NUS | Computing
National University of Singapore

CS5228: Knowledge Discovery and Data Mining

Lecture 7 — Classification & Regression III

Course Logistics — Update

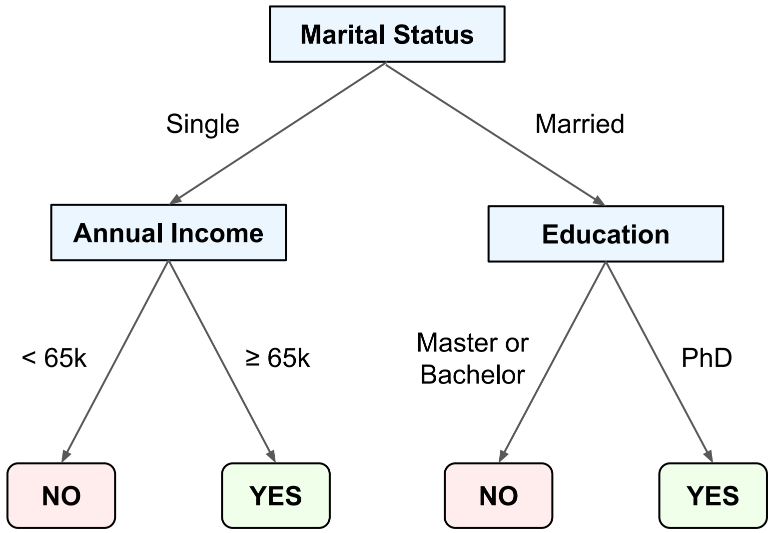
- Assignment 3
  - Available on Canvas (since Oct 13)
  - Submission deadline: Thu Oct 24, 11.59 pm

- Project
  - Progress reports completed + feedback provided to almost most team
    (there will be an announcement with a short summary)
  - 1st TEAMMATES session live (deadline: Oct 17, 11.59 pm)

Quick Recap — Decision Trees

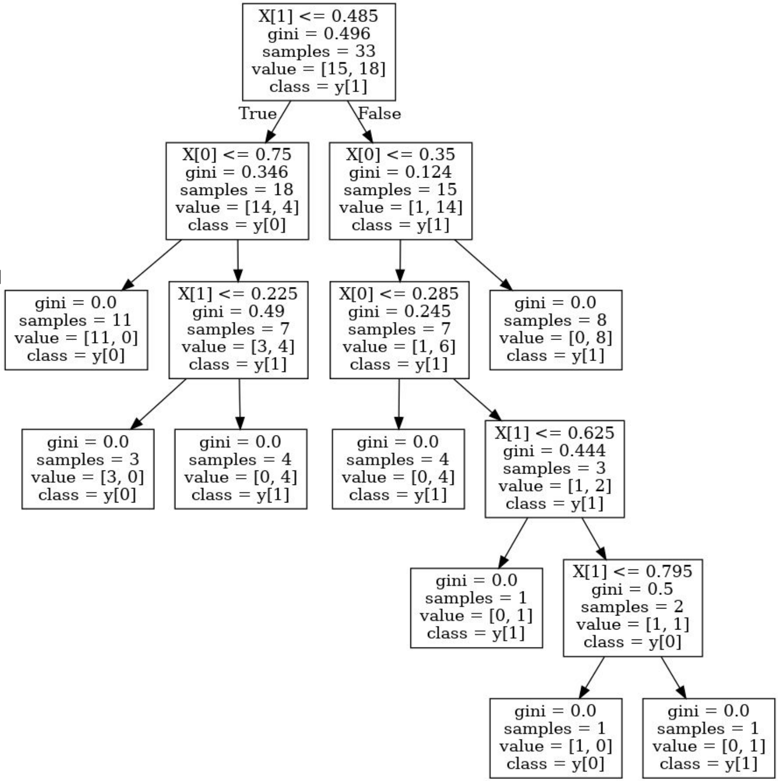
- Decision Trees
  - Flowchart-like structure mapping input features to output labels or values
  - Applicable to classification & regression tasks
  - Support for categorical & numerical features
  - Typically quite interpretable

- Building Decision Trees
  - Greedy algorithm iteratively finding the best splits
  - Best split = split that minimizes impurity



Quick Recap — Decision Trees

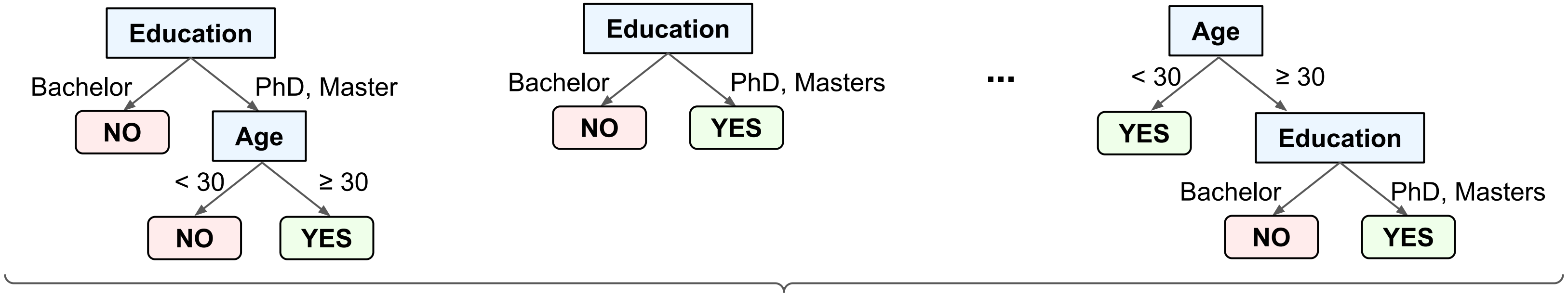
- Challenges
  - Sensitive to small changes in training data
    ➜ High variance
  - High chance of overfitting in case of maximum/complet
    ➜ Pruning of tree to avoid overfitting
  - In practice, Decision Trees do not show state-of-the-art performance



➜ Tree Ensemble methods

Quick Recap — Tree Ensembles

- Tree ensembles: Construct many decision trees and combine their predictions
  - Pros: Higher accuracy, lower variance
  - Cons: Lower interpretability, longer training time
- Ensembles of independent models:
  - Bagging — Train decision trees over re-sampled training data (bootstrap sampling)
  - Random Forests — bootstrap sampling + feature sampling



Prediction using majority vote

Quick Recap — Tree Ensembles

- Ensembles of dependent models (boosting methods)
  - Sequential training of decision trees
  - Next tree tries to improve errors of previous trees
  - Trees have different amount of say in predictions
- Two introduced boosting methods:
  - AdaBoost — resample training data to favour previously misclassified samples
  - Gradient Boosted Trees — start with initial prediction, improve based on predicted errors

Outline

- **Linear Models**
  - Basic setup
- Linear Regression
  - Problem formulation
  - Normal Equation (analytical solution)
  - Gradient Descent (iterative optimization)
  - Polynomial Linear Regression (overfitting, regularization)
  - Interpretation of Coefficients
- Logistic Regression
  - Problem formulation
  - Gradient Descent

Linear Models

Age	Edu-cation	Marital Status	Income Level	Credit Approval	Credit Limit
23	Masters	Single	Mid	No	$S5,000
35	College	Married	High	Yes	$S7,000
26	Masters	Single	High	No	$S9,000
...	...	...	...	...	...

- Basic setup
  - Dataset of *n* samples $\{(x_i, y_i)\}_{i=1}^{n}$
  - Input data with *d* features $x_i = (x_{i1}, x_{i2}, ..., x_{id})$

- Assumption
  - There exists linear relationship between x_i and dependent variable y_i

$$\hat{y}_i = h_\theta(x_i) = f(\theta_0 x_{i0} + \theta_1 x_{i1} + \theta_2 x_{i2} + ... + \theta_d x_{id})$$

Predicted value which is hopefully close to y_i

$$\theta = \{\theta_0, \theta_1, \theta_2, ..., \theta_d\},\ \theta_i \in \mathbb{R}$$

Linear Models

- Vector representation
  - Introduce constant feature x_{i0}

$$h_\theta(x_i) = f(\theta_0 \underbrace{x_{i0}}_{= 1} + \theta_1 x_{i1} + \theta_2 x_{i2} + \ldots + \theta_d x_{id})$$

  - Represent x_i with new constant feature

$$x_i = (1, x_{i1}, x_{i2}, \ldots, x_{id})$$

  - Rewrite linear relationship using vectors representing x_i and θ

$$h_\theta(x_i) = f(\theta^T x_i)$$

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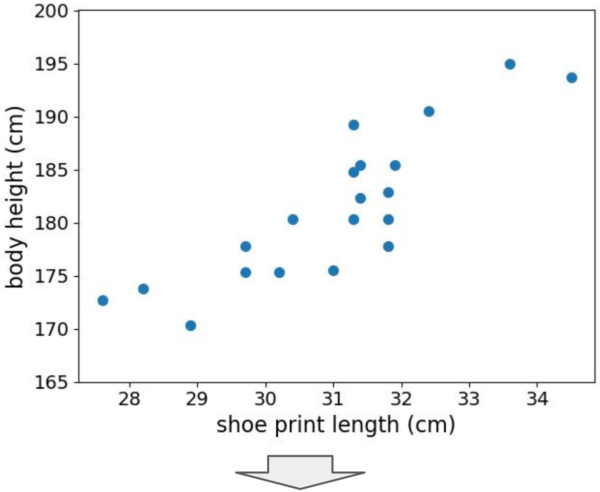
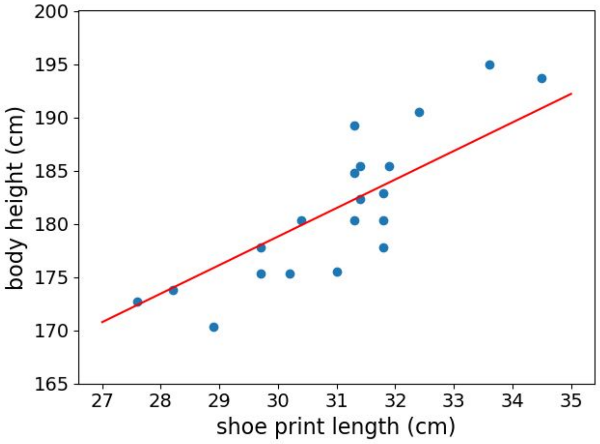
Linear Regression — Simple Example

- Crime scene investigation (CSI)
  - Found a shoe print of size 32.2cm
  - What is the estimated height of the suspect?





- Approach: Linear Regression
  - Collect a dataset of (size, height)-pairs
  - Quantify linear relationship between shoe print size and body height ➜ $h_\theta(size) = \theta_0 + \theta_1 size$
  - Predict suspect's height via $\hat{y} = h_\theta(32.2)$

Linear Regression

- Regression ➜ Real-valued predictions
  - Function f is the identity function f(x) = x

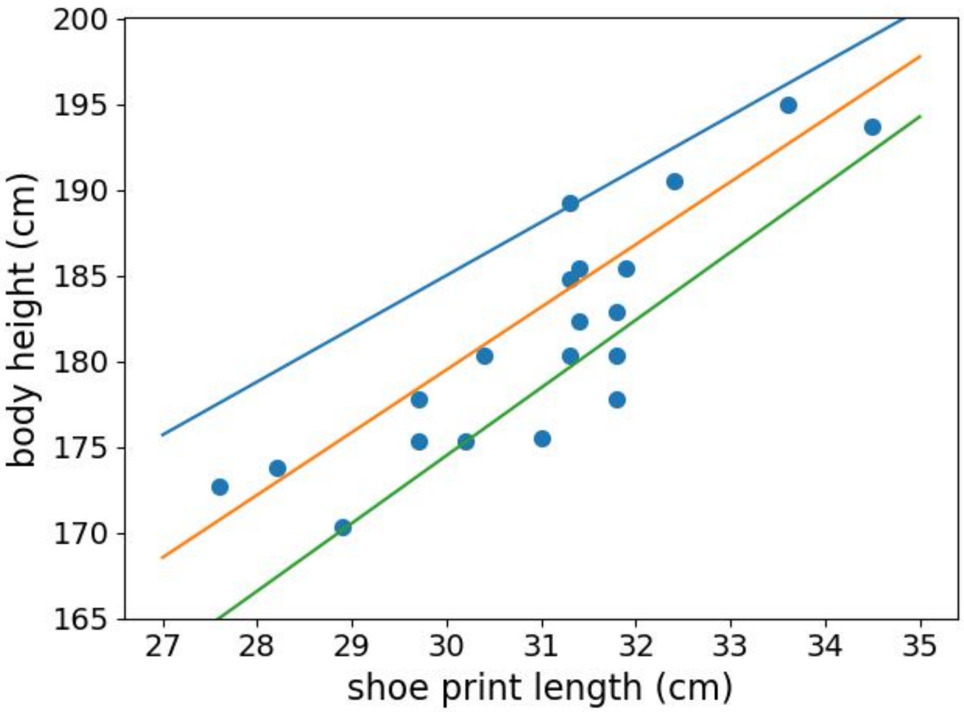
$$\hat{y}_i = h_\theta(x_i) = f(\theta^T x_i) = \theta^T x_i$$

$$\hat{y}_i = \theta^T x_i$$

$$\hat{y} = X\theta$$

$$\hat{y} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} \qquad X = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1d} \\ 1 & x_{21} & x_{22} & \dots & x_{2d} \\ 1 & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{nd} \end{bmatrix} \qquad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$$

Quick Quiz



Which is the best line?

Why?

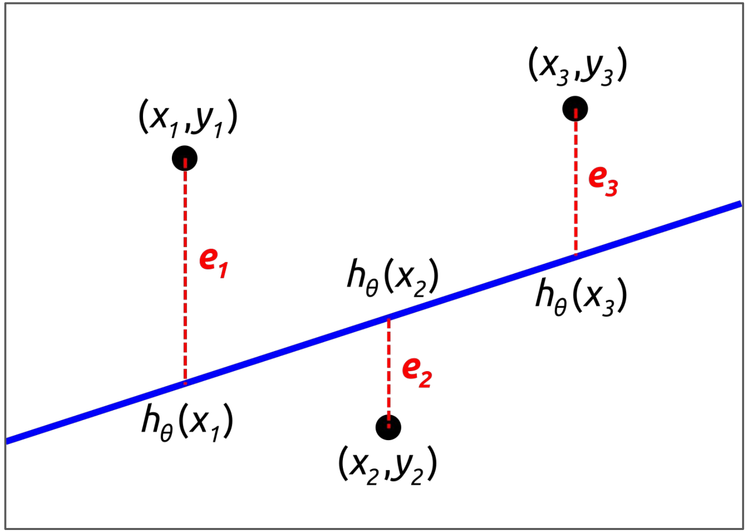
How to find it?

Linear Regression — Loss Function

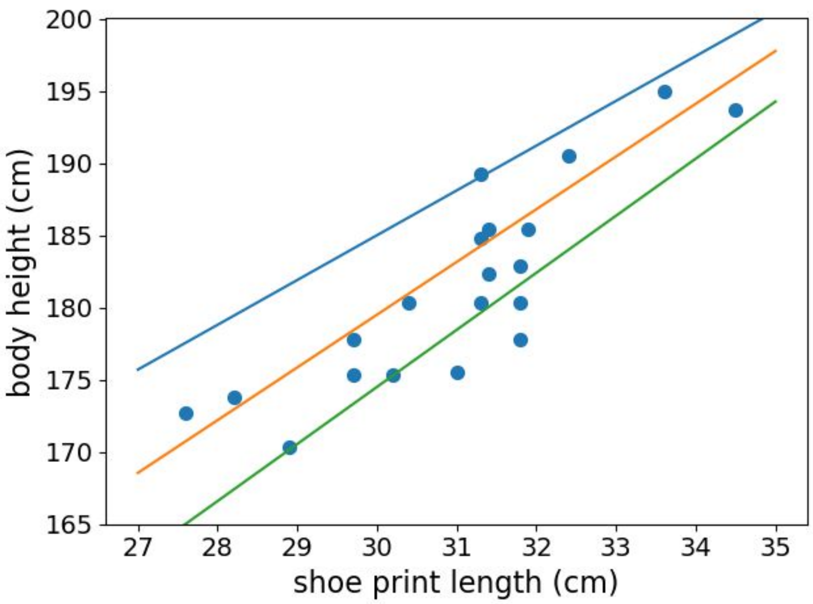
- **Loss function** (also: cost function, error function)
  - Quantifies how good or bad a given set of values for θ is?
  - Measures the difference between predictions $\hat{y}$ and true values y

- Loss function for Linear Regression:
  Mean Squared Error (MSE)

$$L = \frac{1}{n}\sum_{i=1}^{n} e_i^2 = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$$



Losses for CSI Example



$$
\begin{aligned}
h_{blue} &= 92 + 3.10 \cdot x \\
h_{orange} &= 69 + 3.61 \cdot x \\
h_{green} &= 56 + 3.95 \cdot x \\
h_{random} &= 100 - 5.00 \cdot x
\end{aligned}
$$

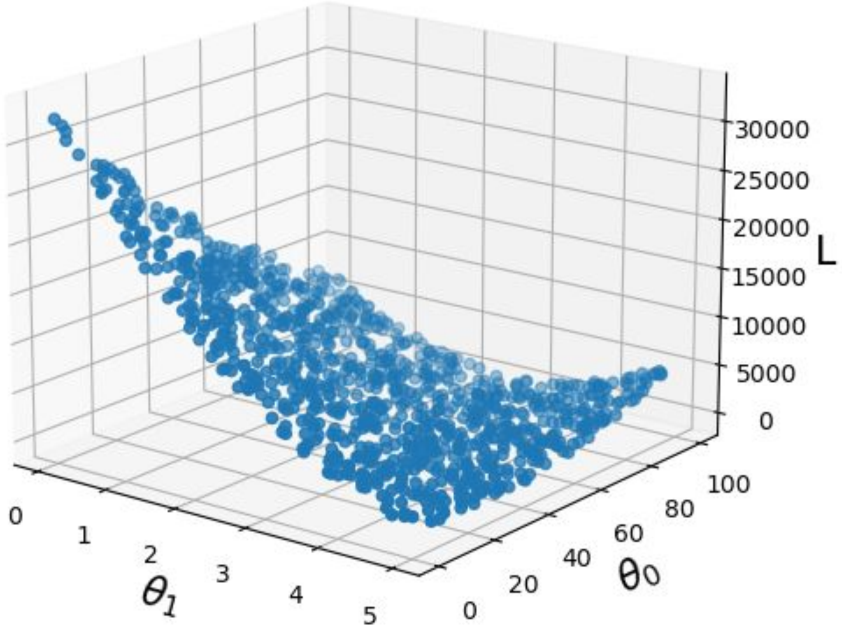
$$
\begin{aligned}
L_{blue} &= 57.47 \\
L_{orange} &= \mathbf{12.12} \\
L_{green} &= 20.83 \\
L_{random} &= 56,129.23
\end{aligned}
$$

➜ How to find the best values for θ?

Method 1: Random Search (the "stupid" way)

- Repeat "enough" times
  - Select random values for $\theta = \{\theta_0, \theta_1, ..., \theta_d\}$
  - Calculate loss L for current θ
- Return θ with smallest loss

Plot of 1,000 losses



- Limitation:
  - Not practical beyond toy examples

➜ Don't do that! :)

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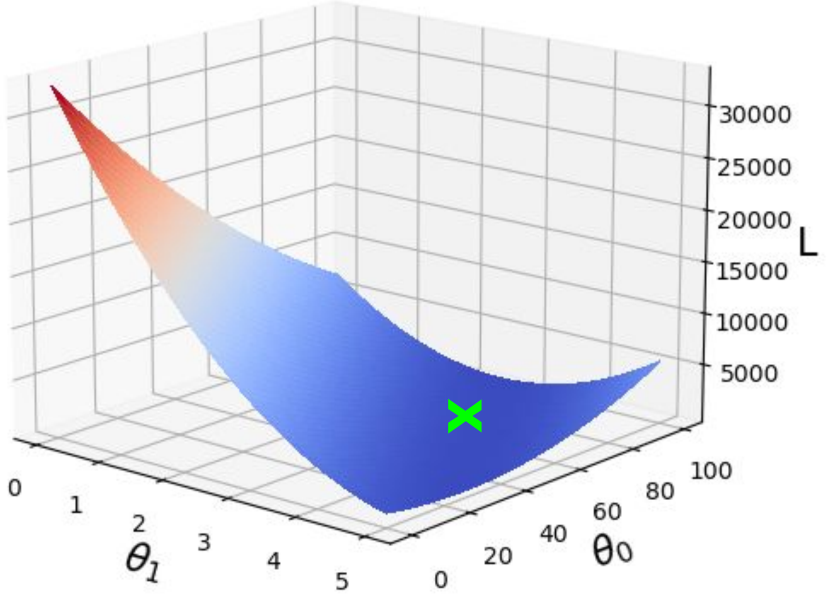
Method 2: Find Minimum of *L* Analytically (the proper way)

- Minimum of loss function L ➜ Calculus to the rescue!
  - Partial derivatives w.r.t. to all θ_i are 0

$$\frac{\partial L}{\partial \theta_0} = 0, \ \frac{\partial L}{\partial \theta_1} = 0, \ \ldots, \ \frac{\partial L}{\partial \theta_d} = 0$$

  - *d*+1 equations with *d*+1 unknowns
  - (no need to check if minimum or maximum)



Method 2: Find Minimum of *L* Analytically (the proper way)

- Rewrite loss function *L*
  - Vector representation mathematically more convenient to handle
  - Avoids dealing with d equations

$$L = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2 = \frac{1}{n}\sum_{i=1}^{n}(\theta^T x_i - y_i)^2 = \frac{1}{n}\|X\theta - y\|^2$$

- Derive *L* w.r.t. to θ
  - Using chain rule

$$\frac{\partial L}{\partial \theta} = \frac{2}{n}X^T(X\theta - y)$$

- Set $\partial L/\partial\theta$ to 0

$$\frac{2}{n}X^T(X\theta - y) \stackrel{!}{=} \vec{0}$$

Linear Regression — Normal Equation

- Solve for θ

$$\frac{2}{n} X^T (X\theta - y) = \vec{0}$$

$$X^T X \theta = X^T y$$

$$(X^T X)^{-1} X^T X \theta = (X^T X)^{-1} X^T y$$

$$\theta = (X^T X)^{-1} X^T y$$

$$\theta = X^\dagger y, \text{ with } \underbrace{X^\dagger = (X^T X)^{-1} X^T}_{\text{"pseudo inverse" of } X}$$

Pseudo Inverse $X^\dagger$

$$X^\dagger = (X^T X)^{-1} X^T$$

$$\overset{X^T}{\begin{bmatrix} (d+1) \times n \end{bmatrix}} \overset{X}{\begin{bmatrix} n \times (d+1) \end{bmatrix}} = \overset{X^T X}{\begin{bmatrix} (d+1) \times (d+1) \end{bmatrix}} \Rightarrow \underbrace{\overset{(X^T X)^{-1}}{\begin{bmatrix} (d+1) \times (d+1) \end{bmatrix}^{-1}} \overset{X^T}{\begin{bmatrix} (d+1) \times n \end{bmatrix}}}_{(d+1) \times n}$$

- Performance analysis
  - Most expensive operation: calculating the inverse of $(X^T X)^{-1}$
  - Calculation of inverse depends on number of features *d*, not on number of data samples *n*
  - Complexity of calculating inverse of a $d \times d$ matrix: $O(d^3)$

Quick Quiz

What condition is **not required** for a matrix A to be **invertible**?

A The determinant of A is non-zero

B A is a square matrix

C A has full rank

D All diagonal values are non-zero

Quick Quiz

When will $X^T X$ **not** be invertible?

A There are more features *d* than data samples *n*

B The data is not normalized

C In practice, $X^T X$ will always be invertible

D X has no determinant

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Method 2: Find Minimum of *L* Analytically (the proper way)

- Algorithm
  - Construct matrix *X* and vector *y* from data
  - Calculate pseudo inverse $X^\dagger = (X^T X)^{-1} X^T$
  - Return $\theta = X^\dagger y$

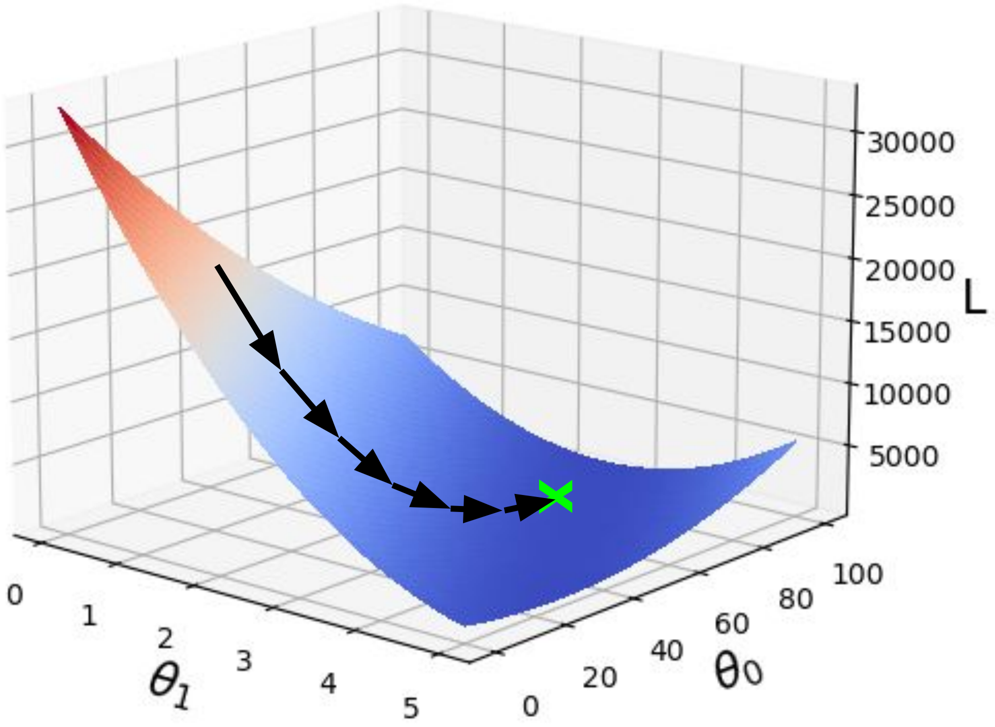
- For the CSI example:

$$\theta = \begin{bmatrix} 20.0 & 620.2 \\ 620.0 & 19284.9 \end{bmatrix}^{-1} X^T y = \begin{bmatrix} 18.4 & -0.6 \\ -0.6 & 0.02 \end{bmatrix} X^T y = \begin{bmatrix} 69.5 \\ 3.6 \end{bmatrix}$$

$$h_\theta(size) = 69.5 + 3.6 size \qquad h_\theta(32.2) = 185.4$$

Method 3: Gradient Descent

- Core idea
  - Start with a random setting of θ
  - Adjust θ iteratively to minimize L



Gradient — Quick Refresher

- Gradient
  - Vector of partial derivatives of a multivariable function (e.g., $\theta_0, \theta_1, \ldots, \theta_d$)
  - Partial derivative: slope w.r.t. to a single variable given a current set of values for all $\theta_0, \theta_1, \ldots, \theta_d$
  - Points in the direction of the steepest ascent

$$\nabla_\theta L = \frac{\partial L}{\partial \theta} = \begin{bmatrix} \frac{\partial L}{\partial \theta_0} \\ \frac{\partial L}{\partial \theta_1} \\ \frac{\partial L}{\partial \theta_2} \\ \vdots \\ \frac{\partial L}{\partial \theta_d} \end{bmatrix}$$

Gradient for CSI Example

Best value: θ_0 = 69.5, θ_1 = 3.6

- Assume θ_0 = 60 and θ_1 = 4

$$\nabla_\theta L = \frac{2}{n} X^T (X\theta - y) = \frac{2}{n} X^T \left(X \cdot \begin{bmatrix} 60 \\ 4 \end{bmatrix} - y\right) = \begin{bmatrix} 5.2 \\ 163.9 \end{bmatrix}$$

- Interpretation of $\nabla_\theta L = \begin{bmatrix} 5.2 \\ 163.9 \end{bmatrix}$
  - Both values positive: a small increase of θ_0 or θ_1 will increase the loss
  - A small change in θ_1 affects the loss more than the same change in θ_0
  - Absolute values of gradient not a direct indicator of how to update θ

Gradient Descent Algorithm

- Important concept: learning rate
  - Scaling factor for gradient (typical range: 0.01 - 0.0001)

$$\textbf{Input} : \text{data}\,(X, y),\ \text{loss function}\ L,\ \text{learning rate}\,\eta$$

$$\textbf{Initialization} : \text{Set}\,\theta\ \text{to random values}$$

$$\textbf{while true} :$$

$$\qquad \text{Calculate gradient}\ \nabla_\theta L$$

$$\qquad \theta \leftarrow \theta - (\eta \cdot \nabla_\theta L)$$

In practice: stop loop when θ converges

Gradient Descent for CSI Example

- Input
  - η = 0.0001
- Initialization
  - θ_0 = 100
  - θ_1 = 50

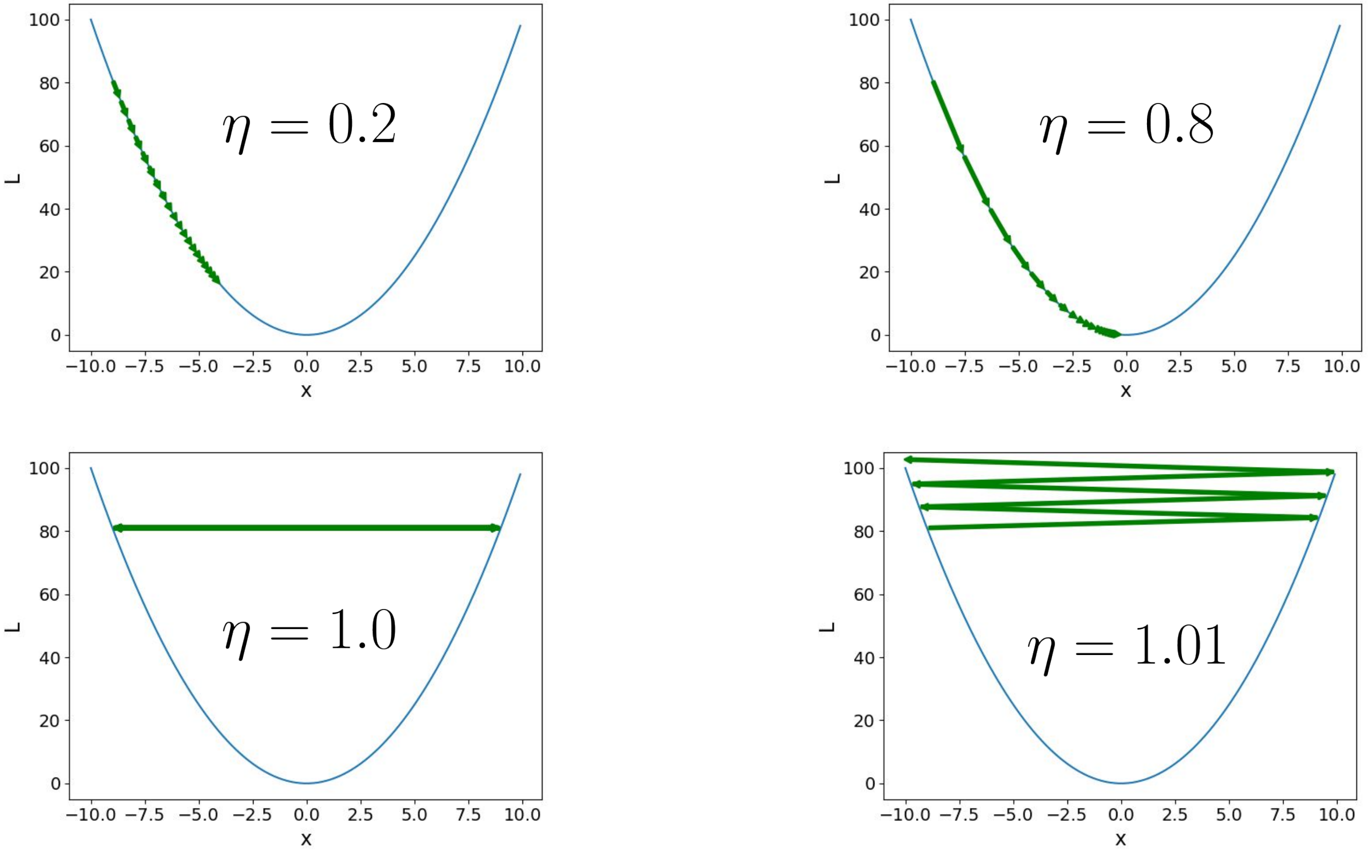
```
[001] theta0=99.70619, theta1=40.86448, loss=2163825.04200
[002] theta0=99.46909, theta1=33.49256, loss=1409025.31406
[003] theta0=99.27776, theta1=27.54378, loss=917521.53239
[004] theta0=99.12336, theta1=22.74340, loss=597468.46605
[005] theta0=98.99877, theta1=18.86972, loss=389059.15347
[006] theta0=98.89823, theta1=15.74385, loss=253349.02868
[007] theta0=98.81709, theta1=13.22143, loss=164978.51518
[008] theta0=98.75161, theta1=11.18595, loss=107434.18922
[009] theta0=98.69877, theta1=9.54342, loss=69962.98624
[010] theta0=98.65613, theta1=8.21798, loss=45562.82115
[011] theta0=98.62172, theta1=7.14841, loss=29674.13840
[012] theta0=98.59395, theta1=6.28532, loss=19327.88711
[013] theta0=98.57153, theta1=5.58885, loss=12590.70710
[014] theta0=98.55344, theta1=5.02683, loss=8203.65008
[015] theta0=98.53884, theta1=4.57330, loss=5346.92525
[016] theta0=98.52706, theta1=4.20733, loss=3486.70856
[017] theta0=98.51754, theta1=3.91201, loss=2275.38917
[018] theta0=98.50986, theta1=3.67370, loss=1486.61298
[019] theta0=98.50366, theta1=3.48140, loss=972.98470
[020] theta0=98.49866, theta1=3.32622, loss=638.52480
```

...

```
[098] theta0=98.47656, theta1=2.67760, loss=14.17658
[099] theta0=98.47655, theta1=2.67760, loss=14.17658
[100] theta0=98.47653, theta1=2.67760, loss=14.17658
```

Quick Quiz: Why not just increase the learning rate to speed things up?

Effects of Learning Rate for $L = x^2, \ \frac{\partial L}{\partial x} = 2x, \ 20 \text{ steps}$



Gradient Descent — Variations

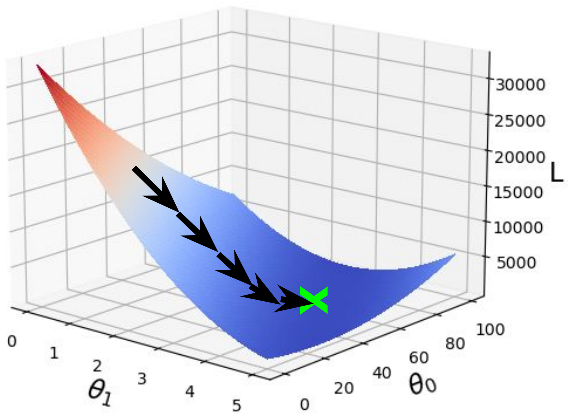
- (Basic) Gradient Descent
  - Calculate gradient und update θ for whole dataset

- Stochastic Gradient Descent (SGD)
  - Calculate gradient und update θ for each data sample

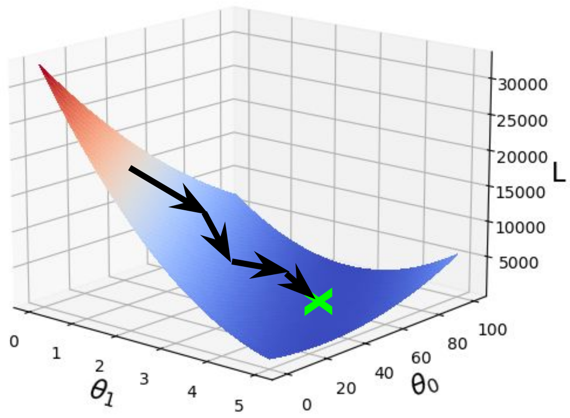
- Mini-batch Gradient Descent
  - Calculate gradient und update θ for batches of sample
  - e.g., batch = 64 data samples
  - In practice often referred to as SGD

Gradient Descent — Variations

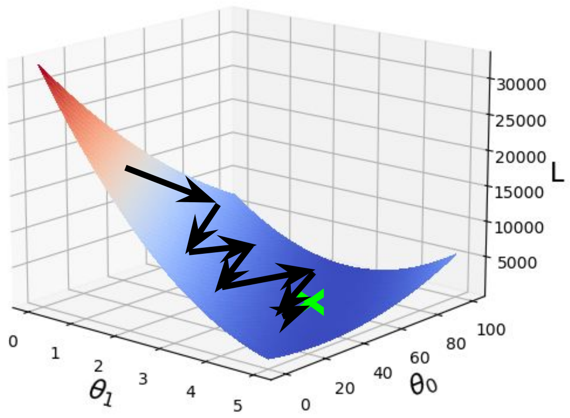
Gradient Descent



Mini-Batch Gradient Descent



Stochastic Gradient Descent



Gradient averaged over <u>all</u> data items

- Smooth descent
- Small(er) gradients
- Small(er) update steps

Gradient averaged over <u>some</u> data items

- Well, "somewhere in-between" :)

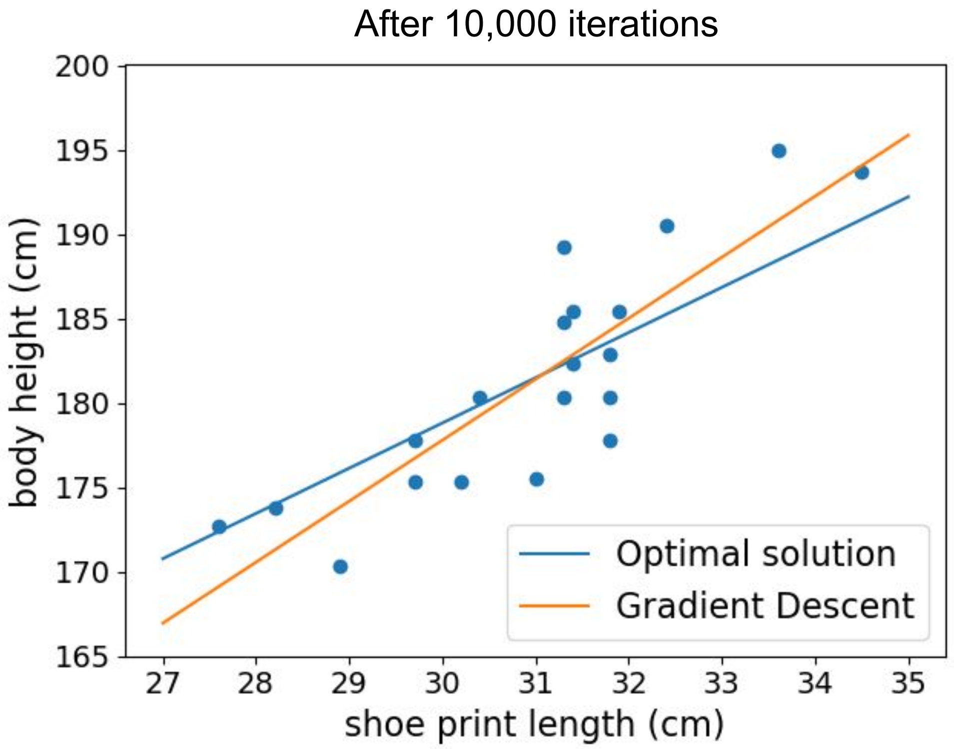
Gradient for each data item considered

- Choppy descent
- Large(r) gradients
- Large(r) steps

Normal Equation vs. Gradient Descent

- Gradient Descent
  - Works well even if d is large
  - Works even if X^TX is non-invertible
  - Iterative process; may not find optimal solution in practice
  - Learning rate a critical hyperparameter
- Normal Equation
  - Finds optimal solutions
  - Non-iterative; no need of learning rate
  - Calculation of $(X^TX)^{-1}$ in $O(d^3)$

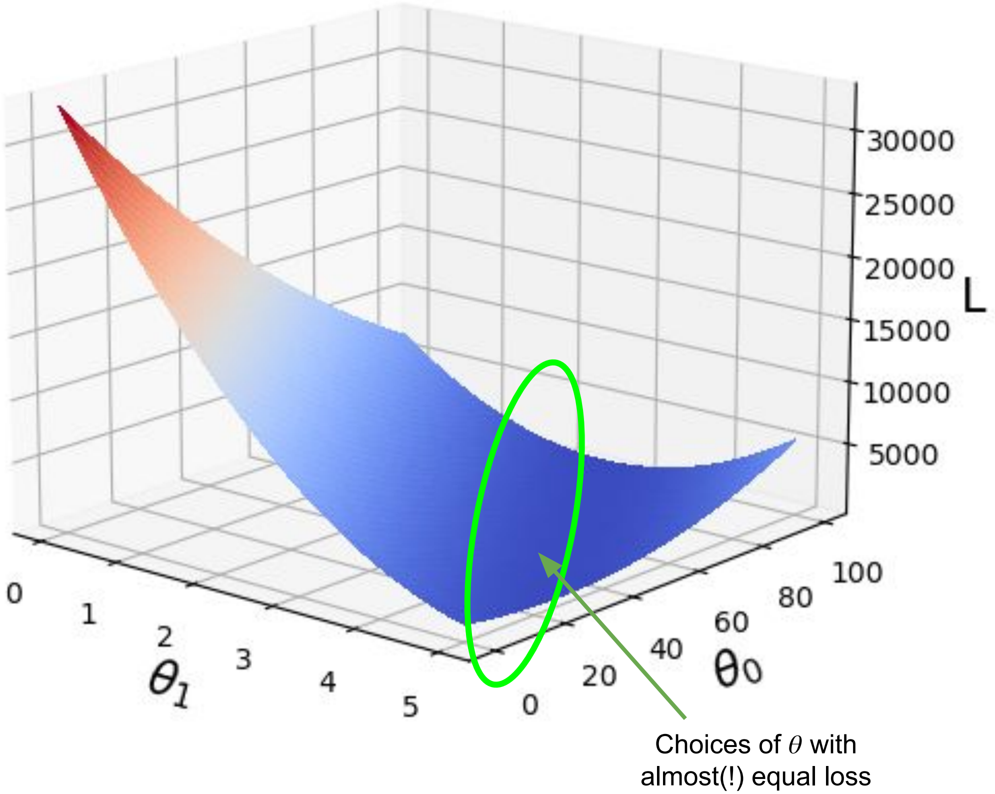
Quick Quiz



Gradient Descent not reaching optimal solution after 10k iterations.

Why?

Quick Quiz



Region of "near-plateau":

➜ Gradient $\nabla_\theta L$ very small

➜ Step $\eta \nabla_\theta L$ extremely small

➜ Very slow convergence

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Polynomial Linear Regression

- Linear Regression $\not\rightarrow$ line / plane / hyperplane

- Polynomial Linear Regression
  - Allows to capture nonlinear relationships between *X* and *y*
  - Polynomial regression model for 1 input feature

Still linear in θ!

$$\hat{y}_i = \theta_0 1 + \theta_1 x_i + \theta_2 x_i^2 + \ldots + \theta_p x_i^p$$

  - Matrix representation (again, 1 input feature!)

$$X^{(1)} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \quad X^{(2)} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix} \quad X^{(3)} = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 \end{bmatrix} \quad X^{(p)} = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & \ldots & x_1^p \\ 1 & x_2 & x_2^2 & x_2^3 & \ldots & x_2^p \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 & \ldots & x_n^p \end{bmatrix}$$

Polynomial Linear Regression

- Example: 1 input feature, 3 data samples

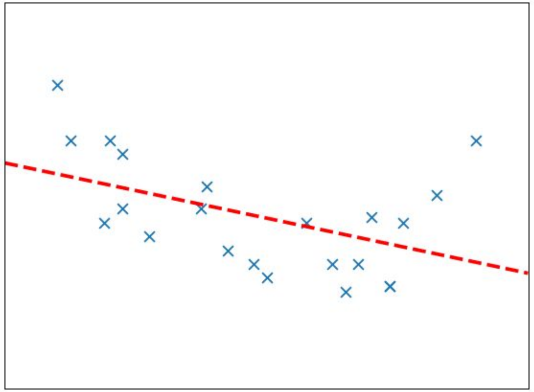
$$X^{(1)} = \begin{bmatrix} 1 & 2 \\ 1 & 3 \\ 1 & 1 \end{bmatrix} \qquad X^{(2)} = \begin{bmatrix} 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 1 & 1 \end{bmatrix} \qquad X^{(3)} = \begin{bmatrix} 1 & 2 & 4 & 8 \\ 1 & 3 & 9 & 27 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

➜ Polynomial terms "look the same" as additional features

➜ Finding best θ using the Normal Equation or Gradient Descent

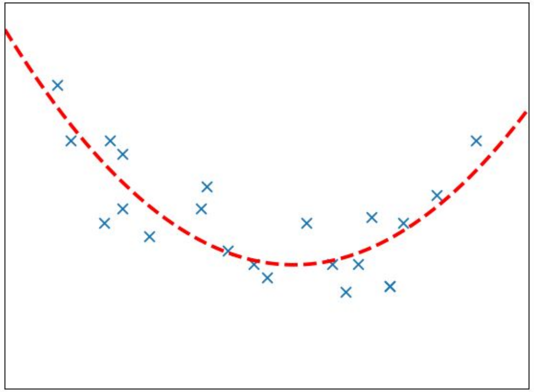
Polynomial Linear Regression — Example

$p = 1$



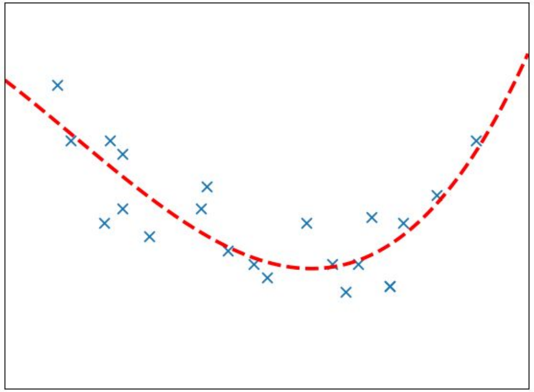
Underfitting

$p = 2$



Good fit

$p = 3$



Overfitting?

Polynomial Linear Regression — Overfitting

- Increasing degree of polynomial *p*
  - More capacity to capture nonlinear relationships
  - Much higher sensitivity to noise and outliers

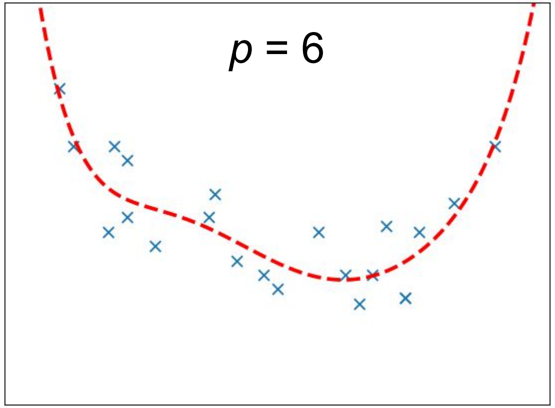
- Countermeasure: **Regularization**
  - Extend loss function to "punish" large values of θ

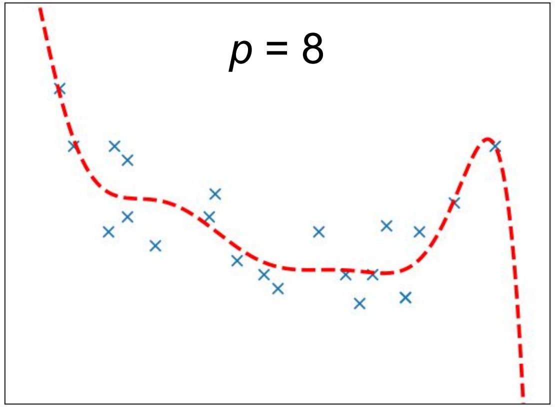
$$L = \frac{1}{n}\|X\theta - y\|^2 + \lambda\frac{1}{n}\|\theta\|_2^2$$

Regularization parameter

$$\|\theta\|_2^2 = \sum_{i=1}^{d} \theta_i^2$$

Note: excludes θ_0!





Polynomial Linear Regression — Minimizing Loss *L*

- Normal Equation

$$\theta = (X^T X + \lambda \begin{array}{c} \text{(d+1) × (d+1)} \\ \begin{bmatrix} 0 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix} \end{array})^{-1} X^T y$$

- Gradient Descent

$$\nabla_\theta L = \frac{2}{n} X^T (X\theta - y) + \lambda \frac{2}{n} \theta$$

Polynomial Linear Regression — More than 1 Feature

- Polynomial of degree *p*=2 and two input features (*d*=2)

$$\hat{y}_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} + \theta_3 x_{i1}^2 + \theta_4 x_{i2}^2 + \theta_5 \underbrace{x_{i1} x_{i2}}_{\text{interaction terms (cross terms)}}$$

- Polynomial of degree *p*=3 and two input features (*d*=2)

$$\hat{y}_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} + \theta_3 x_{i1}^2 + \theta_4 x_{i2}^2 + \theta_5 x_{i1}^3 + \theta_6 x_{i2}^3 + \\ \theta_7 x_{i2}^2 x_{i1} + \theta_8 x_{i2} x_{i1}^2 + \theta_9 x_{i2} x_{i1}$$

- Polynomial of degree *p*=2 and two input features (*d*=3)

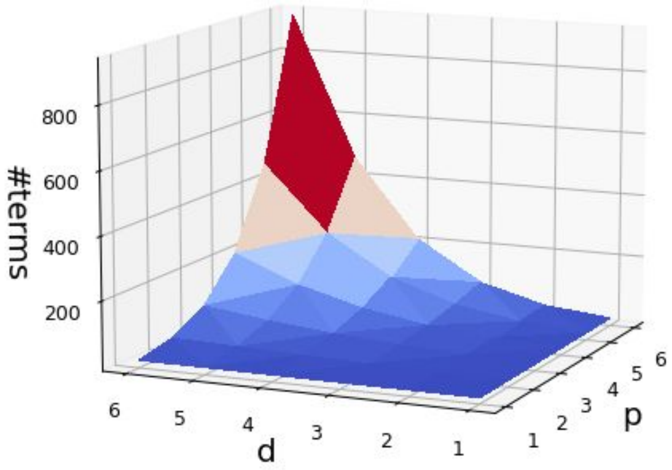
$$\hat{y}_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} + \theta_3 x_{i3} + \theta_4 x_{i1}^2 + \theta_5 x_{i2}^2 + \theta_6 x_{i3}^2 \\ \theta_7 x_{i2} x_{i1} + \theta_8 x_{i3} x_{i1} + \theta_9 x_{i3} x_{i2}$$

Polynomial Linear Regression — More than 1 Feature

- Number of terms in multivariate polynomial given given p, d

$$\theta_i,\ 0 \leq i \leq M, \quad \text{with } M = \binom{p+d}{p}$$

$$\boxed{\binom{n}{k} = \frac{n!}{k!(n-k)!}}$$



- Practical considerations
  - Limited to small number of features and small polynomial degrees
  - In principle, terms can be dropped (e.g., all interaction terms)

risk of overfitting + low interpretability

justification typically not obvious

Outline

- Linear Models
  - Basic setup
- **Linear Regression**
  - Problem formulation
  - Normal Equation (analytical solution)
  - Gradient Descent (iterative optimization)
  - Polynomial Linear Regression (overfitting, regularization)
  - **Interpretation of Coefficients**
- Logistic Regression
  - Problem formulation
  - Gradient Descent

Linear Regression — Interpretation of θ_i

- Example: prediction of house prices

$$\left.\begin{array}{l} price = \theta_0 + \theta_1(\#rooms) + \theta_2(area) + \theta_3(floor) + \ldots \\ price' = \theta_0 + \theta_1(\#rooms + 1) + \theta_2(area) + \theta_3(floor) + \ldots \end{array}\right\} \Delta(price) = price' - price = \theta_1$$

- Interpretation
  - Change of value of feature *i* by 1 unit ➜ change of output value by θ_i
  - Assumption: all other features values remain the same

➜ What about normalizing the data?

Data Normalization — Yes or No? (standardization, min-max scaling)

- Data normalization does not affect model performance
  (assuming basic Linear Regression without regularization)

- In favor of "No"
  - Preserves unit of feature *i* ➜ direct interpretation of θ_i
  - Better for comparing θ_i for the same features across different datasets

- In favour of "Yes"
  - When using regularization
  - When using Polynomial Linear Regression
  - Better for comparing θ_i within a model (e.g., $\theta_i > \theta_j$ ➜ feature *i* more important than feature *j*)

Quick Quiz

Which of the statements regarding Linear Regression is **True**?

A It's impossible to overfit given a dataset with only 1 feature

B Scaling the data will change the coefficients

C Gradient Descent can get stuck in local minimum

D Regularization can improve the training loss/error

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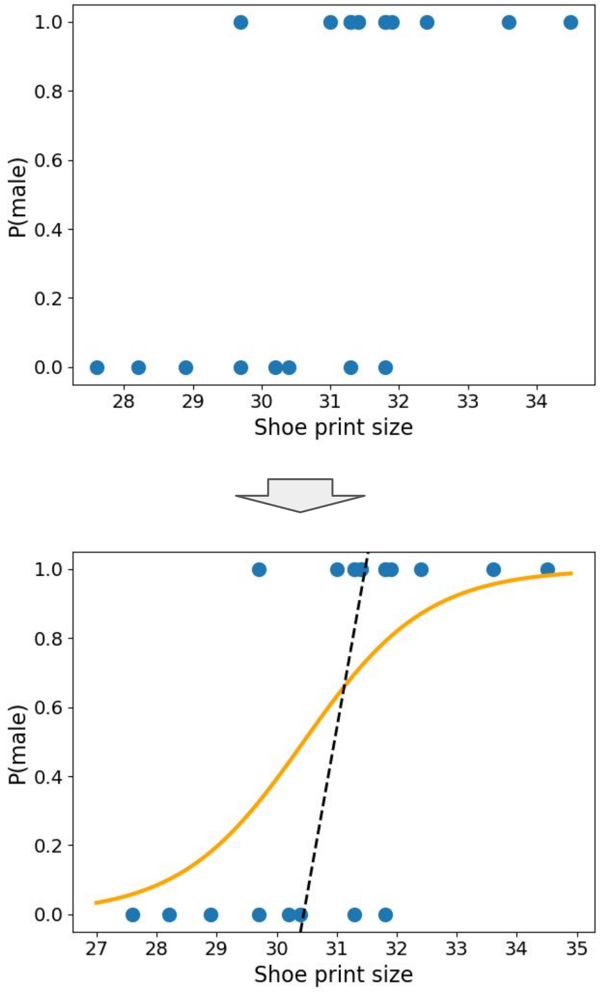
Logistic Regression — Simple Example

- Crime scene investigation (CSI)
  - Found a shoe print of size 32.2cm
  - Is the suspect a male or not?

- Approach: Logistic Regression for binary classification $y_i \in \{0,1\}$
  - Collect a dataset of (size, sex)-pairs
  - Train linear classifier such that

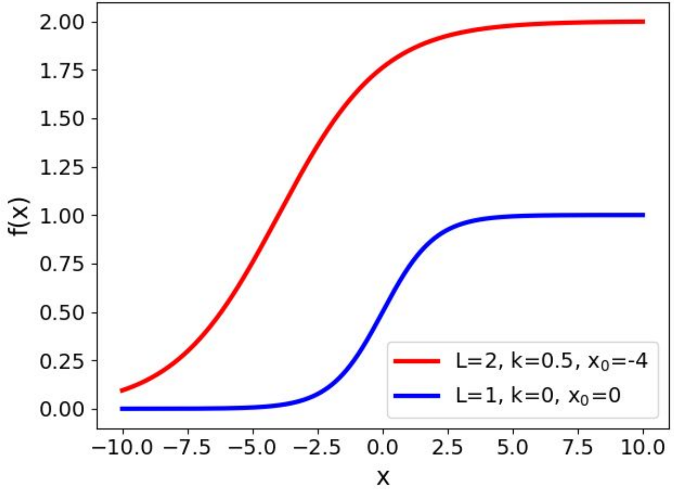
$$0 \leq h_\theta(x_i) \leq 1$$



Logistic Regression

- Logistic Regression ➜ Real-valued predictions interpreted as probability
  - Function *f* is the standard **Logistic Function** (Sigmoid function)

$$f(x) = \frac{L}{1 + e^{-k(x - x_0)}} \xrightarrow{L=1,\ k=1,\ x_0=0} f(x) = \frac{1}{1+e^{-x}}$$



Logistic Regression — Probabilistic Interpretation

- $\hat{y}$ interpreted as a probability

$$\hat{y} = h_\theta(x) = f(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}} \qquad \text{with} \quad \hat{y} \in [0, 1]$$

➜ $\hat{y} = h_\theta(x)$ is the estimated probability that $y_i = 1$ (male) given x and θ

$$\hat{y} = P(y = 1 | x, \theta)$$

➜ Given only discrete 2 outcomes: $P(y = 1|x, \theta) + P(y = 0|x, \theta) = 1$

$$\hat{y} = 1 - P(y = 0|x, \theta)$$

Logistic Regression — Probabilistic Interpretation

$$\hat{y} = P(y = 1|x, \theta) = 1 - P(y = 0|x, \theta)$$

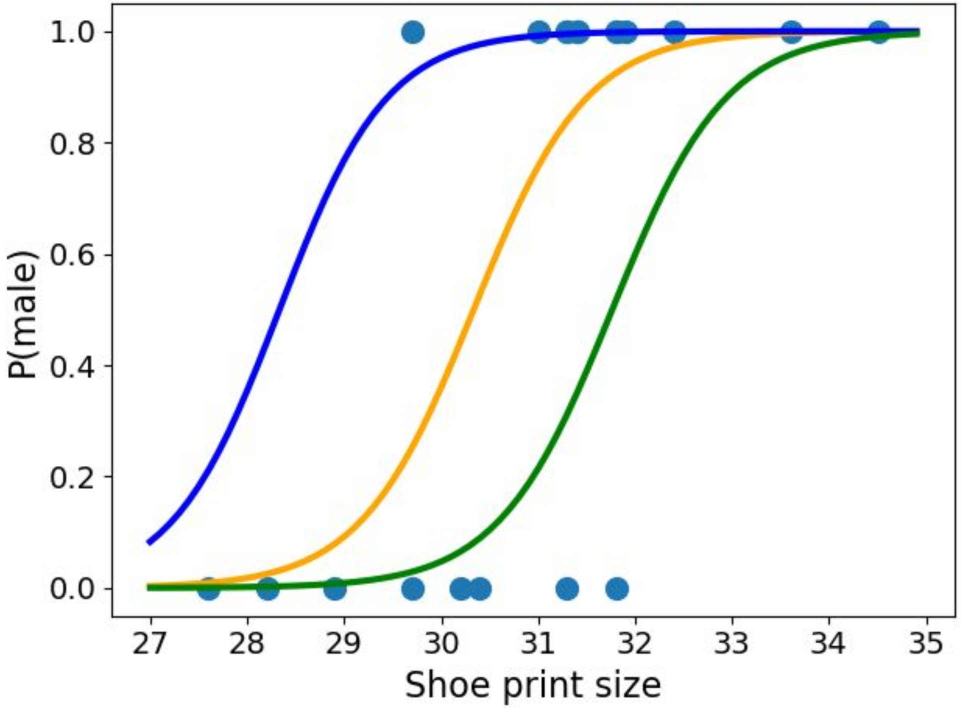
➜ *P(y|x)* is a Bernoulli distribution

$$P(y|x) = \begin{cases} \hat{y} & , y = 1 \\ 1 - \hat{y} & , y = 0 \end{cases}$$

$$P(y|x) = \hat{y}^y (1 - \hat{y})^{1-y}$$

$$\boxed{\hat{y} = \frac{1}{1 + e^{-\theta^T x}}}$$

Logistic Regression



Which $h_\theta(x)$ is the best?

How to find it θ?

Logistic Regression — Loss Function

$$\boxed{\hat{y} = \frac{1}{1 + e^{-\theta^T x}}}$$

- Goal: Maximize probability of true *y* label given training sample *x*
  - Find θ that **maximizes**

$$P(y|x) = \hat{y}^y (1 - \hat{y})^{1-y}$$

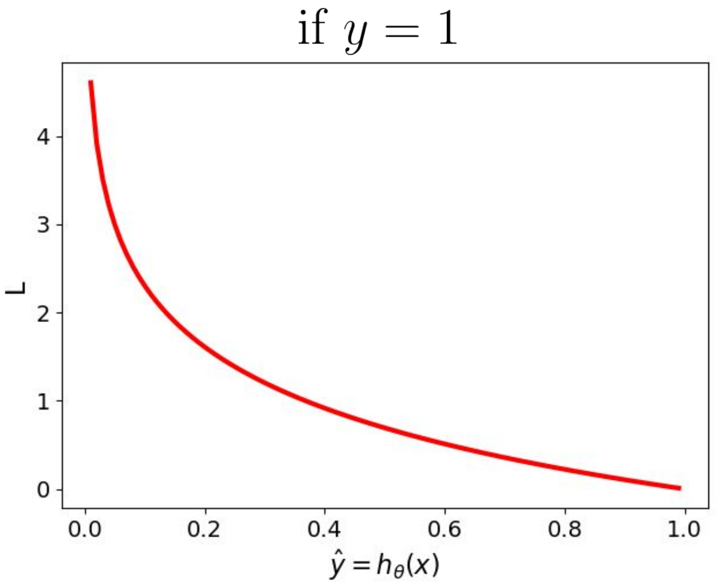
$$\begin{aligned}\log P(y|x) &= \log \left[\hat{y}^y (1 - \hat{y})^{1-y}\right] \\ &= y \log \hat{y} + (1 - y) \log (1 - \hat{y})\end{aligned}$$

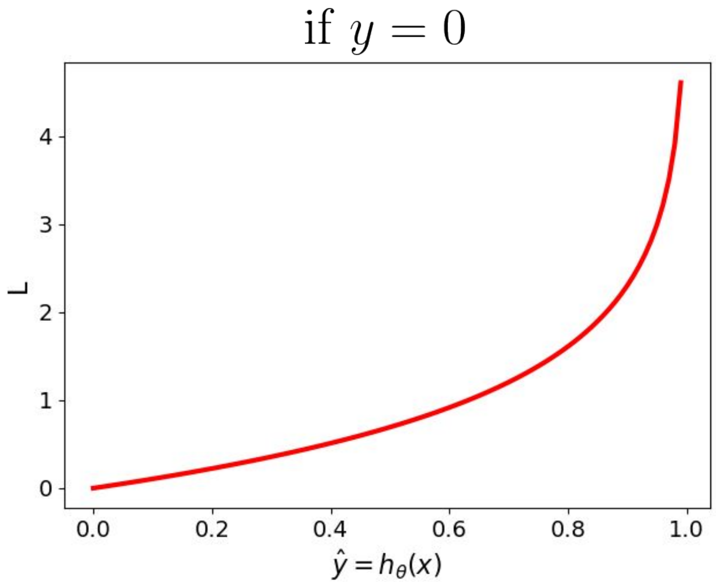
  - Find θ that **minimizes**

$$L = -P(y|x) = \underbrace{-\left[y \log \hat{y} + (1 - y) \log (1 - \hat{y})\right]}_{\textbf{Cross-Entropy Loss}}$$

Cross-Entropy Loss — Visualization

$$L = -\left[y \log \hat{y} + (1-y)\log(1-\hat{y})\right]$$





Quick Quiz

What happens if Logistic Regression gets a training sample **correct**?

- **A** No loss will be calculated
- **B** The loss will be 0
- **C** The loss will be small
- **D** The loss will be large

Overview

- Linear Models
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  - Interpretation of Coefficients

- **Logistic Regression**
  - Problem formulation
  - **Gradient Descent**

Logistic Regression — Loss Function

$$\hat{y} = \frac{1}{1 + e^{-\theta^T x}}$$

- Loss for all training samples

$$
\begin{aligned}
L &= -\frac{1}{n}\sum_{i=1}^{n}\left[y_i \log \hat{y}_i + (1 - y_i)\log(1 - \hat{y}_i)\right] \\
&= -\frac{1}{n}\sum_{i=1}^{n}\left[y_i \log h_\theta(x_i) + (1 - y_i)\log(1 - h_\theta(x_i))\right] \\
&= -\frac{1}{n}\sum_{i=1}^{n}\left[y_i \log \frac{1}{1 + e^{\theta^T x_i}} + (1 - y_i)\log(1 - \frac{1}{1 + e^{\theta^T x_i}})\right]
\end{aligned}
$$

- Required for minimizing the loss: $\nabla_\theta L = \frac{\partial L}{\partial \theta} = ???$

Logistic Regression — Loss Function

- After lots of tedious math…

$$\frac{\partial L}{\partial \theta_j} = \frac{1}{n} \sum_{i=1}^{n} \left[h_\theta(x_i) - y_i \right] x_{ij}$$

$$\nabla_\theta L = \frac{1}{n} X^T (h_\theta(X) - y)$$

- Problem: $\frac{1}{n} X^T (h_\theta(X) - y) \overset{!}{=} 0$ has no closed-form solution for θ

➜ Gradient Descent!

Logistic Regression in Practice (CSI Example)

Vanilla implementation

```
Start training for 1,000,000 iterations...
Loss: 0.6931471805599453        0.0%
Loss: 0.765069661957756         10.0%
Loss: 0.6093119537276577        20.0%
Loss: 0.5066673325457598        30.0%
Loss: 0.4551164039897514        40.0%
Loss: 0.4280635319707213        50.0%
Loss: 0.415438904268411         60.0%
Loss: 0.4152887492109594        70.0%
Loss: 0.4151849953246913        80.0%
Loss: 0.41511286000667447       90.0%
loss: 0.41506245481850296       100.0%
Training finished in 0:00:09.617970
```

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} -43.45 \\ 1.42 \end{bmatrix}$$

sklearn.linear_model.LogisticRegression
(with default L-BFGS-B solver)

```
Start training...
Training finished in 0:00:00.000035 (#iterations: 21)
```

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} -44.91 \\ 1.47 \end{bmatrix}$$

See https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

Logistic Regression in Practice (CSI Example)

Vanilla implementation

```
Start training for 78,000 iterations...
Loss: 0.6931471805599453        0.0%
Loss: 0.6565544350291496        10.0%
Loss: 0.647547882511651 7       20.0%
Loss: 0.6389819932273285        30.0%
Loss: 0.6308342158505089        40.0%
Loss: 0.6230827400881452        50.0%
Loss: 0.6157065622831859        60.0%
Loss: 0.6086855316895313        70.0%
Loss: 0.6020003798552925        80.0%
Loss: 0.5956327355164103        90.0%
loss: 0.5895658866765062        100.0%
Training finished in 0:00:00.784118
```

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} -5.44 \\ 0.19 \end{bmatrix}$$

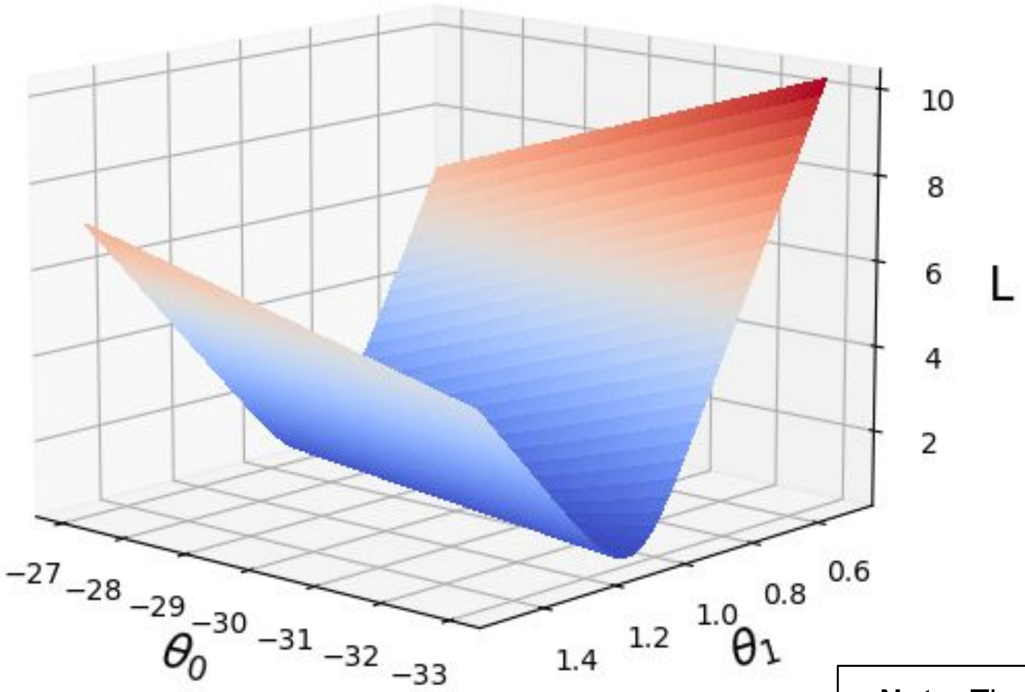
sklearn.linear_model.LogisticRegression
(with SAG solver)

```
Start training...
Training finished in 0:00:00.007022 (#iterations: 5820)
```

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} -5.45 \\ 0.19 \end{bmatrix}$$

See https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

Logistic Regression in Practice (CSI Example)



Region of "near-plateau":

➜ Gradient $\nabla_\theta L$ very small

➜ Step $\eta \nabla_\theta L$ extremely small

➜ Very slow convergence

Note: The Cross-Entropy loss of Logistic Regression is convex

➜ There always exists exactly one minimum (global minimum)!

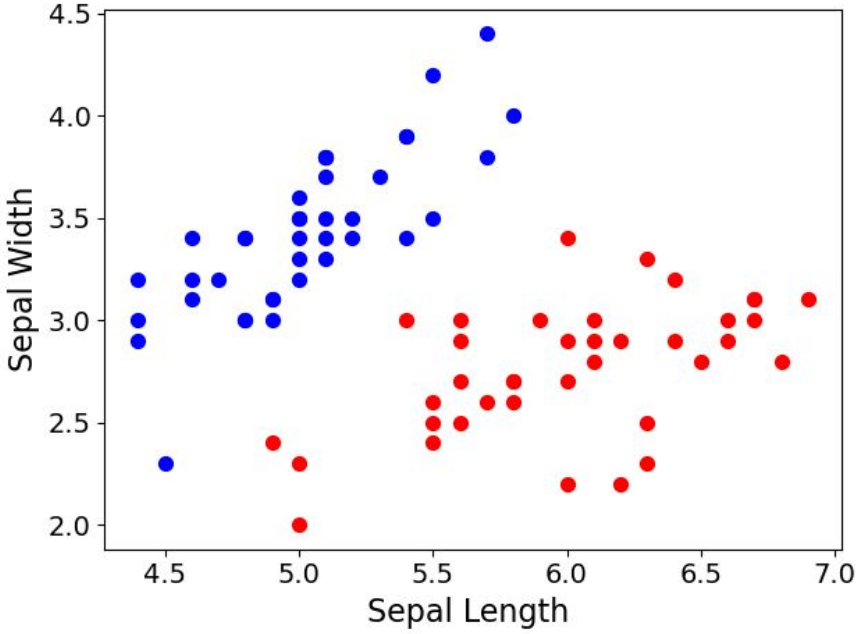
Logistic Regression in Practice

- Logistic Regression with vanilla Gradient Descent (also Linear Regression)
  - Works in principle — the math is sound!
  - Often poor performance compared to more sophisticated implementations

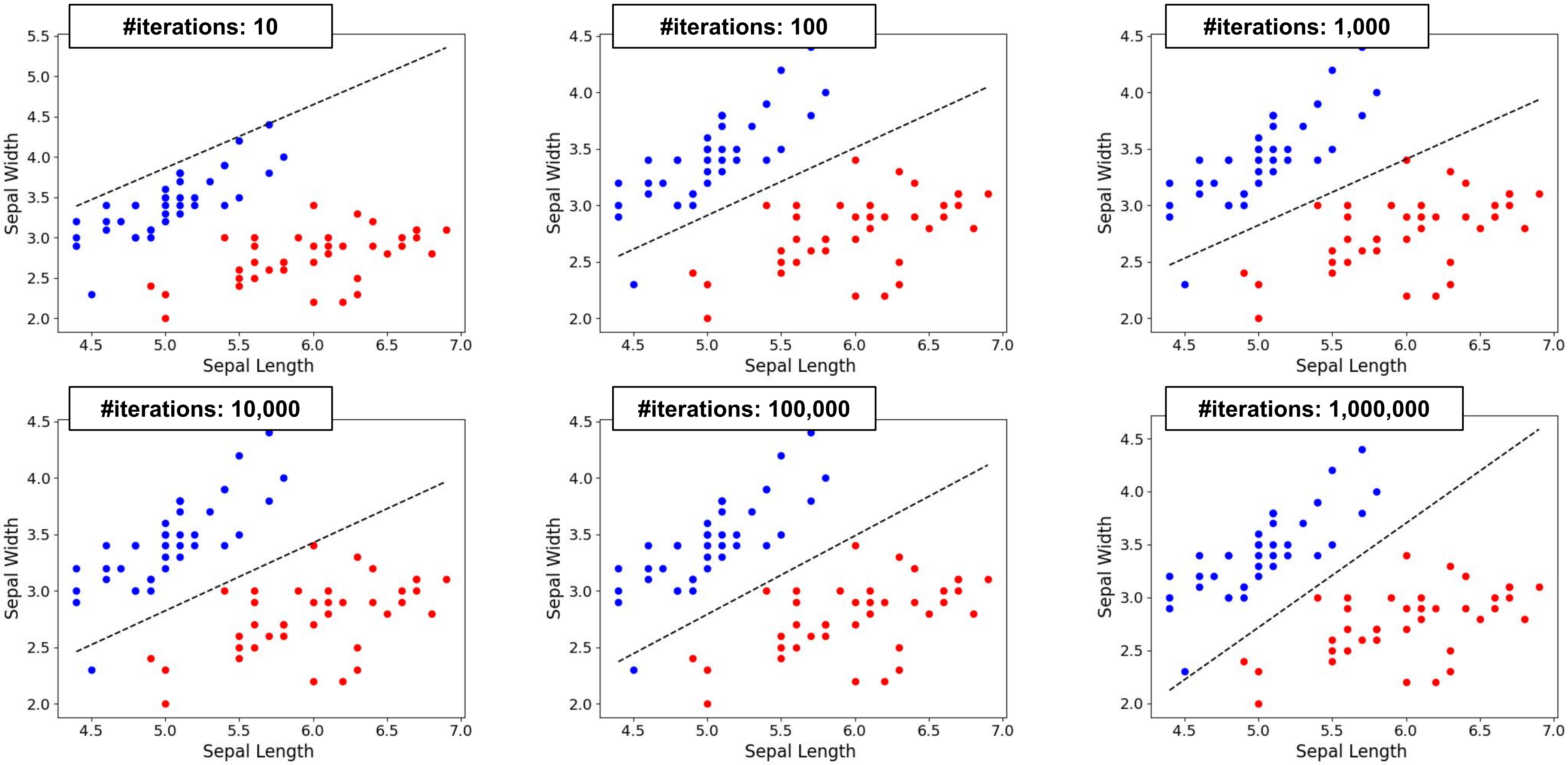
- Many techniques to boost performance
  - Smart(er) initialization of θ
  - Adaptive learning rates
  - Extensions to Gradient Descent
  - Regularization
  - ...and others

Logistic Regression — 2D Example

- IRIS dataset
  - 3 classes of Iris plants
    (only 2 considered)
  - 50 samples per class
  - 4 continuous features
    (only sepal length/width considered)



Logistic Regression — 2D Example (Vanilla Gradient Descent)



Polynomial Logistic Regression

- Analogous to Polynomial Linear Regression
  - Allows to capture nonlinear relationships between *X* and *y*
  - Polynomial Logistic Regression model for 1 input feature

$$\hat{y}_i = \frac{1}{1 + e^{-\theta^T x_i}}, \quad \text{with } \theta^T x_i = \theta_0 + \theta_1 x_i + \theta_2 x_i^2 + ... + \theta_p x_i^p$$

- Identical practical considerations
  - Solve using Gradient Descent as usual
    (optionally with regularization to avoid overfitting)
  - Limited to small number of features
    and small polynomial degrees

$$\nabla_\theta L = \frac{1}{n} X^T (h_\theta(X) - y) + \lambda \frac{2}{n} \theta$$

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- Logistic Regression
  - Problem formulation
  - Gradient Descent

Summary

- Linear Models
  - Assume linear relationship between input features and output
    (i.e., output = sum of weighted feature values)
  - However, regression line / decision boundary not always a line/plane/hyperplane
    (data transformation to add polynomial terms based on input features)
  - Generally good interpretability

- Linear Regression & Logistic Regression
  - Very fundamental and popular regression and classification methods
  - Gradient Descent to solve both tasks + Normal Equation to solve Linear Regression
  - Effects of data normalization mainly(!) on explainability / interpretability of results
  - Straightforward extension of Logistic Regression beyond 2 classes (not covered here)

Solutions to Quick Quizzes

- Slide 13: Yellow (smallest average error)
- Slide 22: D
- Slide 23: A
- Slide 35: "near plateau" ➜ very small gradients and updates
- Slide 48: B
- Slide 57: C