


Machine Learning Department
School of Computer Science
Carnegie Mellon University

# Linear Regression

Matt Gormley
Lecture 7
Sep. 18, 2023

# Reminders

- Homework 3: KNN, Perceptron, Lin.Reg.
  - Out: Fri, Sep. 15
  - Due: Sat, Sep. 23 at 11:59pm
  - (only two grace/late days permitted)
- Exam conflicts form

# Q&A

| | |
|---|---|
| **Q:** | I have a medical emergency or family emergency or disability or other compelling reason and am unable to attend office hours in-person this week. Can an exception be made so I can attend office hours remotely? |
| **A:** | Yes. Please email the Education Associate(s) and request a period of remote office hours. We will reply with instructions on how to utilize them during the approved time period. |

# Q&A

**Q:** How do we build Decision Trees with real-valued features?

**A:** Great question! I made a 7 minute video about that.

**Q:** How do we prove the Perceptron Mistake Bound?

**A:** Great question! I'm going to make a 15 minute video about that.

# DECISION TREES WITH REAL-VALUED FEATURES

# Q&A

**Q:** How do we learn a Decision Tree with real-valued features?

**A:**

## Decision Boundary Example

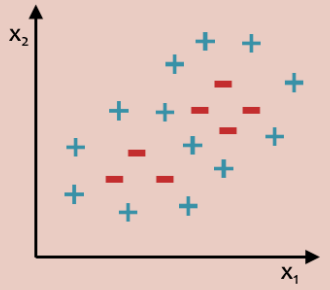
**Dataset:** Outputs {+,-}; Features $x_1$ and $x_2$

### In-Class Exercise

*Question:*

A. Can a **k-Nearest Neighbor classifier with k=1** achieve **zero training error** on this dataset?

B. **If 'Yes'**, draw the learned decision boundary. **If 'No'**, why not?




*Question:*

A. Can a **Decision Tree classifier** achieve **zero training error** on this dataset?

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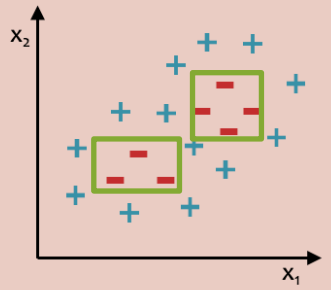


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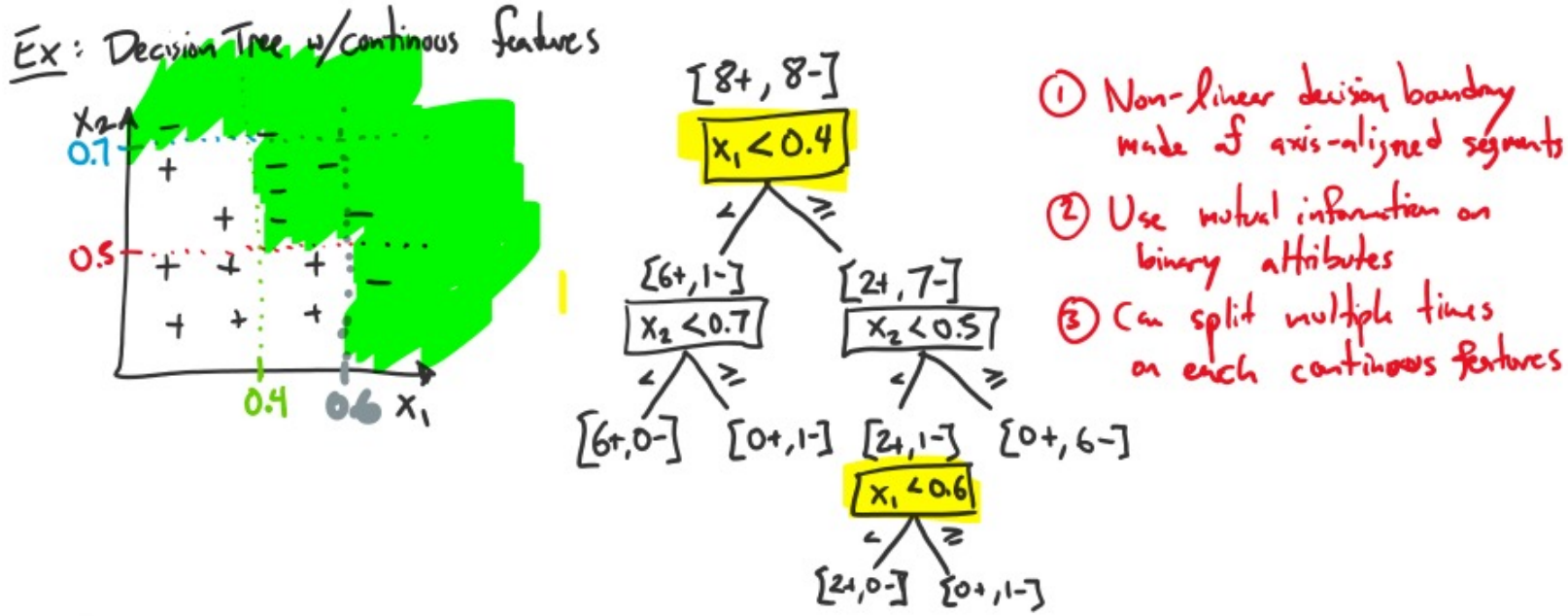
# Q&A

**Q:** How do we learn a Decision Tree with real-valued features?

**A:** Make new discrete features out of the real-valued features and then learn the Decision Tree as normal! Here's an example…

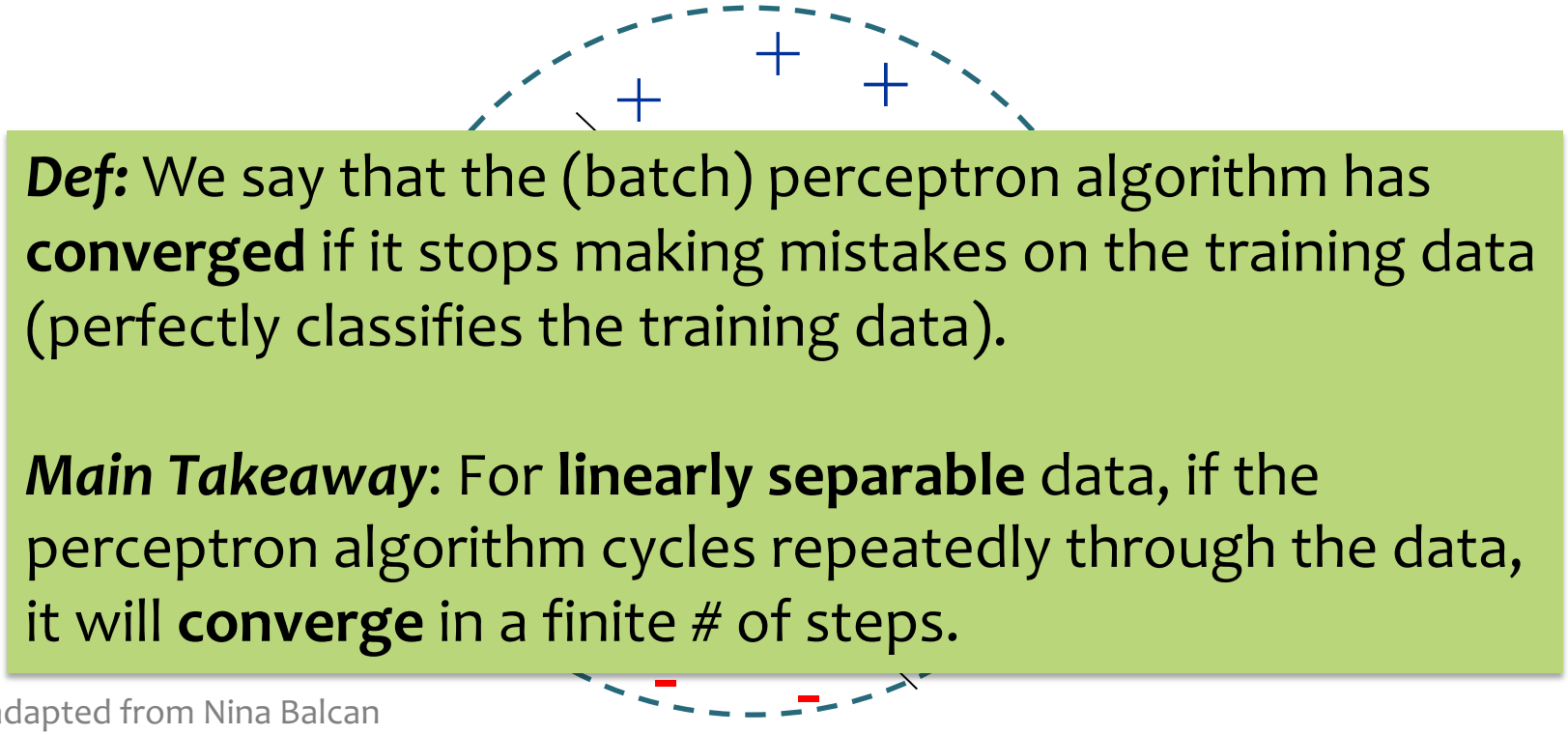


# PERCEPTRON MISTAKE BOUND

# Perceptron Mistake Bound

**Guarantee:** if some data has margin $\gamma$ and all points lie inside a ball of radius $R$ rooted at the origin, then the online Perceptron algorithm makes $\leq (R/\gamma)^2$ mistakes

(Normalized margin: multiplying all points by 100, or dividing all points by 100, doesn't change the number of mistakes! The algorithm is invariant to scaling.)



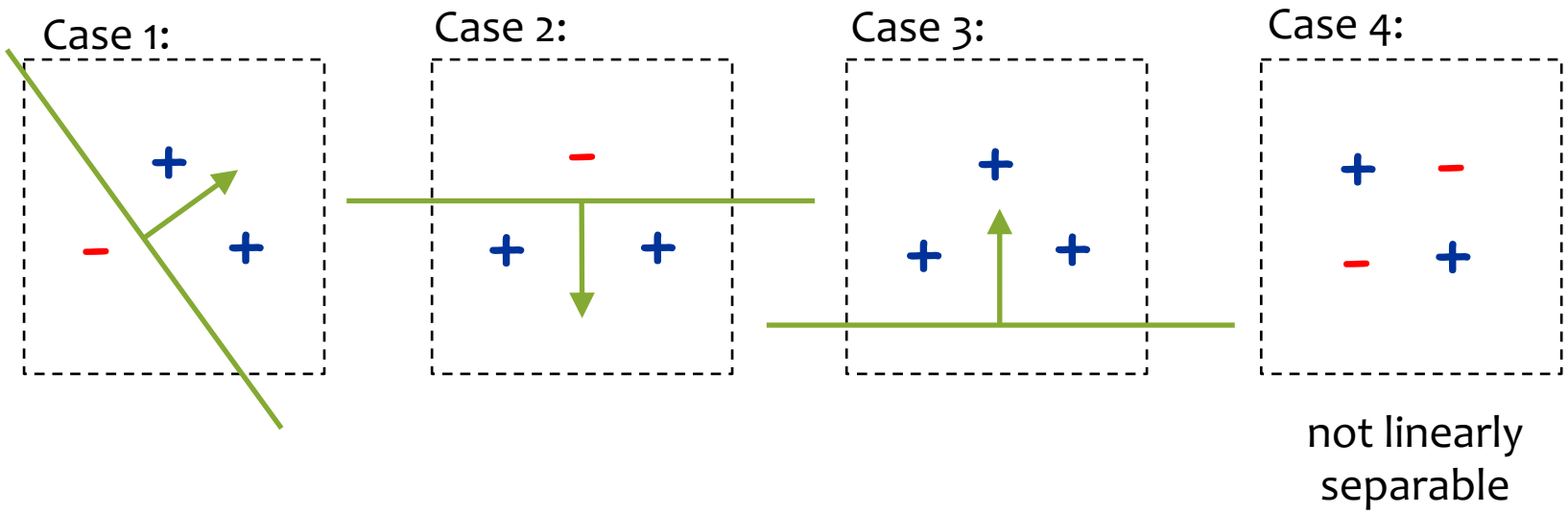
***Def:*** We say that the (batch) perceptron algorithm has **converged** if it stops making mistakes on the training data (perfectly classifies the training data).

***Main Takeaway***: For **linearly separable** data, if the perceptron algorithm cycles repeatedly through the data, it will **converge** in a finite # of steps.

Slide adapted from Nina Balcan

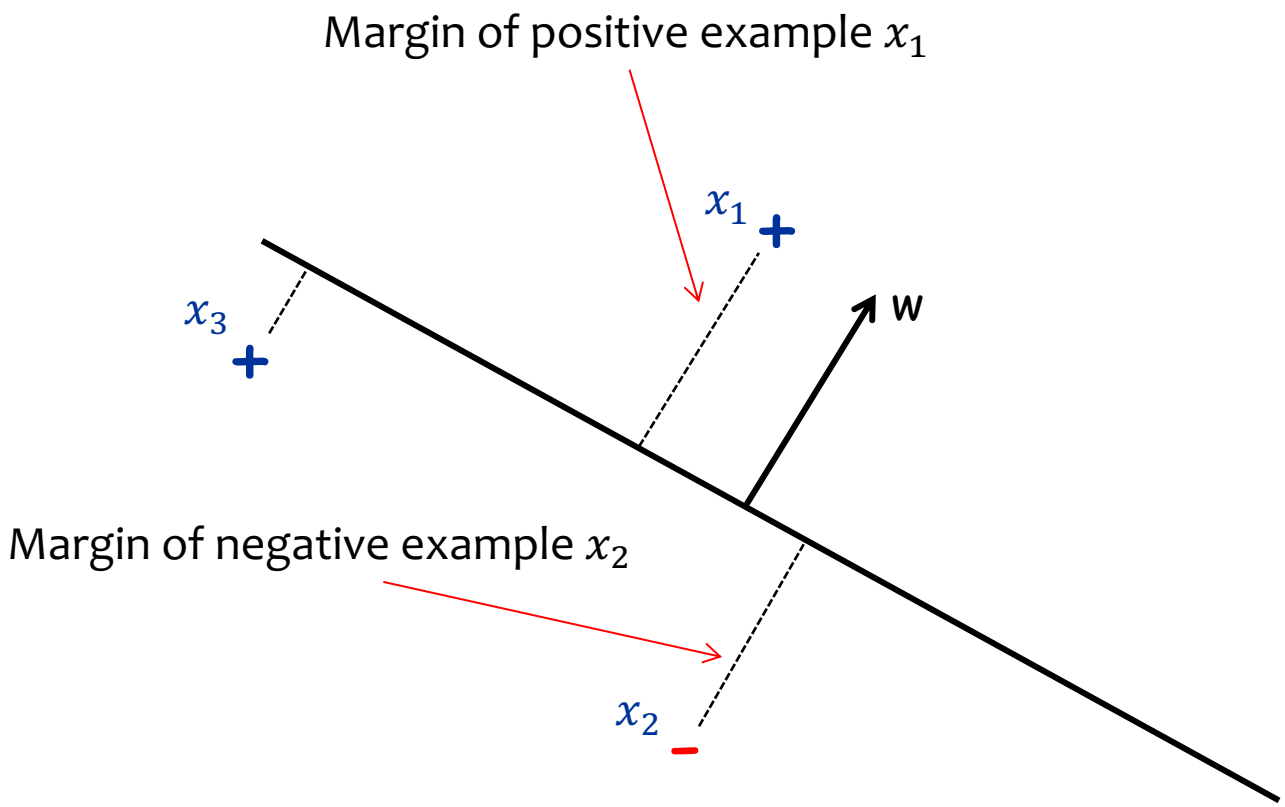
# Linear Separability

***Def:*** For a **binary classification** problem, a set of examples $S$ is **linearly separable** if there exists a linear decision boundary that can separate the points



# Geometric Margin

**Definition:** The margin of example $x$ w.r.t. a linear separator $w$ is the distance from $x$ to the plane $w \cdot x = 0$ (or the negative if on wrong side)

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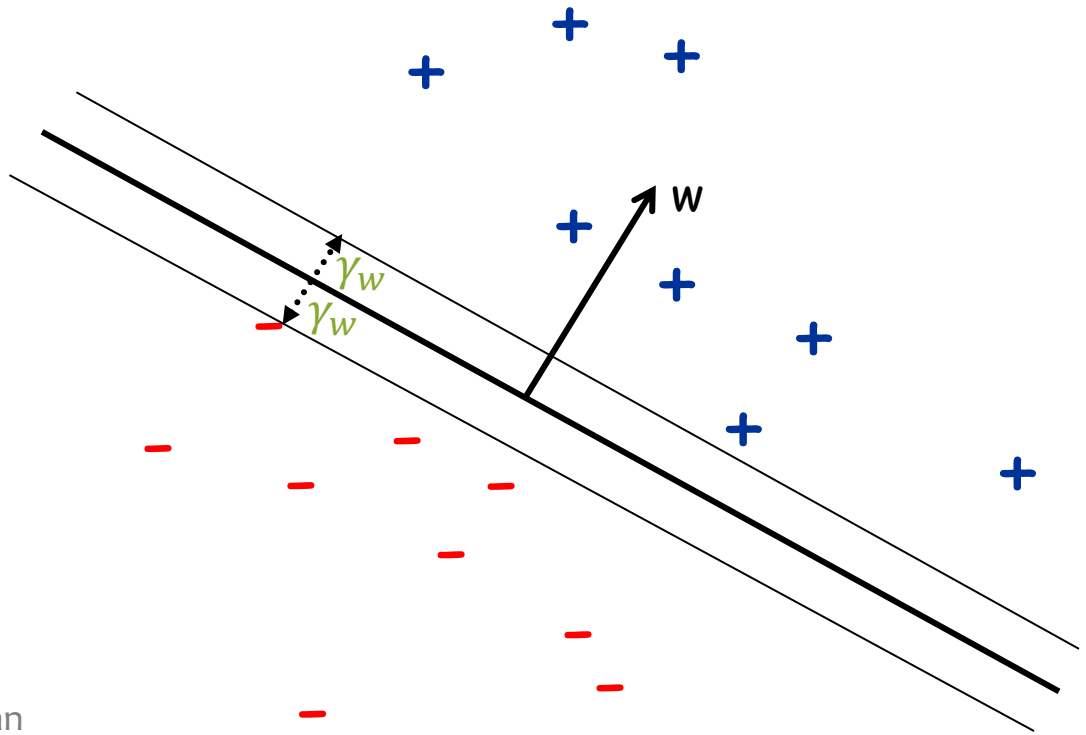


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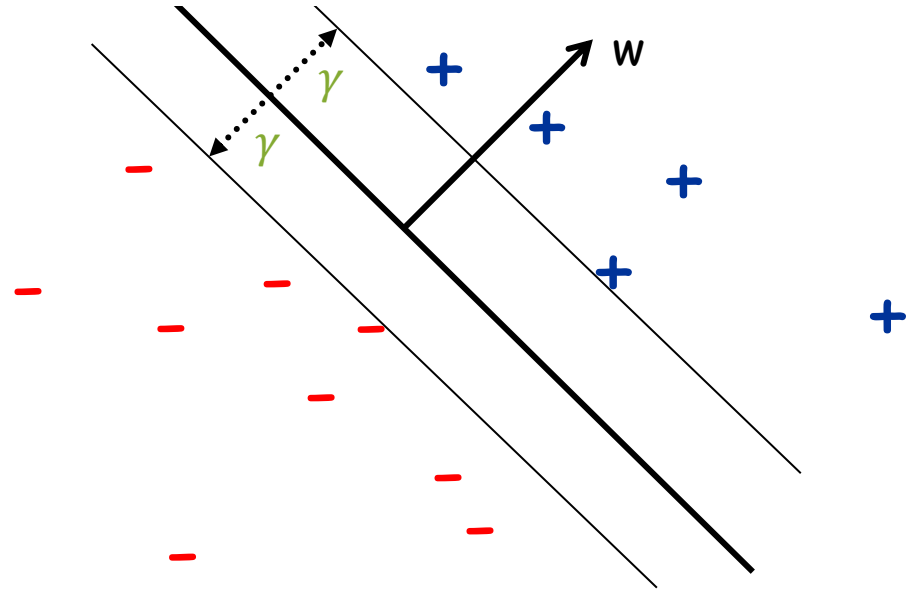
**Definition:** The margin $\gamma$ of a set of examples $S$ is the maximum $\gamma_w$ over all linear separators $w$.




Slide from Nina Balcan

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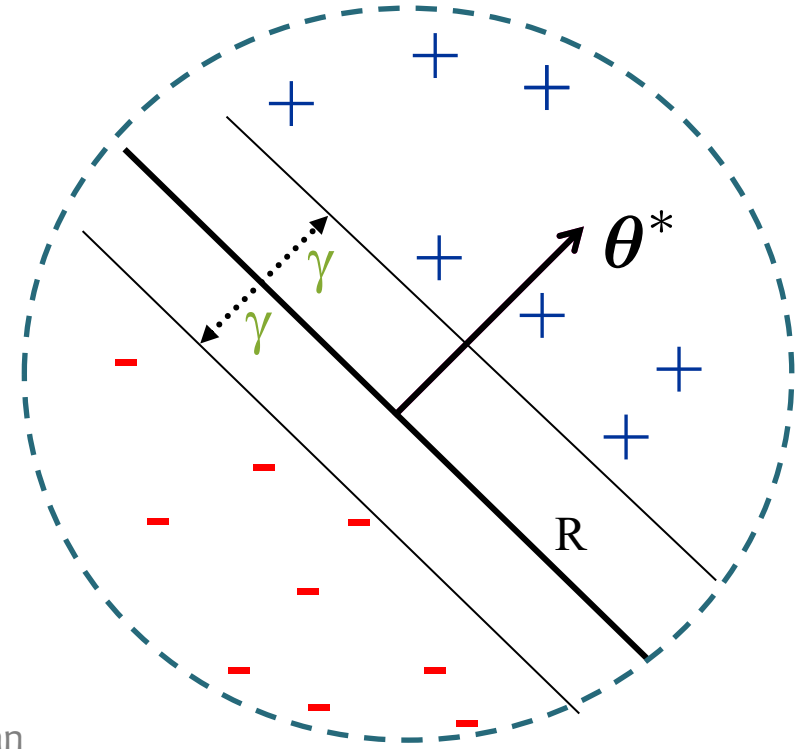


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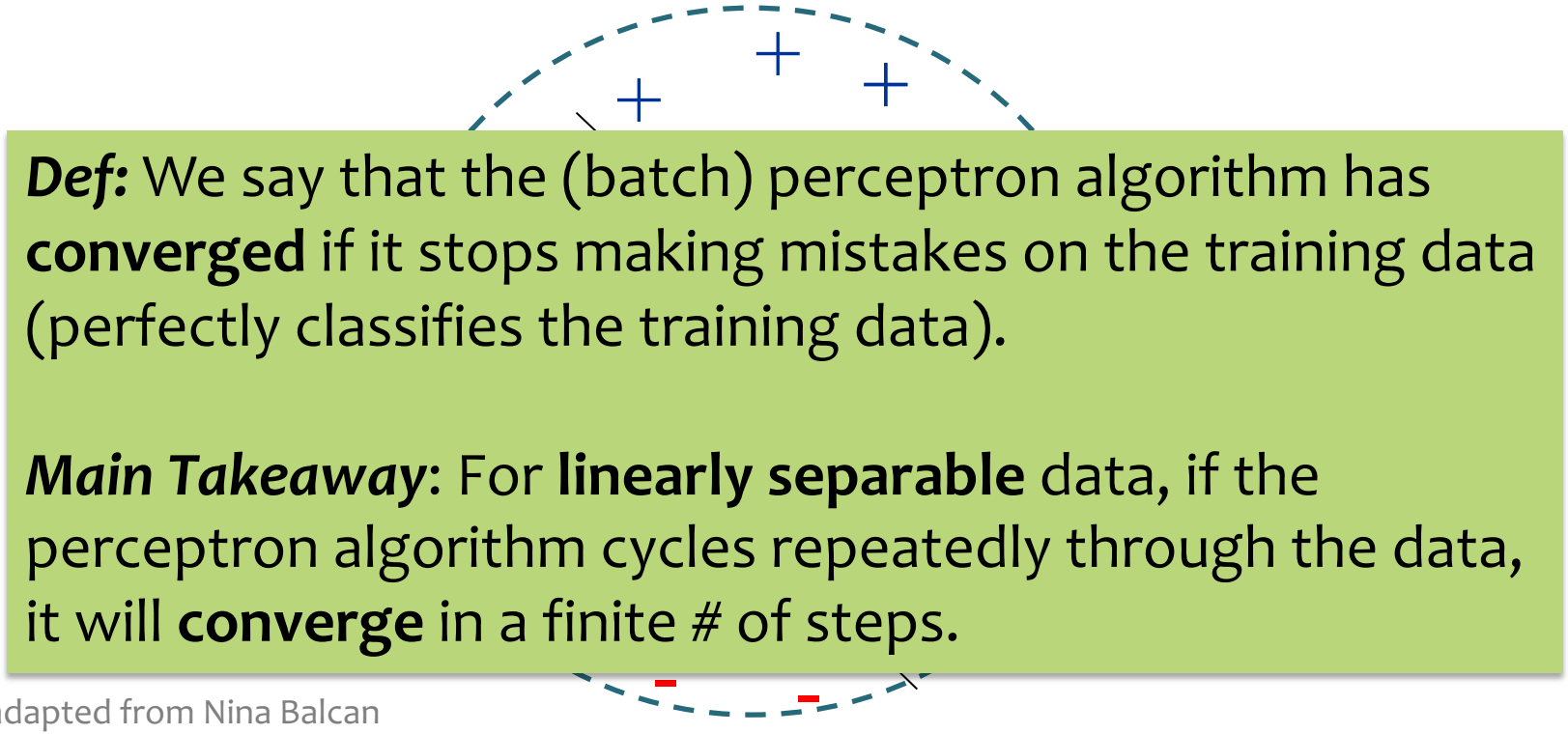

***Def:*** We say that the (batch) perceptron algorithm has **converged** if it stops making mistakes on the training data (perfectly classifies the training data).

***Main Takeaway***: For **linearly separable** data, if the perceptron algorithm cycles repeatedly through the data, it will **converge** in a finite # of steps.

Slide adapted from Nina Balcan

# PROOF OF THE MISTAKE BOUND

# Analysis: Perceptron

**Perceptron Mistake Bound**

**Theorem 0.1** (Block (1962), Novikoff (1962)).

*Given dataset:* $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$.

*Suppose:*

1. *Finite size inputs:* $||x^{(i)}|| \leq R$
2. *Linearly separable data:* $\exists \boldsymbol{\theta}^*$ *s.t.* $||\boldsymbol{\theta}^*|| = 1$ *and* $y^{(i)}(\boldsymbol{\theta}^* \cdot \mathbf{x}^{(i)}) \geq \gamma, \forall i$ *and some* $\gamma > 0$

*Then: The number of mistakes made by the Perceptron algorithm on this dataset is*

$$k \leq (R/\gamma)^2$$

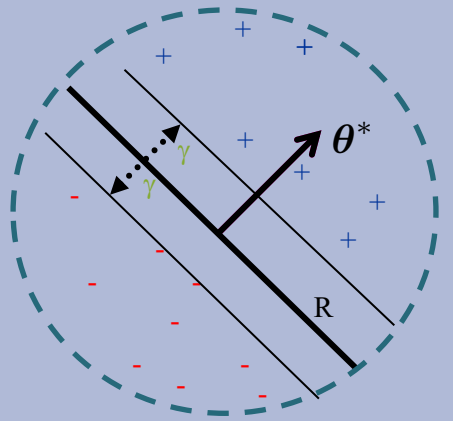


Figure from Nina Balcan

# Analysis: Percept

**Common Misunderstanding:** The **radius** is **centered at the origin**, not at the center of the points.

**Perceptron Mistake Boun**

**Theorem 0.1** (Block (1962), Novikoff (19

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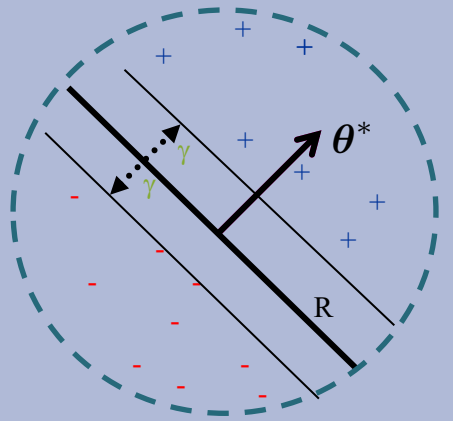


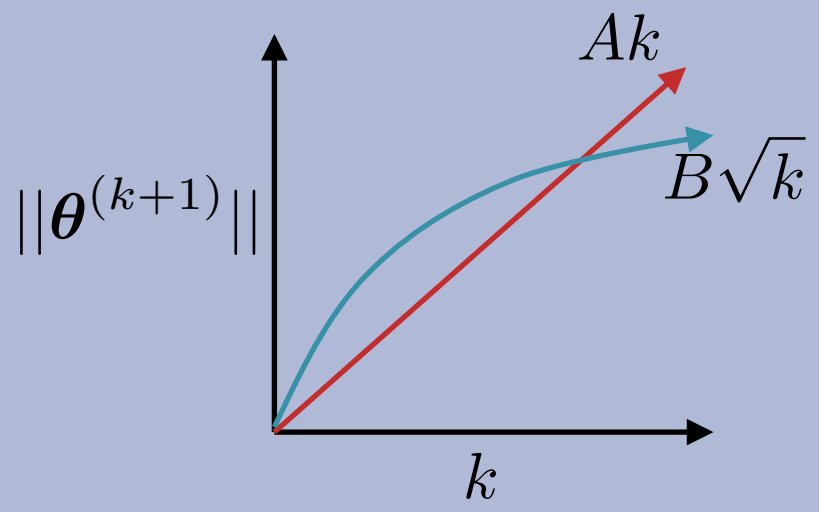

Figure from Nina Balcan

# Analysis: Perceptron

**Proof of Perceptron Mistake Bound:**

We will show that there exist constants A and B s.t.

$$Ak \leq ||\boldsymbol{\theta}^{(k+1)}|| \leq B\sqrt{k}$$



# Analysis: Perceptron

**Theorem 0.1** (Block (1962), Novikoff (1962)).
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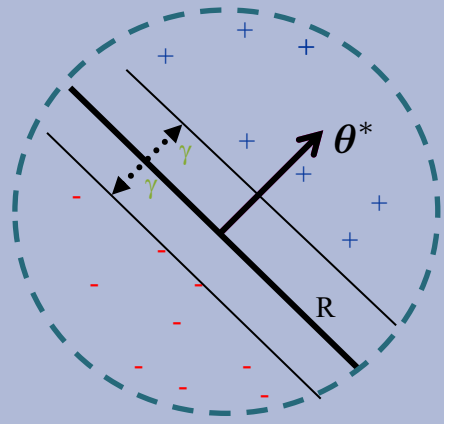



**Algorithm 1** Perceptron Learning Algorithm (Online)

**procedure** PERCEPTRON($\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots\}$)
  $\boldsymbol{\theta} \leftarrow \mathbf{0}, k = 1$ ▷ Initialize parameters
  **for** $i \in \{1, 2, \ldots\}$ **do** ▷ For each example
    **if** $y^{(i)}(\boldsymbol{\theta}^{(k)} \cdot \mathbf{x}^{(i)}) \leq 0$ **then** ▷ If mistake
      $\boldsymbol{\theta}^{(k+1)} \leftarrow \boldsymbol{\theta}^{(k)} + y^{(i)}\mathbf{x}^{(i)}$ ▷ Update parameters
      $k \leftarrow k + 1$
  **return** $\boldsymbol{\theta}$

# Analysis: Perceptron

**Proof of Perceptron Mistake Bound:**

Part 1: for some A, $Ak \leq ||\boldsymbol{\theta}^{(k+1)}||$

$$\boldsymbol{\theta}^{(k+1)} \cdot \boldsymbol{\theta}^* = (\boldsymbol{\theta}^{(k)} + y^{(i)}\mathbf{x}^{(i)})\boldsymbol{\theta}^*$$

by Perceptron algorithm update

$$= \boldsymbol{\theta}^{(k)} \cdot \boldsymbol{\theta}^* + y^{(i)}(\boldsymbol{\theta}^* \cdot \mathbf{x}^{(i)})$$

$$\geq \boldsymbol{\theta}^{(k)} \cdot \boldsymbol{\theta}^* + \gamma$$

by assumption

$$\Rightarrow \boldsymbol{\theta}^{(k+1)} \cdot \boldsymbol{\theta}^* \geq k\gamma$$

by induction on $k$ since $\theta^{(1)} = \mathbf{0}$

$$\Rightarrow ||\boldsymbol{\theta}^{(k+1)}|| \geq k\gamma$$

since $||\mathbf{w}|| \times ||\mathbf{u}|| \geq \mathbf{w} \cdot \mathbf{u}$ and $||\theta^*|| = 1$

Cauchy-Schwartz inequality

# Analysis: Perceptron

**Proof of Perceptron Mistake Bound:**

Part 2: for some B, $||\boldsymbol{\theta}^{(k+1)}|| \leq B\sqrt{k}$

$$||\boldsymbol{\theta}^{(k+1)}||^2 = ||\boldsymbol{\theta}^{(k)} + y^{(i)}\mathbf{x}^{(i)}||^2$$

by Perceptron algorithm update

$$= ||\boldsymbol{\theta}^{(k)}||^2 + (y^{(i)})^2||\mathbf{x}^{(i)}||^2 + 2y^{(i)}(\boldsymbol{\theta}^{(k)} \cdot \mathbf{x}^{(i)})$$

$$\leq ||\boldsymbol{\theta}^{(k)}||^2 + (y^{(i)})^2||\mathbf{x}^{(i)}||^2$$

since $k$th mistake $\Rightarrow y^{(i)}(\boldsymbol{\theta}^{(k)} \cdot \mathbf{x}^{(i)}) \leq 0$

$$= ||\boldsymbol{\theta}^{(k)}||^2 + R^2$$

since $(y^{(i)})^2||\mathbf{x}^{(i)}||^2 = ||\mathbf{x}^{(i)}||^2 = R^2$ by assumption and $(y^{(i)})^2 = 1$

$$\Rightarrow ||\boldsymbol{\theta}^{(k+1)}||^2 \leq kR^2$$

by induction on $k$ since $(\theta^{(1)})^2 = 0$

$$\Rightarrow ||\boldsymbol{\theta}^{(k+1)}|| \leq \sqrt{k}R$$

# Analysis: Perceptron

**Proof of Perceptron Mistake Bound:**

Part 3: Combining the bounds finishes the proof.

$$k\gamma \leq ||\boldsymbol{\theta}^{(k+1)}|| \leq \sqrt{k}R$$

$$\Rightarrow k \leq (R/\gamma)^2$$

The total number of mistakes must be less than this

# Analysis: Perceptron

**What if the data is *not* linearly separable?**

1. Perceptron will **not converge** in this case (it can't!)
2. However, Freund & Schapire (1999) show that by projecting the points (hypothetically) into a higher dimensional space, we can achieve a similar bound on the number of mistakes made on **one pass** through the sequence of examples

**Theorem 2.** *Let* $\langle (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m) \rangle$ *be a sequence of labeled examples with* $\|\mathbf{x}_i\| \leq R$. *Let* $\mathbf{u}$ *be any vector with* $\|\mathbf{u}\| = 1$ *and let* $\gamma > 0$. *Define the deviation of each example as*

$$d_i = \max\{0, \gamma - y_i(\mathbf{u} \cdot \mathbf{x}_i)\},$$

*and define* $D = \sqrt{\sum_{i=1}^{m} d_i^2}$. *Then the number of mistakes of the online perceptron algorithm on this sequence is bounded by*

$$\left(\frac{R + D}{\gamma}\right)^2.$$

# Summary: Perceptron

- Perceptron is a **linear classifier**
- **Simple learning algorithm:** when a mistake is made, add / subtract the features
- Perceptron will converge if the data are **linearly separable**, it will **not** converge if the data are **linearly inseparable**
- For linearly separable and inseparable data, we can **bound the number of mistakes** (geometric argument)
- **Extensions** support nonlinear separators and structured prediction

# Perceptron Learning Objectives

*You should be able to…*

- Explain the difference between online learning and batch learning
- Implement the perceptron algorithm for binary classification [CIML]
- Determine whether the perceptron algorithm will converge based on properties of the dataset, and the limitations of the convergence guarantees
- Describe the inductive bias of perceptron and the limitations of linear models
- Draw the decision boundary of a linear model
- Identify whether a dataset is linearly separable or not
- Defend the use of a bias term in perceptron

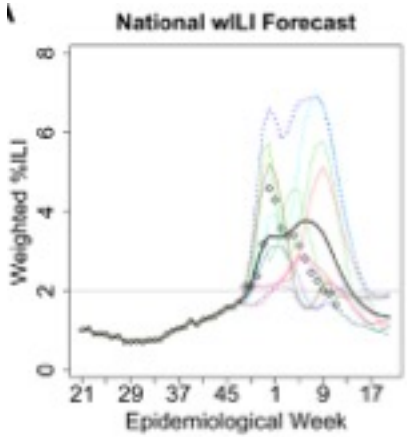
# REGRESSION

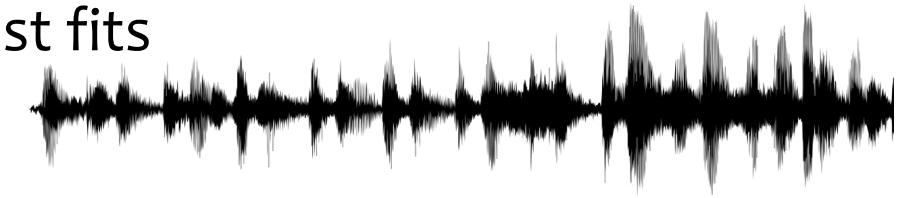
# Regression

This is what differentiates *regression* from *classification*

**Goal:**

- Given a training dataset of pairs (**x**,y) where
  - **x** is a vector
  - y is a scalar
- Learn a function (aka. curve or line) y' = h(x) that best fits the training data



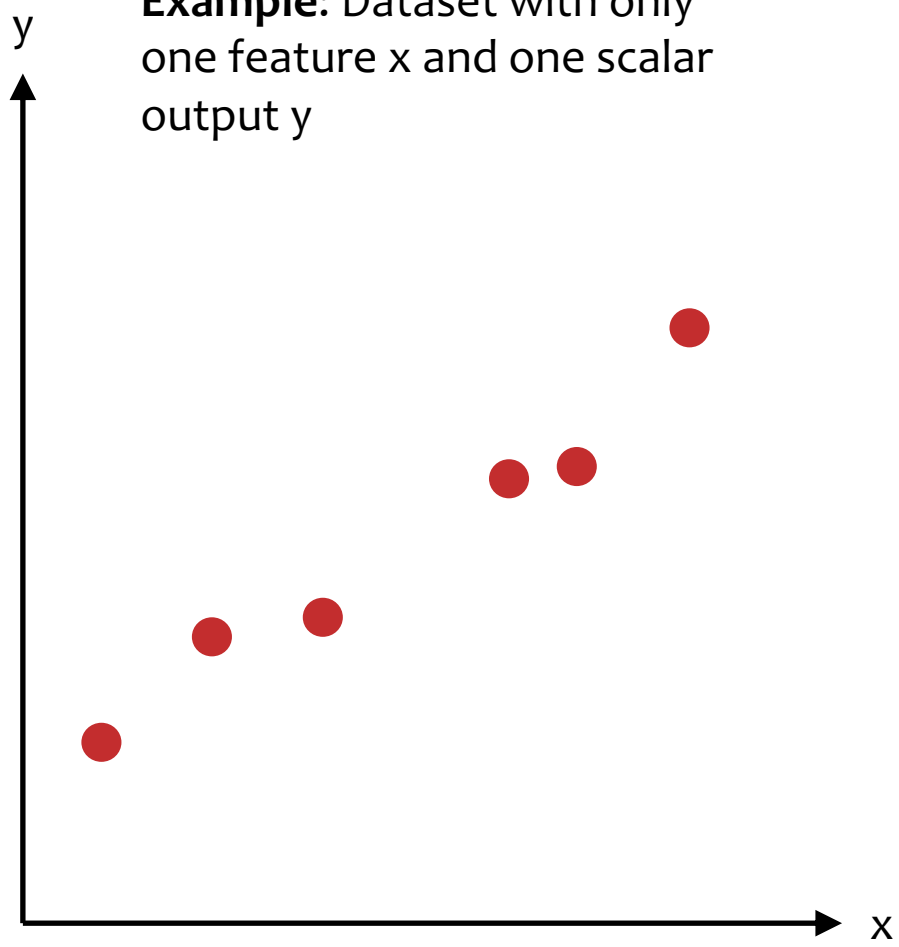



**Example Applications:**

- Stock price prediction
- Forecasting epidemics
- Speech synthesis
- Generation of images (e.g. *Deep Dream*)

# Regression

**Example:** Dataset with only one feature x and one scalar output y

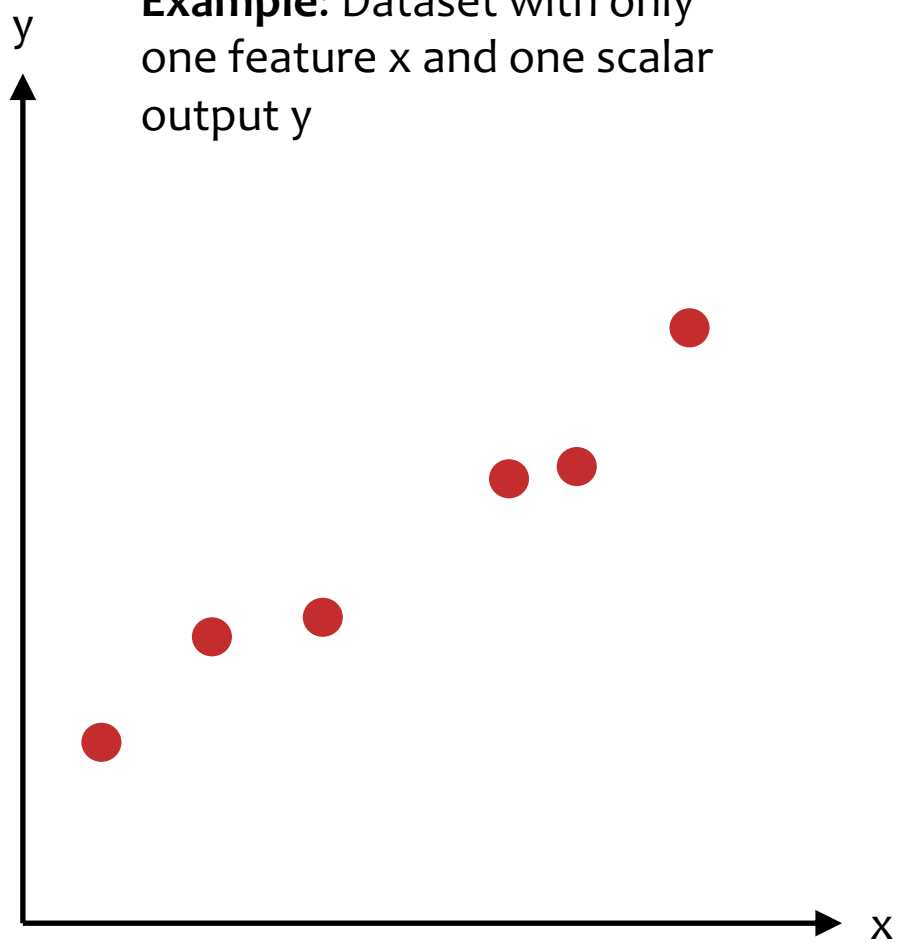



**Q: What is the function that best fits these points?**

# K-NEAREST NEIGHBOR REGRESSION

# k-NN Regression

**Example:** Dataset with only one feature x and one scalar output y




**Algorithm 1: k=1 Nearest Neighbor Regression**

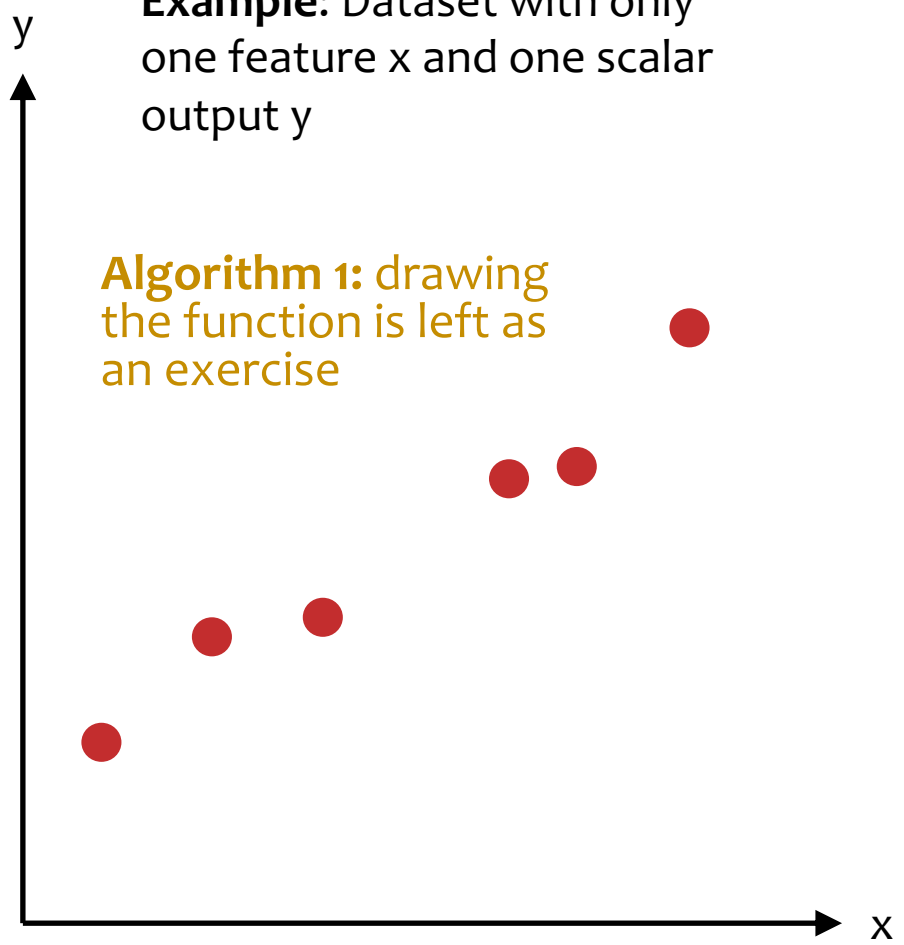
- *Train*: store all (x, y) pairs
- *Predict*: pick the nearest x in training data and return its y

**Algorithm 2: k=2 Nearest Neighbors Distance Weighted Regression**

- *Train*: store all (x, y) pairs
- *Predict*: pick the nearest two instances $x^{(n1)}$ and $x^{(n2)}$ in training data and return the weighted average of their y values

# k-NN Regression

**Example:** Dataset with only one feature x and one scalar output y




**Algorithm 1:** drawing the function is left as an exercise

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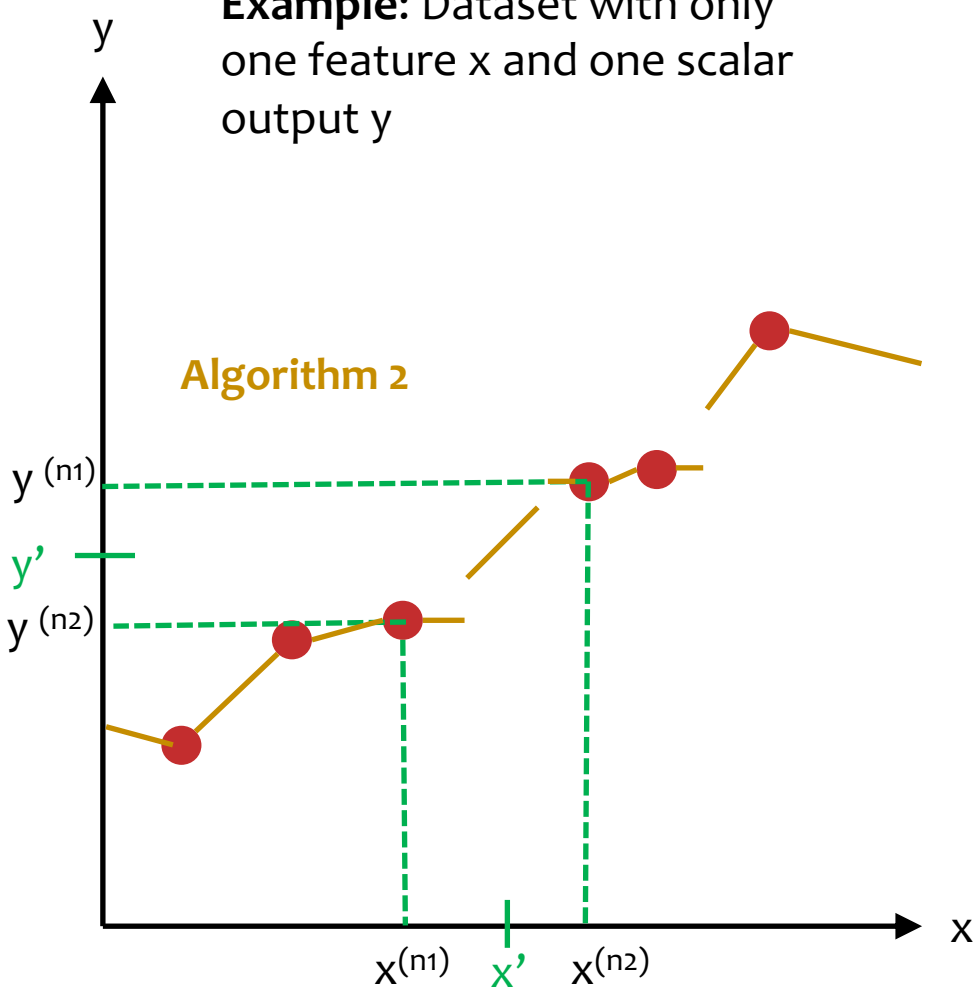


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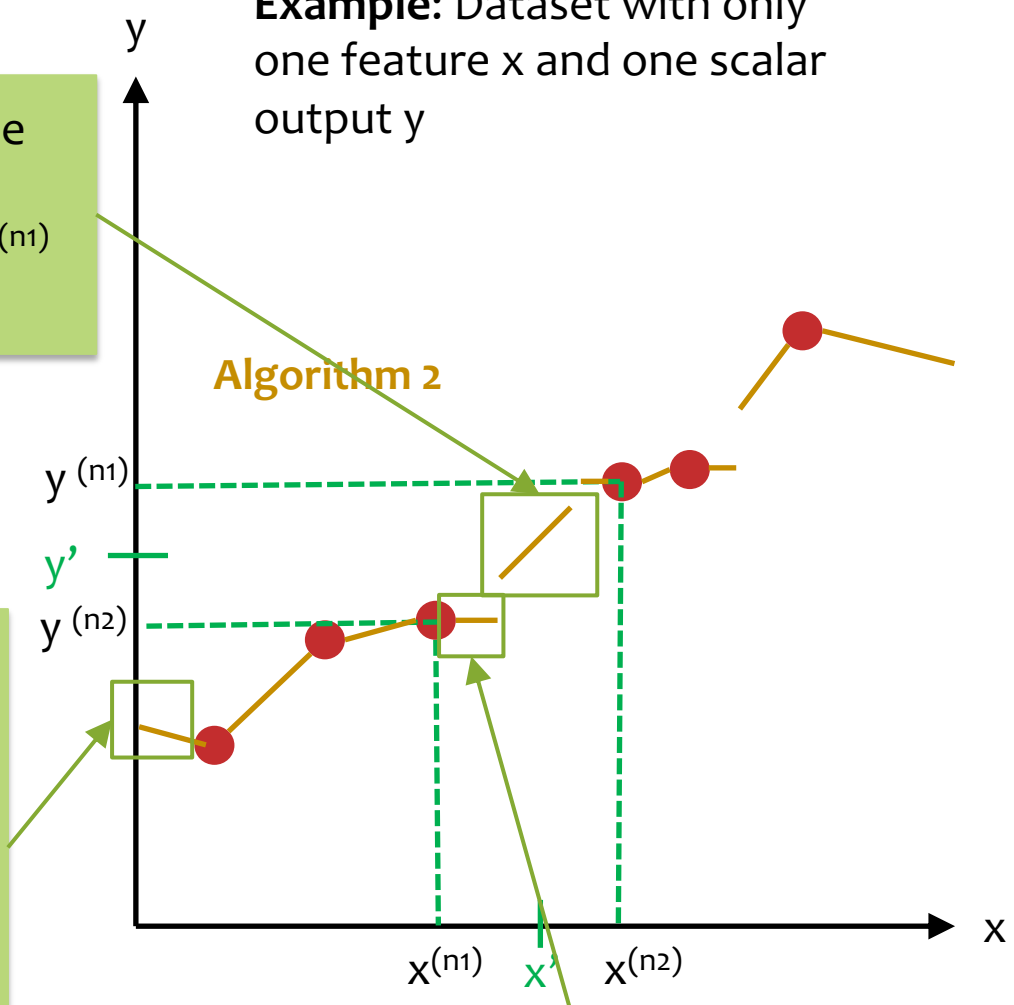


The distance weighted average of $x^{(n1)}$ and $x^{(n2)}$

This tends toward the average height of the leftmost two points

This region is closer to the two points to the left

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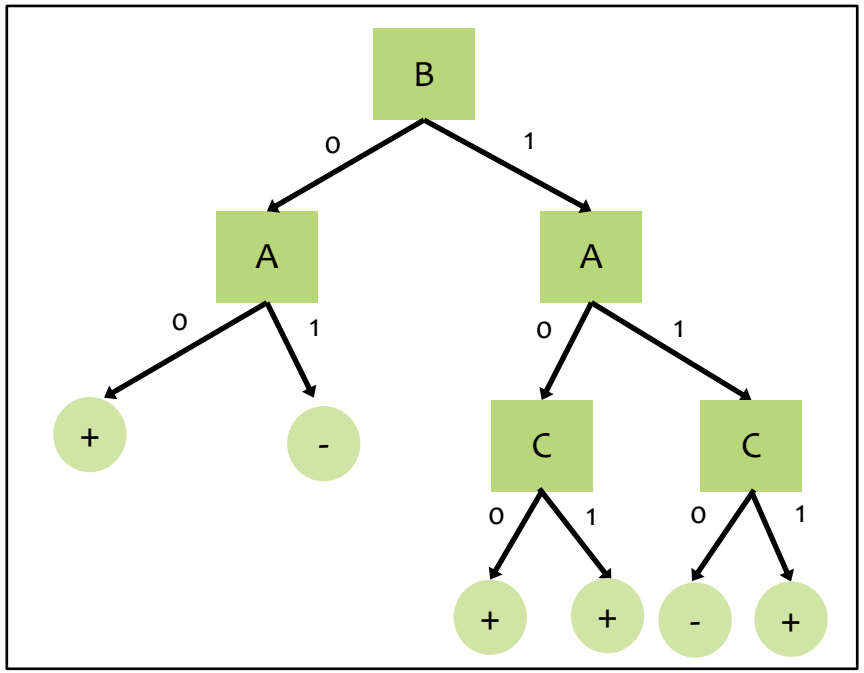
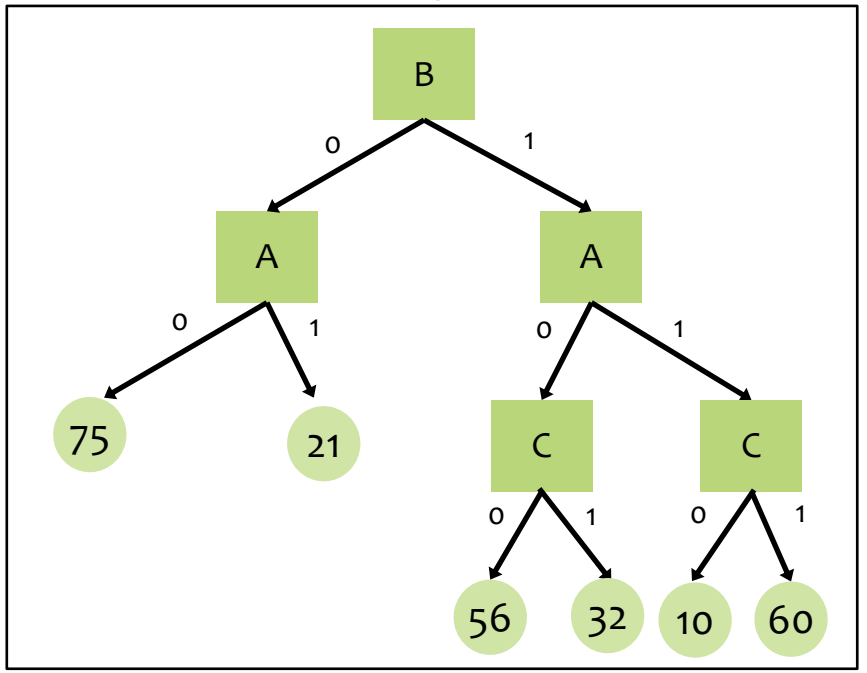
# DECISION TREE REGRESSION

# Decision Tree Regression

Decision Tree for Classification




Decision Tree for Regression

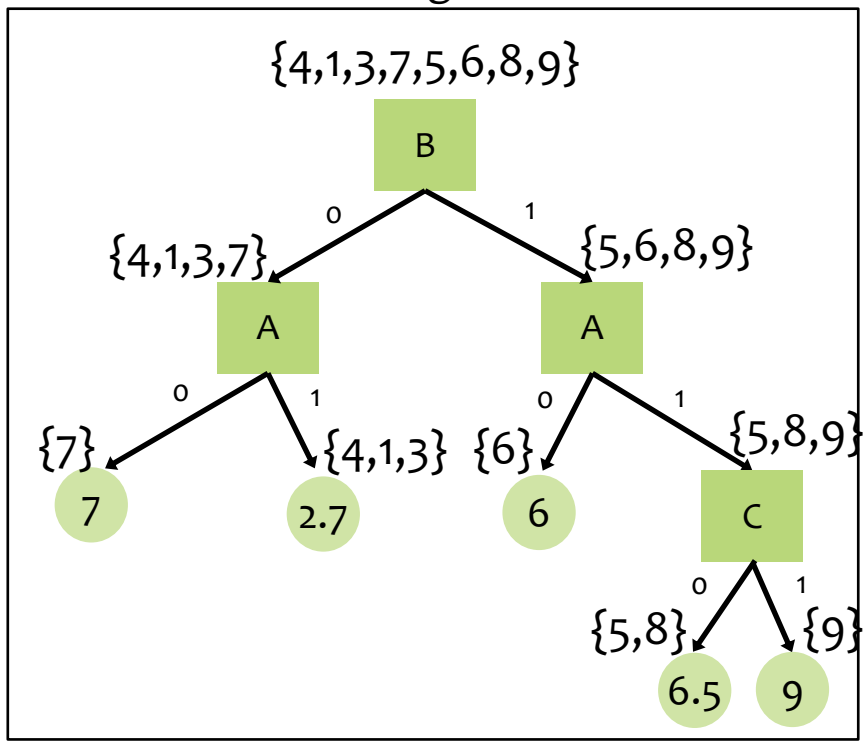


# Decision Tree Regression

Dataset for Regression

| Y | A | B | C |
|---|---|---|---|
| 4 | 1 | 0 | 0 |
| 1 | 1 | 0 | 1 |
| 3 | 1 | 0 | 0 |
| 7 | 0 | 0 | 1 |
| 5 | 1 | 1 | 0 |
| 6 | 0 | 1 | 1 |
| 8 | 1 | 1 | 0 |
| 9 | 1 | 1 | 1 |

Decision Tree for Regression




During learning, choose the attribute that minimizes an appropriate splitting criterion (e.g. mean squared error, mean absolute error)

# LINEAR FUNCTIONS, RESIDUALS, AND MEAN SQUARED ERROR

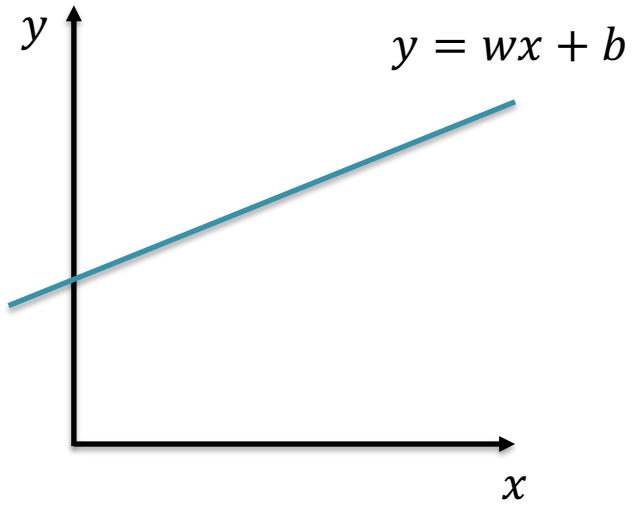
# Linear Functions

*Def:* Regression is predicting real-valued outputs

$$\mathcal{D} = \left\{\left(\mathbf{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{n} \text{ with } \mathbf{x}^{(i)} \in \mathbb{R}^M, y^{(i)} \in \mathbb{R}$$

***Common Misunderstanding*:**

Linear functions ≠ Linear decision boundaries



# Linear Functions

*Def:* Regression is predicting real-valued outputs

$$\mathcal{D} = \left\{\left(\mathbf{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{n} \text{ with } \mathbf{x}^{(i)} \in \mathbb{R}^M, y^{(i)} \in \mathbb{R}$$

***Common Misunderstanding*:**

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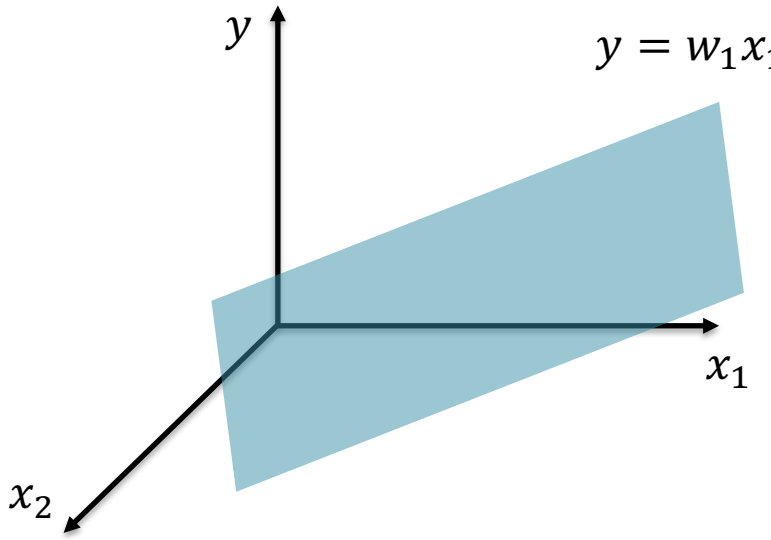



$$y = w_1 x_1 + w_2 x_2 + b$$

- A general linear function is
  $$y = \mathbf{w}^T \mathbf{x} + b$$
- A general linear decision boundary is
  $$y = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$$

# Key Idea of Linear Regression

**Residuals**

**Key Idea of Linear Regression**

**Mean squared error**

The Big Picture

# OPTIMIZATION FOR ML

# Unconstrained Optimization

- *Def*: In **unconstrained optimization,** we try minimize (or maximize) a function with *no constraints* on the inputs to the function

Given a function $J(\boldsymbol{\theta}), J : \mathbb{R}^M \rightarrow \mathbb{R}$

Our goal is to find $\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta} \in \mathbb{R}^M}{\operatorname{argmin}} J(\boldsymbol{\theta})$

For ML, these are the parameters

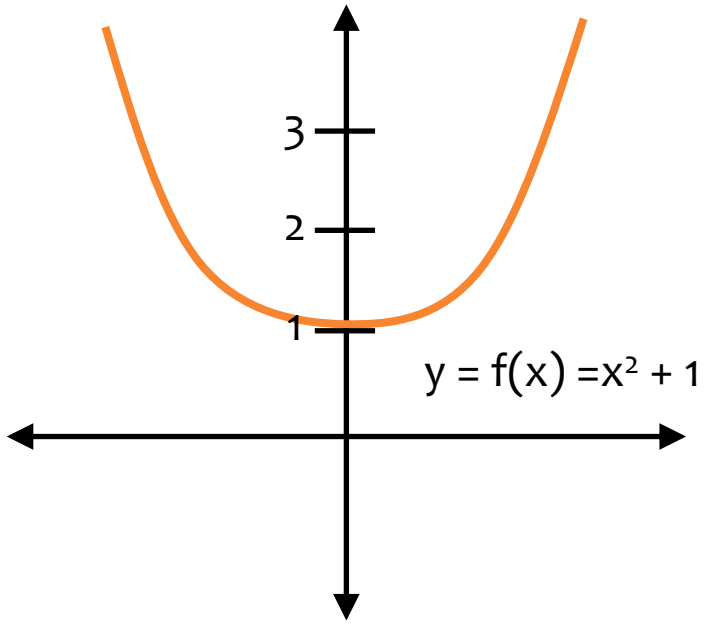
For ML, this is the objective function

# Optimization for ML

Not quite the same setting as other fields…

- Function we are optimizing might not be the true goal
  (e.g. likelihood vs generalization error)
- Precision might not matter
  (e.g. data is noisy, so optimal up to 1e-16 might not help)
- Stopping early can help generalization error
  (i.e. "early stopping" is a technique for regularization – discussed more next time)

# min vs. argmin




$v^* = \min_x f(x)$

$x^* = \text{argmin}_x f(x)$

1. Question: What is v*?

2. Question: What is x*?

# OPTIMIZATION METHOD #0: RANDOM GUESSING

# Notation Trick: Folding in the Intercept Term

$$\mathbf{x}' = [1, x_1, x_2, \ldots, x_M]^T$$

$$\boldsymbol{\theta} = [b, w_1, \ldots, w_M]^T$$

*Notation Trick*: fold the bias *b* and the weights ***w*** into a single vector **θ** by prepending a constant to **x** and increasing dimensionality by one!

$$h_{\mathbf{w},b}(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

$$h_{\boldsymbol{\theta}}(\mathbf{x}') = \boldsymbol{\theta}^T\mathbf{x}'$$

This convenience trick allows us to more compactly talk about linear functions as a simple dot product (without explicitly writing out the intercept term every time).



55

# Linear Regression as Function Approximation

$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N}$
where $\mathbf{x} \in \mathbb{R}^M$ and $y \in \mathbb{R}$

1. Assume $\mathcal{D}$ generated as:

$$\mathbf{x}^{(i)} \sim p^*(\cdot)$$
$$y^{(i)} = h^*(\mathbf{x}^{(i)})$$

2. Choose hypothesis space, $\mathcal{H}$:
*all linear functions in $M$-dimensional space*

$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}, \boldsymbol{\theta} \in \mathbb{R}^M\}$$

3. Choose an objective function:
*mean squared error (MSE)*

$$J(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N} e_i^2$$
$$= \frac{1}{N}\sum_{i=1}^{N} \left(y^{(i)} - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})\right)^2$$
$$= \frac{1}{N}\sum_{i=1}^{N} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)})\right)^2$$

4. Solve the unconstrained optimization problem via favorite method:

- *gradient descent*
- *closed form*
- *stochastic gradient descent*
- ...

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, J(\boldsymbol{\theta})$$

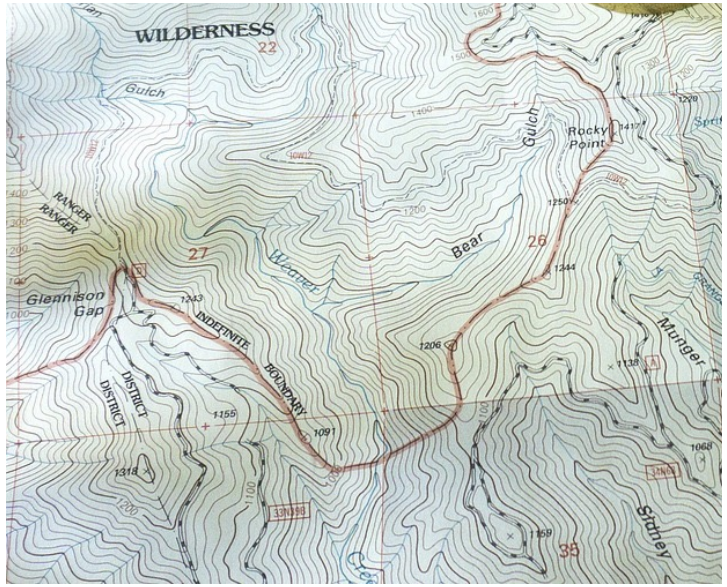
5. Test time: given a new $\mathbf{x}$, make prediction $\hat{y}$

$$\hat{y} = h_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) = \hat{\boldsymbol{\theta}}^T \mathbf{x}$$

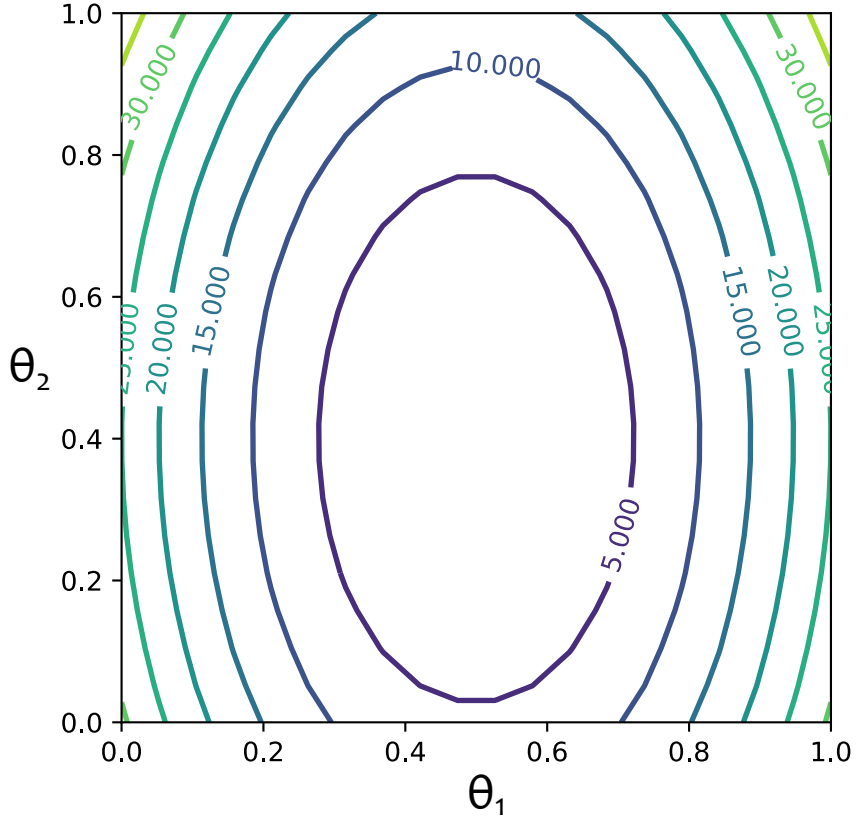
# Contour Plots

**Contour Plots**

1. Each level curve labeled with value
2. Value label indicates the value of the function for all points lying on that level curve
3. Just like a topographical map, but for a function




$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = (10(\theta_1 - 0.5))^2 + (6(\theta_1 - 0.4))^2$

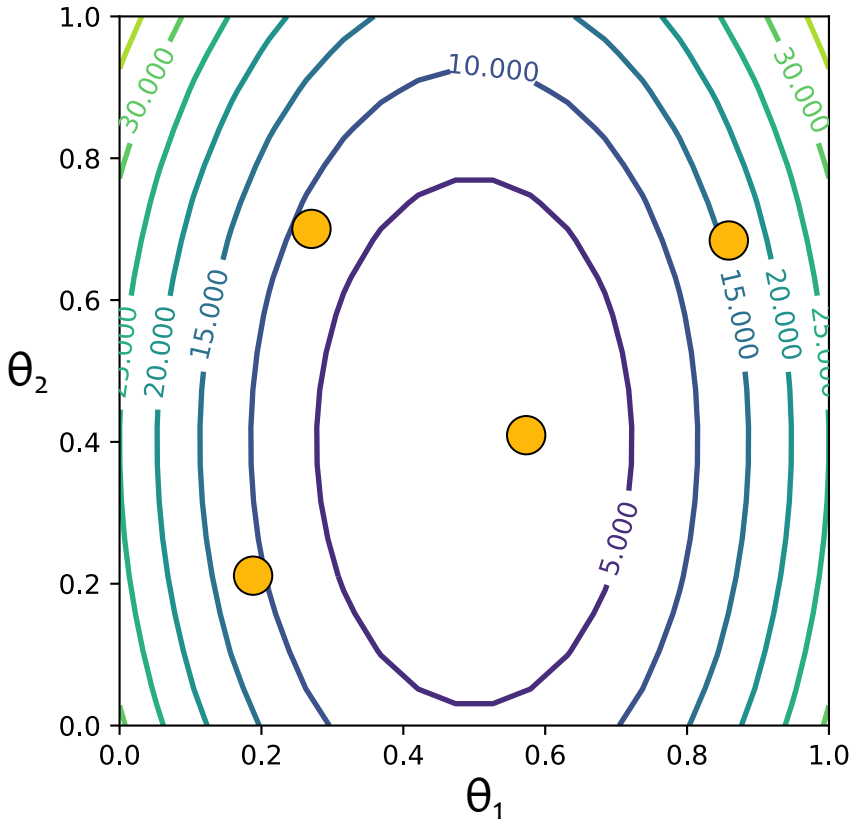


# Optimization by Random Guessing

**Optimization Method #0: Random Guessing**

1. Pick a random $\boldsymbol{\theta}$
2. Evaluate $J(\boldsymbol{\theta})$
3. Repeat steps 1 and 2 many times
4. Return $\boldsymbol{\theta}$ that gives smallest $J(\boldsymbol{\theta})$

$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = (10(\theta_1 - 0.5))^2 + (6(\theta_1 - 0.4))^2$$




| t | $\theta_1$ | $\theta_2$ | $J(\theta_1, \theta_2)$ |
|---|---|---|---|
| 1 | 0.2 | 0.2 | 10.4 |
| 2 | 0.3 | 0.7 | 7.2 |
| 3 | 0.6 | 0.4 | 1.0 |
| 4 | 0.9 | 0.7 | 16.2 |

# Optimization by Random Guessing

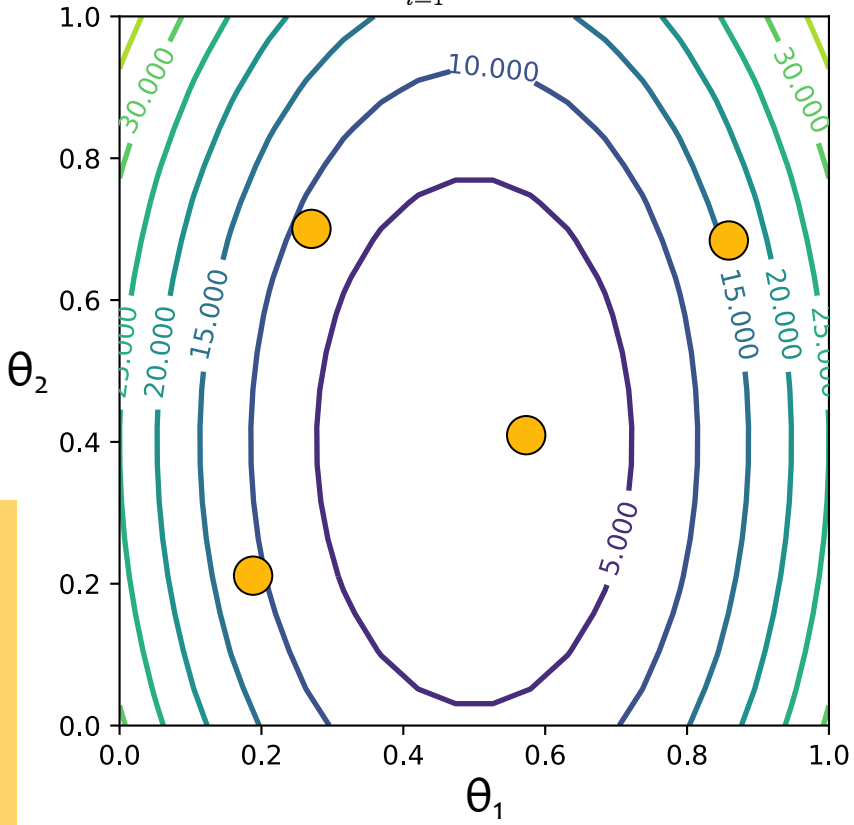
**Optimization Method #0: Random Guessing**

1. Pick a random **θ**
2. Evaluate J(**θ**)
3. Repeat steps 1 and 2 many times
4. Return **θ** that gives smallest J(**θ**)

**For Linear Regression:**

- **objective function** is Mean Squared Error (MSE)
- MSE = J(w, b)
  = $J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2$
- contour plot: each line labeled with MSE – **lower means a better fit**
- **minimum** corresponds to parameters (w,b) = ($\theta_1$, $\theta_2$) that **best fit** some training dataset

$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2$

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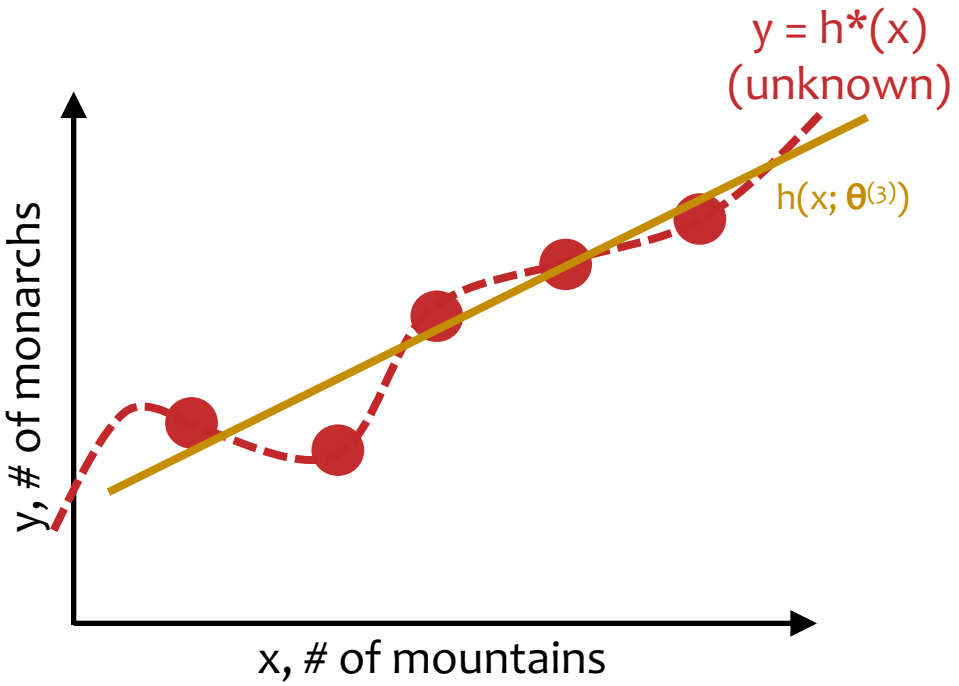
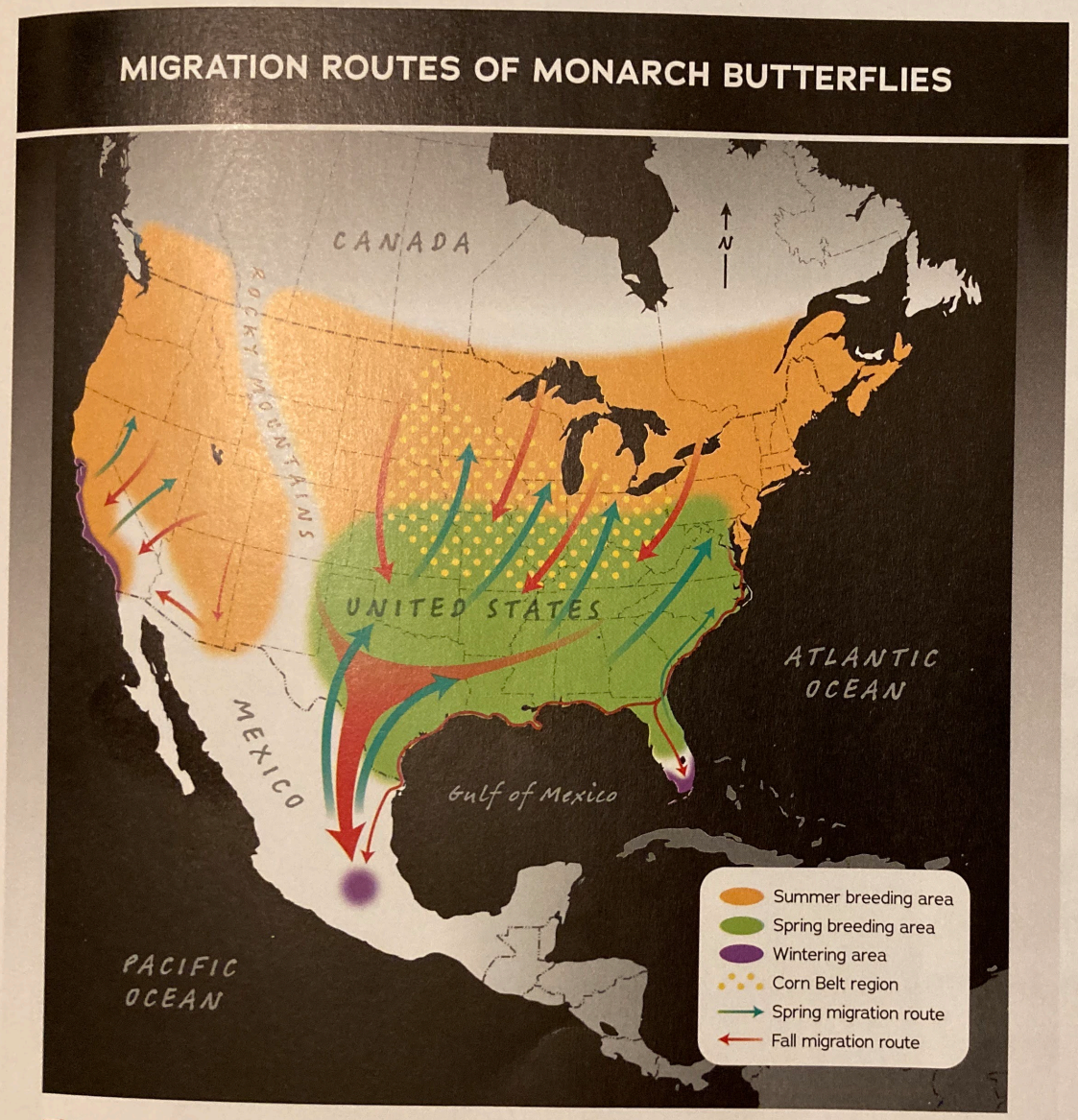
# Linear Regression: Running Example

# Counting Butterflies



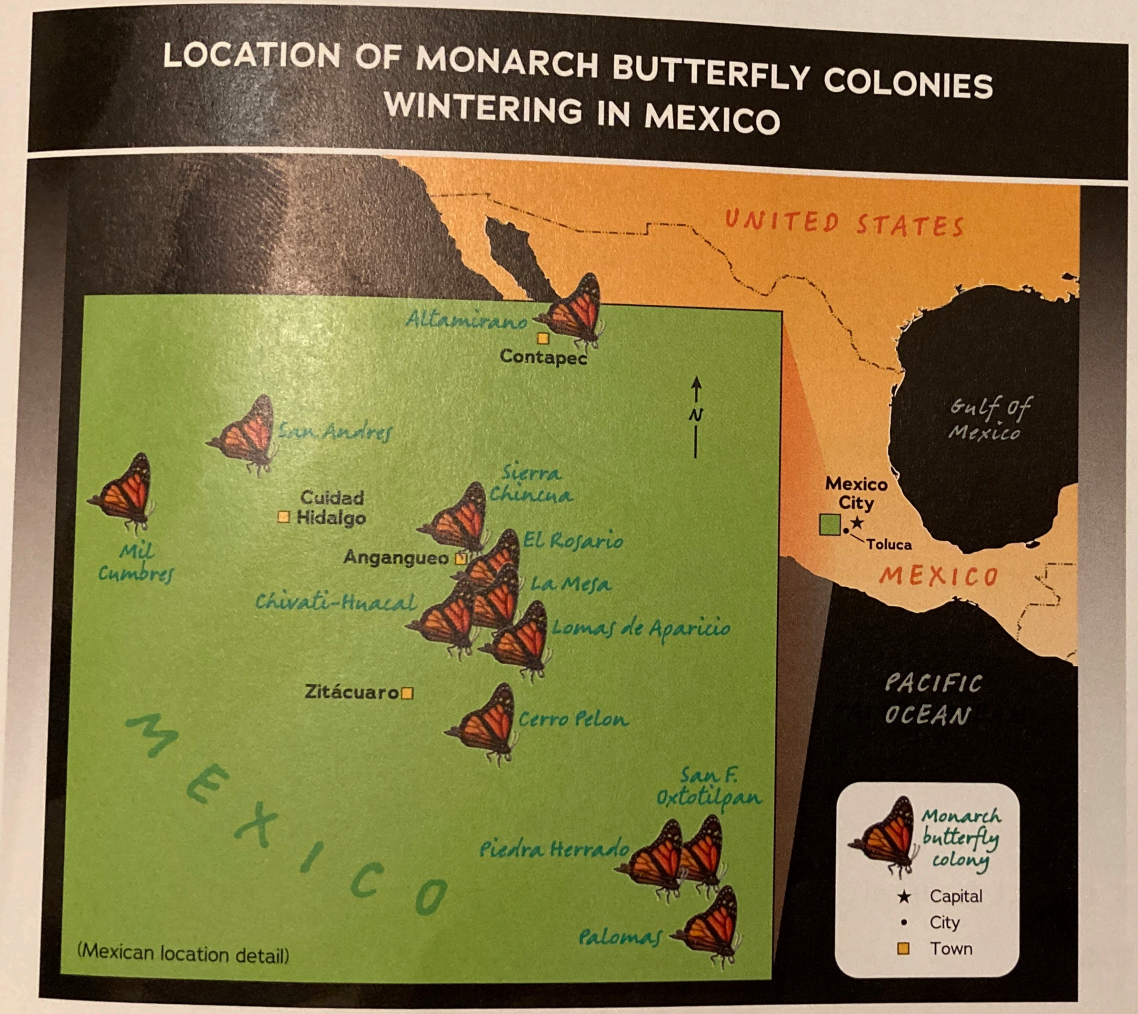
breed only in places where milkweed grows. When the last ice age ended, and the cold and glaciers retreated, milkweed may have gradually spread northward, and monarchs may have followed. But the monarch butterfly remained a tropical creature, unable to survive the severe northern winters. So every year as winter approached, monarchs left their summer fields of milkweed and flew south again. To this day, every spring and summer, monarchs travel north to their breeding grounds across the eastern United States and Canada. Every winter, they return to Mexico.



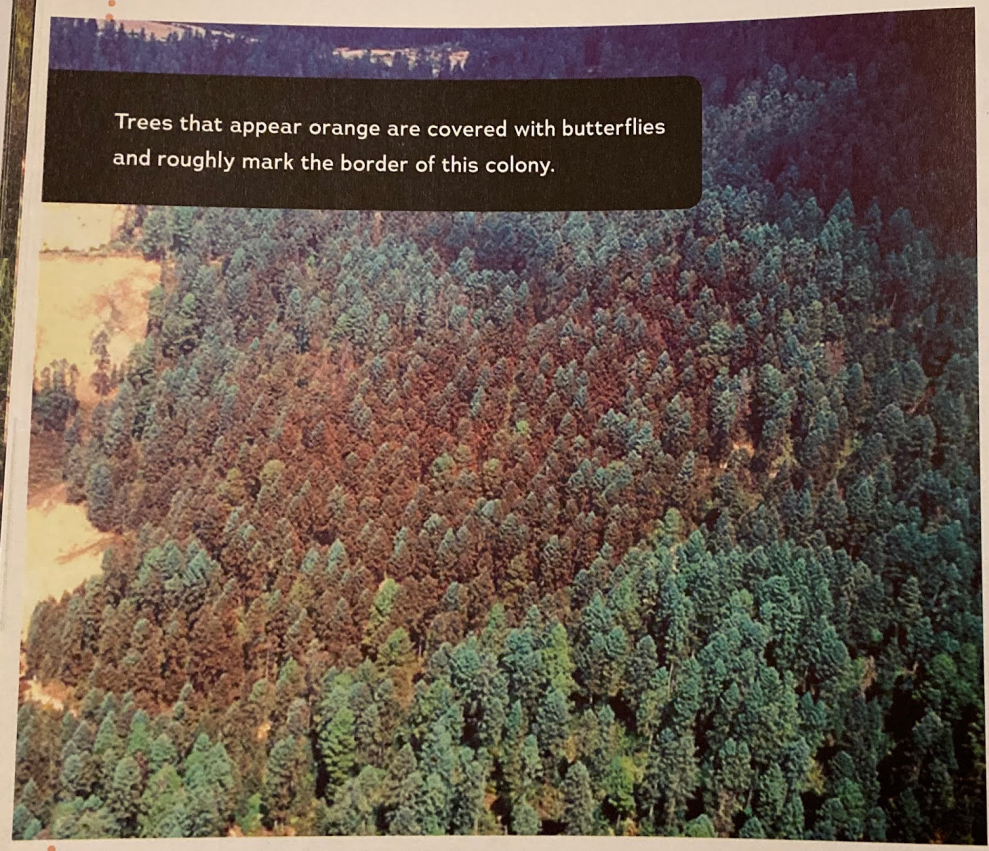

This map shows migration routes of fall and spring migrations, both east and west of the Rocky Mountains.

Researchers began taking measurements in 1993. The highest year on record came in 1997, when the colonies covered about 45 acres (18 ha), an area equal to about thirty-four football fields. Scientists aren't sure exactly how many butterflies that represented, but one estimate is that there were one billion monarchs in the colonies that winter.

But as researchers measured the colonies year after year, they noticed that the colonies were shrinking. By 2014 the colonies measured just 1.7 acres (0.7 ha), or less than one and a half football fields. That year there may have been only about thirty-five million monarchs in the colonies.




The eastern monarchs migrate to just twelve mountaintops, all located in central Mexico.



Trees that appear orange are covered with butterflies and roughly mark the border of this colony.

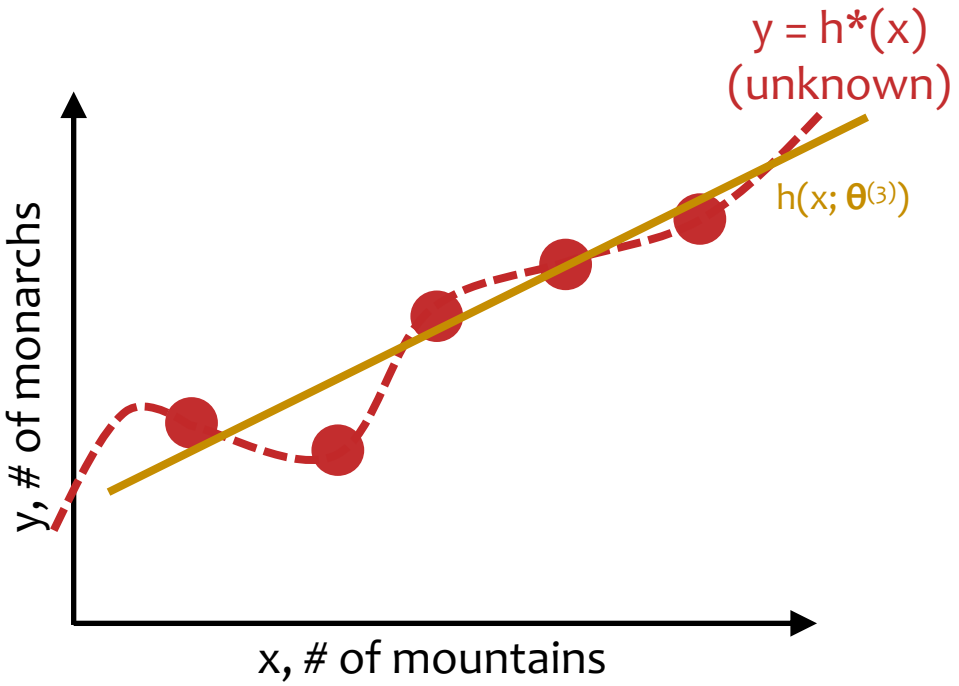
Many scientists were worried. The population of eastern monarchs had dropped more than 90 percent in just seventeen years.

At the same time, scientists in California reported that the number of western monarchs was dropping as well. From 1997 to 2014, the number of monarchs overwintering along the California coast had fallen by 74 percent.

Populations of overwintering monarchs were falling fast. By 2014 their numbers had fallen so far that people wondered whether the monarch butterfly should be listed as an endangered species—a species in danger of becoming extinct, or disappearing forever.

Losing monarchs could be bad for our world because monarchs play an important part in the food web. Despite the milkweed toxins in their bodies, they are food for songbirds, spiders, and insects. Monarchs visit many flowers and act as pollinators.

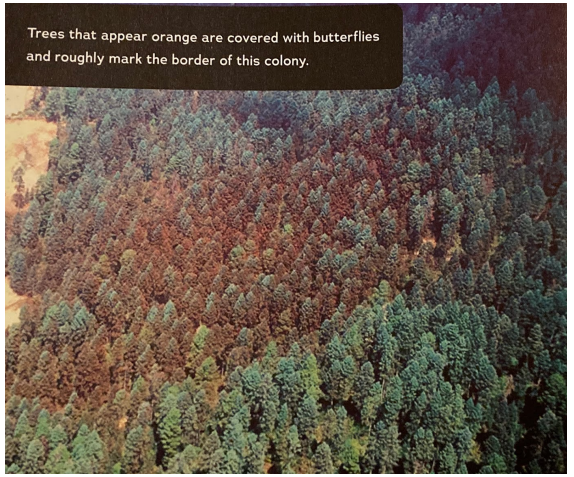
# Counting Butterflies



# Linear Regression in High Dimensions

- In our discussions of linear regression, we will always assume there is just one output, y
- But our inputs will usually have many features:

  $\mathbf{x} = [x_1, x_2, \ldots, x_M]^T$
- For example:
  - suppose we had a drone take pictures of each section of forest
  - each feature could correspond to a pixel in this image such that $x_m = 1$ if the pixel is orange and $x_m = 0$ otherwise
  - the output y would be the number of butterflies in each picture




**Q:** How would you obtain ground truth data?

# Linear Regression by Rand. Guessing

**Optimization Method #0: Random Guessing**

1. Pick a random $\boldsymbol{\theta}$
2. Evaluate $J(\boldsymbol{\theta})$
3. Repeat steps 1 and 2 many times
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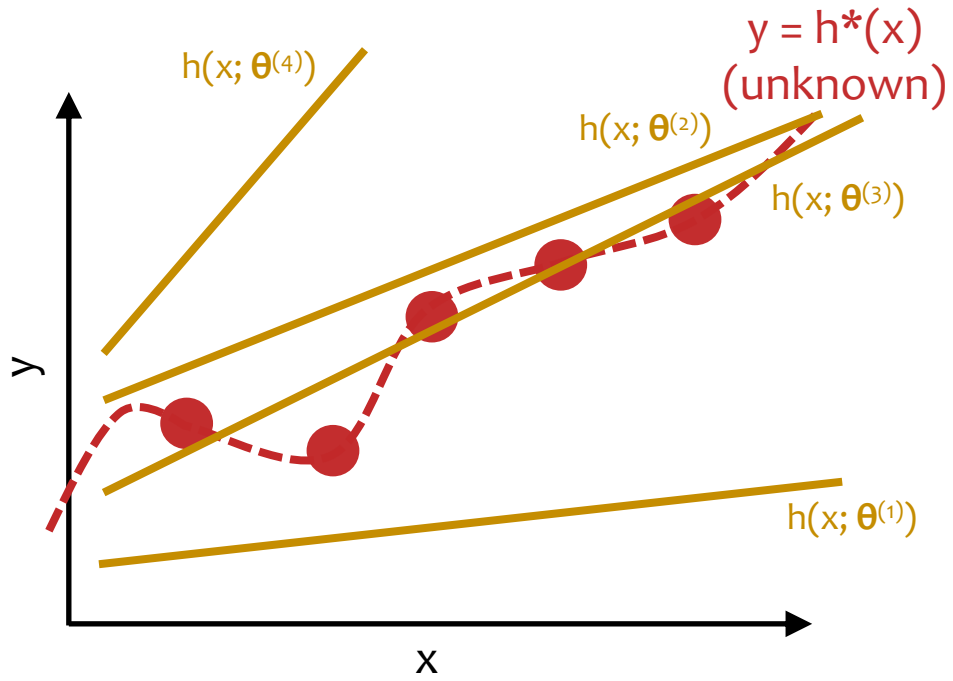


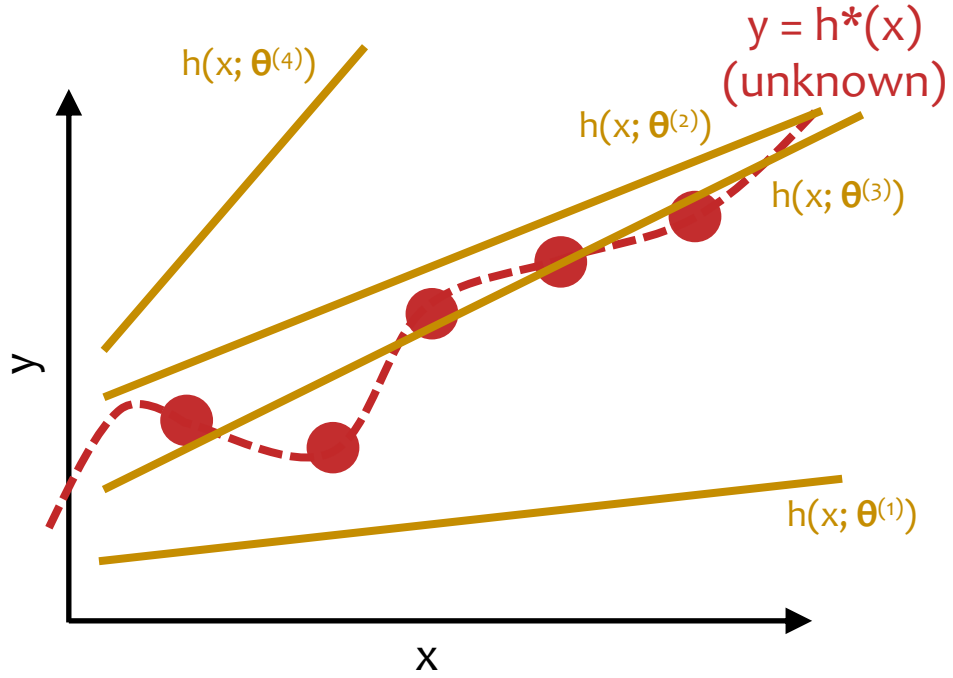

**For Linear Regression:**

- target function h*(x) is **unknown**
- only have access to h*(x) through **training examples** $(x^{(i)},y^{(i)})$
- want $h(x; \boldsymbol{\theta}^{(t)})$ that **best approximates** h*(x)
- **enable generalization** w/inductive bias that restricts hypothesis class to **linear functions**

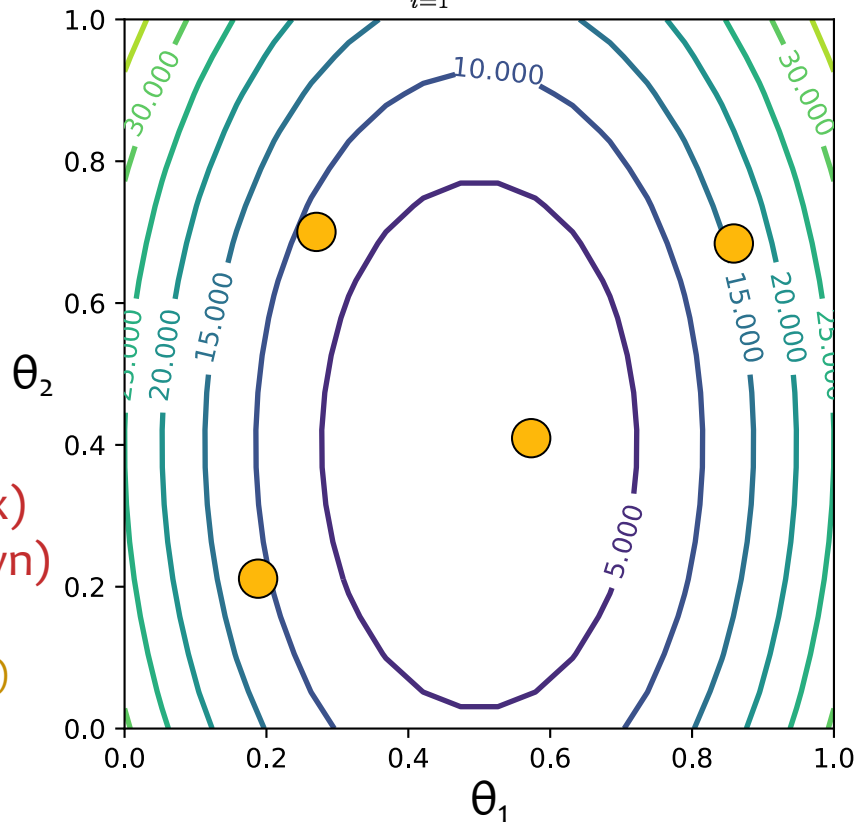
# Linear Regression by Rand. Guessing

**Optimization Method #0: Random Guessing**

1. Pick a random **θ**
2. Evaluate J(**θ**)
3. Repeat steps 1 and 2 many times
4. Return **θ** that gives smallest J(**θ**)




$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2$$

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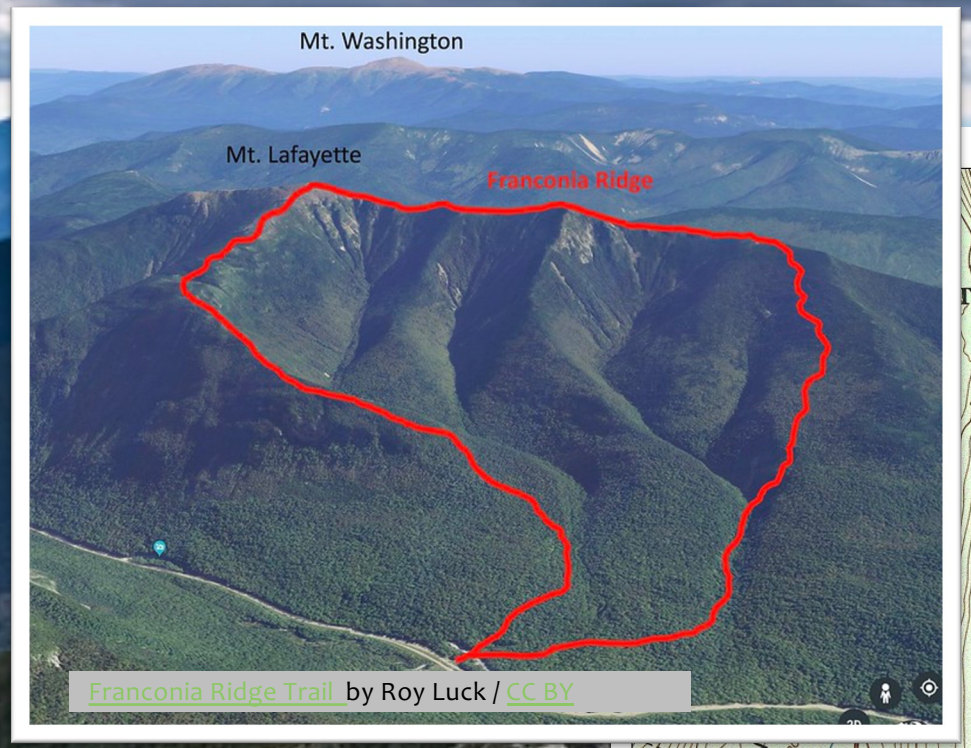
# OPTIMIZATION METHOD #1: GRADIENT DESCENT

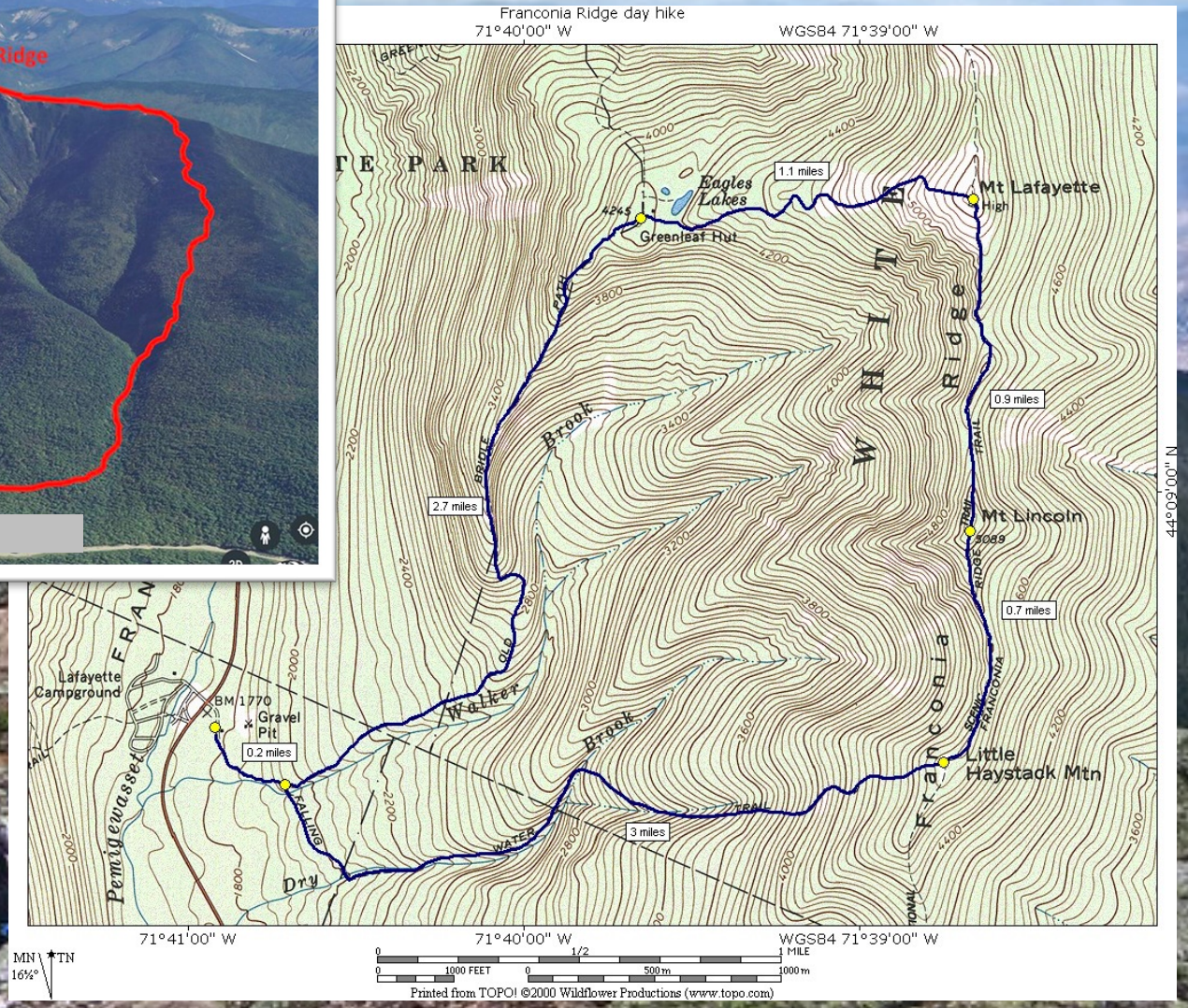
# Derivatives

# Gradient

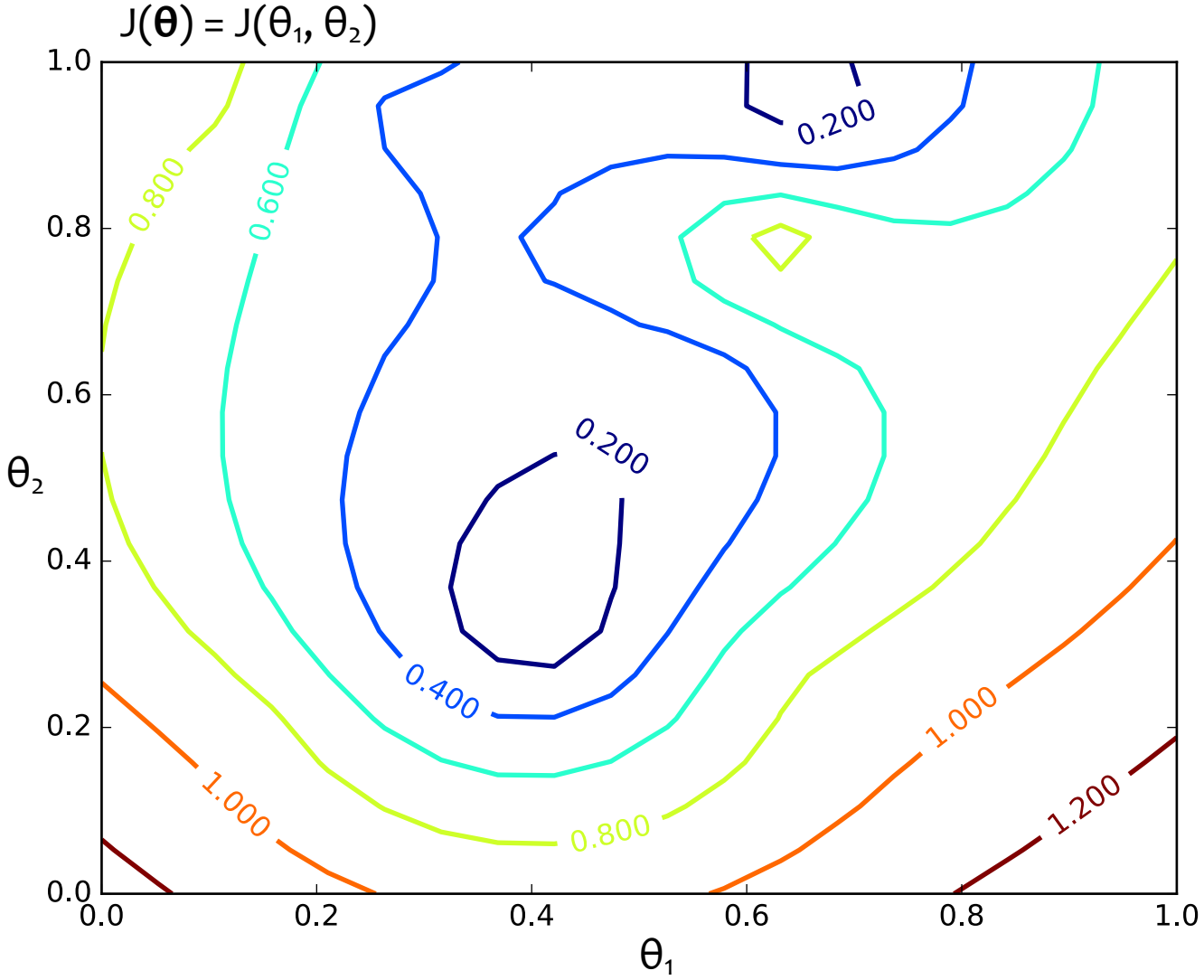
# Topographical Maps

# Topographical Maps

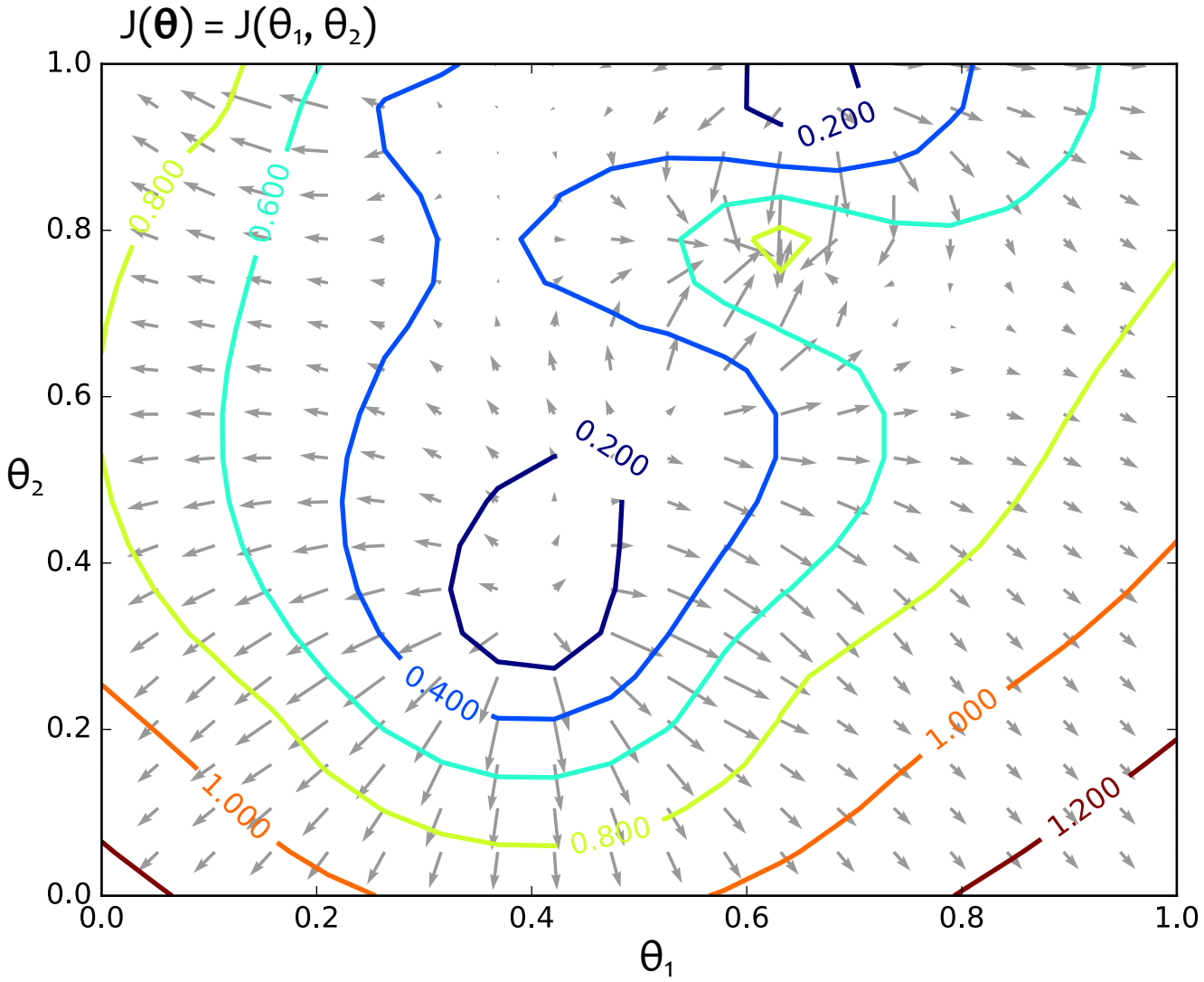


# Gradients

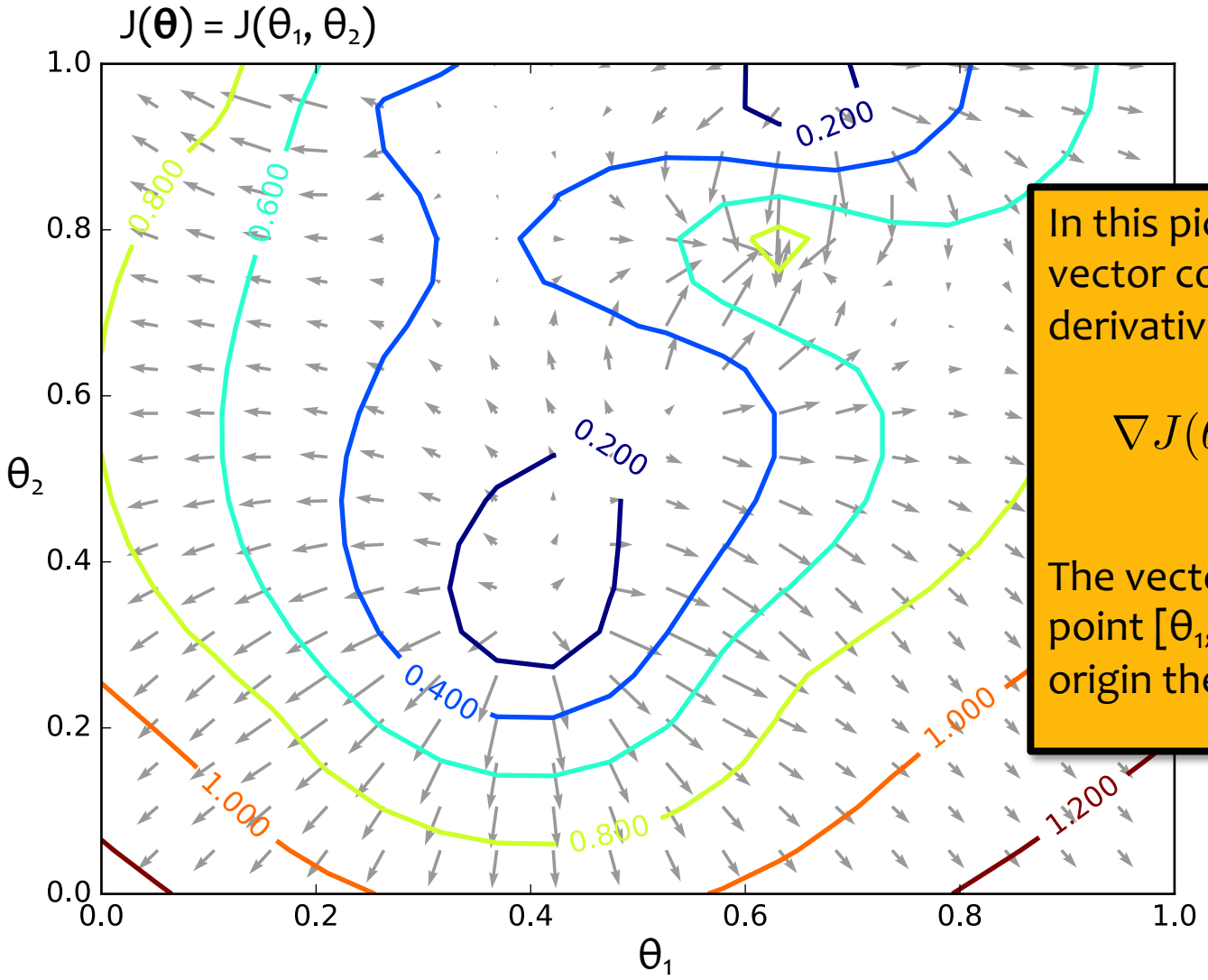

J(θ) = J(θ1, θ2)
1.0
0.8
0.6
0.4
0.2
0.0
θ2
0.0
0.2
0.4
0.6
0.8
1.0
θ1
0.200
0.800
0.600
0.200
0.400
1.000
0.800
1.000
1.200

# Gradients




These are the **gradients** that Gradient **Ascent** would follow.

# Gradients



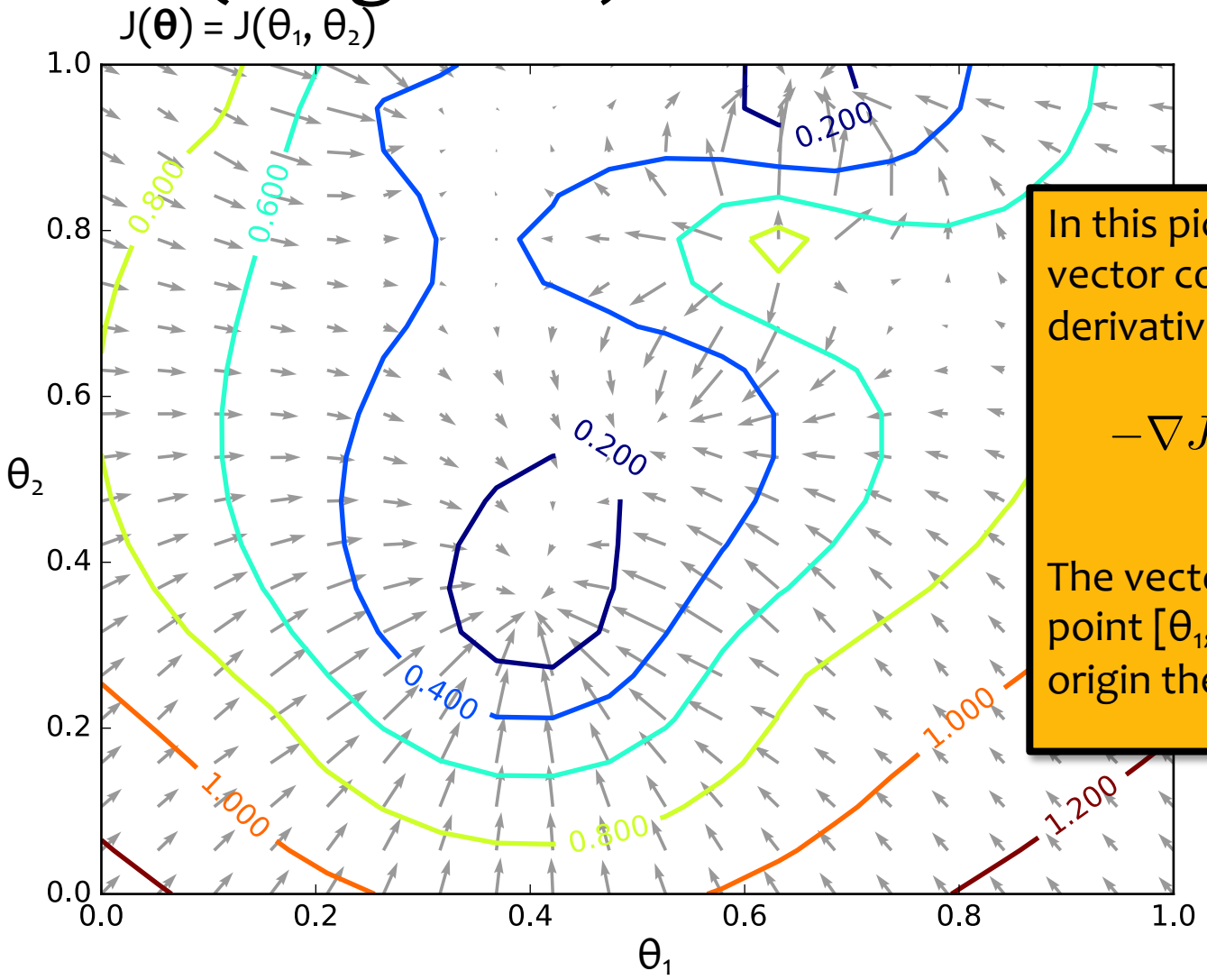

In this picture, each arrow is a 2D vector consisting of two partial derivatives.

$$\nabla J(\theta_1, \theta_2) = \begin{bmatrix} \frac{\partial J}{\partial \theta_1} \\ \\ \frac{\partial J}{\partial \theta_2} \end{bmatrix}$$

The vector is evaluated at the point $[\theta_1, \theta_2]^T$ and plotted with its origin there as well.

These are the **gradients** that Gradient **Ascent** would follow.

# (Negative) Gradients



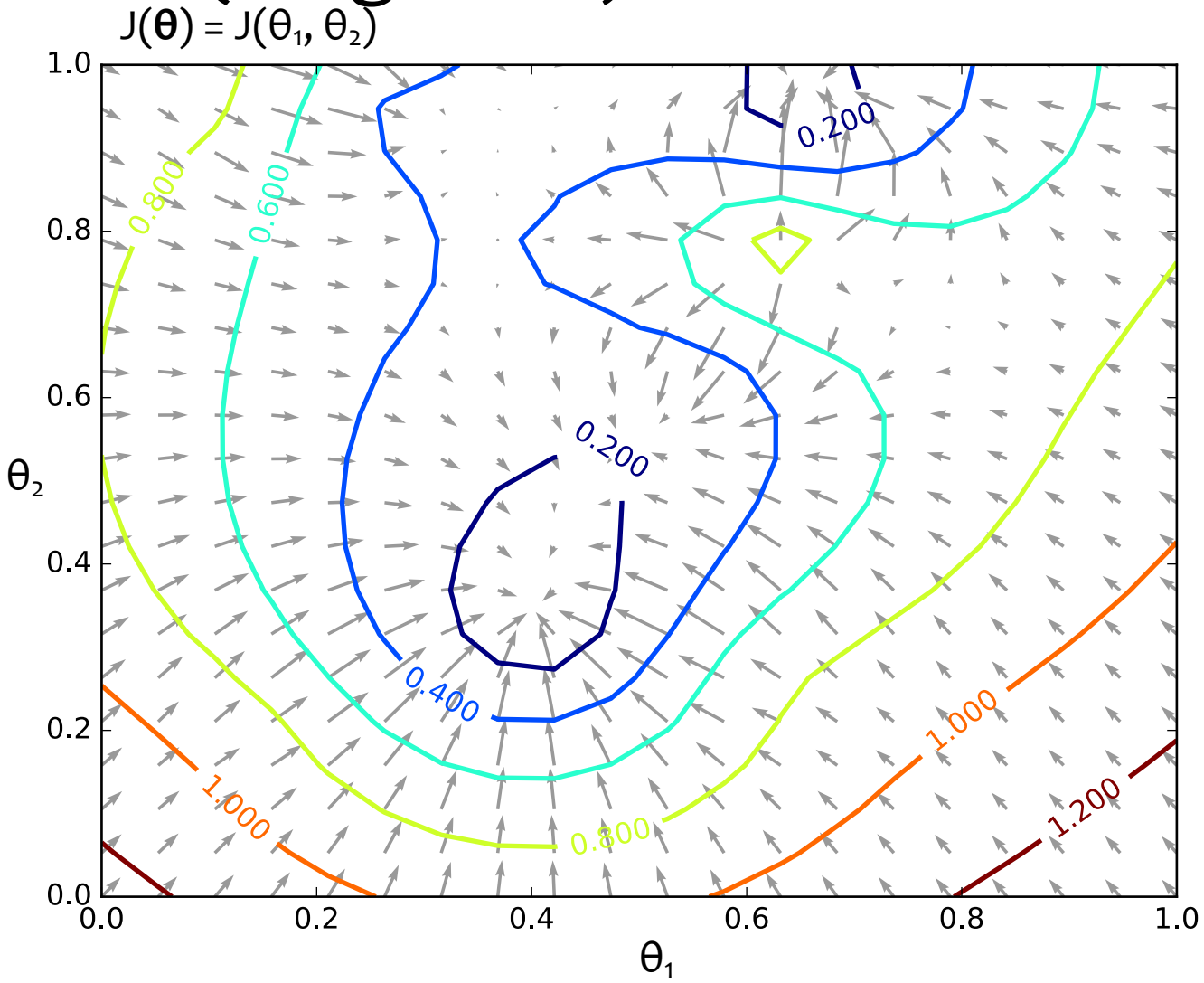

In this picture, each arrow is a 2D vector consisting of two partial derivatives.

$$-\nabla J(\theta_1, \theta_2) = \begin{bmatrix} -\frac{\partial J}{\partial \theta_1} \\ -\frac{\partial J}{\partial \theta_2} \end{bmatrix}$$

The vector is evaluated at the point $[\theta_1, \theta_2]^T$ and plotted with its origin there as well.

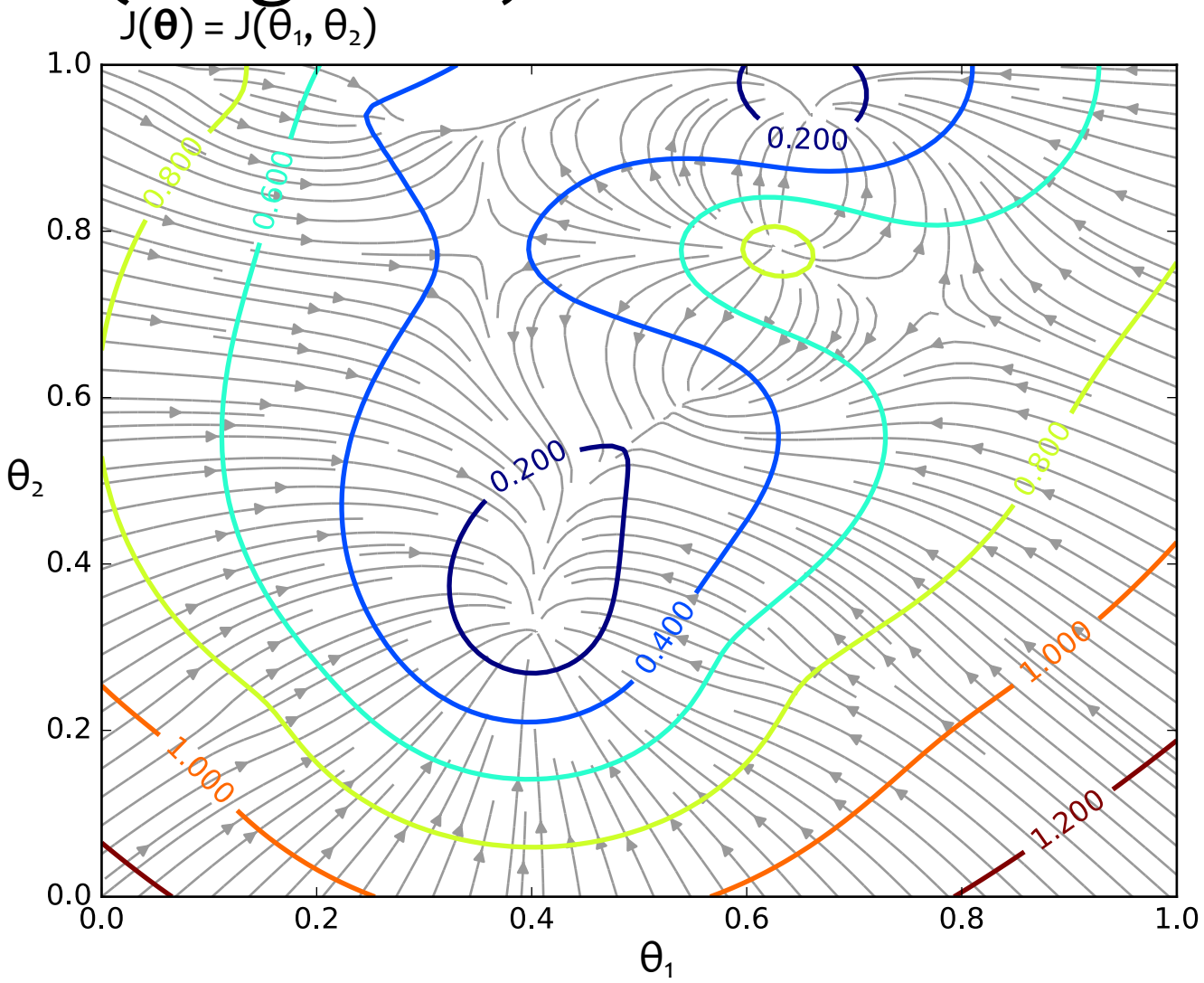
These are the **negative** gradients that Gradient **Descent** would follow.

# (Negative) Gradients




These are the **negative** gradients that Gradient **Descent** would follow.

# (Negative) Gradient *Paths*




Shown are the **paths** that Gradient Descent would follow if it were making **infinitesimally small steps.**

# Gradient Descent

**Gradient Descent Algorithm**

**Remarks**

# Gradient Descent: Step Size

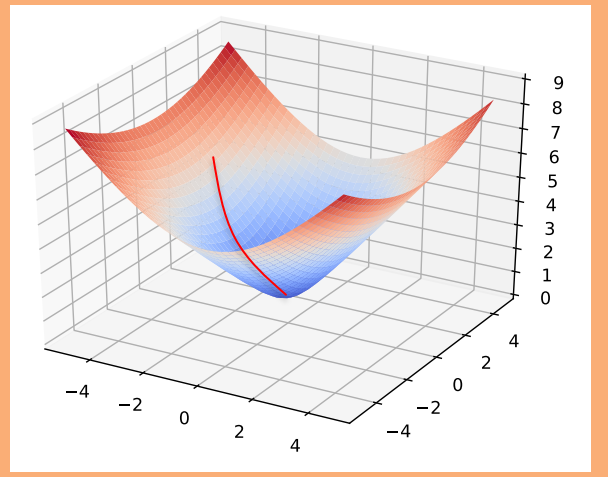
**Question:**
In gradient descent, what could go wrong if we *always* use the same step size (or step size schedule) for every problem we encounter?

**Answer:**

# Gradient Descent

**Algorithm 1** Gradient Descent

1: **procedure** GD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
2: $\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
3: $\quad$**while** not converged **do**
4: $\quad\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
5: $\quad$**return** $\boldsymbol{\theta}$




In order to apply GD to Linear Regression all we need is the **gradient** of the objective function (i.e. vector of partial derivatives).

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_M} J(\boldsymbol{\theta}) \end{bmatrix}$$

# Gradient Descent

**Algorithm 1** Gradient Descent

1: **procedure** GD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
2: $\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
3: $\quad$**while** not converged **do**
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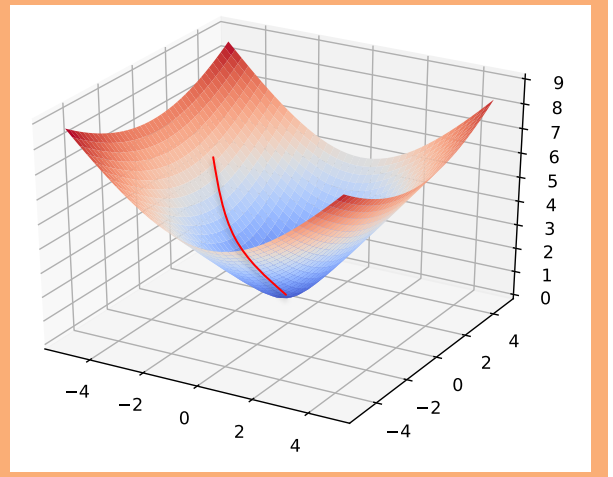



There are many possible ways to detect **convergence**. For example, we could check whether the L2 norm of the gradient is below some small tolerance.

$$||\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})||_2 \leq \epsilon$$

Alternatively we could check that the reduction in the objective function from one iteration to the next is small.

# GRADIENT DESCENT FOR LINEAR REGRESSION

# Linear Regression as Function Approximation

$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N}$
where $\mathbf{x} \in \mathbb{R}^M$ and $y \in \mathbb{R}$

1. Assume $\mathcal{D}$ generated as:

$$\mathbf{x}^{(i)} \sim p^*(\cdot)$$
$$y^{(i)} = h^*(\mathbf{x}^{(i)})$$

2. Choose hypothesis space, $\mathcal{H}$:
*all linear functions in $M$-dimensional space*

$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}, \boldsymbol{\theta} \in \mathbb{R}^M\}$$

3. Choose an objective function:
*mean squared error (MSE)*

$$J(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N} e_i^2$$
$$= \frac{1}{N}\sum_{i=1}^{N} \left(y^{(i)} - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})\right)^2$$
$$= \frac{1}{N}\sum_{i=1}^{N} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)})\right)^2$$

4. Solve the unconstrained optimization problem via favorite method:

- *gradient descent*
- *closed form*
- *stochastic gradient descent*
- ...

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, J(\boldsymbol{\theta})$$

5. Test time: given a new $\mathbf{x}$, make prediction $\hat{y}$

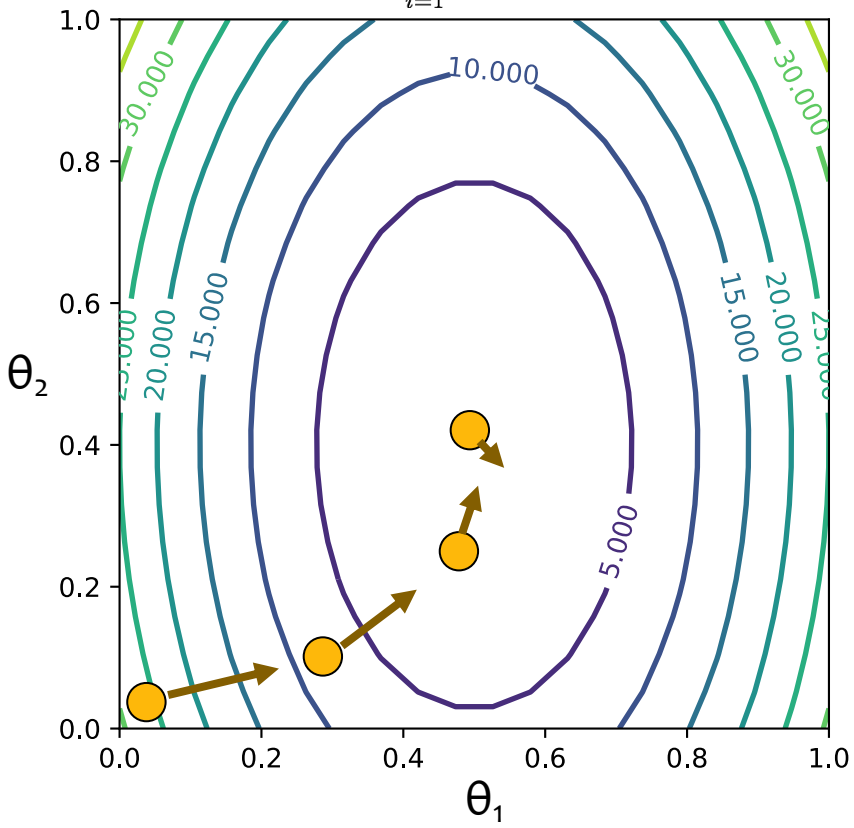
$$\hat{y} = h_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) = \hat{\boldsymbol{\theta}}^T \mathbf{x}$$

# Linear Regression by Gradient Desc.

**Optimization Method #1: Gradient Descent**

1. Pick a random **θ**
2. Repeat:
   a. Evaluate gradient ∇J(**θ**)
   b. Step opposite gradient
3. Return **θ** that gives smallest J(**θ**)

$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2$$




| t | $\theta_1$ | $\theta_2$ | $J(\theta_1, \theta_2)$ |
|---|---|---|---|
| 1 | 0.01 | 0.02 | 25.2 |
| 2 | 0.30 | 0.12 | 8.7 |
| 3 | 0.51 | 0.30 | 1.5 |
| 4 | 0.59 | 0.43 | 0.2 |

# Linear Regression by Gradient Desc.

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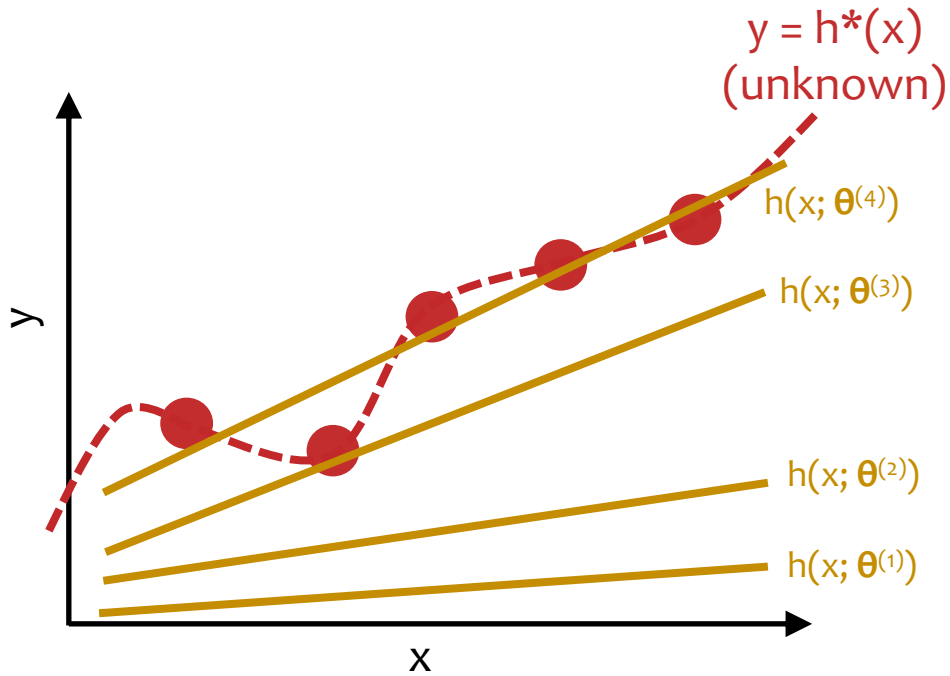


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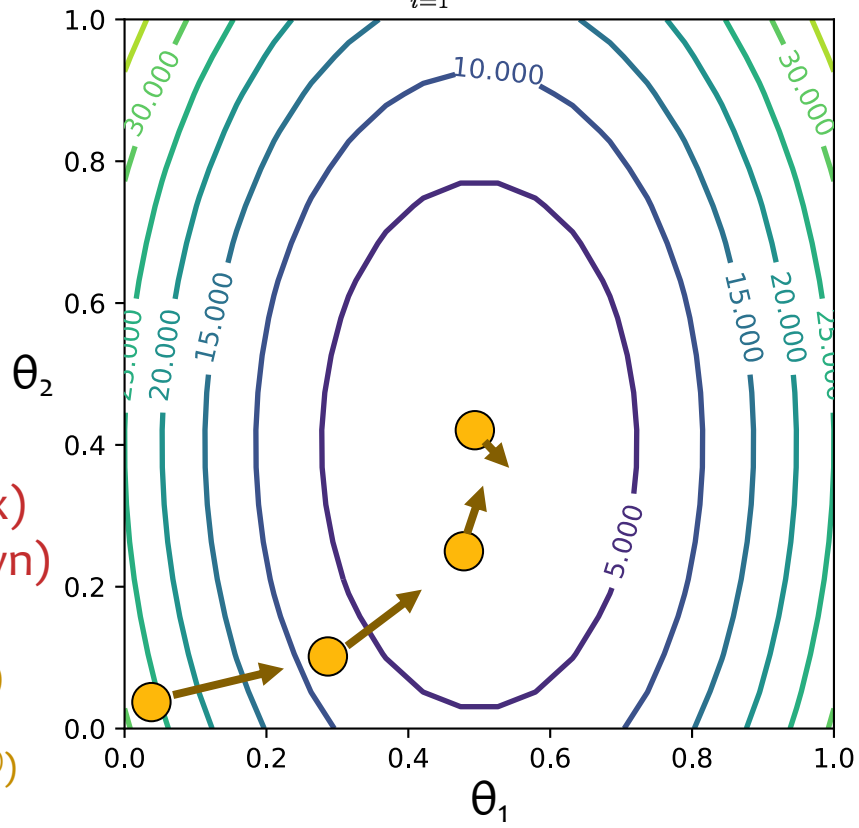


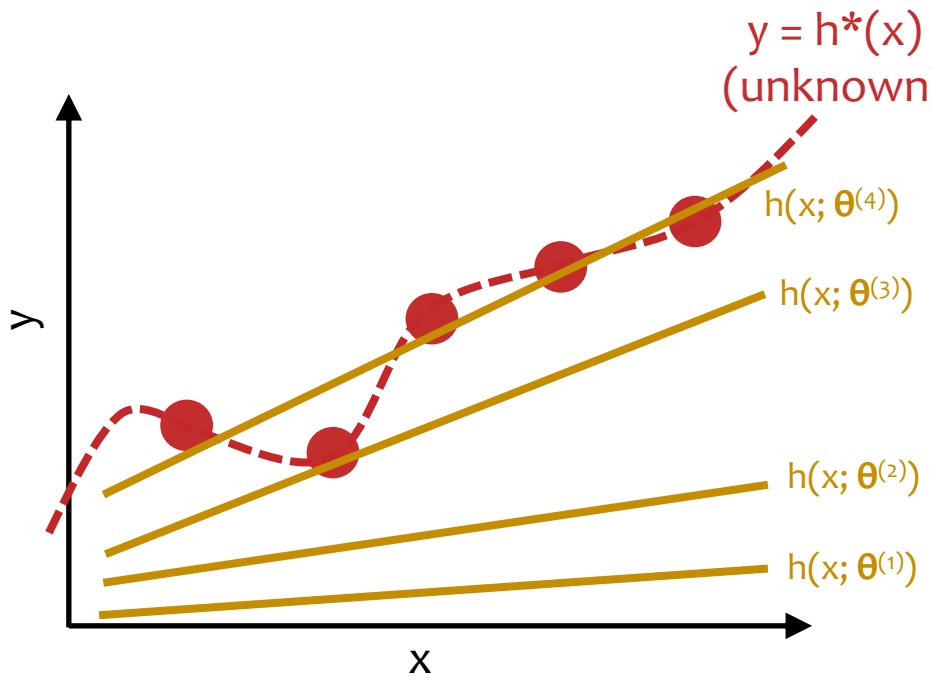


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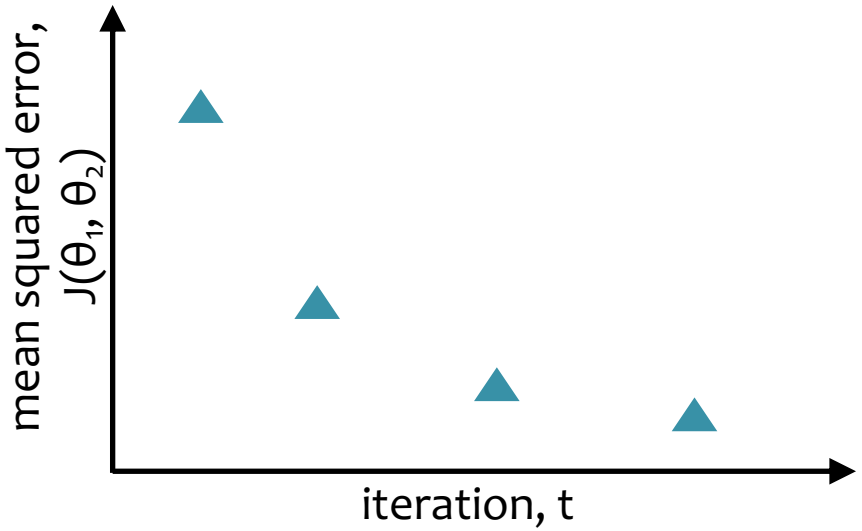


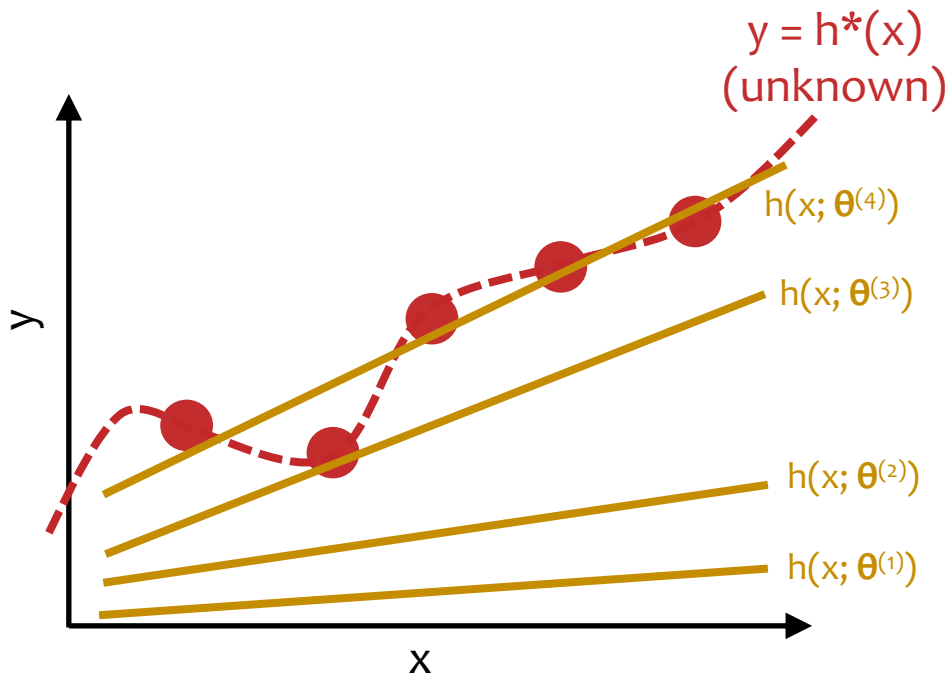


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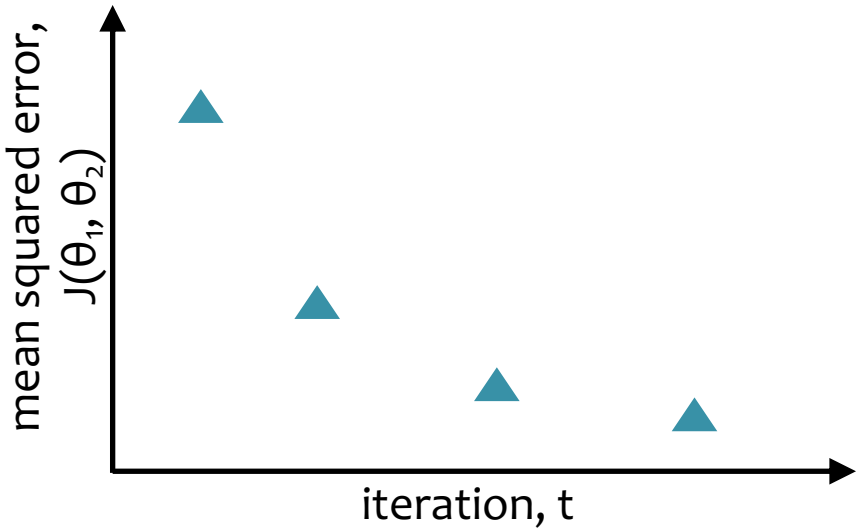


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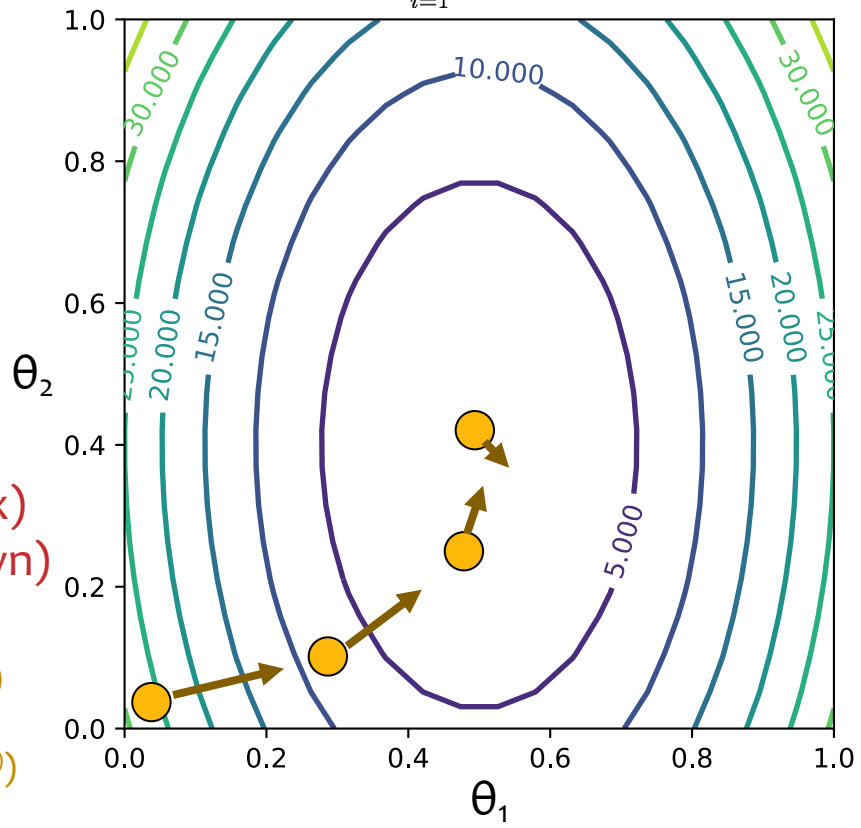


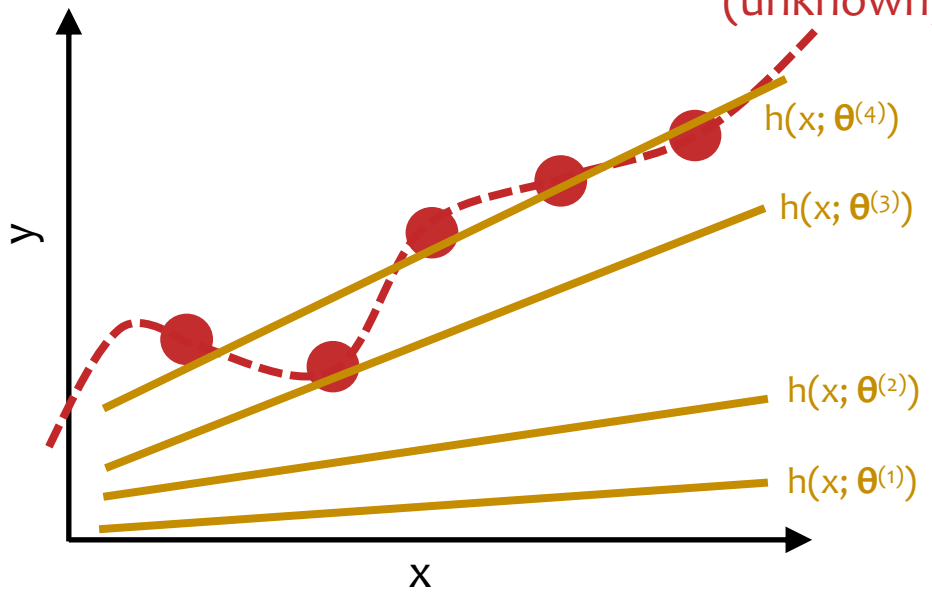


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# Gradient Calculation for Linear Regression

# Gradient Calculation for Linear Regression

Derivative of $J^{(i)}(\boldsymbol{\theta})$:

$$\begin{aligned}
\frac{d}{d\theta_k} J^{(i)}(\boldsymbol{\theta}) &= \frac{d}{d\theta_k} \frac{1}{2} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2 \\
&= \frac{1}{2} \frac{d}{d\theta_k} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2 \\
&= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \frac{d}{d\theta_k} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \\
&= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \frac{d}{d\theta_k} \left( \sum_{j=1}^{K} \theta_j x_j^{(i)} - y^{(i)} \right) \\
&= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_k^{(i)}
\end{aligned}$$

Derivative of $J(\boldsymbol{\theta})$:

$$\begin{aligned}
\frac{d}{d\theta_k} J(\boldsymbol{\theta}) &= \sum_{i=1}^{N} \frac{d}{d\theta_k} J^{(i)}(\boldsymbol{\theta}) \\
&= \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_k^{(i)}
\end{aligned}$$

Gradient of $J(\boldsymbol{\theta})$ [used by Gradient Descent]

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) &= \begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_M} J(\boldsymbol{\theta}) \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_1^{(i)} \\ \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_2^{(i)} \\ \vdots \\ \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_M^{(i)} \end{bmatrix} \\
&= \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}
\end{aligned}$$

# GD for Linear Regression

Gradient Descent for Linear Regression repeatedly takes steps opposite the gradient of the objective function

**Algorithm 1** GD for Linear Regression

1: **procedure** GDLR($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
2: $\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$ ▷ Initialize parameters
3: $\quad$**while** not converged **do**
4: $\quad\quad\mathbf{g} \leftarrow \sum_{i=1}^{N}(\boldsymbol{\theta}^T\mathbf{x}^{(i)} - y^{(i)})\mathbf{x}^{(i)}$ ▷ Compute gradient
5: $\quad\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma\mathbf{g}$ ▷ Update parameters
6: $\quad$**return** $\boldsymbol{\theta}$