Optimization

CMPUT 296: Basics of Machine Learning

Textbook §4.1-4.4

Logistics

Reminders:

- Thought Question 1 due **TODAY, September 17, by 11:59pm**
  - To be handed in via eClass
- Assignment 1 (due **Thursday, September 24**)

Tutorial:

- Python tutorial from yesterday is available on eClass

Recap: Estimators

- An **estimator** is a random variable representing a procedure for estimating the value of an unobserved quantity based on observed data
- **Concentration inequalities** let us bound the probability of a given estimator being at least ϵ from the estimated quantity
- An estimator is **consistent** if it **converges in probability** to the estimated quantity

Recap: Sample Complexity

- **Sample complexity** is the **number of samples** needed to attain a desired error bound ϵ at a desired probability $1 - \delta$
- The **mean squared error** of an estimator **decomposes** into **bias** (squared) and **variance**
- Using a **biased** estimator can have **lower error** than an unbiased estimator
  - Bias the estimator based some **prior information**
  - *But this only helps if the prior information is* ***correct***
  - Cannot reduce error by adding in arbitrary bias

Outline

1. Recap & Logistics
2. Optimization by Gradient Descent
3. Multivariate Gradient Descent
4. Adaptive Step Sizes
5. Optimization Properties

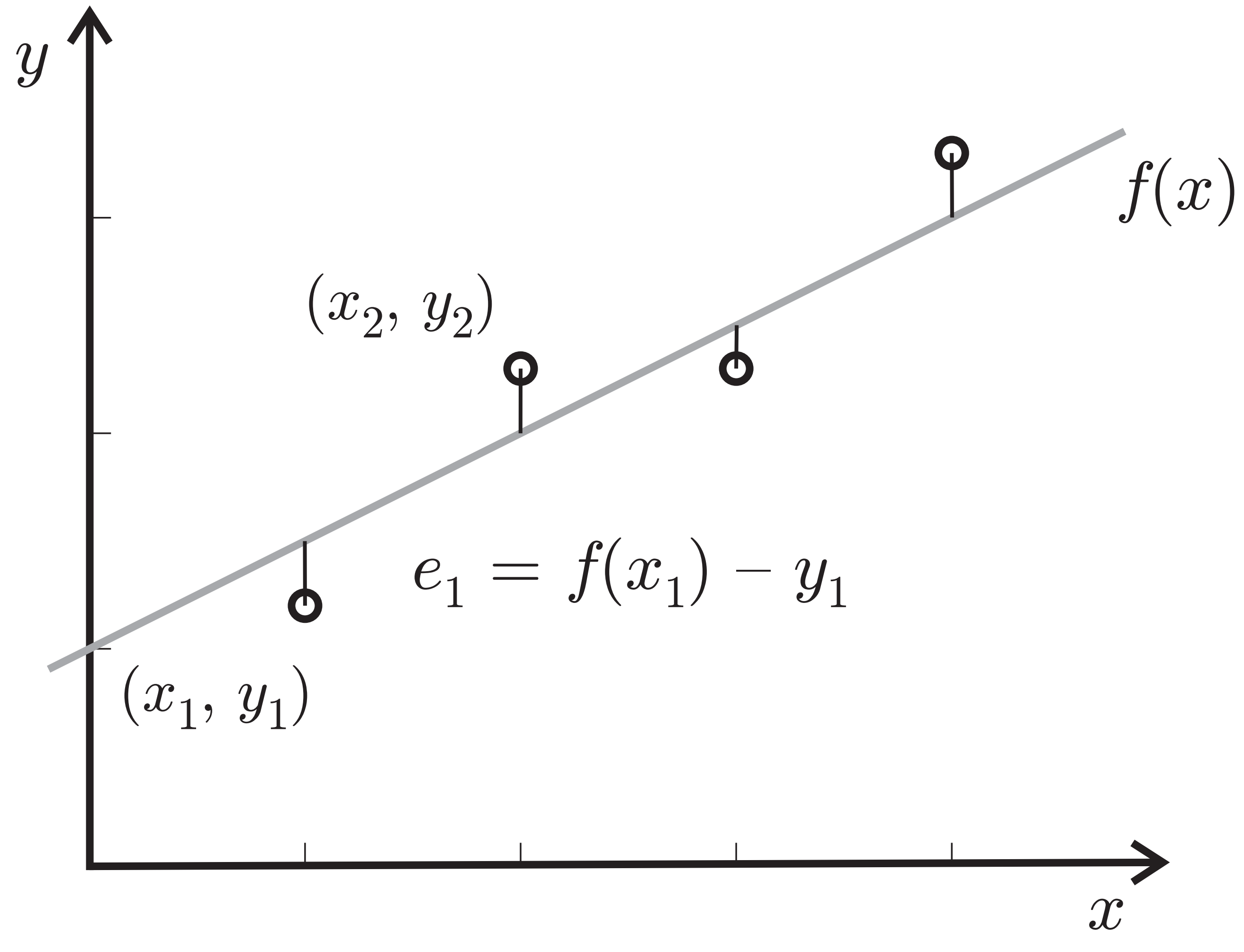
Optimization

We often want to find the argument w^* that **minimizes** an **objective function** c

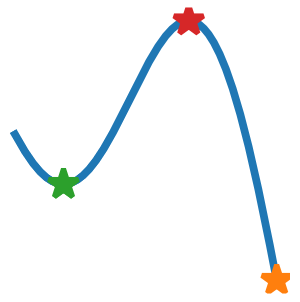
$$\mathbf{w}^* = \arg\min_{\mathbf{w}} c(\mathbf{w})$$

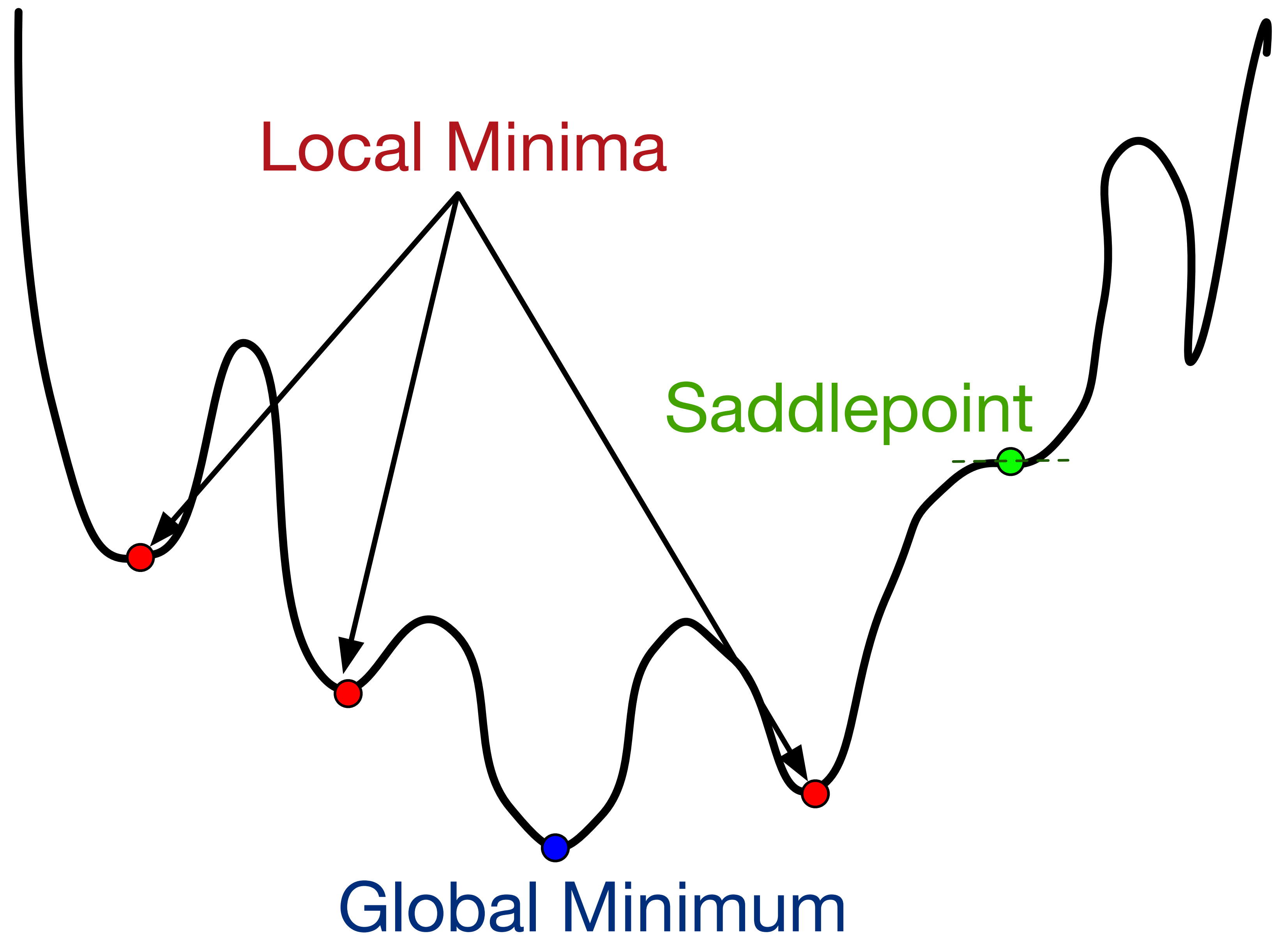
Example: Using linear regression to fit a dataset $\left\{(x_i, y_i)\right\}_{i=1}^{n}$

- Estimate the targets by $\hat{y} = f(x) = w_0 + w_1 x$
- Each vector $\mathbf{w}$ specifies a particular f
- Objective is the **total error** $c(\mathbf{w}) = \sum_{i=1}^{n} (f(x_i) - y_i)^2$



Stationary Points

- Recall that every minimum of an everywhere-differentiable function $c(w)$ must* occur at a **stationary point**: A point at which $c'(w) = 0$
  - ✳ **Question:** What is the exception? 
- However, not every stationary point is a minimum
- Every stationary point is either:
  - A **local minimum**
  - A **local maximum**
  - A **saddlepoint**
- The **global minimum** is either a local minimum, or a boundary point



Numerical Optimization

- So a simple recipe for optimizing a function is to find its stationary points; one of those must be the minimum (as long as domain is unbounded)
  - **Question:** Why don't we always just do that?
- We will *almost never* be able to **analytically** compute the minimum of the functions that we want to optimize
  - ✴ (Linear regression is an important exception)
- Instead, we must try to find the minimum **numerically**
- Main techniques: First-order and second-order **gradient descent**

Taylor Series

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Definition: A **Taylor series** is a way of approximating a function c in a small neighbourhood around a point a:

$$c(w) \approx c(a) + c'(a)(w-a) + \frac{c''(a)}{2}(w-a)^2 + \cdots + \frac{c^{(k)}(a)}{k!}(w-a)^k$$

$$= c(a) + \sum_{i=1}^{k} \frac{c^{(i)}(a)}{i!}(w-a)^i$$

- *Intuition:* Following tangent line of the function approximates how it changes
  - i.e., following a function with the same first derivative
  - Following a function with the same first and second derivatives is a better approximation; with the same first, second, third derivatives is even better; etc.

Second-Order Gradient Descent (Newton-Raphson Method)

1. Approximate the target function with a **second-order Taylor series** around the current guess w_t:

$$\hat{c}(w) = c(w_t) + c'(w_t)(w - w_t) + \frac{c''(w_t)}{2}(w - w_t)^2$$

2. Find the stationary point of the approximation

$$\boxed{w_{t+1} \leftarrow w_t - \frac{c'(w_t)}{c''(w_t)}}$$

3. If the stationary point of the approximation is a (good enough) stationary point of the objective, then stop. Else, goto 1.

$$\begin{aligned}
0 &= \frac{d}{dw}\left[c(a) + c'(a)(w-a) + \frac{c''(a)}{2}(w-a)^2\right] \\
&= c'(a) + 2\frac{c''(a)}{2}w - 2\frac{c''(a)}{2}a \\
&= c'(a) + c''(a)(w-a) \\
\iff &\quad -c'(a) = c''(a)(w-a) \\
\iff &\quad (w-a) = -\frac{c'(a)}{c''(a)} \\
\iff &\quad w = a - \frac{c'(a)}{c''(a)}
\end{aligned}$$

(First-Order) Gradient Descent

- We can run Newton-Raphson whenever we have access to both the first and second derivatives of the target function
- Often we want to only use the **first derivative** (**why?**)
- **First-order gradient descent:** Replace the **second derivative** with a constant $\frac{1}{\eta}$ (the **step size**) in the approximation:

$$\hat{c}(w) = c(w_t) + c'(w_t)(w - w_t) + \frac{c''(w_t)}{2}(w - w_t)^2$$

$$\hat{c}(w) = c(w_t) + c'(w_t)(w - w_t) + \frac{1}{2\eta}(w - w_t)^2$$

- By exactly the same derivation as before:

$$\boxed{w_{t+1} \leftarrow w_t - \eta c'(w_t)}$$

Partial Derivatives

- **So far:** Optimizing univariate function $c : \mathbb{R} \rightarrow \mathbb{R}$
- **But actually:** Optimizing multivariate function $c : \mathbb{R}^d \rightarrow \mathbb{R}$
  - d is typically **HUGE** ($d \gg 10{,}000$ is not uncommon)
- First derivative of a multivariate function is a vector of partial derivatives

Definiton:

The **partial derivative** $\frac{\partial f}{\partial x_i}(x_1, \ldots, x_d)$

of a function $f(x_1, \ldots, x_d)$ at $x_1, \ldots, x_d$ with respect to x_i **is** $g'(x_i)$, where

$$g(y) = f(x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_d)$$

Gradients

The multivariate analog to a **first derivative** is called a **gradient**.

Definition:

The **gradient** $\nabla f(\mathbf{x})$ of a function $f : \mathbb{R}^d \to \mathbb{R}$ at $\mathbf{x} \in \mathbb{R}^d$ is a vector of all the partial derivatives of f at $\mathbf{x}$:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial_{x_1}}(\mathbf{x}) \\ \frac{\partial f}{\partial_{x_2}}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial_{x_d}}(\mathbf{x}) \end{bmatrix}$$

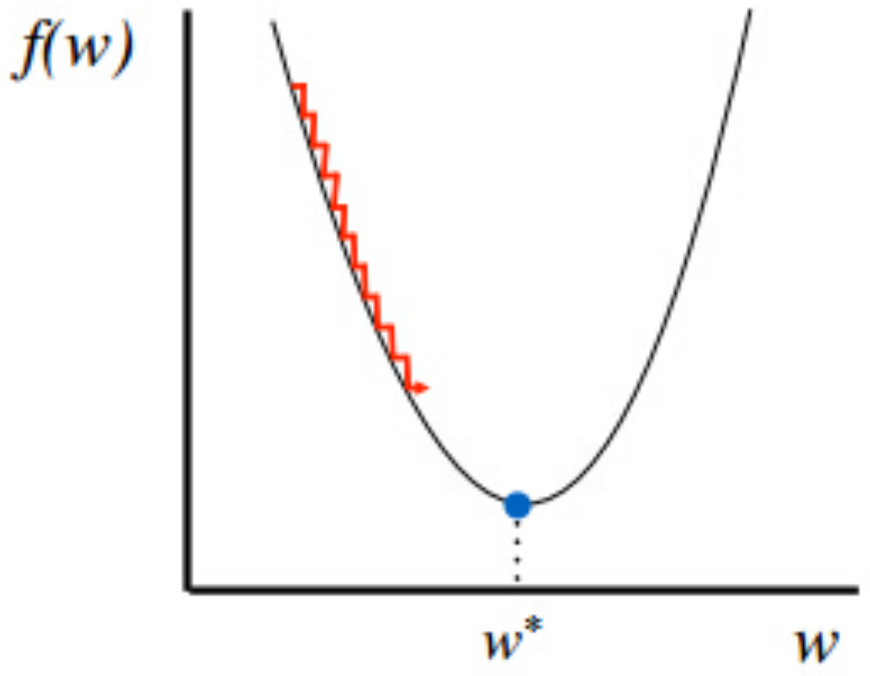
Multivariate Gradient Descent

First-order gradient descent for multivariate functions $c : \mathbb{R} \rightarrow \mathbb{R}$ is just:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \nabla c(\mathbf{w}_t)$$

- Notice the t subscript on η
- We can choose a **different** η_t for each iteration
  - Indeed, for univariate functions, Newton-Raphson can be understood as first-order gradient descent that chooses a step size of $\eta_t = \dfrac{1}{c''(w_t)}$ at each iteration.
- Choosing a good step size is crucial to efficiently using first-order gradient descent

Adaptive Step Sizes



(a) Step-size too small

- If the step size is **too small**, gradient descent will "work", but take forever
- **Too big**, and we can overshoot the optimum
- Ideally, we would choose $\eta_t = \arg\min_{\eta \in \mathbb{R}^+} c\left(\mathbf{w}_t - \eta \nabla c(\mathbf{w}_t)\right)$
  - But that's another optimization!
- There are some heuristics that we can use to **adaptively** guess good values for η_t

Line Search

A simple heuristic: **line search**

1. Try some largest-reasonable step size $\eta_t^{(0)} = \eta_{\max}$
2. Is $c\left(w_t - \eta_t^{(s)} \nabla c(w_t)\right) < c(w_t)$?
   If yes, $w_{t+1} \leftarrow w_t - \eta_t^{(s)} \nabla c(w_t)$
3. Otherwise, try $\eta_t^{(s+1)} = \tau \eta_t^{(s)}$
   (for $\tau < 1$) and goto 2

Intuition:

- Big step sizes are better so long as they don't overshoot
- Try a big step size! If it increases the objective, try a smaller one.
- Keep trying smaller ones until you decrease the objective; then start iteration $t+1$ from $\eta_{\max}$ again.

- Typically $\tau \in [0.5, 0.9]$

Optimization Properties

1. **Maximizing** $c(w)$ is the same as minimizing $-c(w)$:

$$\arg\max_{w} c(w) = \arg\min_{w} - c(w)$$

2. **Convex functions** have a **global** minimum at **every** stationary point

$$c \text{ is convex} \iff c(t\mathbf{w}_1 + (1-t)\mathbf{w}_2) \leq tc(\mathbf{w}_1) + (1-t)c(\mathbf{w}_2)$$

3. **Identifiability:** Sometimes we want the actual **global minimum**; other times we want a good-enough minimizer (i.e., **local minimum** might be OK).

4. **Equivalence under constant shifts:** Adding, subtracting, or multiplying by a positive constant **does not change** the minimizer of a function:

$$\arg\min_{w} c(w) = \arg\min_{w} c(w)+k = \arg\min_{w} c(w)-k = \arg\min_{w} kc(w) \quad \forall k \in \mathbb{R}^+$$

Summary

- We often want to find the argument w^* that **minimizes** an **objective function** c:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} c(\mathbf{w})$$

- Every interior minimum is a **stationary point**, so check the stationary points
- Stationary points usually identified **numerically**
  - Typically, by **gradient descent**
- Choosing the **step size** is important for efficiency and correctness
  - Common approach: Adaptive step size
  - E.g., by **line search**