

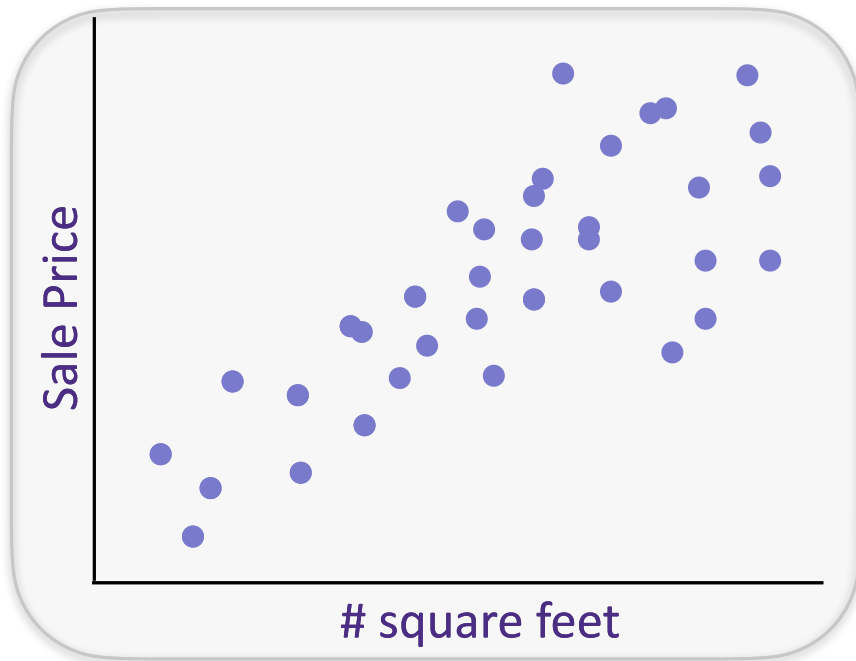
Linear Regression

The regression problem, 1-dimensional

Given past sales data on [zillow.com](https://www.zillow.com), predict:

$y =$ House sale price from

$x = \{\# \text{ sq. ft.}\}$



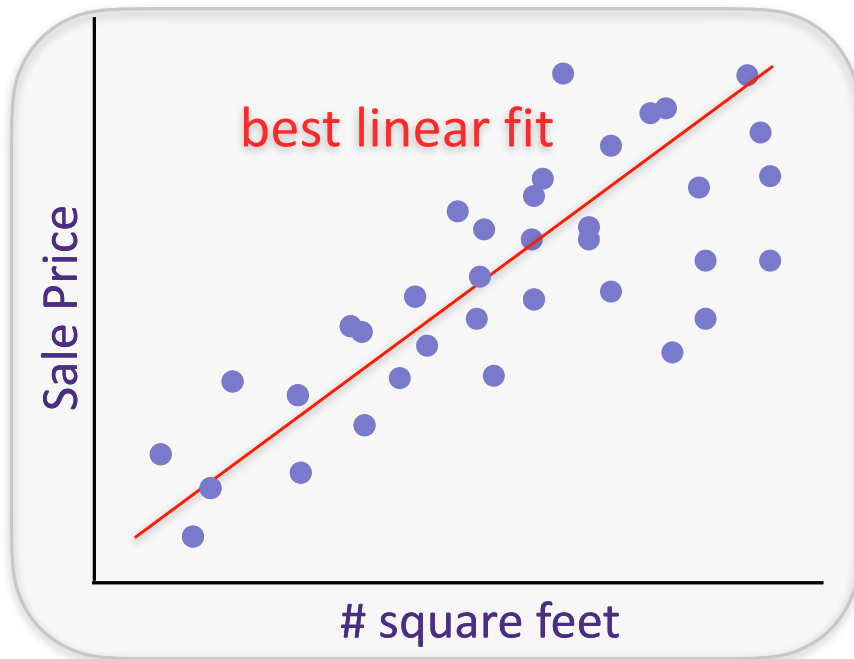
Training Data: $x_i \in \mathbb{R}$
 $\{(x_i, y_i)\}_{i=1}^n$ $y_i \in \mathbb{R}$

Fit a function to our data, 1-d

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Hypothesis/Model: linear

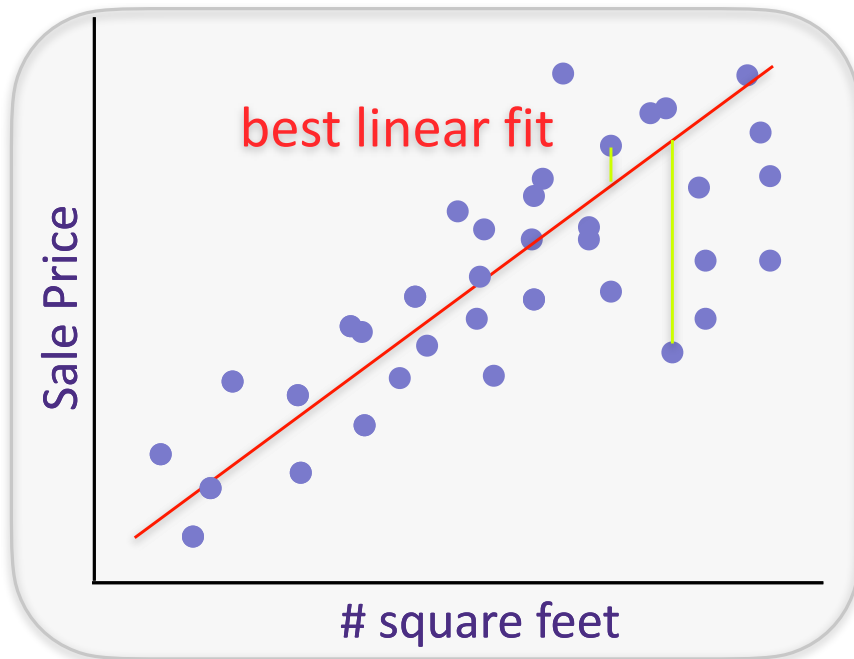
$$y_i = x_i w + \epsilon_i \quad \epsilon_i \stackrel{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$$

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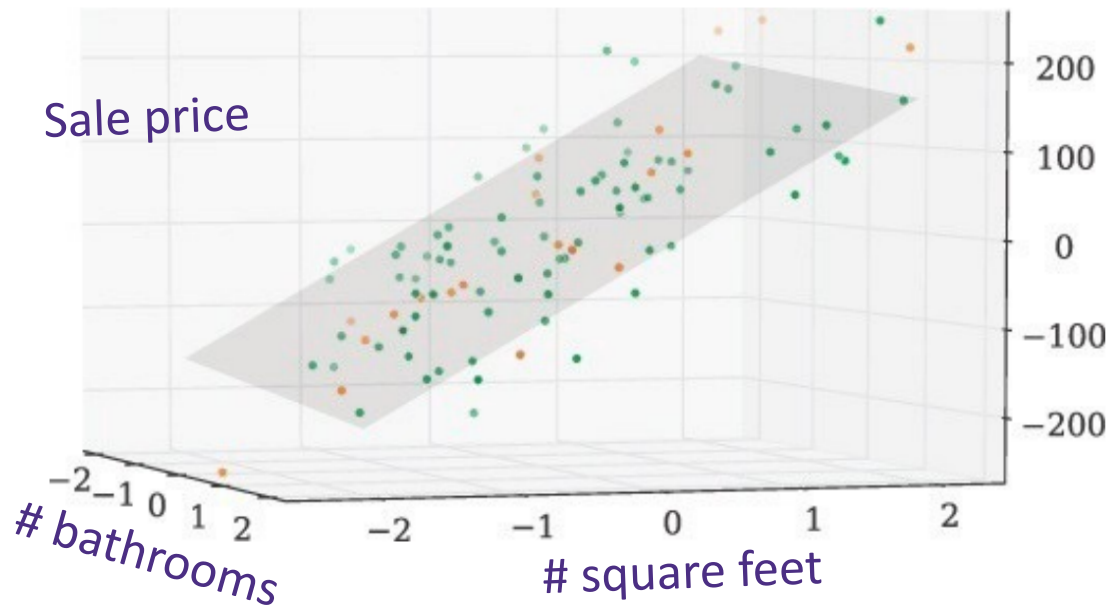
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The regression problem, d-dim

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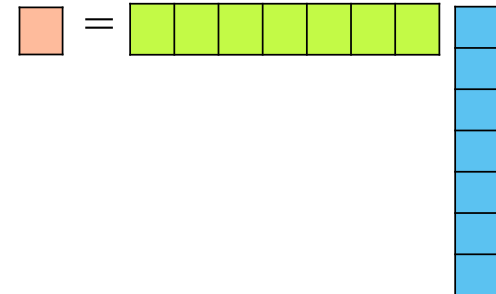
$x =$ {# sq. ft., zip code, date of sale, etc.}



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

Hypothesis/Model: linear

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

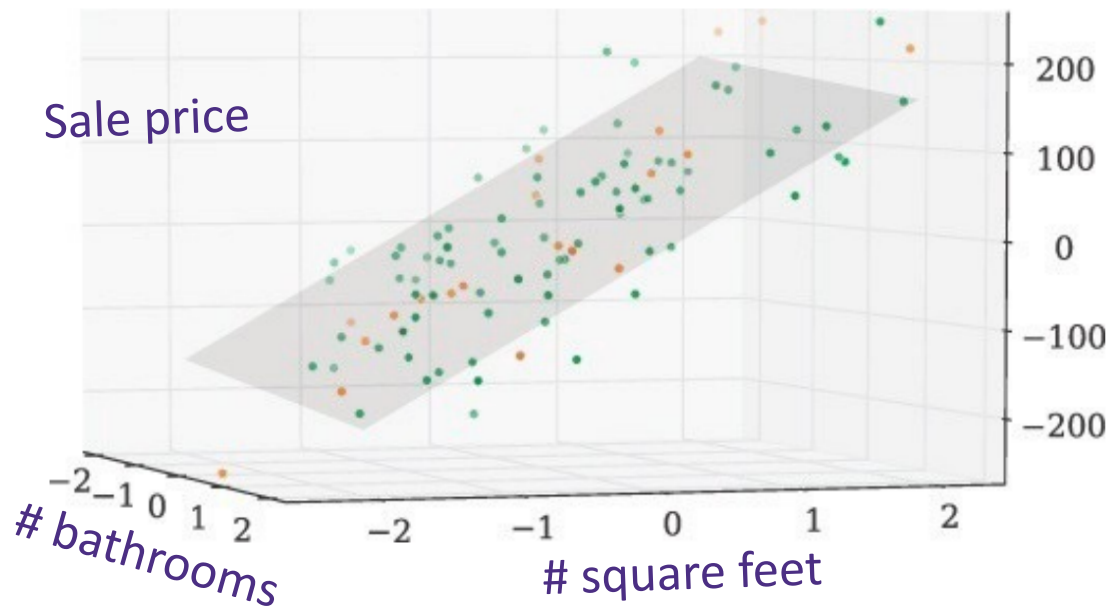


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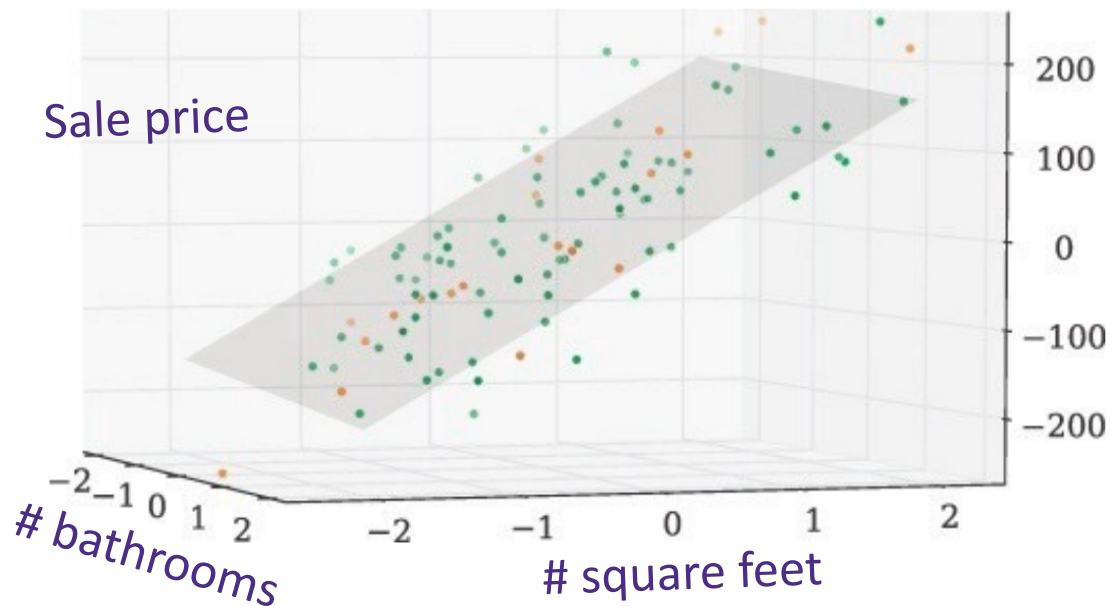
$$p(y|x, w, \sigma) =$$

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

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

Maximizing log-likelihood

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

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

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

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 $X \sim f(\cdot; \hat{\theta}_{MLE})$

Maximizing log-likelihood

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

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

The regression problem in matrix notation

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

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

d : # of features

n : # of examples/datapoints

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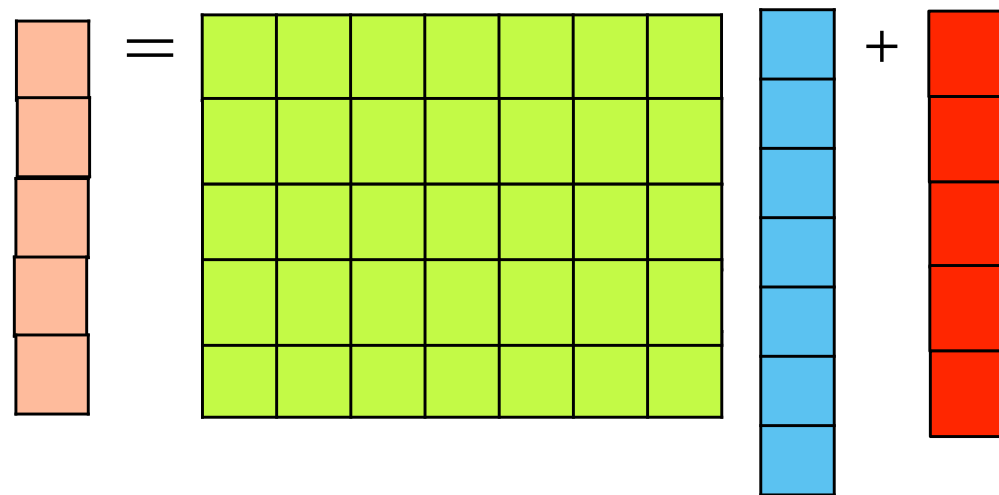
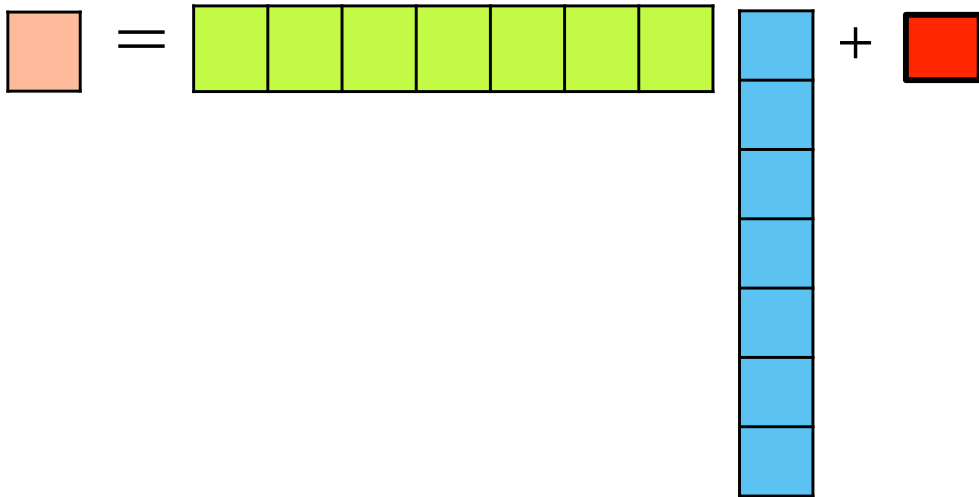
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$$y_i = x_i^\top w + \epsilon_i$$

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



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

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

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$$\mathbf{X}^\top \mathbf{X} = \sum_{i=1}^n x_i x_i^\top$$

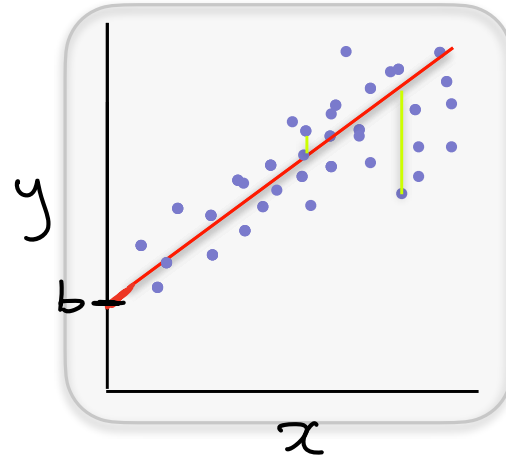
$$\mathbf{X}^\top \mathbf{y} = \sum_{i=1}^n x_i y_i$$

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

The regression problem in matrix notation

$$\underline{y_i \approx x_i^T w}$$

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



What about an offset?

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

$$y \approx w^T x + b$$

↑
offset

Dealing with an offset

$$\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

↓

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

$$\nabla_w \|y - (Xw + \mathbf{1}b)\|_2^2 = 2 X^T (y - \underline{Xw + b\mathbf{1}}) = 0$$

$$X^T X \hat{w}_{MLE} + X^T \mathbf{1} \hat{b}_{MLE} = X^T y$$

Dealing with an offset

$$\tilde{x}_i = \begin{bmatrix} x_i \\ 1 \end{bmatrix} \quad \tilde{w} = \begin{bmatrix} w \\ b \end{bmatrix}$$

$$\tilde{x}_i^T \tilde{w} = x_i^T w + b$$

$$\|Y - \tilde{X}\tilde{w}\|_2^2$$

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

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

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

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

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

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

$$\dot{\mathbf{X}} = \mathbf{X} - \mathbf{1}\mu^T$$

$$\dot{\mathbf{X}}^T \mathbf{1} = 0$$

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

$$\underbrace{\mathbf{1} \mu^T}_{n \times d}$$

$$\mathbf{X}$$

$n \times d$

$$y_i \approx (x_i - \mu)^T \hat{w} + \hat{b} = x_i^T \hat{w} + (\hat{b} - \mu^T \hat{w})$$

$$\begin{bmatrix} \mathbf{X}^T \mathbf{X} & \mathbf{X}^T \mathbf{1} \\ \mathbf{1}^T \mathbf{X} & \mathbf{1}^T \mathbf{1} \end{bmatrix} \begin{bmatrix} \hat{w} \\ \hat{b} \end{bmatrix} = \begin{bmatrix} \mathbf{X}^T \mathbf{y} \\ \mathbf{1}^T \mathbf{y} \end{bmatrix}$$

$$\mathbf{1} \in \mathbb{R}^n$$

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

$$\mu \in \mathbb{R}^d$$

Make Predictions

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

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

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

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

Process

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

Find the function which fits the data best

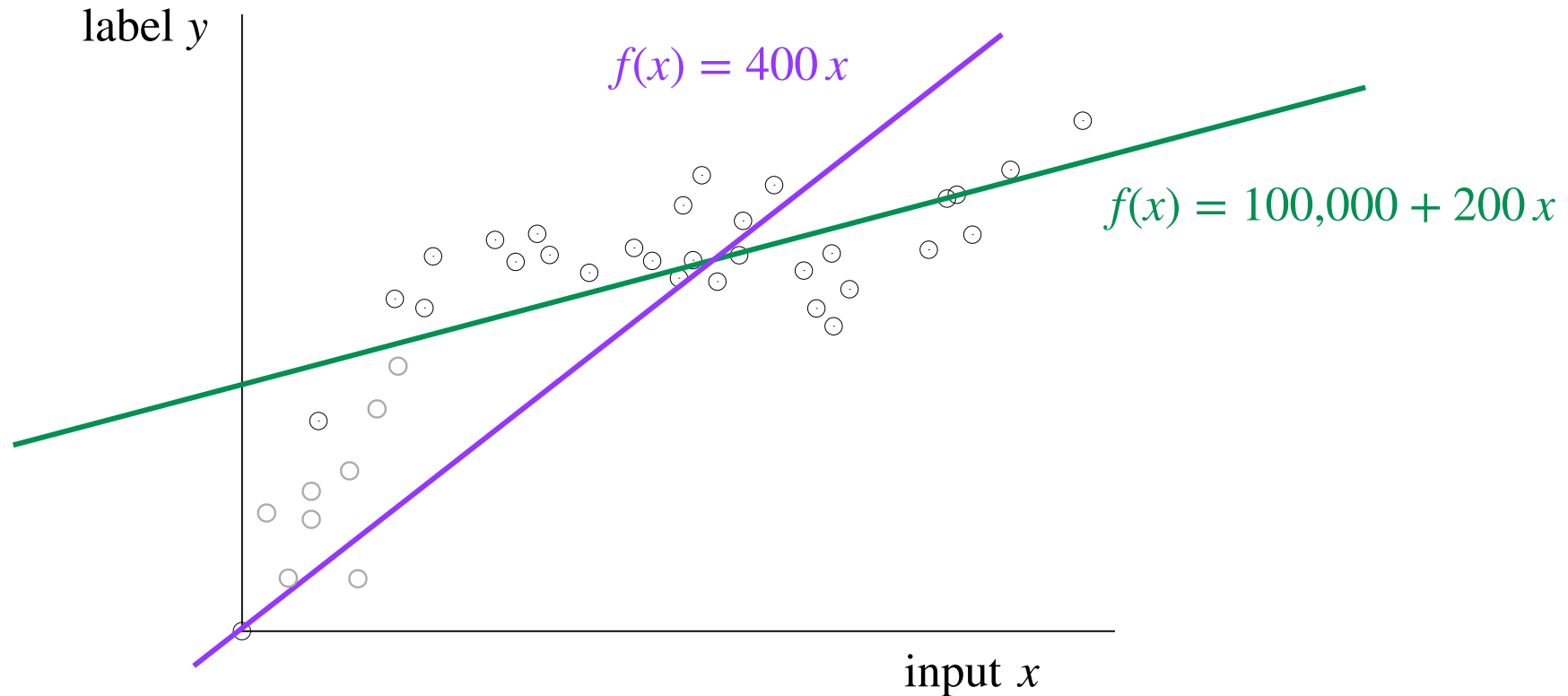
Choose a loss function- least squares

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 $y_i \simeq w^T x_i + b$, or equivalently $y_i = w^T x_i + b + \epsilon_i$ with model parameters $(w \in \mathbb{R}^d, b \in \mathbb{R})$ that minimizes ℓ_2 -loss

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

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:

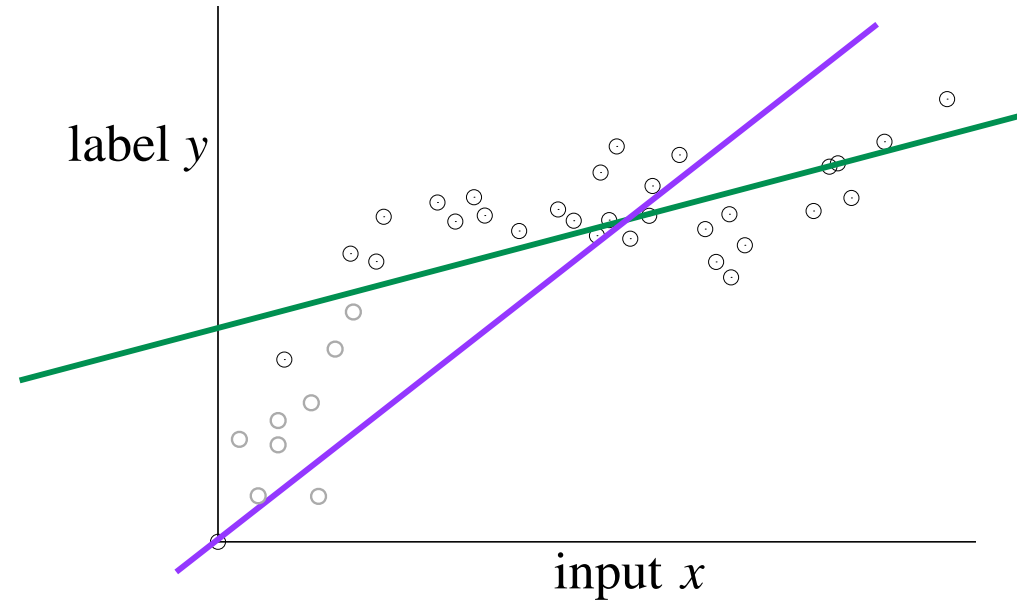
$$\begin{bmatrix} \hat{\mathbf{w}}_{\text{LS}} \\ \hat{b}_{\text{LS}} \end{bmatrix} = \left(\begin{bmatrix} \mathbf{X}^T \\ \mathbf{1}^T \end{bmatrix} [\mathbf{X} \quad \mathbf{1}] \right)^{-1} \begin{bmatrix} \mathbf{X}^T \\ \mathbf{1}^T \end{bmatrix} \mathbf{y}$$

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) :**

- $\hat{y}_i = \underline{b + w_1 x_i}$



Quadratic regression in 1-dimension

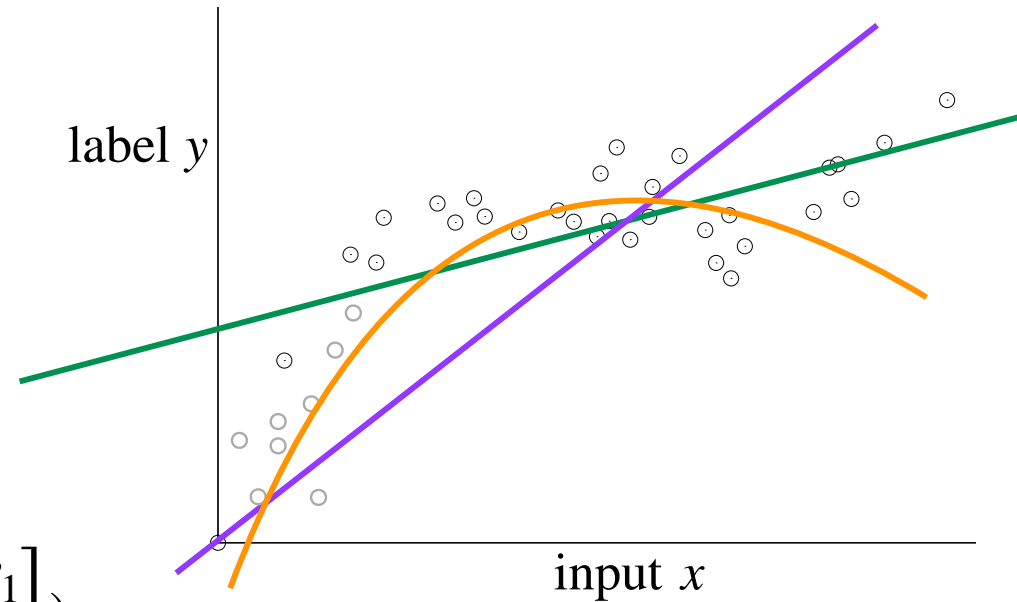
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- **Quadratic model with parameter $(b, w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix})$:**

- $\hat{y}_i = \underline{b + w_1 x_i + w_2 x_i^2}$



$$\sum_{i=1}^n (y_i - ([x_i]^\top w + b))^2$$

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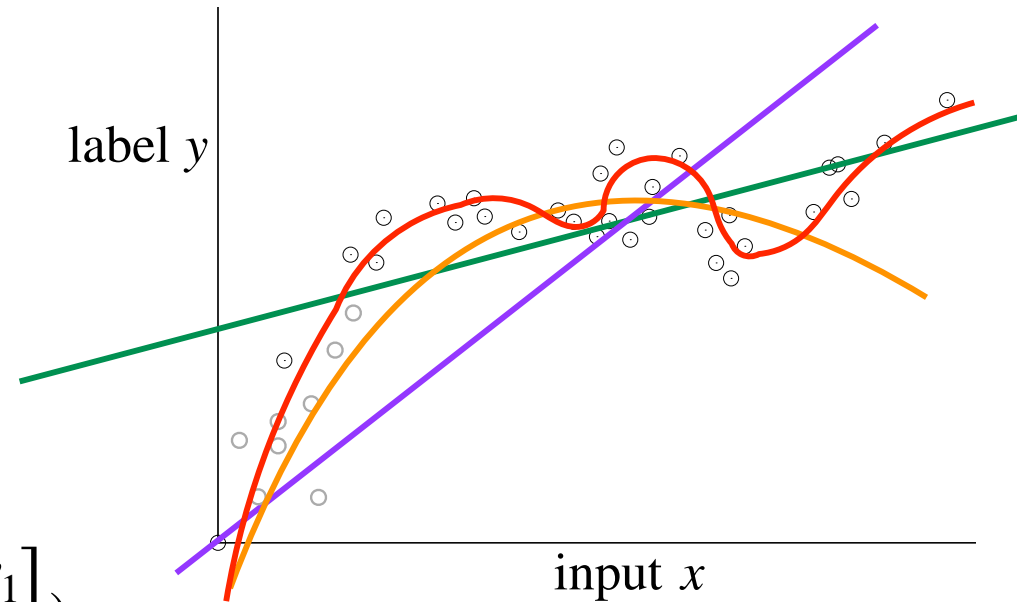
- $\hat{y}_i = b + w_1 x_i$

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

- $\hat{y}_i = b + w_1 x_i + w_2 x_i^2$

- Degree- p polynomial model with parameter $(b, w = \begin{bmatrix} w_1 \\ \vdots \\ w_p \end{bmatrix})$:

- $\hat{y}_i = b + w_1 x_i + w_2 x_i^2 + \dots + w_p x_i^p$



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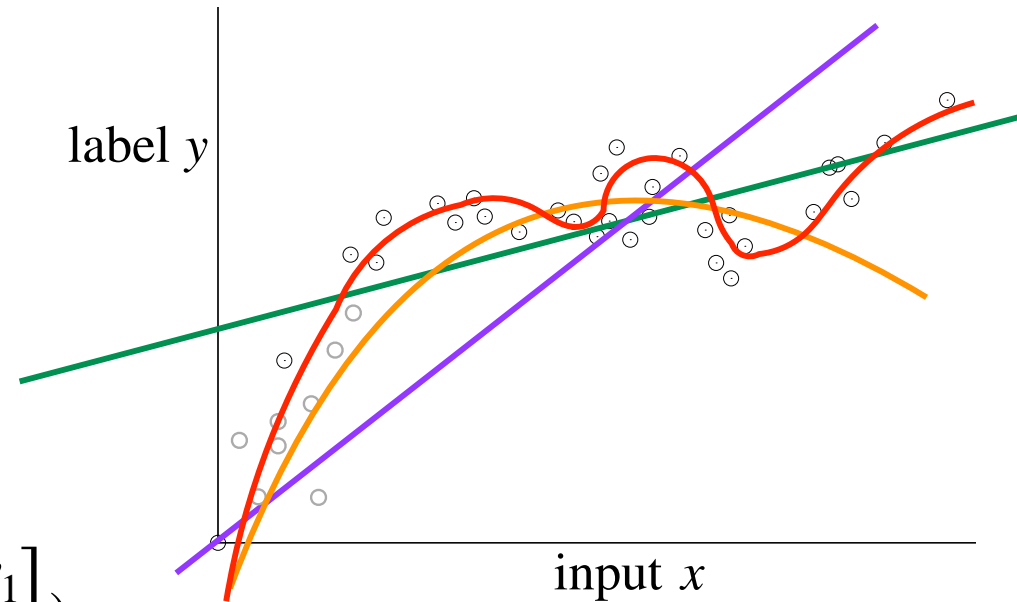
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- **General p-features with parameter $w = \begin{bmatrix} w_1 \\ \vdots \\ w_p \end{bmatrix}$:**

- $\hat{y}_i = \langle w, h(x_i) \rangle$ where $h : \mathbb{R} \rightarrow \mathbb{R}^p$



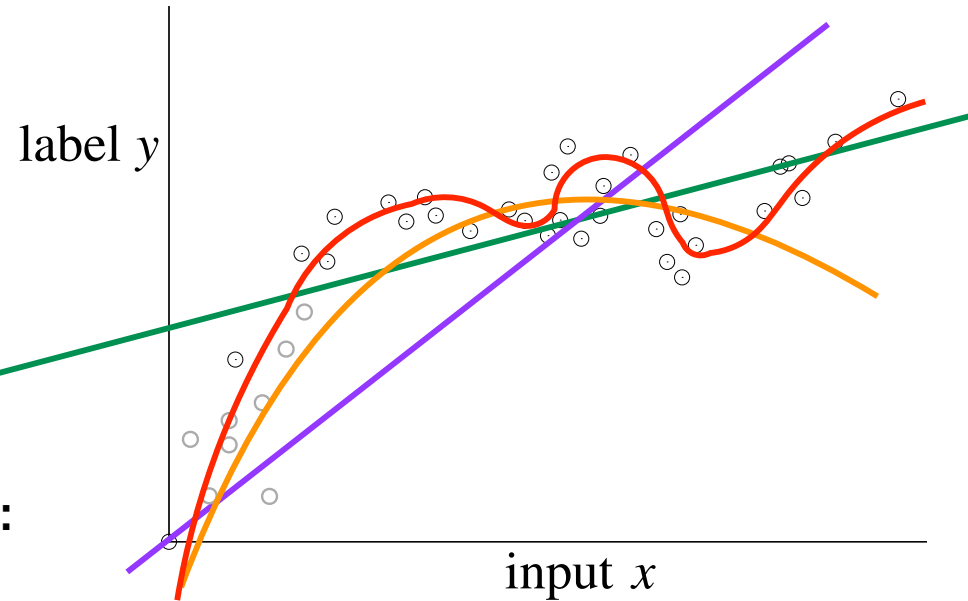
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Note: h can be arbitrary non-linear functions!

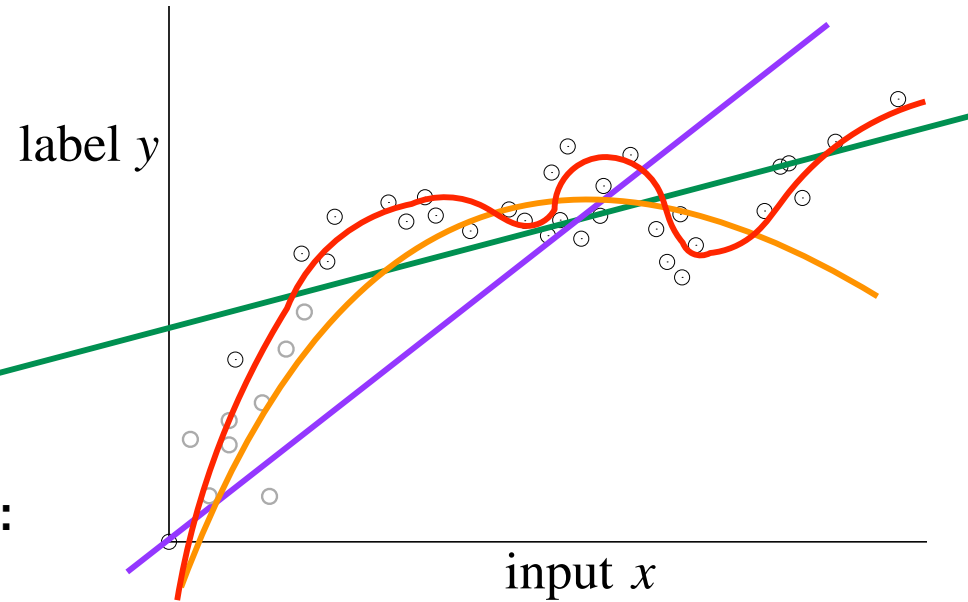
$$h(x) = \left[\log(x), x^2, \sin(x), \sqrt{x} \right]^T$$



Quadratic regression in 1-dimension

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How do we learn w ?

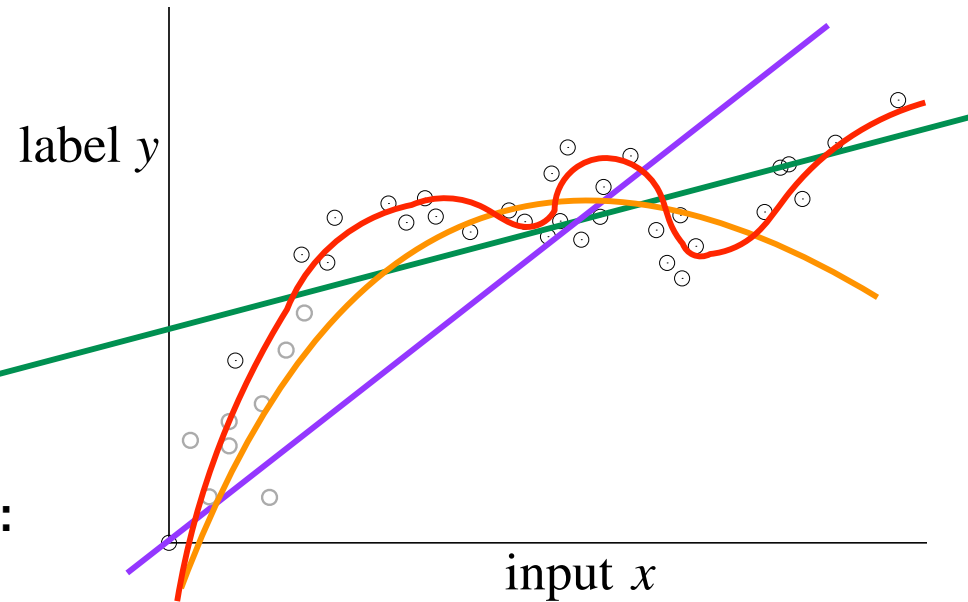
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How do we learn w ?

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

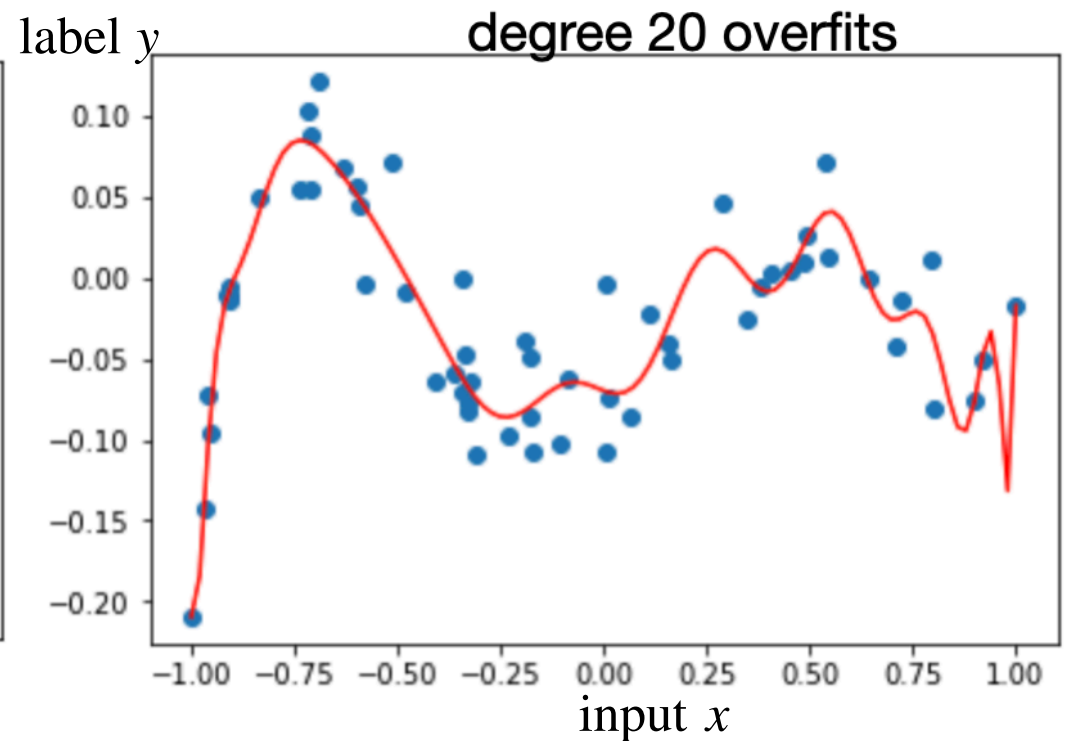
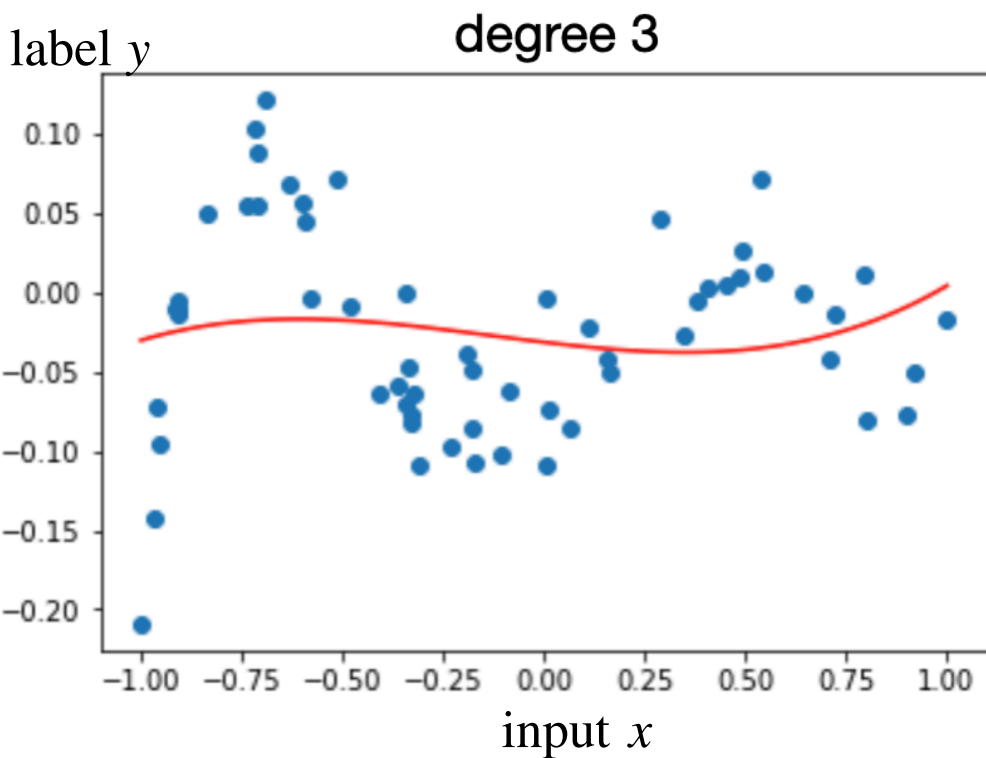


$$\hat{w} = \arg \min_w \|\mathbf{H}w - \mathbf{y}\|_2^2$$

For a new test point x , predict
 $\hat{y} = \langle \hat{w}, h(x) \rangle$

Which p should we choose?

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



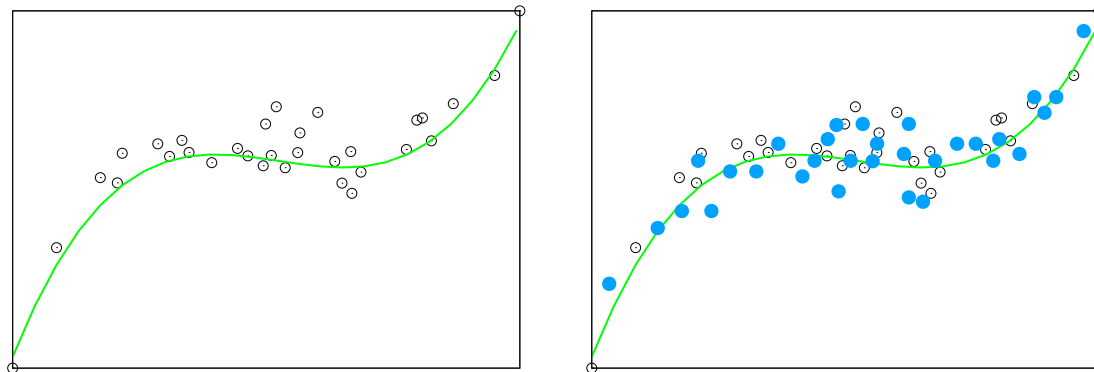
- How do we determine which is better model?

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

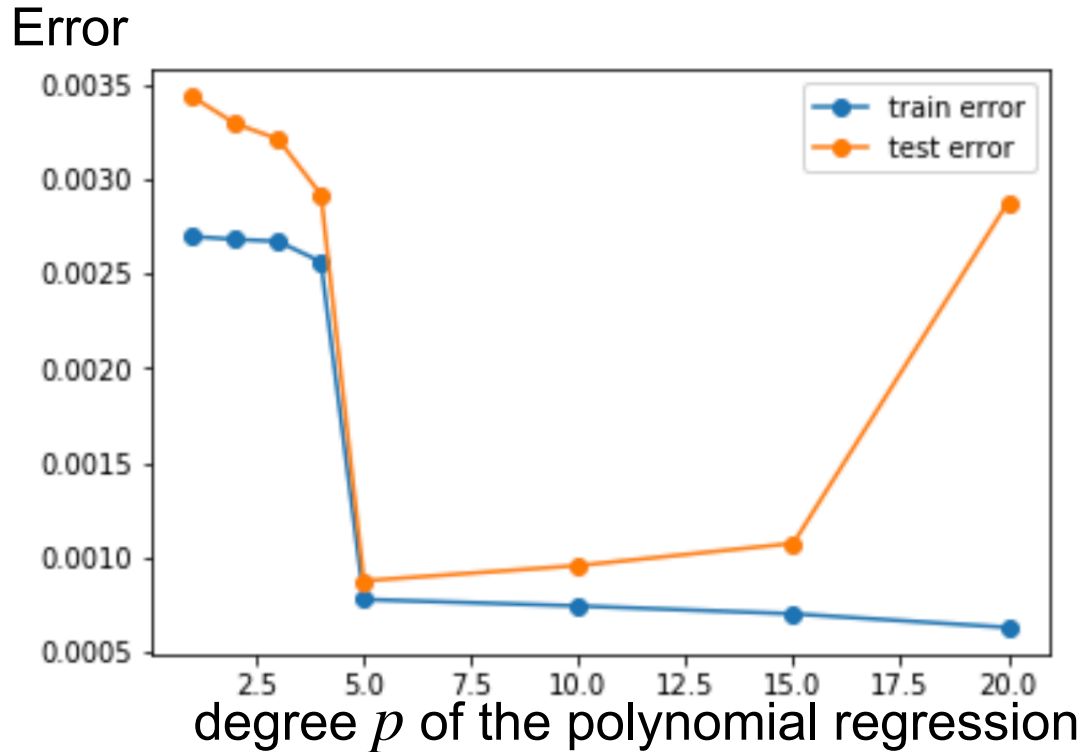
- minimize $\mathcal{L}_{\text{train}}(w) = \frac{1}{|S_{\text{train}}|} \sum_{i \in S_{\text{train}}} (y_i - x_i^T w)^2$

- **test set** used to evaluate the model

- $\mathcal{L}_{\text{test}}(w) = \frac{1}{|S_{\text{test}}|} \sum_{i \in S_{\text{test}}} (y_i - x_i^T w)^2$

- 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

