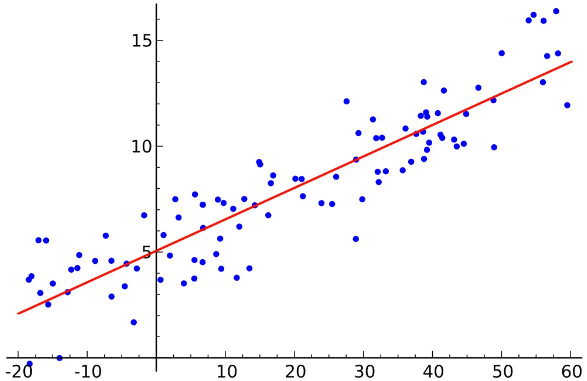
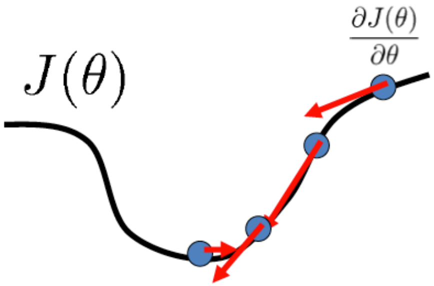
Tufts COMP 135: Introduction to Machine Learning
https://www.cs.tufts.edu/comp/135/2020f/

Gradient Descent





Many slides attributable to:
Erik Sudderth (UCI)
Finale Doshi-Velez (Harvard)
James, Witten, Hastie, Tibshirani (ISL/ESL books)

Prof. Mike Hughes

Today’s Objectives (day 06)

Gradient descent

- Key idea: Find optimal (or close to optimal) parameters for an objective by repeatedly stepping downhill
- Benefits:
  - Widely useful for many ML tasks. Likely useful for any objective that is differentiable
  - In contrast, exact solutions (like our formulas for optimal weights for least squares) are hard to derive for most objectives
- Practical problems:
  - Local vs. global minima
  - How to pick step size
  - How to assess convergence
  - Initialization

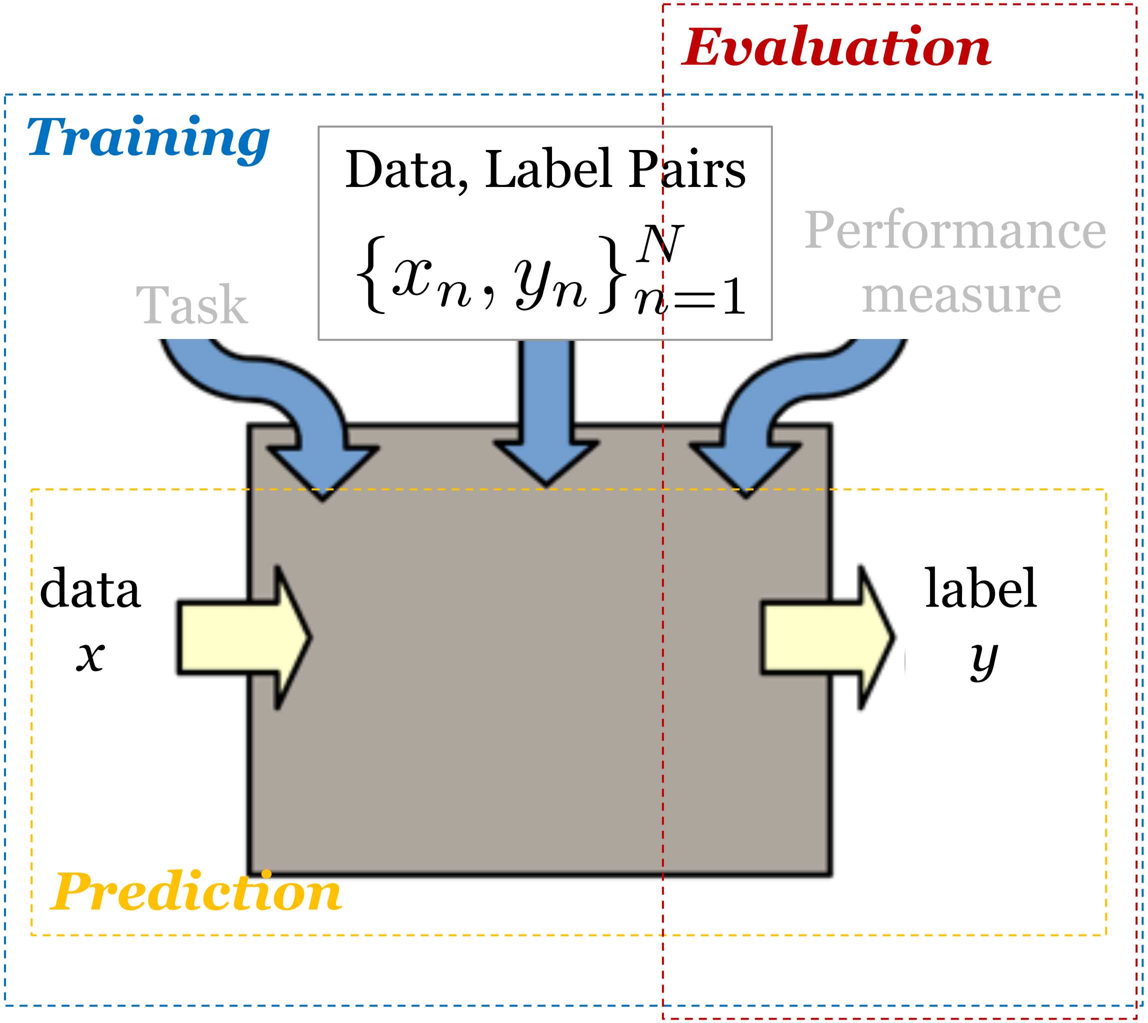
- Lab: Gradient descent for linear regression

What will we learn?

Supervised Learning

Unsupervised Learning

Reinforcement Learning



Task: Regression

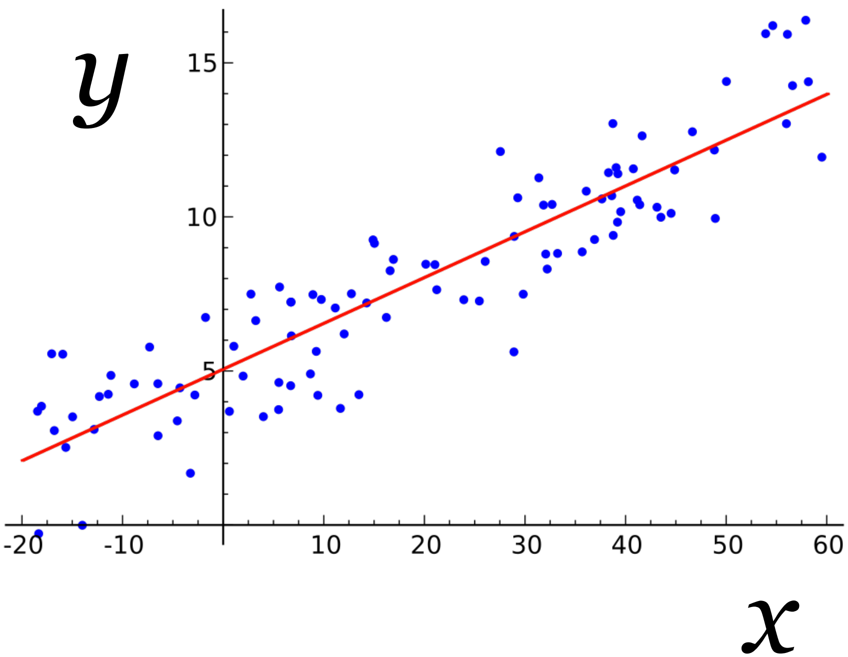
Supervised Learning

regression

Unsupervised Learning

Reinforcement Learning

y is a numeric variable e.g. sales in $$



Linear Regression

Optimization problem: “Least Squares”

$$\min_{\theta \in \mathbb{R}^{F+1}} \quad \sum_{n=1}^{N} (y_n - \hat{y}(x_n, \theta))^2$$

$$\tilde{X} = \begin{bmatrix} x_{11} & \dots & x_{1F} & 1 \\ x_{21} & \dots & x_{2F} & 1 \\ & & \dots & \\ x_{N1} & \dots & x_{NF} & 1 \end{bmatrix}$$

$$\min_{\theta \in \mathbb{R}^{F+1}} \quad \underbrace{(y - \tilde{X}\theta)^T (y - \tilde{X}\theta)}_{J(\theta)}$$

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

We can solve **this particular** optimization problem exactly.

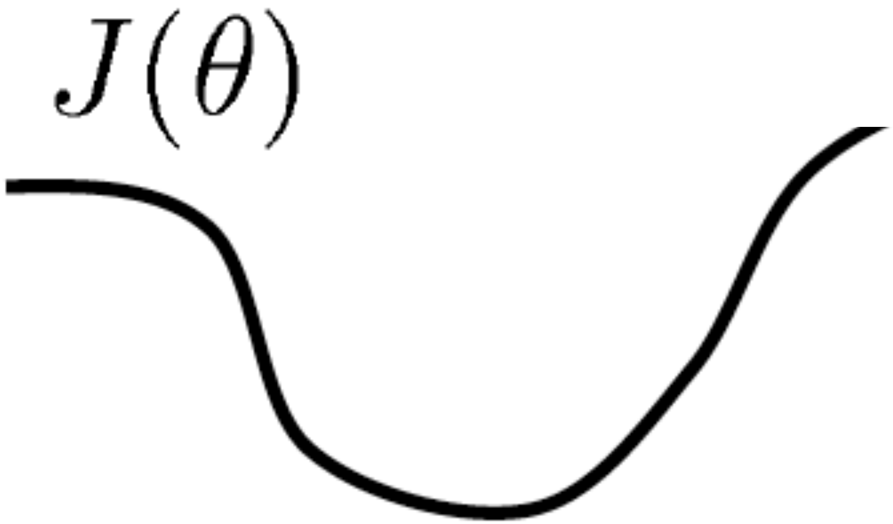
However, what happens when:

- We want to use another error than squared error?
- We want to add an L1 penalty?
- We have so many dimensions (F > 1 million) that solving the linear system exactly is prohibitive
- We want to change the objective in some other way

Is there a general purpose way to solve optimization problems like

$$\min_{\theta} \quad J(\theta)$$

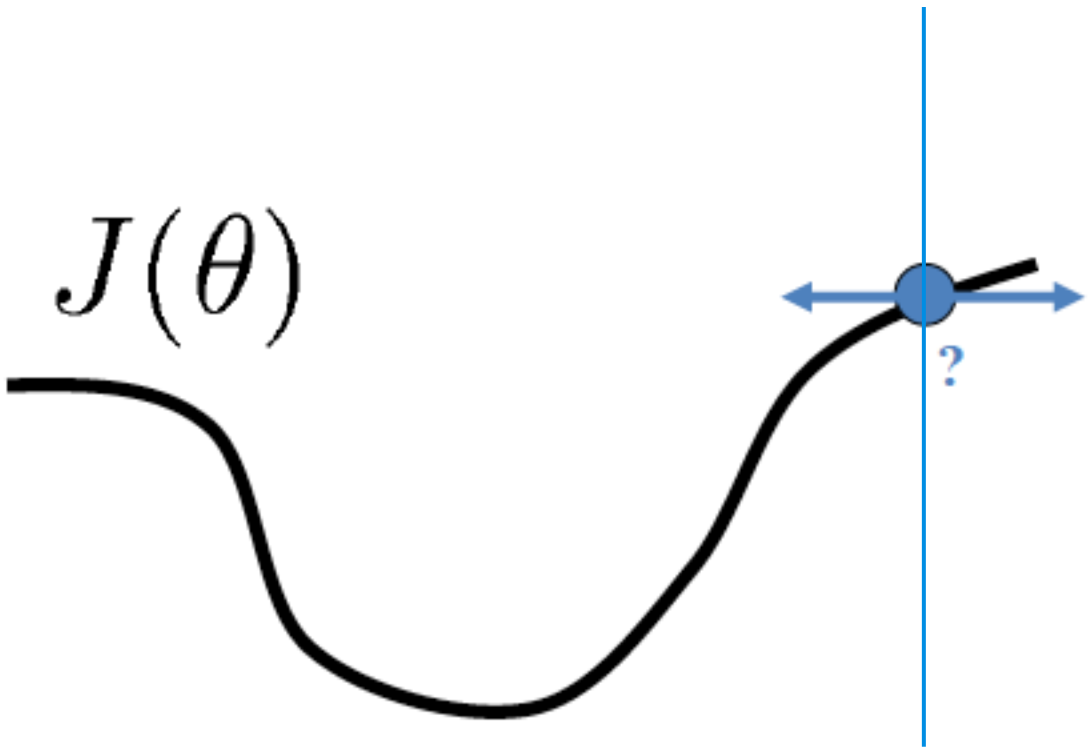
Assumptions



- Loss function J is smooth and deterministic
- We can evaluate our loss function at any value of parameter theta
- We can evaluate the first derivative ("gradient") of our loss at any value of parameter theta

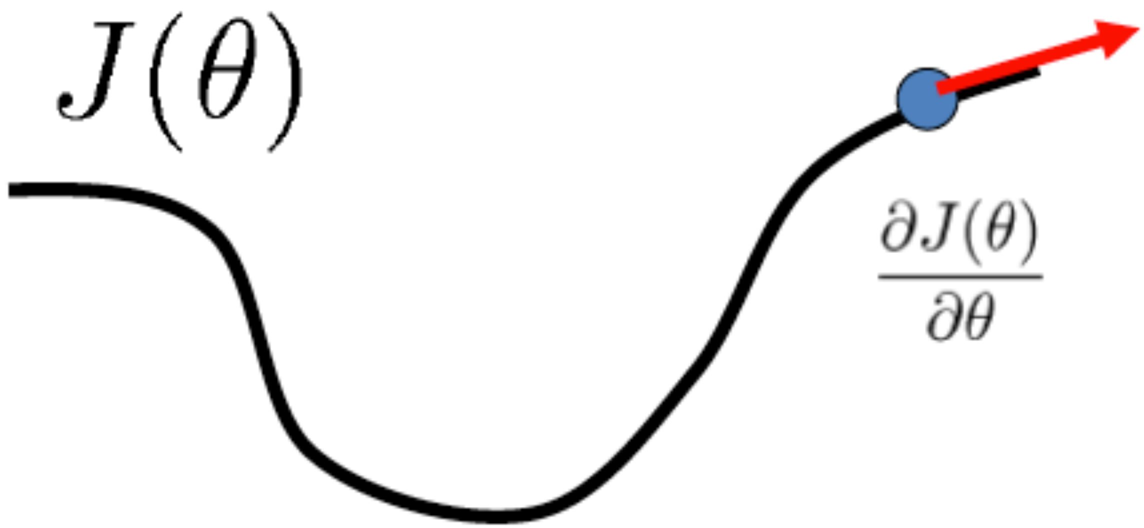
$$\frac{\partial J(\theta)}{\partial \theta}$$

Idea: Optimize via small steps

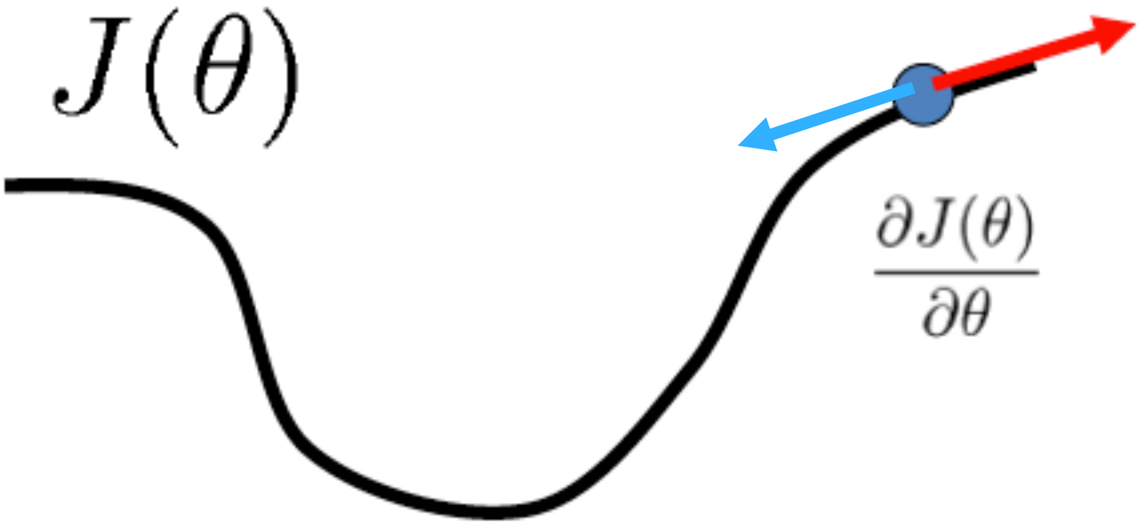


Current "guess" for
parameter theta

Derivatives point **uphill**



To minimize, go **downhill**



Step in the opposite **direction** of the derivative

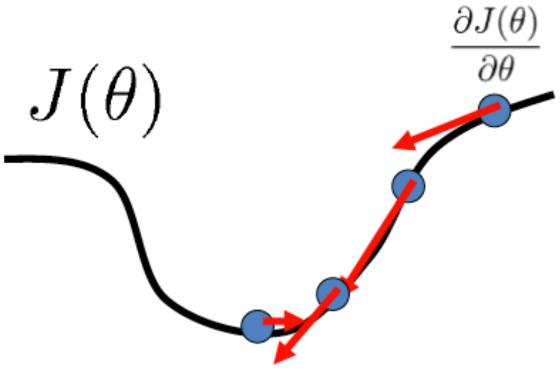
Steepest descent algorithm

input: initial $\theta \in \mathbb{R}$

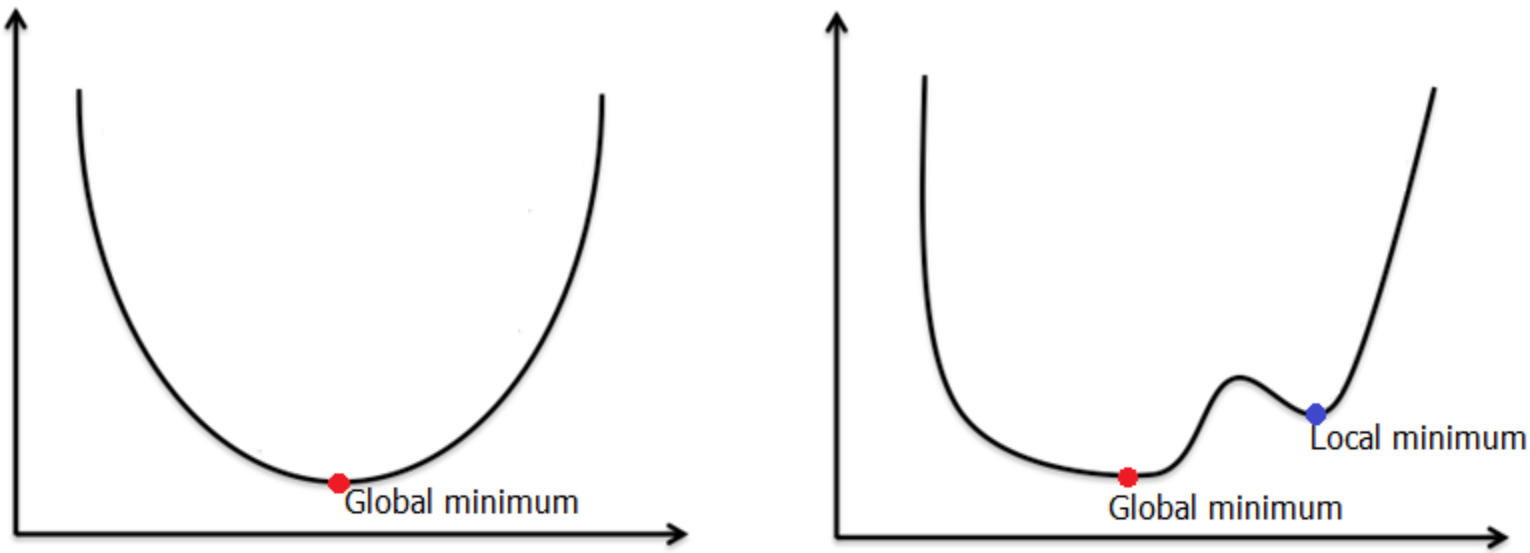
input: step size $\alpha \in \mathbb{R}_+$

while not converged:

$$\theta \leftarrow \theta - \alpha \frac{d}{d\theta} J(\theta)$$



Will gradient descent always find same solution?



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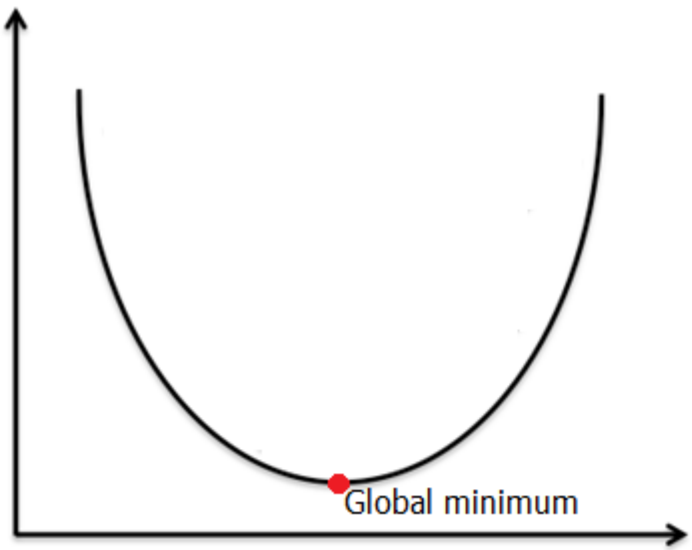
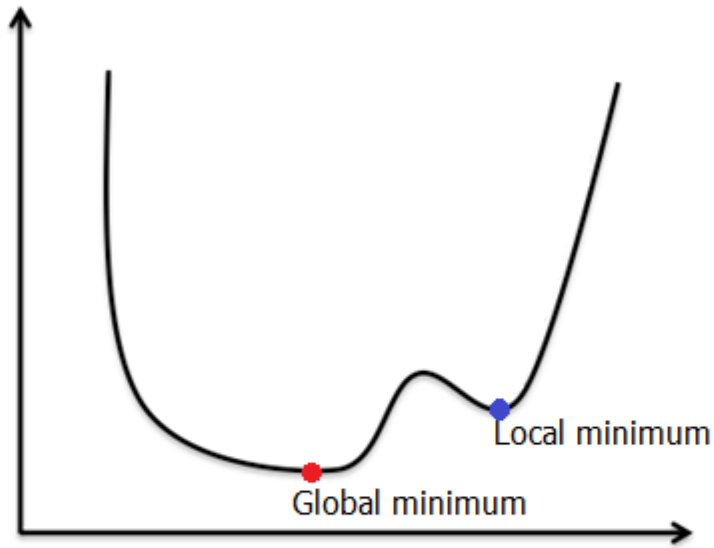
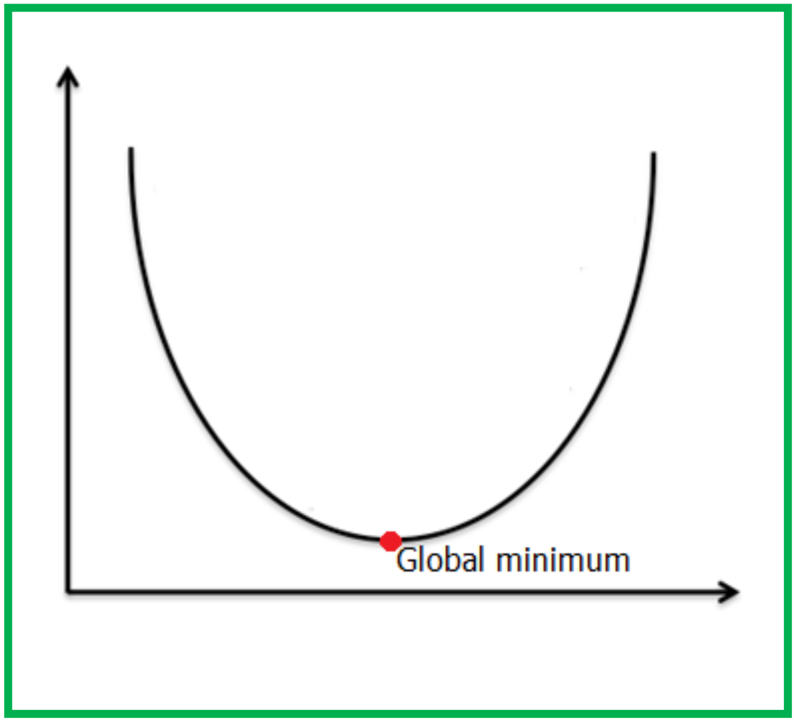


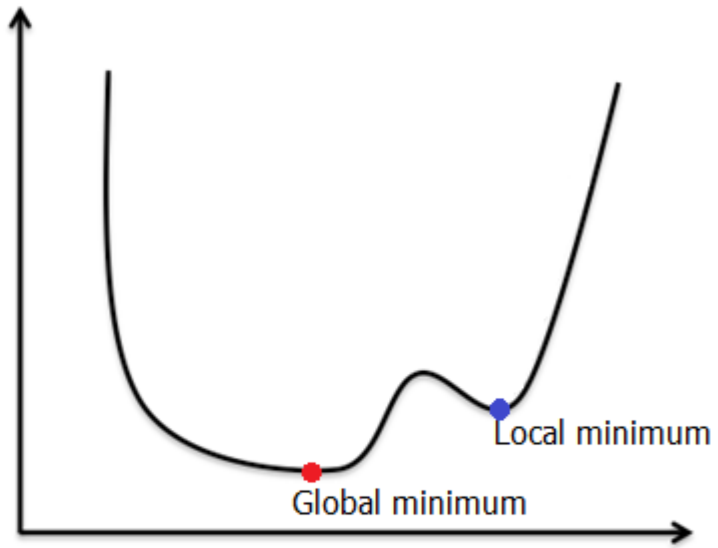
Yes, if loss looks like this



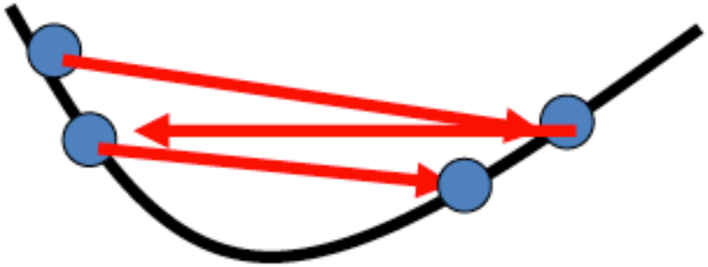
Not if multiple local minima exist

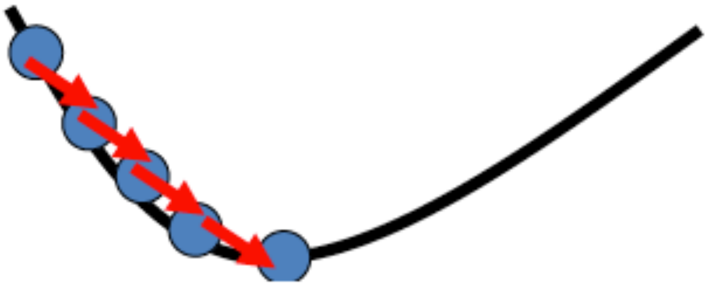
Linear Regression is convex!





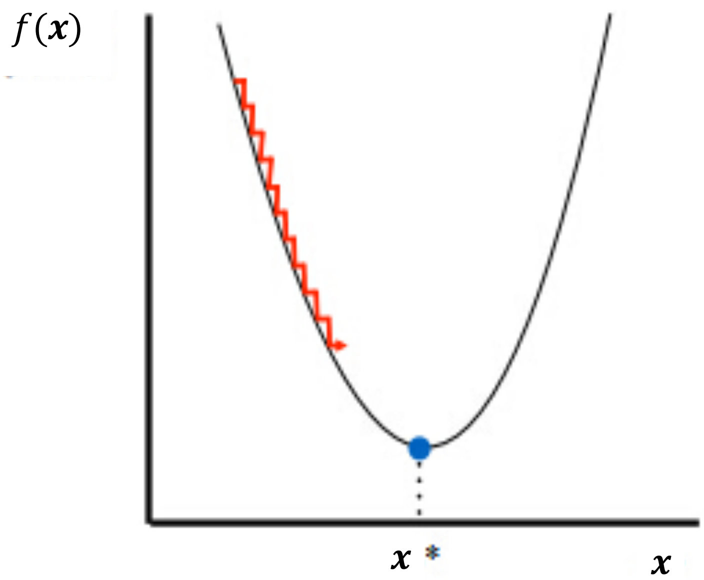
How to set step size?



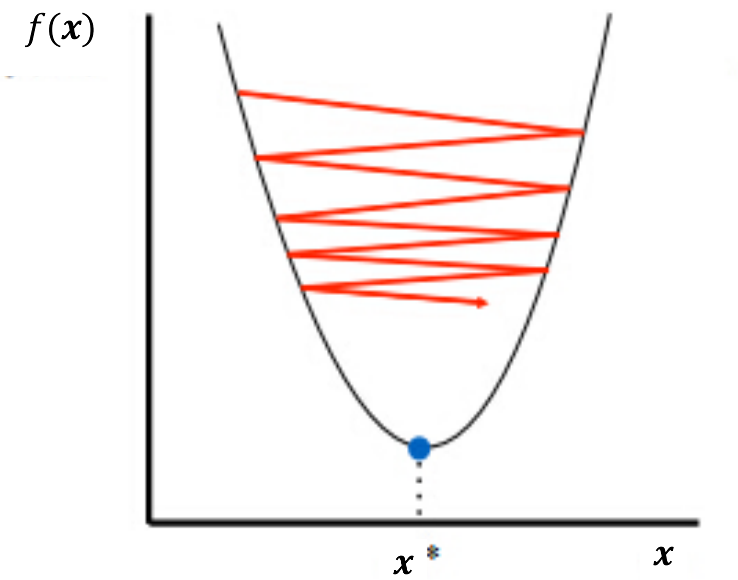


Intuition: 1D gradient descent

Choosing good step size matters!



Too small: converge very slowly



Too big: overshoot and even diverge

Debugging: loss vs iterations

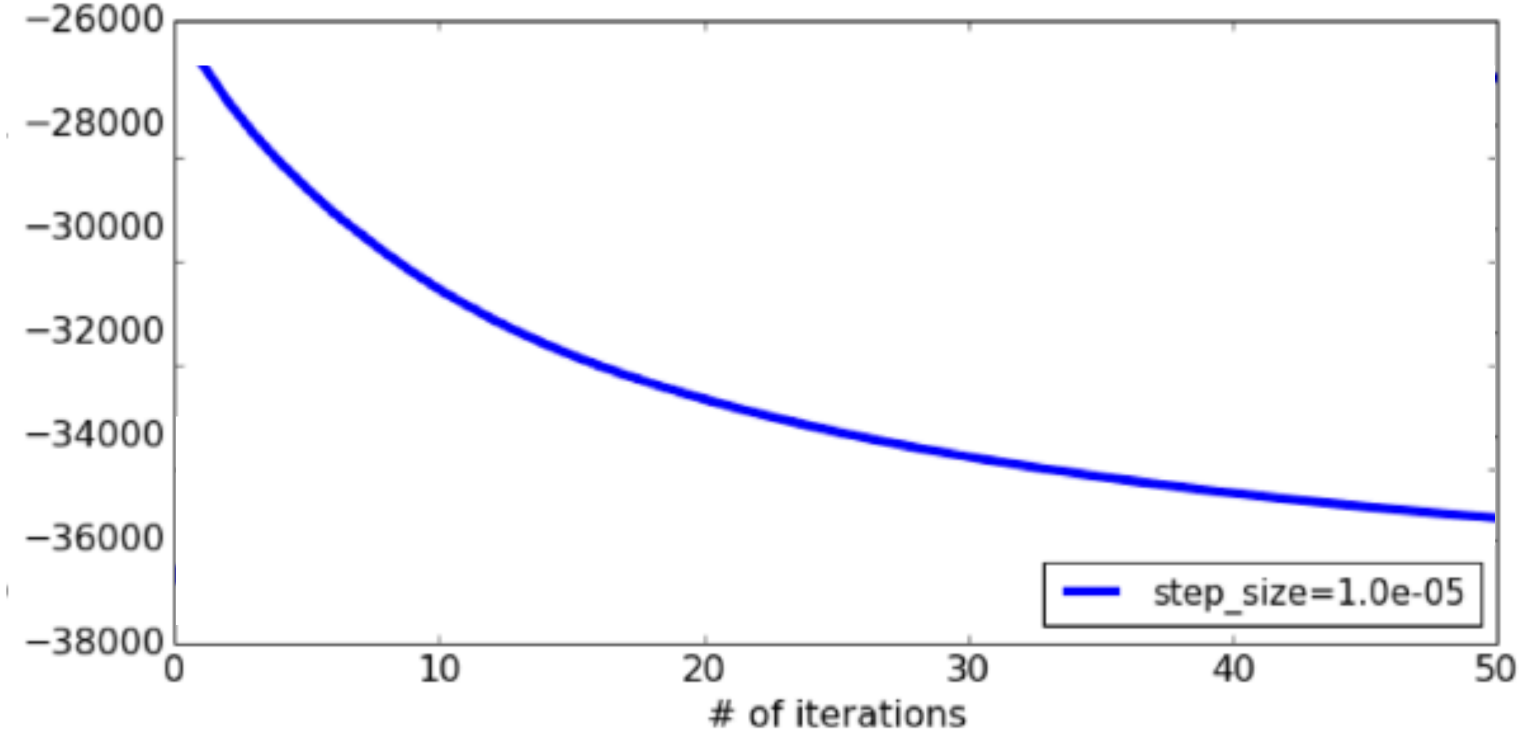


Figure Credit: Emily Fox (UW)

If step size is **too small**

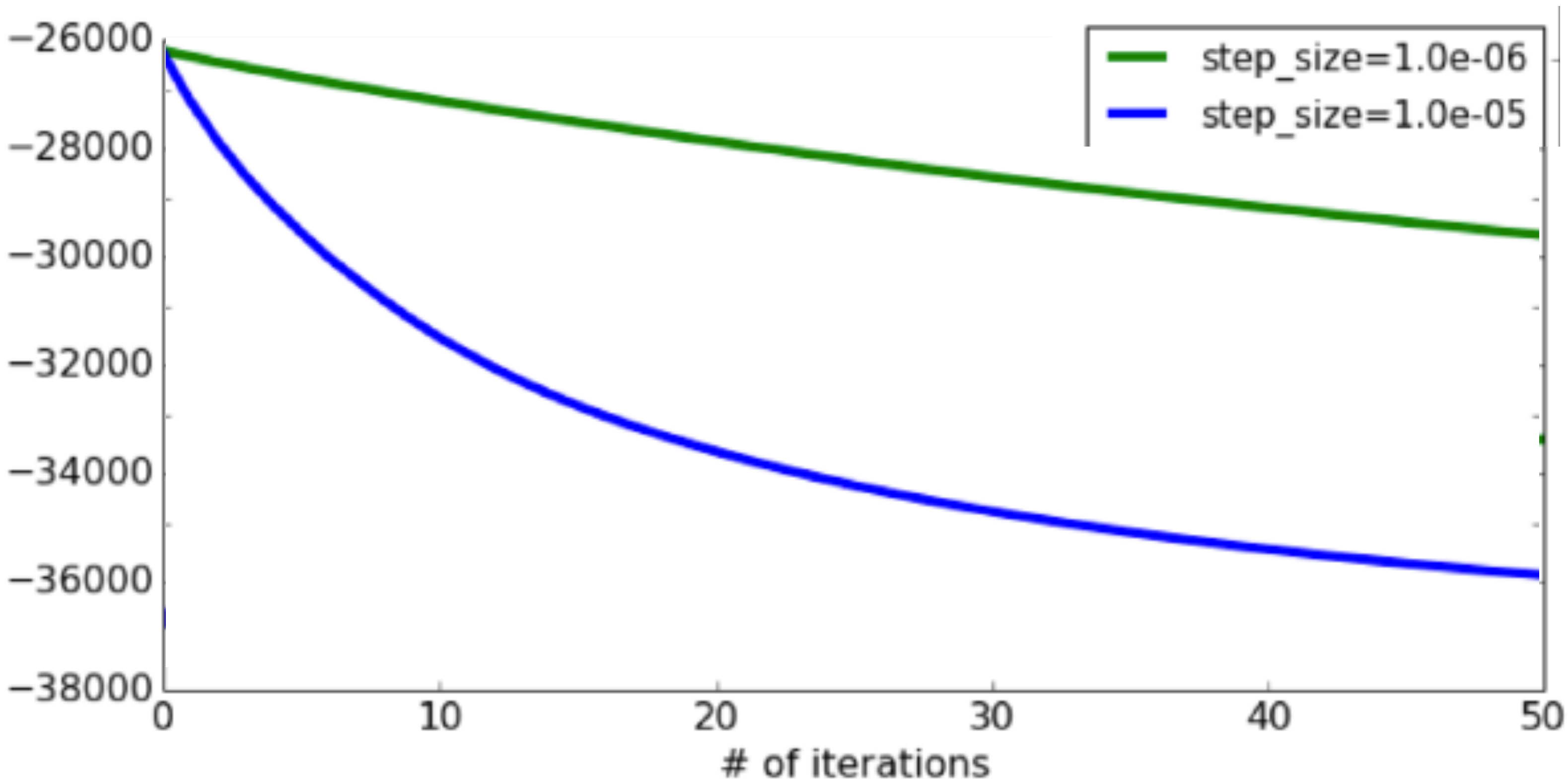


Figure Credit: Emily Fox (UW)

If step size is **large**

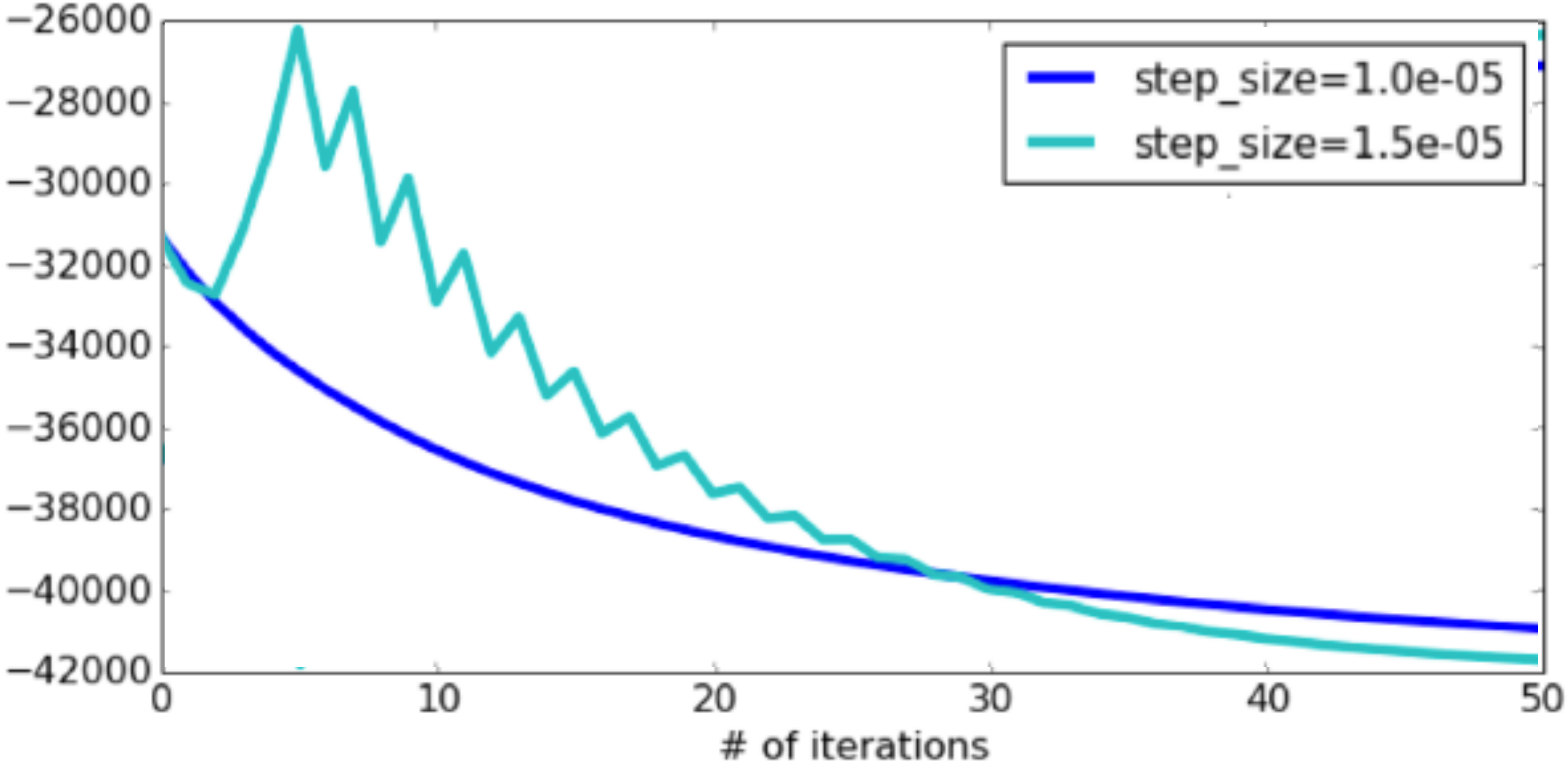
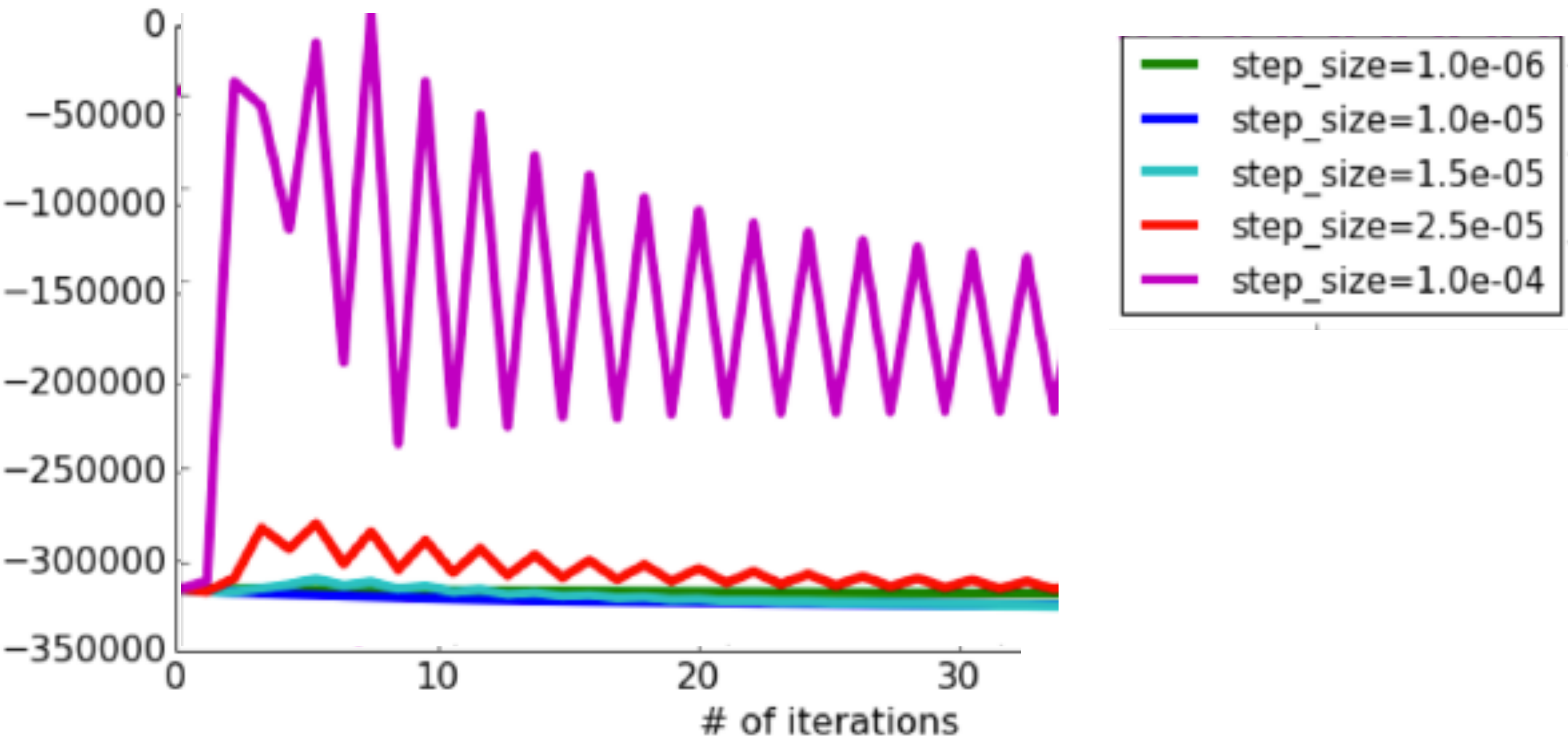


Figure Credit: Emily Fox (UW)

If step size is **way too large**



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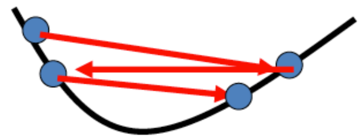
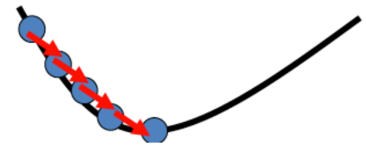
Hints for picking step sizes





- Don’t blindly trust the default
- Don’t try just one!

- Try several values (spaced like 10^{-4}, 10^{-2}, 1, 100) until
  - Find one clearly too small
  - Find one clearly too large (oscillation / divergence)
  - Then focus on finding “just right” value in between

- Always make trace plots!
  - loss vs iteration
  - gradient vs iteration
  - parameter vs iteration

- Smarter choices for step size (advanced material, beyond today’s class)
  - Decaying methods
  - Line search methods
  - Second-order methods
  - Adaptive methods

How to assess convergence?

- Ideal: stop when derivative equals zero

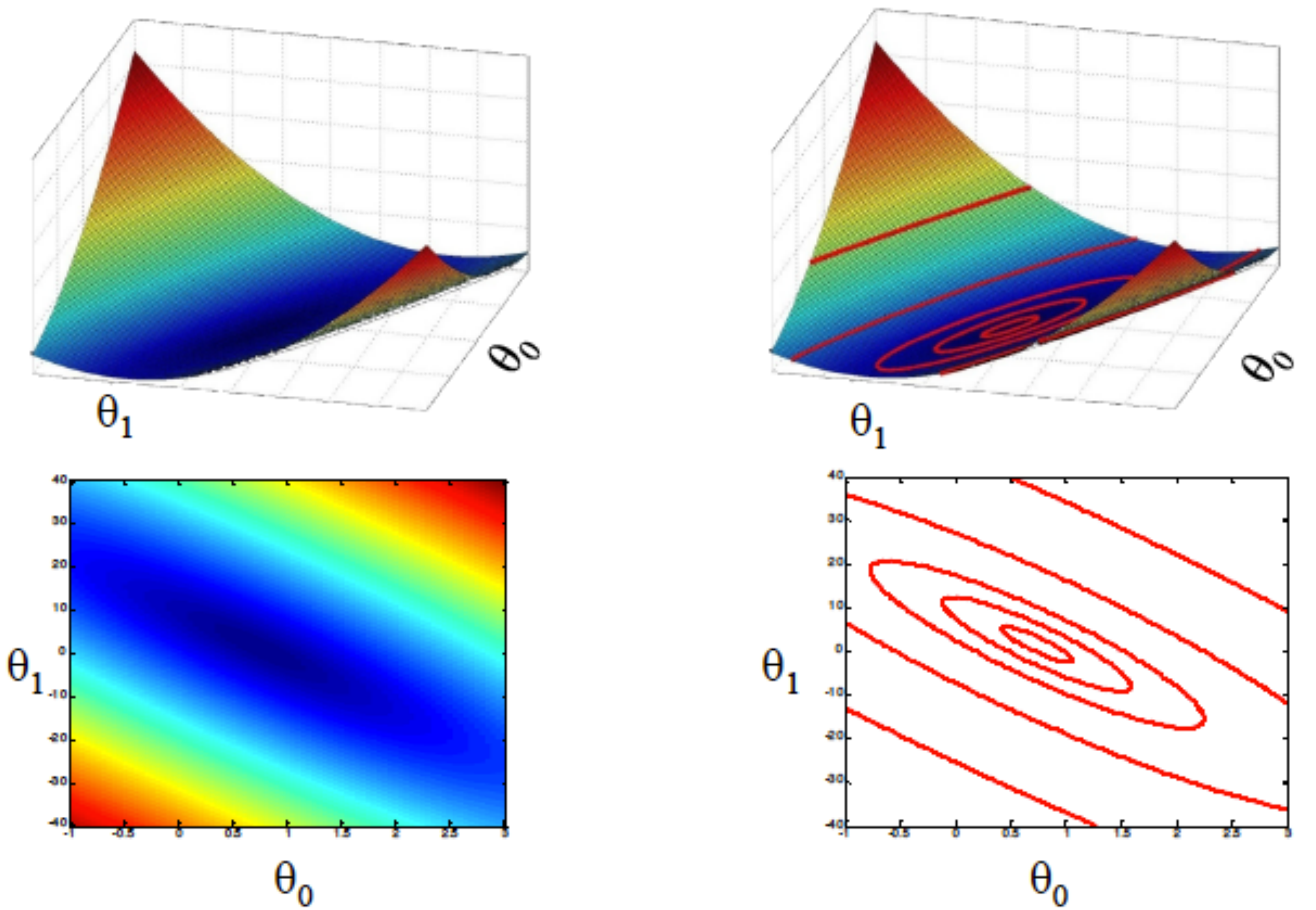
- Practical heuristics: stop when …
  - change in loss becomes "small enough"

$$|J(\theta_t) - J(\theta_{t-1})| < \epsilon$$

  - net step size is indistinguishable from zero

$$\alpha \left|\frac{d}{d\theta} J(\theta)\right| < \epsilon$$

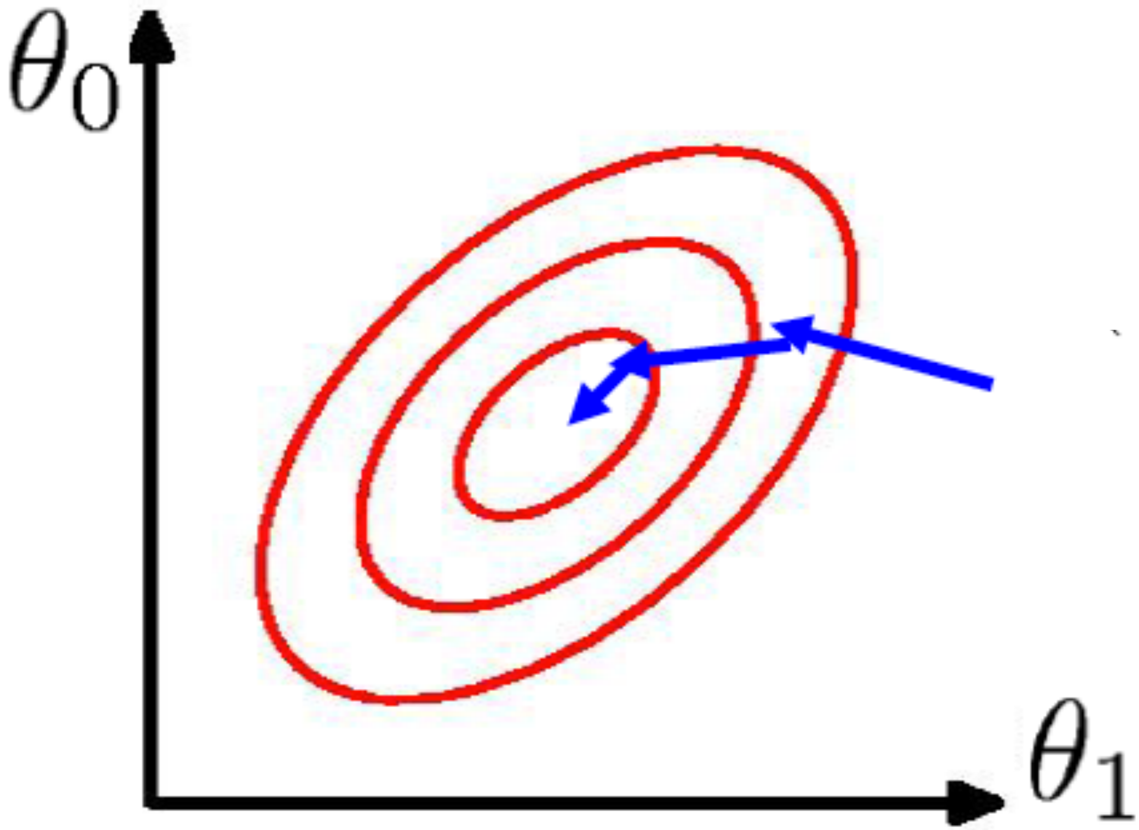
Visualizing loss function when parameter has 2 dimensions



"Level set" contours : all points with same function value

Gradient descent when parameter has 2 dimensions

gradient = vector of partial derivatives



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- Lab: Gradient descent for linear regression with one slope parameter