CSE 446/546
Lec 2: Linear Regression

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Maximum Likelihood Estimation

Observe $X_1, X_2, \ldots, X_n$ 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) $\widehat{\theta}_{MLE} = \arg\max_{\theta} L_n(\theta)$

MLE for Gaussian

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

$$P(\mathcal{D}|\mu,\sigma) = P(x_1,\ldots,x_n|\mu,\sigma)$$
$$= \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \prod_{i=1}^{n} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- 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?

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

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

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

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

MLE for variance

$$\frac{d}{d\sigma}\sigma^{-2} = -2\sigma^{-3}$$

- Again, set derivative to zero:

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

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

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

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

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

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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?

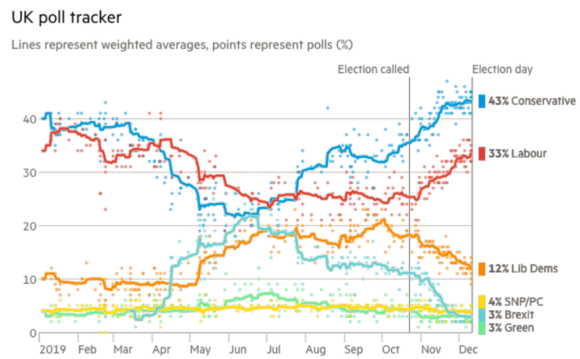
- **Estimation** of the parameters θ_* is the goal
- Help **interpret** or summarize large datasets
- Make **predictions** about future data
- **Generate** new data $X \sim f(\,\cdot\,;\widehat{\theta}_{MLE})$

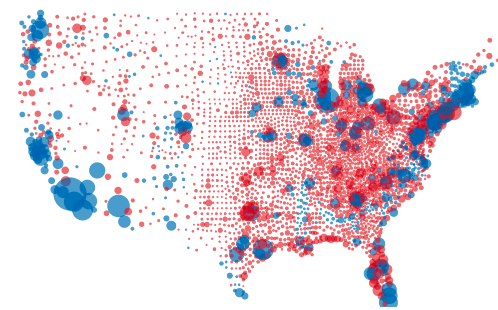
Estimation

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?

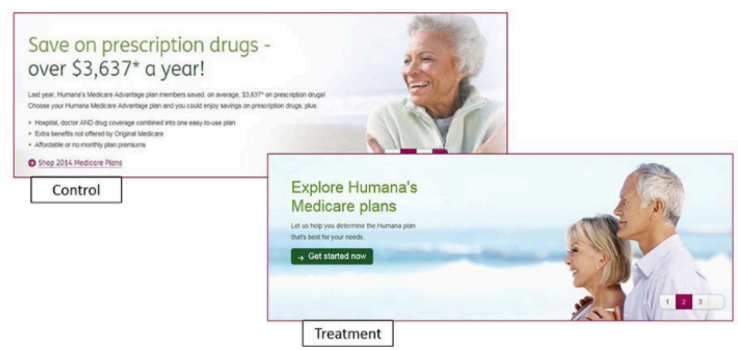
- θ_* is "true" average opinion
- $X_1, X_2, \ldots$ are sample calls





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"

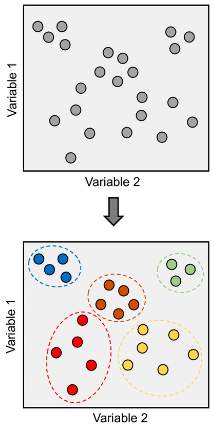


Interpret

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

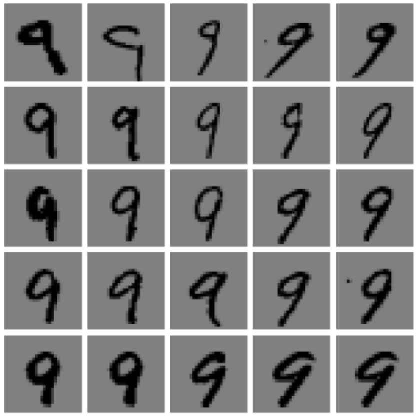
Customer segmentation / clustering
Can we identify distinct groups of customers by their behavior?

- 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

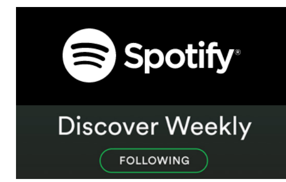


Predict

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

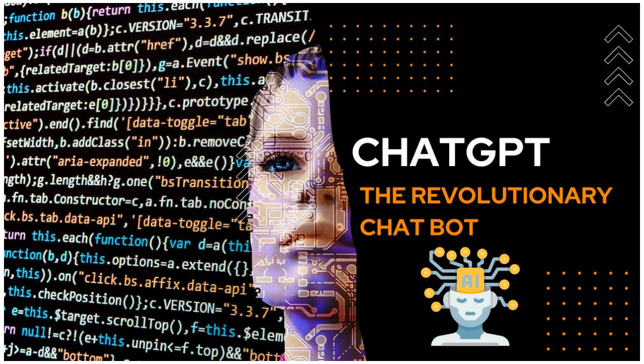
Generate

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/

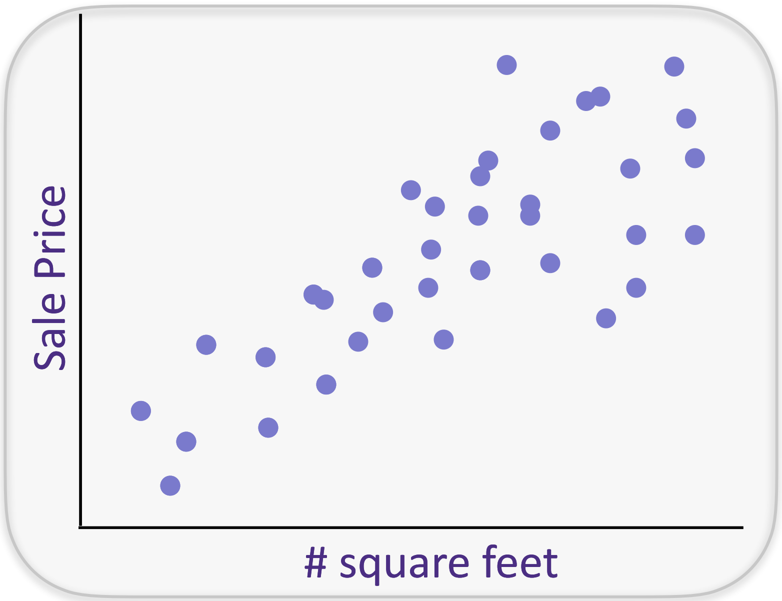
Linear Regression

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

Given past sales data on zillow.com, predict:

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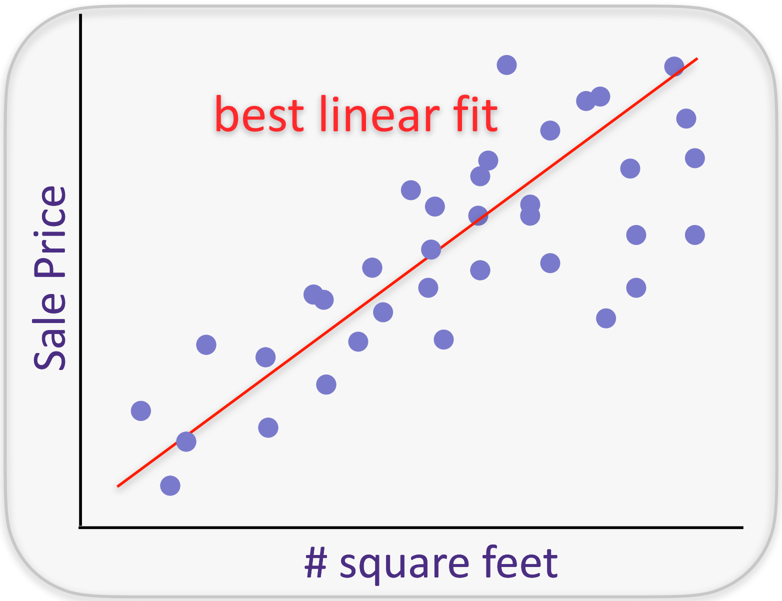
x = **{# sq. ft.}**



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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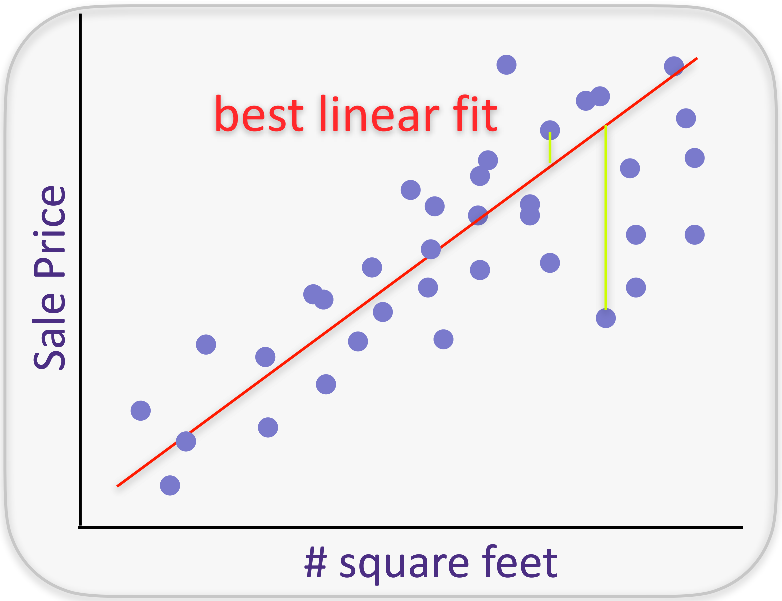

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The regression problem, d-dim

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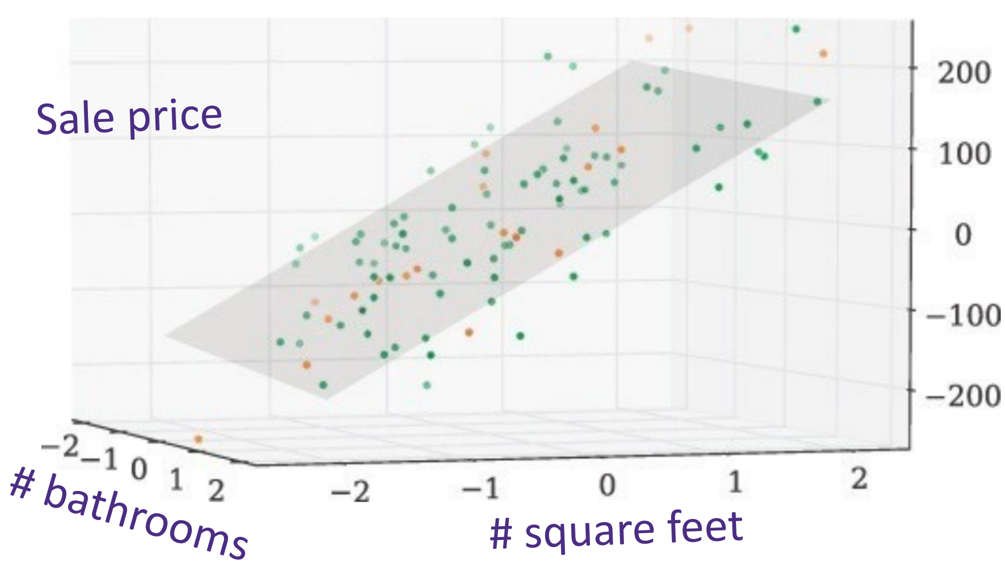
x = **{# sq. ft., zip code, date of sale, etc.}**



Training Data: $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$

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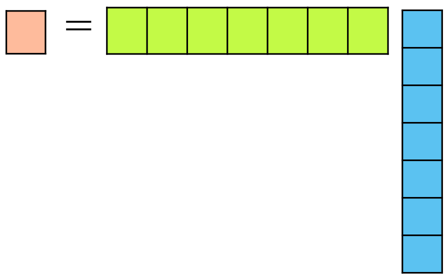

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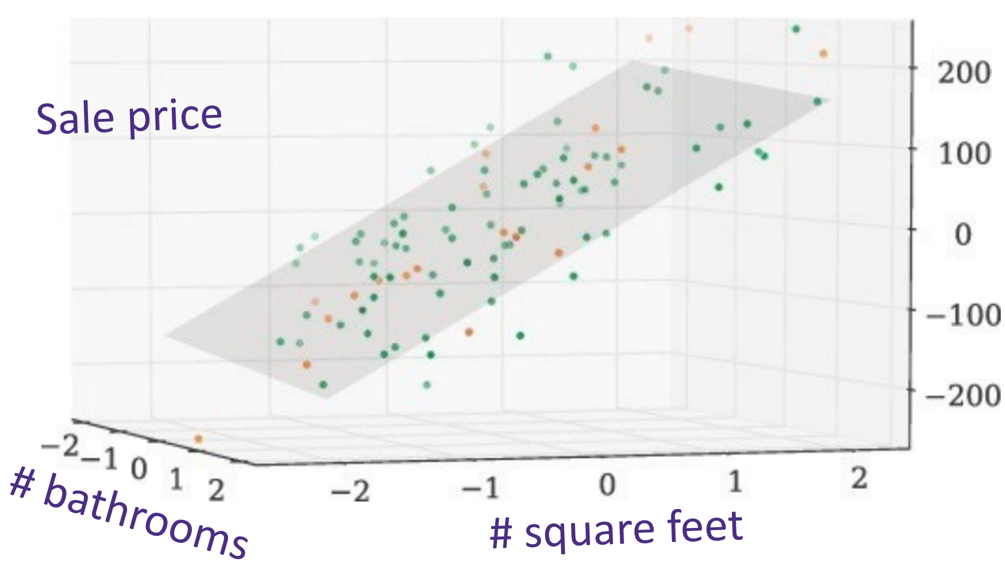

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$$p(y|x, w, \sigma) =$$

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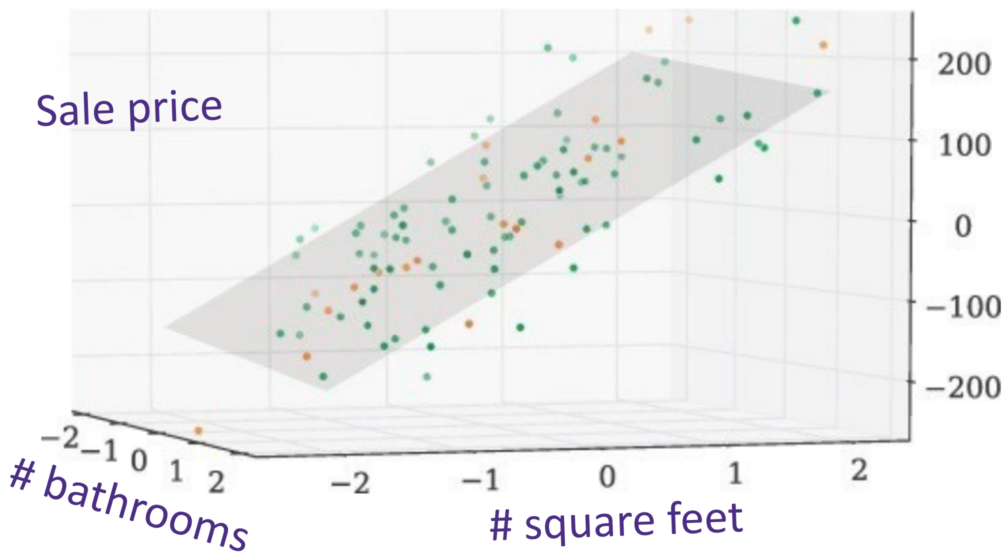

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Maximizing log-likelihood

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

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

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

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

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Set derivate=0, solve for w

Maximizing log-likelihood

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Set derivate=0, solve for w

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

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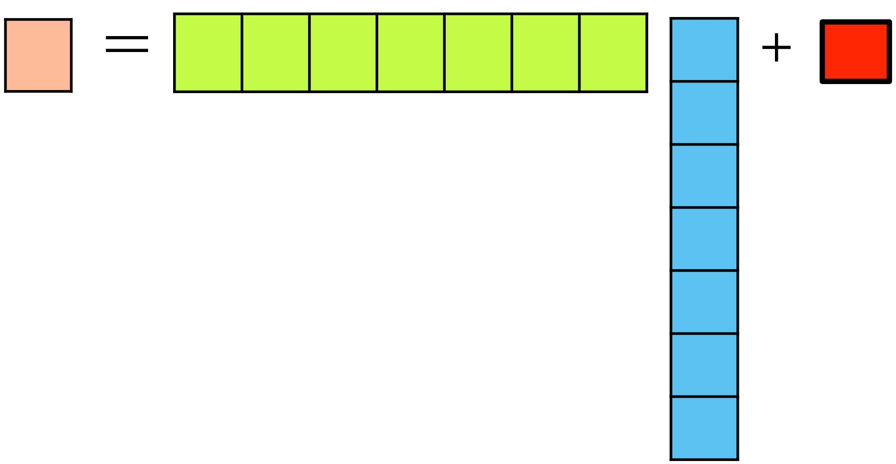
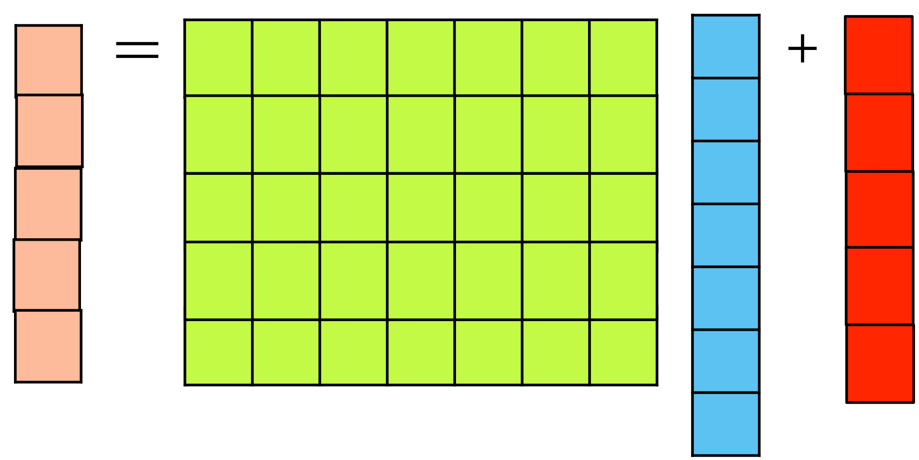
$$y_i = x_i^T w + \epsilon_i$$



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



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

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

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

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

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

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

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

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

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

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

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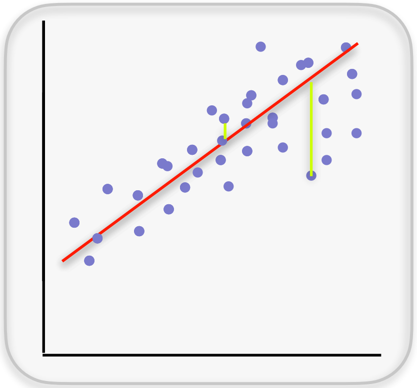

What about an offset?

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

Dealing with an offset

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

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

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

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

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

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

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