Recitation 1

Gradients and Directional Derivatives

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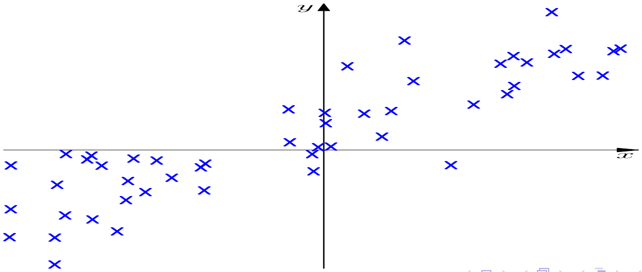
Intro Question

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 $\mathcal{F} = \{h_\theta(x) = \theta^T x \mid \theta \in \mathbb{R}^d\}$ and the loss function $\ell(a, y) = (a - y)^2$. Given an initial guess $\tilde{\theta}$ for the empirical risk minimizing parameter vector, how could we improve our guess?



Intro Solution

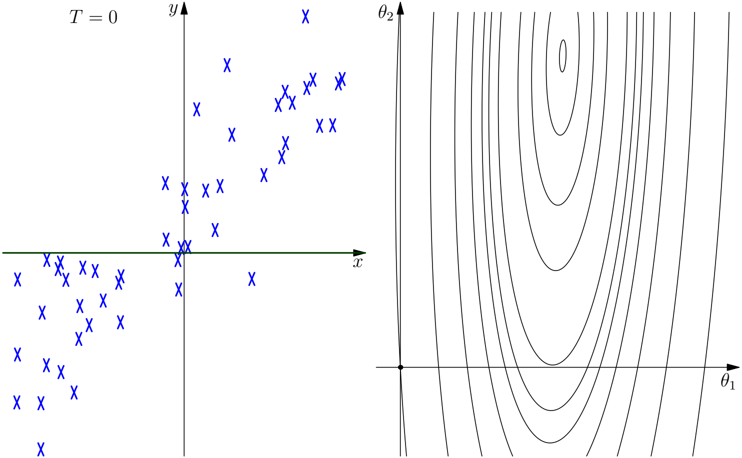
Solution

- The empirical risk is given by

$$J(\theta) := \hat{R}_n(h_\theta) = \frac{1}{n}\sum_{i=1}^{n}\ell(h_\theta(x_i), y_i) = \frac{1}{n}\sum_{i=1}^{n}(\theta^T x_i - y_i)^2 = \frac{1}{n}\|X\theta - y\|_2^2,$$

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

Negative Gradient Steps



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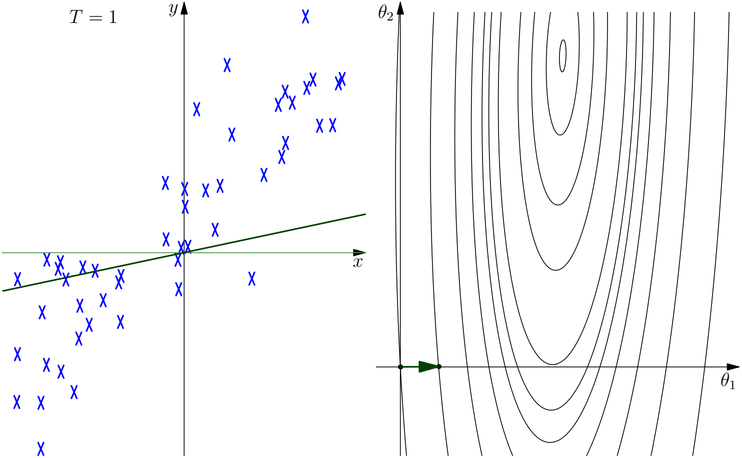

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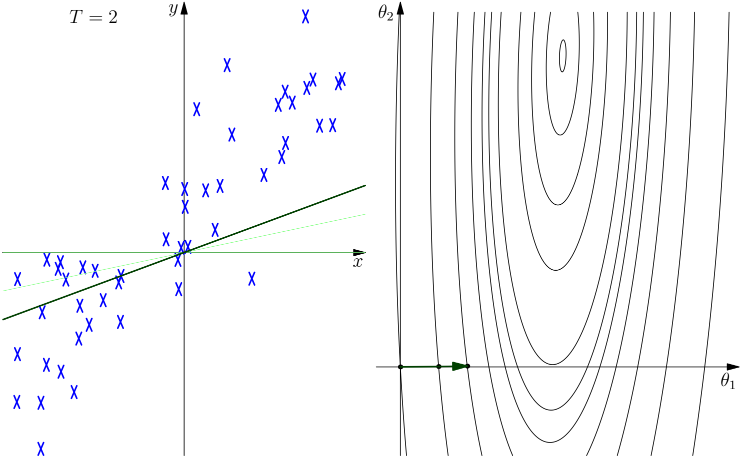

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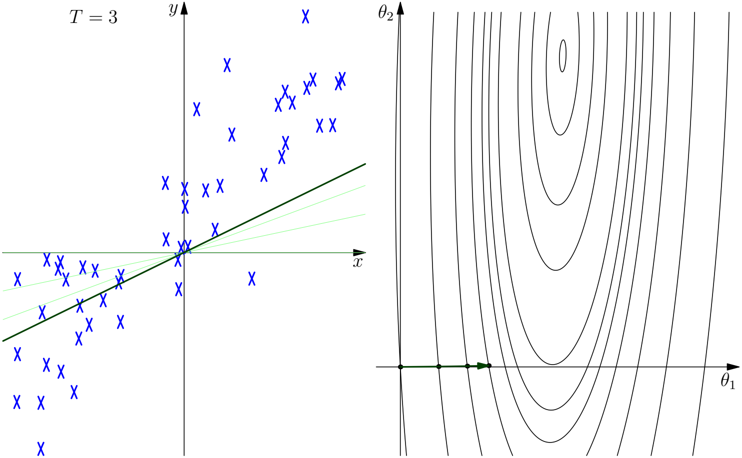

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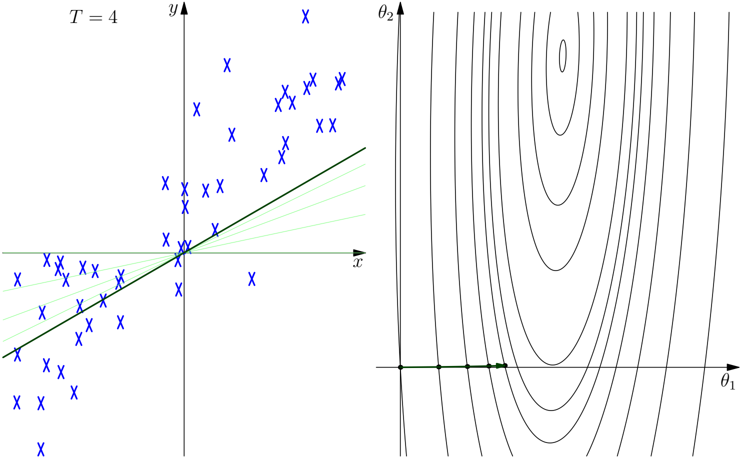

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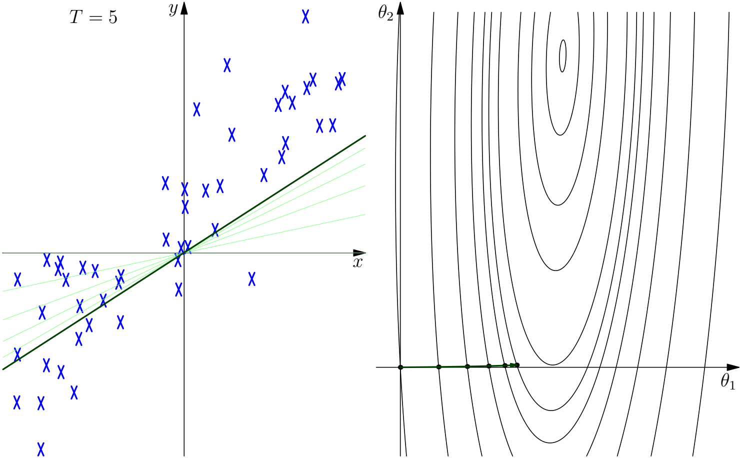

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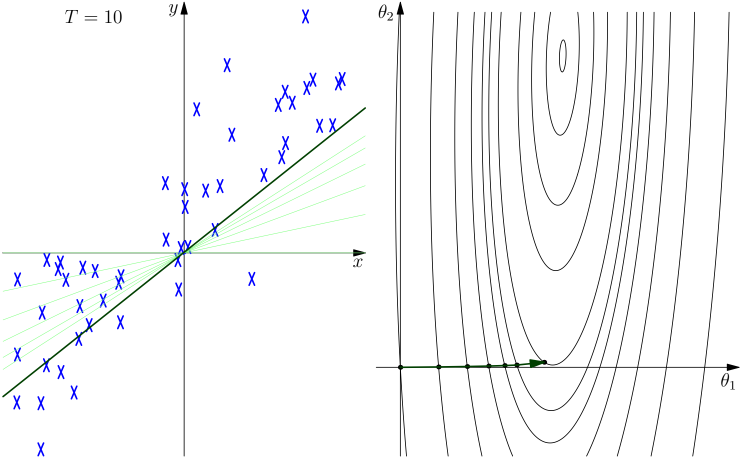

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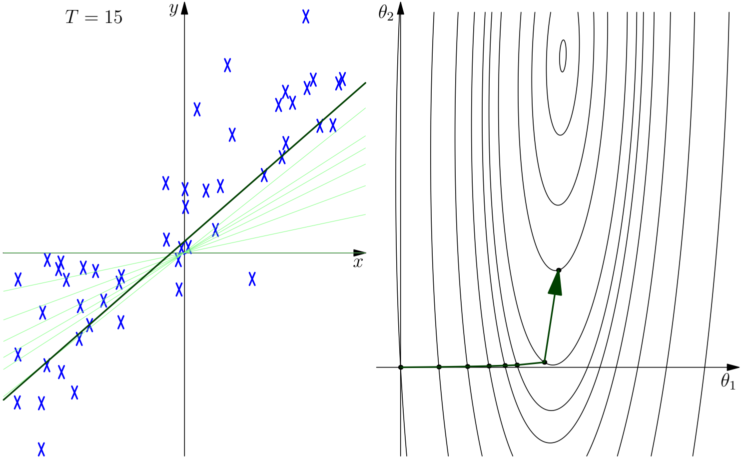

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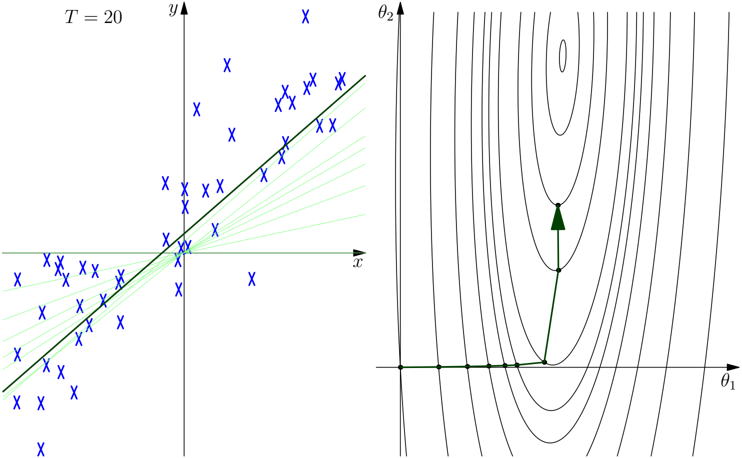

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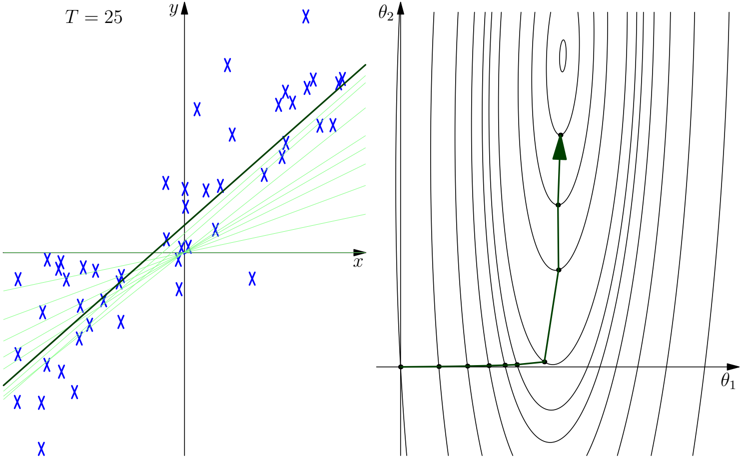

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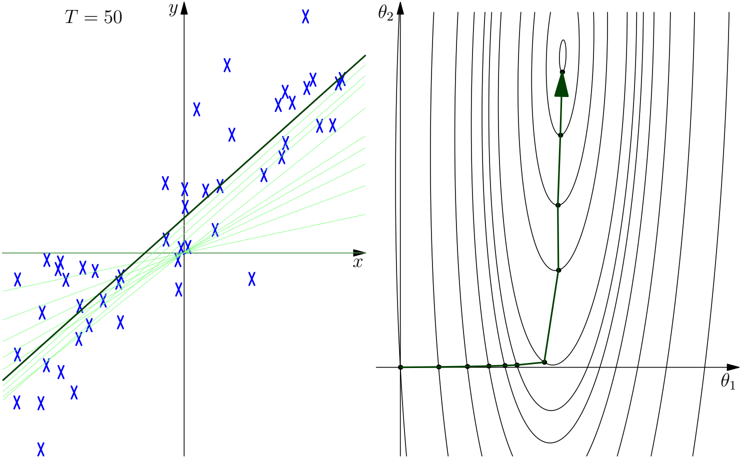


Single Variable Differentiation

- Calculus lets us turn non-linear problems into linear algebra.
- For $f : \mathbb{R} \to \mathbb{R}$ differentiable, the derivative is given by

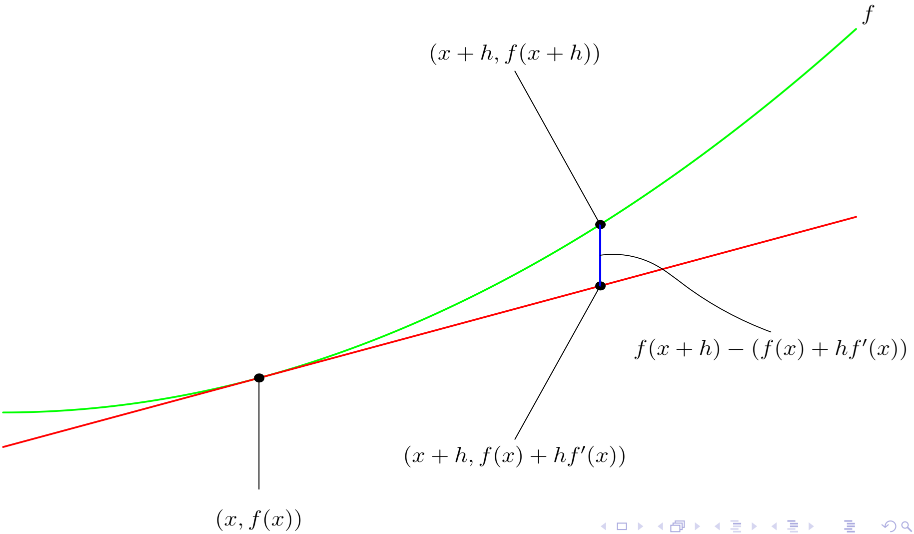
$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}.$$

- 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*.

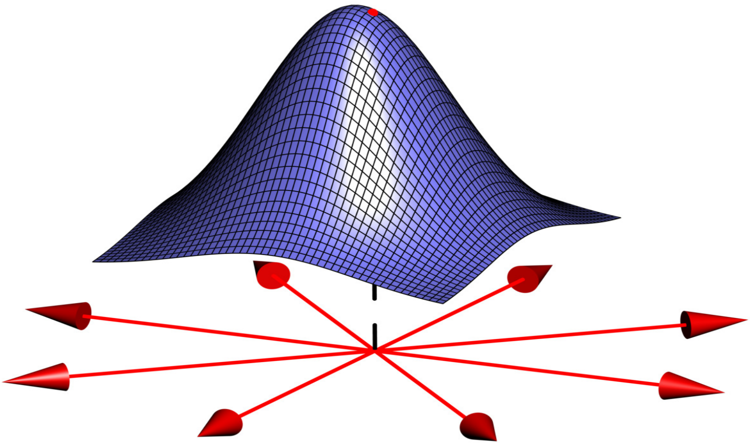
1D Linear Approximation By Derivative



Multivariable Differentiation

- Consider now a function $f : \mathbb{R}^n \to \mathbb{R}$ with inputs of the form $x = (x_1, \ldots, x_n)^T \in \mathbb{R}^n$.
- 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 $f : \mathbb{R}^2 \to \mathbb{R}$



Multivariable Differentiation

1. We will look at two (related) methods for understanding multivarible differentiation:
    1. Directional Derivatives: Derivative computed along a single direction
    2. Gradient: Gives multidimensional linear approximation and the steepest ascent direction

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

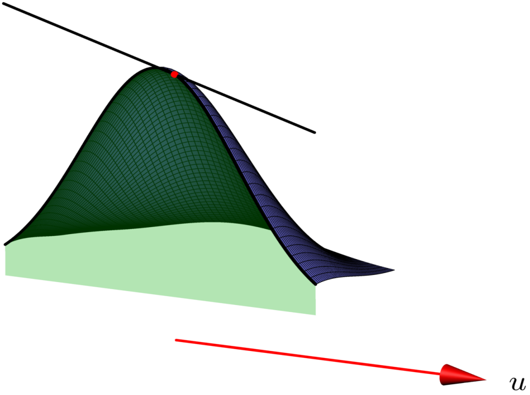
$$f'(x; u) = \lim_{h \to 0} \frac{f(x + hu) - f(x)}{h}.$$

- 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 $f'(x; u) < 0$.
- Taking a small enough step in a descent direction causes the function value decreases.

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 $\partial_{x_i} f(x)$? For example, what does a large value of $\partial_{x_3} f(x)$ imply?

Differentiability and Gradients

- 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 $x \in \mathbb{R}^{p+q}$ into parts $w \in \mathbb{R}^p$ and $z \in \mathbb{R}^q$ so that $x = (w, z)$.
- Define the partial gradients

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

Linear Approximation and Tangent Plane

- Gradient gives us a linear approximation of f near the point x:

$$f(x+v) \approx f(x) + \nabla f(x)^T v.$$

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

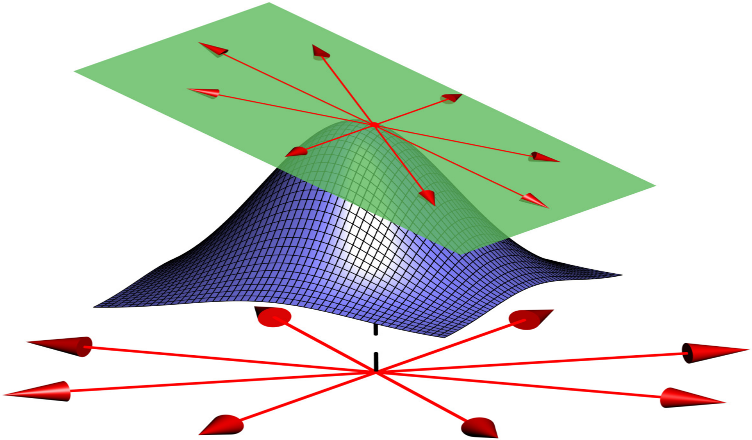
$$f(x+v) = f(x) + \nabla f(x)^T v + o(\|v\|_2).$$

- The gradient approximation can be seen as a tangent plane given by

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

- Methods like gradient descent approximate a function locally by its tangent plane, and then take a step accordingly.

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



Directional Derivatives from Gradients

- If f is differentiable we obtain a formula for any directional derivative in terms of the gradient

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

- This means a direction is a descent direction if and only if it makes an acute angle with the negative gradient.
- If $\nabla f(x) \neq 0$ applying Cauchy-Schwarz gives

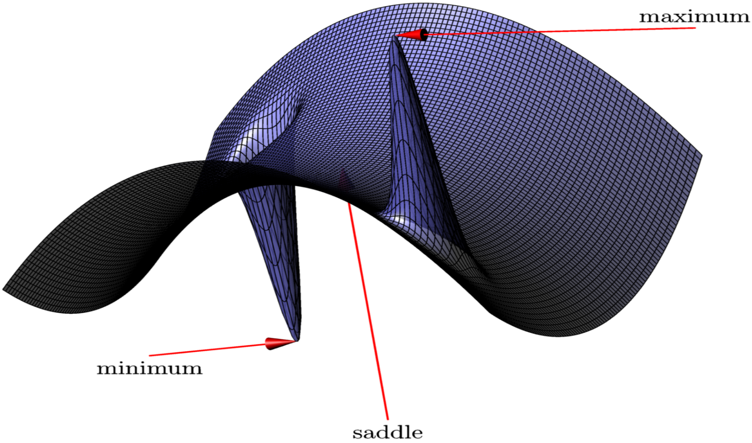
$$\arg\max_{\|u\|_2=1} f'(x;u) = \frac{\nabla f(x)}{\|\nabla f(x)\|_2} \quad \text{and} \quad \arg\min_{\|u\|_2=1} f'(x;u) = -\frac{\nabla f(x)}{\|\nabla f(x)\|_2}.$$

- 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 in the course 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 $f : \mathbb{R}^2 \to \mathbb{R}$



Recap

- To find a good decision function we will minimize the empirical loss on the training data.
- Having fixed a hypothesis space parameterized by θ, finding a good decision function means finding a good θ.
- Given a current guess for θ, we will use the gradient of the empirical loss (w.r.t. θ) to get a local linear approximation.
- If the gradient is non-zero, taking a small step in the direction of the negative gradient is guaranteed to decrease the empirical loss.
- This motivates the minimization algorithm called gradient descent.

Computing Gradients

Question

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

1. $J : \mathbb{R}^3 \to \mathbb{R}$ is given by
$$J(\theta_1, \theta_2, \theta_3) = \log(1 + e^{\theta_1 + 2\theta_2 + 3\theta_3}).$$
2. $J : \mathbb{R}^n \to \mathbb{R}$ is given by
$$J(\theta) = \|X\theta - y\|_2^2 = (X\theta - y)^T(X\theta - y) = \theta^T X^T X\theta - 2y^T X\theta + y^T y,$$
for some $X \in \mathbb{R}^{m \times n}$ and $y \in \mathbb{R}^m$.
3. Assume X in the previous question has full column rank. What is the critical point of J?

$J(\theta_1, \theta_2, \theta_3) = \log(1 + e^{\theta_1+2\theta_2+3\theta_3})$ Solution 1

We can compute the partial derivatives directly:

$$\begin{aligned}
\partial_{\theta_1} J(\theta_1, \theta_2, \theta_3) &= \frac{e^{\theta_1+2\theta_2+3\theta_3}}{1 + e^{\theta_1+2\theta_2+3\theta_3}} \\
\partial_{\theta_2} J(\theta_1, \theta_2, \theta_3) &= \frac{2e^{\theta_1+2\theta_2+3\theta_3}}{1 + e^{\theta_1+2\theta_2+3\theta_3}} \\
\partial_{\theta_3} J(\theta_1, \theta_2, \theta_3) &= \frac{3e^{\theta_1+2\theta_2+3\theta_3}}{1 + e^{\theta_1+2\theta_2+3\theta_3}}
\end{aligned}$$

and obtain

$$\nabla J(\theta_1, \theta_2, \theta_3) = \begin{pmatrix} \frac{e^{\theta_1+2\theta_2+3\theta_3}}{1 + e^{\theta_1+2\theta_2+3\theta_3}} \\ \frac{2e^{\theta_1+2\theta_2+3\theta_3}}{1 + e^{\theta_1+2\theta_2+3\theta_3}} \\ \frac{3e^{\theta_1+2\theta_2+3\theta_3}}{1 + e^{\theta_1+2\theta_2+3\theta_3}} \end{pmatrix}.$$

$J(\theta_1, \theta_2, \theta_3) = \log(1 + e^{\theta_1 + 2\theta_2 + 3\theta_3})$ Solution 2

- Spot the linear algebra!
- Let $w = (1, 2, 3)^T$.
- Write $J(\theta) = \log(1 + e^{w^T\theta})$.
- Apply a version of the chain rule:

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

Theorem (Chain Rule)

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

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

$J(\theta) = \|X\theta - y\|_2^2$ Solution

- We could use techniques similar to the previous problem, but instead we show a different method using directional derivatives.
- For arbitrary $t \in \mathbb{R}$ and $\theta, v \in \mathbb{R}^n$ we have

$$\begin{aligned}
&J(\theta + tv)\\
&= (\theta + tv)^T X^T X(\theta + tv) - 2y^T X(\theta + tv) + y^T y\\
&= \underline{\theta^T X^T X\theta} + t^2 v^T X^T Xv + 2t\theta^T X^T Xv - \underline{2y^T X\theta} - 2ty^T Xv + \underline{y^T y}\\
&= \underline{J(\theta)} + t(2\theta^T X^T X - 2y^T X)v + t^2 v^T X^T Xv.
\end{aligned}$$

- This gives

$$J'(\theta; v) = \lim_{t \to 0} \frac{J(\theta + tv) - J(\theta)}{t} = (2\theta^T X^T X - 2y^T X)v = \nabla J(\theta)^T v$$

- Thus $\nabla J(\theta) = 2(X^T X\theta - X^T y) = 2X^T(X\theta - y)$.
- Data science interpretation of $\nabla J(\theta)$ (assuming columns of X are centered)?

Critical Points of $J(\theta) = \|X\theta - y\|_2^2$

- Need $\nabla J(\theta) = 2X^TX\theta - 2X^Ty = 0$.
- Since X is assumed to have full column rank, we see that X^TX is invertible.
- Thus we have $\theta = (X^TX)^{-1}X^Ty$.
- As we will see later, this function is strictly convex (Hessian $\nabla^2 J(\theta) = 2X^TX$ 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 $\partial_i f : \mathbb{R}^n \to \mathbb{R}$ is continuous for $i = 1, \ldots, n$. Then f is differentiable.