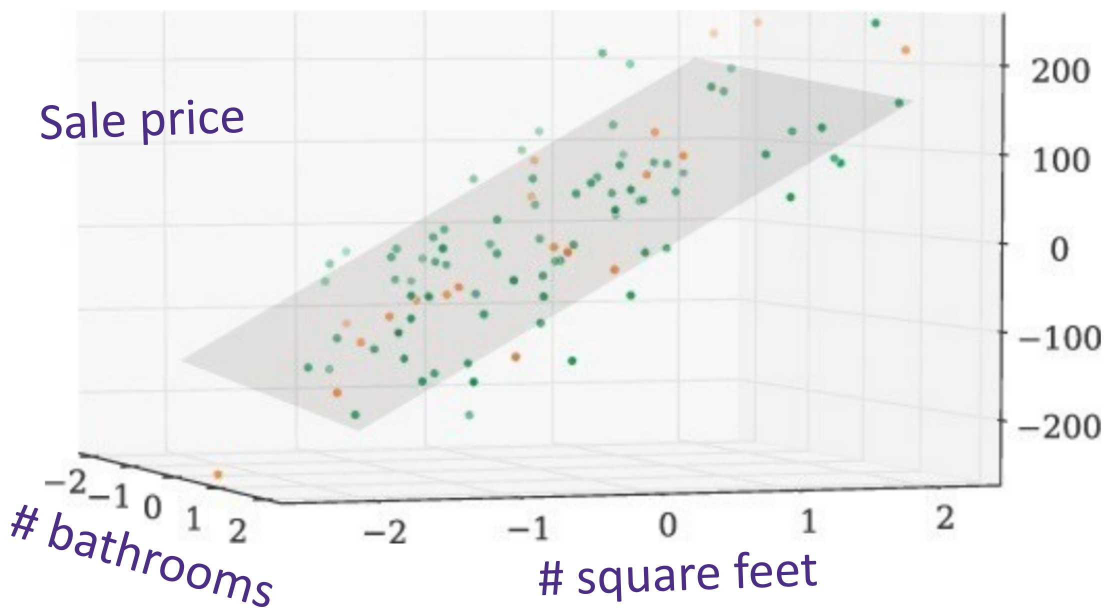

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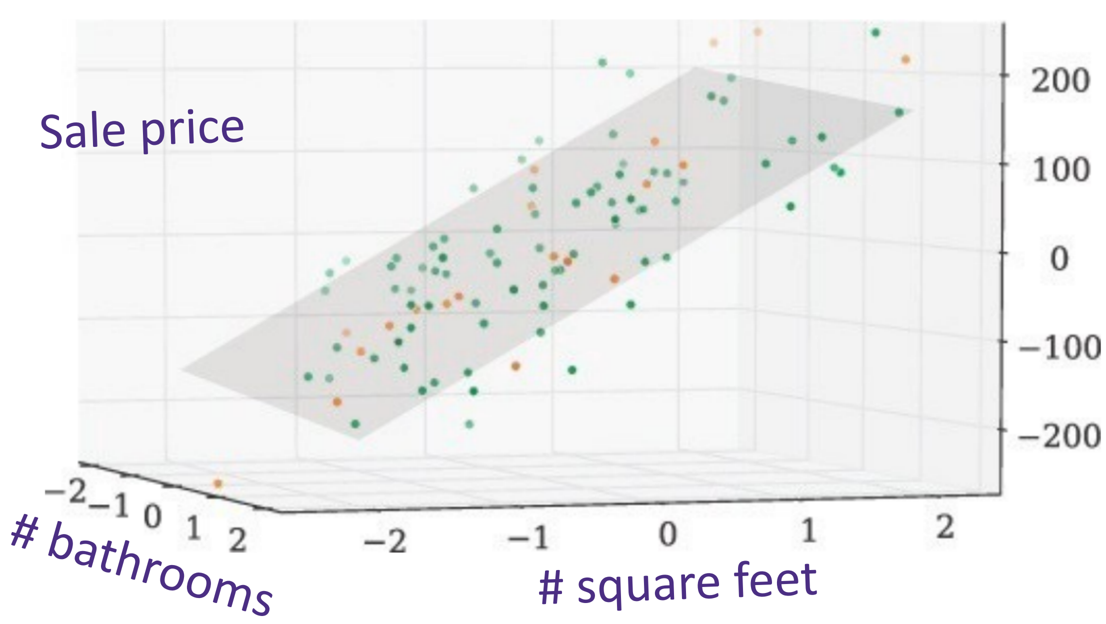

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$$p(y|x, w, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(y - x^\top w)^2 / 2\sigma^2}$$

Maximizing log-likelihood

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Likelihood: $$P(\mathcal{D}|w,\sigma) = \prod_{i=1}^n p(y_i|x_i,w,\sigma) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(y_i-x_i^\top w)^2/2\sigma^2}$$

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Set derivate=0, solve for w

Maximizing log-likelihood

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$$\boxed{\widehat{w}_{MLE} = \left(\sum_{i=1}^{n} x_i x_i^\top \right)^{-1} \sum_{i=1}^{n} x_i y_i}$$

The regression problem in matrix notation

$$\widehat{w}_{MLE} = \arg\min_w \sum_{i=1}^n (y_i - x_i^\top w)^2$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix}$$

d : # of features

n : # of examples/datapoints

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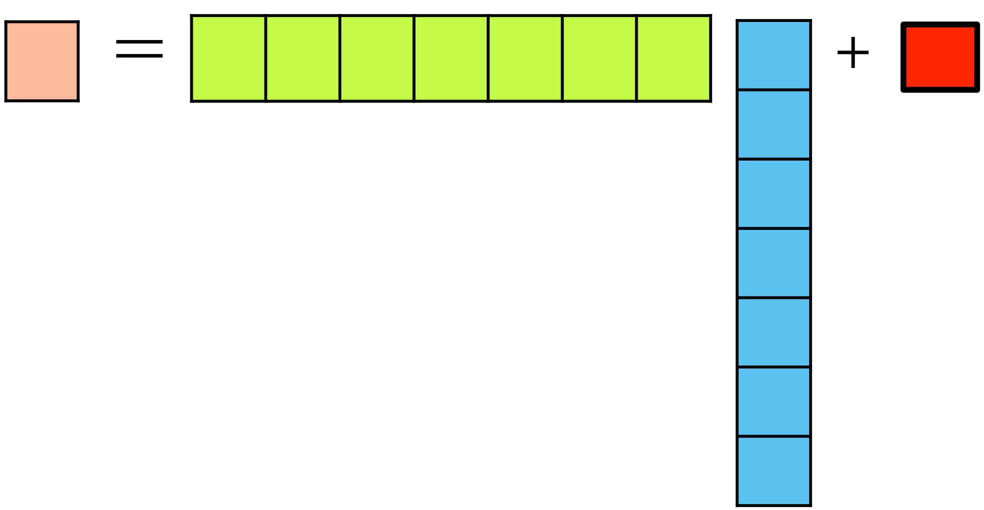
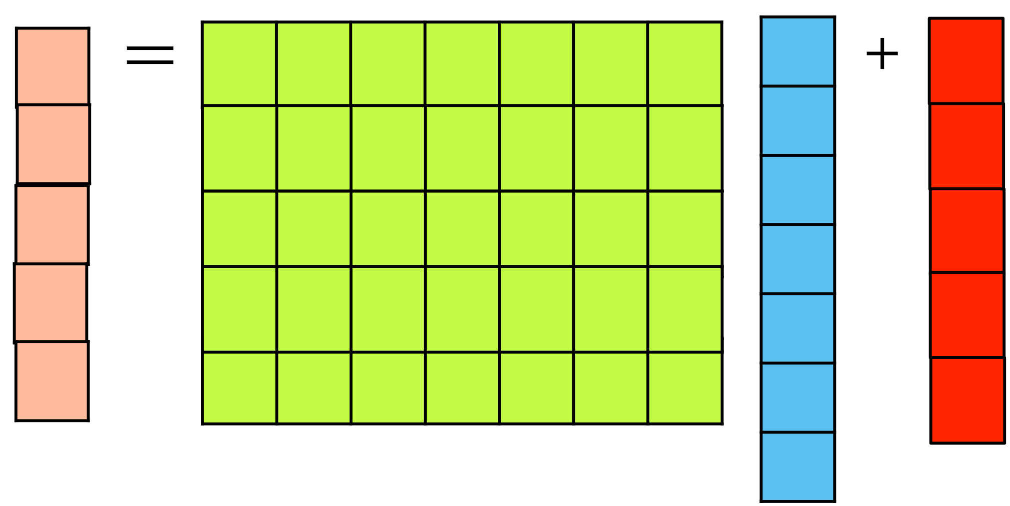


$$\mathbf{y} = \mathbf{X}w + \epsilon$$



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$$\mathbf{y} = \mathbf{X}w + \epsilon$$

$$\begin{aligned} \widehat{w}_{LS} &= \arg\min_w ||\mathbf{y} - \mathbf{X}w||_2^2 \\ &= \arg\min_w (\mathbf{y} - \mathbf{X}w)^T(\mathbf{y} - \mathbf{X}w) \end{aligned}$$

$$\boxed{\ell_2 \text{ norm: } \|z\|_2 = \sqrt{\textstyle\sum_{i=1}^n z_i^2} = \sqrt{z^\top z}}$$

The regression problem in matrix notation

$$\widehat{w}_{MLE} = \arg\min_w \sum_{i=1}^{n} (y_i - x_i^\top w)^2$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix}$$

d : # of features

n : # of examples/datapoints

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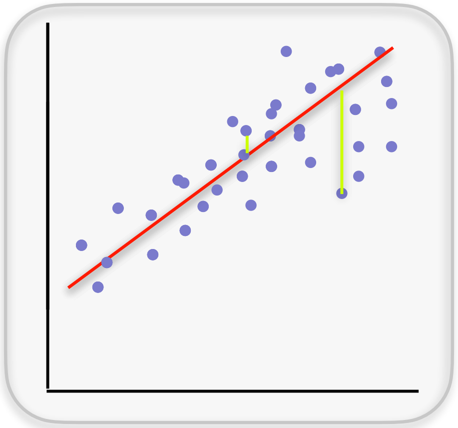
$$\boxed{\widehat{w}_{LS} = \widehat{w}_{MLE} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}}$$

The regression problem in matrix notation

$$\widehat{w}_{LS} = \arg\min_w ||\mathbf{y} - \mathbf{X}w||_2^2$$
$$= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$



What about an offset?

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} \sum_{i=1}^{n} \left(y_i - (x_i^T w + b)\right)^2$$
$$= \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2$$

Dealing with an offset

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2$$

Dealing with an offset

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2$$

$$\mathbf{X}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{X}^T\mathbf{1} = \mathbf{X}^T\mathbf{y}$$
$$\mathbf{1}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{1}^T\mathbf{1} = \mathbf{1}^T\mathbf{y}$$

If $\mathbf{X}^T\mathbf{1} = 0$ (i.e., if each feature is mean-zero) then

$$\widehat{w}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

$$\widehat{b}_{LS} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

Make Predictions

$$\widehat{w}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

$$\widehat{b}_{LS} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

A new house is about to be listed. What should it sell for?

$$\hat{y}_{\text{new}} = x_{\text{new}}^T \hat{w}_{LS} + \hat{b}_{LS}$$

Process

Decide on a **model** for the likelihood function $f(x;\theta)$

Find the function which fits the data best

Choose a loss function- least squares

Pick the function which minimizes loss on data

Use function to make prediction on new examples