10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Linear Regression

+

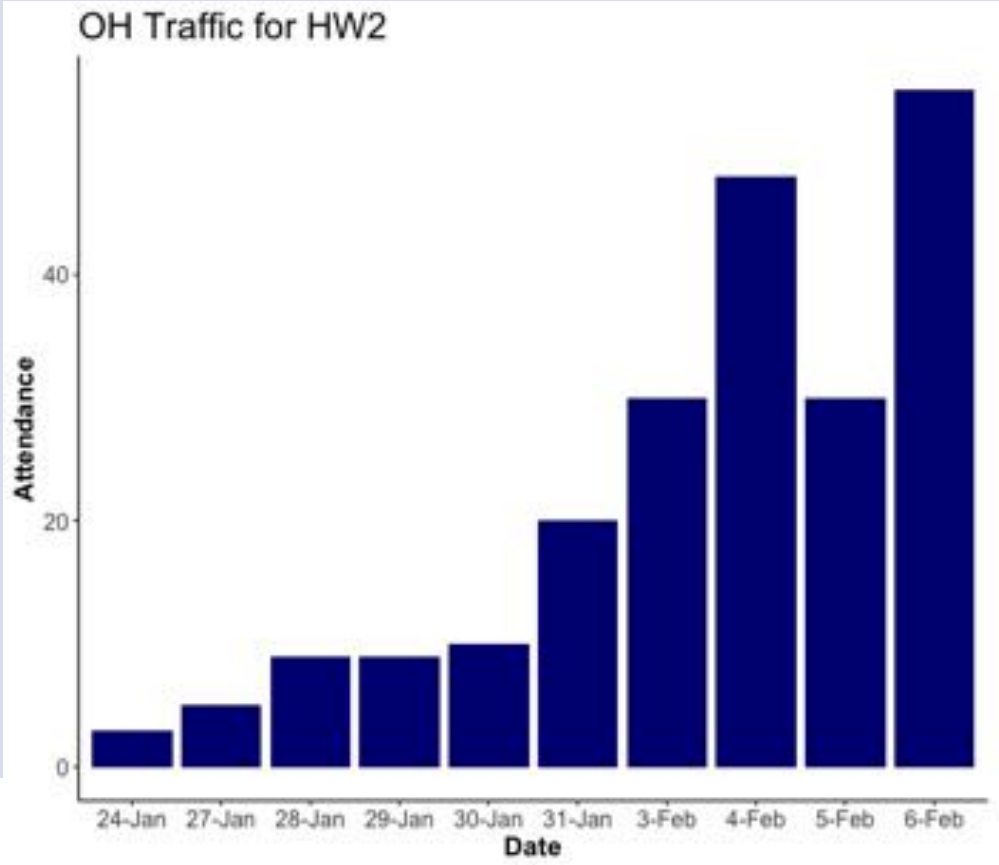
Optimization for ML

Matt Gormley
Lecture 8
Feb. 07, 2020

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!



Reminders

- Homework 3: KNN, Perceptron, Lin.Reg.
  - Out: Wed, Feb. 05 (+ 1 day)
  - Due: Wed, Feb. 12 at 11:59pm
- Today's In-Class Poll
  - http://p8.mlcourse.org

LINEAR REGRESSION

Regression Problems

Chalkboard

- Definition of Regression
- Linear functions
- Residuals
- Notation trick: fold in the intercept

The Big Picture

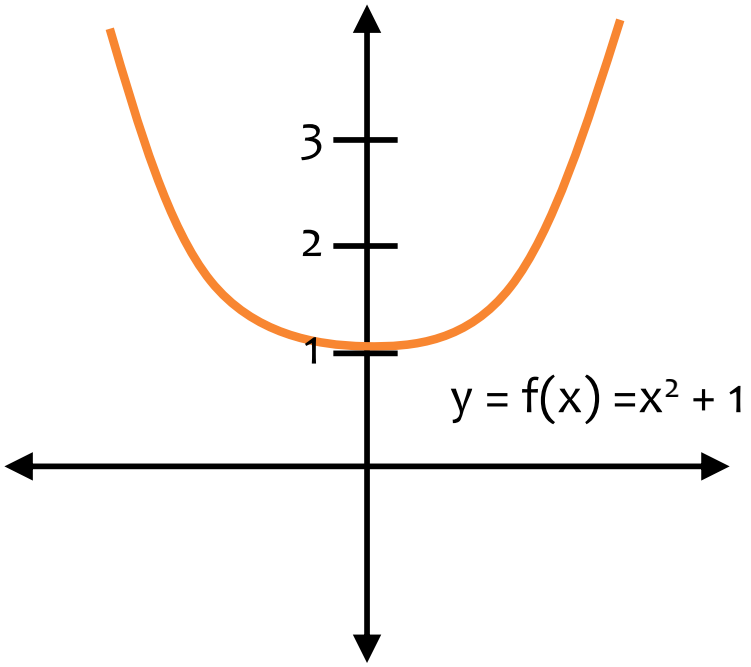
OPTIMIZATION FOR ML

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. Q: What is v*?

   v* = 1, the minimum value of the function

2. Q: What is x*?

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

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*
- ...

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

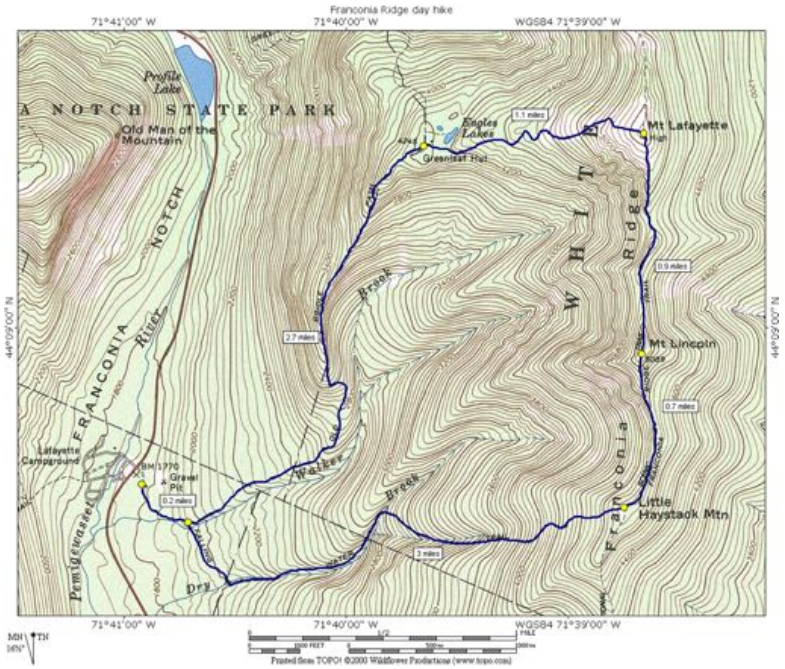
5. Test time: given a new $\mathbf{x}$, make prediction $\hat{y}$

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

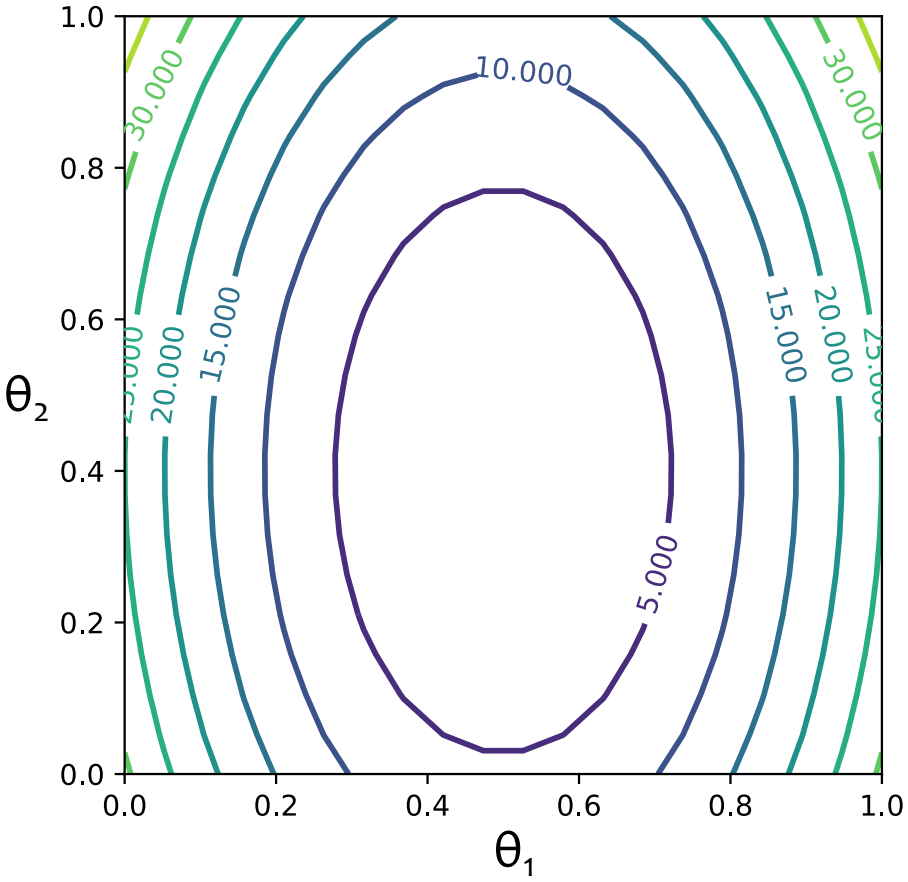
Contour Plots

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 $J(\boldsymbol{\theta})$

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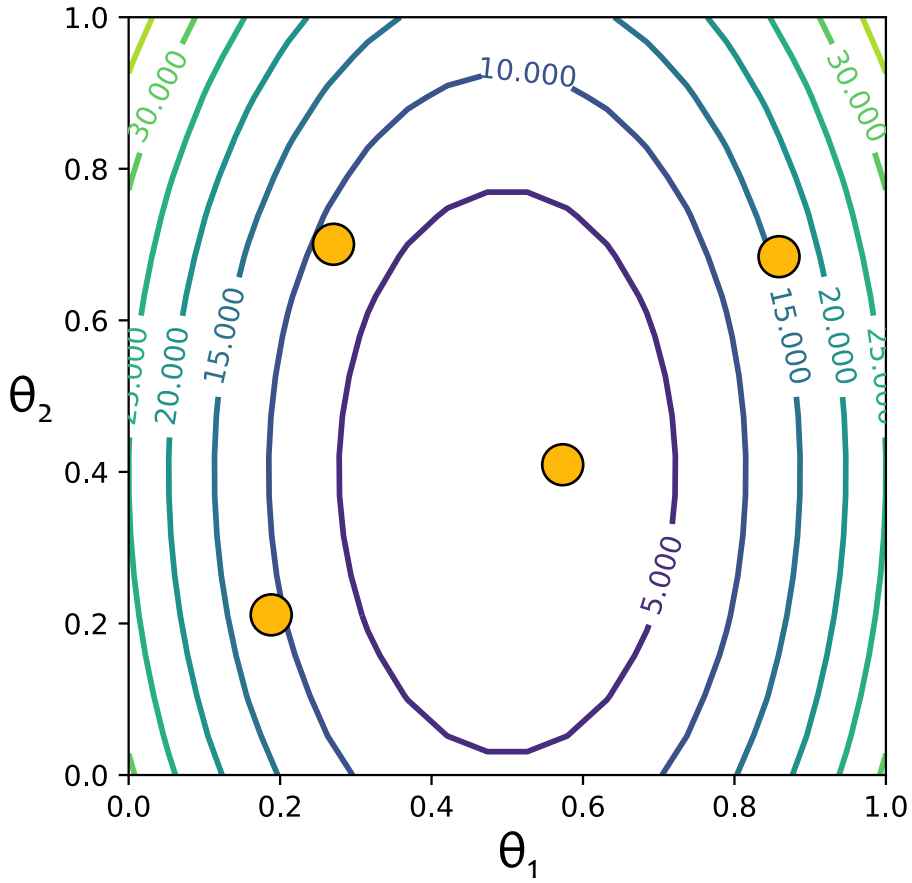

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1	0.2	0.2	10.4
2	0.3	0.7	7.2
3	0.6	0.4	1.0
4	0.9	0.7	19.2

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2. Evaluate J(**θ**)
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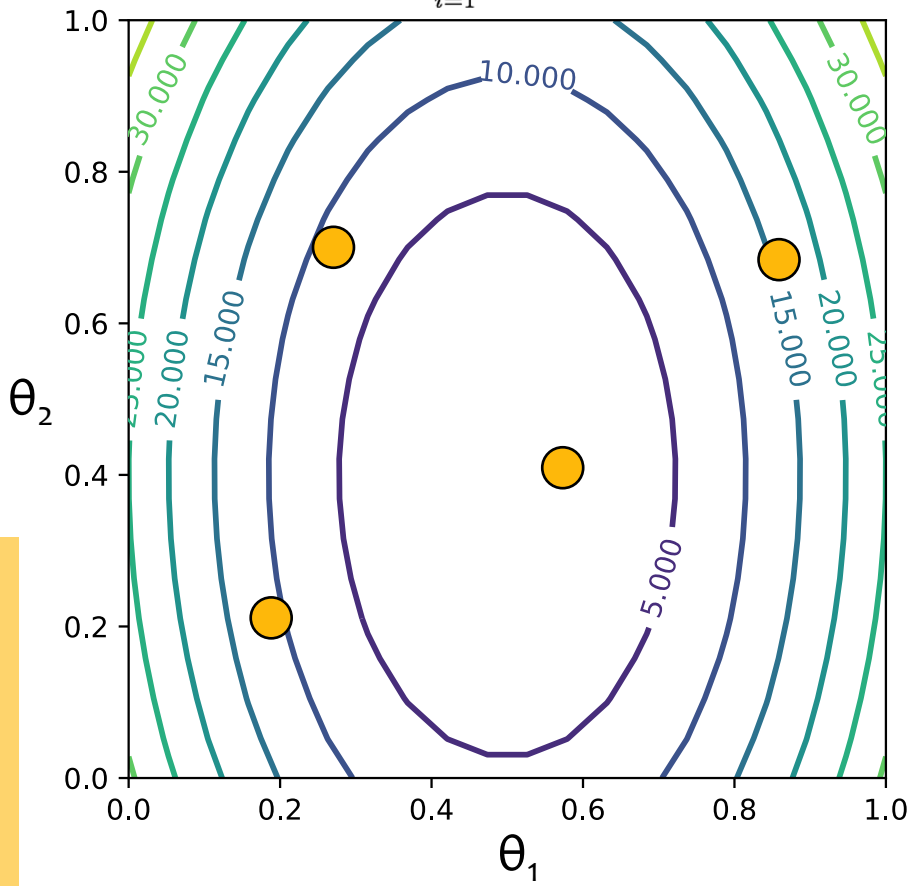
For Linear Regression:

- **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) = (θ_1, θ_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 by Rand. Guessing

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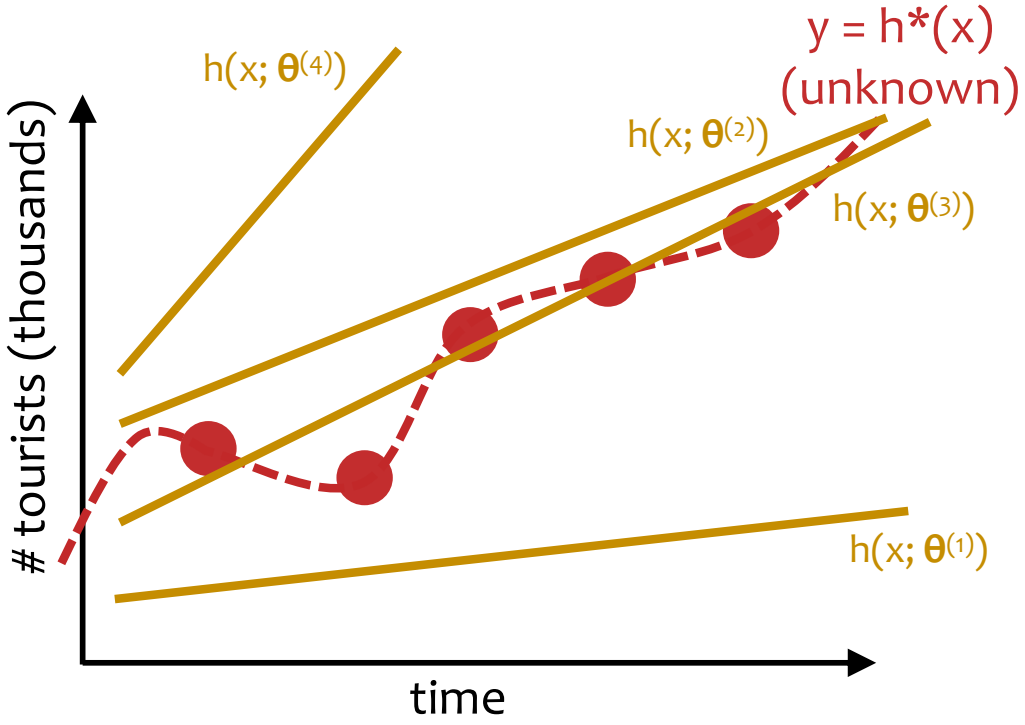

For Linear Regression:

- 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**
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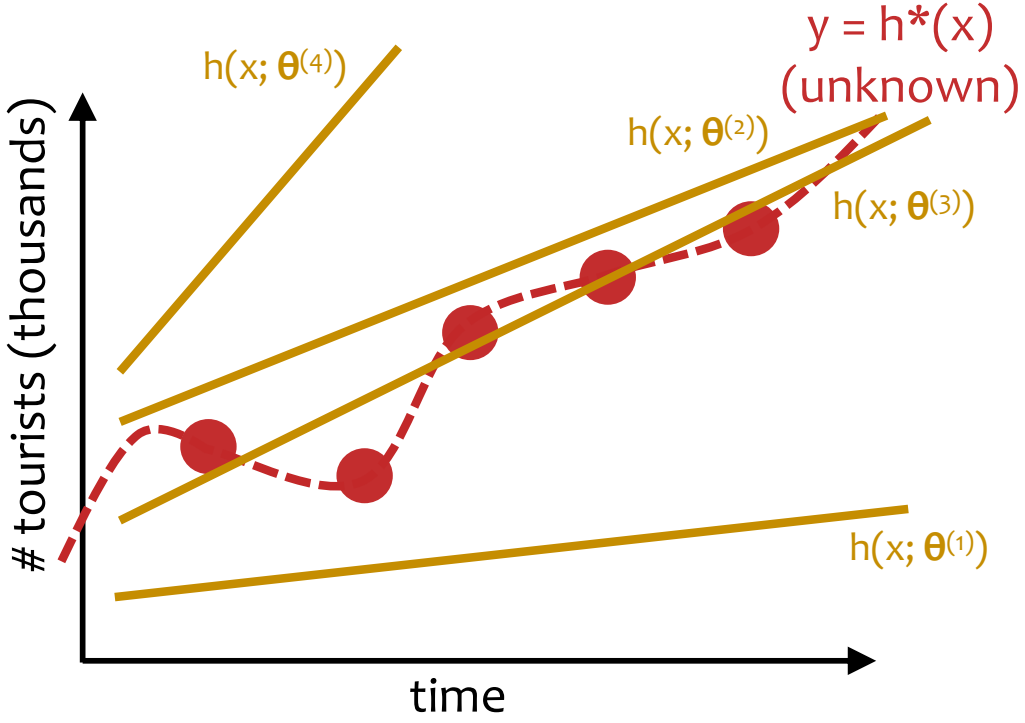

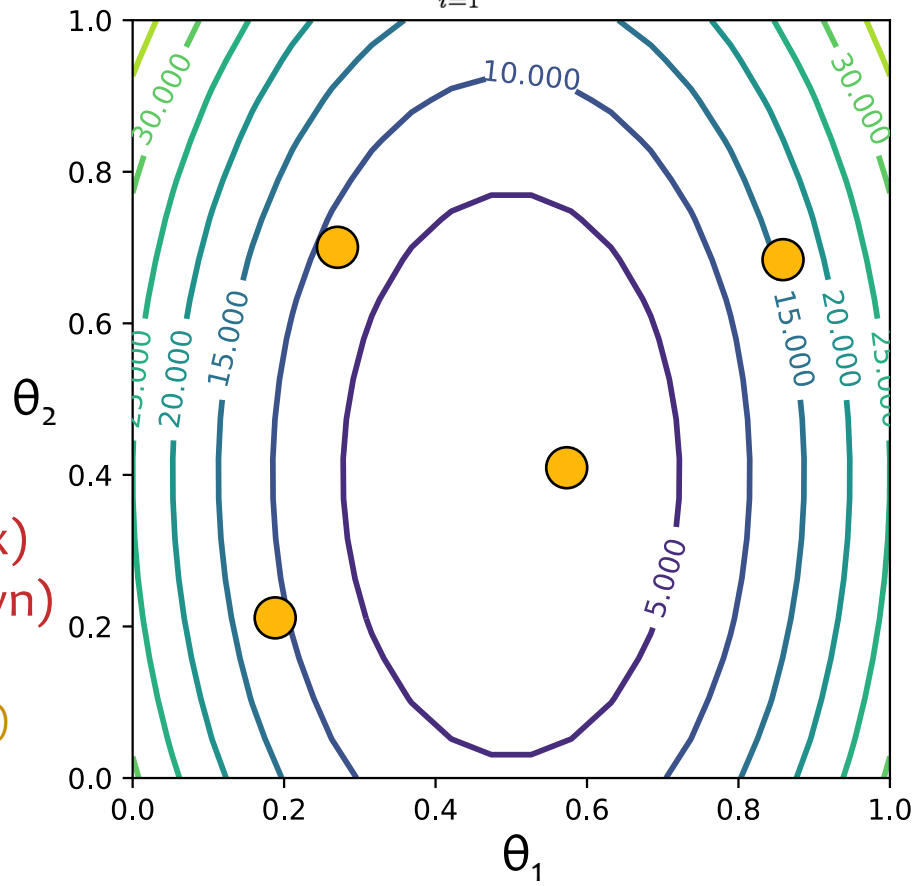

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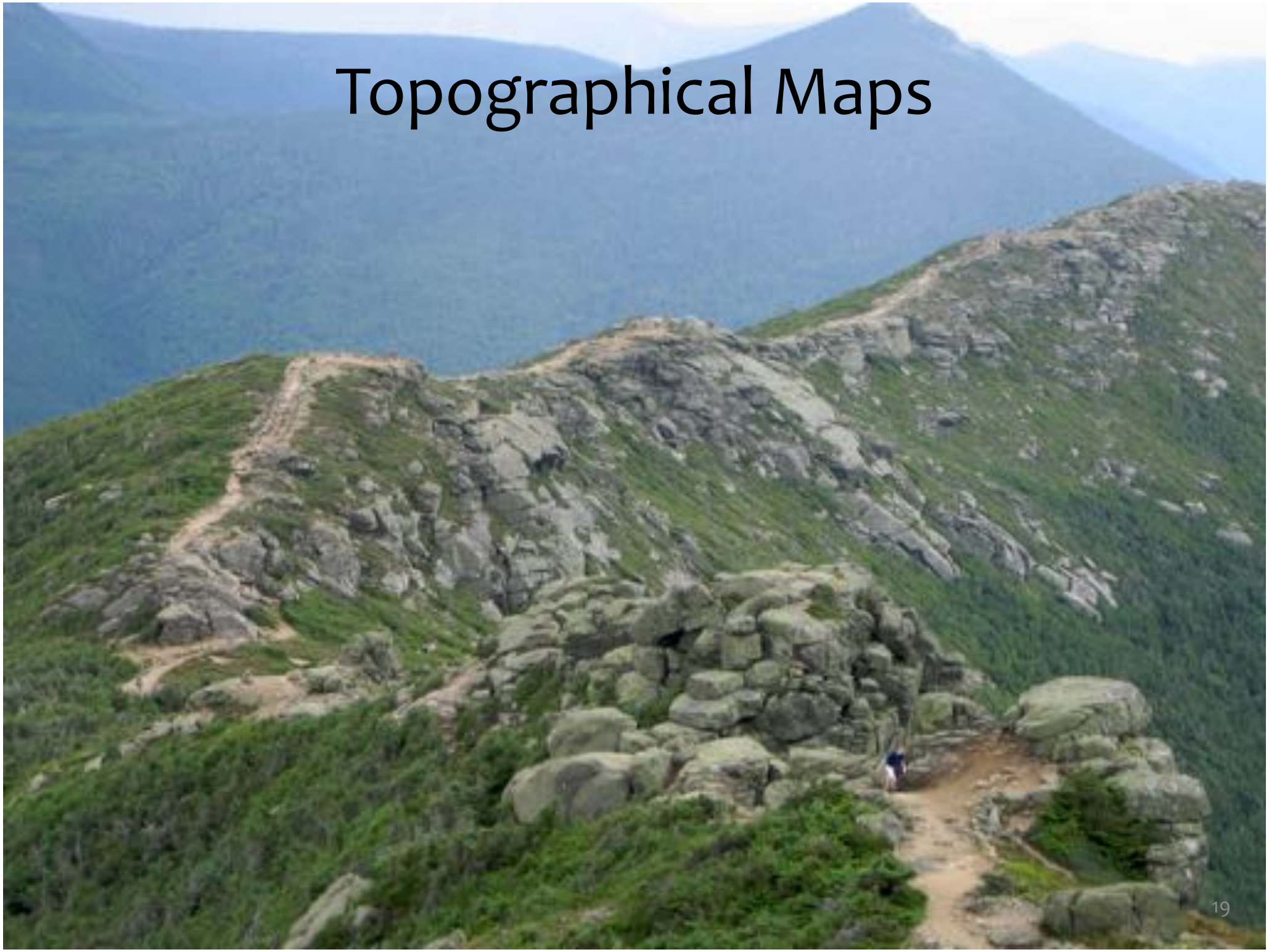
OPTIMIZATION METHOD #1: GRADIENT DESCENT

Optimization for ML

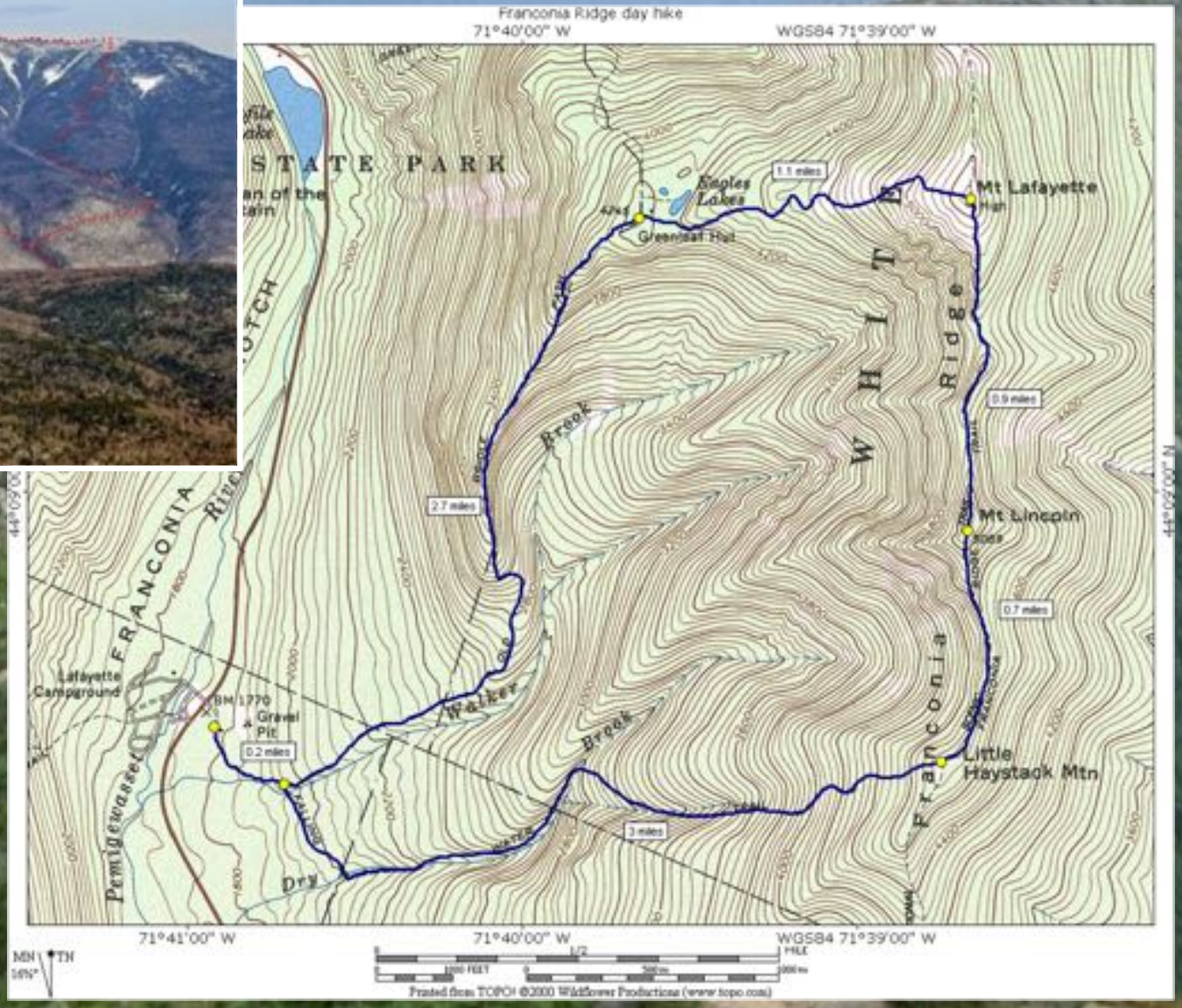
Chalkboard

- Unconstrained optimization
- Derivatives
- Gradient

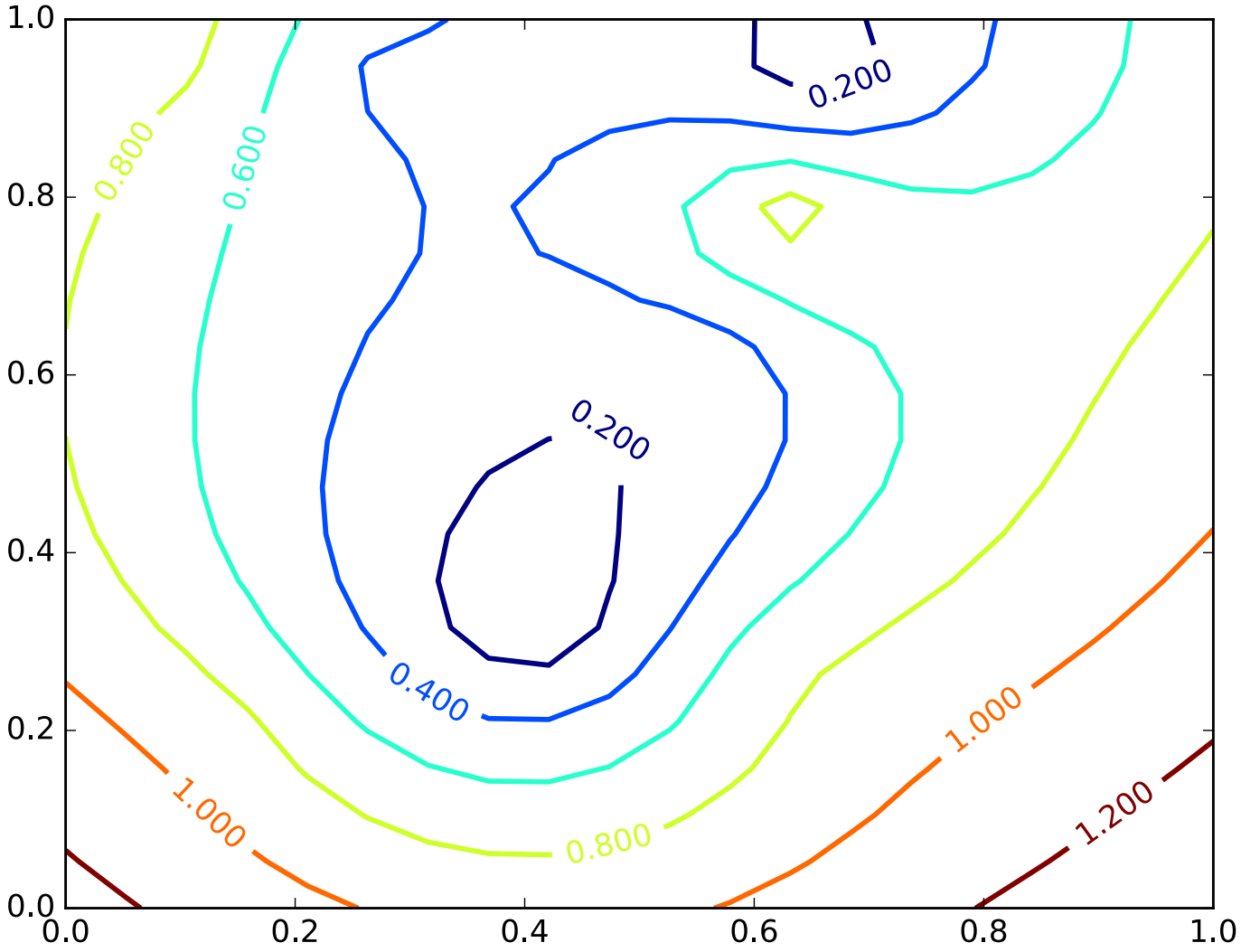
Topographical Maps



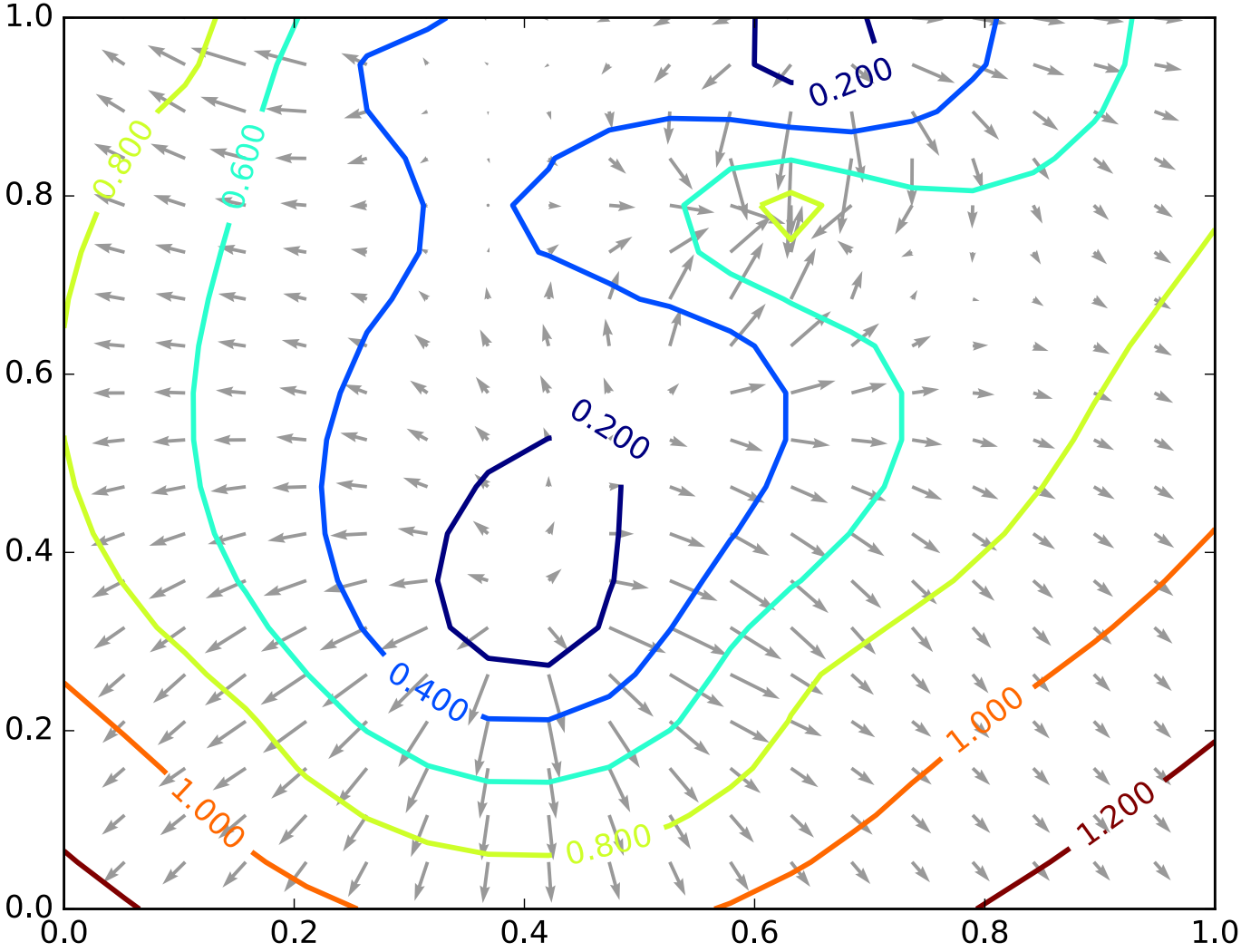
Topographical Maps



Gradients

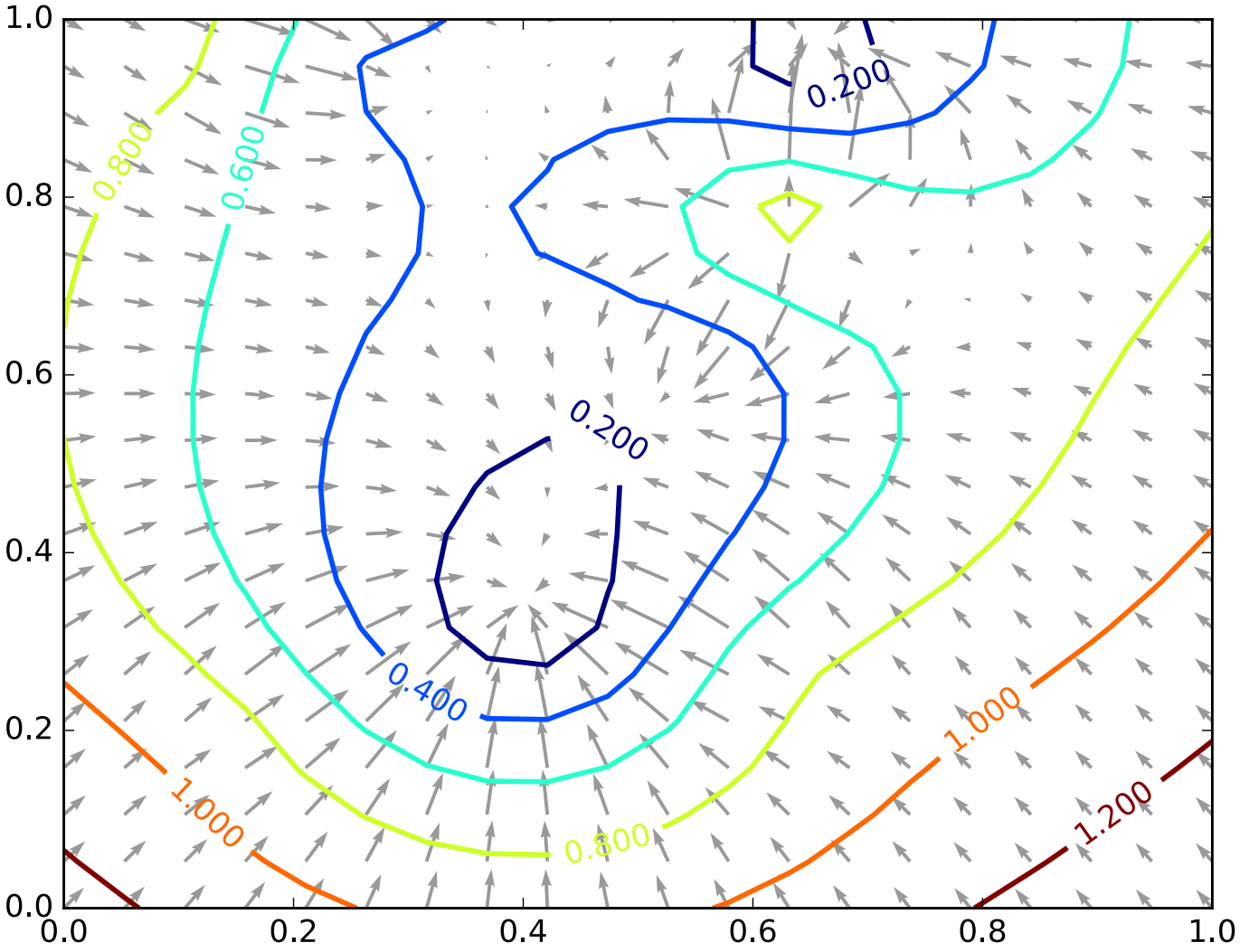

1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
0.800
0.600
0.200
0.200
0.400
1.000
0.800
1.000
1.200

Gradients



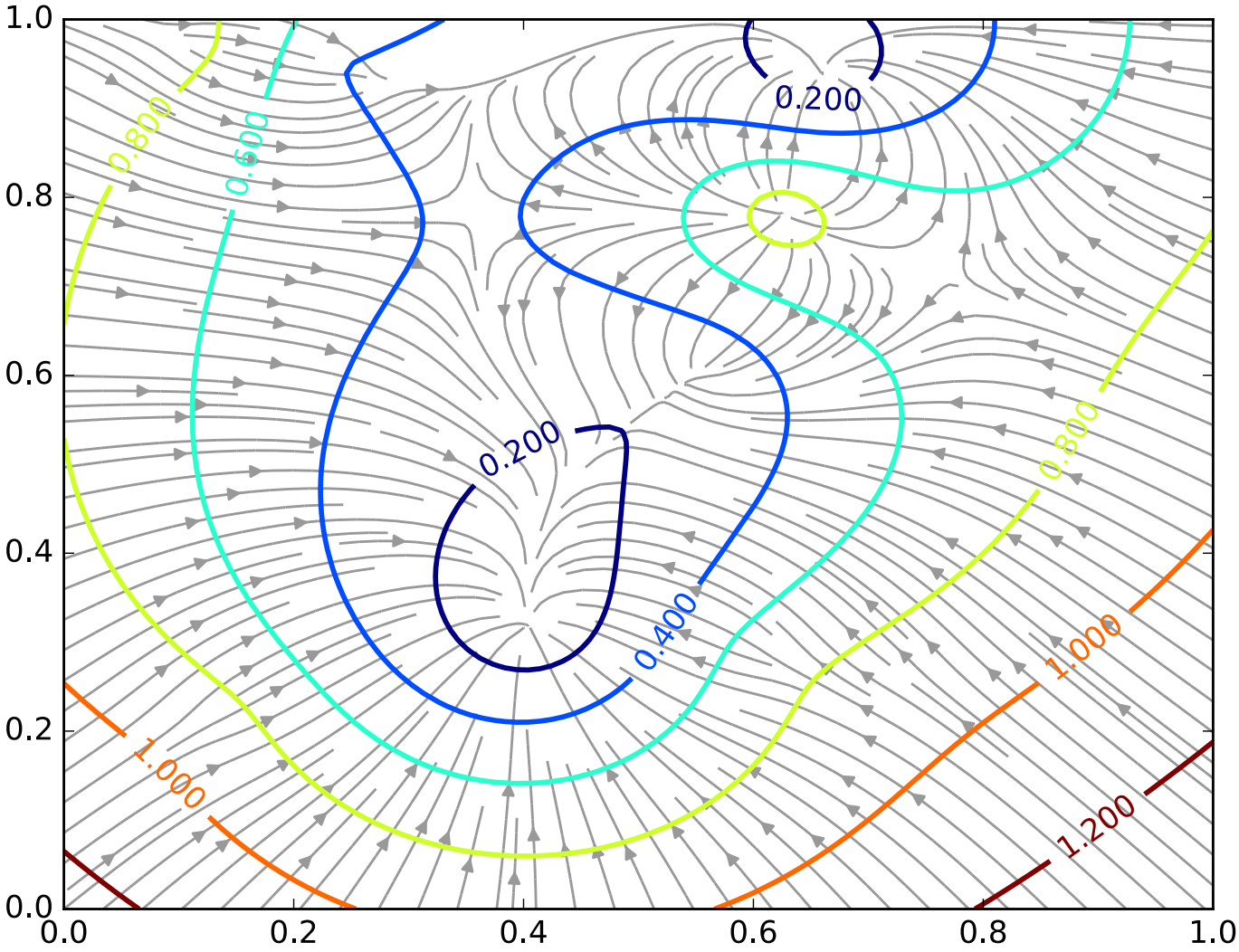
These are the **gradients** that
Gradient **Ascent** would follow.

(Negative) Gradients



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

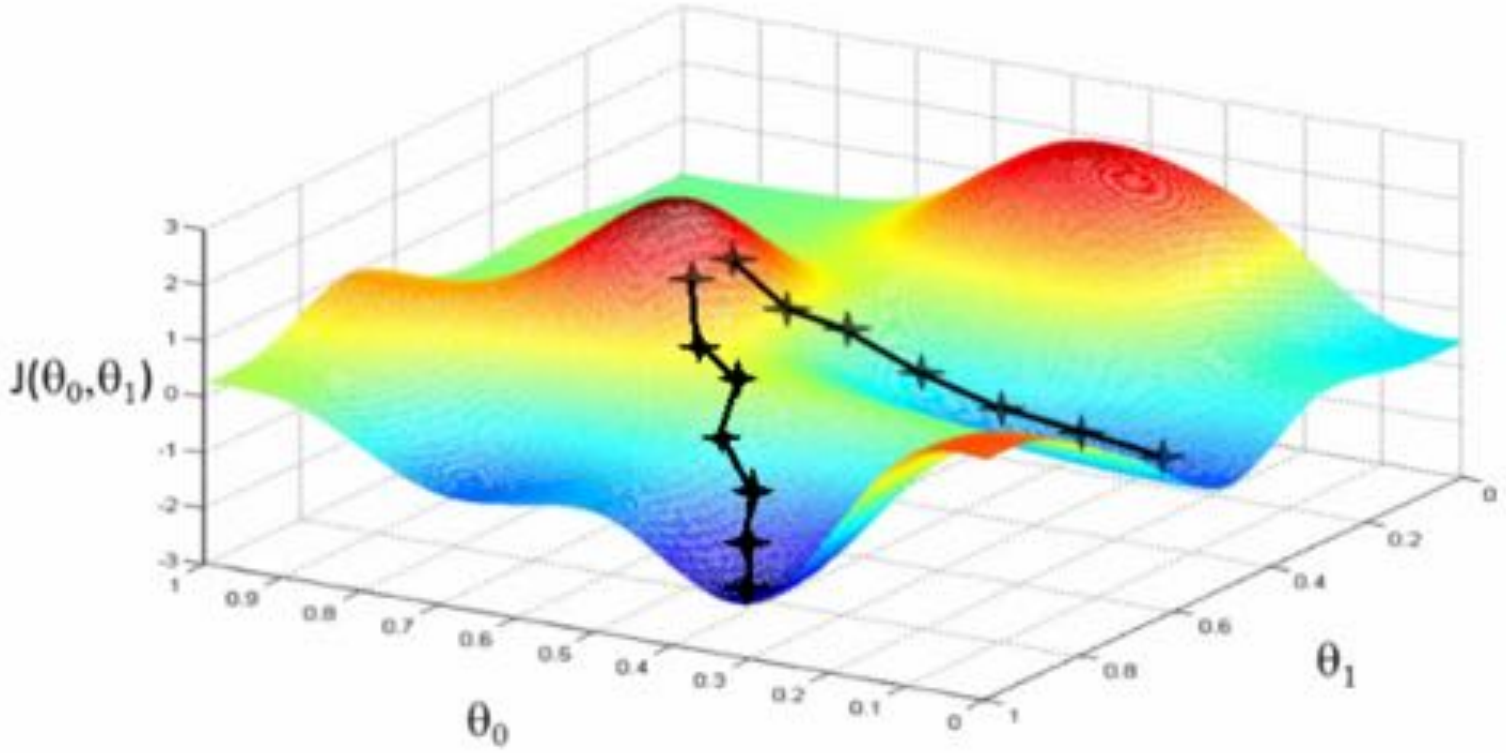
(Negative) Gradient *Paths*



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

Pros and cons of gradient descent

- Simple and often quite effective on ML tasks
- Often very scalable
- Only applies to smooth functions (differentiable)
- Might find a local minimum, rather than a global one



Slide courtesy of William Cohen

Gradient Descent

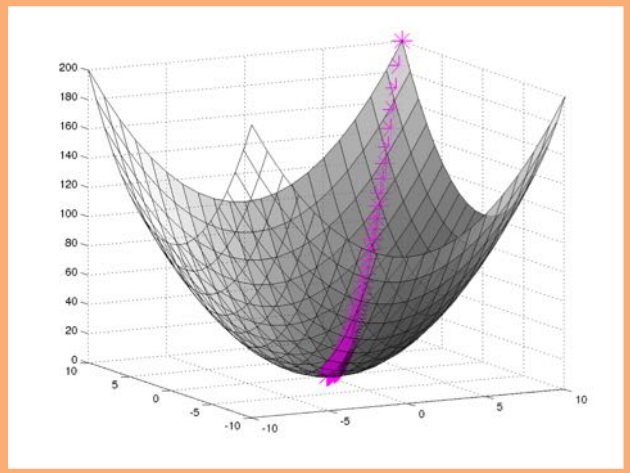
Chalkboard

- Gradient Descent Algorithm
- Details: starting point, stopping criterion, line search

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

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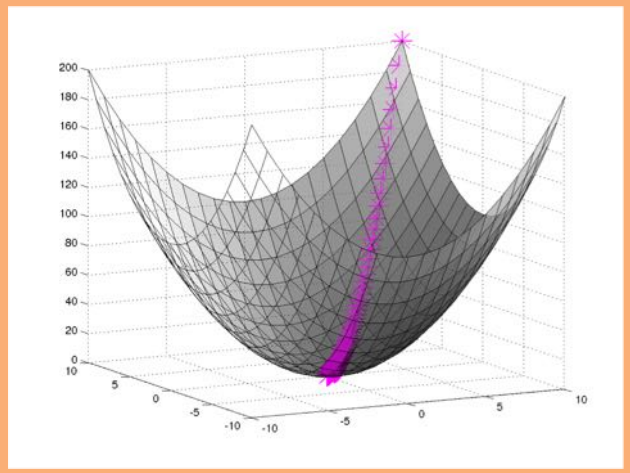

There are many possible ways to detect **convergence**. For example, we could check whether the L2 norm of the gradient is below some small tolerance.

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

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

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Linear Regression by Gradient Desc.

Optimization Method #1: Gradient Descent

1. Pick a random $\boldsymbol{\theta}$
2. Repeat:
   a. Evaluate gradient $\nabla J(\boldsymbol{\theta})$
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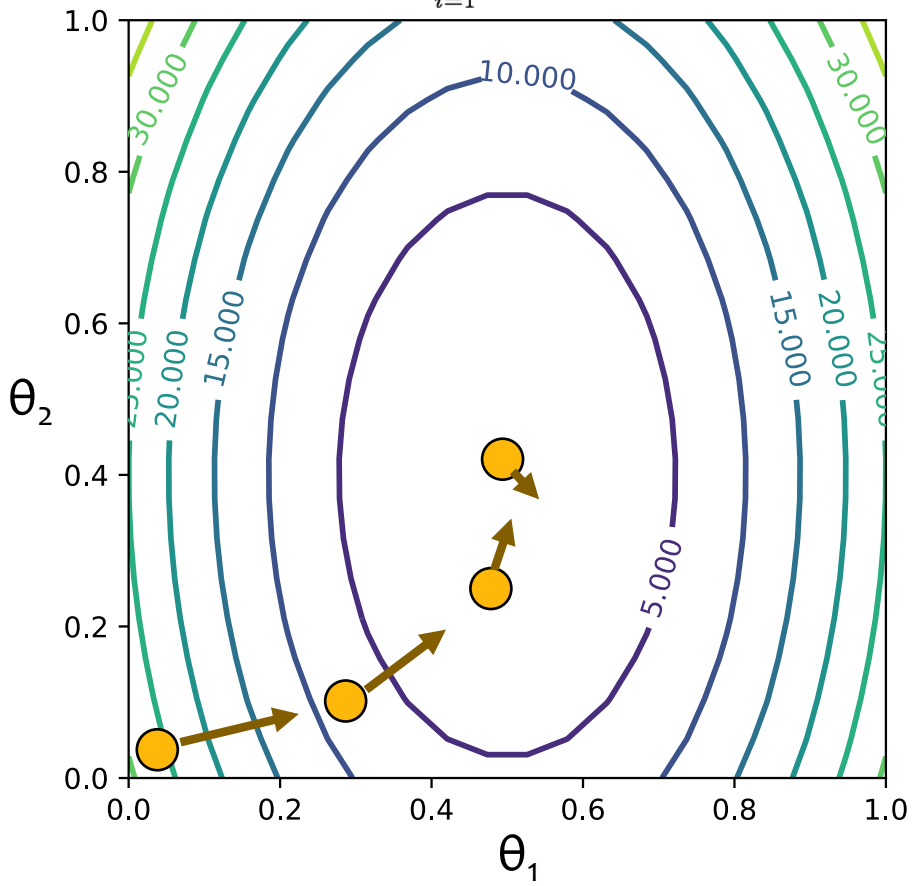

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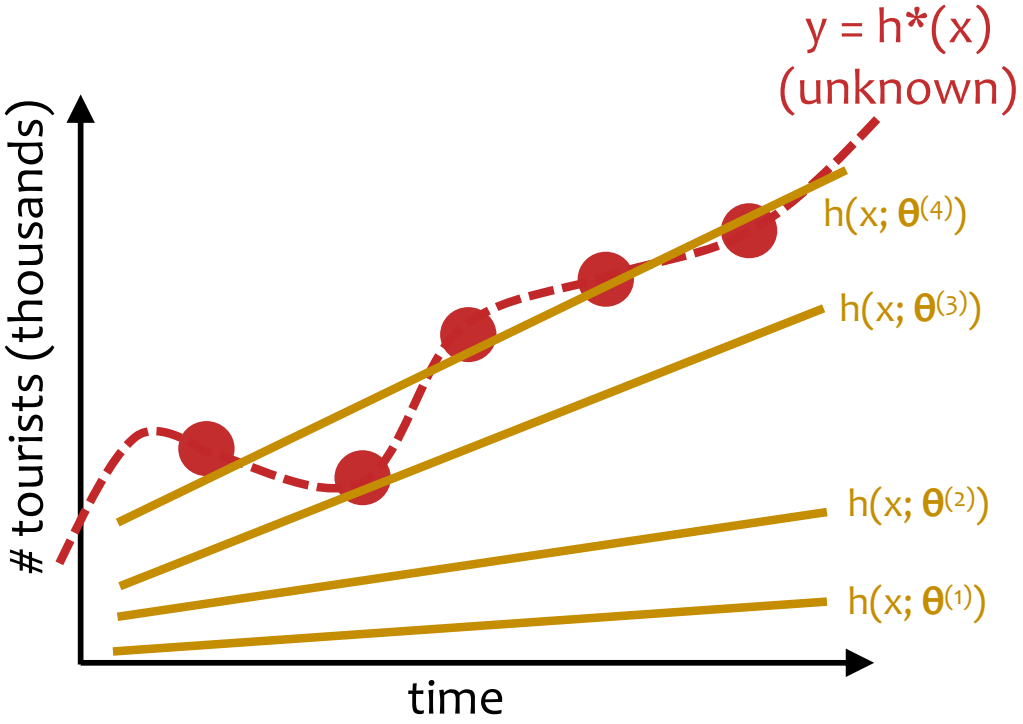

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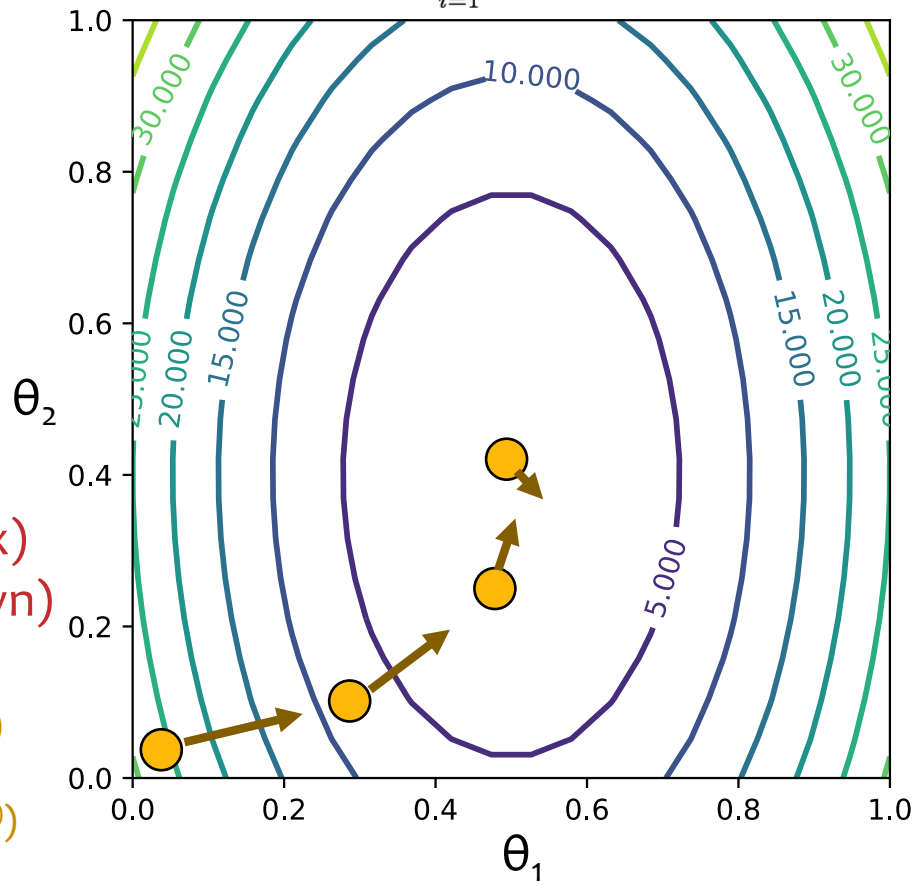

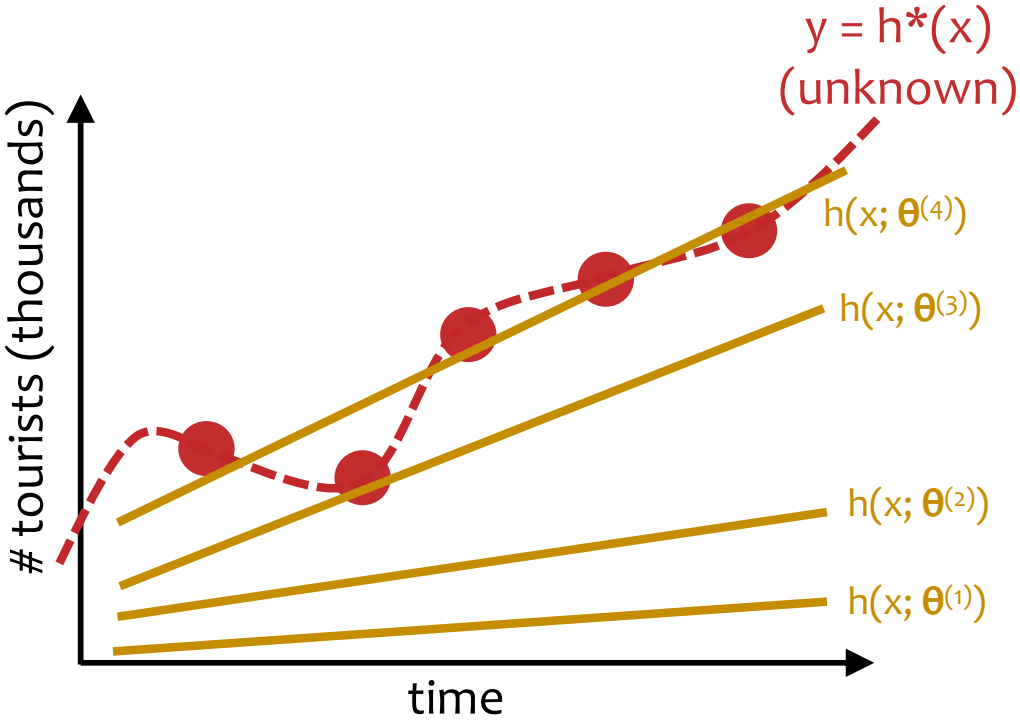

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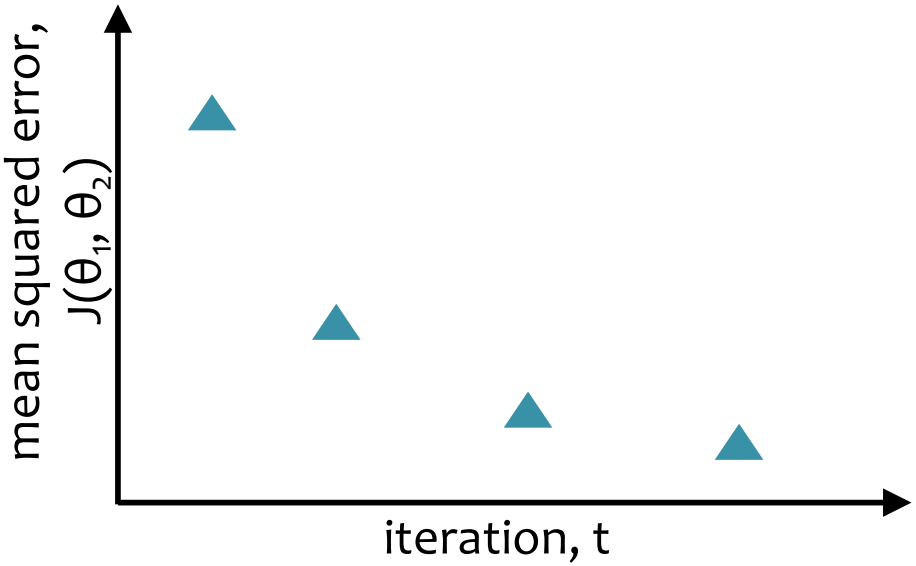

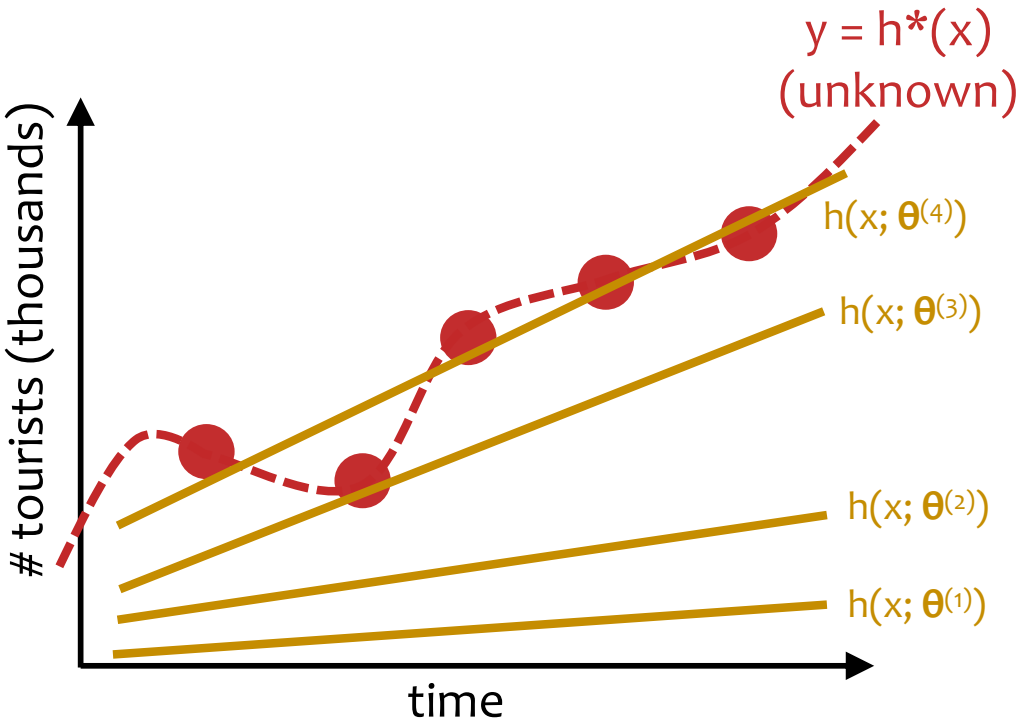

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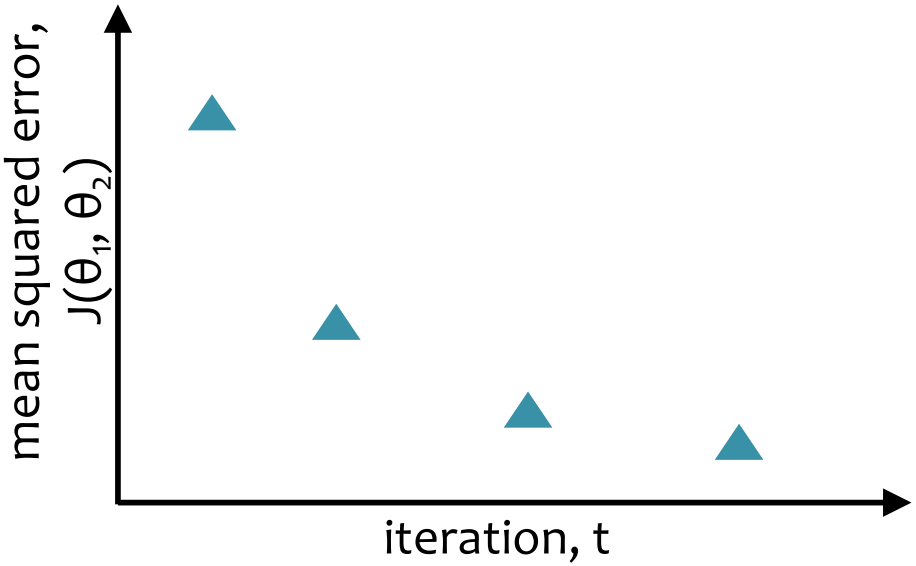

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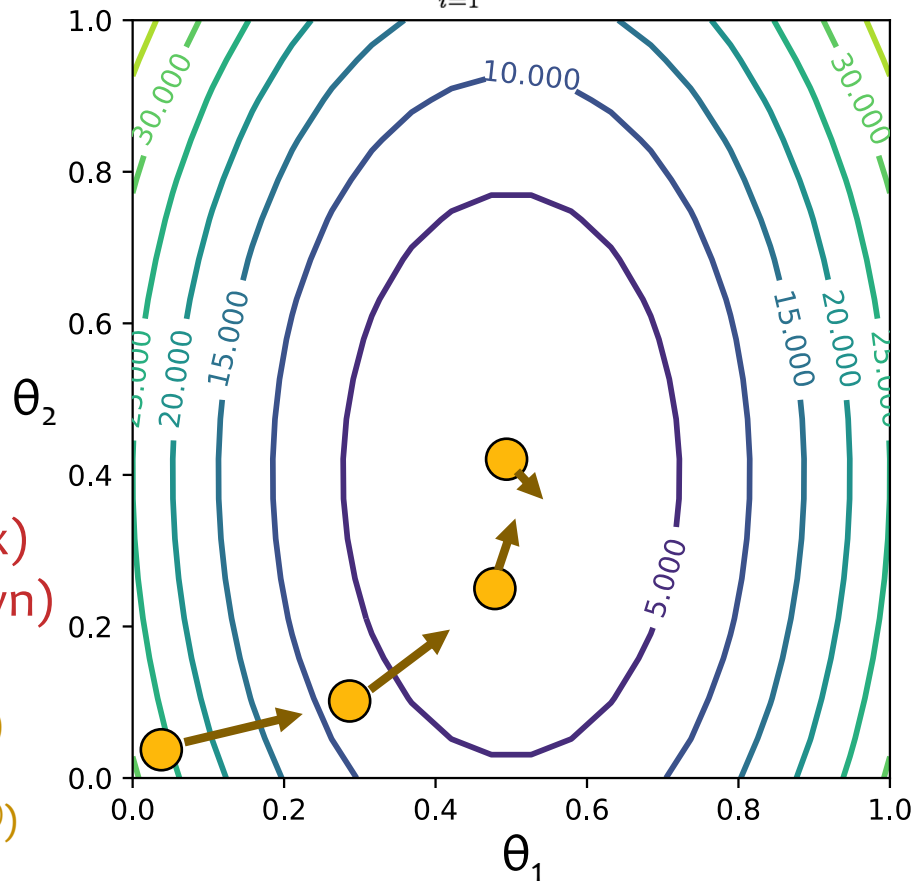

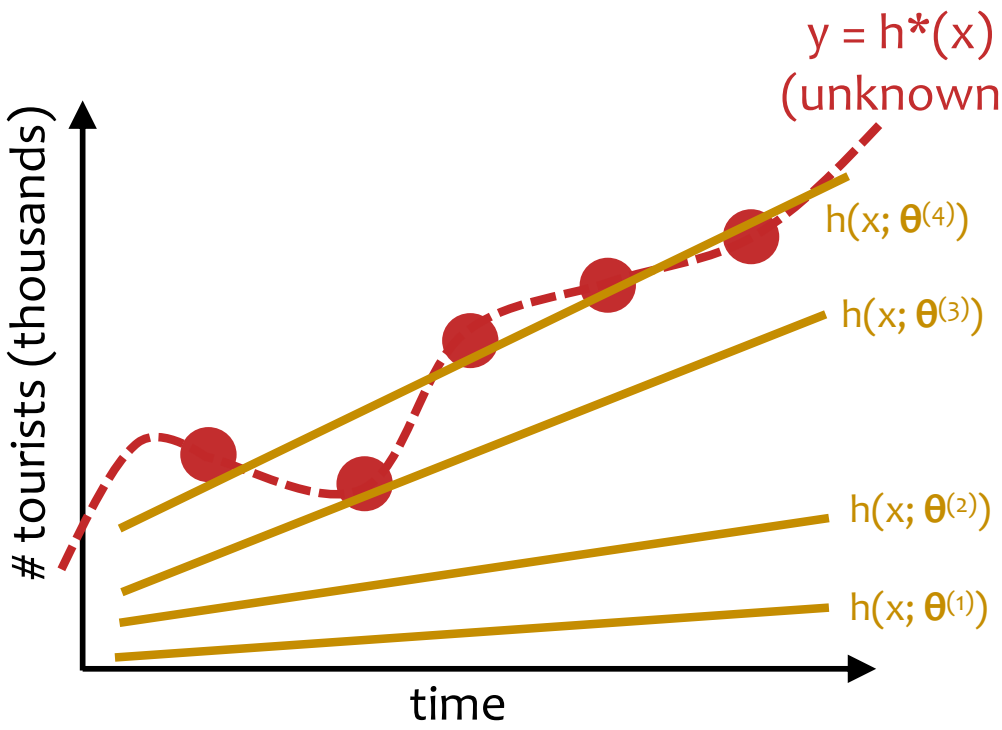

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Optimization for Linear Regression

Chalkboard

- Computing the gradient for Linear Regression
- Gradient Descent 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]

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

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

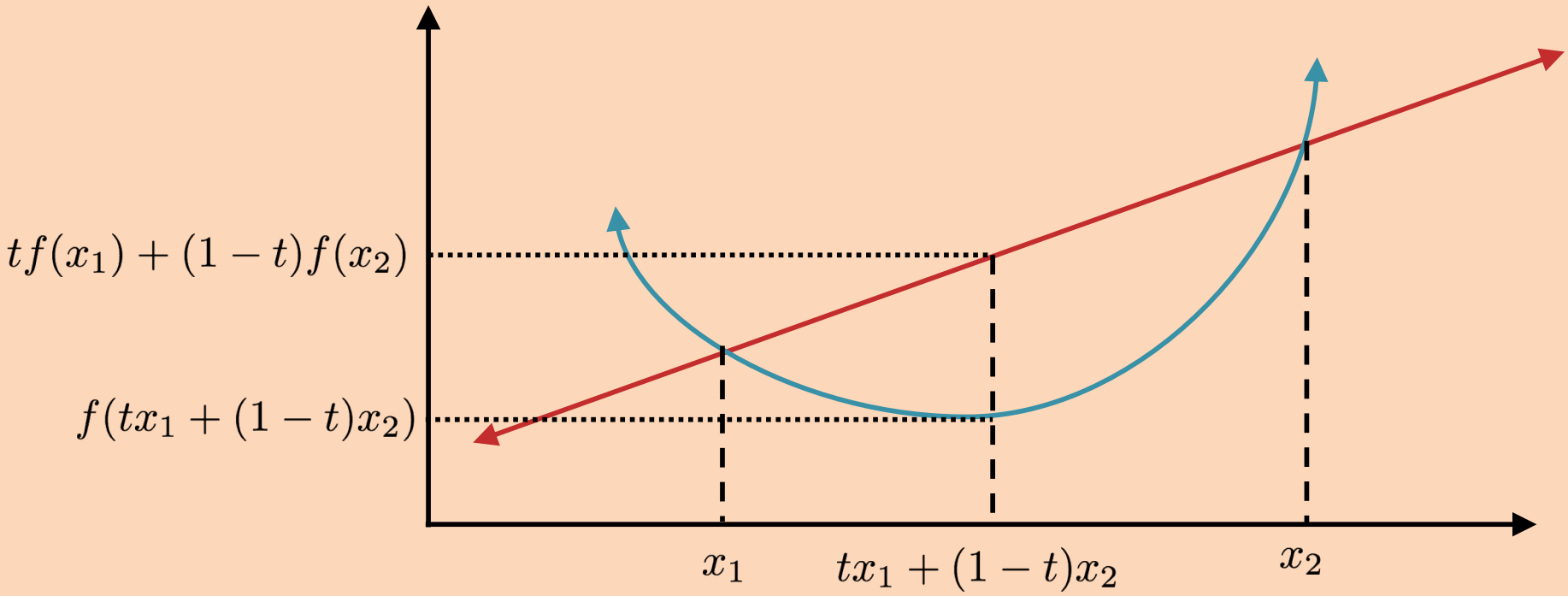
1: **procedure** GDLR($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
2: $\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$ ▷ Initialize parameters
3: $\quad$**while** not converged **do**
4: $\quad\quad\mathbf{g} \leftarrow \sum_{i=1}^{N}(\boldsymbol{\theta}^T\mathbf{x}^{(i)} - y^{(i)})\mathbf{x}^{(i)}$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

CONVEXITY

Convexity

Function $f : \mathbb{R}^M \rightarrow \mathbb{R}$ is **convex**
if $\forall\ \mathbf{x}_1 \in \mathbb{R}^M, \mathbf{x}_2 \in \mathbb{R}^M, 0 \leq t \leq 1$:

$$f(t\mathbf{x}_1 + (1-t)\mathbf{x}_2) \leq tf(\mathbf{x}_1) + (1-t)f(\mathbf{x}_2)$$

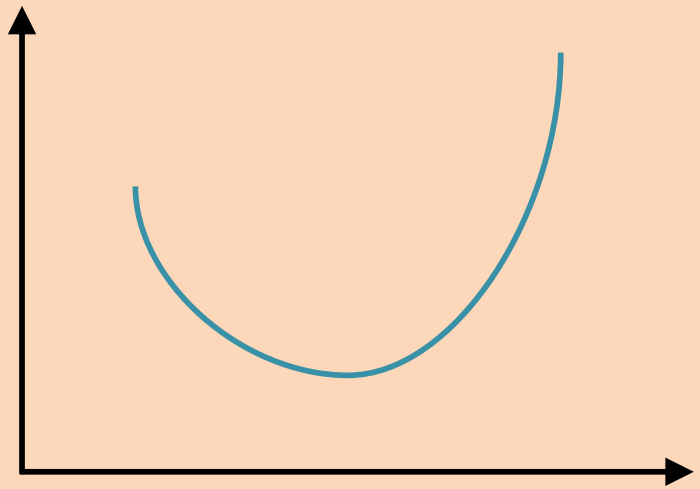


Convexity

Suppose we have a function $f(x) : \mathcal{X} \rightarrow \mathcal{Y}$.

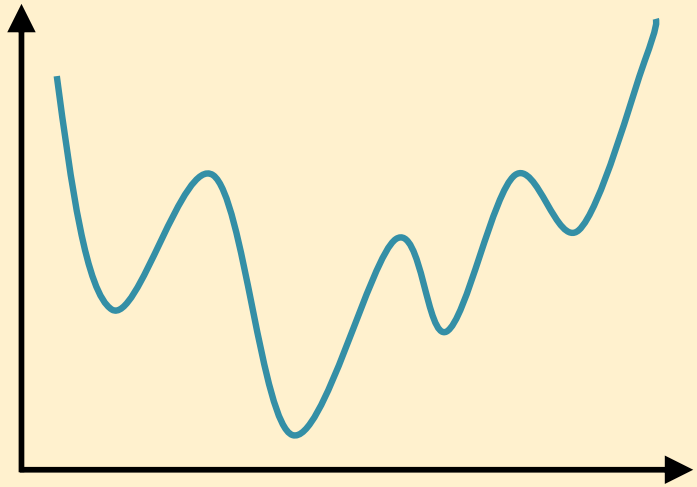
- The value x^* is a **global minimum** of f iff $f(x^*) \leq f(x), \forall x \in \mathcal{X}$.
- The value x^* is a **local minimum** of f iff $\exists \epsilon$ s.t. $f(x^*) \leq f(x), \forall x \in [x^* - \epsilon, x^* + \epsilon]$.

Convex Function



- Each **local minimum** is a **global minimum**

Nonconvex Function

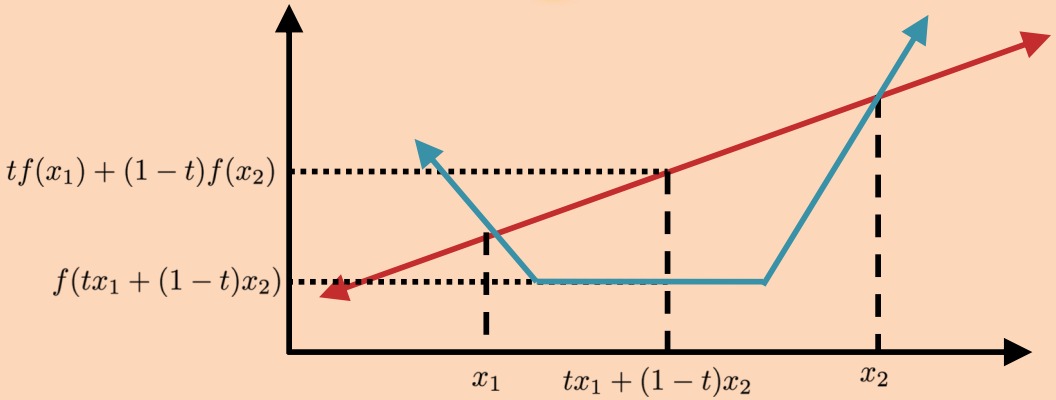


- A *nonconvex* function is **not convex**
- Each **local minimum** is **not** necessarily a **global minimum**

Convexity

Function $f : \mathbb{R}^M \to \mathbb{R}$ is **convex**
if $\forall\ \mathbf{x}_1 \in \mathbb{R}^M, \mathbf{x}_2 \in \mathbb{R}^M, 0 \leq t \leq 1$:

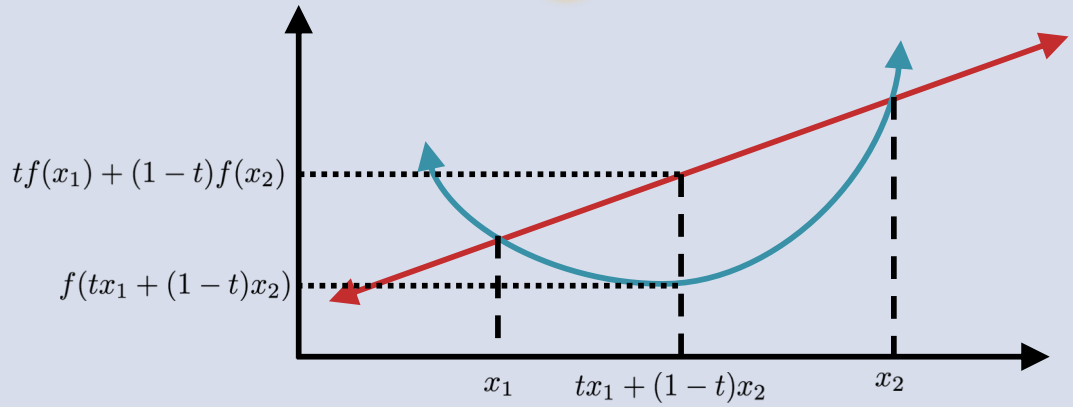
$$f(t\mathbf{x}_1 + (1-t)\mathbf{x}_2) \leq tf(\mathbf{x}_1) + (1-t)f(\mathbf{x}_2)$$



Each **local minimum** of a **convex** function is also a **global minimum.**

Function $f : \mathbb{R}^M \to \mathbb{R}$ is **strictly convex**
if $\forall\ \mathbf{x}_1 \in \mathbb{R}^M, \mathbf{x}_2 \in \mathbb{R}^M, 0 \leq t \leq 1$:

$$f(t\mathbf{x}_1 + (1-t)\mathbf{x}_2) < tf(\mathbf{x}_1) + (1-t)f(\mathbf{x}_2)$$



A **strictly convex** function has a **unique global minimum.**

CONVEXITY AND LINEAR REGRESSION

Convexity and Linear Regression

The **Mean Squared Error** function, which we minimize for learning the parameters of Linear Regression, **is convex**!

…but in the general case it is **not strictly convex**.

Regression Loss Functions

In-Class Exercise:

Which of the following could be used as loss functions for training a linear regression model?

Select all that apply.

A. $\ell(\hat{y}, y) = ||\hat{y} - y||_2$

B. $\ell(\hat{y}, y) = |\hat{y} - y|$

C. $\ell(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$

D. $\ell(\hat{y}, y) = \frac{1}{4}(\hat{y} - y)^4$

E. $\ell(\hat{y}, y) = \begin{cases} \frac{1}{2}(\hat{y} - y)^2 & \text{if } |\hat{y} - y| \leq \delta \\ \delta|\hat{y} - y| - \frac{1}{2}\delta^2 & \text{otherwise} \end{cases}$

F. $\ell(\hat{y}, y) = \log(\cosh(\hat{y} - y))$

Solving Linear Regression

Question:

True or False: If Mean Squared Error (i.e. $\frac{1}{N}\sum_{i=1}^{N}(y^{(i)} - h(\mathbf{x}^{(i)}))^2$) has a unique minimizer (i.e. argmin), then Mean Absolute Error (i.e. $\frac{1}{N}\sum_{i=1}^{N}|y^{(i)} - h(\mathbf{x}^{(i)})|$) must also have a unique minimizer.

Answer:

OPTIMIZATION METHOD #2: CLOSED FORM SOLUTION

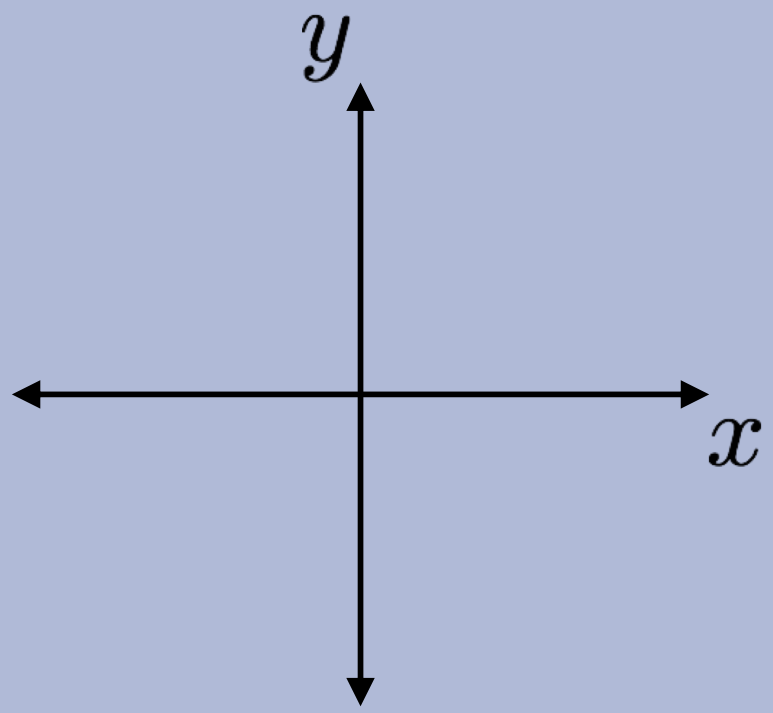
Calculus and Optimization

In-Class Exercise

Plot three functions:

1. $f(x) = x^3 - x$
2. $f'(x) = \frac{\partial y}{\partial x}$
3. $f''(x) = \frac{\partial^2 y}{\partial x^2}$

Answer Here:



Optimization: Closed form solutions

Chalkboard

- Zero Derivatives
- Example: 1-D function
- Example: higher dimensions

CLOSED FORM SOLUTION 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: Closed Form

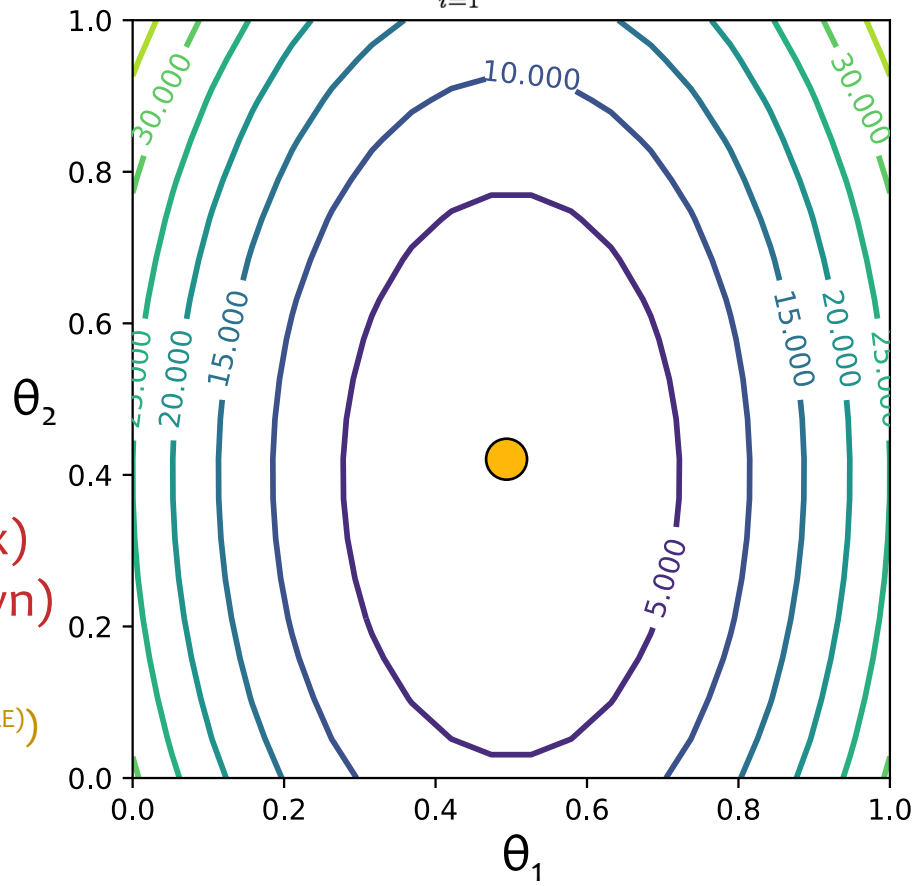
Optimization Method #2: Closed Form

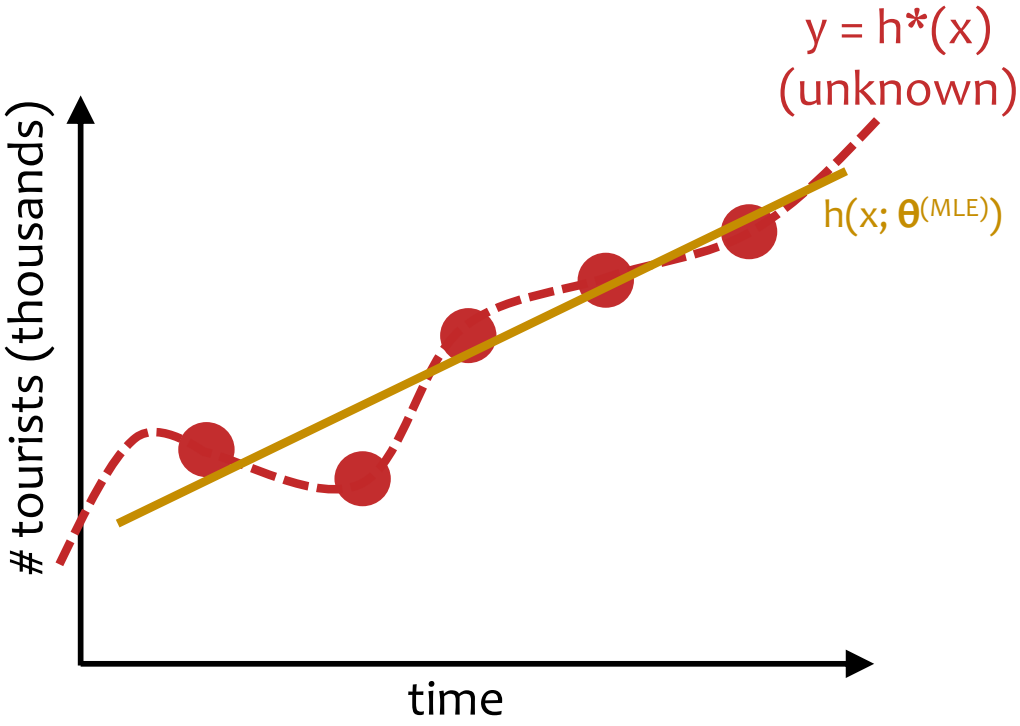
1. Evaluate

$$\boldsymbol{\theta}^{\text{MLE}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

2. Return $\boldsymbol{\theta}^{\text{MLE}}$

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





t	θ_1	θ_2	$J(\theta_1, \theta_2)$
MLE	0.59	0.43	0.2

Optimization for Linear Regression

Chalkboard

– Closed-form (Normal Equations)

Computational Complexity of OLS

To solve the Ordinary Least Squares problem we compute:

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}(y^{(i)} - (\boldsymbol{\theta}^T\mathbf{x}^{(i)}))^2$$
$$= (\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{Y})$$

The resulting shape of the matrices:

$$\underbrace{(\underbrace{\mathbf{X}^T}_{M\times N}\ \underbrace{\mathbf{X}}_{N\times M})^{-1}}_{M\times M}\ \underbrace{(\underbrace{\mathbf{X}^T}_{M\times N}\ \underbrace{\mathbf{Y}}_{N\times 1})}_{M\times 1}$$

Background: Matrix Multiplication Given matrices $\mathbf{A}$ and $\mathbf{B}$

- If $\mathbf{A}$ is $q \times r$ and $\mathbf{B}$ is $r \times s$, computing $\mathbf{AB}$ takes $O(qrs)$
- If $\mathbf{A}$ and $\mathbf{B}$ are $q \times q$, computing $\mathbf{AB}$ takes $O(q^{2.373})$
- If $\mathbf{A}$ is $q \times q$, computing A^{-1} takes $O(q^{2.373})$.

Computational Complexity of OLS:

$\mathbf{X}^T\mathbf{X}$	$O(M^2N)$
$(\quad)^{-1}$	$O(M^{2.373})$
$\mathbf{X}^T\mathbf{Y}$	$O(MN)$
$(\quad)^{-1}(\quad)$	$O(M^2)$
total	$O(M^2N + M^{2.373})$

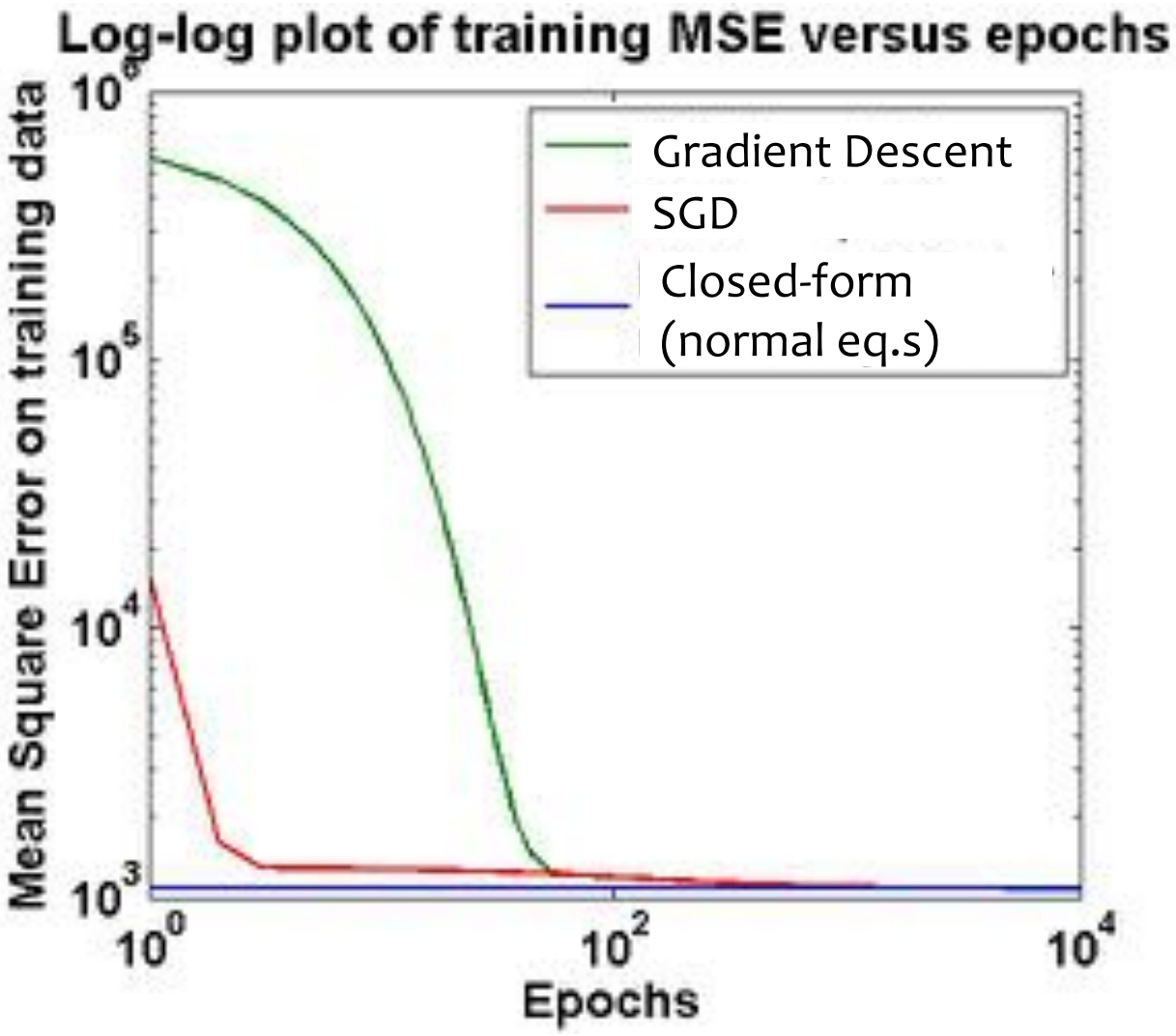
Linear in # of examples, N
Polynomial in # of features, M

Gradient Descent

Cases to consider gradient descent:

1. What if we **can not** find a closed-form solution?
2. What if we **can**, but it's inefficient to compute?
3. What if we **can**, but it's numerically unstable to compute?

Convergence Curves



- *Def*: an **epoch** is a single pass through the training data

1. For GD, only **one update** per epoch
2. For SGD, ***N* updates** per epoch
   N = (# train examples)

- SGD reduces MSE much more rapidly than GD
- For GD / SGD, training MSE is initially large due to uninformed initialization

Figure adapted from Eric P. Xing