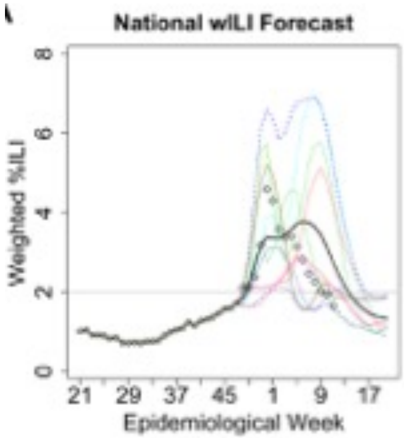
10-301/601: Introduction to Machine Learning Lecture 7 – Linear Regression

Henry Chai & Matt Gormley & Hoda Heidari

2/7/24

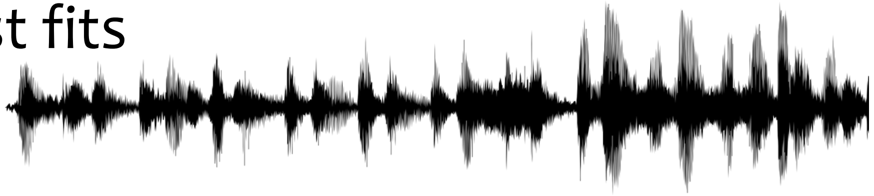
Regression



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

This is what differentiates *regression* from *classification*

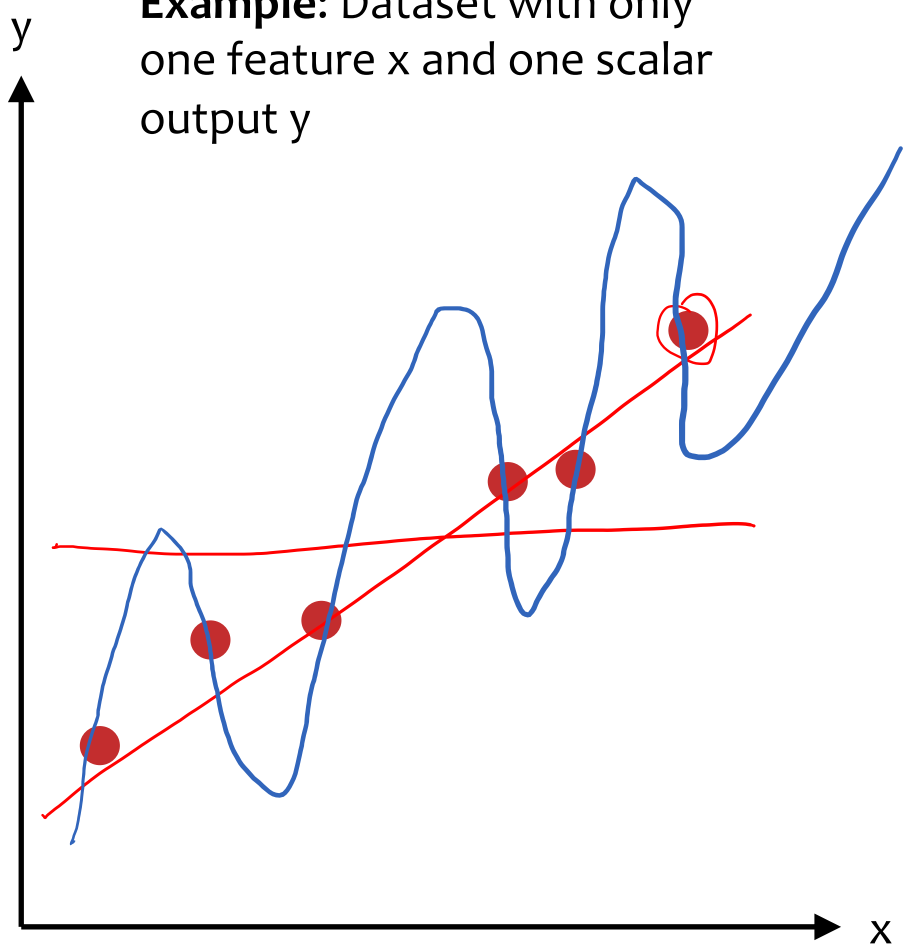


Example Applications:

- 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

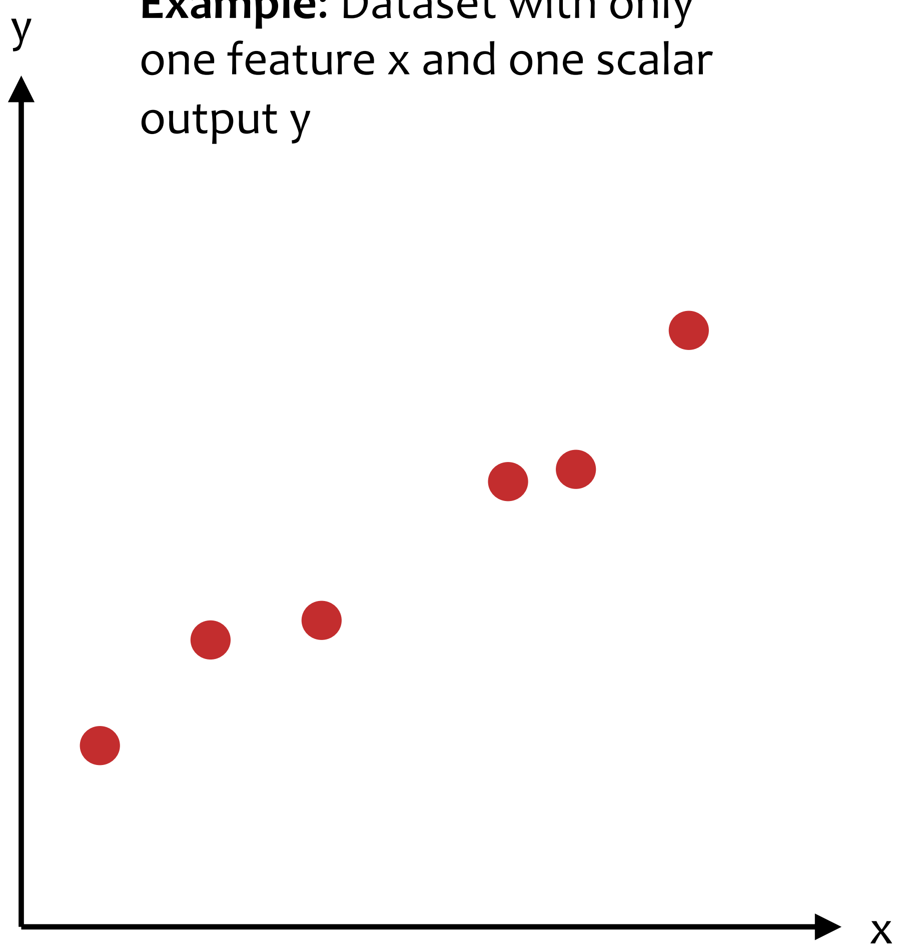


Q: What is the function that best fits these points?

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

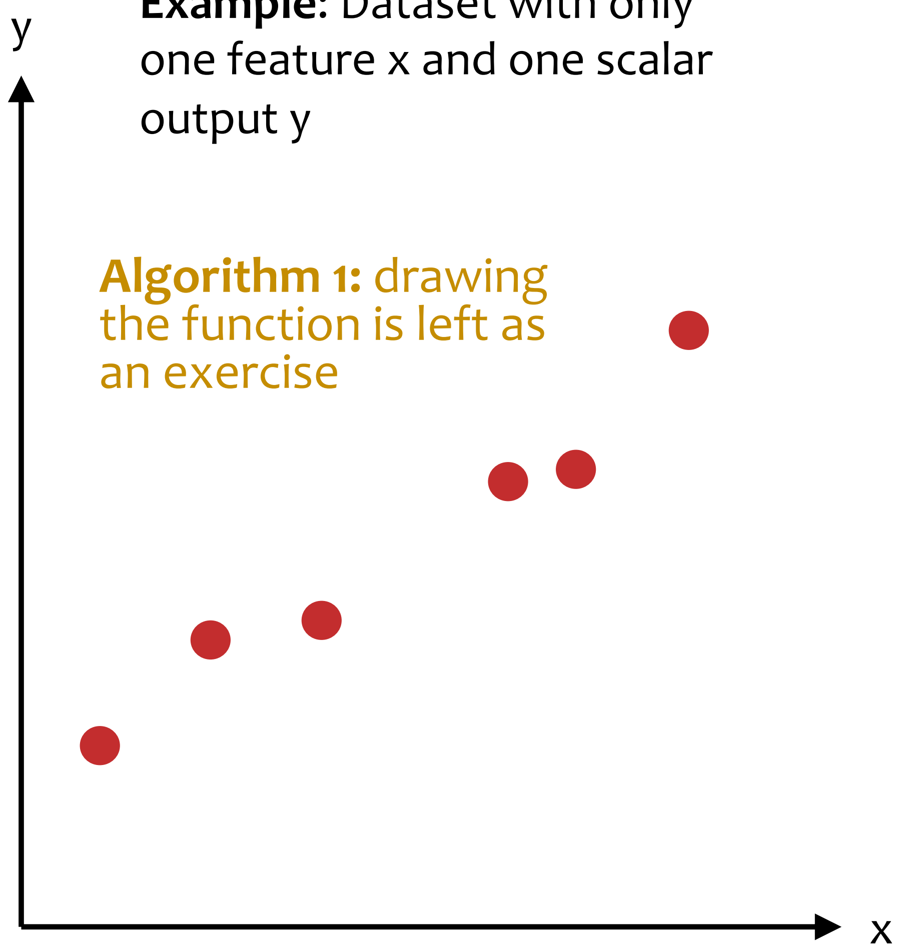
- *Train*: store all (x, y) pairs
- *Predict*: pick the nearest x in training data and return its y

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: k=1 Nearest Neighbor Regression

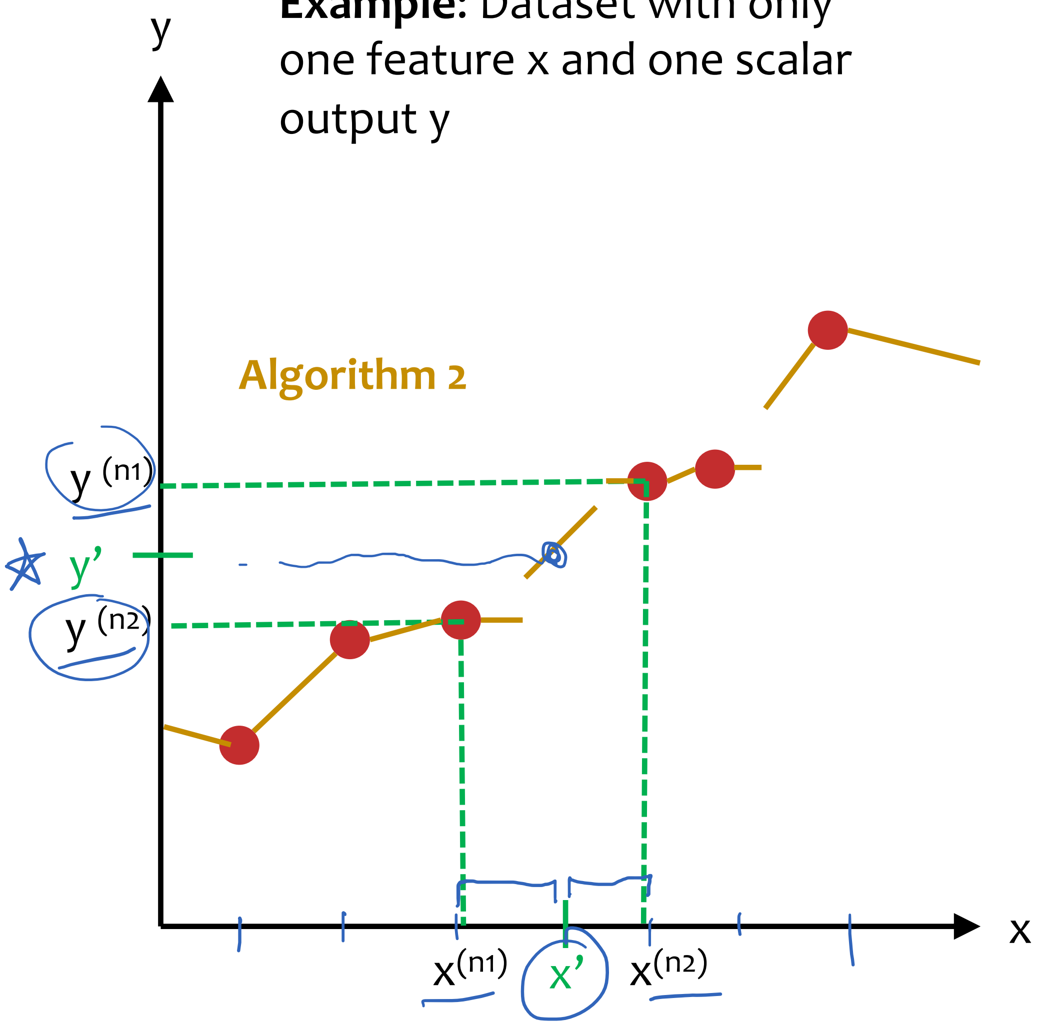
- *Train*: store all (x, y) pairs
- *Predict*: pick the nearest x in training data and return its y

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



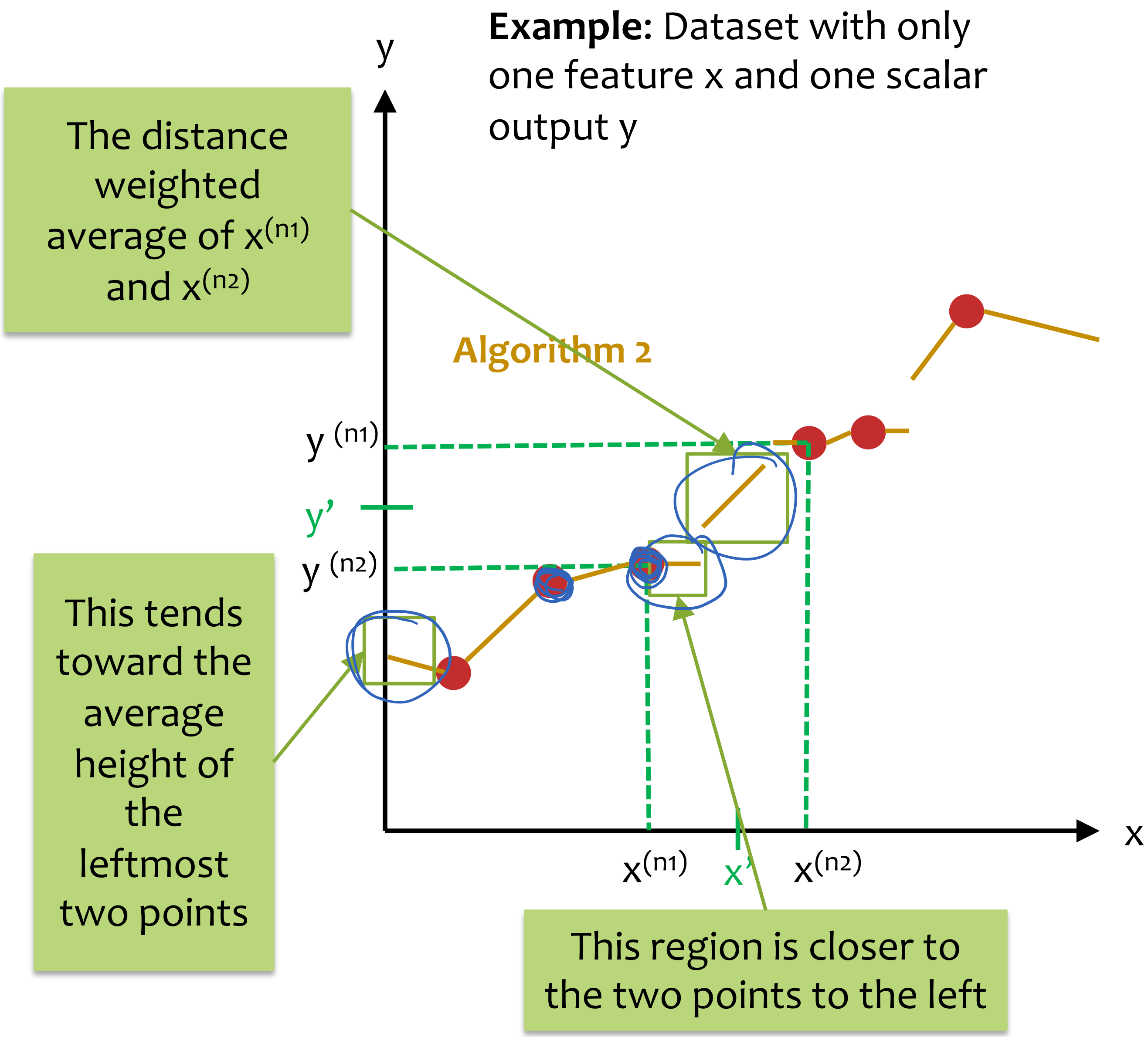
Algorithm 1: k=1 Nearest Neighbor Regression

- *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



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

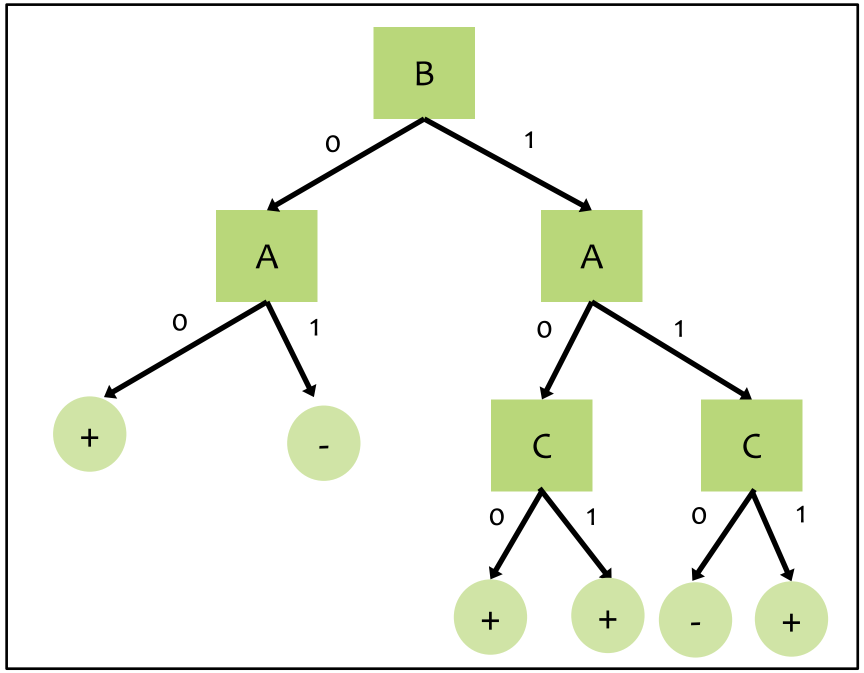
Algorithm 2: k=2 Nearest Neighbors Distance Weighted Regression

- *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

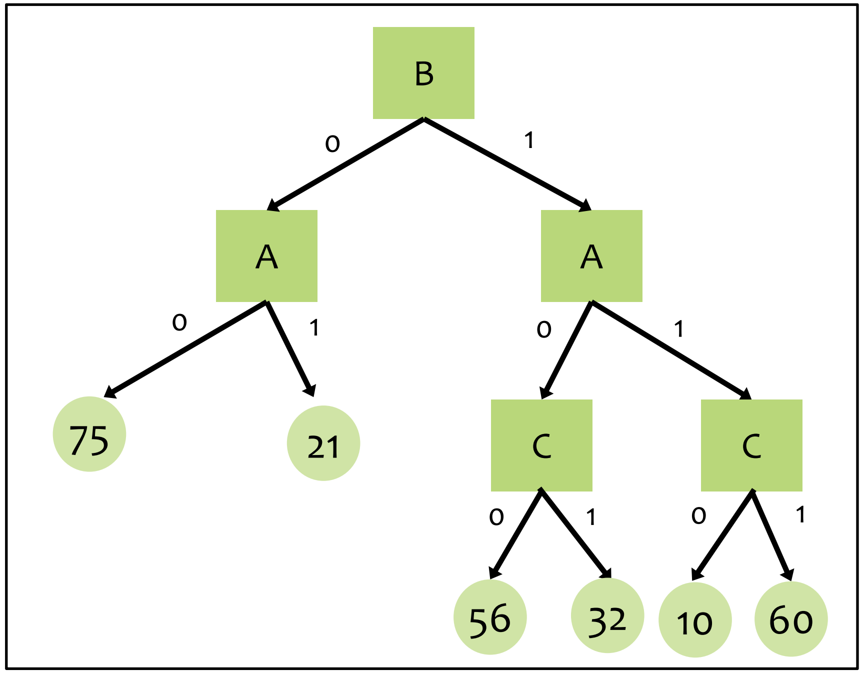
DECISION TREE REGRESSION

Decision Tree Regression

Decision Tree for Classification



Decision Tree for Regression

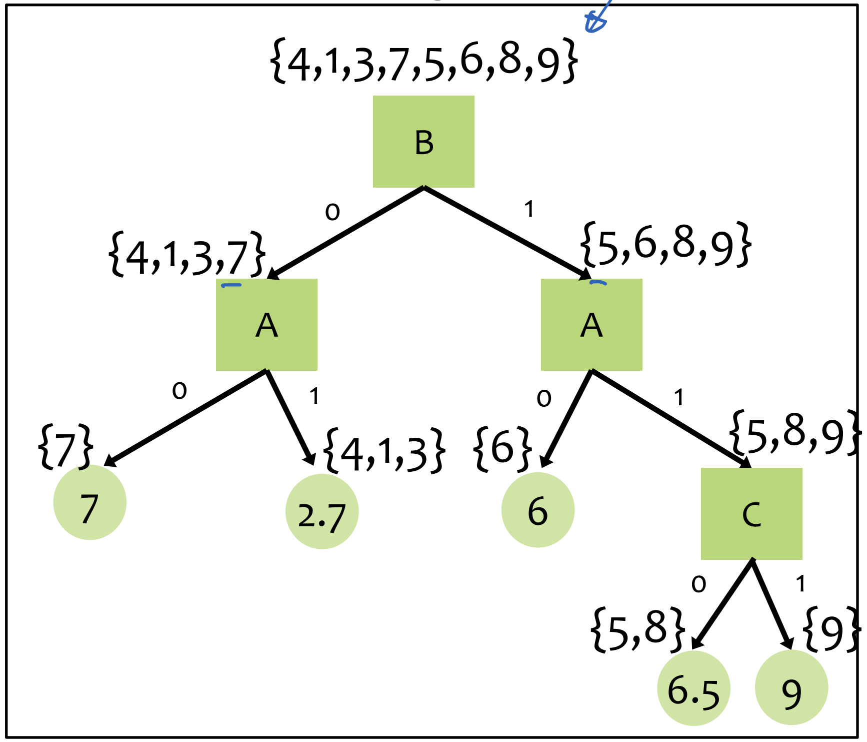


Decision Tree Regression

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

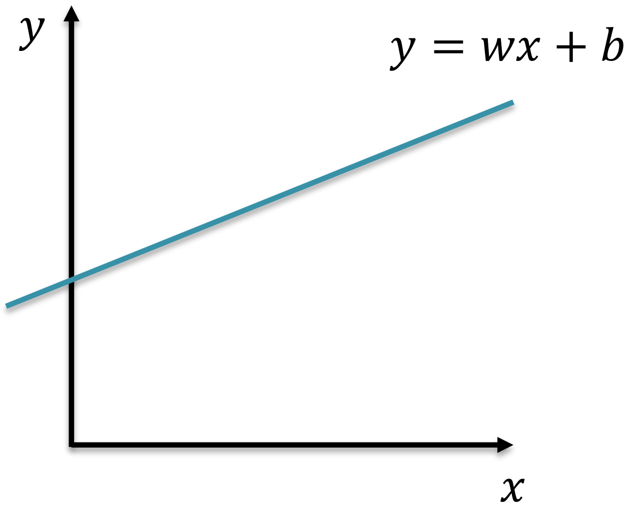
Linear Functions

<u>Def</u>: 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 ≠ Linear decision boundaries



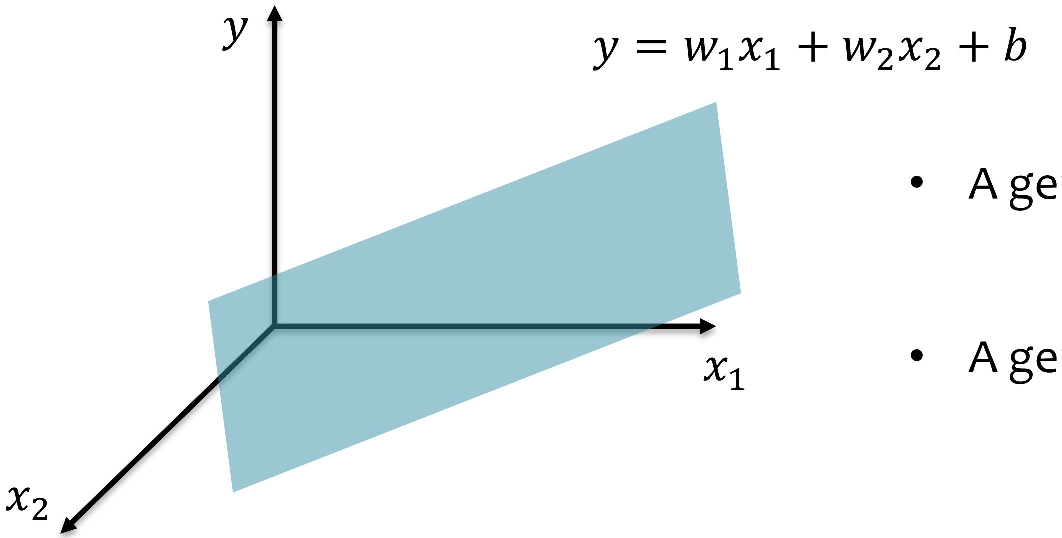
Linear Functions

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

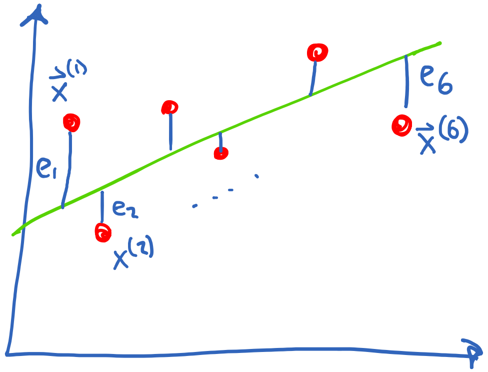


- A general linear function is
  $$y = \mathbf{w}^T \mathbf{x} + b$$
- A general linear decision boundary is
  $$y = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$$

Key Idea of Linear Regression

Residuals

Def: a residual is the distance
from observed
to predicted value y



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

Key Idea of Linear Regression

Find the linear function h (w/parameters $\vec{w}, b$) that minimizes the $\boxed{\text{squares of the residuals}}$ for a training set

only one option

Mean squared error (MSE)

Def: MSE Objective Function

$$J_D(\vec{w}, b) = \frac{1}{N}\sum_{i=1}^{N} (e_i)^2$$
$$= \frac{1}{N}\sum_{i=1}^{N} (y^{(i)} - (\vec{w}^T\vec{x}^{(i)} + b))^2$$

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 $\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta} \in \mathbb{R}^M}{\text{argmin}}\, J(\boldsymbol{\theta})$

For ML, these are the parameters

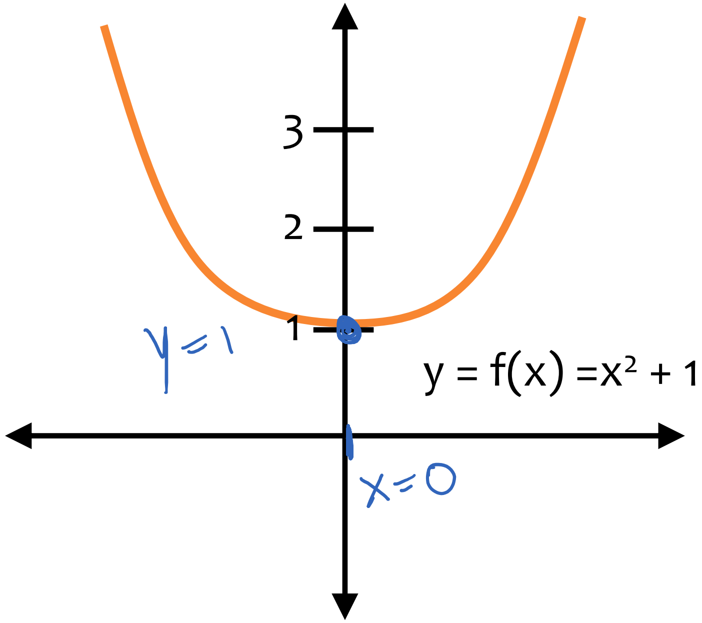
For ML, this is the objective function

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



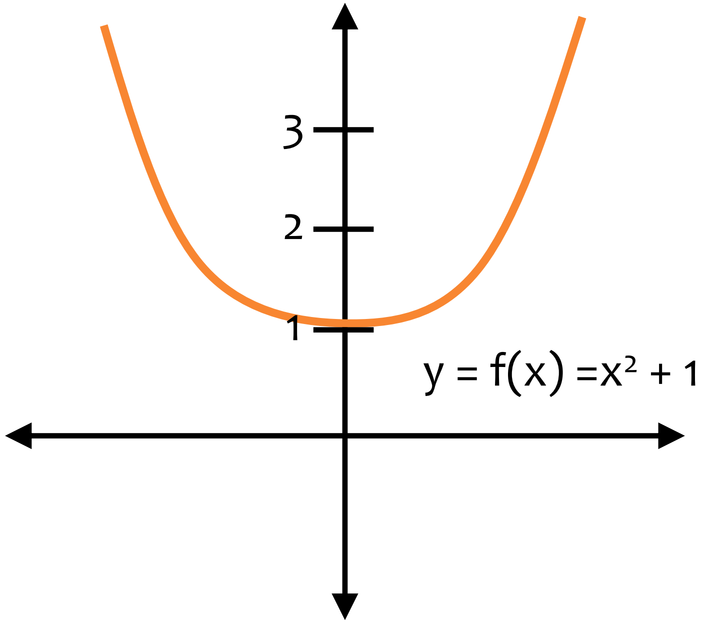
$v^* = \min_x f(x)$

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

Q1 1. Question: What is v*?

Q2 2. Question: What is x*?

min vs. argmin



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

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

1. Question: What is v*?

   $v^* = 1$, the minimum value of the function

2. Question: What is x*?

   $x^* = 0$, the argument that yields the minimum value

OPTIMIZATION METHOD #0: RANDOM GUESSING

Notation Trick: Folding in the Intercept Term

$M = |\theta|$

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

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

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!

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

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

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:

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

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*
   - ...

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

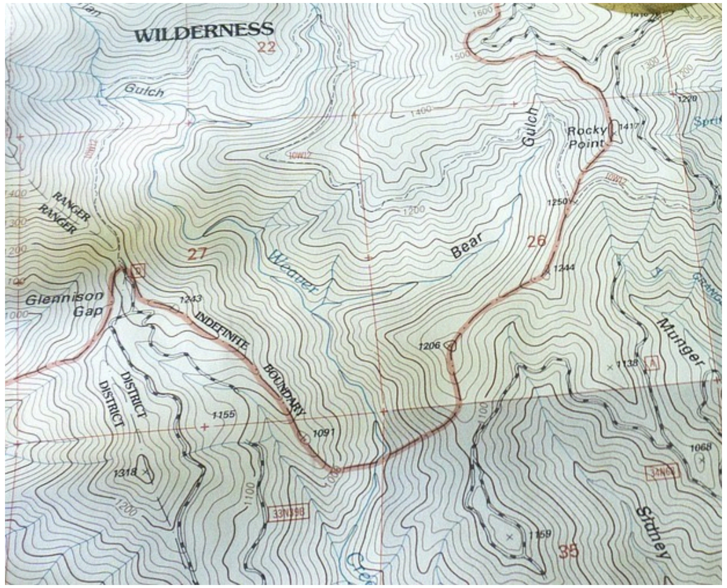
5. Test time: given a new $\mathbf{x}$, make prediction $\hat{y}$

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

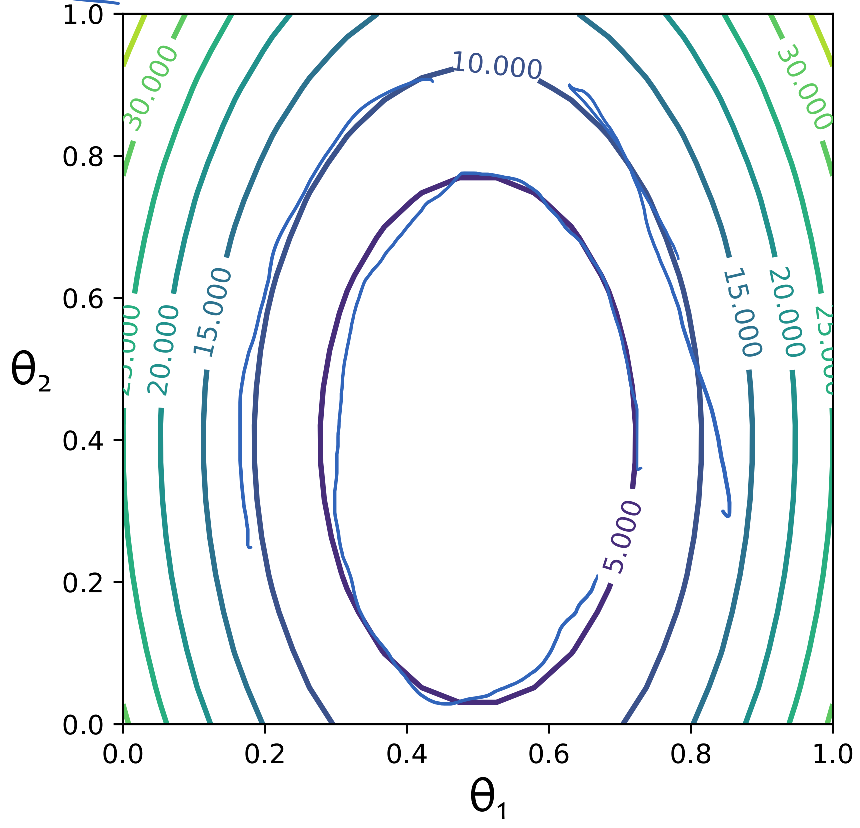
Contour Plots

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



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

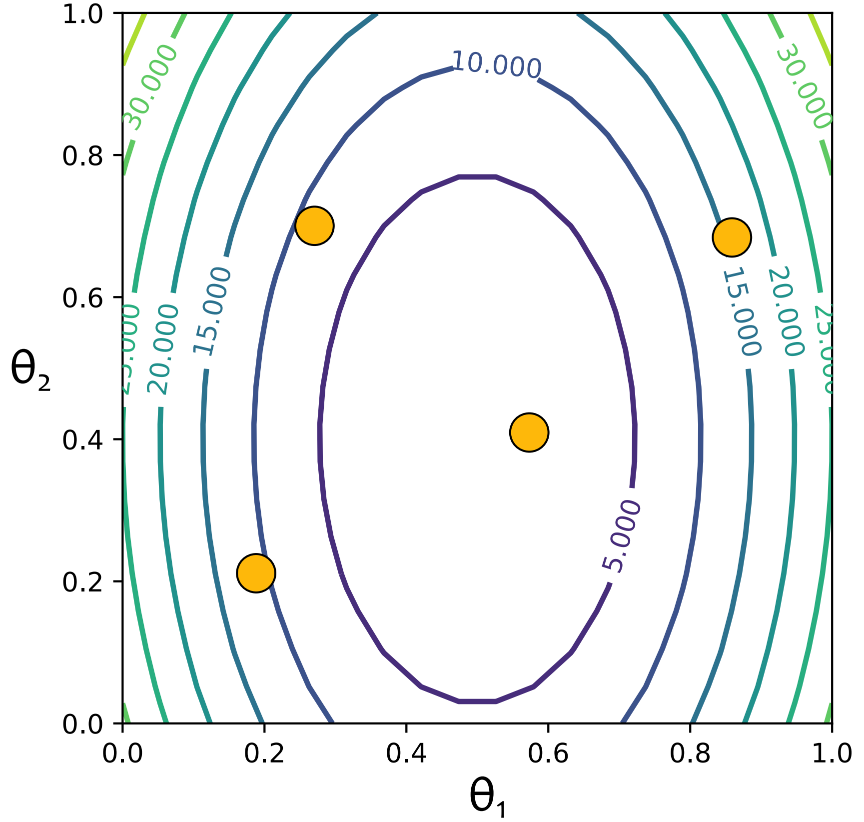


Optimization by Random Guessing

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	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

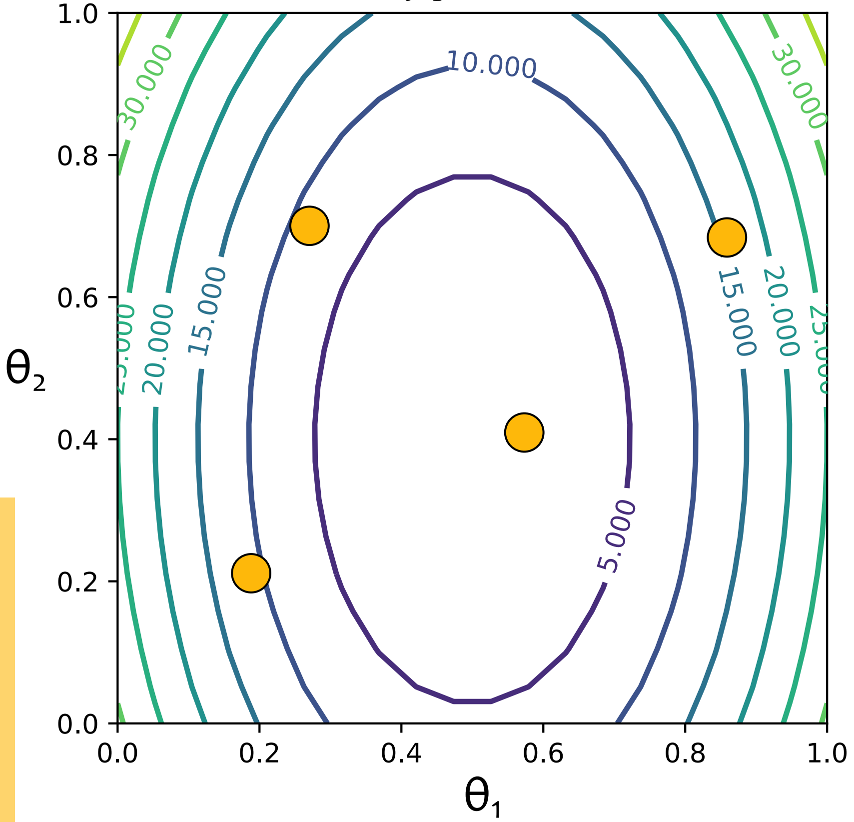
Optimization Method #0: Random Guessing

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 $J(\boldsymbol{\theta})$

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

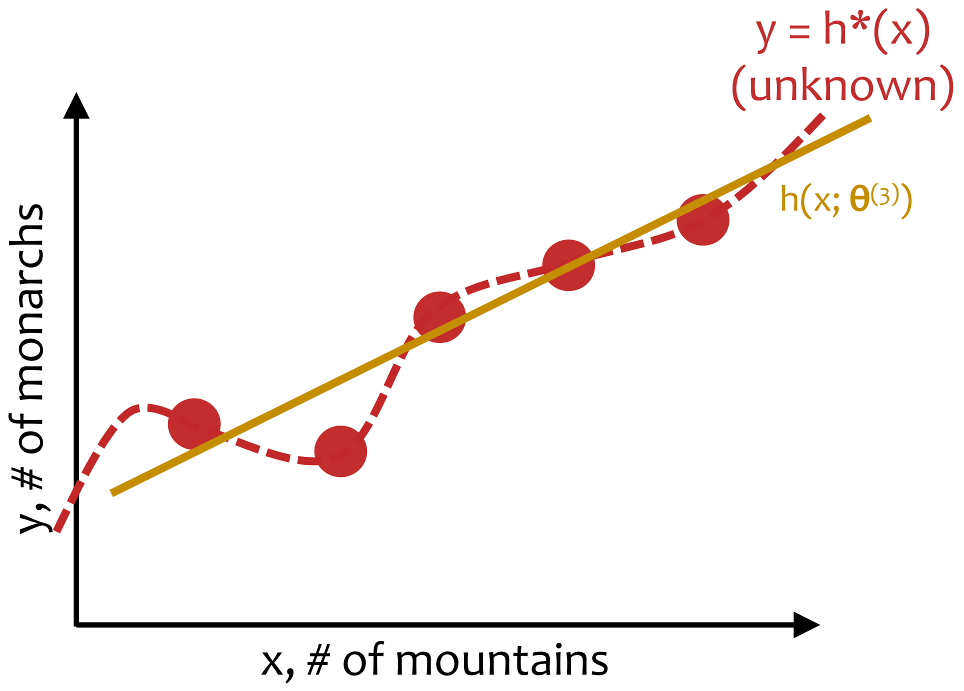
$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2$$



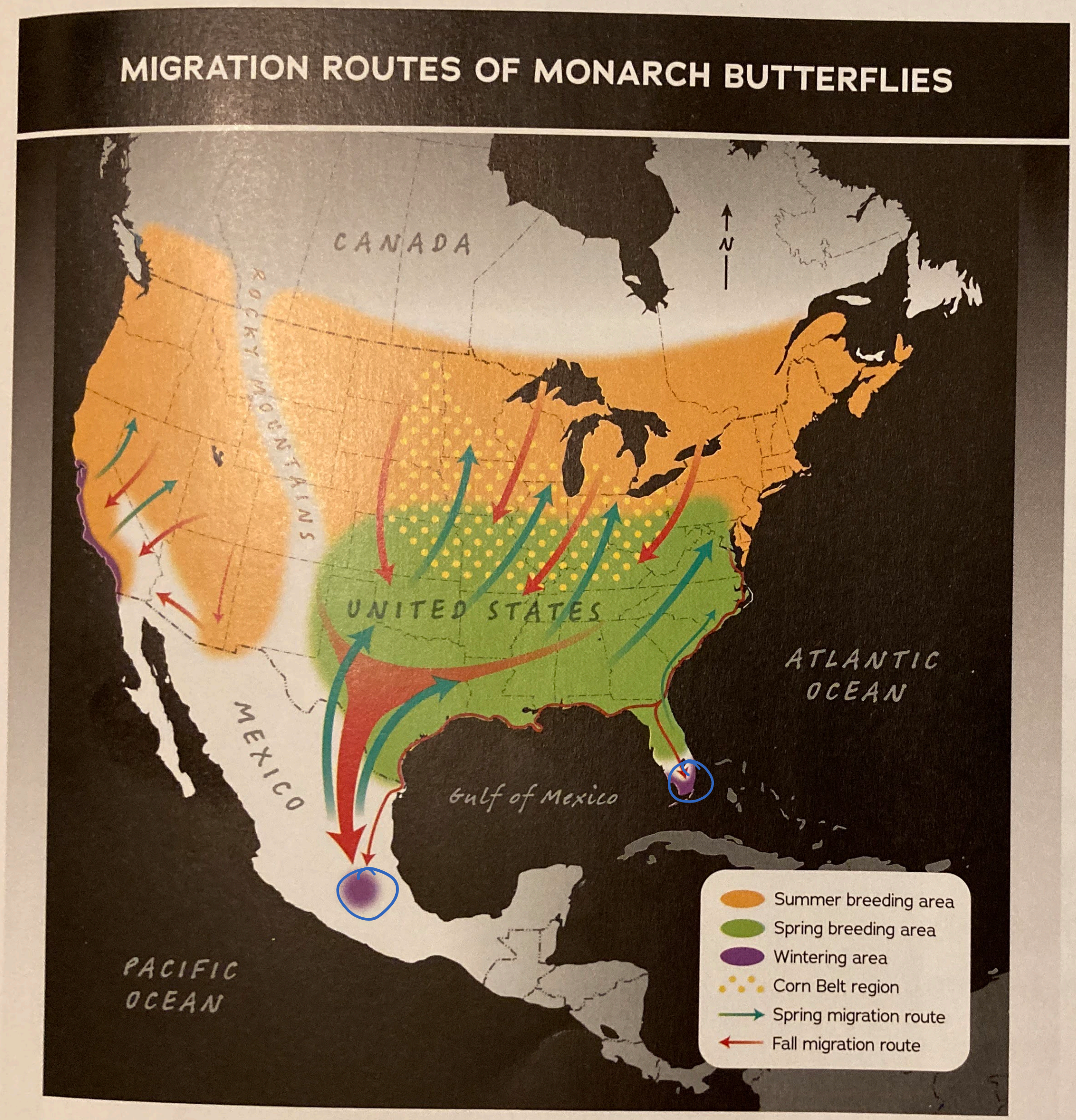
t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.2	0.2	10.4
2	0.3	0.7	7.2
3	0.6	0.4	1.0
4	0.9	0.7	16.2

Linear Regression: Running Example

Counting Butterflies



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.

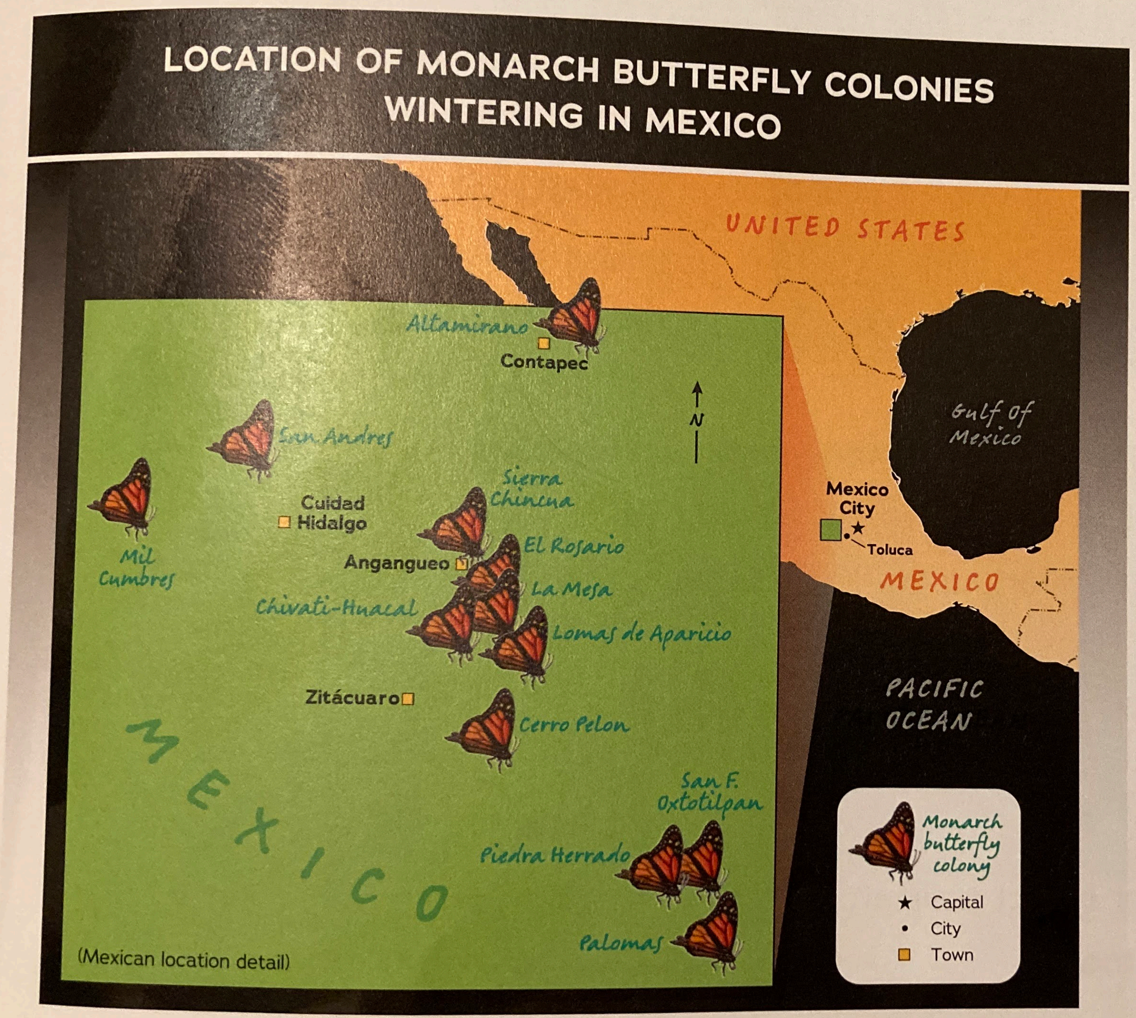


This map shows migration routes of fall and spring migrations, both east and west of the Rocky Mountains.

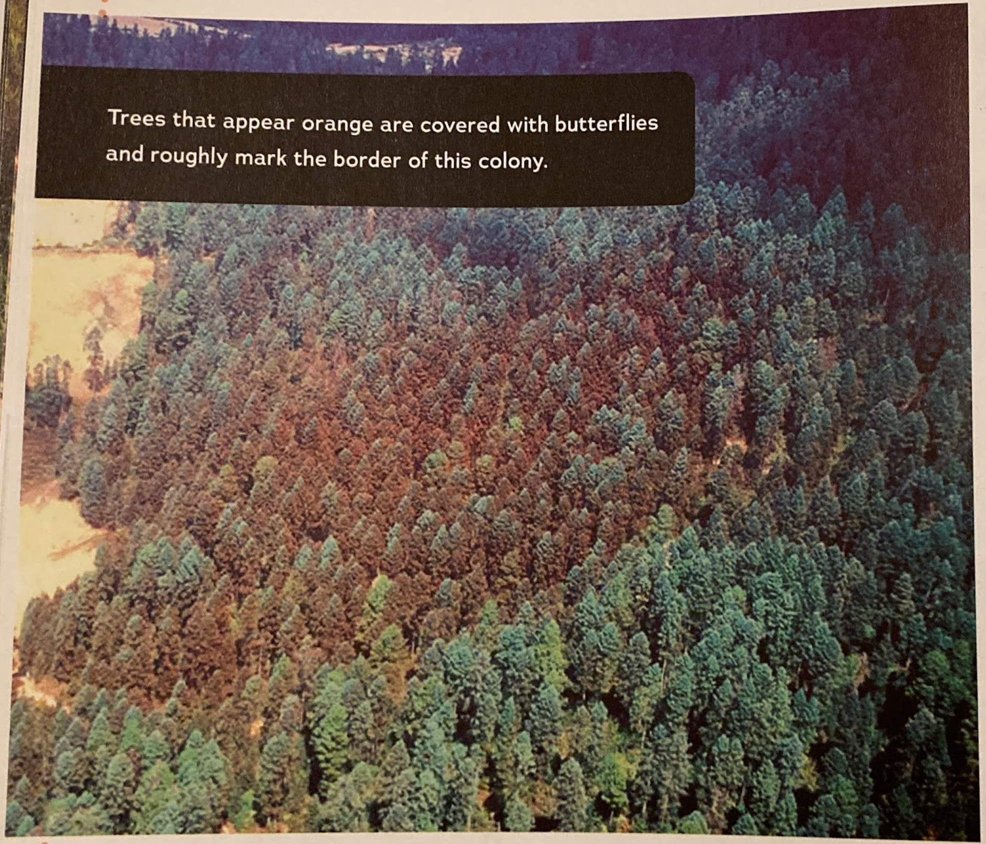
...reveal about the eastern monarchs?

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 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.

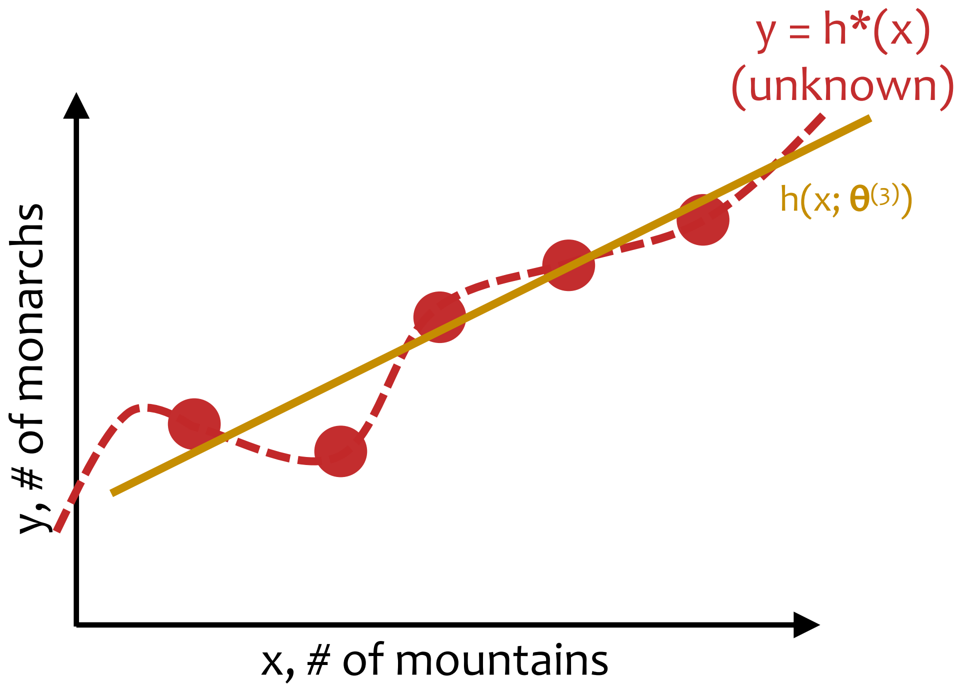
Many scientists were worried. The population of eastern monarchs had dropped more than 90 percent in just seventeen years.

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.

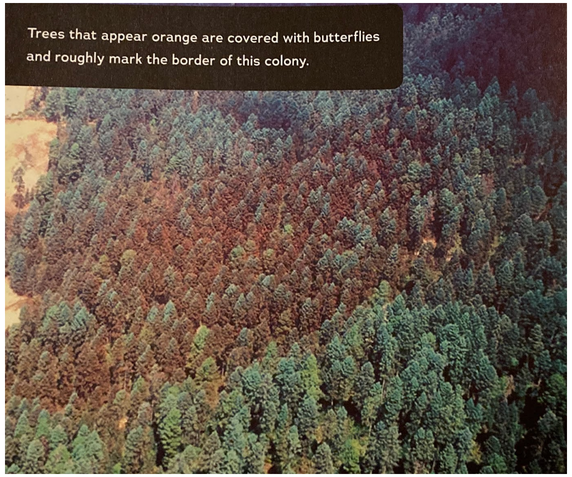
Counting Butterflies



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

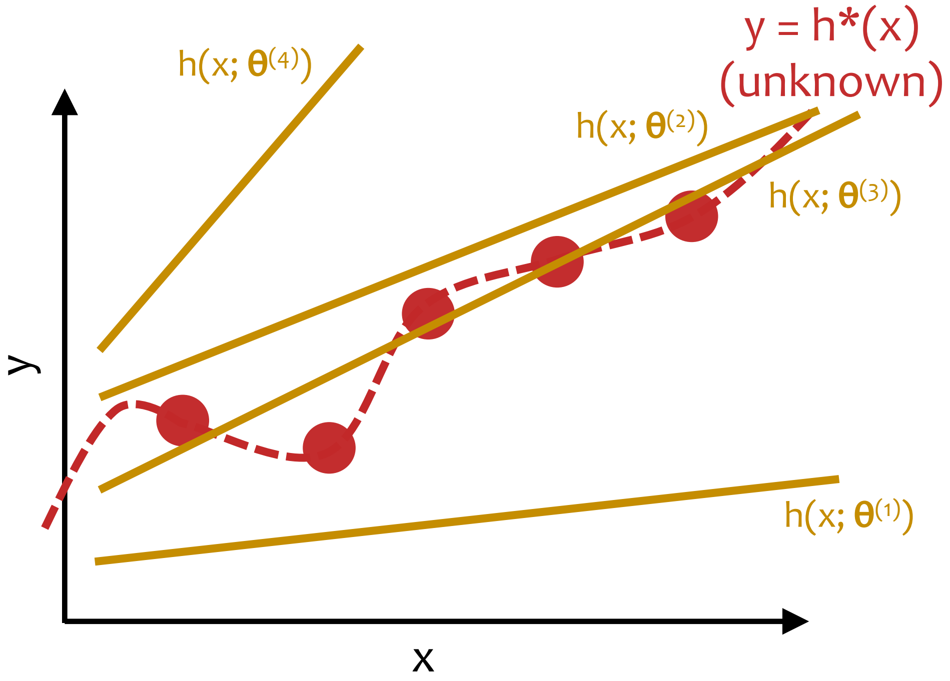


Q: How would you obtain ground truth data?

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
4. Return $\boldsymbol{\theta}$ that gives smallest $J(\boldsymbol{\theta})$



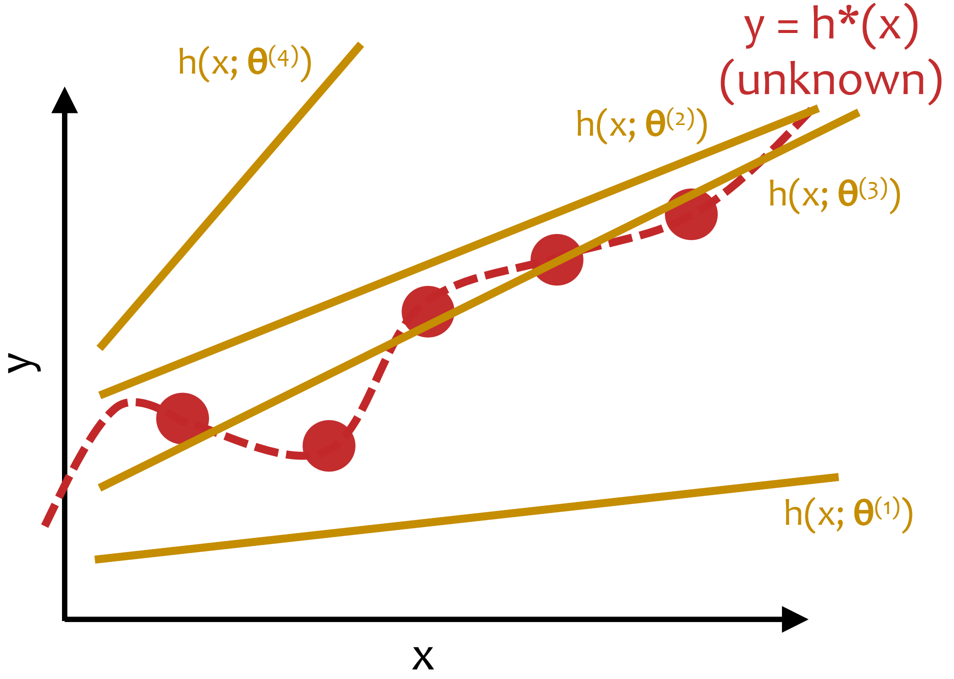
For Linear Regression:

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

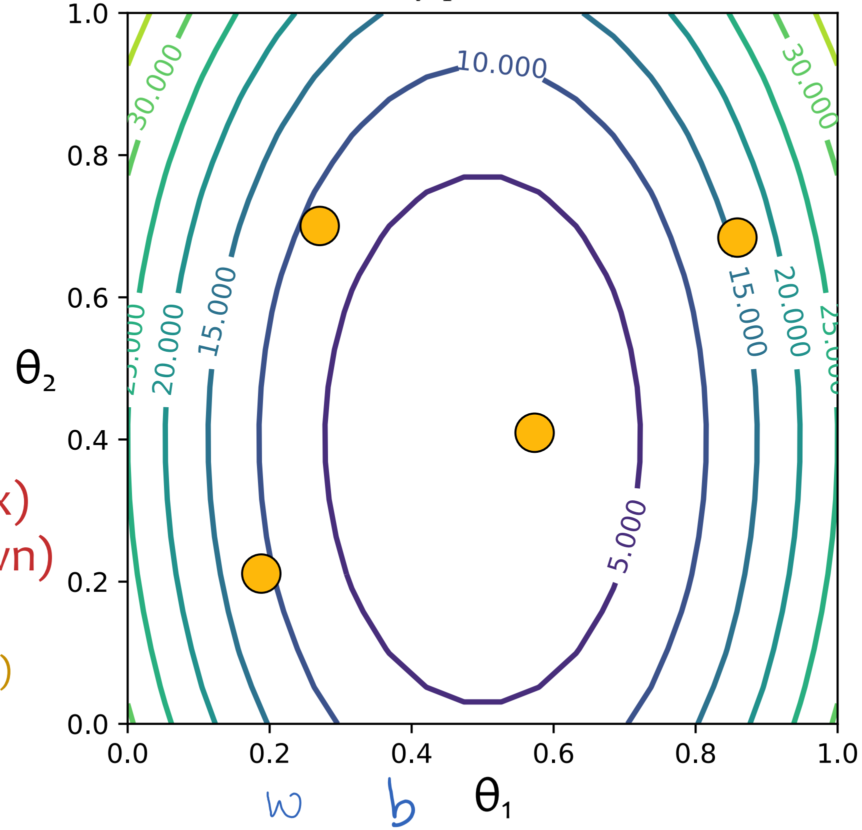
Linear Regression by Rand. Guessing

Optimization Method #0: Random Guessing

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



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

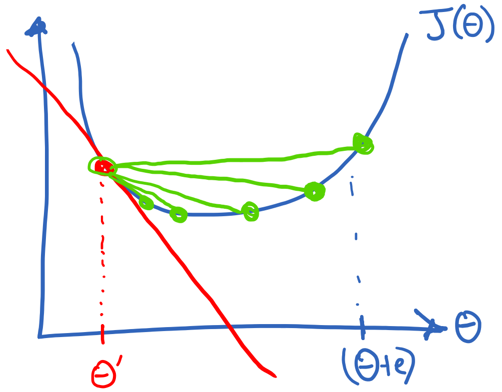


t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.2	0.2	10.4
2	0.3	0.7	7.2
3	0.6	0.4	1.0
4	0.9	0.7	16.2

OPTIMIZATION METHOD #1: GRADIENT DESCENT

Derivatives

① Deriv. as a Slope



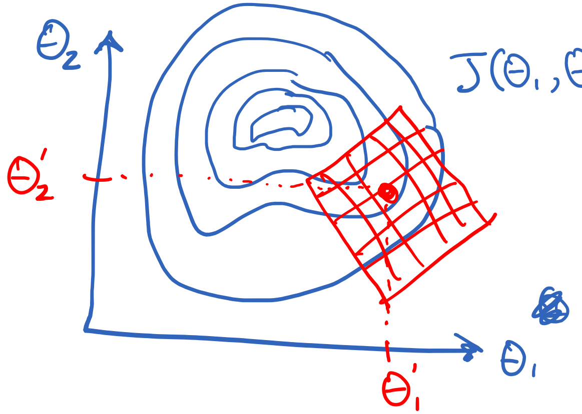
$$\text{slope} = \frac{\partial J(\theta)}{\partial \theta}$$

② Deriv as a Limit

$$\frac{\partial J(\theta)}{\partial \theta} = \boxed{\lim_{e \to 0}} \frac{J(\theta + e) - J(\theta)}{e}$$

limit of the secants is the tangent

③ Deriv as a Tangent Plane



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

$$|\vec{\theta}| = 2$$

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

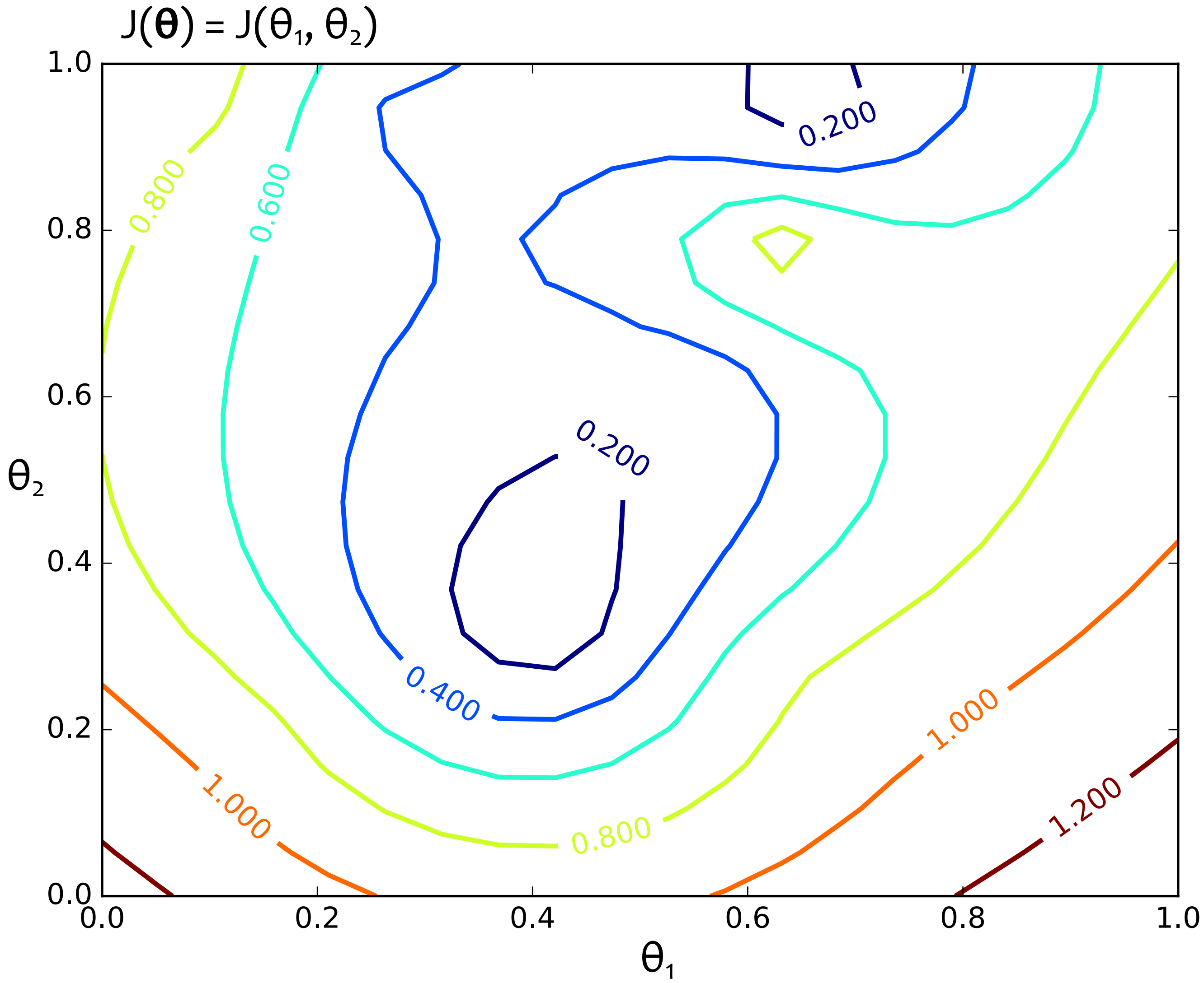
Gradient

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

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

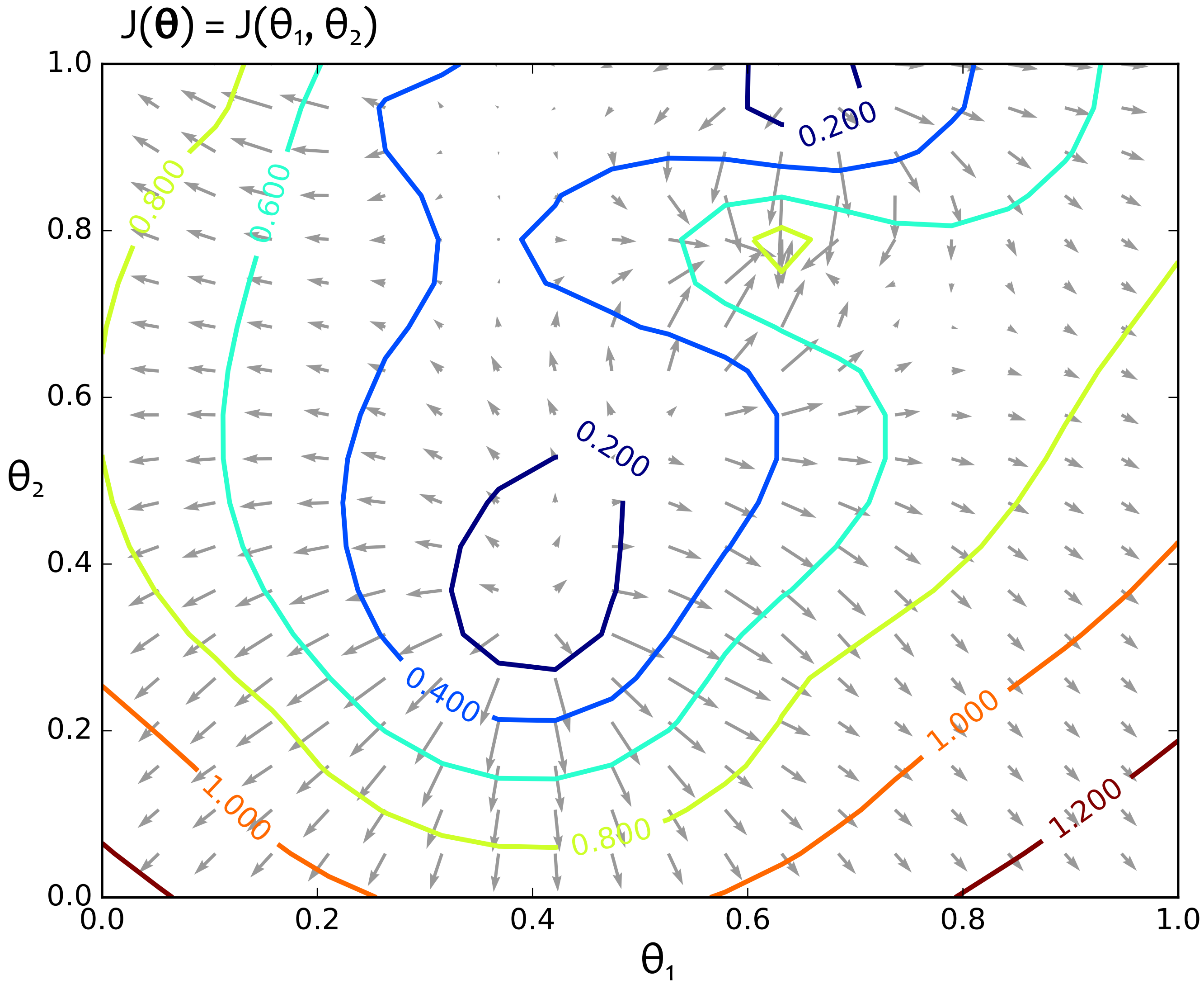
first-order partial derivative

Gradients



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

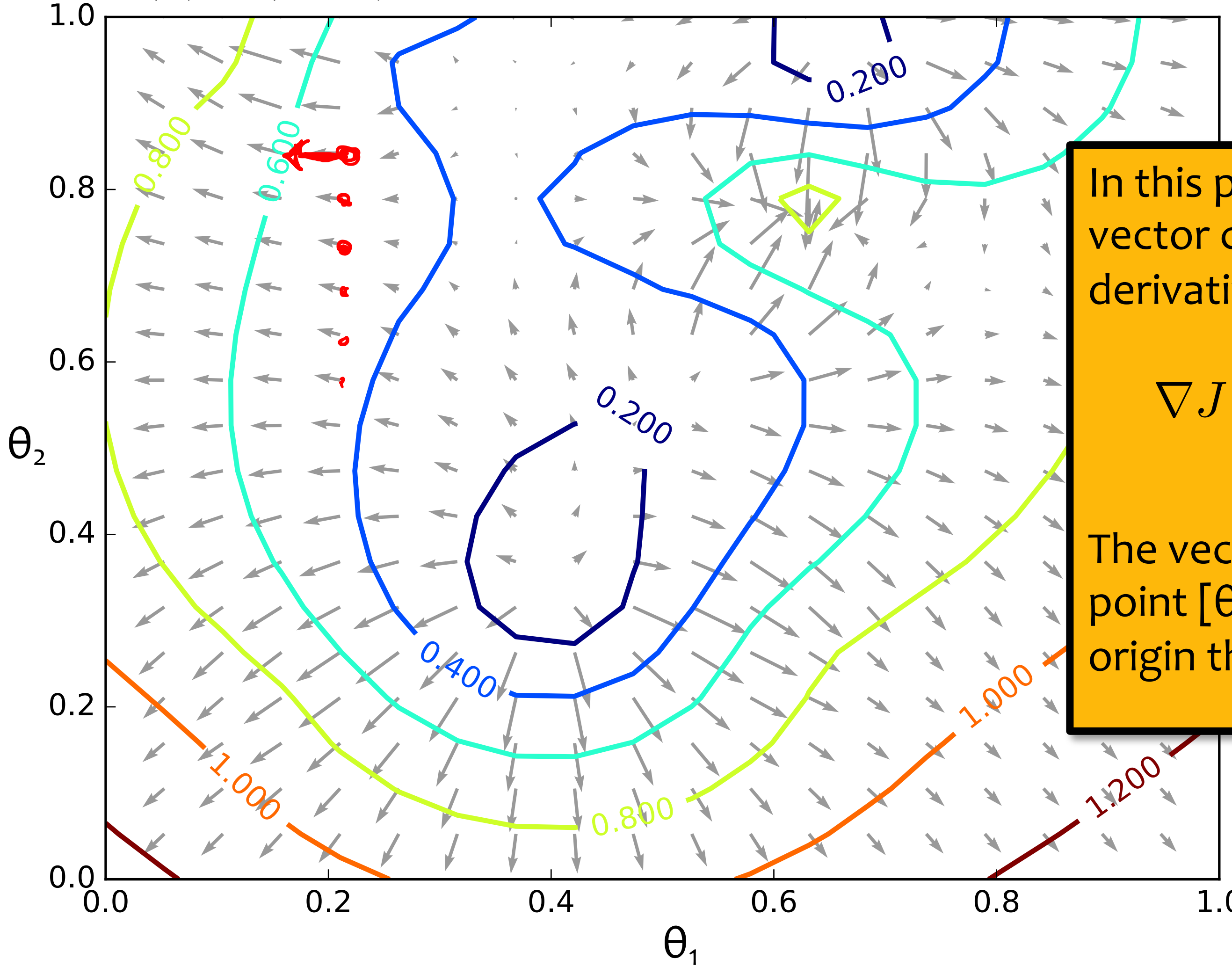
Gradients



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

Gradients

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



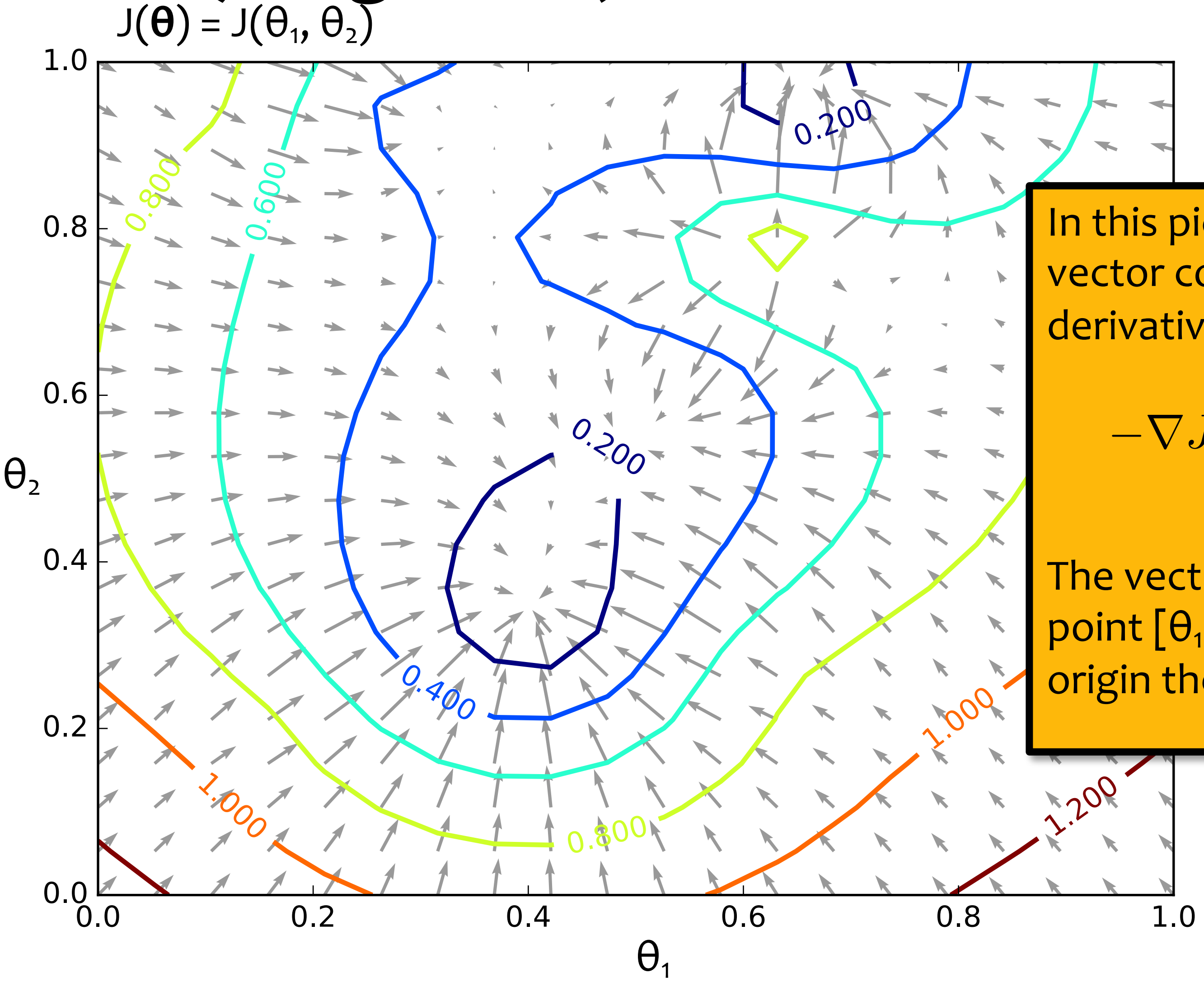
In this picture, each arrow is a 2D vector consisting of two partial derivatives.

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

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



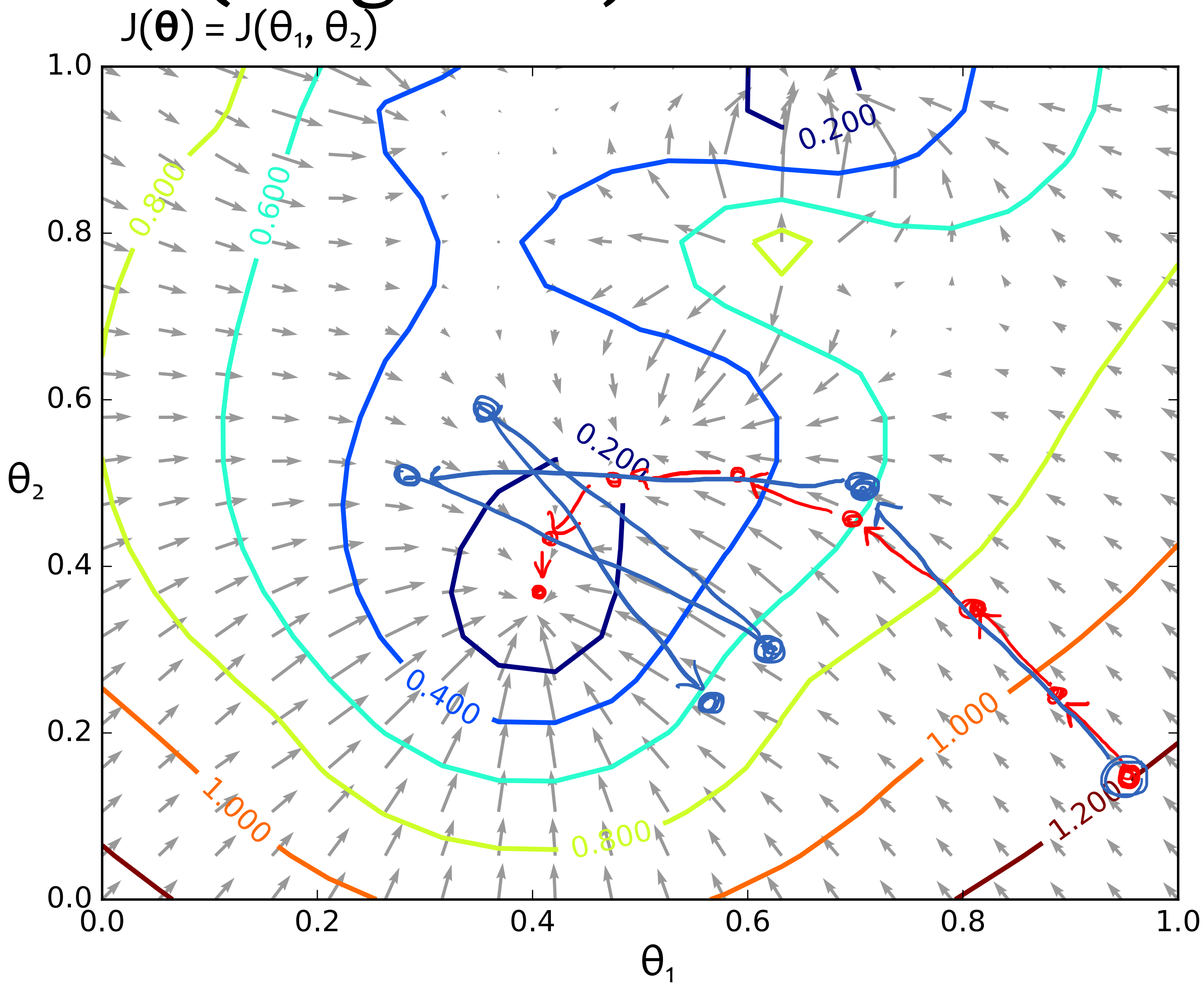
In this picture, each arrow is a 2D vector consisting of two partial derivatives.

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

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

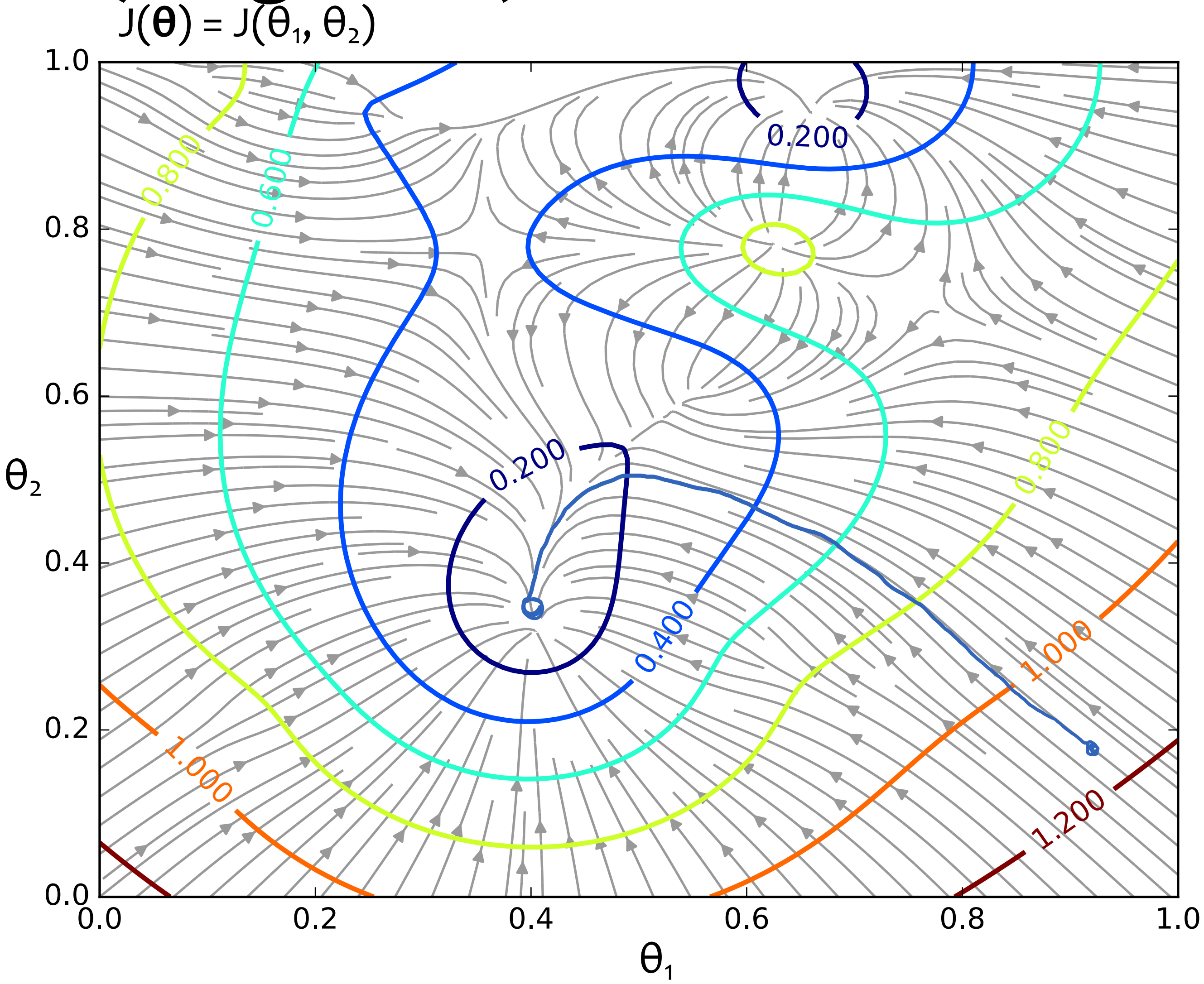
These are the **negative** gradients that Gradient **Descent** would follow.

(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

① Choose initial point $\vec{\theta}$

② Repeat $t = 1, 2, 3, \ldots, T$

a) Compute gradient $\vec{g} = \nabla J(\vec{\theta})$

b) Select step size γ_t

c) Update params $\vec{\theta} \leftarrow \vec{\theta} - \gamma_t \vec{g}$

③ Return $\vec{\theta}$ when stopping criterion reached

Remarks

Initial Point

- randomly
- $\vec{\theta}$ = all zeroes

Step Size

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

Stopping Criterion

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

Gradient Descent: Step Size

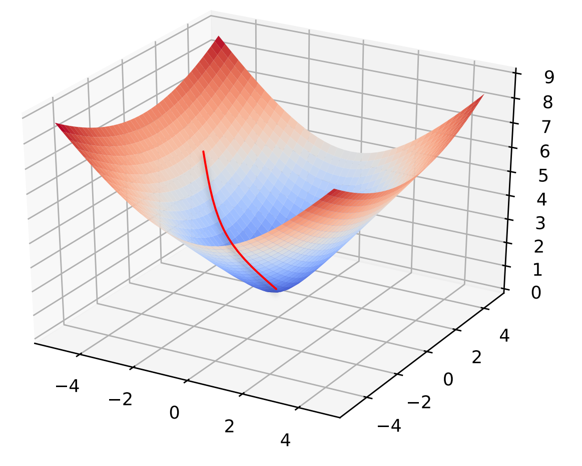
Question:
In gradient descent, what could go wrong if we *always* use the same step size (or step size schedule) for every problem we encounter?

Answer:

Gradient Descent

Algorithm 1 Gradient Descent

procedure GD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
  while not converged **do**
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
  return $\boldsymbol{\theta}$



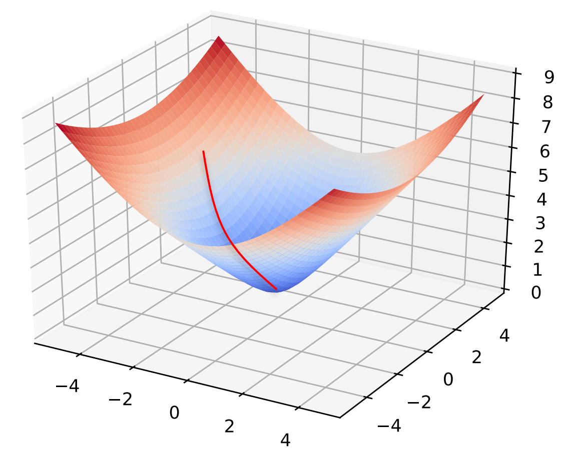
In order to apply GD to Linear Regression all we need is the **gradient** of the objective function (i.e. vector of partial derivatives).

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

Gradient Descent

Algorithm 1 Gradient Descent

procedure GD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
  while not converged **do**
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
  return $\boldsymbol{\theta}$



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.

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

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)

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

4. Solve the unconstrained optimization problem via favorite method:
   - *gradient descent*
   - *closed form*
   - *stochastic gradient descent*
   - ...

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

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

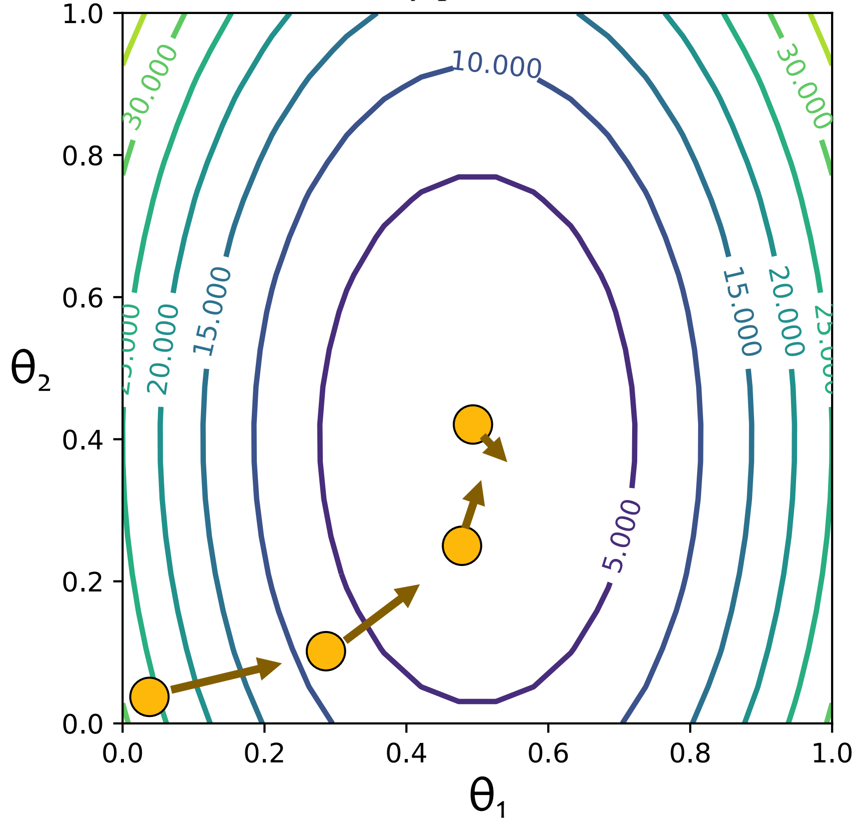
$$\hat{y} = h_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) = \hat{\boldsymbol{\theta}}^T\mathbf{x}$$

Linear Regression by Gradient Desc.

Optimization Method #1: Gradient Descent

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

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

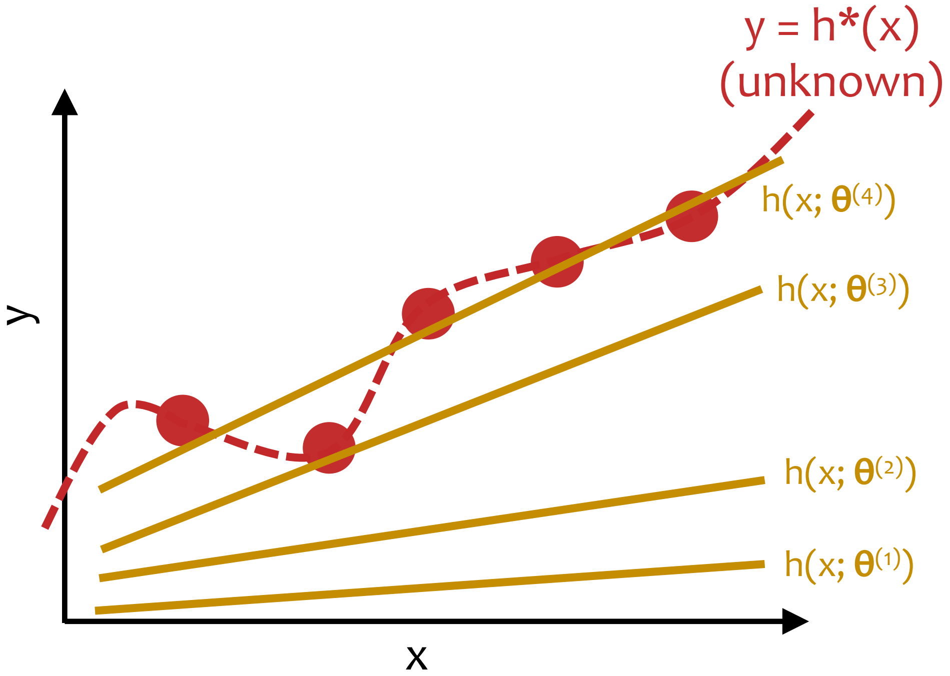


t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

Linear Regression by Gradient Desc.

Optimization Method #1: Gradient Descent

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

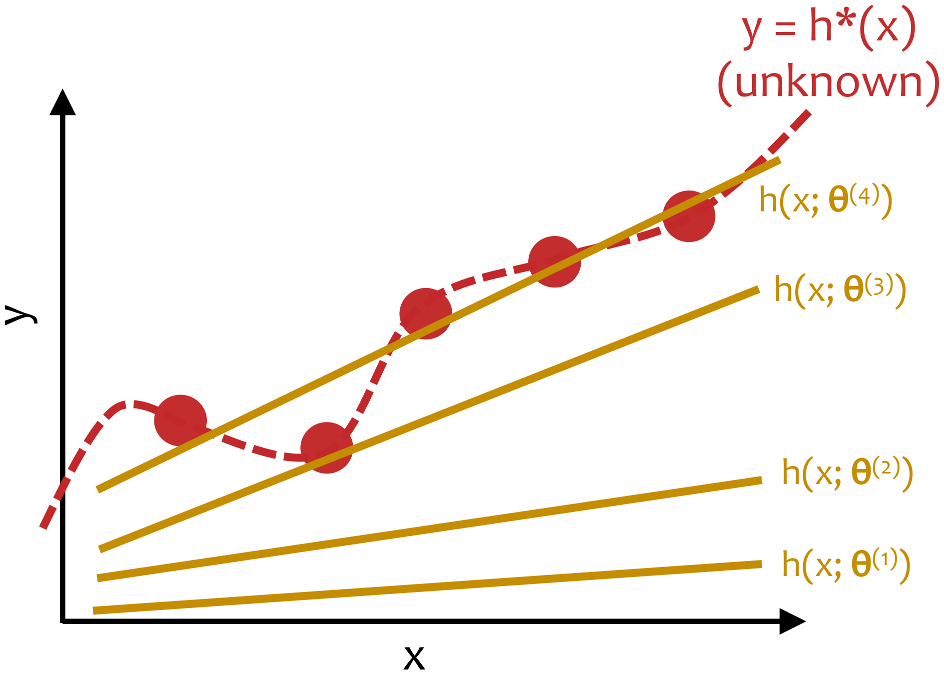


t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

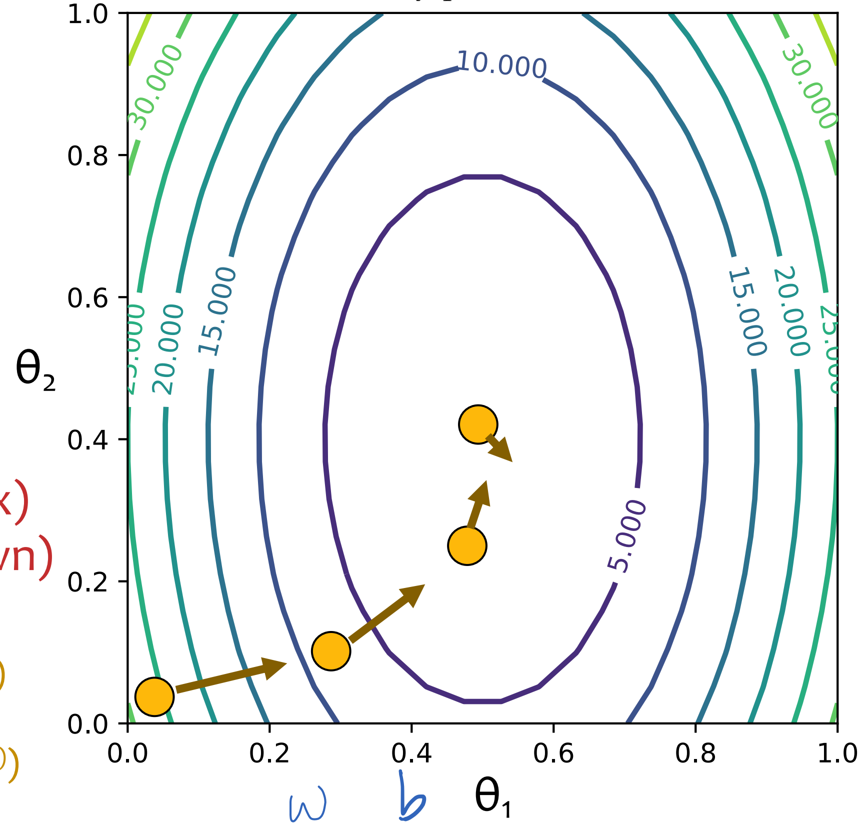
Linear Regression by Gradient Desc.

Optimization Method #1: Gradient Descent

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

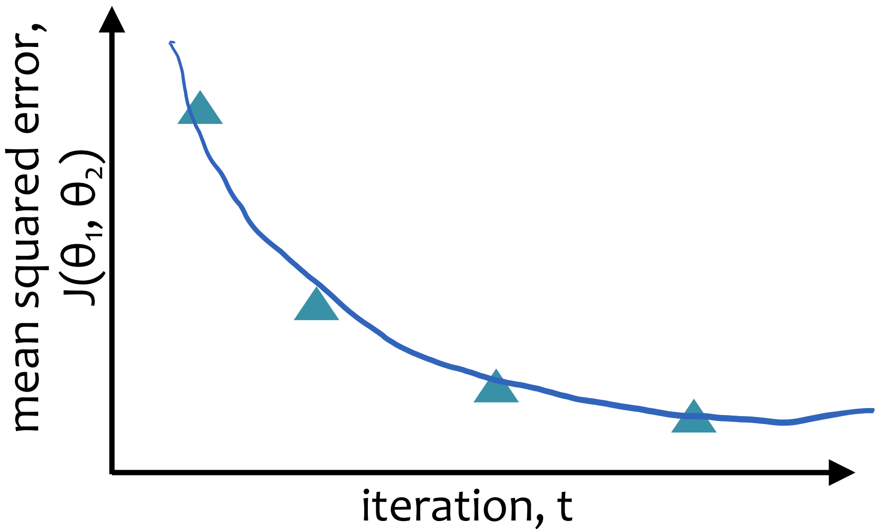


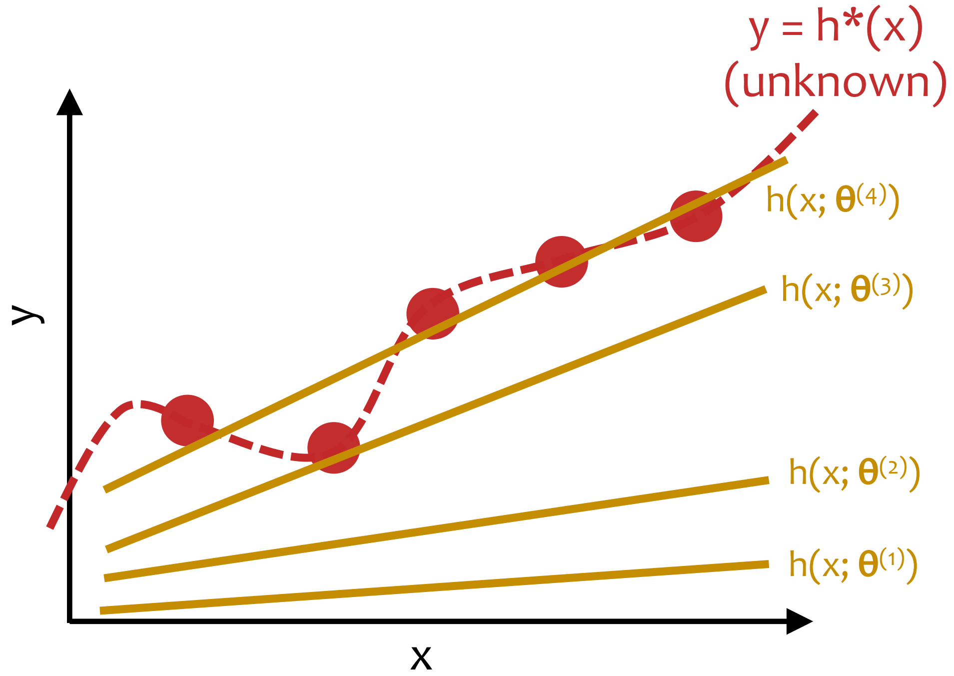
$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2$$



t	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

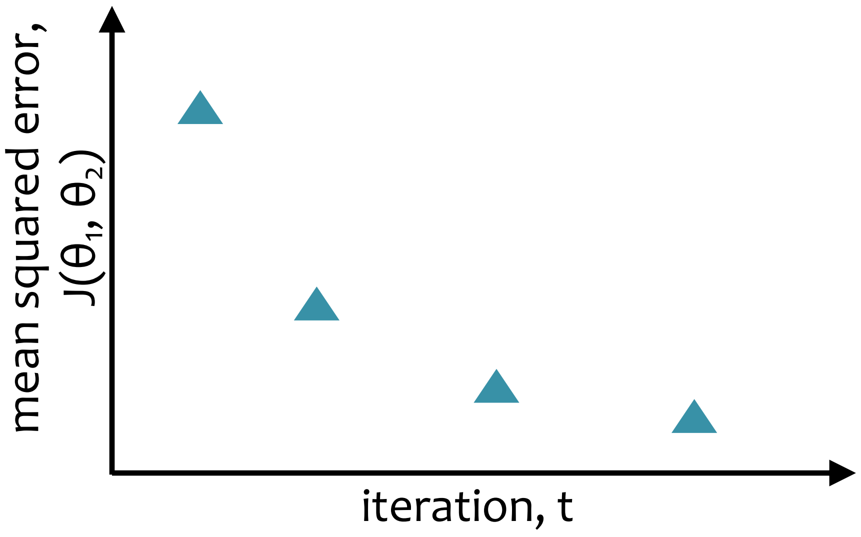
Linear Regression by Gradient Desc.



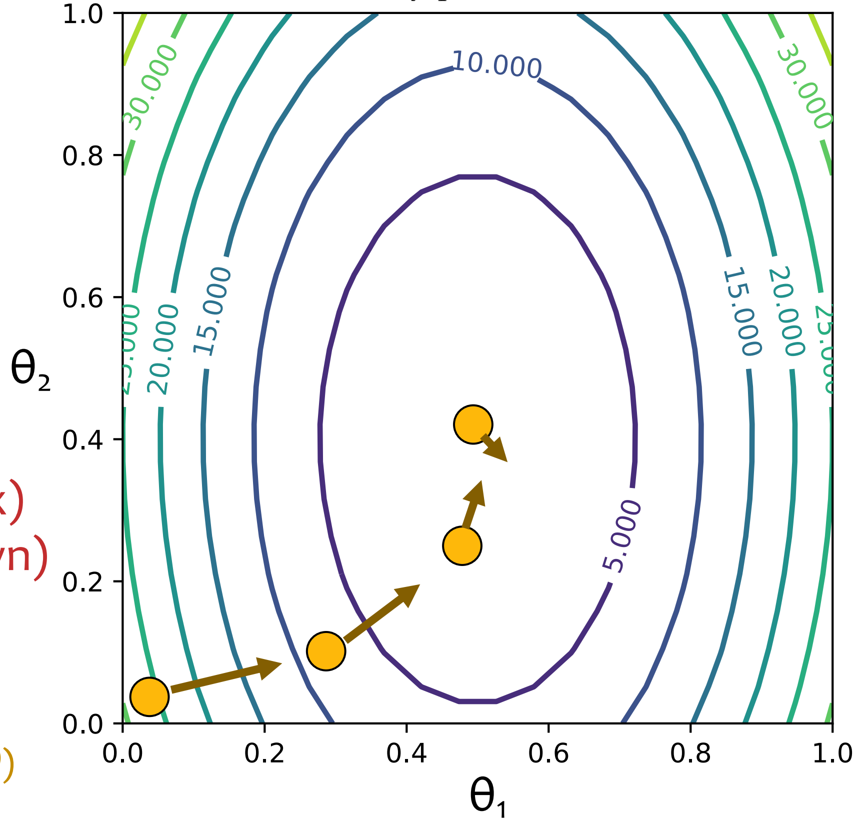


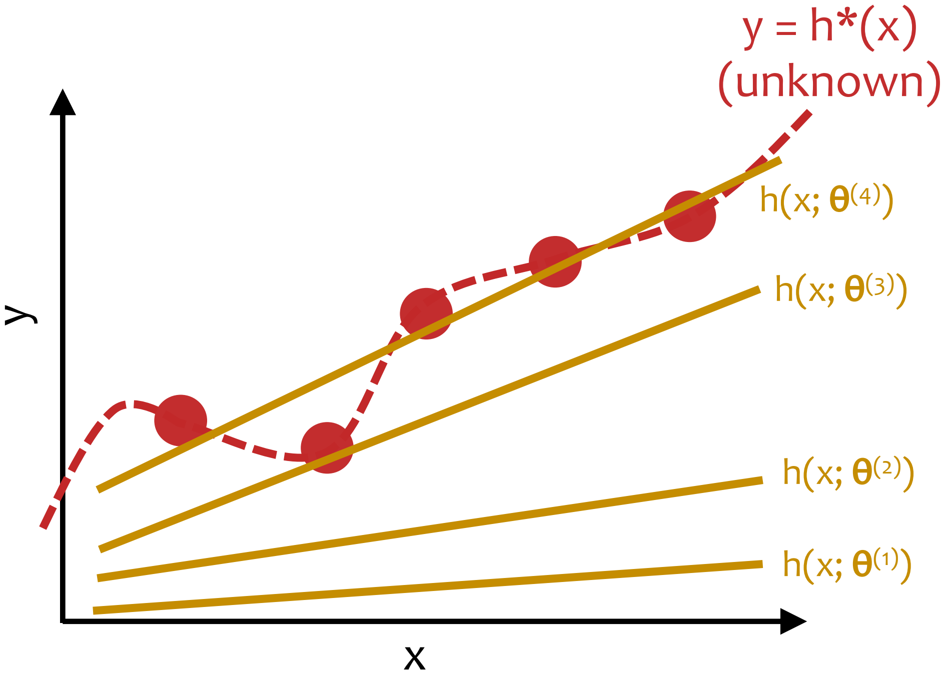
t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

Linear Regression by Gradient Desc.



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





t	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

$\vec{\theta} = [\theta_1, \ldots, \theta_M]^T$

Gradient Calculation for Linear Regression

MSE:

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

does not change the argmin

Partial Derivs

$$\frac{\partial J^{(i)}(\vec{\theta})}{\partial \theta_j} = \frac{\partial}{\partial \theta_j}\left(\frac{1}{2}\left(y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}\right)^2\right)$$

$$= \cancel{\frac{1}{2} \cdot 2}\left(y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}\right) \frac{\partial}{\partial \theta_j}\left(y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}\right)$$

$$= \left(y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}\right) \frac{\partial}{\partial \theta_j}\left(y^{(i)} - \sum_{m=1}^{M} \theta_m x_m^{(i)}\right)$$

$$= -\left(y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}\right) x_j^{(i)}$$

Gradient

$$\nabla J^{(i)}(\theta) = \begin{bmatrix} \partial J / \partial \theta_1 \\ \vdots \\ \partial J / \partial \theta_M \end{bmatrix} = \underbrace{-\left(y^{(i)} - \theta^T x^{(i)}\right)}_{\text{scalar}} \underbrace{\vec{x}^{(i)}}_{\text{vector}}$$

$$\nabla J(\theta) = \nabla\left(\frac{1}{N}\sum_{i=1}^{N} J^{(i)}(\theta)\right)$$

$$= \frac{1}{N}\sum_{i=1}^{N} \nabla J^{(i)}(\theta)$$

$$= \frac{1}{N}\sum_{i=1}^{N} -\left(y^{(i)} - \vec{\theta}^T \vec{x}^{(i)}\right) \vec{x}^{(i)}$$

constants from D

Gradient Calculation for Linear Regression

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

$$\frac{d}{d\theta_k} J^{(i)}(\boldsymbol{\theta}) = \frac{d}{d\theta_k} \frac{1}{2} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2$$

$$= \frac{1}{2} \frac{d}{d\theta_k} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2$$

$$= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \frac{d}{d\theta_k} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})$$

$$= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \frac{d}{d\theta_k} \left(\sum_{j=1}^{K} \theta_j x_j^{(i)} - y^{(i)} \right)$$

$$= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_k^{(i)}$$

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

$$\frac{d}{d\theta_k} J(\boldsymbol{\theta}) = \sum_{i=1}^{N} \frac{d}{d\theta_k} J^{(i)}(\boldsymbol{\theta})$$

$$= \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_k^{(i)}$$

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

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

$$= \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}$$

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

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