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:

- *You*: The probability is:

- *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

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

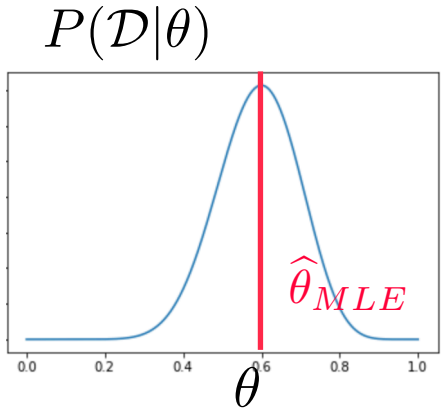
Maximum Likelihood Estimation

- **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:

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



Your first learning algorithm

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

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

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

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

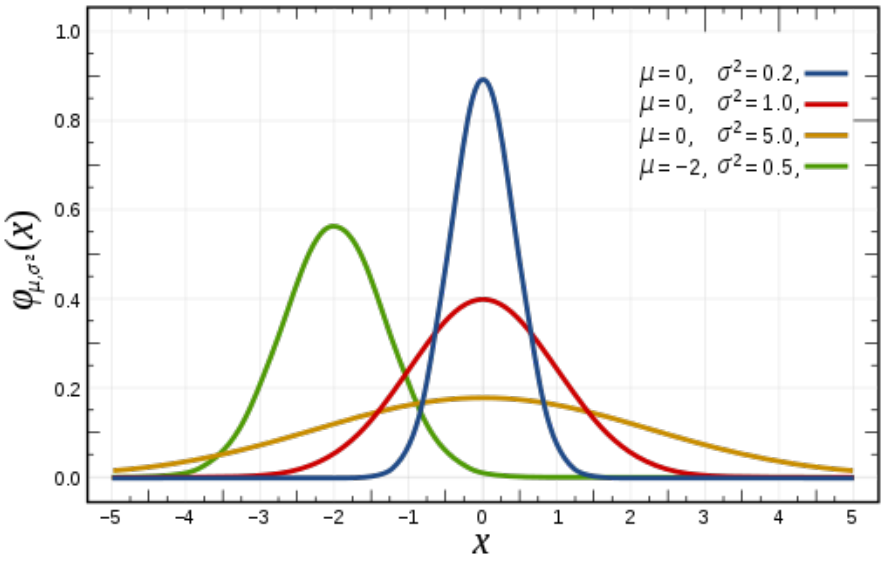
Recap

- 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…**

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



Some properties of Gaussians

- affine transformation (multiplying by scalar and adding a constant)
  - $X \sim N(\mu, \sigma^2)$
  - $Y = aX + b \quad \rightarrow \quad Y \sim N(a\mu+b, a^2\sigma^2)$

- 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

- 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?

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

MLE for variance

- Again, set derivative to zero:

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

Learning Gaussian parameters

- MLE:

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

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

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

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

- Unbiased variance estimator:

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

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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

UNIVERSITY of WASHINGTON

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

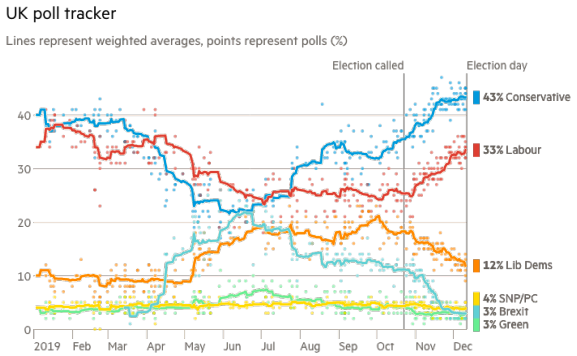
- **Estimation** of the parameters θ_* is the goal
- Help **interpret** or summarize large datasets
- Make **predictions** about future data
- **Generate** new data $X \sim f(\cdot\,; \widehat{\theta}_{MLE})$

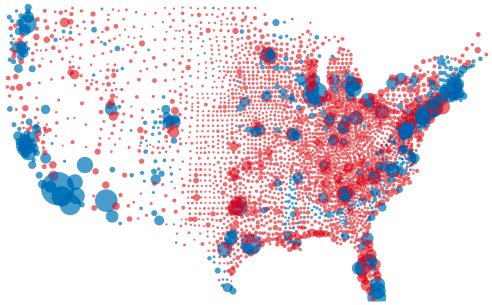
Estimation

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?

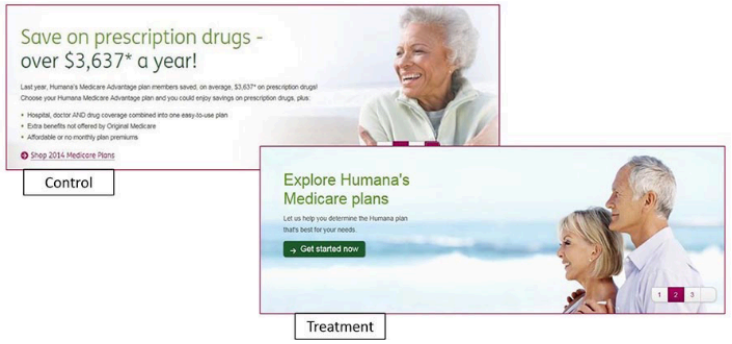
- θ_* is "true" average opinion
- $X_1, X_2, \ldots$ are sample calls





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

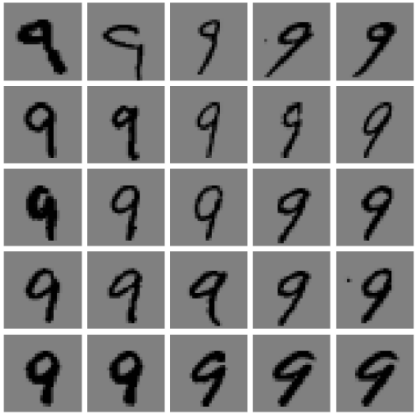
Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

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

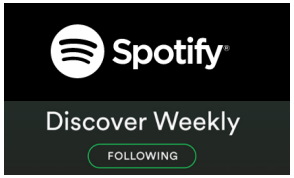


Predict

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

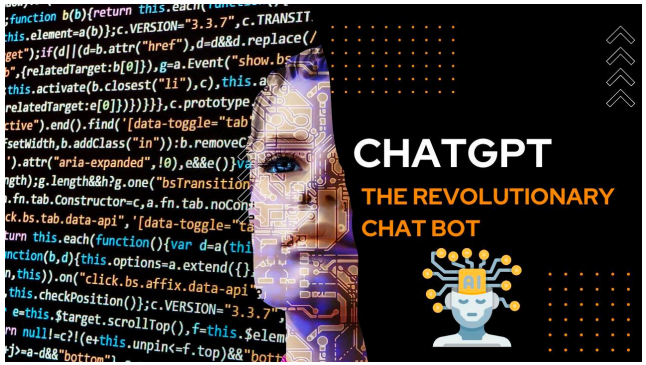
Generate

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/

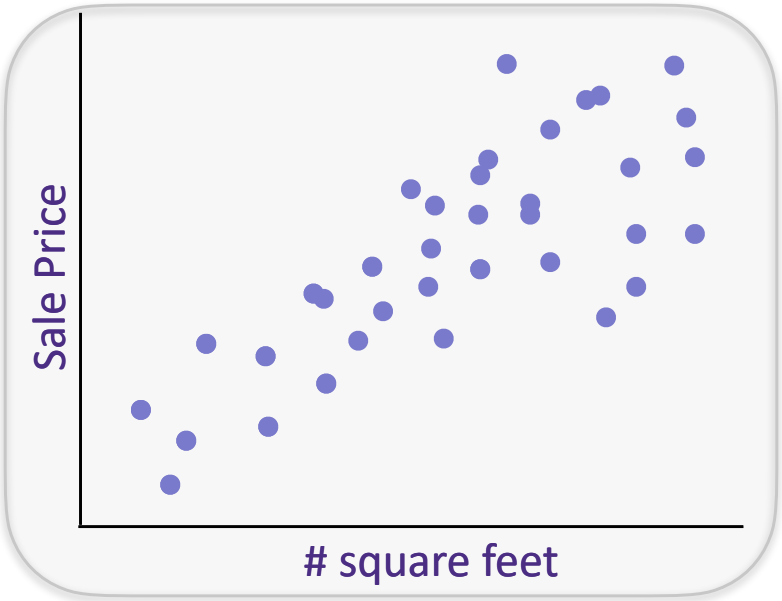
Linear Regression

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

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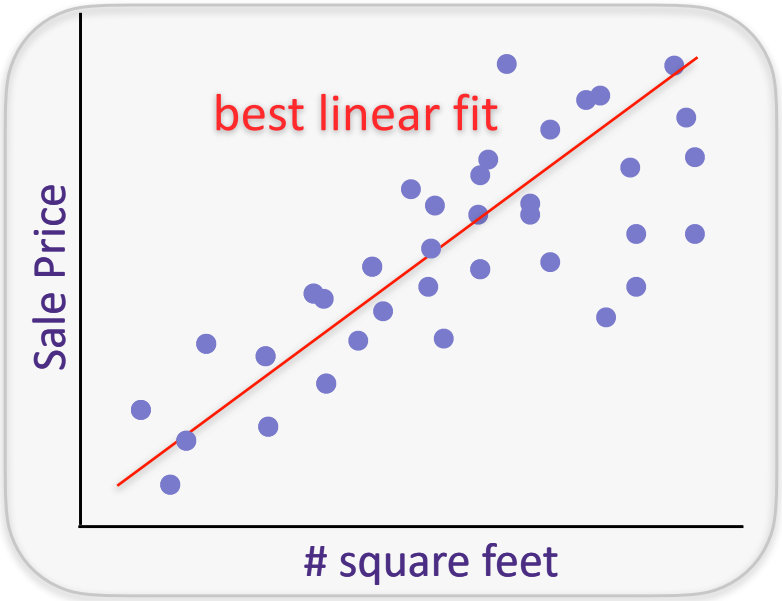

Training Data: $\{(x_i, y_i)\}_{i=1}^{n}$ $x_i \in \mathbb{R}$ $y_i \in \mathbb{R}$

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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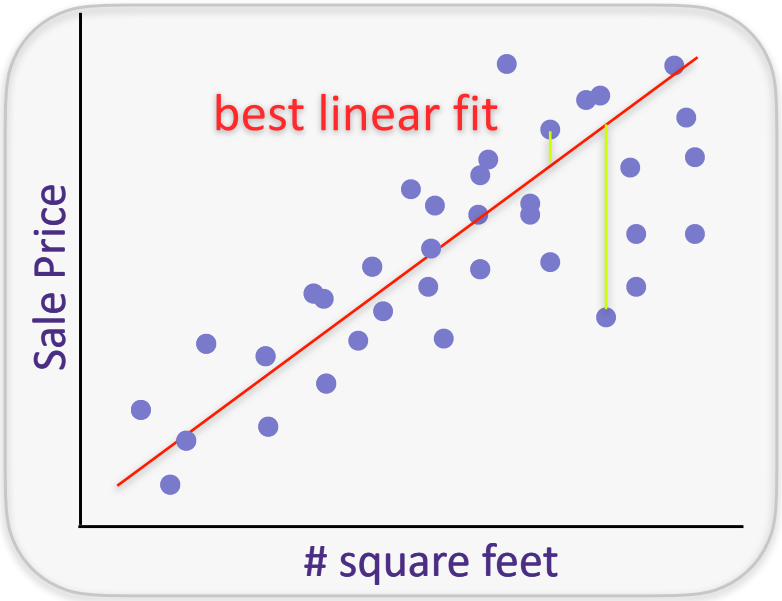

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The regression problem, d-dim

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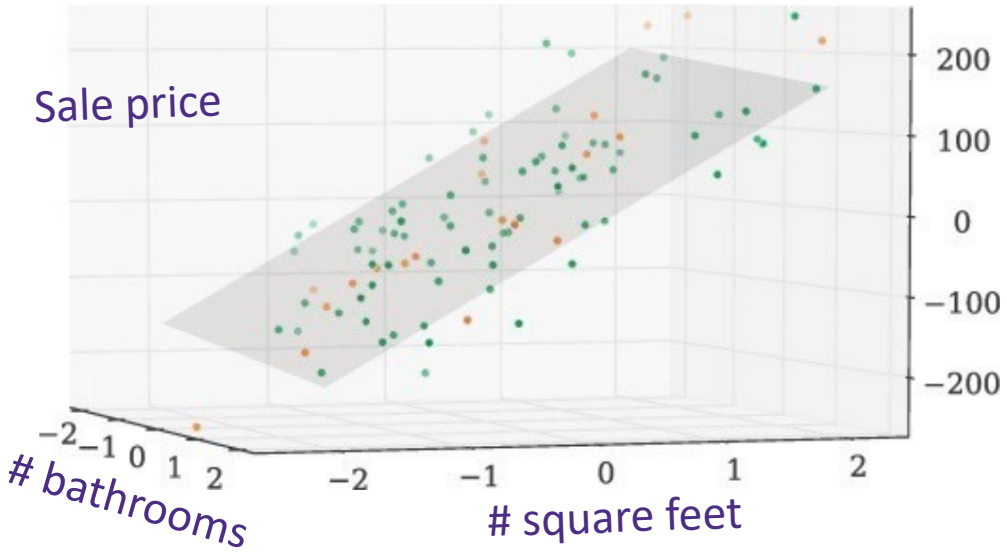
***x* = {# sq. ft., zip code, date of sale, etc.}**



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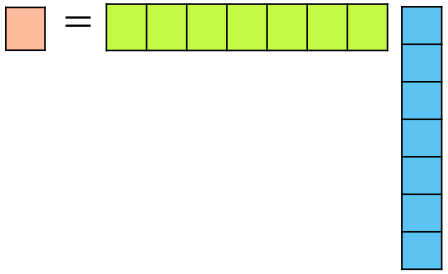

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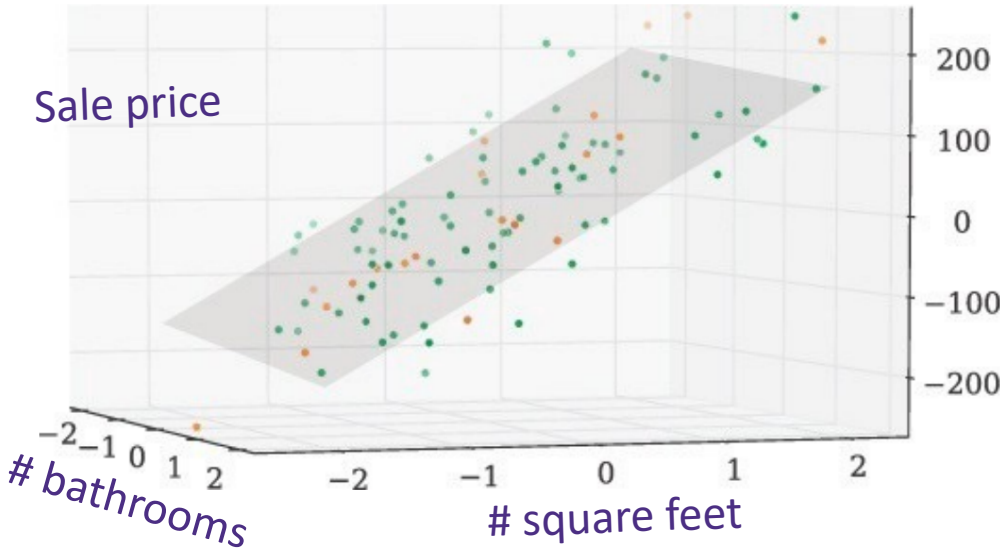

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$$p(y|x, w, \sigma) =$$

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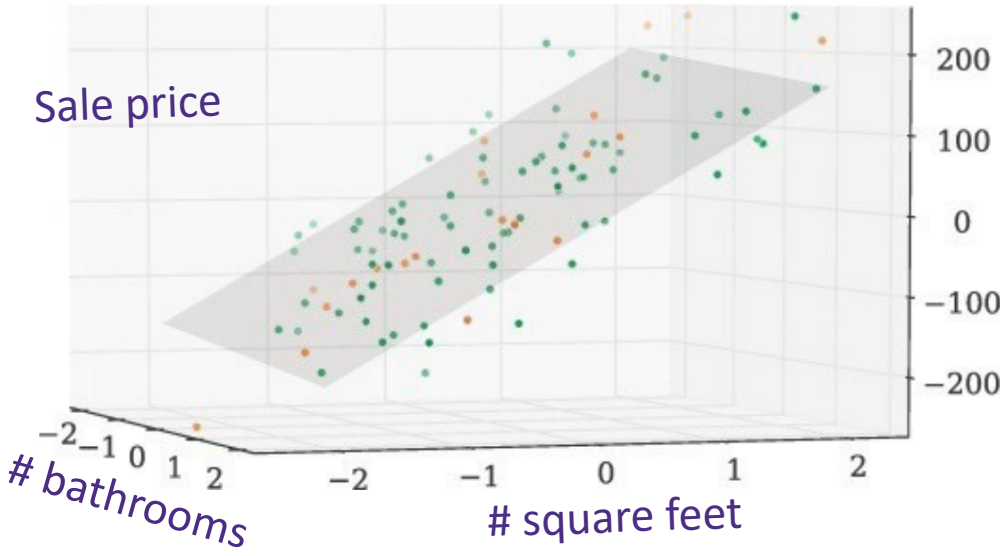

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$$p(y|x, w, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(y - x^\top w)^2 / 2\sigma^2}$$

Maximizing log-likelihood

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

The regression problem in matrix notation

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

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

d : # of features

n : # of examples/datapoints

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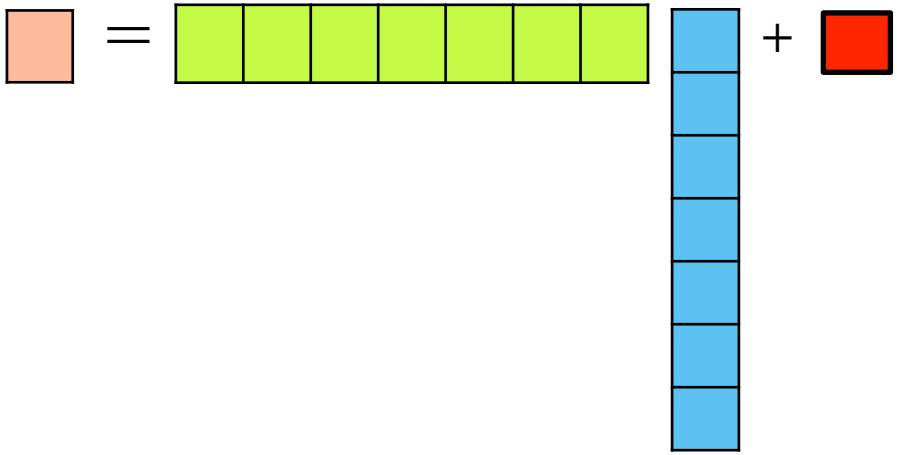

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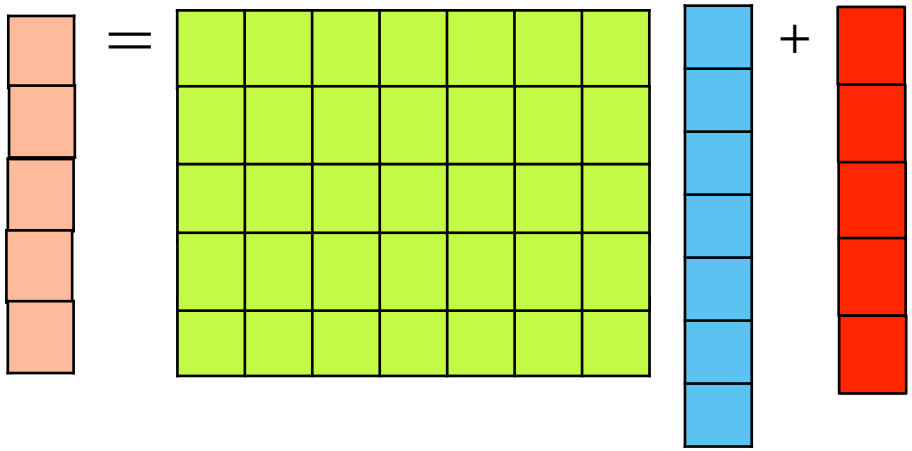

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ℓ_2 norm: $\|z\|_2 = \sqrt{\sum_{i=1}^{n} z_i^2} = \sqrt{z^\top z}$

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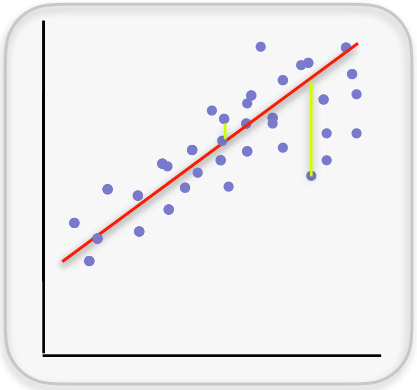
The regression problem in matrix notation

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



What about an offset?

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

Dealing with an offset

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

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

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

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

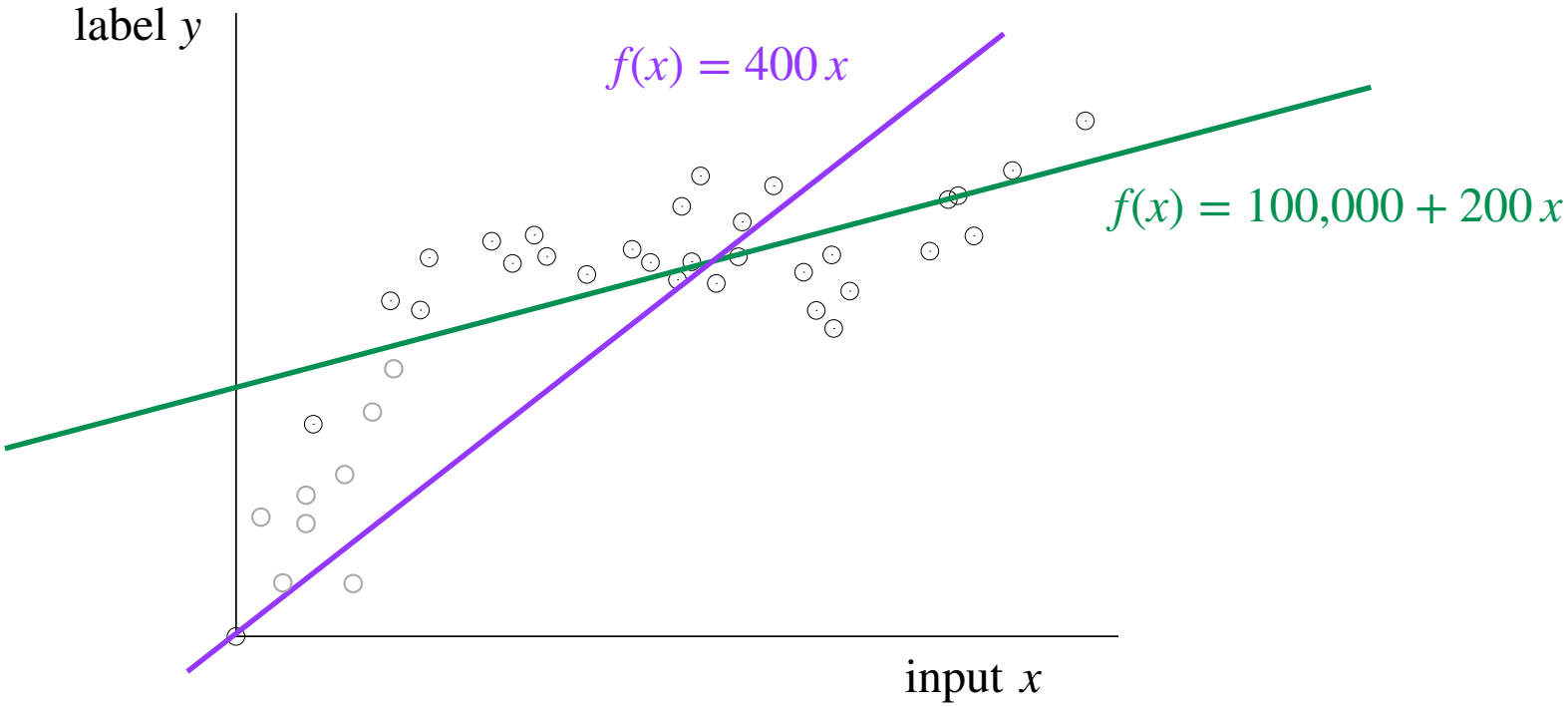
Choose a loss function- least squares

Pick the function which minimizes loss on data

Use function to make prediction on new examples

Linear regression with non-linear basis functions

Recap: Linear Regression



- In general high-dimensions, we fit a linear model with intercept

$$y_i \simeq w^T x_i + b\,, \quad \text{or equivalently} \quad y_i = w^T x_i + b + \epsilon_i$$

with model parameters $(w \in \mathbb{R}^d, b \in \mathbb{R})$ that minimizes ℓ_2-loss

$$\mathscr{L}(w,b) \;=\; \sum_{i=1}^{n} \underbrace{(y_i - (w^T x_i + b))^2}_{\text{error } \epsilon_i}$$

Recap: Linear Regression

- The least squares solution, i.e. the minimizer of the ℓ_2-loss can be written in a **closed form** as a function of data $\mathbf{X}$ and $\mathbf{y}$ as

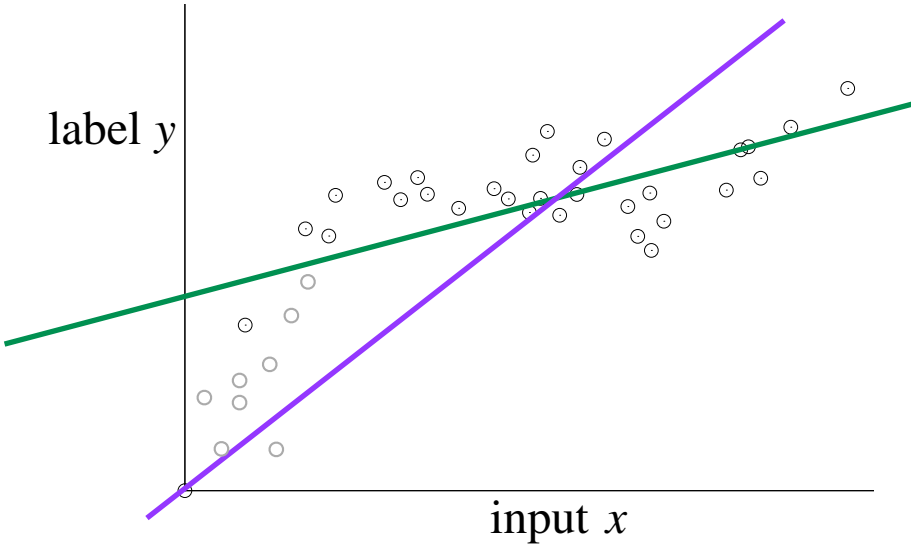
or equivalently using straightforward linear algebra by setting the gradient to zero:

$$\begin{bmatrix} \widehat{w}_{\text{LS}} \\ \widehat{b}_{\text{LS}} \end{bmatrix} = \left(\begin{bmatrix} \mathbf{X}^T \\ \mathbf{1}^T \end{bmatrix} \begin{bmatrix} \mathbf{X} & \mathbf{1} \end{bmatrix} \right)^{-1} \begin{bmatrix} \mathbf{X}^T \\ \mathbf{1}^T \end{bmatrix} \mathbf{y}$$

Quadratic regression in 1-dimension

- **Data:** $\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$

- **Linear model with parameter** (b, w_1)**:**
  - $\hat{y}_i = b + w_1 x_i$



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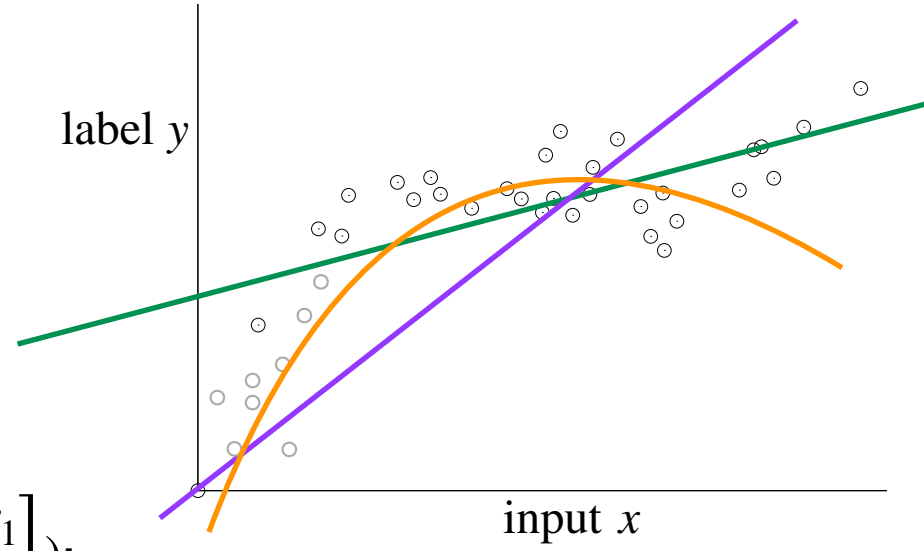

- **Linear model with parameter** (b, w_1)**:**
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- **Quadratic model with parameter** $(b, w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix})$**:**
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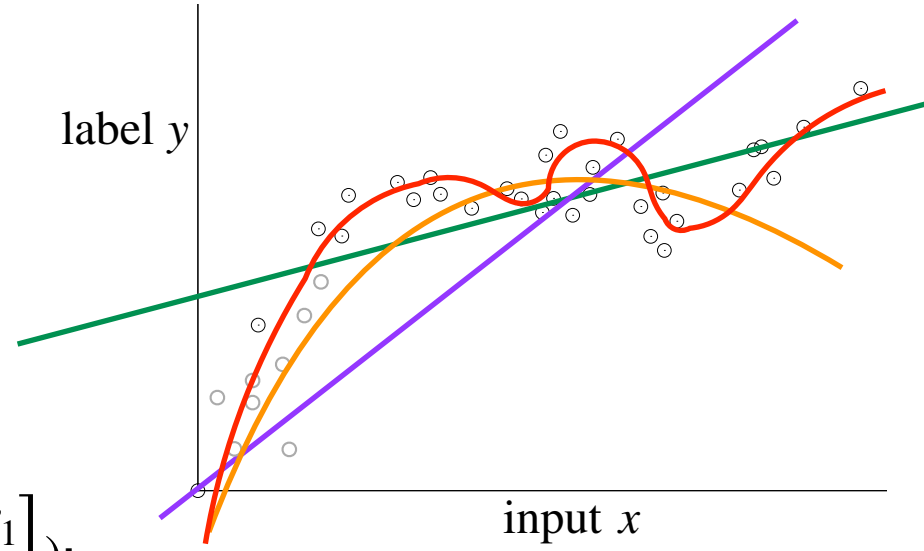

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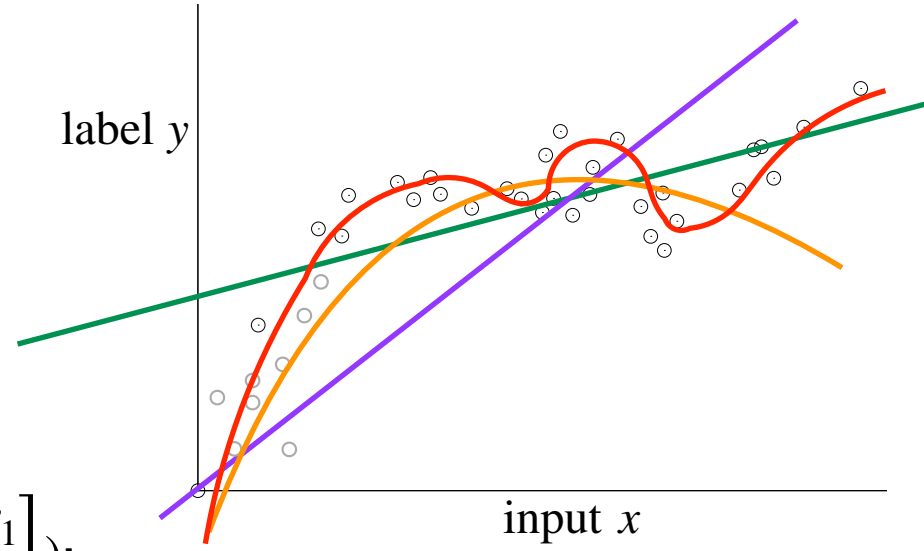

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Quadratic regression in 1-dimension

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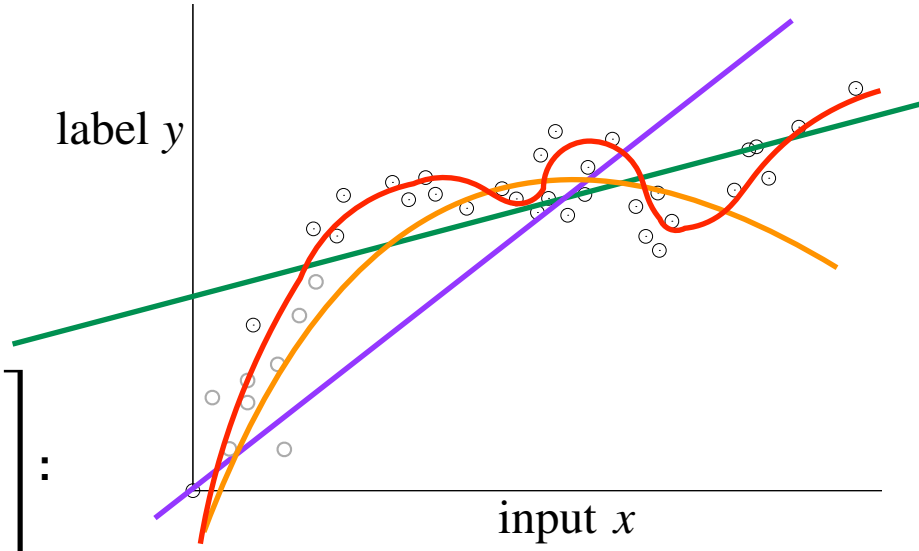

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Note: h can be arbitrary non-linear functions!

$$h(x) = \left[\log(x), x^2, \sin(x), \sqrt{x}\right]^\top$$

Quadratic regression in 1-dimension

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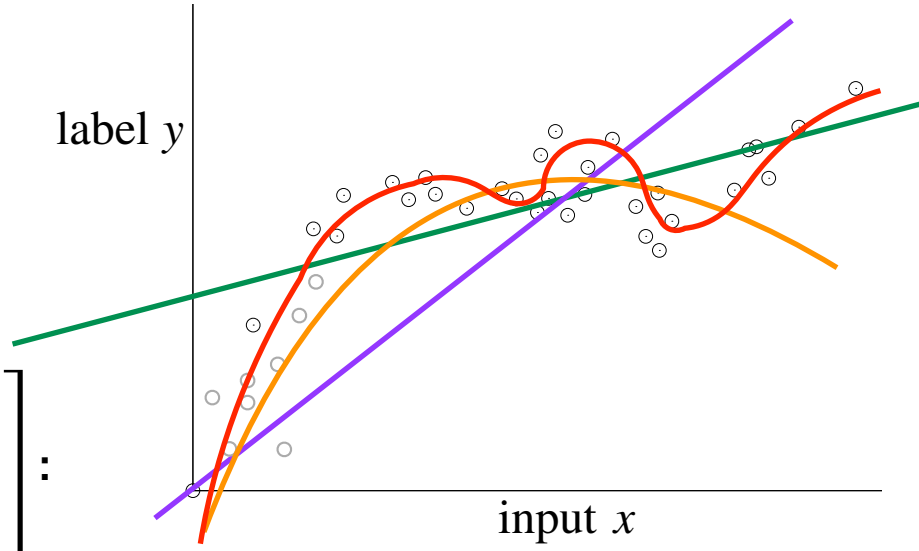

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How do we learn w?

Quadratic regression in 1-dimension

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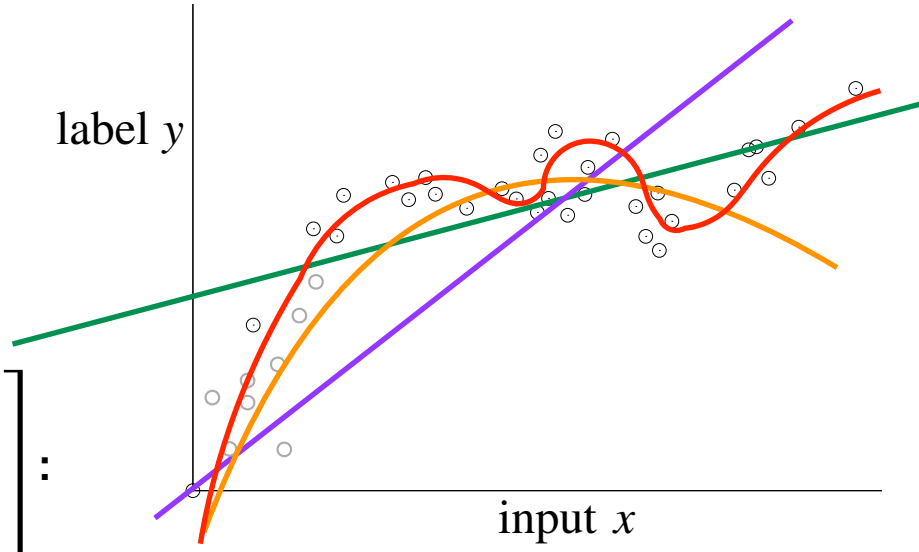

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How do we learn w?

$$\mathbf{H} = \begin{bmatrix} - - h(x_1)^\top - - \\ \vdots \\ - - h(x_n)^\top - - \end{bmatrix} \in \mathbb{R}^{n \times p}$$

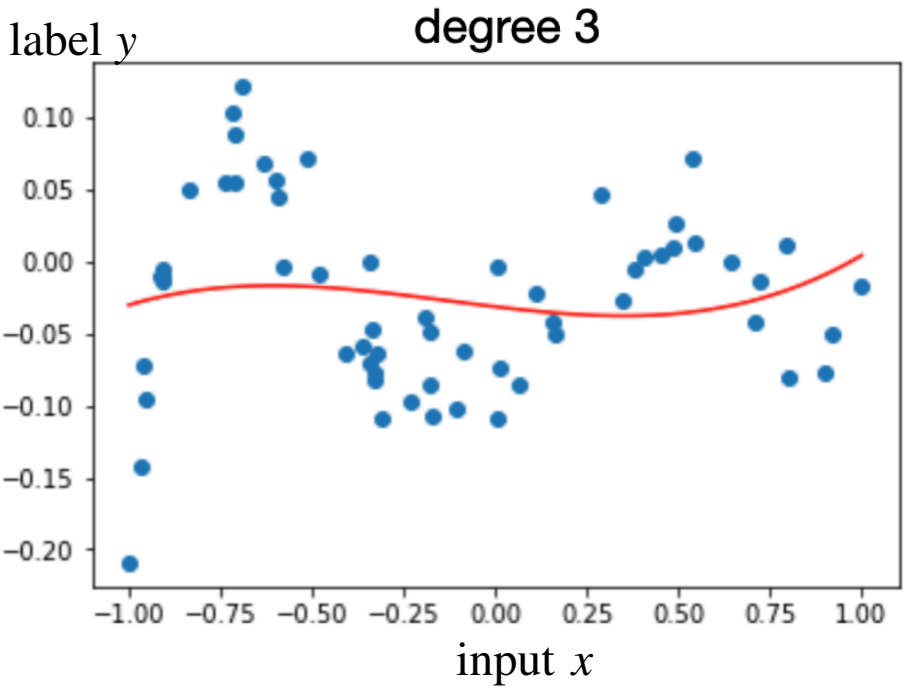
$$\widehat{w} = \arg\min_w \|\mathbf{H}w - \mathbf{y}\|_2^2$$

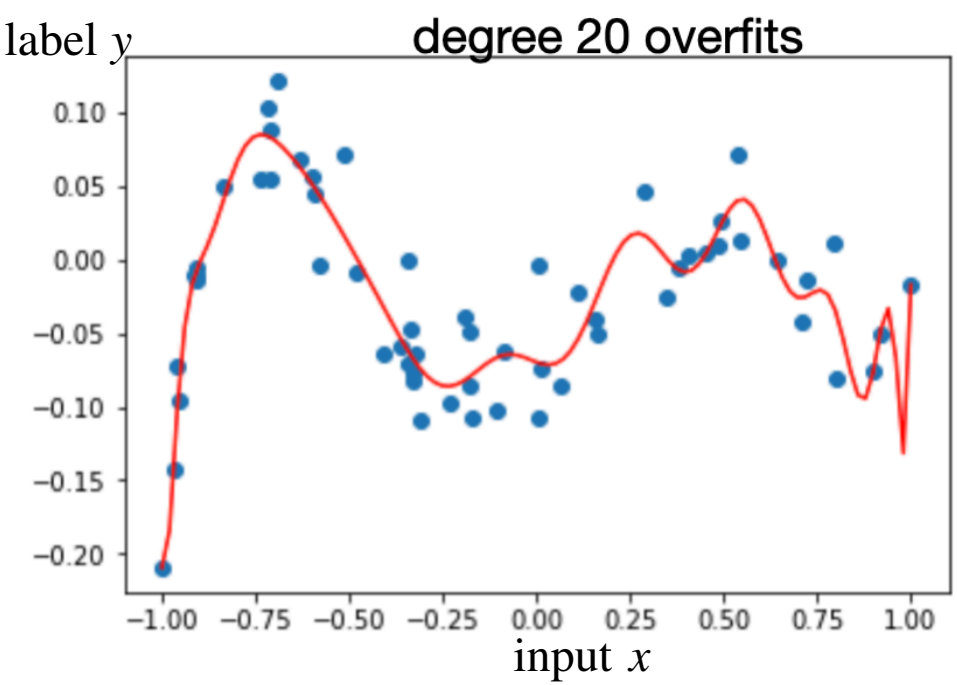
For a new test point x, predict

$\hat{y} = \langle \widehat{w}, h(x) \rangle$

Which p should we choose?

- First instance of class of models with different representation power = model complexity





- How do we determine which is better model?

Generalization

- we say a predictor **generalizes** if it performs as well on unseen data as on training data (we will formalize the next lecture)
- the data used to train a predictor is **training data** or **in-sample data**
- we want the predictor to work on **out-of-sample data**
- we say a predictor **fails to generalize** if it performs well on in-sample data but does not perform well on out-of-sample data

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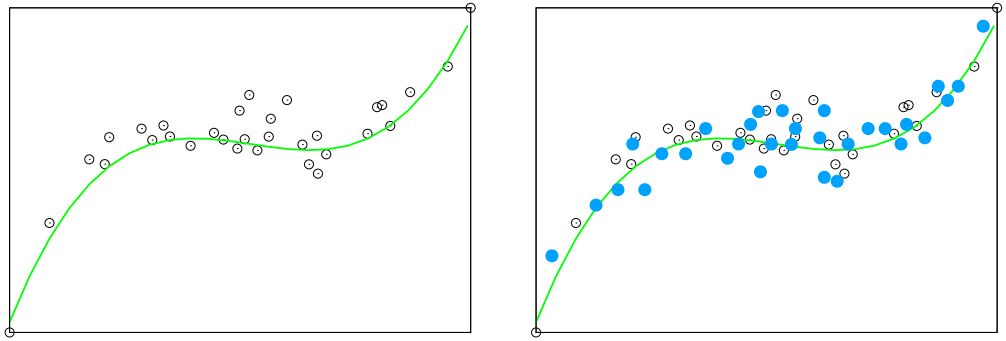
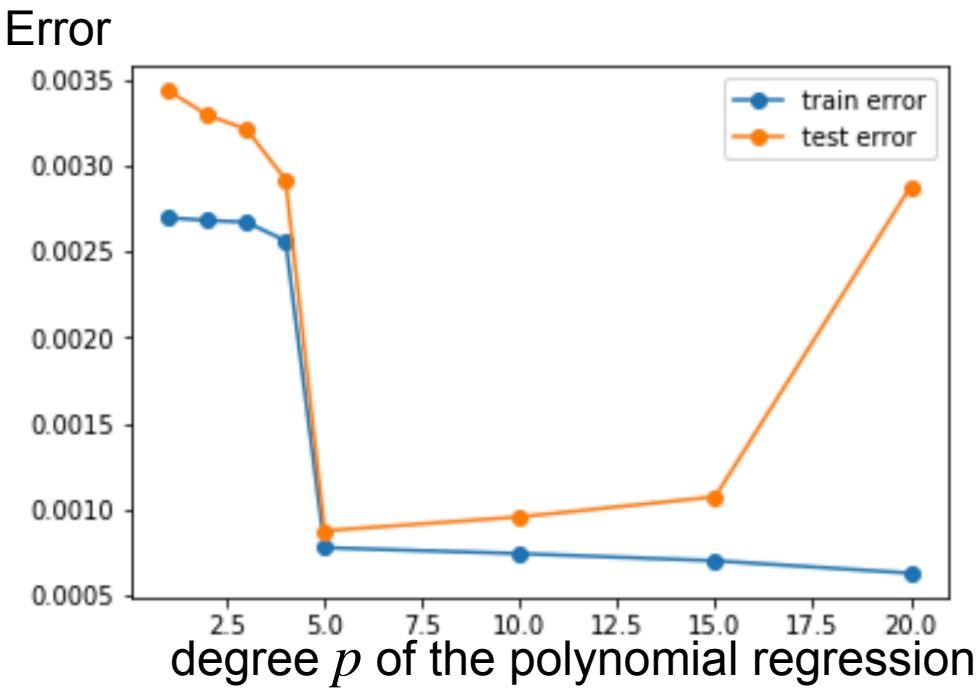


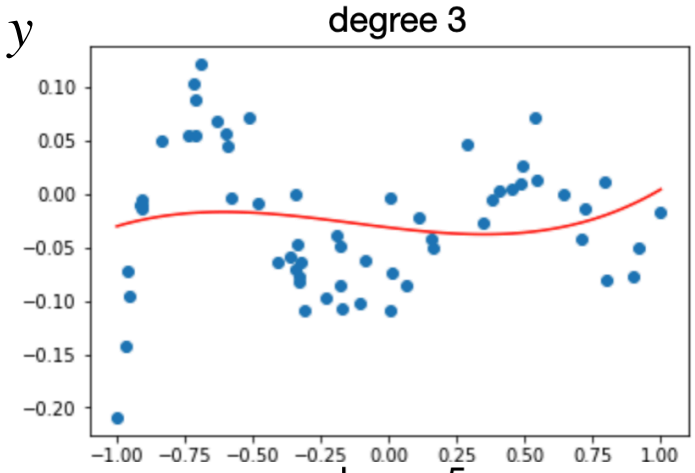
- **train** a cubic predictor on 32 (**in-sample**) white circles: Mean Squared Error (MSE) 174
- **predict** label y for 30 (**out-of-sample**) blue circles: MSE 192
- conclude this predictor/model generalizes, as in-sample MSE $\simeq$ out-of-sample MSE

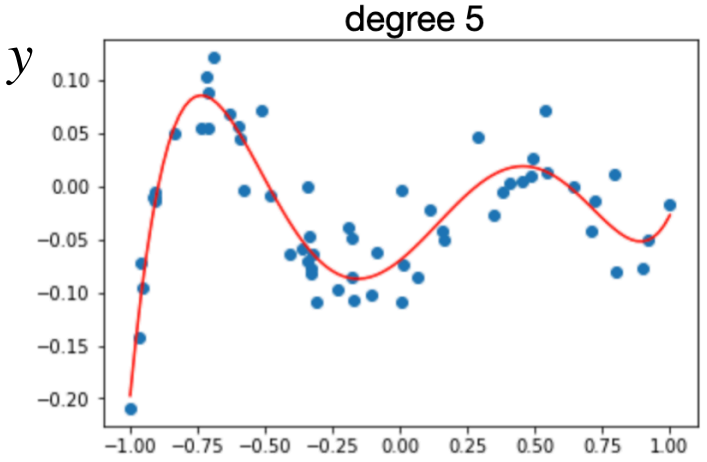
Split the data into training and testing

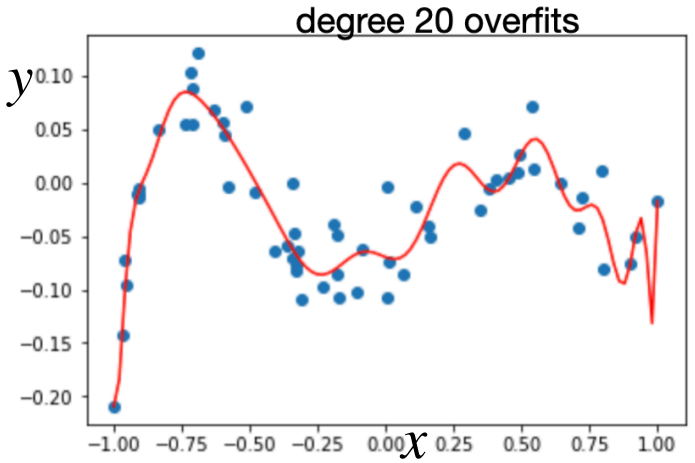
- a way to mimic how the predictor performs on unseen data
- given a single dataset $S = \{(x_i, y_i)\}_{i=1}^{n}$
- we split the dataset into two: training set and test set (e.g., 90/10)
- **training set** used to train the model
  - $$\text{minimize} \quad \mathscr{L}_{\text{train}}(w) = \frac{1}{|S_{\text{train}}|} \sum_{i \in S_{\text{train}}} (y_i - x_i^T w)^2$$
- **test set** used to evaluate the model
  - $$\mathscr{L}_{\text{test}}(w) = \frac{1}{|S_{\text{test}}|} \sum_{i \in S_{\text{test}}} (y_i - x_i^T w)^2$$
- this assumes that test set is similar to unseen data
- **test set should never be used in training or picking unknowns**

Train/test error vs. complexity









- Degree $p = 5$, since it achieves **minimum test error**
- **Train error** monotonically decreases with model complexity
- **Test error** has a U shape

test set should never be used in training or picking degree