Lecture 2: MLE for Gaussian and linear regression

Sewoong Oh

Ed Discussion:

Recap: Maximum Likelihood Estimation

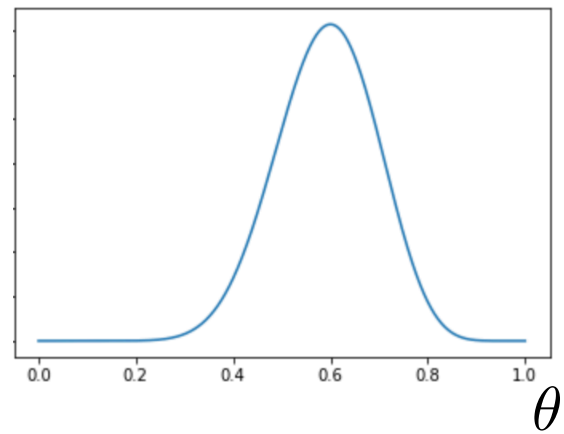
H T ... H $\qquad X_i \sim \text{Binomial}(\theta)$

- **Observe** $\mathscr{D} = X_1, X_2, \ldots, X_n$ drawn i.i.d. from $P(X_i; \theta)$ for some ground truth $\theta = \theta^*$, unknown to us
- **Maximize log-likelihood** when we observe k heads in n flips

$$\log P(\mathscr{D}; \theta) = \log\left(\theta^k (1-\theta)^{n-k}\right)$$

$$= k \cdot \log\theta + (n-k)\log(1-\theta)$$

$P(\mathscr{D}; \theta)$ when $\overset{3}{\overset{\parallel}{k}}$ heads obsereved in $\overset{5}{\overset{\parallel}{n}}$ flips

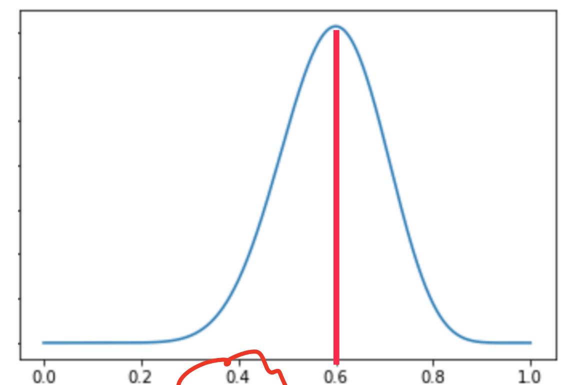


Recap: Maximum Likelihood Estimation

- **Observe** $\mathscr{D} = X_1, X_2, \ldots, X_n$ drawn i.i.d. from $P(X_i; \theta)$ for some ground truth $\theta = \theta^*$, unknown to us
- **Maximize log-likelihood** when we observe k heads in n flips

$$\log P(\mathscr{D}; \theta) \;=\; k \log(\theta) + (n-k) \log(1-\theta)$$

$P(\mathscr{D}; \theta)$ when $\overset{3}{k}$ heads obsereved in $\overset{5}{n}$ flips



- Maximum likelihood Estimate (MLE)

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

$\frac{k}{n} = \widehat{\theta}_{MLE}$

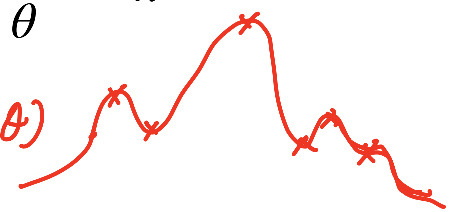
- Use the fact that derivative is zero at maxima (and also minima)
- Set derivative to zero,

  and find θ satisfying: $$\frac{d}{d\theta} \log P(\mathscr{D}; \theta) = 0$$

Maximum Likelihood Estimation

- **Observe** $X_1, X_2, \ldots, X_n$ drawn i.i.d. from $P(X_i; \theta)$ for some true $\theta = \theta^*$
- **Likelihood function**: $L_n(\theta) = \prod_{i=1}^{n} P(X_i; \theta)$
- **Log-likelihood function**: $\ell_n(\theta) = \log L_n(\theta) = \sum_{i=1}^{n} \log P(X_i; \theta)$
- **Maximum Likelihood Estimator (MLE)**: $\widehat{\theta}_{\text{MLE}} = \arg\max_{\theta} \ell_n(\theta)$

$\sum_{i=1}^{n} \log P(X_i; \theta)$



- Warning when setting the derivative to zero to find the MLE:
  - The solution includes maxima, minima, and stationary points ⇒ needs to be checked
  - It does not always lead to an explicit expression in a closed form ⇒ alternative methods

week 3

What about continuous variables?

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

normal = Gaussian

  - A Gaussian random variable is written as $X \sim \mathcal{N}(\mu, \sigma^2)$ with mean $\mu \triangleq \mathbb{E}[X]$ and variance $\sigma^2 \triangleq \mathbb{E}\left[(X - \mathbb{E}[X])^2\right]$
  - The p.d.f. (Probability Density Function) of X is

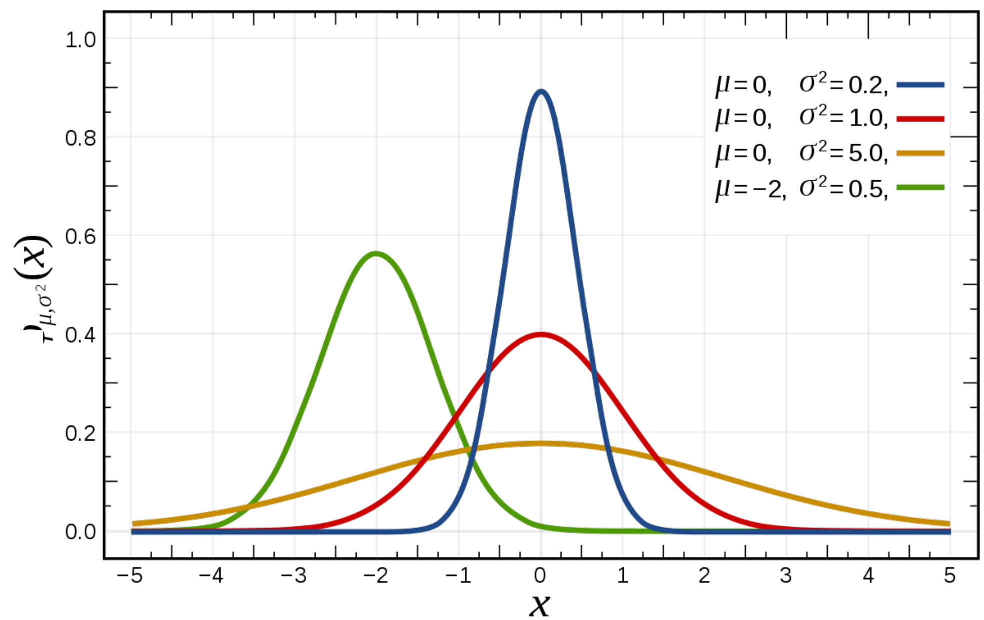
$$\boxed{P(x; \mu, \sigma^2)} = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$\boxed{P(x \mid \mu, \sigma^2)} = \frac{P(x, \mu, \sigma^2)}{P(\mu, \sigma^2)}$$

· Conditional on

· Given

Bayes Rule



[EdDiscussion Question: What distributions do we need to memorize?]

Binomial (θ)

Gaussian (μ, σ^2)

Some useful properties of Gaussians

- Affine transformation
  (multiplying by scalar and adding a constant)
  - $X \sim \mathcal{N}(\mu, \sigma^2)$
  - $Y = aX + b \implies Y \sim \underbrace{\mathcal{N}}_{\text{Gaussian}}(\overbrace{a\mu + b}^{\text{mean}}, \overbrace{a^2\sigma^2}^{\text{variance}})$

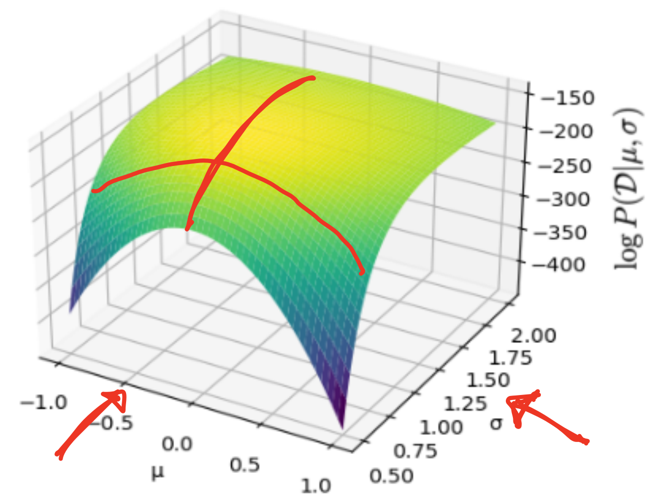
- Sum of Gaussians , Set of Gaussian Distributions is "closed under summation"
  and Poisson
  - $X \sim \mathcal{N}(\mu_X, \sigma_X^2)$
  - $Y \sim \mathcal{N}(\mu_Y, \sigma_Y^2)$
  - $Z = X + Y \implies Z \sim \underbrace{\mathcal{N}}_{\text{Gaussian}}(\overbrace{\mu_X + \mu_Y}, \overbrace{\sigma_X^2 + \sigma_Y^2})$

- [HW0 Questions A3 and A4]

MLE for Gaussian

- **Hypothesis**: i.i.d. samples $\mathscr{D} = \{x_1, x_2, \ldots, x_n\}$ from $\mathcal{N}(\mu, \sigma^2)$

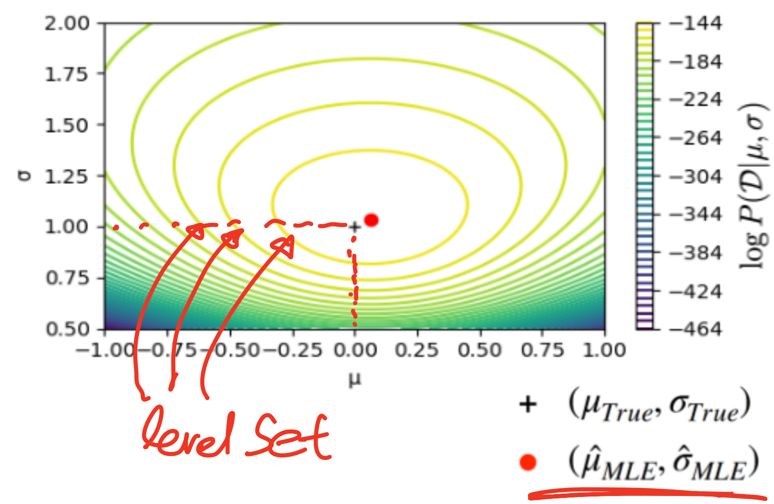
$$\begin{aligned} P(\mathscr{D}; \mu, \sigma^2) &= P(x_1, \ldots, x_n; \mu, \sigma^2) \\ &= P(x_1; \mu, \sigma^2) \times P(x_2; \mu, \sigma^2) \times \cdots P(x_n; \mu, \sigma^2) \\ &= \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}} \end{aligned}$$



- **Log-likelihood** of data:

$$\log P(\mathscr{D}; \underbrace{\mu, \sigma^2}_{\theta}) = \sum_{i=1}^{n} \left\{ -\log(\sigma\sqrt{2\pi}) - \frac{(x_i-\mu)^2}{2\sigma^2} \right\}$$

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



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

Your second learning algorithm:
MLE for mean of a Gaussian distribution

- What's MLE for mean? Set partial derivative to zero:

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

$$\underbrace{\sum_{i=1}^{n}\log(\sigma\sqrt{2\pi})}_{=0}$$

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

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

$$\sum_{i=1}^{n} x_i = n\cdot\mu$$

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

: Empirical mean

$\boxed{\text{Does not depend on } \sigma.}$

MLE for variance of a Gaussian distribution

- Again, set partial derivative to zero:

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

$\hat{\mu}_{MLE}$

$$= \frac{-n}{\sigma} + \sum_{i=1}^{n}\frac{(x_i-\mu)^2}{\sigma^3} = 0$$

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2$$: Empirical Variance.

plug in $\hat{\mu}_{MLE}$

What can we say about the MLE?

- MLE for the mean of a Gaussian is **unbiased**
  - $$\widehat{\mu}_{\mathrm{MLE}} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$\mathbb{E}[\hat{\theta}] = \theta^*$

$x_i \sim N(\mu^*, \sigma_*^2)$

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

$= \frac{1}{n}\sum_{i=1}^{n} \underbrace{\mathbb{E}[x_i]}_{\mu^*} = \mu^*$

- MLE for the variance of a Gaussian is **biased**
  - $$\widehat{\sigma}^2_{\mathrm{MLE}} = \frac{1}{n}\sum_{i=1}^{n} (x_i - \widehat{\mu}_{\mathrm{MLE}})^2$$
  - $\mathbb{E}[\widehat{\sigma}^2_{\mathrm{MLE}}] \neq \sigma^2$

$\mathbb{E}[\hat{\sigma}^2_{MLE}] = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}[(x_i - \hat{\mu})^2]$

$= \frac{1}{n}\sum_{i=1}^{n}\left\{\underbrace{\mathbb{E}\, x_i^2}_{\sigma^2+\mu^2} - 2\underbrace{\mathbb{E}[x_i]}_{\mu^*}\hat{\mu} + \hat{\mu}^2\right\}$

$= \sigma^2 + (\mu - \hat{\mu})^2$

Maximum Likelihood Estimation

- **Observe** $X_1, X_2, \ldots, X_n$ drawn i.i.d. from $P(X_i; \theta)$ for some true $\theta = \theta^*$
- **Likelihood function**: $L_n(\theta) = \prod_{i=1}^{n} P(X_i; \theta)$
- **Log-likelihood function**: $\ell_n(\theta) = \log L_n(\theta) = \sum_{i=1}^{n} \log P(X_i; \theta)$
- **Maximum Likelihood Estimator (MLE)**: $\widehat{\theta}_{\mathrm{MLE}} = \arg\max_{\theta} \ell_n(\theta)$

- Properties (under benign regularity conditions—smoothness, identifiability, etc.):
  - MLE converges to the ground truths θ^* as the number of samples $n \to \infty$

Linear Regression

Maximum Likelihood Estimation

- **Observe** $X_1, X_2, \ldots, X_n$ drawn i.i.d. from $P(X_i; \theta)$ for some true $\theta = \theta^*$
- **Likelihood function**: $L_n(\theta) = \prod_{i=1}^{n} P(X_i; \theta)$
- **Log-likelihood function**: $\ell_n(\theta) = \log L_n(\theta) = \sum_{i=1}^{n} \log P(X_i; \theta)$
- **Maximum Likelihood Estimator (MLE)**: $\widehat{\theta}_{\mathrm{MLE}} = \arg\max_{\theta} \ell_n(\theta)$

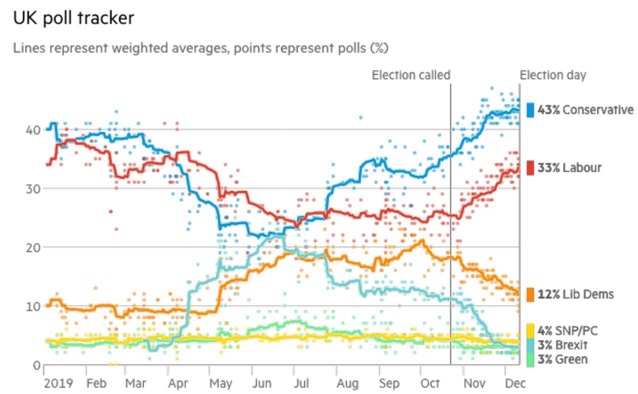
- Why do we care about recovering the "true" parameter θ^*?
  - **Estimation** of the parameter θ^* can be a goal.
  - Help **Interpret** or summarize large datasets.
  - Make **predictions** about future data.
  - **Generate** new data $X \sim f(\,\cdot\,; \hat{\theta}_{\mathrm{MLE}})$

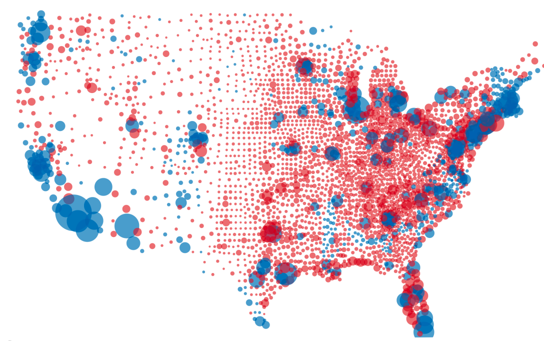
Estimation

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?

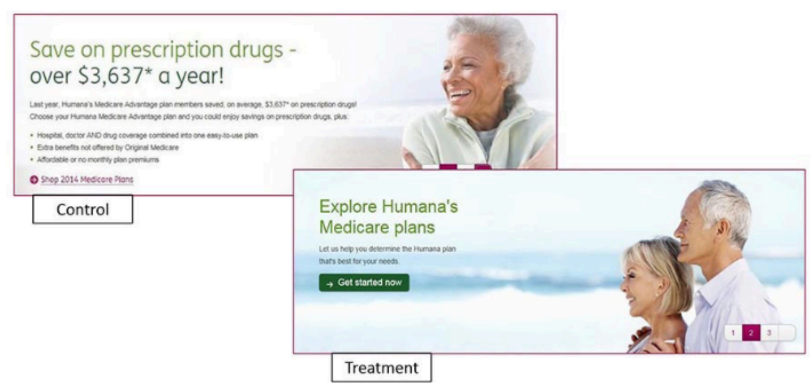
- θ_* is "true" average opinion
- $X_1, X_2, \ldots$ are sample calls





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"

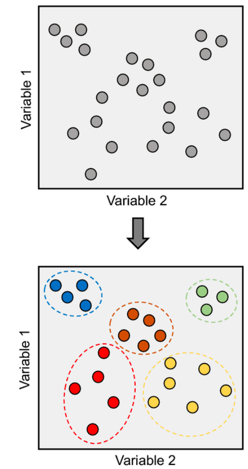


Interpret

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

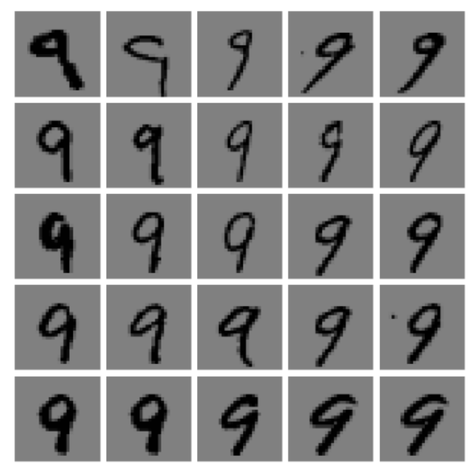
Customer segmentation / clustering
Can we identify distinct groups of customers by their behavior?

- 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

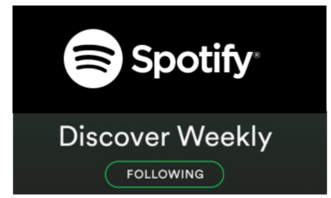


Predict

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

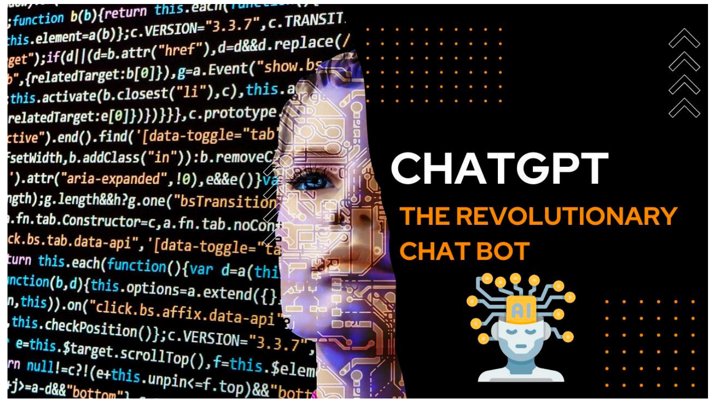
Generate

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ 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/

CSE 446/546

- week 1: **Estimation**
  - Maximum Likelihood Estimation
- week 1~8: **Prediction**
  - week 1~4: Linear regression models
  - week 4~5: Linear classification models (also called Logistic regression)
  - Mideterm
  - week 6~7: Non-linear models
- week 8~9: **Interpretation**
- week 10: **Generation**…(?) $\longrightarrow$ CSE 493S/599 2026sp

Linear regression model, 1-dimensional

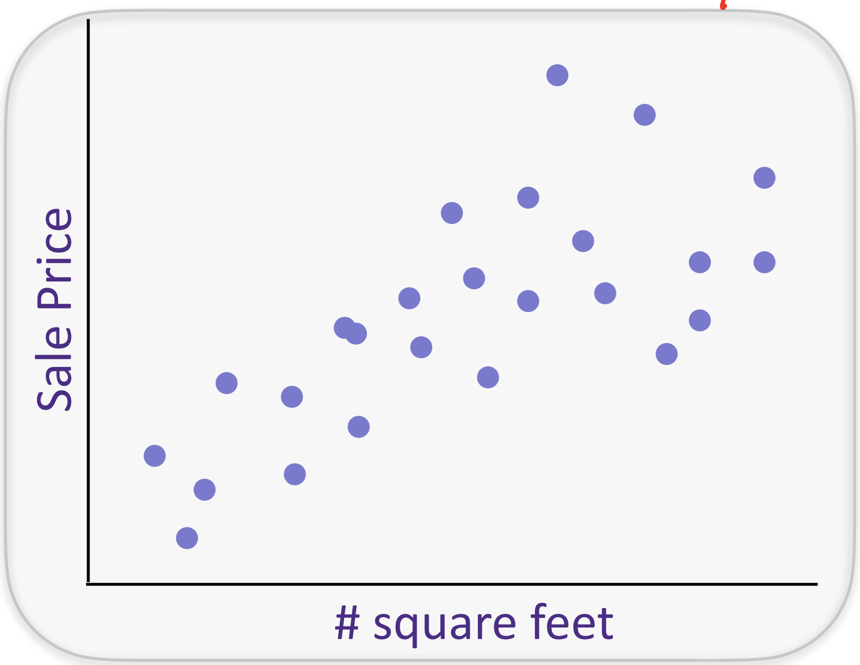
You want to sell your house that is 2,500 sq.ft.

Q. What is the right price?

Collect past sales data on zillow.com:

y = **House sale price** *and* x = **{# sq. ft.}**

label, response, dependent variable / Covariate, input variable, independent variable



Training Data: $x_i \in \mathbb{R} \quad y_i \in \mathbb{R}$

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

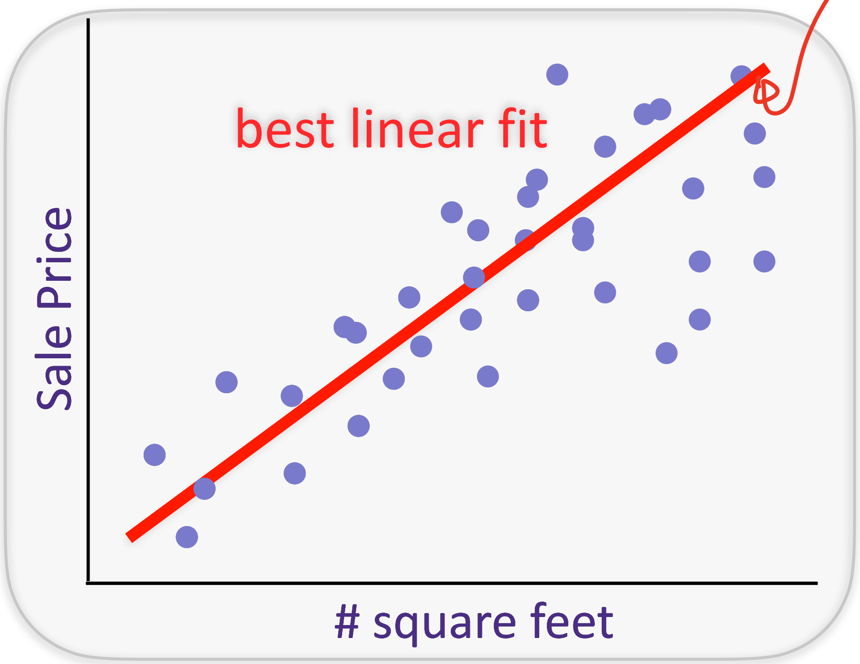
Linear regression model, 1-dimension

Given past sales data on zillow.com, predict:

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

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

w: slope



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

2. Hypothesis/Model: linear model

$$\boxed{y_i = \underbrace{w}_{\mathbb{R}} \cdot x_i + \underbrace{\epsilon_i}_{\mathbb{R}}}$$

Parameter of the model

Noise iid

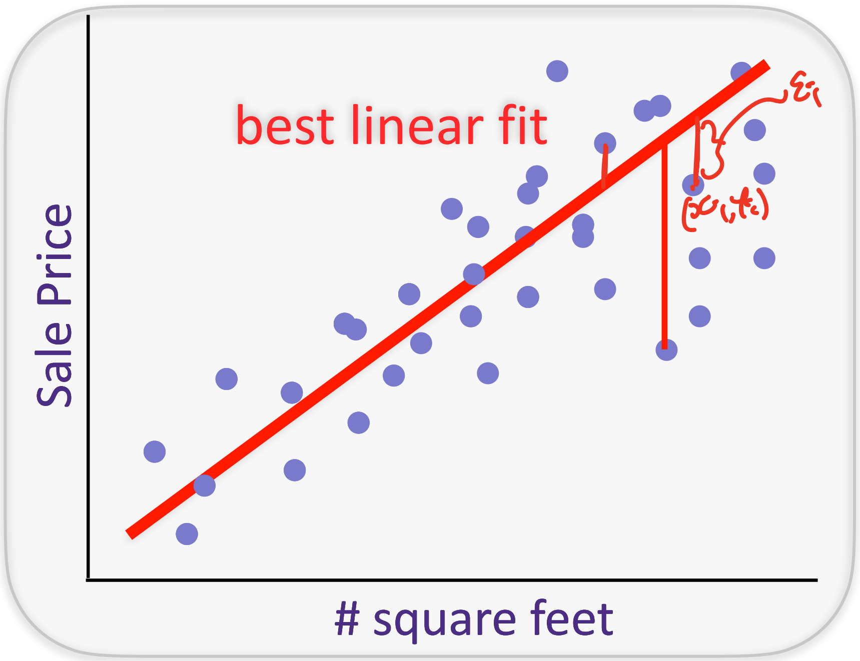
For now we assume there is no y-intercept in the model, and will handle it later

Linear regression model, 1-dimension

Given past sales data on zillow.com, predict:

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

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



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

2. Hypothesis/Model: linear

$$\boxed{y_i = w \cdot x_i + \epsilon_i}$$

3. Noise: i.i.d. Gaussian with

$$\epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

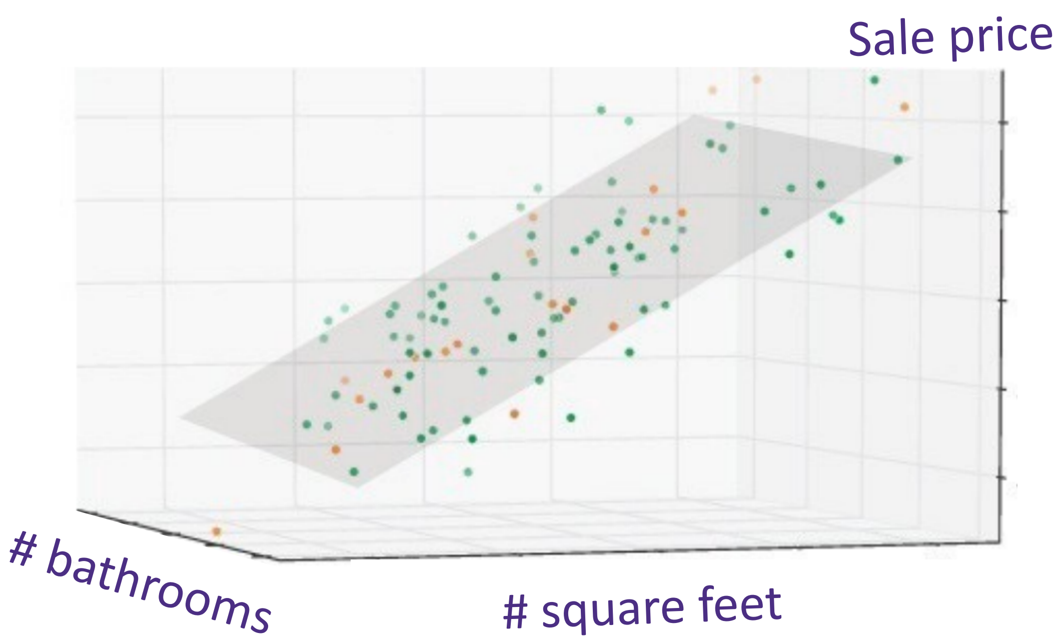
For now we assume there is no y-intercept in the model, and will handle it later

Linear regression model, d-dim

Given past sales data on zillow.com, predict:

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

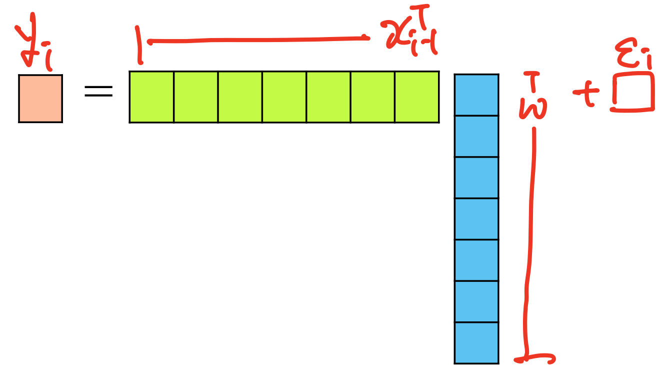
x = **{# sq. ft., zip code, date of sale, etc.}**



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

Hypothesis/Model: linear

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

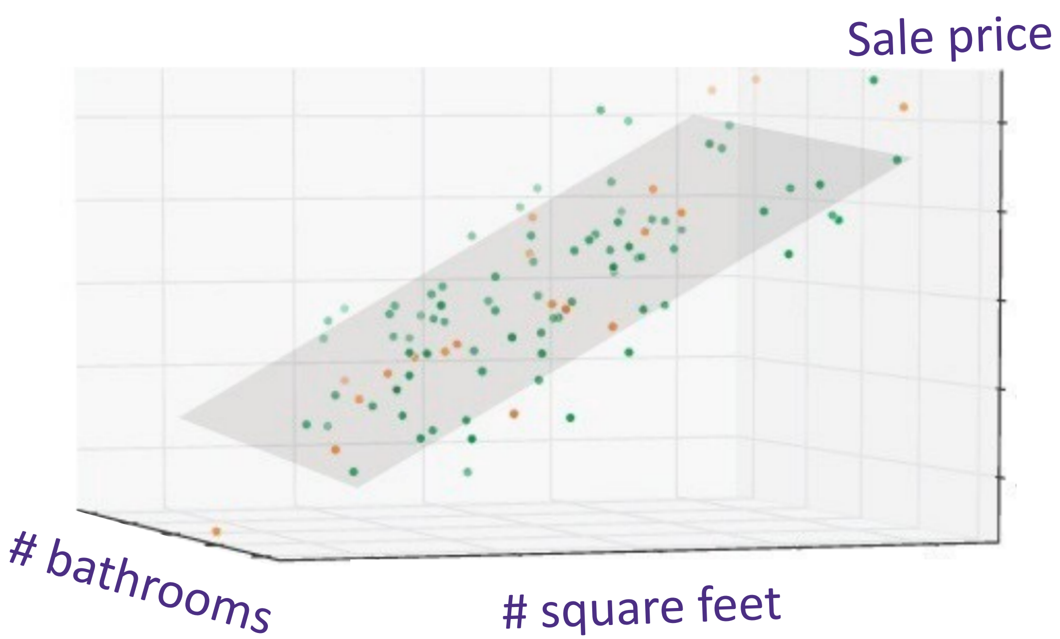


Linear regression model, d-dim

Given past sales data on zillow.com, predict:

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

x = **{# sq. ft., zip code, date of sale, etc.}**



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

Hypothesis/Model: linear

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

$\sim N(x_i^T w, \sigma^2)$

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

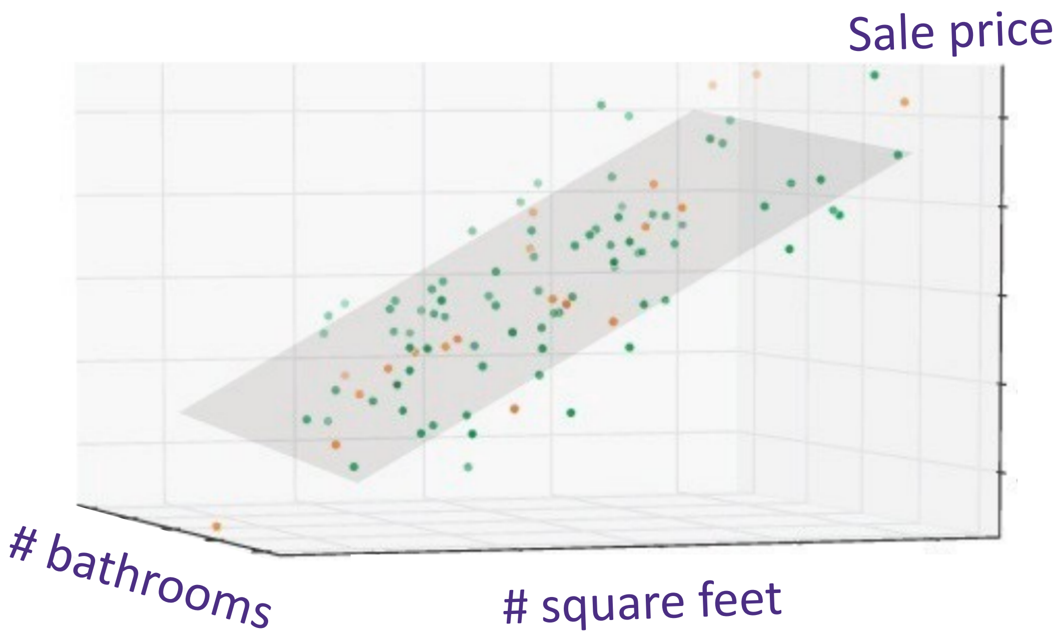
$$= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - x_i^T w)^2}{2\sigma^2}}$$

Linear regression model, d-dim

Given past sales data on zillow.com, predict:

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

x = **{# sq. ft., zip code, date of sale, etc.}**



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

Hypothesis/Model: linear

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

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

Maximizing log-likelihood

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

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

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

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

Maximum Likelihood Estimation

- **Observe** $X_1, X_2, \ldots, X_n$ drawn i.i.d. from $P(X_i; \theta)$ for some true $\theta = \theta^*$
- **Likelihood function**: $L_n(\theta) = \prod_{i=1}^{n} P(X_i; \theta)$
- **Log-likelihood function**: $\ell_n(\theta) = \log L_n(\theta) = \sum_{i=1}^{n} \log P(X_i; \theta)$
- **Maximum Likelihood Estimator (MLE)**: $\widehat{\theta}_{\mathrm{MLE}} = \arg\max_{\theta} \ell_n(\theta)$

- Properties (under benign regularity conditions—smoothness, identifiability, etc.):
  - MLE converges to the ground truths θ^* as the number of samples $n \to \infty$

Maximizing log-likelihood

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

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

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

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

$$\hat{w}_{MLE} = \arg\max_w \sum_{i=1}^n \left\{ \underbrace{-\log\sqrt{2\pi\sigma^2}}_{\text{ignore}} - \frac{(y_i - x_i^\top w)^2}{2\sigma^2} \right\}$$

$$= \arg\min \sum_{i=1}^n (y_i - x_i^\top w)^2$$

Maximizing log-likelihood

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

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

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

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

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

* MLE is minimizing squared error
* Different noise results in different loss

Maximizing log-likelihood

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

Set gradient=0, solve for w

$$\nabla_w f = -\sum_{i=1}^{n} (y_i - x_i^T w)\cdot x_i$$

$\frac{\partial f}{\partial w_i}$ ith

$$\left(\sum_{i=1}^{n} x_i x_i^T\right) w = \sum_{i=1}^{n} y_i x_i$$

$$\boxed{w = \left(\sum_{i=1}^{n} x_i x_i^T\right)^{-1} \cdot \sum_{j=1}^{n} y_i x_i}$$

* if $\sum_{i=1}^{n} x_i x_i^T$ is invertible

Maximizing log-likelihood

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

Set gradient=0, solve for w

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

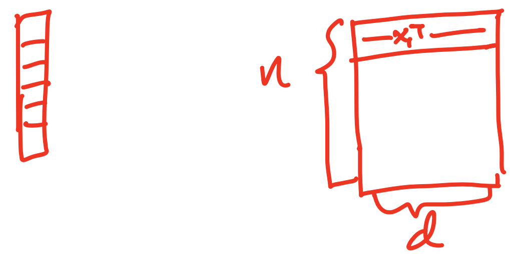
The regression problem in matrix notation

Data:

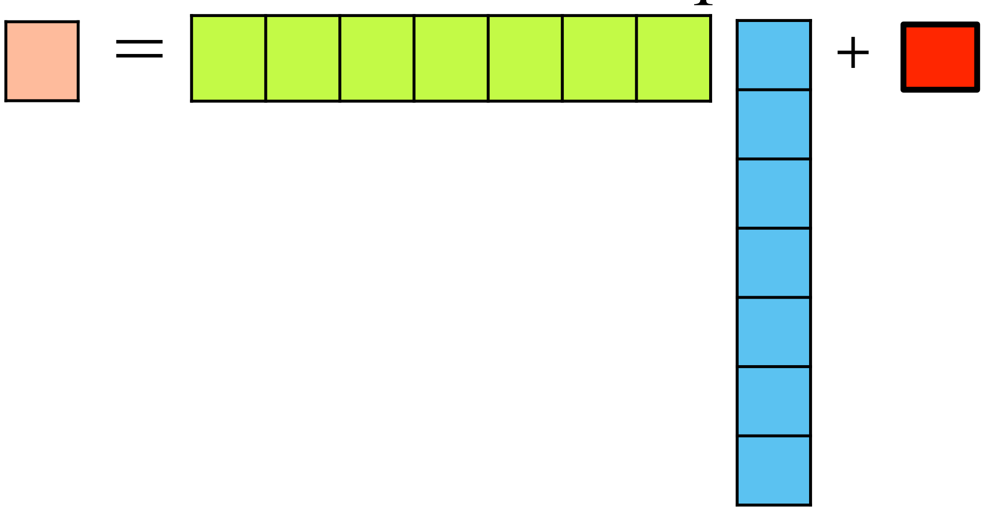
label $\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$ input matrix $\mathbf{X} = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix}$

d : # of features/size of the input

n : # of examples/datapoints

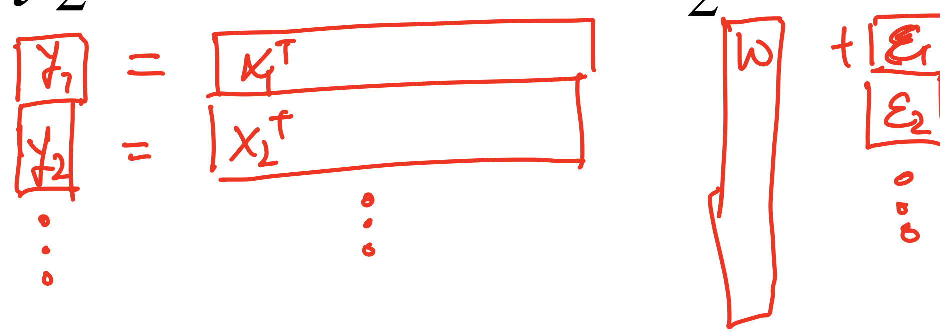


$$y_1 = x_1^T w + \epsilon_1$$



$$y_1 = x_1^T w + \epsilon_1$$

$$y_2 = x_2^T w + \epsilon_2$$



The regression problem in matrix notation

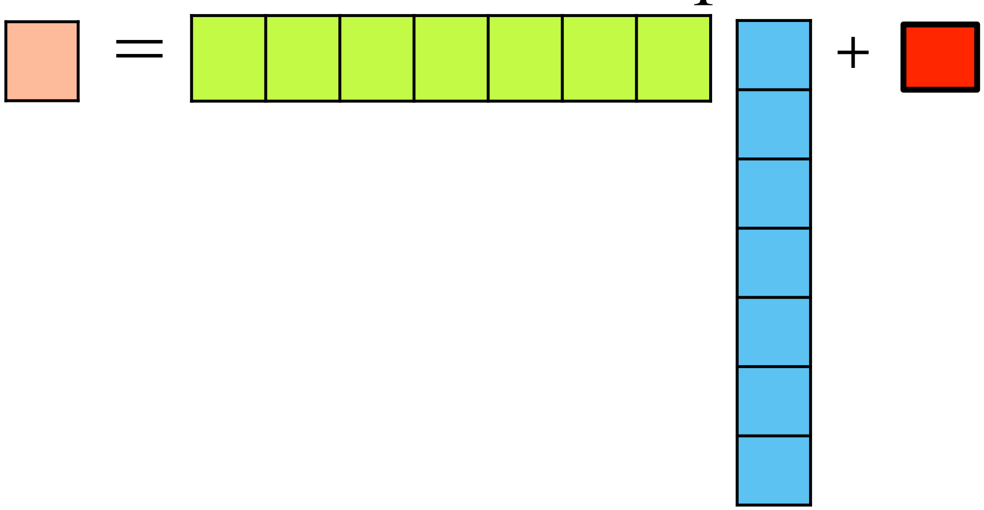
Data:

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

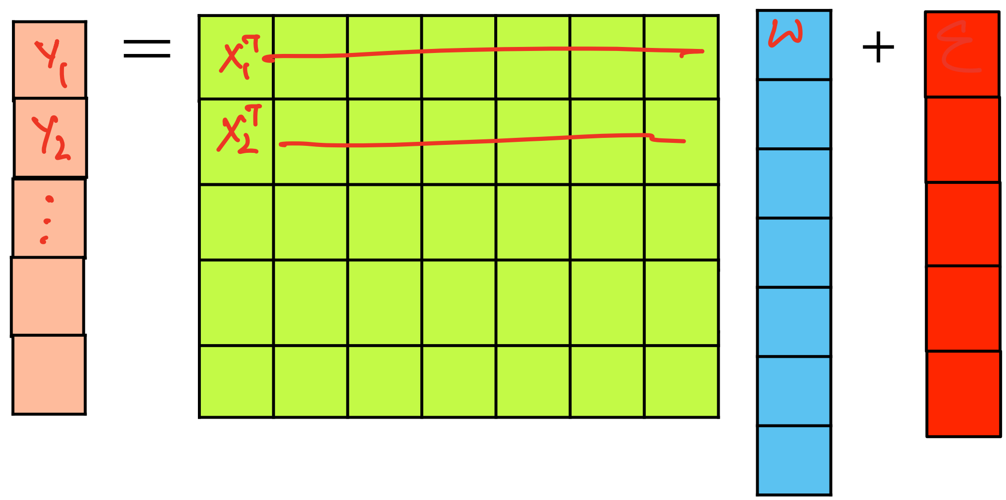
d : # of features/size of the input

n : # of examples/datapoints

$$y_1 = x_1^T w + \epsilon_1$$



$$y = Xw + \epsilon$$



The regression problem in matrix notation

$$\widehat{w}_{MLE} = \arg\min_w \sum_{i=1}^n (y_i - x_i^\top w)^2 = \| y - X \cdot w \|_2^2$$

d : # of features

n : # of examples/datapoints

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

$z =$

$\|z\|_2^2 = \sum_{i=1}^{d} z_i^2$

square of a scalar

we use ℓ_2-norm

$\|z\|_p^2$: ℓ_p-norm.

ℓ_2 norm: $\|z\|_2 = \sqrt{\sum_{i=1}^n z_i^2} = \sqrt{z^\top z}$

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

$$= \arg\min_w (\mathbf{y} - \mathbf{X}w)^T (\mathbf{y} - \mathbf{X}w)$$

[related to HW0 questions A6 and A7]

The regression problem in matrix notation

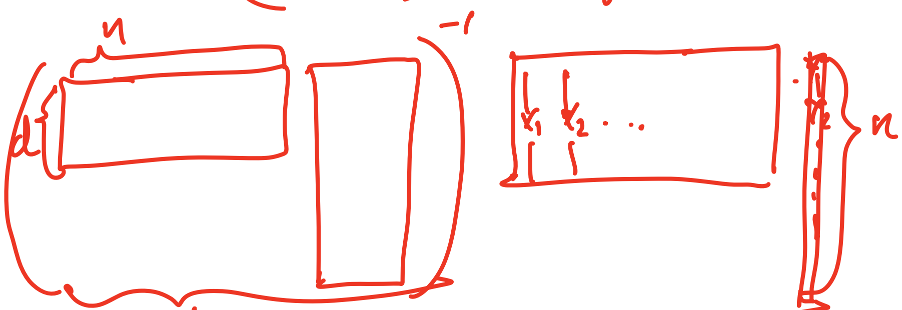
$$= \arg\min_w (\mathbf{y} - \mathbf{X}w)^T (\mathbf{y} - \mathbf{X}w)$$

$$= \quad y^T y - 2 y^T X w + w^T X^T X w.$$

$$\nabla_w f(w) = -2X^T y + 2X^T X w \quad = 0$$

$$X^T y = (X^T X) w$$

$$\hat{w}_{MLE} = (X^T X)^{-1} \cdot X^T y.$$



$$\left(\sum_{i=1}^{n} x_i x_i^T \right)^{-1} \qquad \sum_{i=1}^{n} x_i^T y_i$$

$$\leftarrow \nabla_w w^T w = w$$

$$\nabla_w x^T w = x$$

$$\nabla_w w^T A w = 2 A \cdot w$$

$$\hat{w}_{MLE} = (X^T X)^{-1} X^T y$$

The regression problem in matrix notation

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

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

d : # of features

n : # of examples/datapoints

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

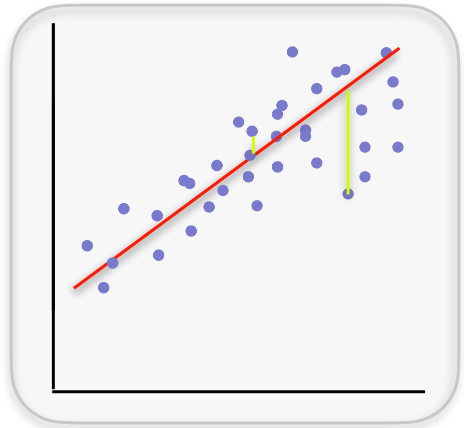
$$\begin{aligned} \widehat{w}_{LS} &= \arg\min_w ||\mathbf{y} - \mathbf{X}w||_2^2 \\ &= \arg\min_w (\mathbf{y} - \mathbf{X}w)^T(\mathbf{y} - \mathbf{X}w) \end{aligned}$$

$$\boxed{\hat{w}_{LS} = \hat{w}_{MLE} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}}$$

The regression problem in matrix notation

Recall that we start with a linear model with no offset

$$y_i = x_i^T w + \epsilon_1$$



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

We can add the offset to the linear model,

with a new parameter b

$\theta = (w \in \mathbb{R}^d, b \in \mathbb{R})$

$$y_i = x_i^T w + b + \epsilon_1$$

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

all 1's vector.

Dealing with an offset

$$y^Ty - 2y^TXw - 2y^T1\cdot b + w^TX^TXw + b^2 1^T1 = f(w,b)$$

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

$$\nabla_w f(w,b) = 0 \longrightarrow \mathbf{X}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{X}^T\mathbf{1} = \mathbf{X}^T\mathbf{y}$$

$$\nabla_b f(w,b) = 0 \longrightarrow \mathbf{1}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{1}^T\mathbf{1} = \mathbf{1}^T\mathbf{y}$$

$$\begin{bmatrix} X^TX & X^T1 \\ 1^TX & 1^T1 \end{bmatrix} \begin{bmatrix} \widehat{w}_{LS} \\ \widehat{b}_{LS} \end{bmatrix} \begin{matrix} \}d \\ \}1 \end{matrix} = \begin{bmatrix} X^Ty \\ \vdots \\ 1^Ty \end{bmatrix}$$

$$\tilde{X} = [X \;\; 1]$$

$$\tilde{X}^T\tilde{X}\tilde{w} = \tilde{X}^Ty$$

$$\tilde{w} = (\tilde{X}^T\tilde{X})^{-1}\tilde{X}^Ty$$

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 $X^T\mathbf{1} = 0$, i.e., if each feature is mean-zero or we pre-processed the data have zero-mean, then

$$\widehat{w}_{LS} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

$$\widehat{b}_{LS} = \frac{1}{n}\sum_{i=1}^{n} y_i \quad \leftarrow \text{Average Response.}$$

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?

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

Questions?