Recitation 1

Gradients and Directional Derivatives

Brett Bernstein

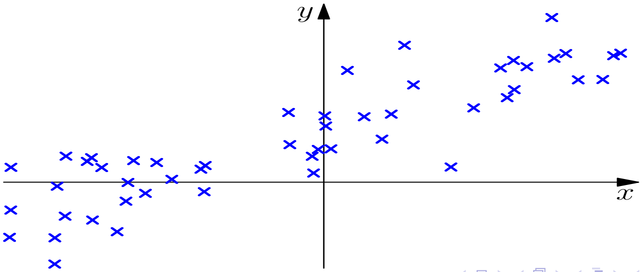
CDS at NYU

January 20, 2018

Intro Question

Question

We are given the data set $(x_1, y_1), \ldots, (x_n, y_n)$ where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$. We want to fit a linear function to this data by performing empirical risk minimization. More precisely, we are using the hypothesis space $\mathcal{F} = \{f(x) = w^T x \mid w \in \mathbb{R}^d\}$ and the loss function $\ell(a, y) = (a - y)^2$. Given an initial guess $\tilde{w}$ for the empirical risk minimizing parameter vector, how could we improve our guess?



Intro Solution

Solution

- The empirical risk is given by

$$\hat{R}_n(f) = \frac{1}{n}\sum_{i=1}^{n}\ell(f(x_i), y_i) = \frac{1}{n}\sum_{i=1}^{n}(w^T x_i - y_i)^2 = \frac{1}{n}\|Xw - y\|_2^2,$$

  where $X \in \mathbb{R}^{n\times d}$ is the matrix whose ith row is given by x_i.
- Can improve a non-optimal guess $\tilde{w}$ by taking a small step in the direction of the negative gradient.

Single Variable Differentiation

- For $f : \mathbb{R} \to \mathbb{R}$ differentiable, the derivative is given by

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

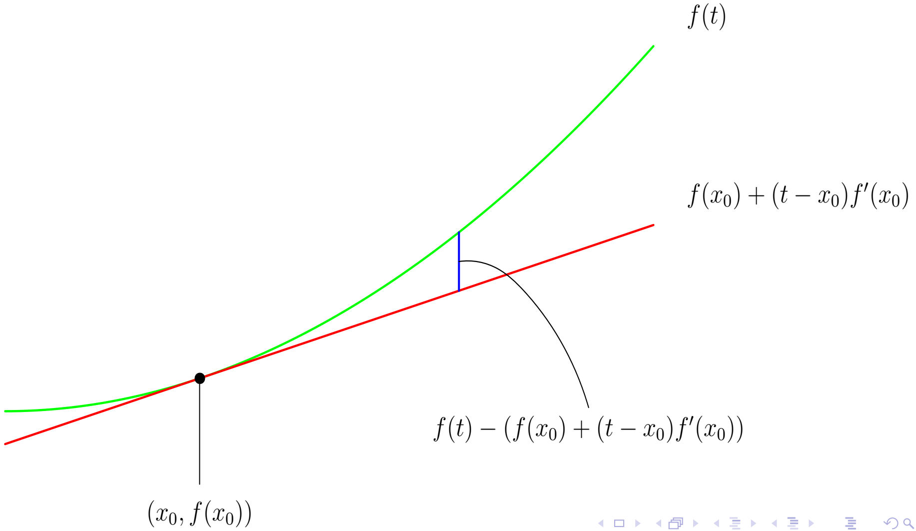
- Can also be written as

$$f(x+h) = f(x) + hf'(x) + o(h) \quad \text{as } h \to 0,$$

where $o(h)$ denotes a function $g(h)$ with $g(h)/h \to 0$ as $h \to 0$.

- Points with $f'(x) = 0$ are called *critical points*.

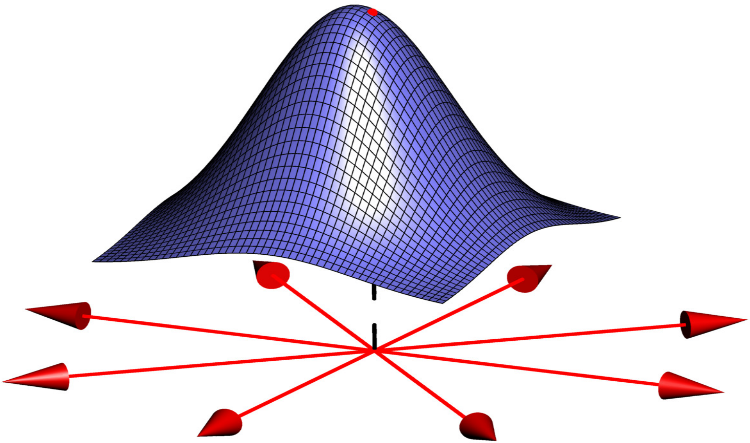
1D Linear Approximation By Derivative



Multivariable Differentiation

- Consider now a function $f : \mathbb{R}^n \to \mathbb{R}$ with inputs of the form $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$.
- Unlike the 1-dimensional case, we cannot assign a single number to the slope at a point since there are many directions we can move in.

Multiple Possible Directions for $f : \mathbb{R}^2 \to \mathbb{R}$



Directional Derivative

Definition

Let $f : \mathbb{R}^n \to \mathbb{R}$. The directional derivative $f'(x; u)$ of f at $x \in \mathbb{R}^n$ in the direction $u \in \mathbb{R}^n$ is given by

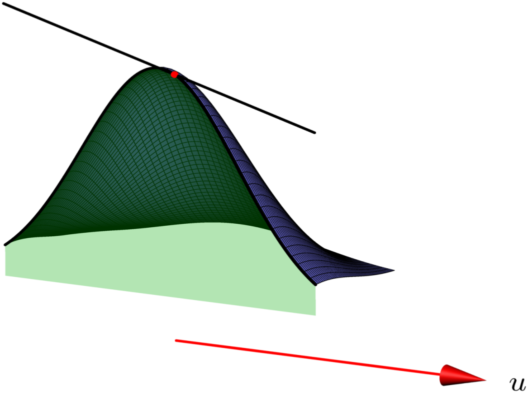
$$f'(x; u) = \lim_{h \to 0} \frac{f(x + hu) - f(x)}{h}.$$

- By fixing a direction u we turned our multidimensional problem into a 1-dimensional problem.
- Similar to 1-d we have

$$f(x + hu) = f(x) + hf'(x; u) + o(h).$$

- We say that u is a *descent direction* of f at x if $f'(x; u) < 0$.

Directional Derivative as a Slope of a Slice



Partial Derivative

- Let $e_i = (\overbrace{0, 0, \ldots, 0}^{i-1}, 1, 0, \ldots, 0)$ denote the ith standard basis vector.
- The ith *partial derivative* is defined to be the directional derivative along e_i.
- It can be written many ways:

$$f'(x; e_i) = \frac{\partial}{\partial x_i} f(x) = \partial_{x_i} f(x) = \partial_i f(x).$$

- What is the intuitive meaning of $\partial_{x_i} f(x)$?

Differentiability

- We say a function $f:\mathbb{R}^n \to \mathbb{R}$ is *differentiable* at $x \in \mathbb{R}^n$ if

$$\lim_{v\to 0} \frac{f(x+v)-f(x)-g^T v}{\|v\|_2} = 0,$$

  for some $g \in \mathbb{R}^n$.

- If it exists, this g is unique and is called the *gradient* of f at x with notation

$$g = \nabla f(x).$$

- It can be shown that

$$\nabla f(x) = \begin{pmatrix} \partial_{x_1} f(x) \\ \vdots \\ \partial_{x_n} f(x) \end{pmatrix}.$$

Useful Convention

- Consider $f : \mathbb{R}^{p+q} \to \mathbb{R}$.
- Split the input to f into parts $w \in \mathbb{R}^p$ and $z \in \mathbb{R}^q$.
- Define the partial gradients

$$\nabla_w f(w,z) := \begin{pmatrix} \partial_{w_1} f(w,z) \\ \vdots \\ \partial_{w_p} f(w,z) \end{pmatrix} \quad \text{and} \quad \nabla_z f(w,z) := \begin{pmatrix} \partial_{z_1} f(w,z) \\ \vdots \\ \partial_{z_q} f(w,z) \end{pmatrix}.$$

Tangent Plane

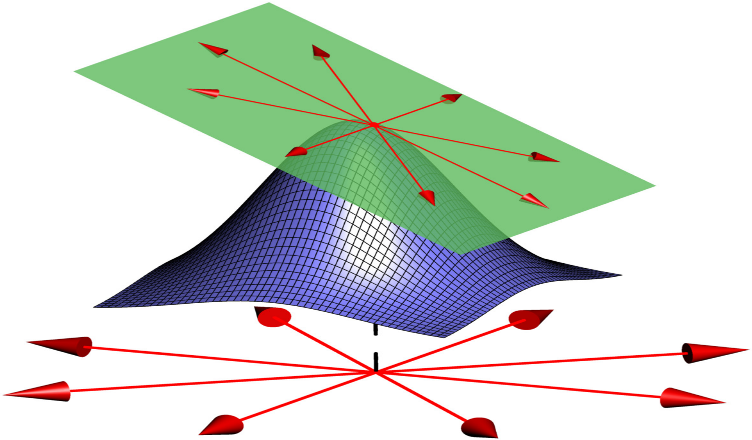
- Analogous to the 1-d case we can express differentiability as

$$f(x+v) = f(x) + \nabla f(x)^T v + o(\|v\|_2).$$

- The approximation $f(x+v) \approx f(x) + \nabla f(x)^T v$ gives a tangent plane at the point x.
- The tangent plane of f at x is given by

$$P = \{(x+v, f(x) + \nabla f(x)^T v) \mid v \in \mathbb{R}^n\} \subseteq \mathbb{R}^{n+1}.$$

Tangent Plane for $f : \mathbb{R}^2 \to \mathbb{R}$



Directional Derivatives from Gradients

- If f is differentiable we have

$$f'(x;u) = \nabla f(x)^T u.$$

- If $\nabla f(x) \neq 0$ this implies that

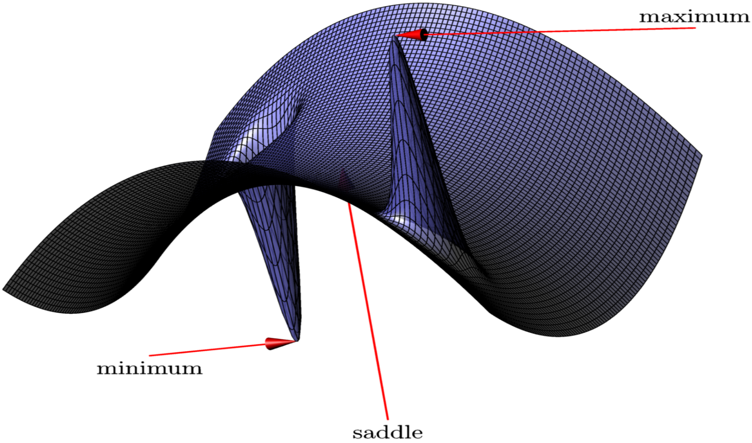
$$\arg\max_{\|u\|_2=1} f'(x;u) = \frac{\nabla f(x)}{\|\nabla f(x)\|_2} \quad \text{and} \quad \arg\min_{\|u\|_2=1} f'(x;u) = -\frac{\nabla f(x)}{\|\nabla f(x)\|_2}.$$

- The gradient points in the direction of steepest ascent.
- The negative gradient points in the direction of steepest descent.

Critical Points

- Analogous to 1-d, if $f : \mathbb{R}^n \to \mathbb{R}$ is differentiable and x is a local extremum then we must have $\nabla f(x) = 0$.
- Points with $\nabla f(x) = 0$ are called *critical points*.
- Later we will see that for a convex differentiable function, x is a critical point if and only if it is a global minimizer.

Critical Points of $f : \mathbb{R}^2 \to \mathbb{R}$



Computing Gradients

Question

For questions 1 and 2, compute the gradient of the given function.

1. $f : \mathbb{R}^3 \to \mathbb{R}$ is given by
$$f(x_1, x_2, x_3) = \log(1 + e^{x_1 + 2x_2 + 3x_3}).$$
2. $f : \mathbb{R}^n \to \mathbb{R}$ is given by
$$f(x) = \|Ax - y\|_2^2 = (Ax - y)^T(Ax - y) = x^T A^T Ax - 2y^T Ax + y^T y,$$
for some $A \in \mathbb{R}^{m \times n}$ and $y \in \mathbb{R}^m$.
3. Assume A in the previous question has full column rank. What is the critical point of f?

$f(x_1, x_2, x_3) = \log(1 + e^{x_1+2x_2+3x_3})$ Solution 1

We can compute the partial derivatives directly:

$$\begin{aligned}
\partial_{x_1} f(x_1, x_2, x_3) &= \frac{e^{x_1+2x_2+3x_3}}{1 + e^{x_1+2x_2+3x_3}} \\
\partial_{x_2} f(x_1, x_2, x_3) &= \frac{2e^{x_1+2x_2+3x_3}}{1 + e^{x_1+2x_2+3x_3}} \\
\partial_{x_3} f(x_1, x_2, x_3) &= \frac{3e^{x_1+2x_2+3x_3}}{1 + e^{x_1+2x_2+3x_3}}
\end{aligned}$$

and obtain

$$\nabla f(x_1, x_2, x_3) = \begin{pmatrix} \frac{e^{x_1+2x_2+3x_3}}{1 + e^{x_1+2x_2+3x_3}} \\ \frac{2e^{x_1+2x_2+3x_3}}{1 + e^{x_1+2x_2+3x_3}} \\ \frac{3e^{x_1+2x_2+3x_3}}{1 + e^{x_1+2x_2+3x_3}} \end{pmatrix}.$$

$f(x_1, x_2, x_3) = \log(1 + e^{x_1+2x_2+3x_3})$ Solution 2

- Let $w = (1, 2, 3)^T$.
- Write $f(x) = \log(1 + e^{w^T x})$.
- Apply a version of the chain rule:

$$\nabla f(x) = \frac{e^{w^T x}}{1 + e^{w^T x}} w.$$

Theorem (Chain Rule)

If $g : \mathbb{R} \to \mathbb{R}$ and $h : \mathbb{R}^n \to \mathbb{R}$ are differentiable then

$$\nabla (g \circ h)(x) = g'(h(x)) \nabla h(x).$$

$f(x) = \|Ax - y\|_2^2$ Solution

- We could use techniques similar to the previous problem, but instead we show a different method using directional derivatives.
- Note that

$$
\begin{aligned}
& f(x+tv) \\
&= (x+tv)^T A^T A(x+tv) - 2y^T A(x+tv) + y^T y \\
&= x^T A^T Ax + t^2 v^T A^T Av + 2tx^T A^T Av - 2y^T Ax - 2ty^T Av + y^T y \\
&= f(x) + t(2x^T A^T A - 2y^T A)v + t^2 v^T A^T Av.
\end{aligned}
$$

- This gives

$$
f'(x;v) = \lim_{t\to 0} \frac{f(x+tv) - f(x)}{t} = (2x^T A^T A - 2y^T A)v
$$

- Thus $\nabla f(x) = 2(A^T Ax - A^T y) = 2A^T(Ax - y)$.

Critical Points of $f(x) = \|Ax - y\|_2^2$

- Need $\nabla f(x) = 2A^T Ax - 2A^T y = 0$.
- Since A is assumed to have full column rank, we see that $A^T A$ is invertible.
- Thus we have $x = (A^T A)^{-1} A^T y$.
- As we will see later, this function is strictly convex (Hessian $\nabla^2 f(x) = A^T A$ is positive definite).
- Thus we have found the unique minimizer (least squares solution).

Technical Aside: Differentiability

- When computing the gradients above we assumed the functions were differentiable.
- Can use the following theorem to be completely rigorous.

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ and suppose $\partial_{x_i} f : \mathbb{R}^n \to \mathbb{R}$ is continuous for $i = 1, \ldots, n$. Then f is differentiable.