



10-301/10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Linear Regression

Matt Gormley
Lecture 7
Sep. 16, 2024

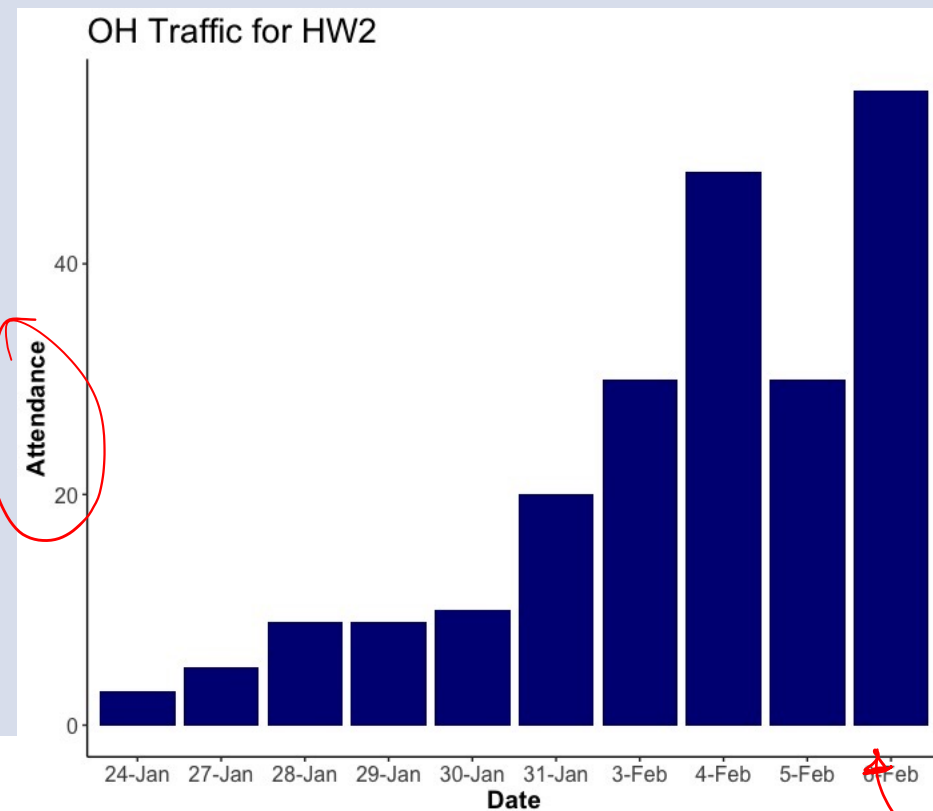
Reminders

- **Homework 2: Decision Trees**
 - Out: Wed, Sep. 4
 - Due: Mon, Sep. 16 at 11:59pm
- **Homework 3: KNN, Perceptron, Lin.Reg.**
 - Out: Mon, Sep. 16
 - Due: Mon, Sep. 23 at 11:59pm
 - (only two grace/late days permitted)
- **Exam conflicts form**

Q&A

Q: How can I get more one-on-one interaction with the course staff?

A: Attend office hours as soon after the homework release as possible!



Q&A

Q: I just asked a question in OH and now my TA is crying quietly -- what did I do wrong?

A: You've just committed the worst of crimes: asking a question that was directly answered in a recitation.

The TA you asked spent hours carefully writing careful recitation notes and solutions, practicing their recitation, responding to criticism / changes from me, etc.

To increase OH efficiency, please review the HW recitation before asking HW questions in OHs.

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 prove the Perceptron Mistake Bound?

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

PROOF OF THE MISTAKE BOUND

Analysis: Perceptron

Perceptron Mistake Bound

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

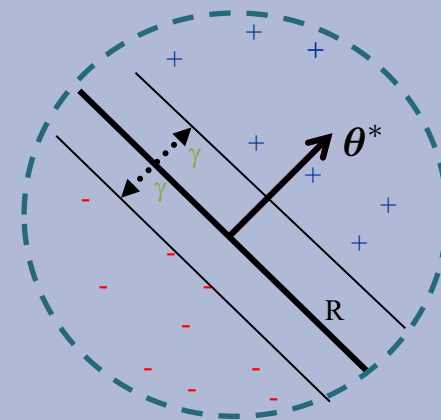
Given dataset: $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$.

Suppose:

1. Finite size inputs: $\|\mathbf{x}^{(i)}\| \leq R$
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

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



Analysis: Perceptron

Common Misunderstanding:

The radius is centered at the origin, not at the center of the points.

Perceptron Mistake Bound

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

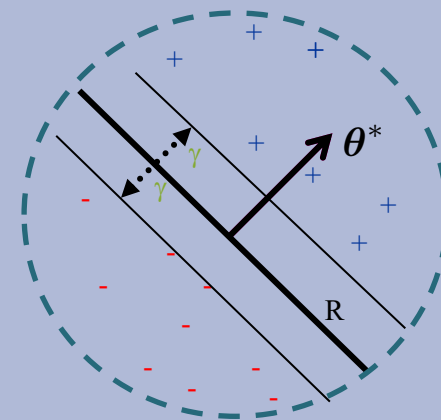
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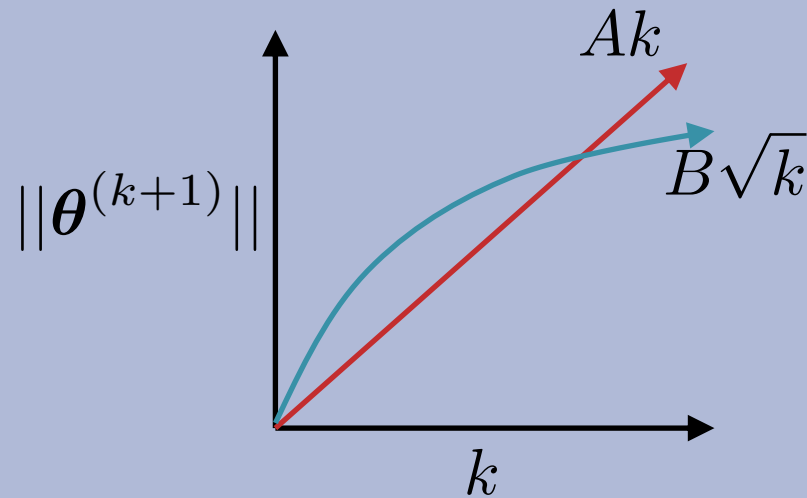


Analysis: Perceptron

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)).

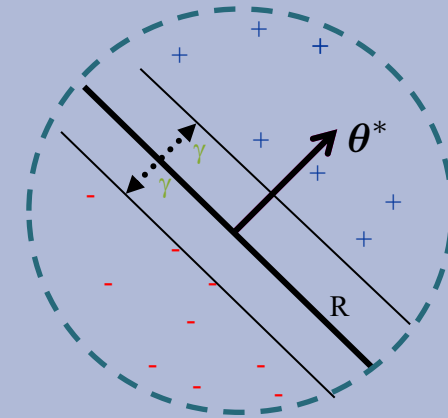
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Algorithm 1 Perceptron Learning Algorithm (Online)

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

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

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

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 $(\boldsymbol{\theta}^{(1)})^2 = 0$

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


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 $\langle (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m) \rangle$ 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

Perceptron Exercise

Question:

Unlike Decision Trees and K-Nearest Neighbors, the Perceptron algorithm **does not suffer from overfitting** because it does not have any hyperparameters that could be over-tuned on the training data.

- A. True
- B. True and False
- C. False

toxic →

Answer:

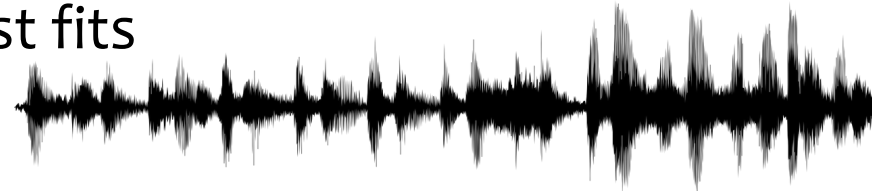
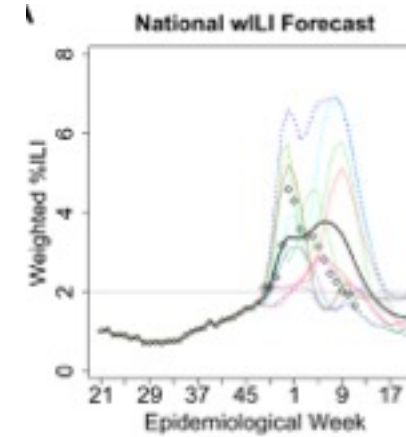
REGRESSION

Regression

Goal:

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

This is what differentiates regression from classification



Example Applications:

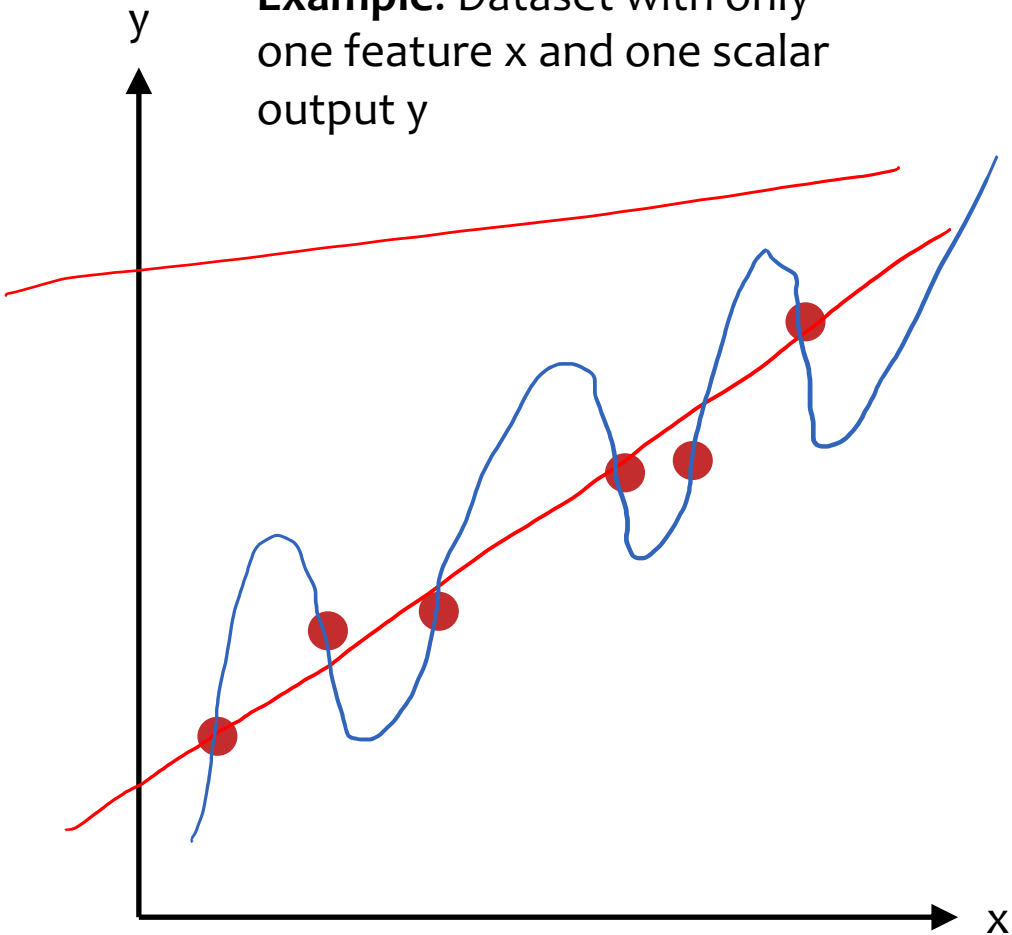
- Stock price prediction
- Forecasting epidemics
- Speech synthesis
- Generation of images (e.g. *Deep Dream*)



Regression

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

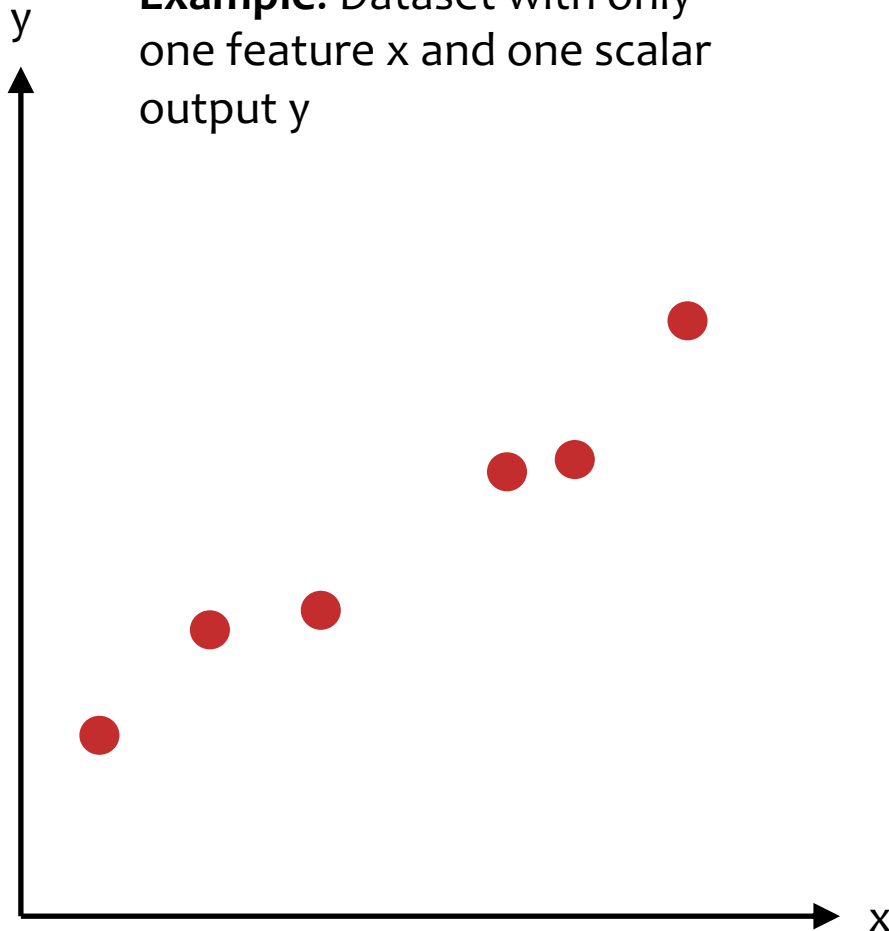
Q: What is the function that best fits these points?



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

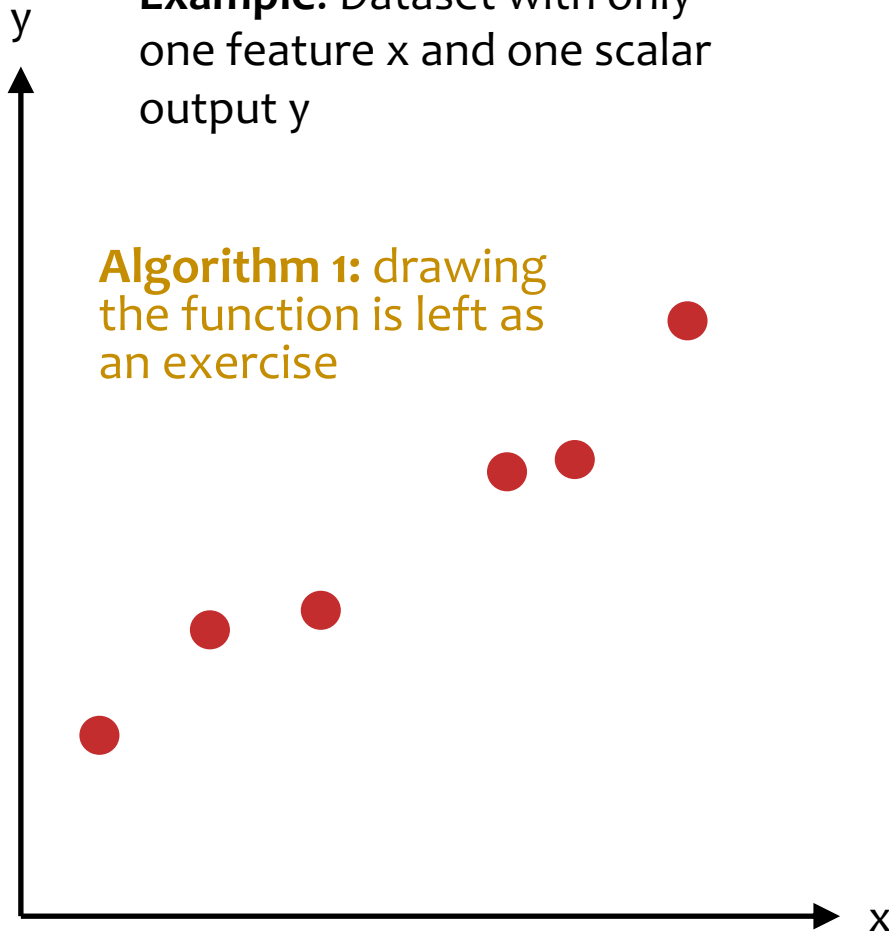
Algorithm 2: $k=2$ Nearest Neighbors Distance Weighted Regression

- *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



Algorithm 1: $k=1$ Nearest Neighbor Regression

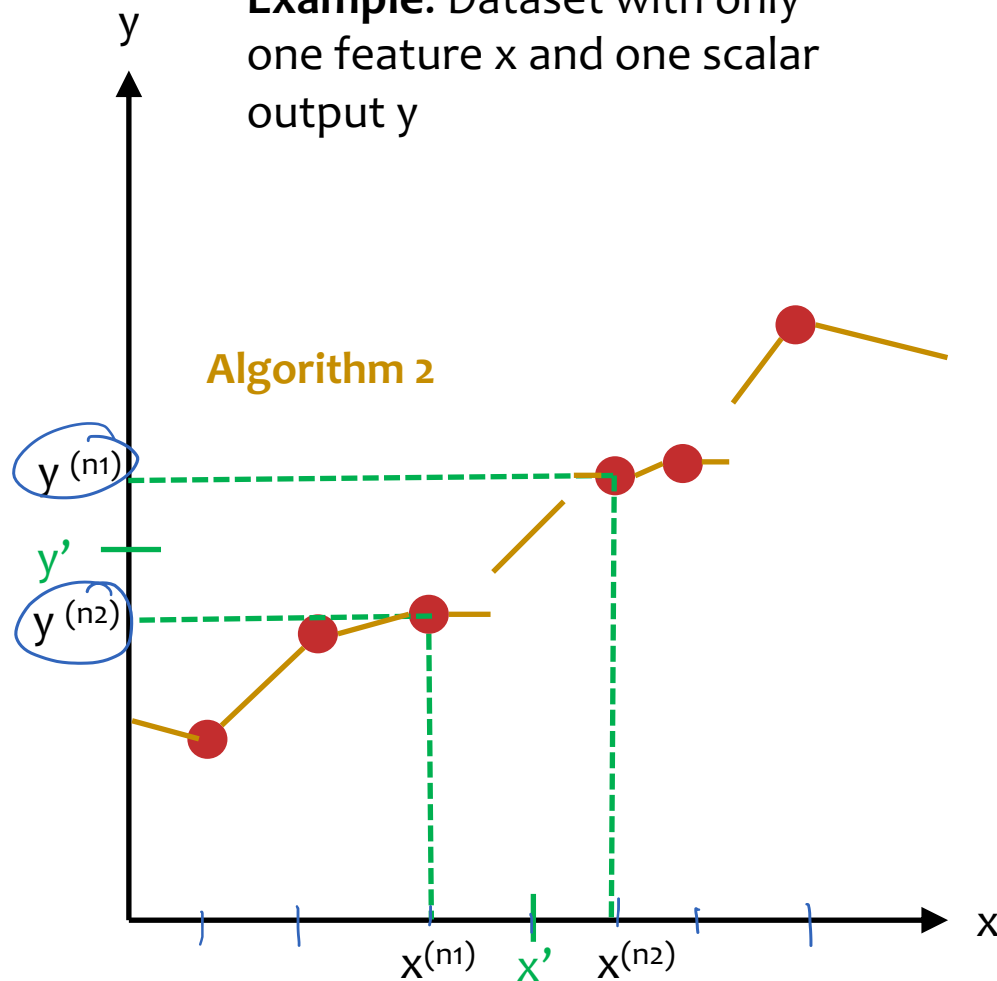
- *Train:* store all (x, y) pairs
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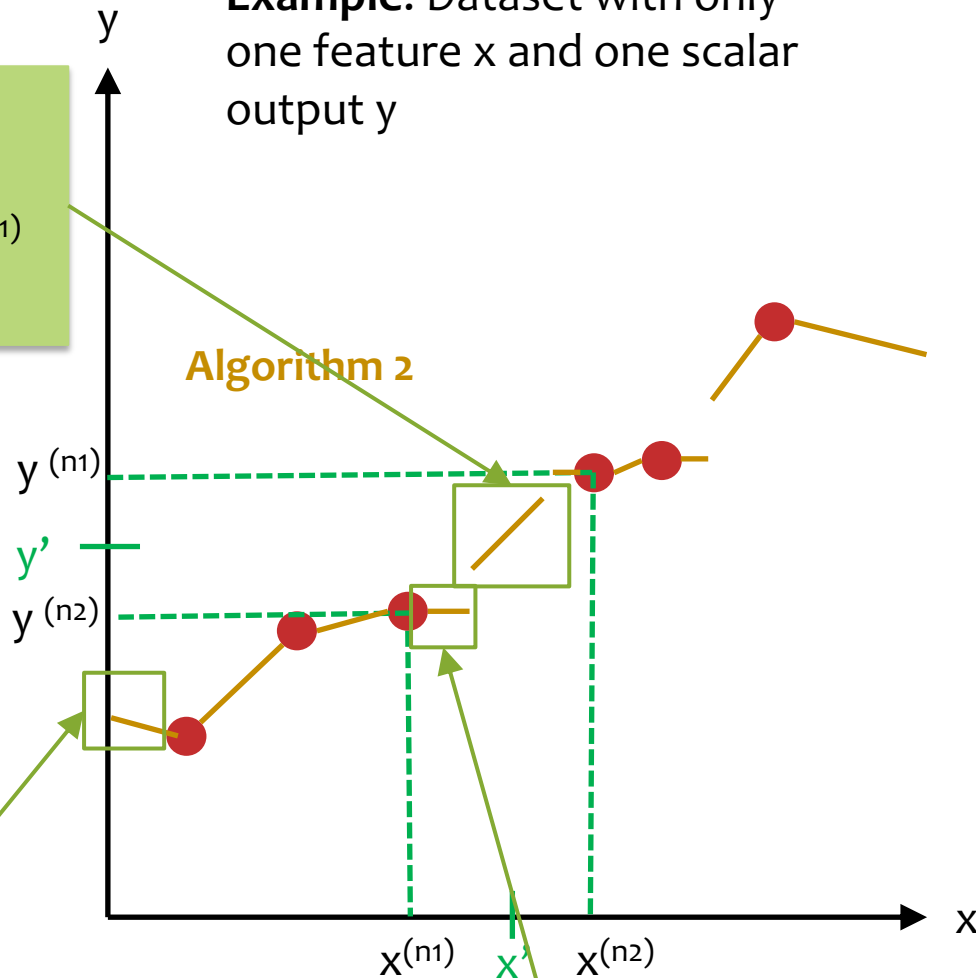
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The distance weighted average of $x^{(n1)}$ and $x^{(n2)}$

Algorithm 2

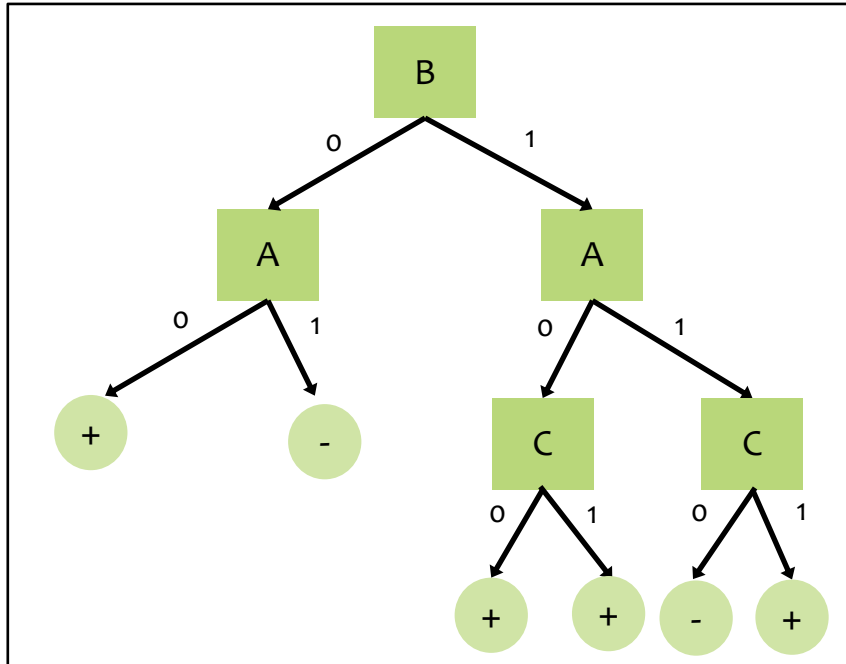
This tends toward the average height of the leftmost two points

This region is closer to the two points to the left

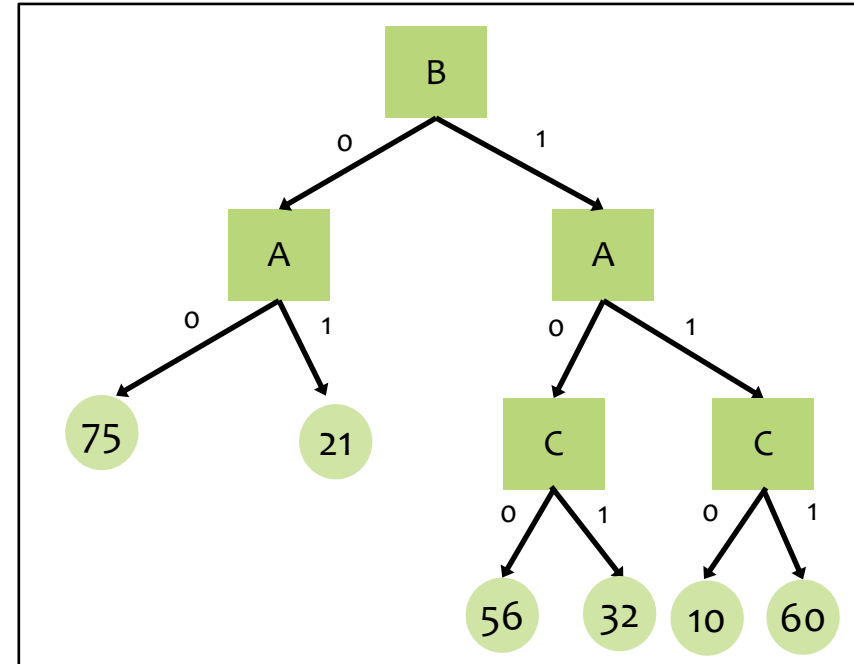
DECISION TREE REGRESSION

Decision Tree Regression

Decision Tree for Classification



Decision Tree for Regression

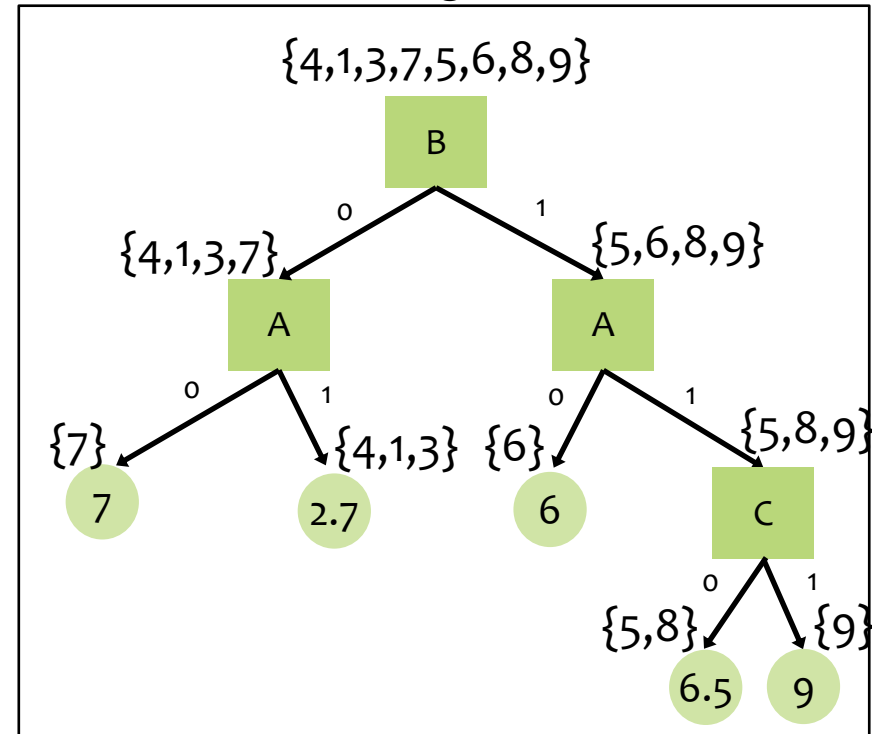


Decision Tree Regression

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

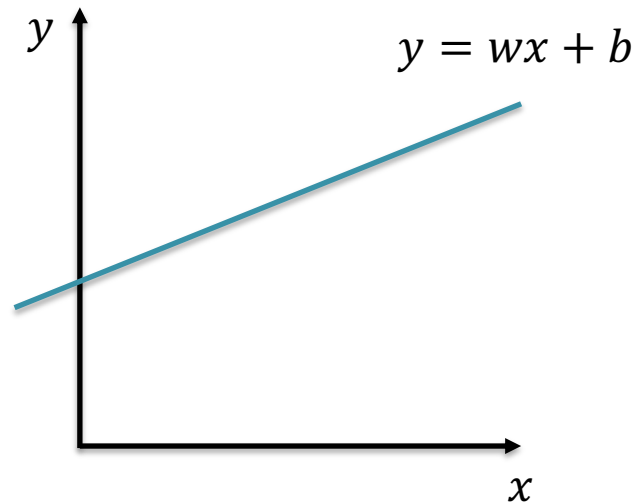
Linear Functions

Def: Regression is predicting real-valued outputs

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

Common Misunderstanding:

Linear functions \neq Linear decision boundaries



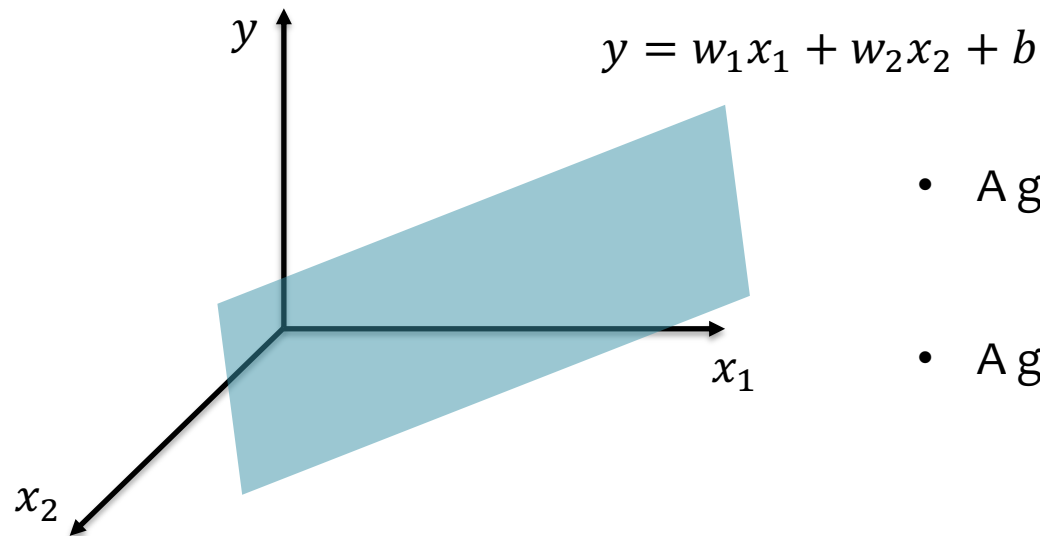
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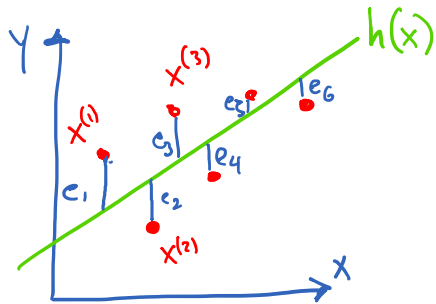
- A general linear function is $y = \mathbf{w}^T \mathbf{x} + b$
- A general linear decision boundary is $y = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$



Key Idea of Linear Regression

Residuals

Def: a residual is the vertical distance from observed value $y^{(i)}$ to predicted value $\hat{y}^{(i)}$



$$\begin{aligned} e_i &= |y^{(i)} - \hat{y}^{(i)}| \\ &= |y^{(i)} - h(\vec{x}^{(i)})| \\ &= |y^{(i)} - (\vec{w}^T \vec{x}^{(i)} + b)| \end{aligned}$$

Key Idea of Linear Regression

Find the linear function h (w/parameter \vec{w}, b) that minimizes the squares of the residuals for some training set

↑ just one option among many

Mean squared error

Def: MSE objective function

$$\begin{aligned} J_0(\vec{w}, b) &= \frac{1}{N} \sum_{i=1}^N (e_i)^2 \\ &= \frac{1}{N} \sum_{i=1}^N (|y^{(i)} - (\vec{w}^T \vec{x}^{(i)} + b)|)^2 \end{aligned}$$

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

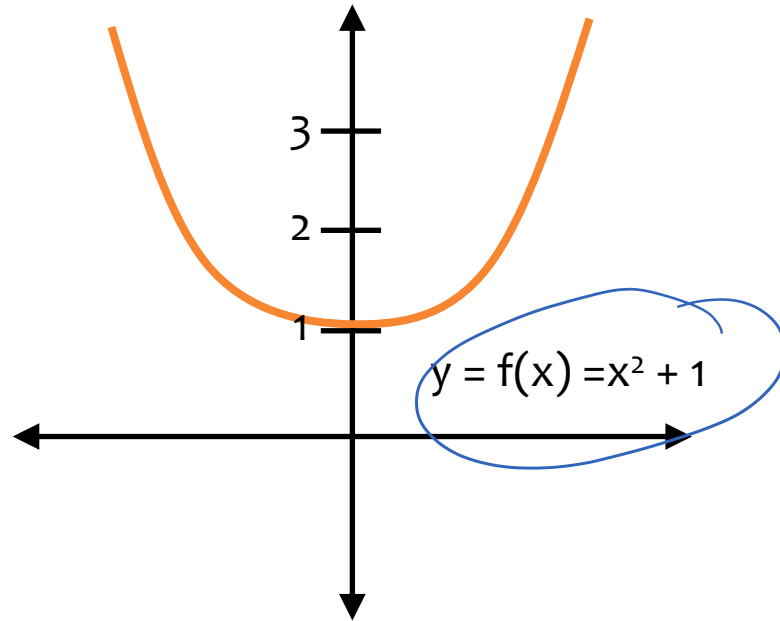
For ML, this is the objective function

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



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

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

Poll 2 :

1. Question: What is v^* ?

Poll 3

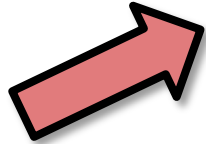
2. Question: What is x^* ?

**OPTIMIZATION METHOD #0:
RANDOM GUESSING**

Notation Trick: Folding in the Intercept Term

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

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



Notation Trick: fold the bias b and the weights \mathbf{w} into a single vector $\boldsymbol{\theta}$ by prepending a constant to \mathbf{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).

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:

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

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)

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

4. Solve the unconstrained optimization problem via favorite method:

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

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

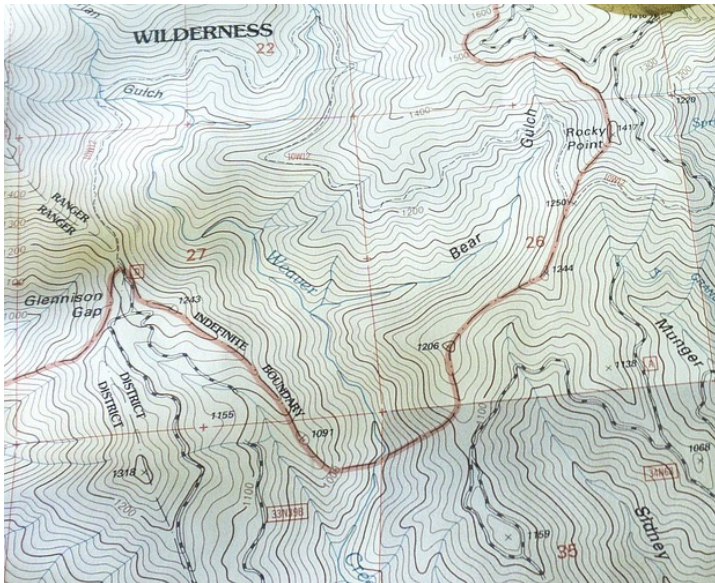
5. Test time: given a new \mathbf{x} , make prediction \hat{y}

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

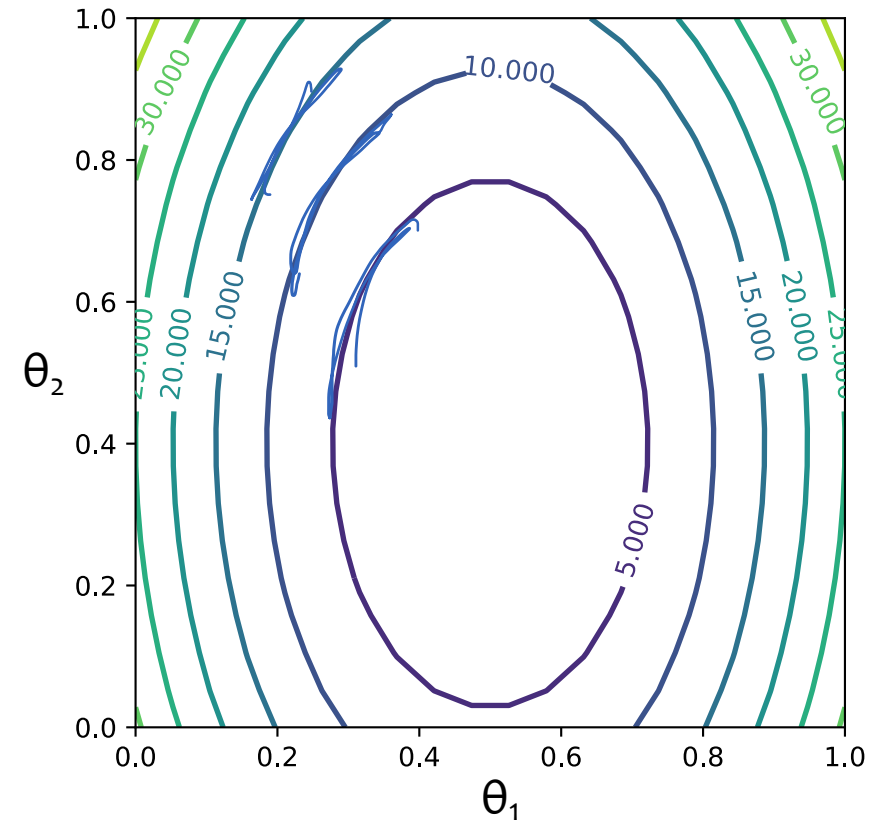
Contour Plots

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



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

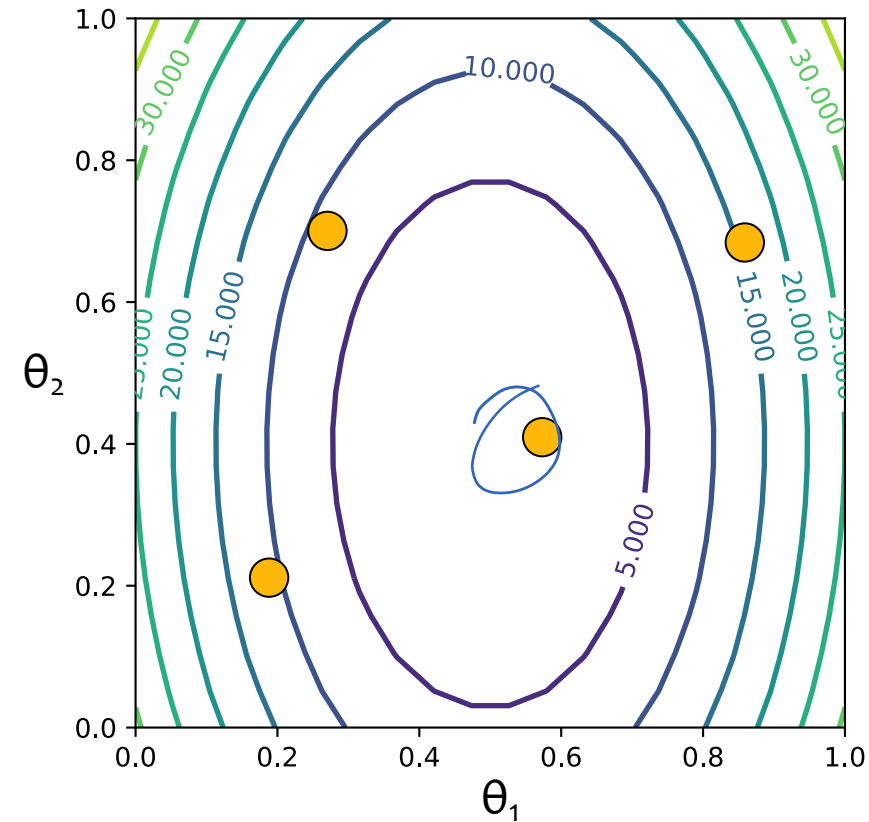


Optimization by Random Guessing

Optimization Method #0: Random Guessing

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

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



t	θ_1	θ_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

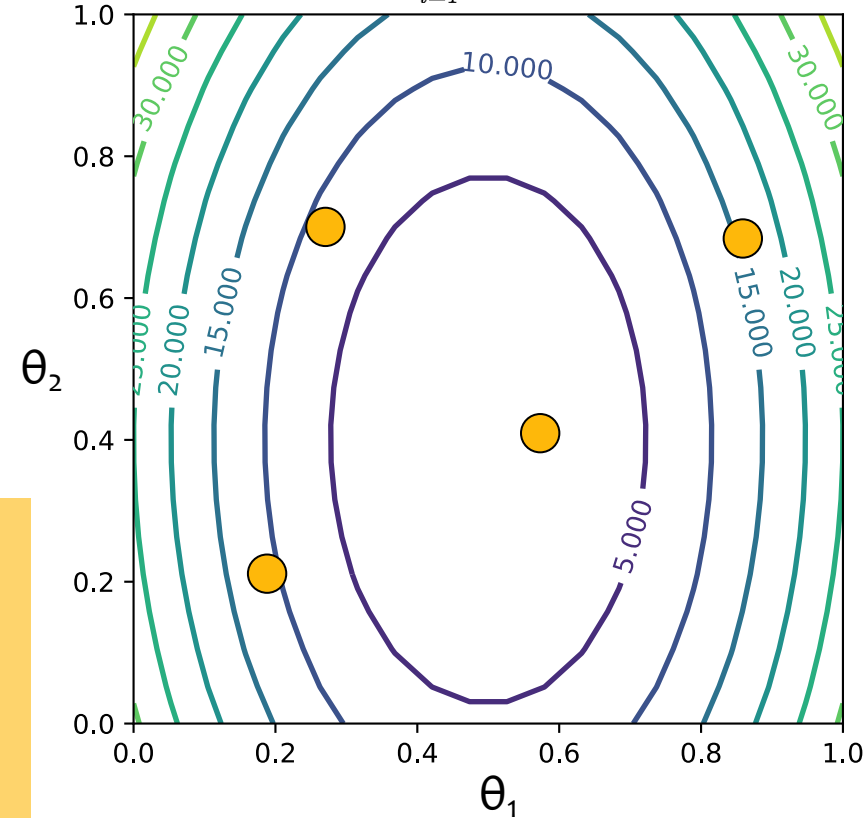
Optimization Method #0: Random Guessing

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For Linear Regression:

- **objective function** is Mean Squared Error (MSE)
- $\text{MSE} = J(w, b)$
 $= J(\theta_1, \theta_2) = \frac{1}{N} \sum_{i=1}^N (y^{(i)} - \theta^T \mathbf{x}^{(i)})^2$
- 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

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

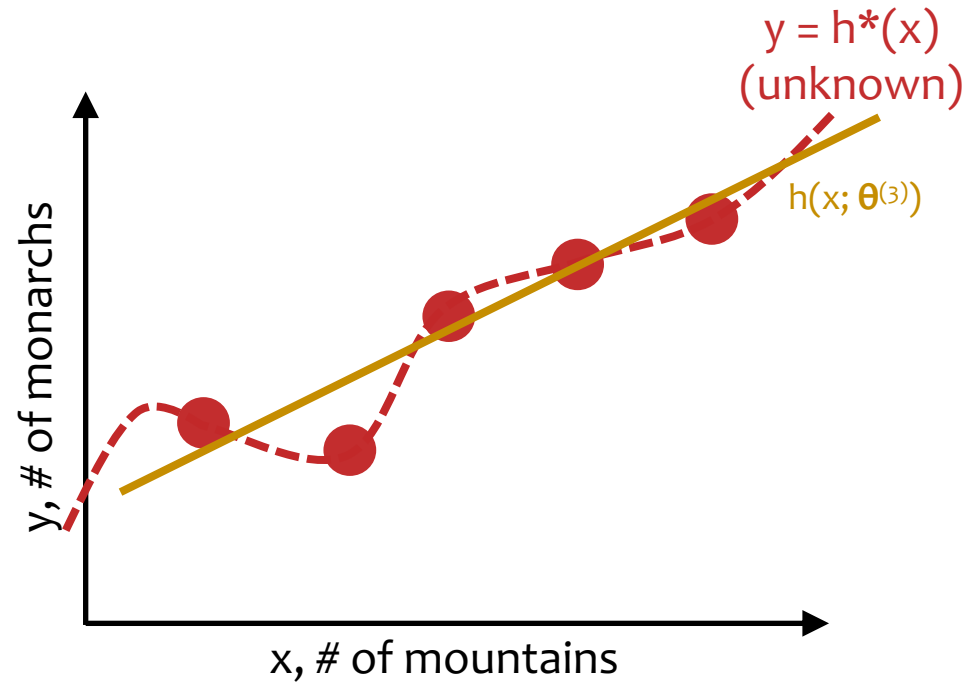


t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.2	0.2	10.4
2	0.3	0.7	7.2
3	0.6	0.4	1.0
4	0.9	0.7	16.2

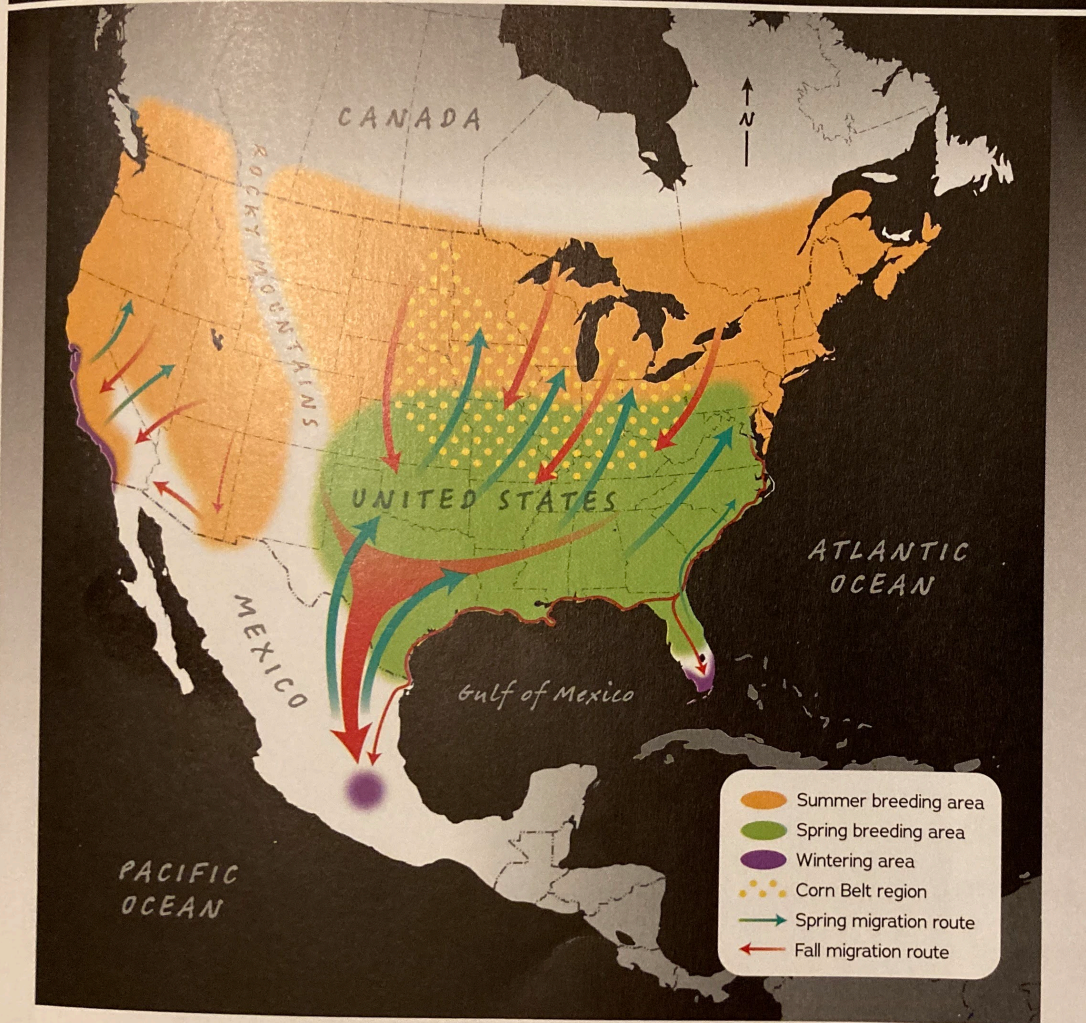
Linear Regression: Running Example



Counting Butterflies



MIGRATION ROUTES OF MONARCH BUTTERFLIES

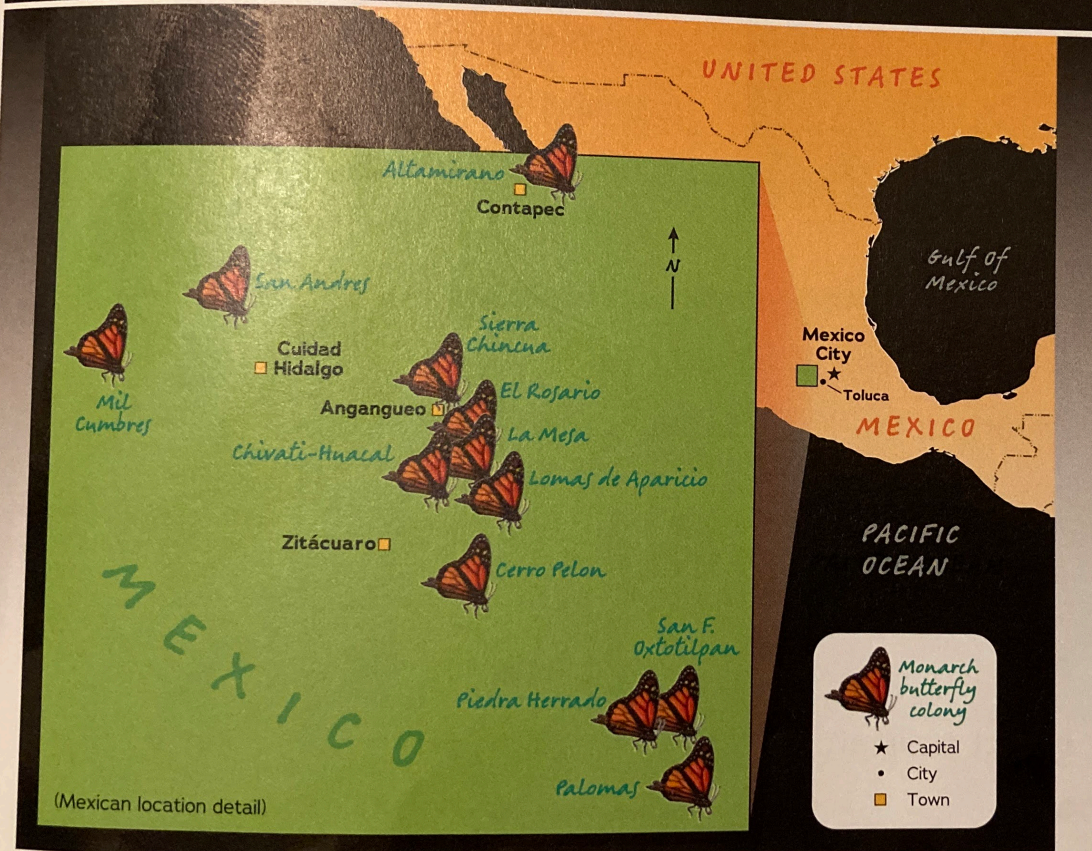


This map shows migration routes of fall and spring migrations, both east and west of the Rocky Mountains.

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.

...imates reveal about the eastern monarchs? 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

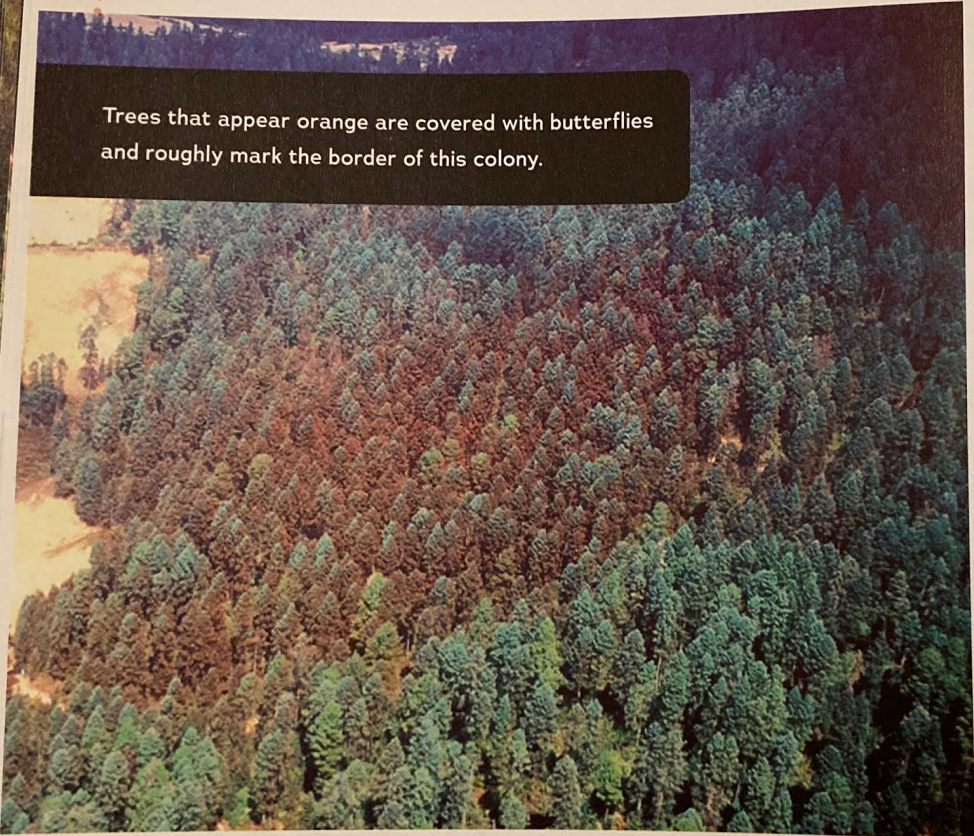
LOCATION OF MONARCH BUTTERFLY COLONIES WINTERING IN MEXICO



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.

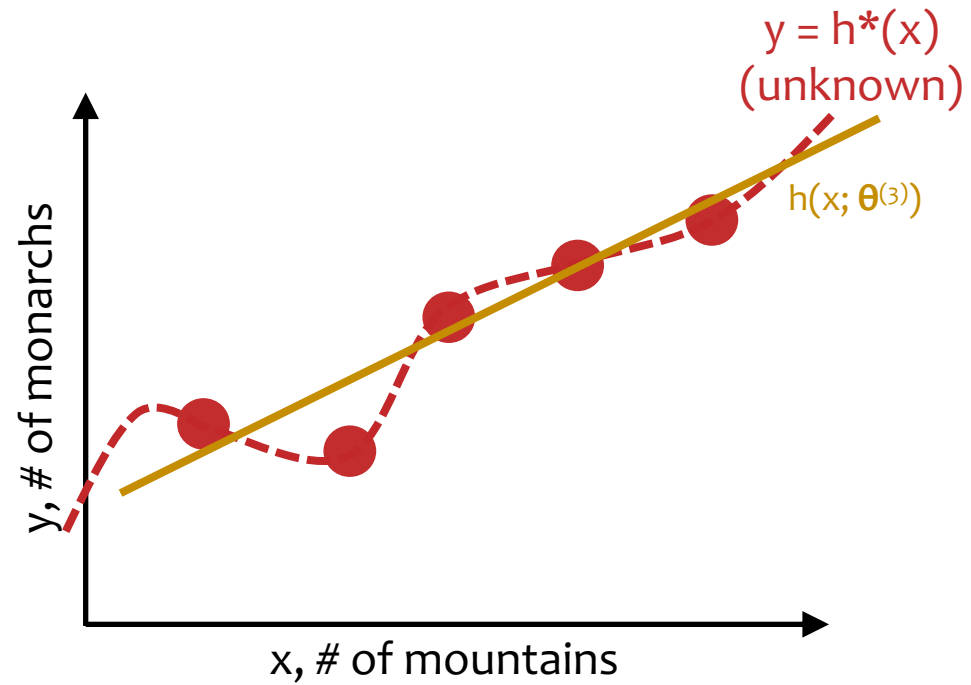
At the same time, scientists in California reported that the number of western monarchs was dropping as well. From 1997 to 2014, the number of monarchs overwintering along the California coast had fallen by 74 percent.

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.

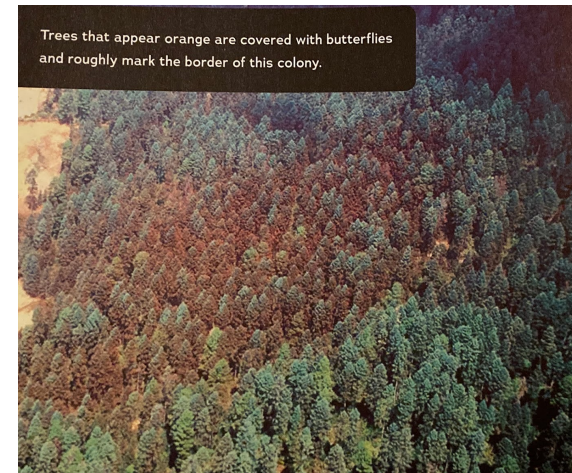
Counting Butterflies



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:
$$\mathbf{x} = [x_1, x_2, \dots, x_M]^T$$
- 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

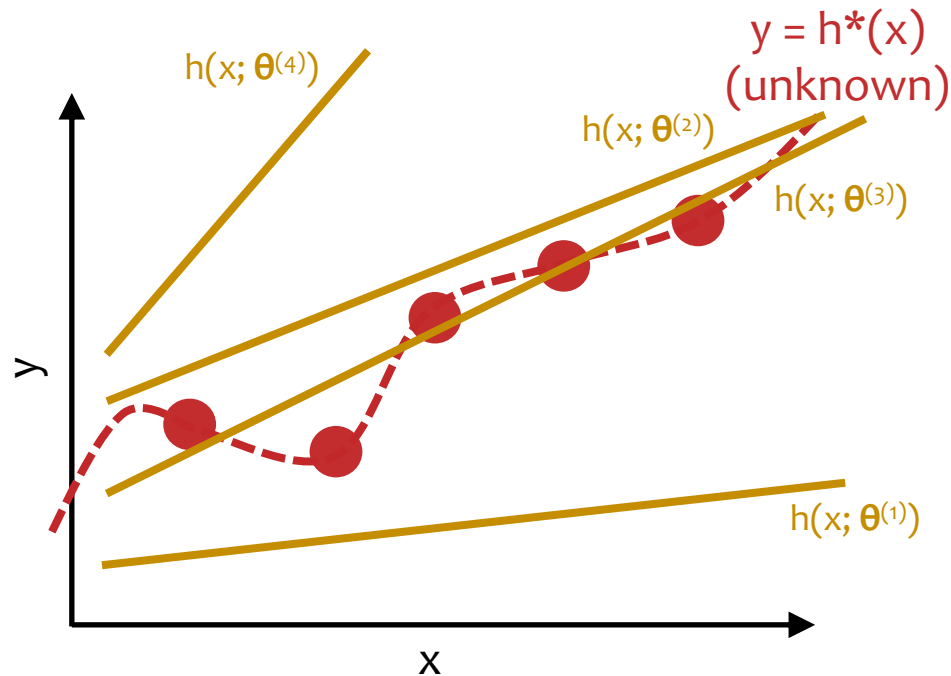
Q: How would you obtain ground truth data?



Linear Regression by Rand. Guessing

Optimization Method #0: Random Guessing

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



For Linear Regression:

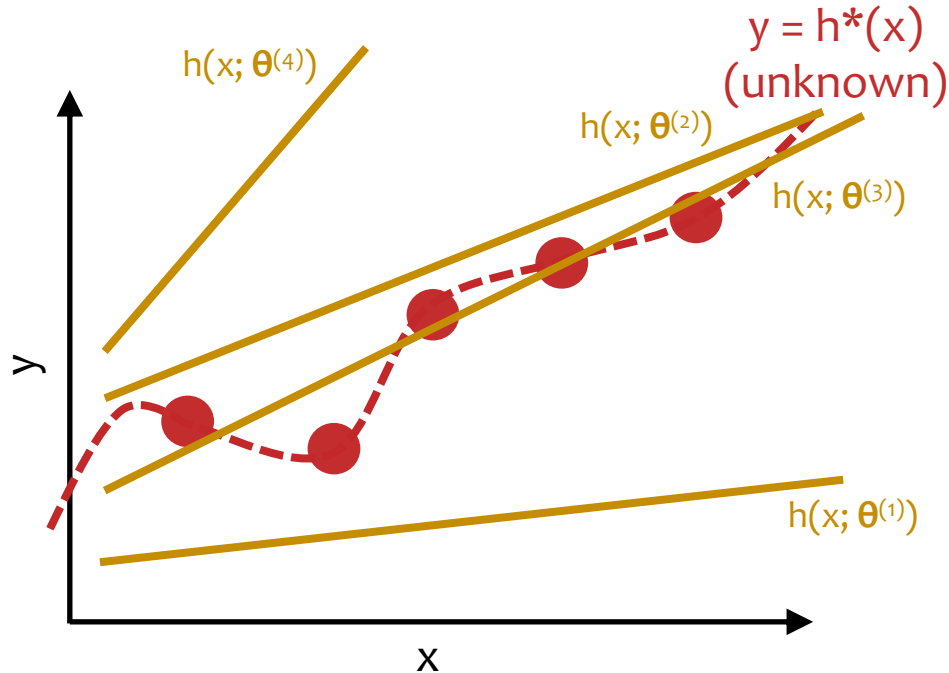
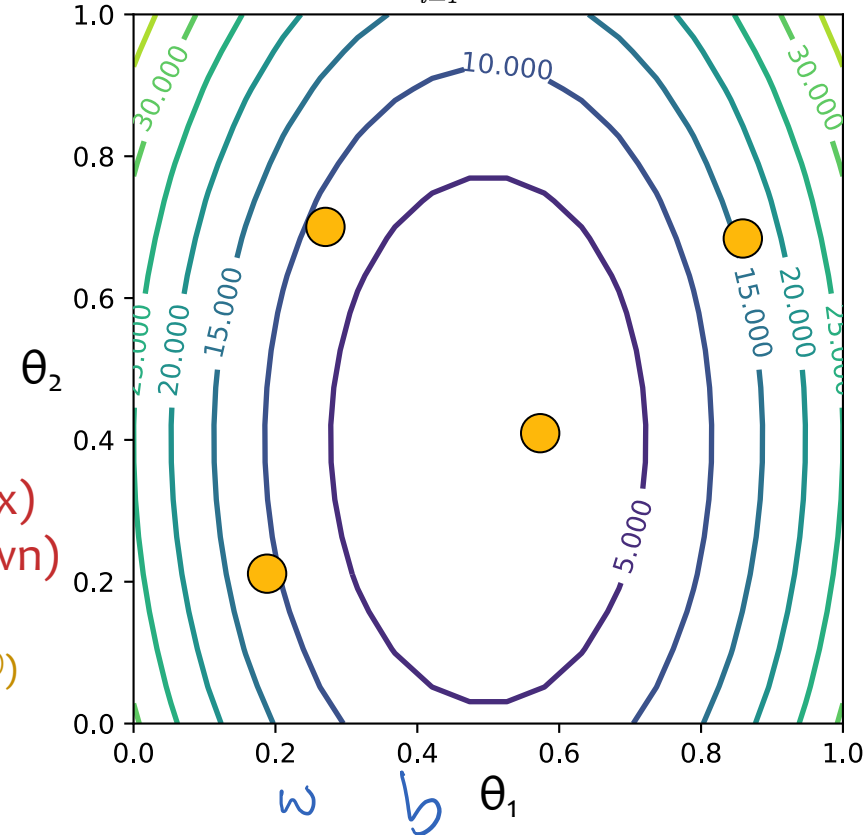
- target function $h^*(x)$ is **unknown**
- only have access to $h^*(x)$ through **training examples** $(x^{(i)}, y^{(i)})$
- want $h(x; \theta^{(t)})$ that **best approximates** $h^*(x)$
- **enable generalization** w/inductive bias that restricts hypothesis class to **linear functions**

Linear Regression by Rand. Guessing

Optimization Method #0: Random Guessing

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

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

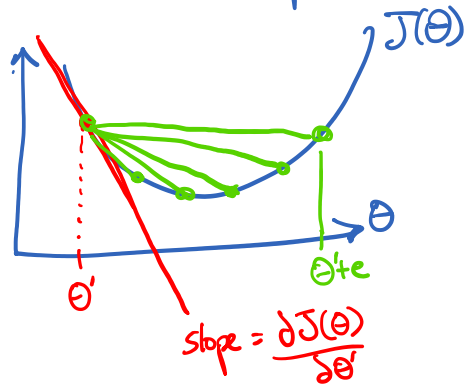


t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.2	0.2	10.4
2	0.3	0.7	7.2
3	0.6	0.4	1.0
4	0.9	0.7	16.2

OPTIMIZATION METHOD #1: GRADIENT DESCENT

Derivatives

① Deriv as a Slope

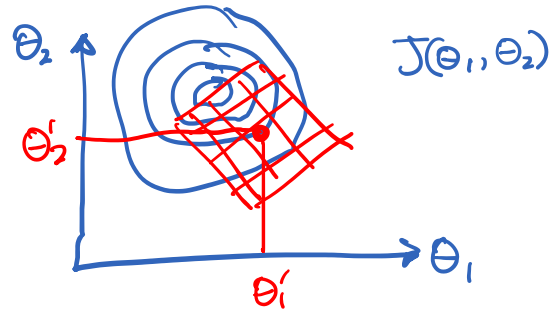


② Deriv as a Limit

$$\frac{\delta J(\theta)}{\delta \theta} = \lim_{e \rightarrow 0} \frac{J(\theta + e) - J(\theta)}{e}$$

limit of the secants
is the tangent

③ Deriv as a Tangent Plane



$$\begin{bmatrix} \frac{\delta J(\theta_1, \theta_2)}{\delta \theta_1} \\ \frac{\delta J(\theta_1, \theta_2)}{\delta \theta_2} \end{bmatrix}$$

Gradient

Def: the gradient of $J: \mathbb{R}^M \rightarrow \mathbb{R}$ is

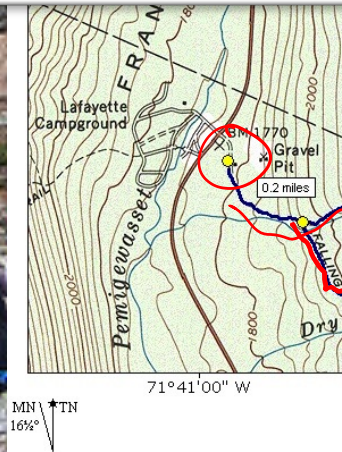
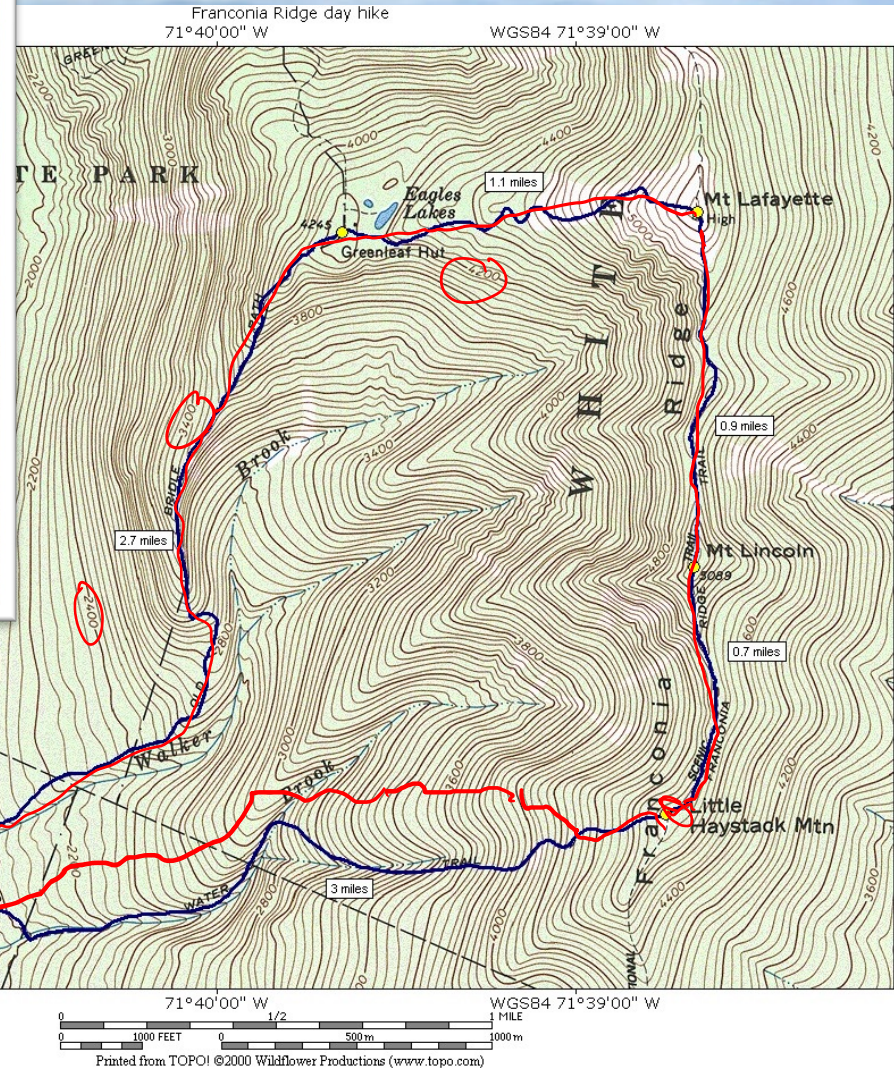
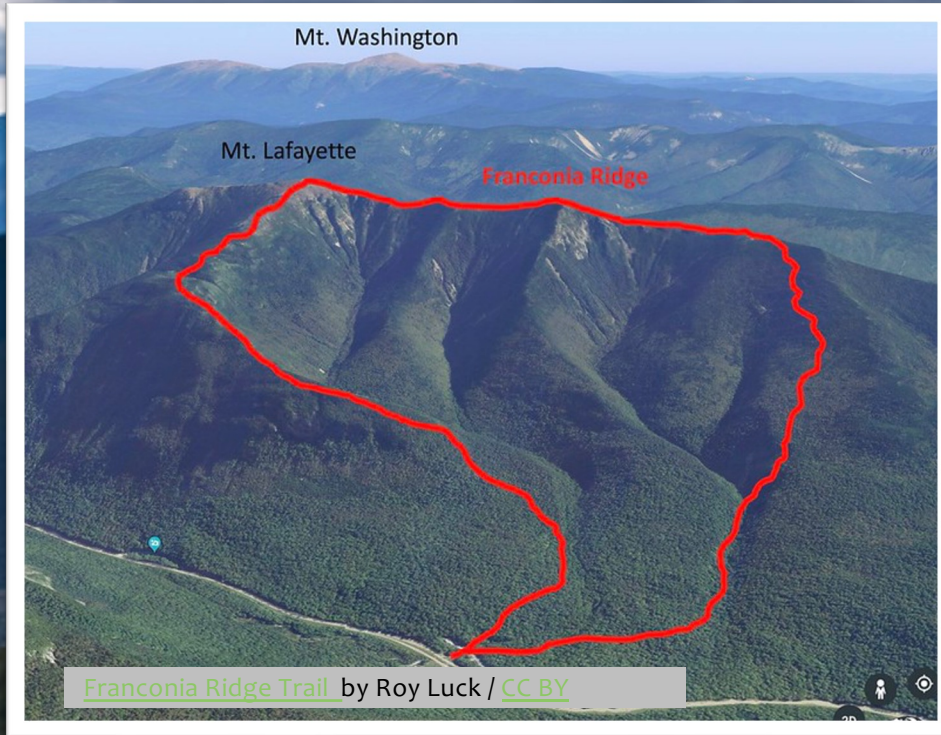
$$\nabla J(\vec{\theta}) = \begin{bmatrix} \delta J(\vec{\theta}) / \delta \theta_1 \\ \delta J(\vec{\theta}) / \delta \theta_2 \\ \vdots \\ \delta J(\vec{\theta}) / \delta \theta_M \end{bmatrix}$$

first order partial derivative

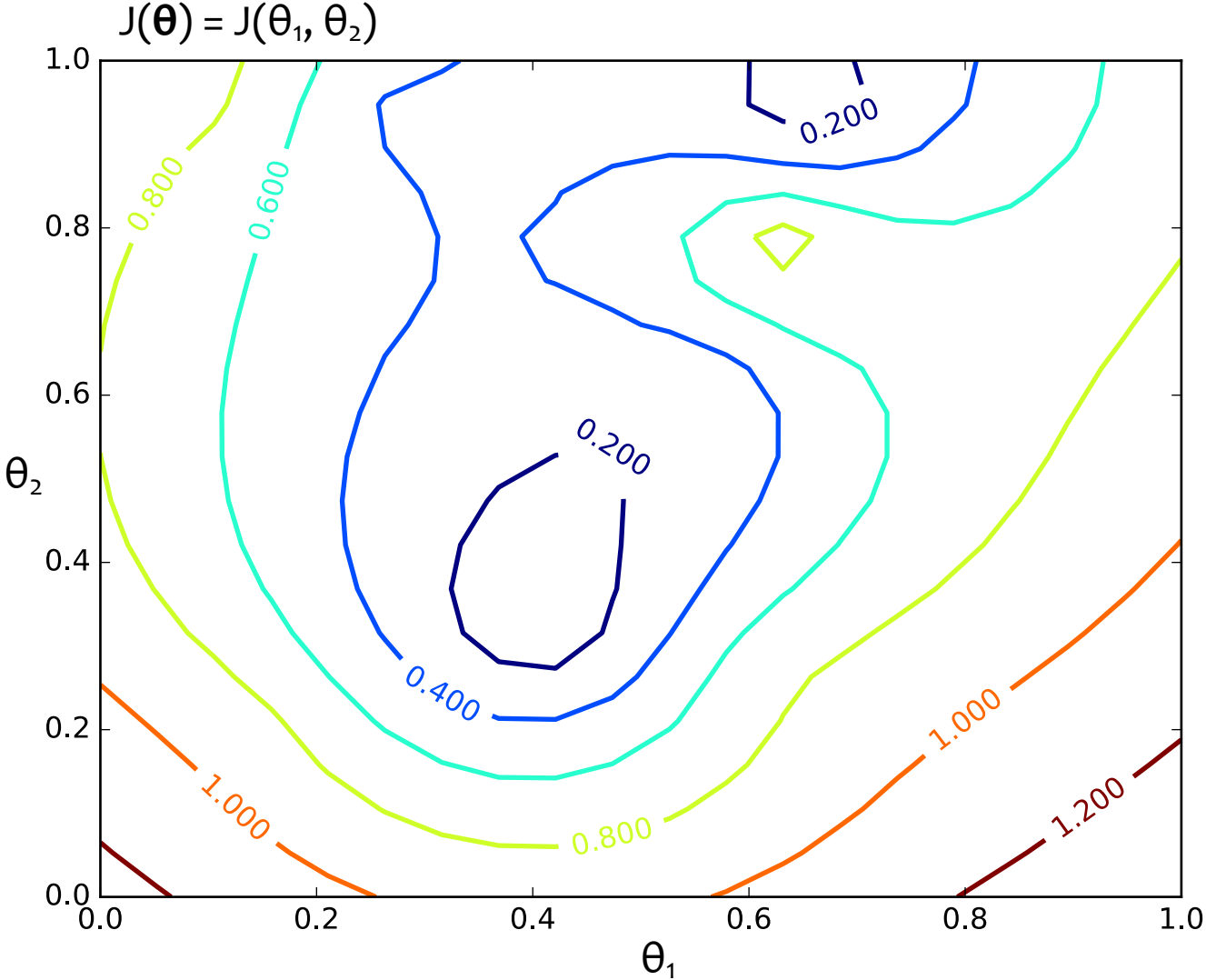
Topographical Maps



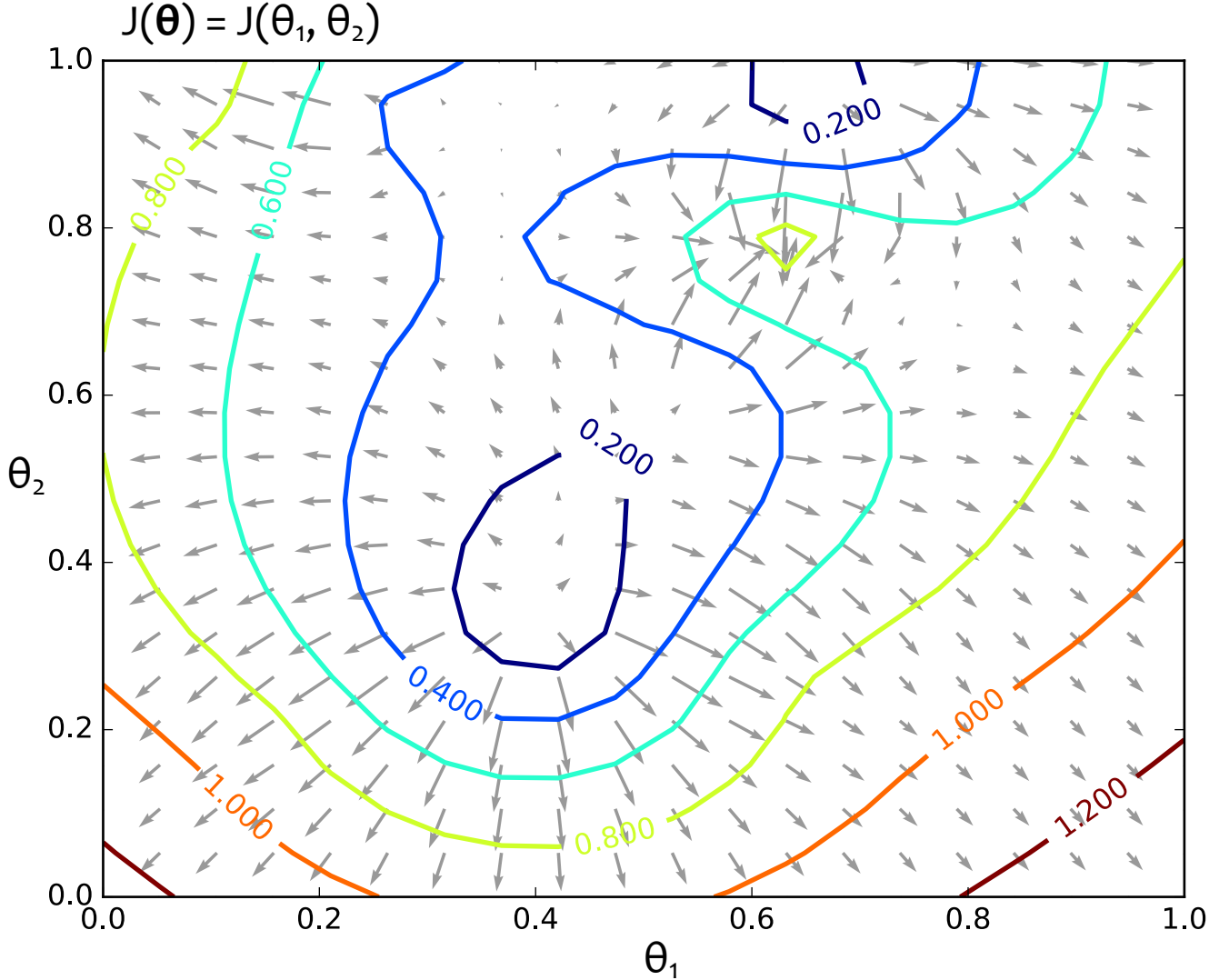
Topographical Maps



Gradients

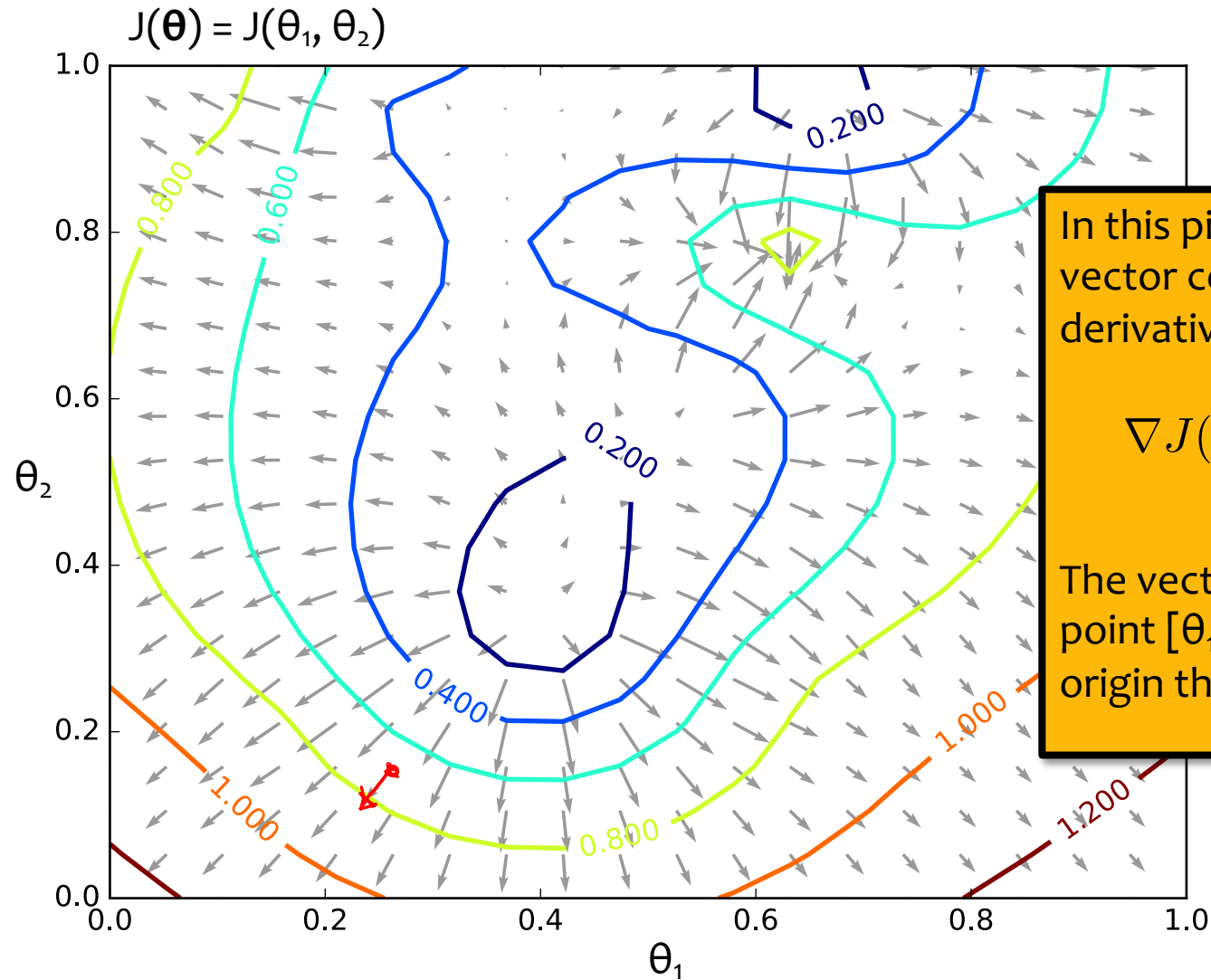


Gradients



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

Gradients



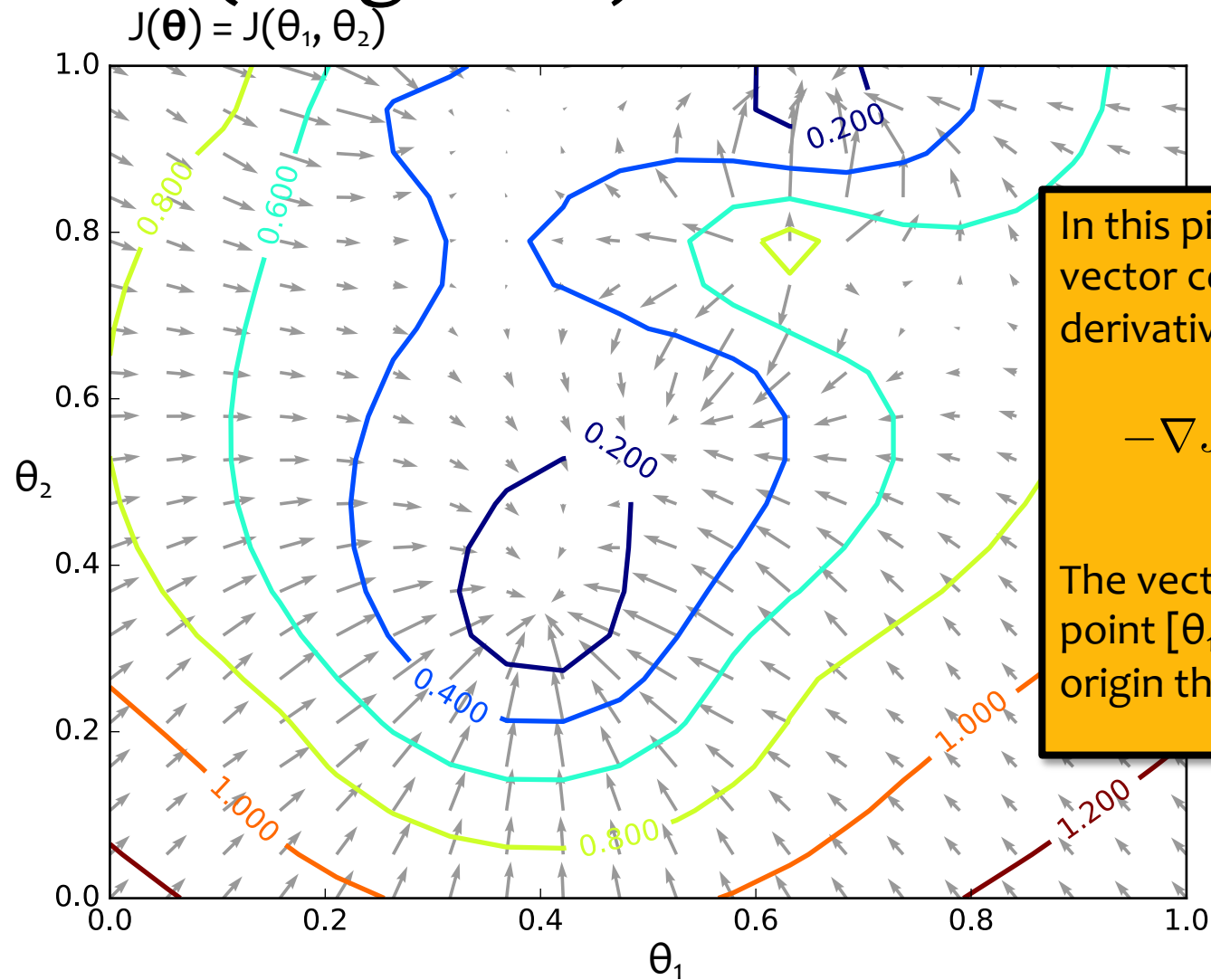
In this picture, each arrow is a 2D vector consisting of two partial derivatives.

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

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



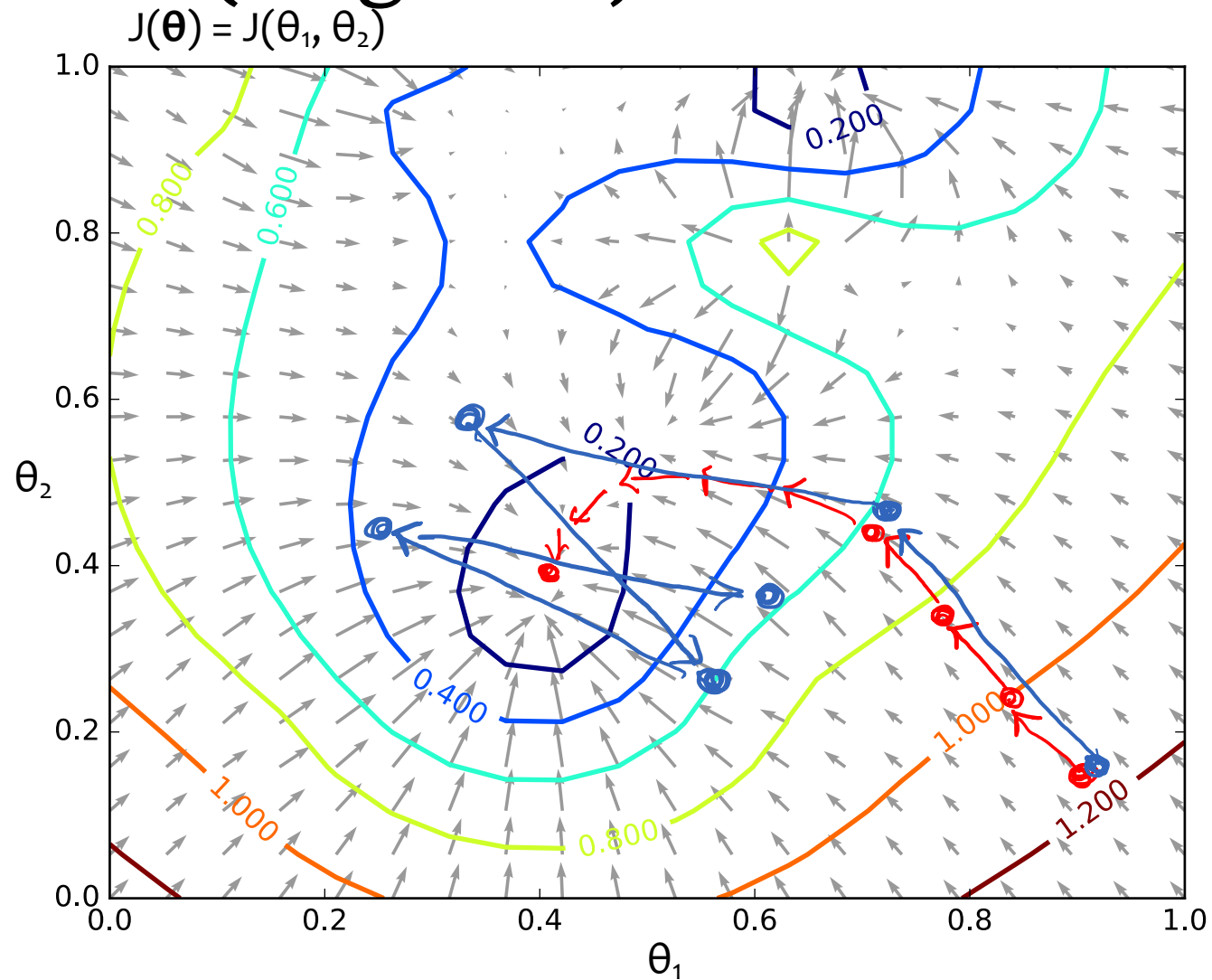
In this picture, each arrow is a 2D vector consisting of two partial derivatives.

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

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 **D**escent would follow.

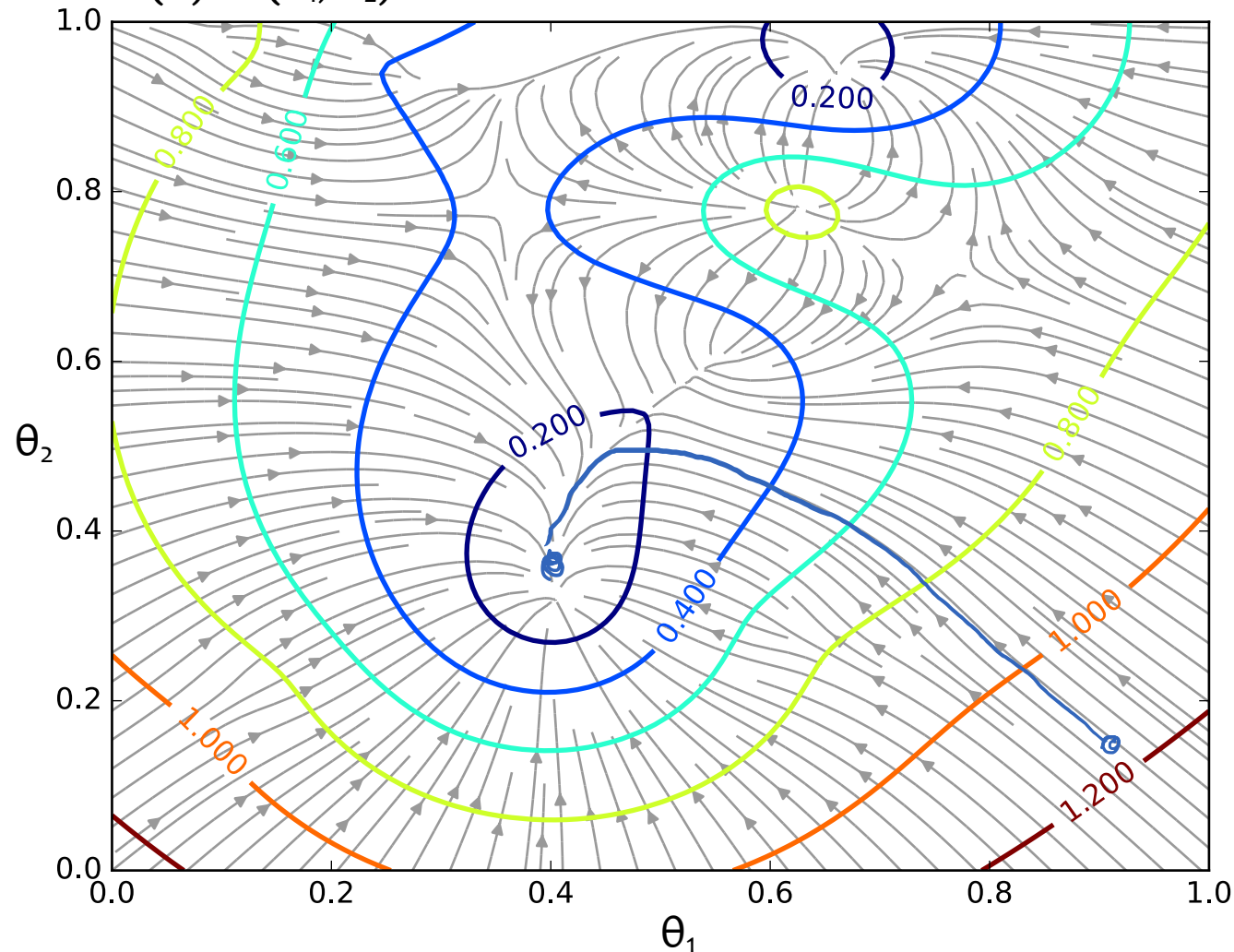
(Negative) Gradients



These are the **negative** gradients that Gradient **D**escent would follow.

(Negative) Gradient Paths

$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2)$$



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

Gradient Descent

Gradient Descent Algorithm

- ① Choose an initial point $\vec{\Theta}$
- ② Repeat $t=1,2,3,\dots$
 - a) Compute gradient $\vec{g} = \nabla J(\vec{\Theta})$
 - b) Select step size $\gamma_t \in \mathbb{R}$
 - c) Update parameters $\vec{\Theta} \leftarrow \vec{\Theta} - \gamma_t \vec{g}$
- ③ Return the best $\vec{\Theta}$ when some stopping criterion is reached

Remarks

Initial Point

- $\vec{\Theta}$ randomly
- Θ all zeros

Step Size

- fixed value $\gamma = 0.1$
- set a schedule $\gamma_t = \frac{\gamma_0}{(t-1)\gamma_0+1}$
- line search

Stopping Criterion

- $\vec{g} \approx 0$
- $\|\nabla J(\vec{\Theta})\|_2 < \epsilon$ for $\epsilon = 10e^{-8}$

Gradient Descent: Step Size

Poll

Question: 4

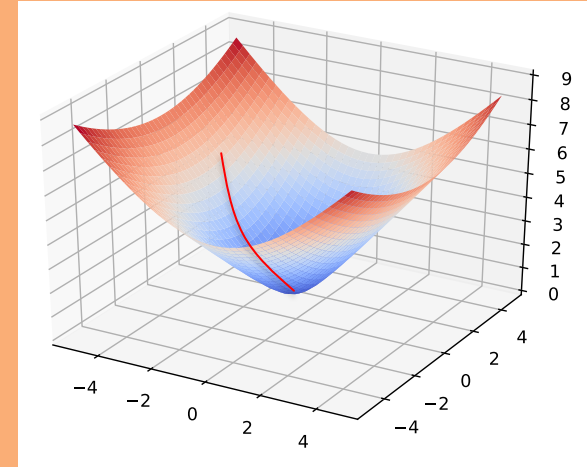
In gradient descent, what could go wrong if we *always* use the same step size (or step size schedule) for every problem we encounter?

Answer:

Gradient Descent

Algorithm 1 Gradient Descent

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



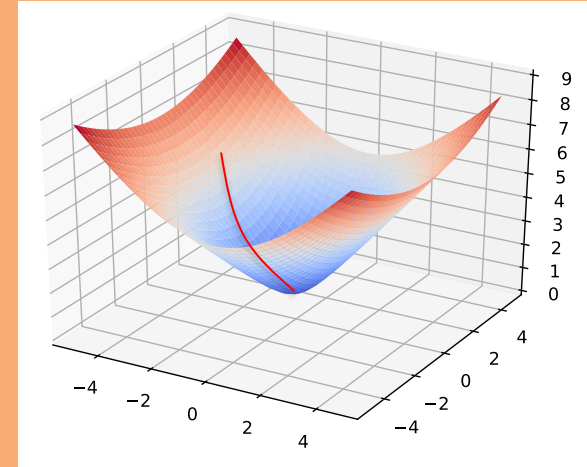
In order to apply GD to Linear Regression all we need is the **gradient** of the objective function (i.e. vector of partial derivatives).

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

Gradient Descent

Algorithm 1 Gradient Descent

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



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.

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

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}

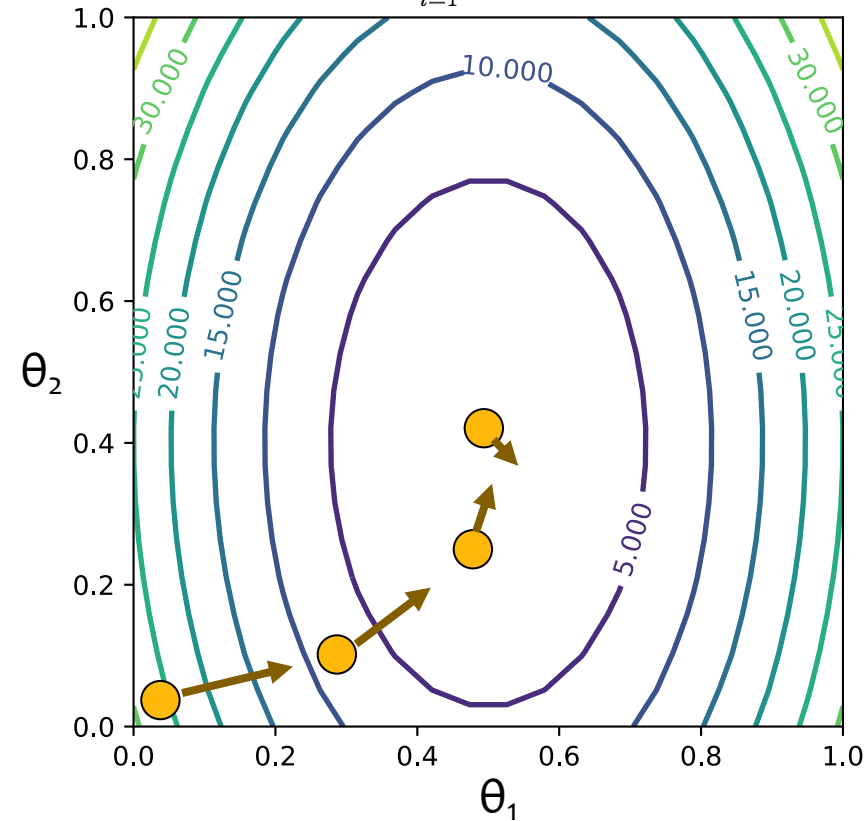
$$\hat{y} = h_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) = \hat{\boldsymbol{\theta}}^T \mathbf{x}$$

Linear Regression by Gradient Desc.

Optimization Method #1: Gradient Descent

1. Pick a random θ
2. Repeat:
 - a. Evaluate gradient $\nabla J(\theta)$
 - b. Step opposite gradient
3. Return θ that gives smallest $J(\theta)$

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

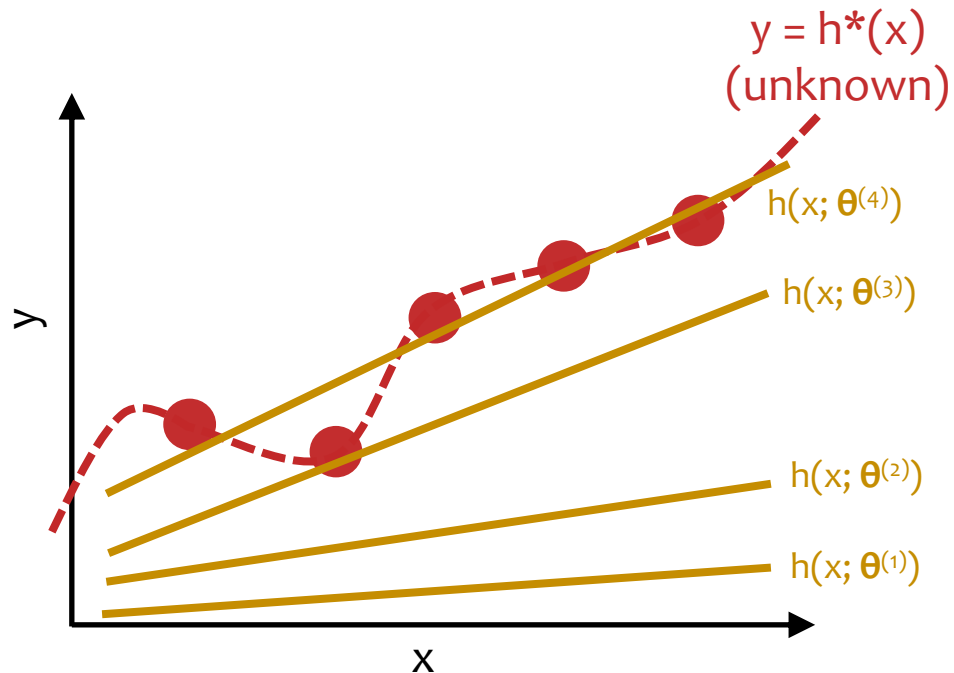


t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

Linear Regression by Gradient Desc.

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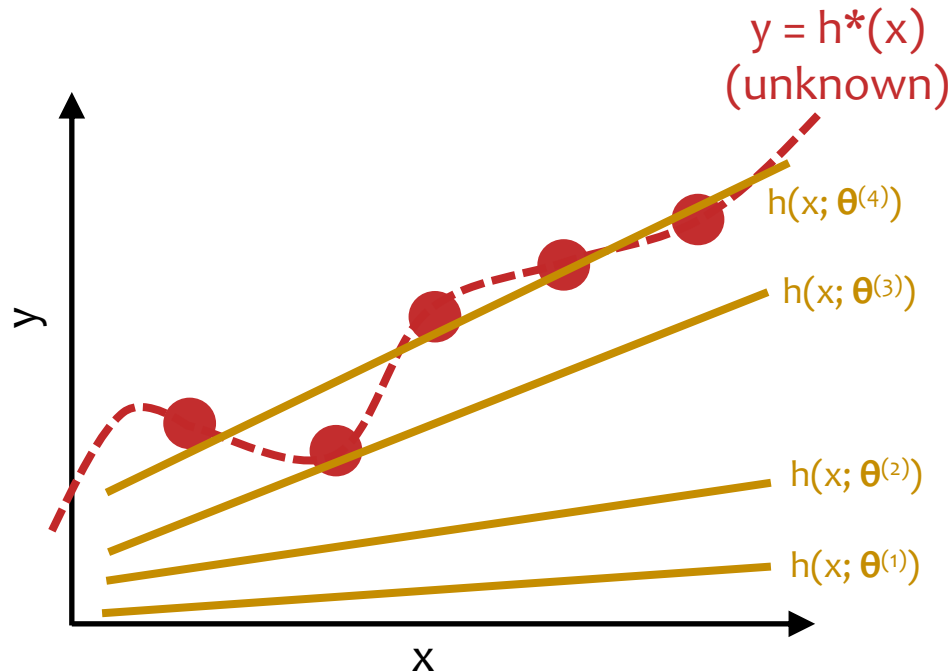


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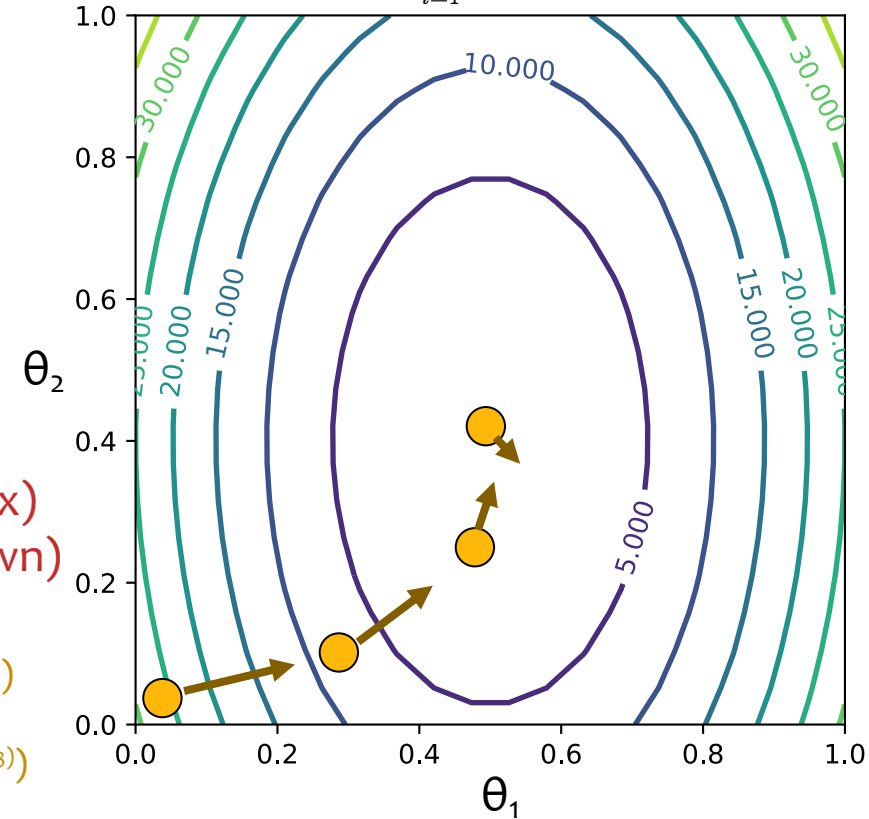
Linear Regression by Gradient Desc.

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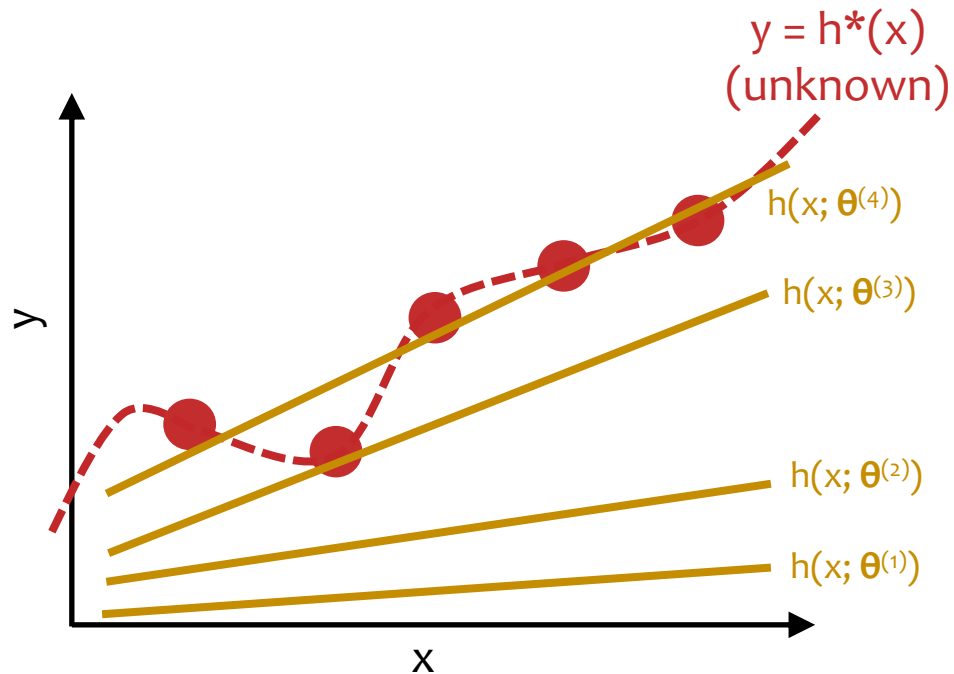
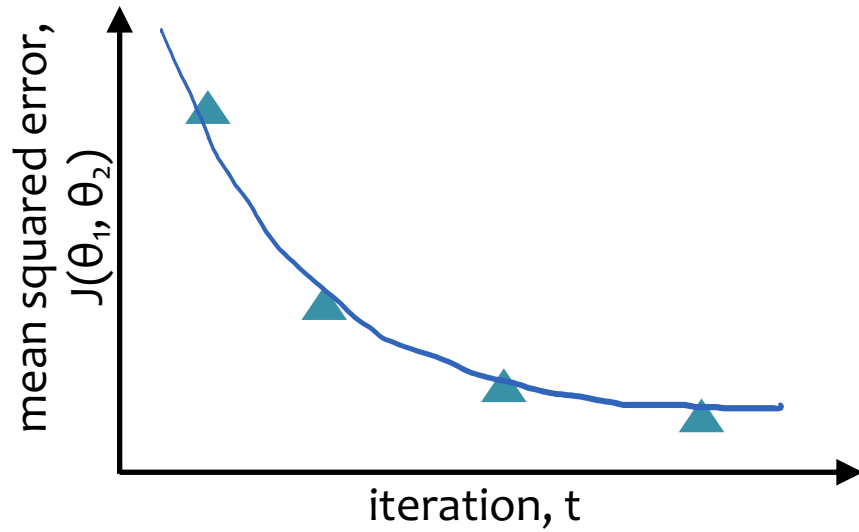


$$J(\theta) = J(\theta_1, \theta_2) = \frac{1}{N} \sum_{i=1}^N (y^{(i)} - \theta^T \mathbf{x}^{(i)})^2$$



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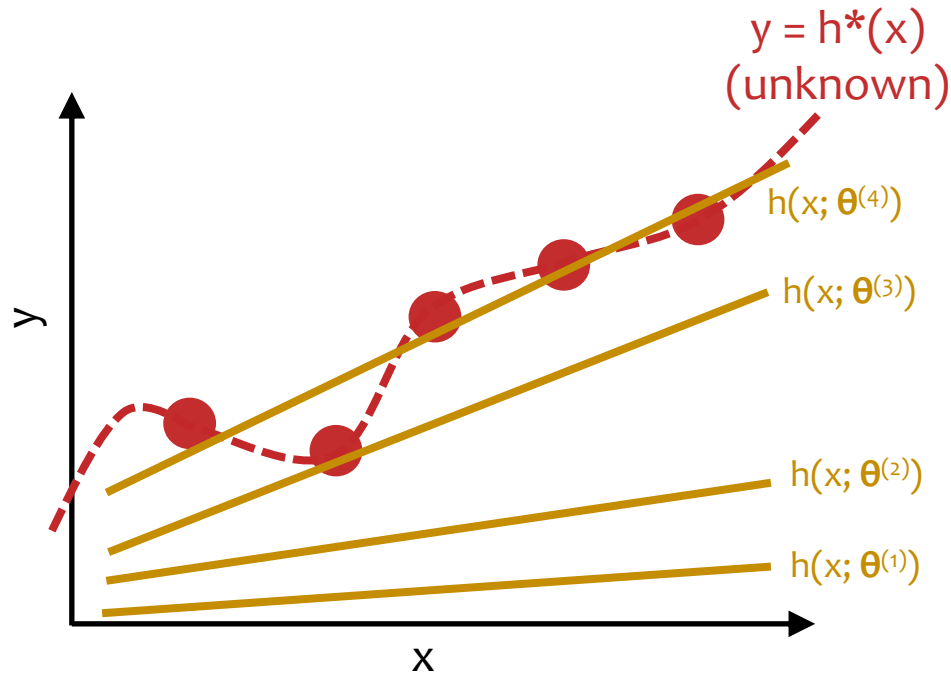
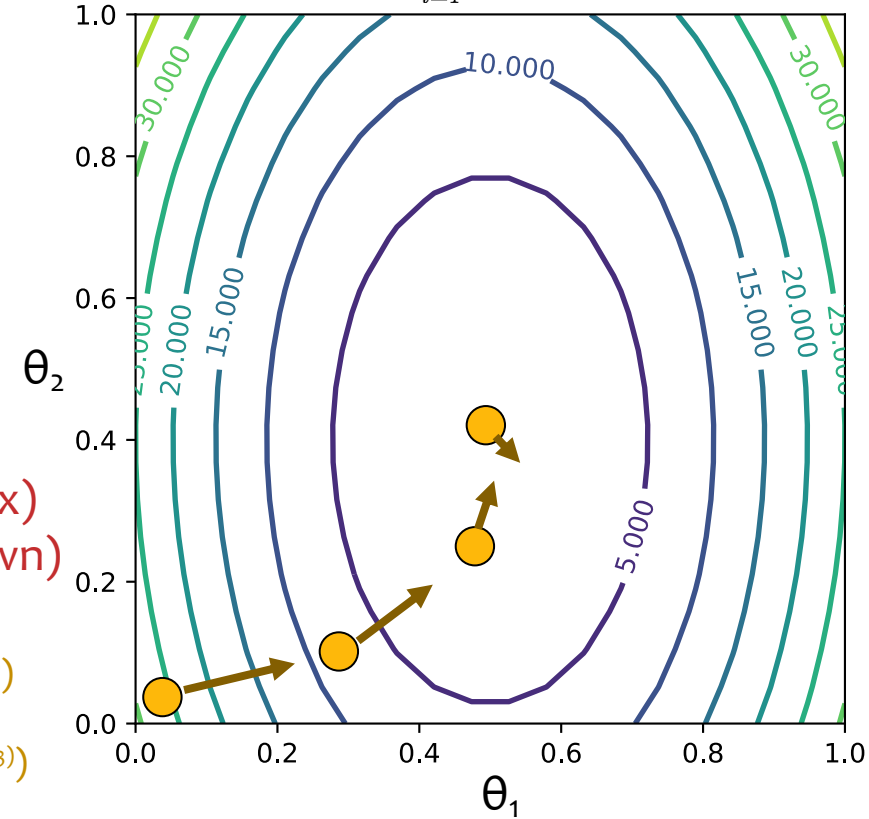
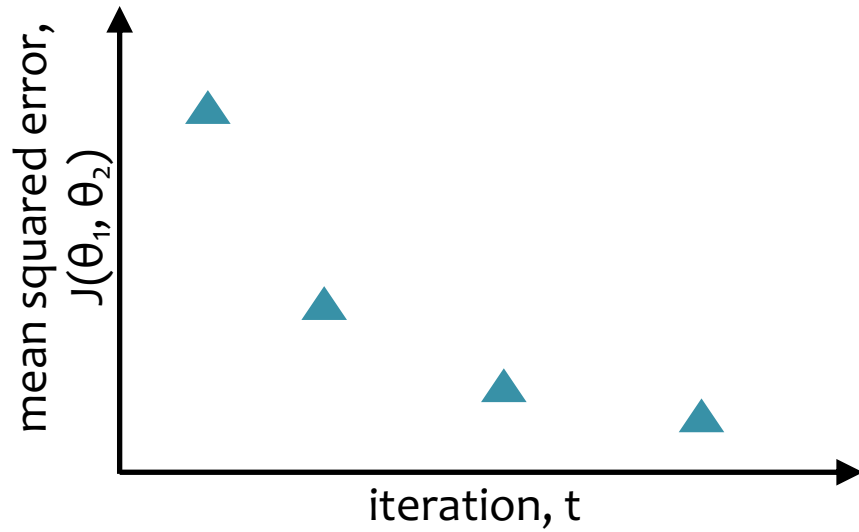
Linear Regression by Gradient Desc.



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Linear Regression by Gradient Desc.

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



t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
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$$\vec{\theta} = [\theta_0, \dots, \theta_M]^T$$

Gradient Calculation for Linear Regression

MSE:

$$J(\vec{\theta}) = \frac{1}{N} \sum_{i=1}^N J^{(i)}(\vec{\theta}) \quad \text{where } J^{(i)}(\vec{\theta}) = \frac{1}{2} (y^{(i)} - \vec{\theta}^T \vec{x}^{(i)})^2$$

← does not change the argmin

Partial Derivs

$$\begin{aligned} \frac{\partial J^{(i)}(\vec{\theta})}{\partial \theta_j} &= \frac{\partial}{\partial \theta_j} \left(\frac{1}{2} (y^{(i)} - \vec{\theta}^T \vec{x}^{(i)})^2 \right) \\ &= \frac{1}{2} \cdot 2 (y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}) \frac{\partial}{\partial \theta_j} (y^{(i)} - \underbrace{\vec{\theta}^T \vec{x}^{(i)}}_{\sum_{m=1}^M \theta_m x_m^{(i)}}) \\ &= - (y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}) x_j^{(i)} \end{aligned}$$

Gradients

$$\nabla J^{(i)}(\vec{\theta}) = \begin{bmatrix} \frac{\partial J^{(i)}}{\partial \theta_0} \\ \vdots \\ \frac{\partial J^{(i)}}{\partial \theta_M} \end{bmatrix} = \underbrace{-(y^{(i)} - \vec{\theta}^T \vec{x}^{(i)})}_{\text{scalar}} \underbrace{\vec{x}^{(i)}}_{\text{vector}}$$

$$\begin{aligned} \nabla J(\vec{\theta}) &= \nabla \left(\frac{1}{N} \sum_{i=1}^N J^{(i)}(\vec{\theta}) \right) \\ &= \frac{1}{N} \sum_{i=1}^N \nabla J^{(i)}(\vec{\theta}) \quad \text{found in D} \\ &= \frac{1}{N} \sum_{i=1}^N - (y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}) \vec{x}^{(i)} \end{aligned}$$

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