10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Optimization for ML

+

Logistic Regression

Matt Gormley

Lecture 8

Sep. 24, 2018

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Probabilistic Learning

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Reminders

- **Homework 3: KNN, Perceptron, Lin.Reg.**
  - Out: Wed, Sep 19
  - Due: Wed, Sep 26 at 11:59pm

GRADIENT DESCENT

Motivation: Gradient Descent

To solve the Ordinary Least Squares problem we compute:

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

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

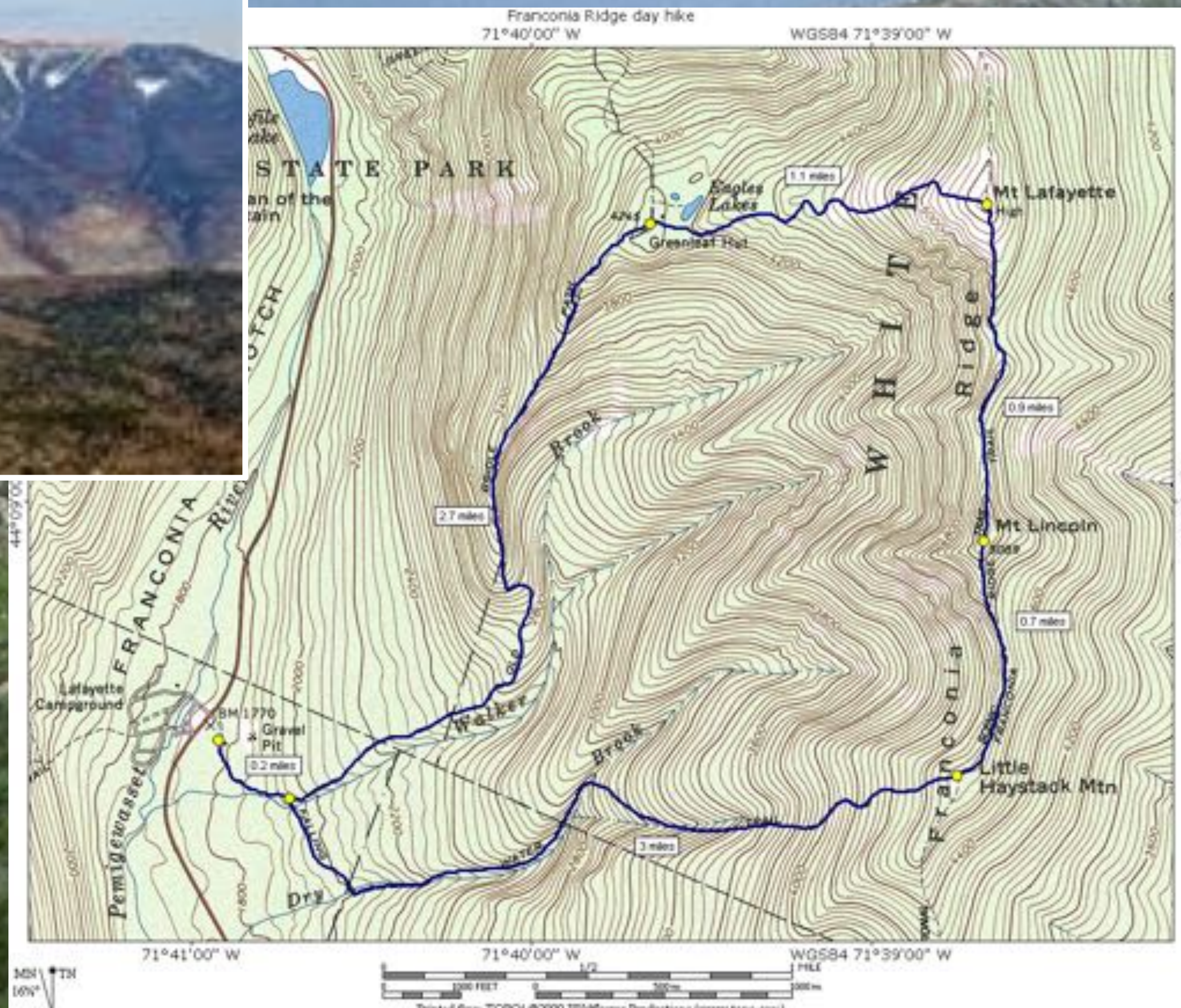
Motivation: Gradient Descent

Cases to consider gradient descent:

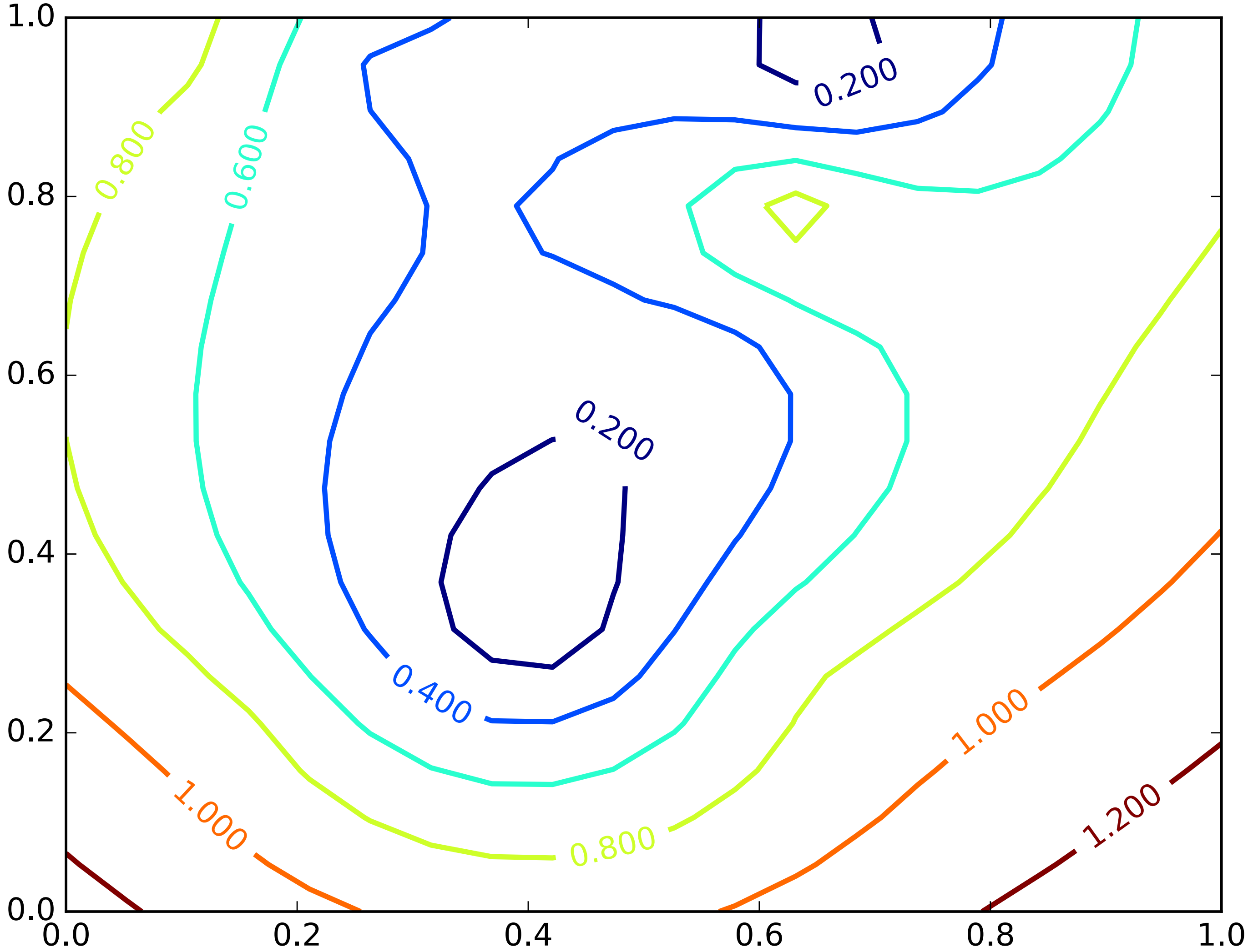
1. What if we **can not** find a closed-form solution?
2. What if we **can**, but it's inefficient to compute?
3. What if we **can**, but it's numerically unstable to compute?

Topographical Maps

Topographical Maps

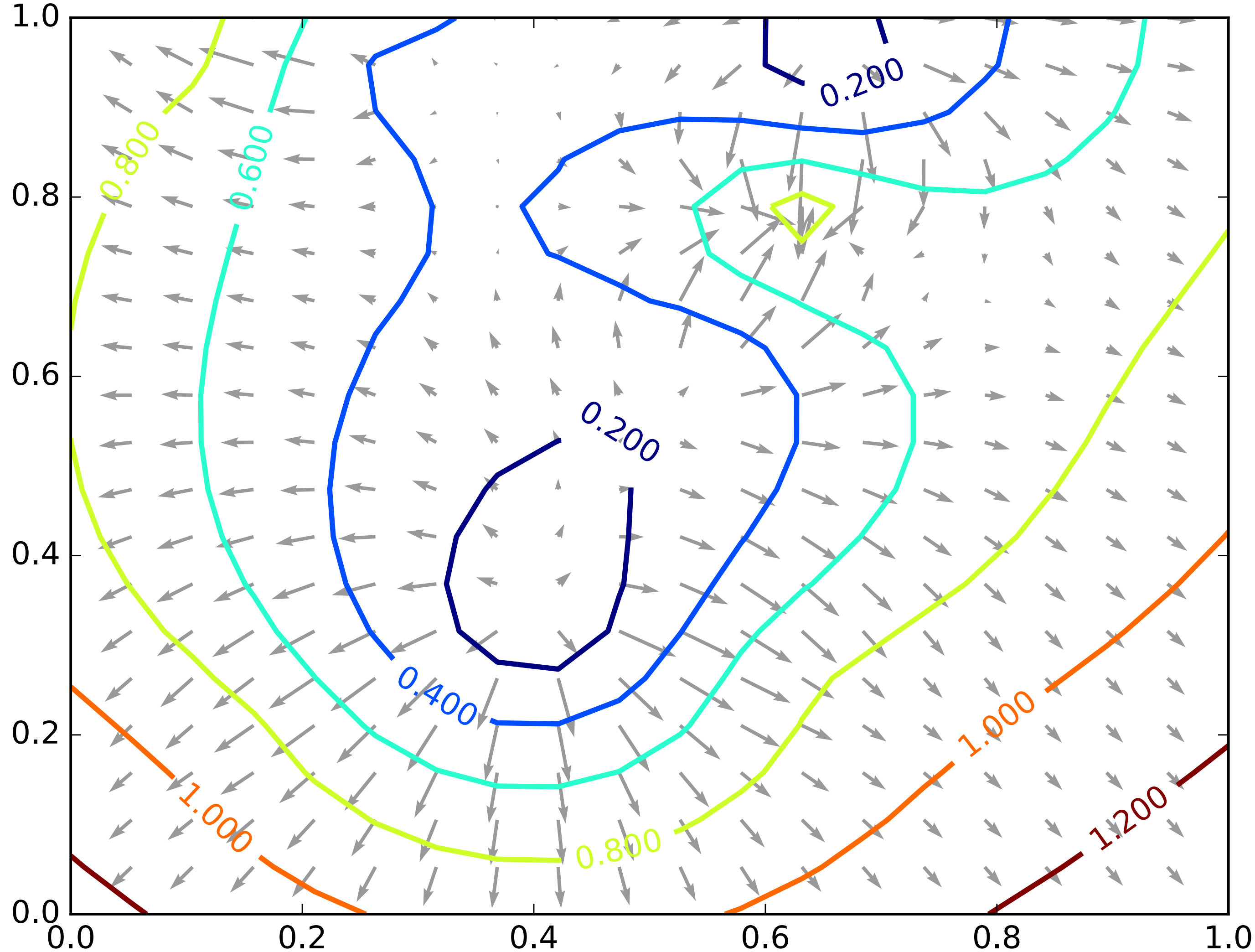


Gradients



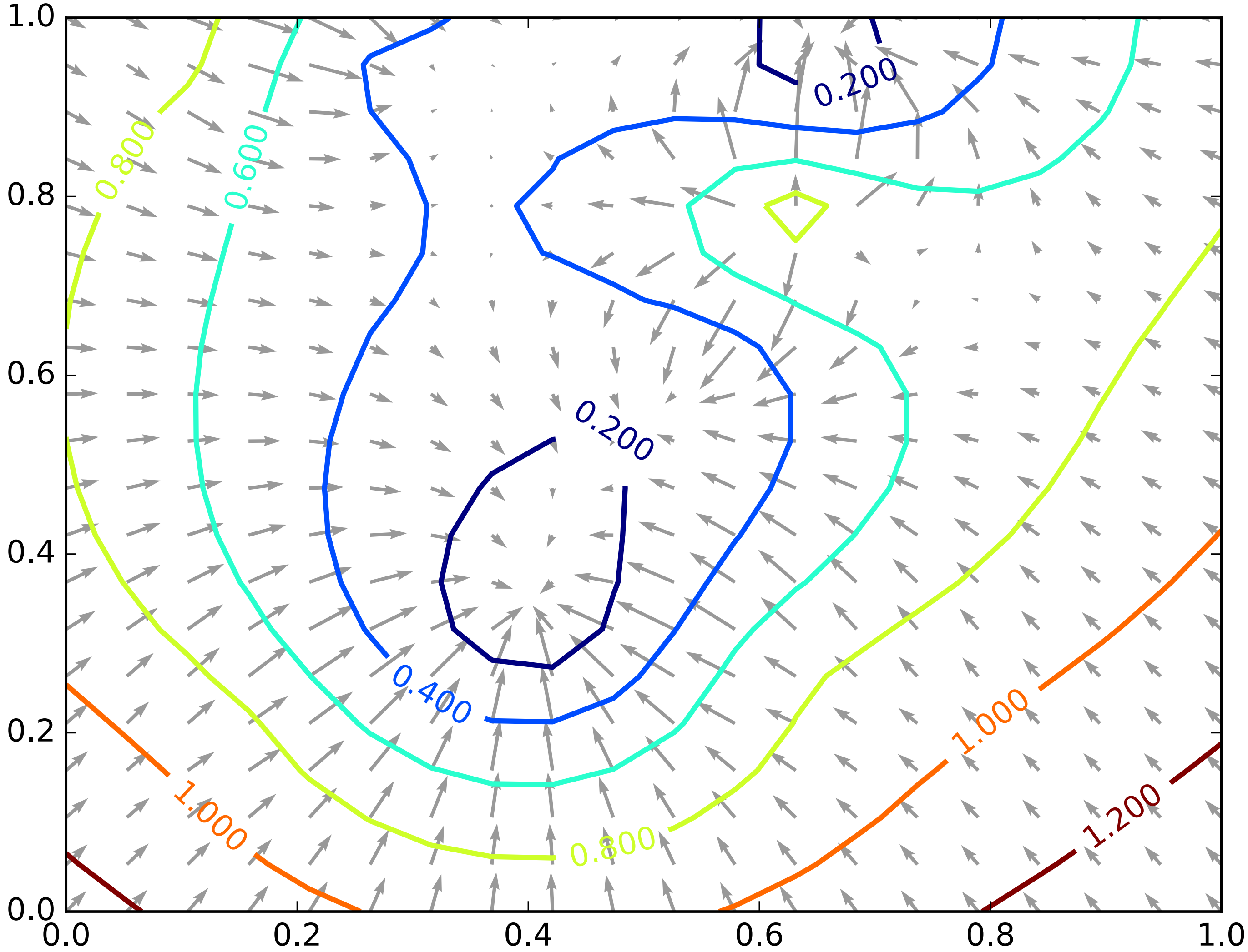
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
0.200
0.200
0.400
0.600
0.800
0.800
1.000
1.000
1.200

Gradients



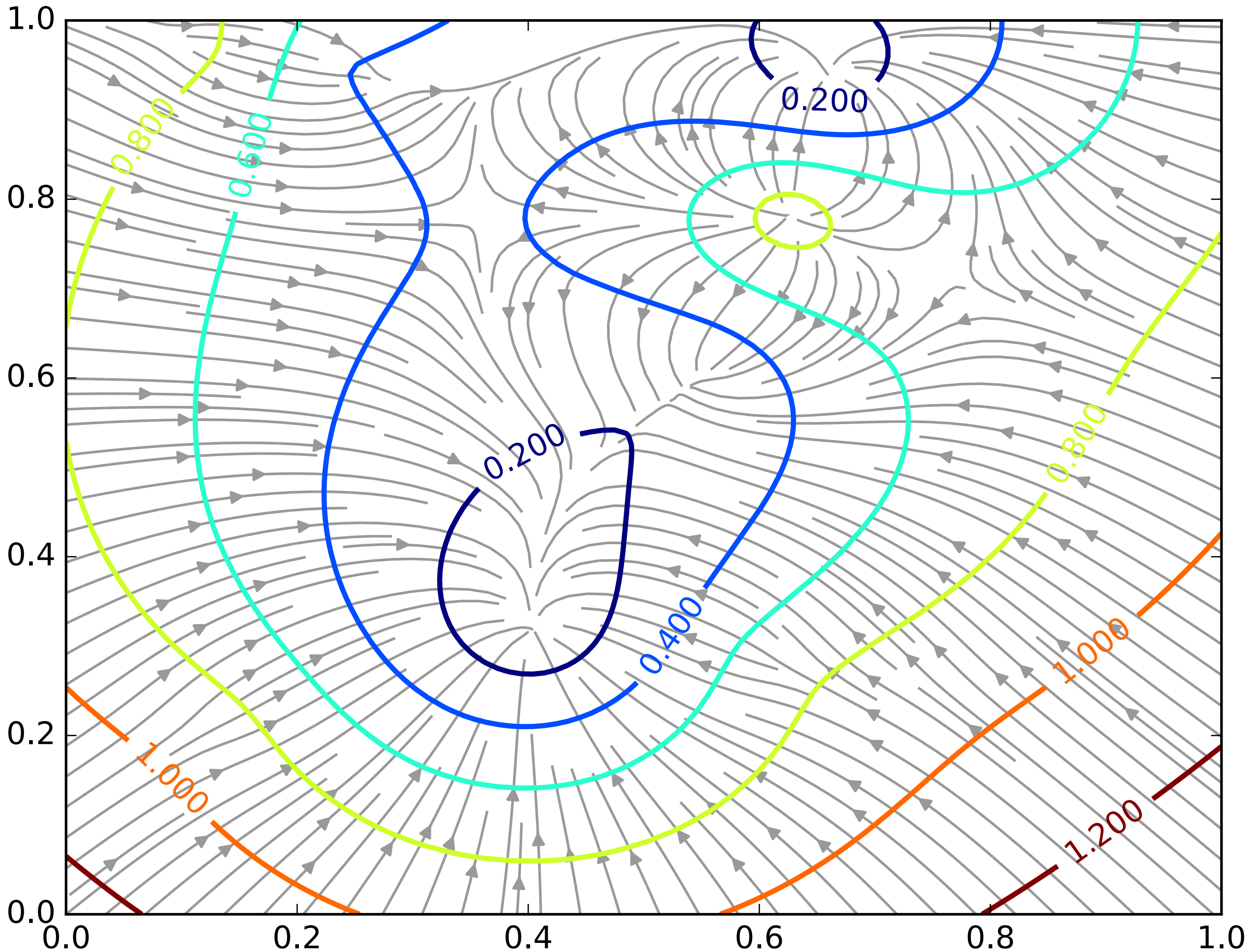
These are the **gradients** that
Gradient **Ascent** would follow.

(Negative) Gradients



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

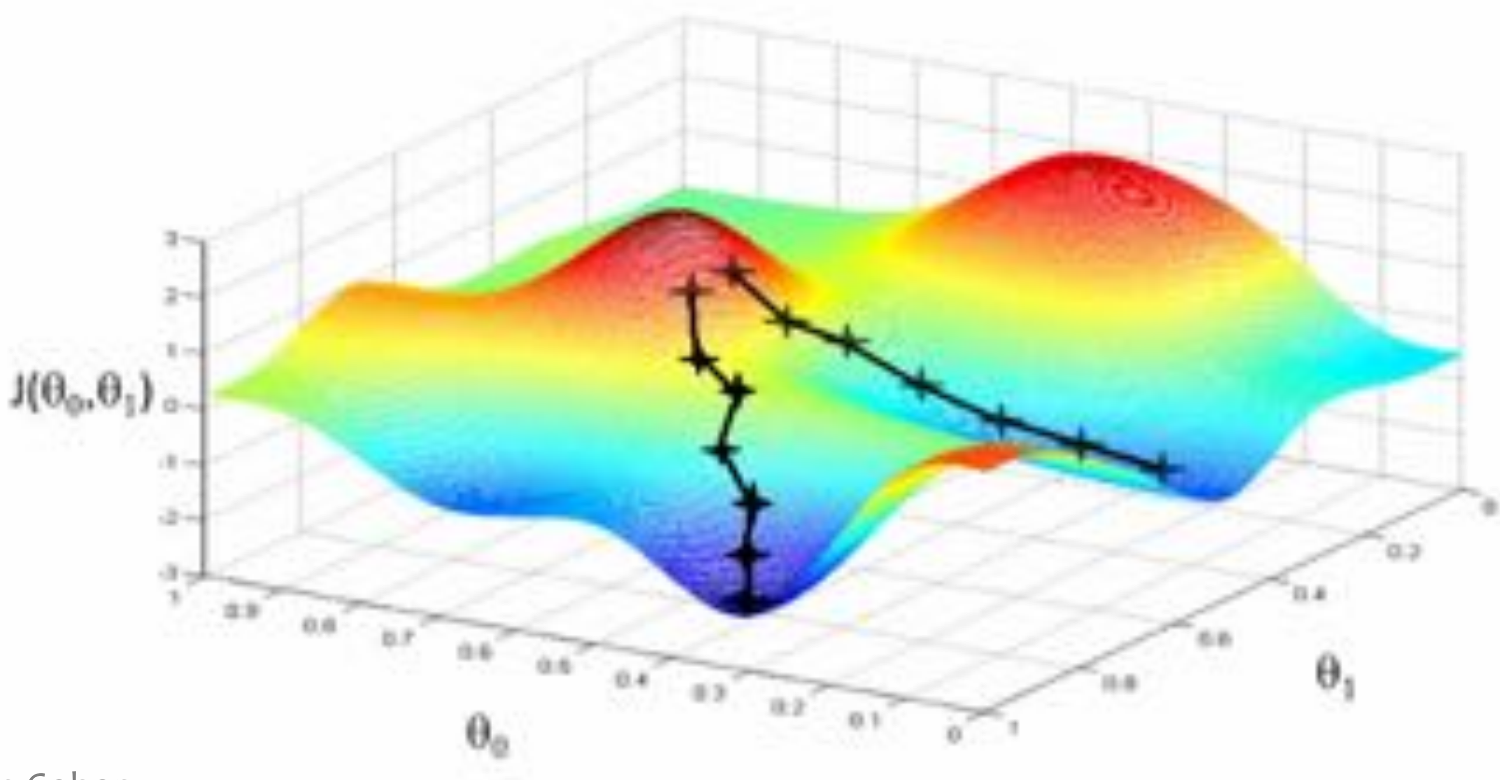
(Negative) Gradient *Paths*



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



Gradient Descent

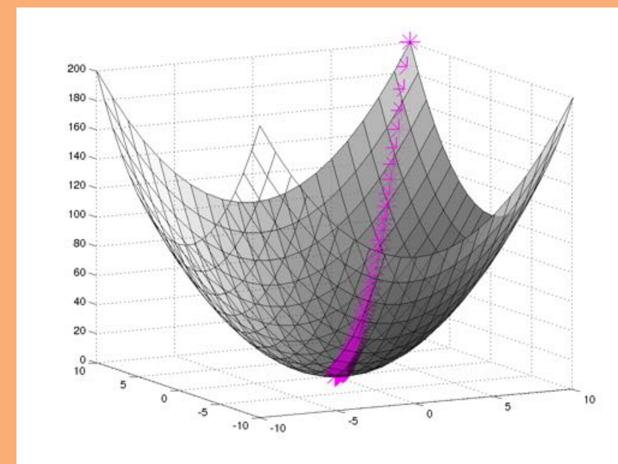
Chalkboard

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

Gradient Descent

Algorithm 1 Gradient Descent

$$
\begin{array}{l}
\textbf{procedure } \mathrm{GD}(\mathcal{D}, \boldsymbol{\theta}^{(0)}) \\
\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)} \\
\quad \textbf{while } \text{not converged } \textbf{do} \\
\quad \quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \\
\quad \textbf{return } \boldsymbol{\theta}
\end{array}
$$



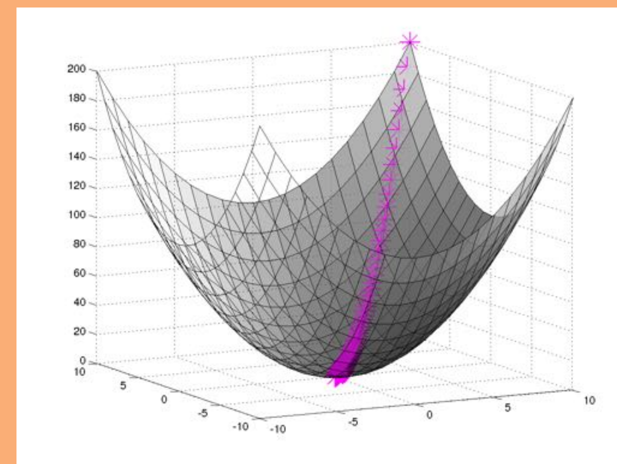
In order to apply GD to Linear Regression all we need is the **gradient** of the objective function (i.e. vector of partial derivatives).

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

Gradient Descent

Algorithm 1 Gradient Descent

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

Optimization for Linear Regression

Chalkboard

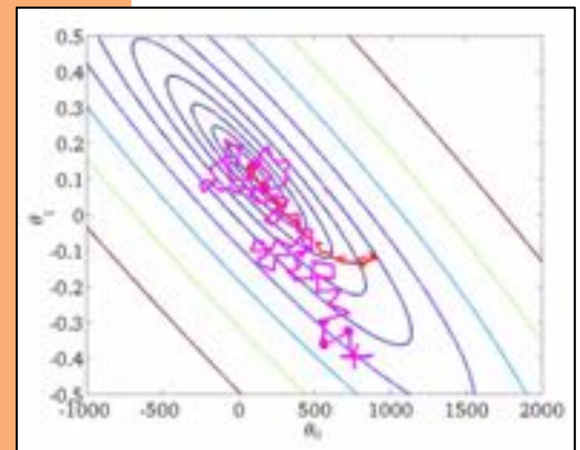
- Computing the gradient for Linear Regression
- Gradient Descent for Linear Regression
- 2D Example in Three Parts:
  1. Line over time
  2. Parameters space over time
  3. Train / test error over time

STOCHASTIC GRADIENT DESCENT

Stochastic Gradient Descent (SGD)

Algorithm 2 Stochastic Gradient Descent (SGD)

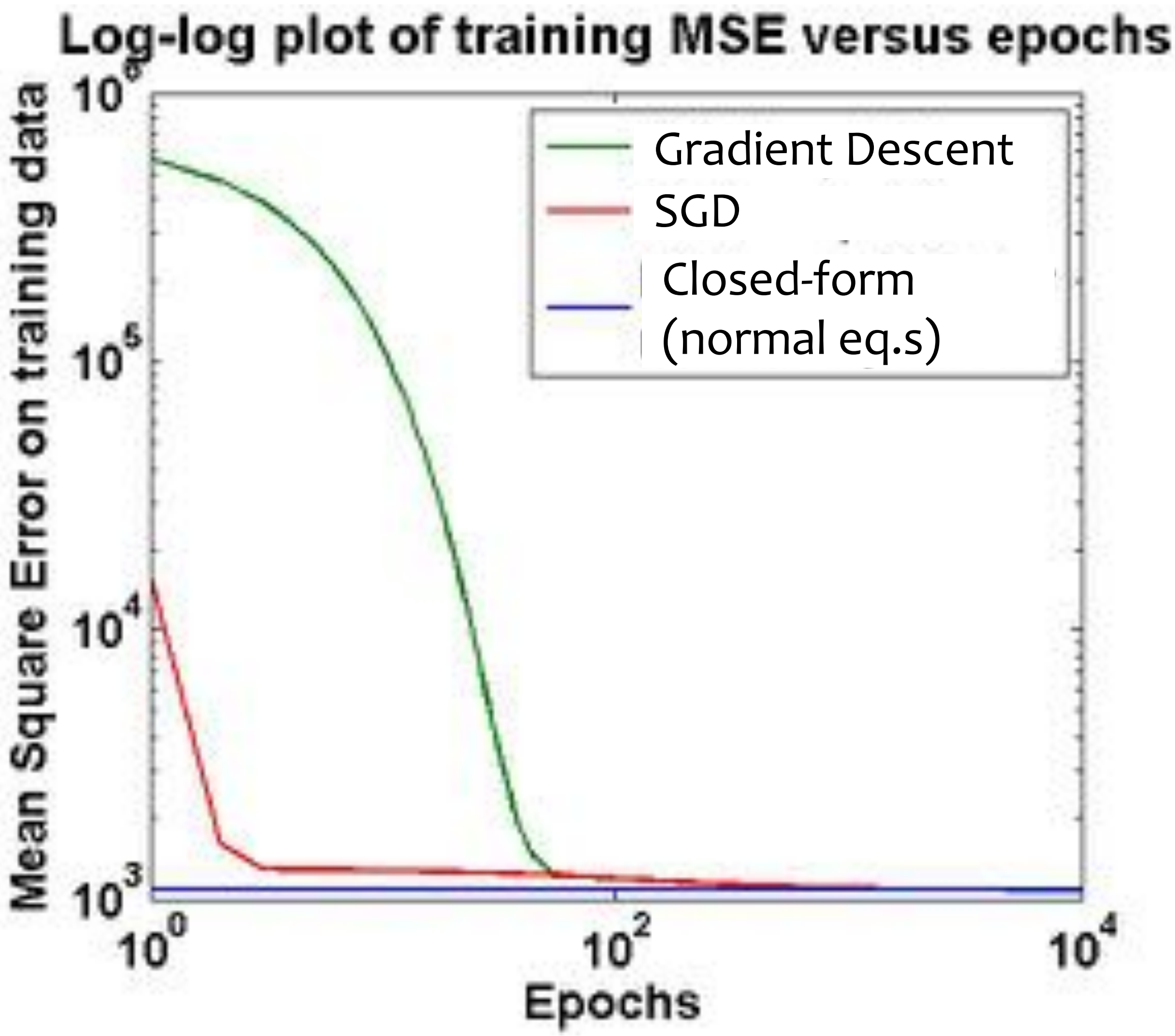
> **procedure** SGD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
> $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
>   **while** not converged **do**
>   **for** $i \in \text{shuffle}(\{1, 2, \ldots, N\})$ **do**
> $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta})$
>   **return** $\boldsymbol{\theta}$



We need a per-example objective:

$$\text{Let } J(\boldsymbol{\theta}) = \sum_{i=1}^{N} J^{(i)}(\boldsymbol{\theta})$$

Convergence Curves

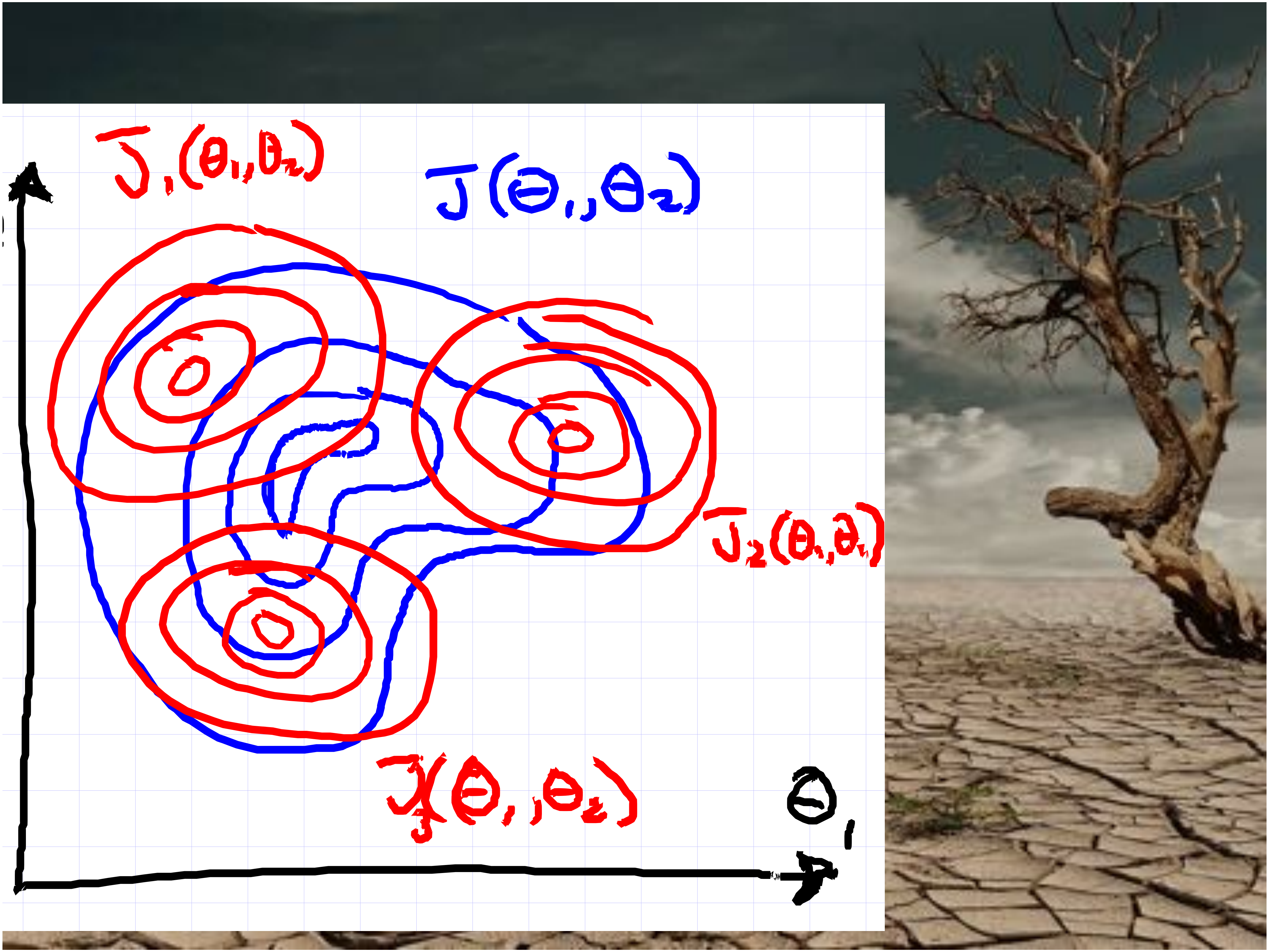


- *Def*: an **epoch** is a single pass through the training data

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



J1(θ1,θ2)
J(θ1,θ2)
J2(θ1,θ2)
J3(θ1,θ2)
θ1

Expectations of Gradients

$$\frac{dJ(\vec{\theta})}{d\theta_j} = \frac{1}{N} \sum_{i=1}^{N} \frac{d}{d\theta_j}\left(J_i(\vec{\theta})\right)$$

$$\nabla J(\vec{\theta}) = \begin{array}{c} \\ j^{th} \end{array} \begin{bmatrix} \vdots \\ \_\_\_\_ \\ \vdots \end{bmatrix} = \frac{1}{N} \sum_{i=1}^{N} \nabla J_i(\vec{\theta})$$

Recall: for any discrete r.v. X

$$E_X[f(X)] \triangleq \sum_x P(X=x) f(x)$$

Q: What is the expected value of a randomly chosen $\nabla J_i(\theta)$?

Let $I \sim \text{Uniform}(\{1, \ldots, N\})$

$\Rightarrow P(I=i) = \frac{1}{N}$ if $i \in \{1 \ldots N\}$

$$E_I[\nabla J_I(\vec{\theta})] = \sum_{i=1}^{N} P(I=i) \nabla J_i(\vec{\theta})$$

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

$$= \nabla J(\vec{\theta})$$

Convergence of Optimizers

Convergence Analysis:

true unknown min

Def: convergence is when $J(\vec{\theta}) - J(\vec{\theta}^*) < \epsilon$

not covered

Methods	Steps to Converge	Computation per iteration
Newton's Method	$O(\ln \ln 1/\epsilon)$	$\nabla J(\theta)$ $\nabla^2 J(\theta) \leftarrow O(NM^2)$
GD	$O(\ln 1/\epsilon)$	$\nabla J(\theta) \leftarrow O(NM)$
SGD	$O(1/\epsilon)$*	$\nabla J_i(\theta) \leftarrow O(M)$

*"almost sure" convergence

lots of caveats and conditions

way less computation

Takeaway: SGD has much slower asymptotic convergence but is often faster in practice.

Optimization Objectives

You should be able to…

- Apply gradient descent to optimize a function
- Apply stochastic gradient descent (SGD) to optimize a function
- Apply knowledge of zero derivatives to identify a closed-form solution (if one exists) to an optimization problem
- Distinguish between convex, concave, and nonconvex functions
- Obtain the gradient (and Hessian) of a (twice) differentiable function

Linear Regression Objectives

You should be able to…

- Design k-NN Regression and Decision Tree Regression
- Implement learning for Linear Regression using three optimization techniques: (1) closed form, (2) gradient descent, (3) stochastic gradient descent
- Choose a Linear Regression optimization technique that is appropriate for a particular dataset by analyzing the tradeoff of computational complexity vs. convergence speed
- Distinguish the three sources of error identified by the bias-variance decomposition: bias, variance, and irreducible error.

PROBABILISTIC LEARNING

Probabilistic Learning

Function Approximation

Previously, we assumed that our output was generated using a **deterministic target function:**

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

Our goal was to learn a hypothesis h(**x**) that best approximates c*(**x**)

Probabilistic Learning

Today, we assume that our output is **sampled** from a conditional **probability distribution:**

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

Our goal is to learn a probability distribution p(y|**x**) that best approximates p*(y|**x**)

Robotic Farming

	Deterministic	**Probabilistic**
Classification (binary output)	Is this a picture of a wheat kernel?	Is this plant drought resistant?
Regression (continuous output)	How many wheat kernels are in this picture?	What will the yield of this plant be?

Bayes Optimal Classifier

Whiteboard

- Bayes Optimal Classifier
- Reducible / irreducible error
- Ex: Bayes Optimal Classifier for 0/1 Loss