06-20416 and 06-12412
(Intro to) Neural Computation

04 – Gradient Descent

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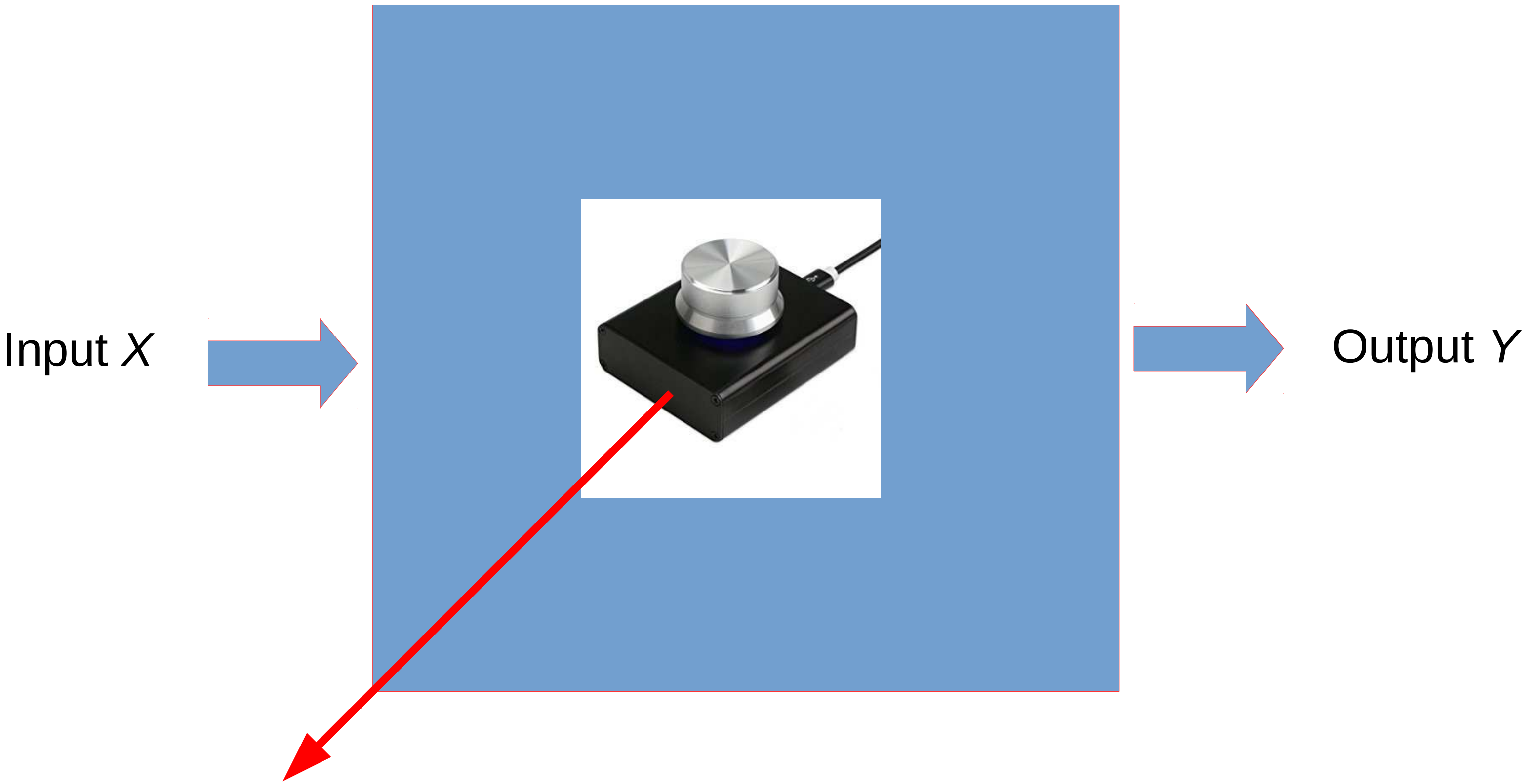
Last lecture

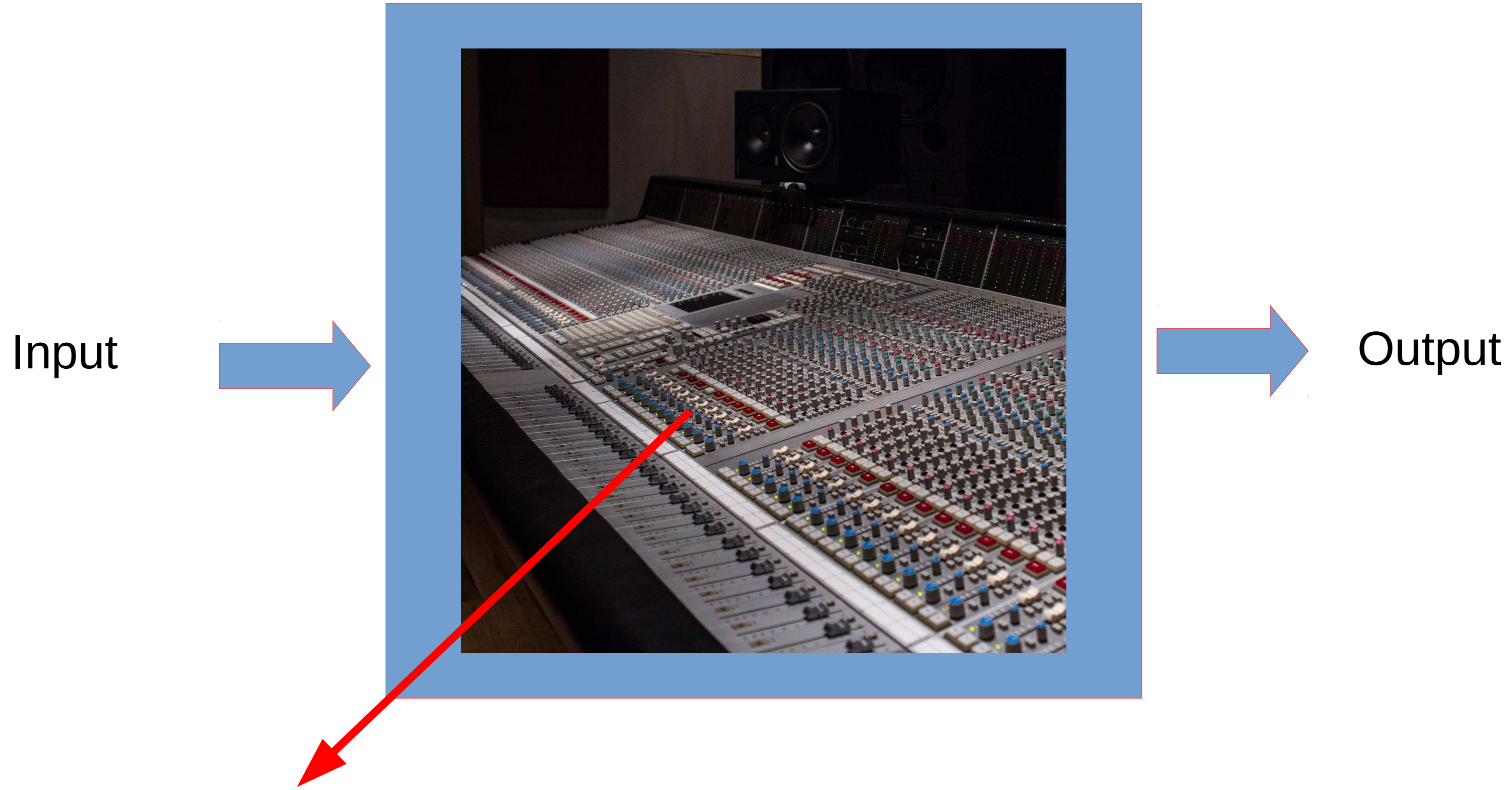
- Probabilistic models
- Some probabilistic concepts
  - Random variable, density function, normal distribution, joint density function, empirical distribution
- Maximum likelihood
  - Likelihood function and Maximum likelihood estimate
  - Learning via log-likelihood. Example: linear regression

So far: Adjusting a single knob



$$J(\Theta) = \mathbb{E}_{(X,Y)\sim\hat{\mathcal{D}}} - \log p_{\mathrm{model}}(Y \mid X; \Theta)$$

Today: Adjusting millions of knobs

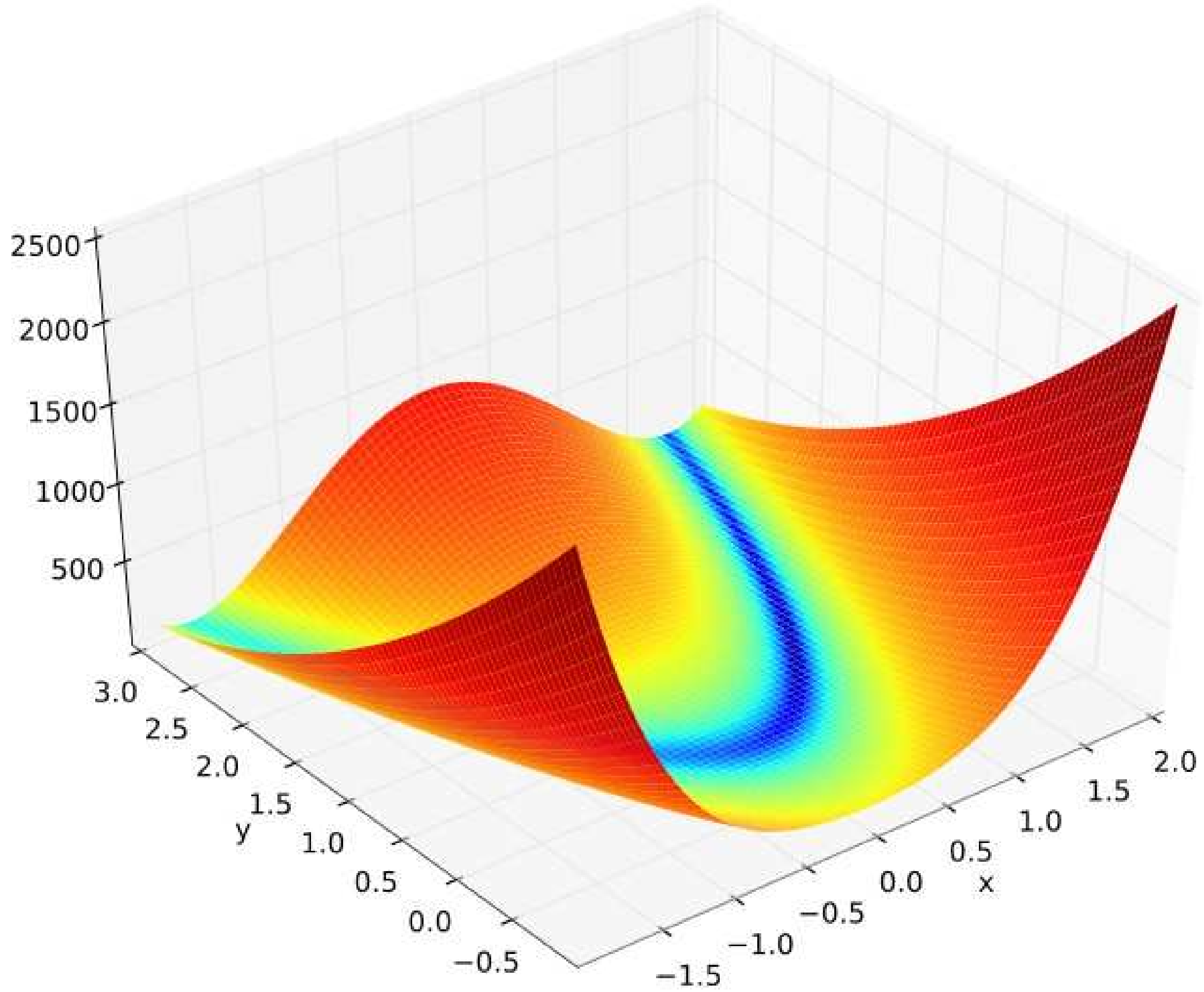


$$J(\Theta) = \mathbb{E}_{(X,Y)\sim\hat{\mathcal{D}}} - \log p_{\text{model}}(Y \mid X; \Theta)$$

Outline

- Functions of multiple variables
- Partial derivatives and the chain rule
- Gradients
  - Direction of steepest ascent
- Gradient descent

Functions of Multiple Variables

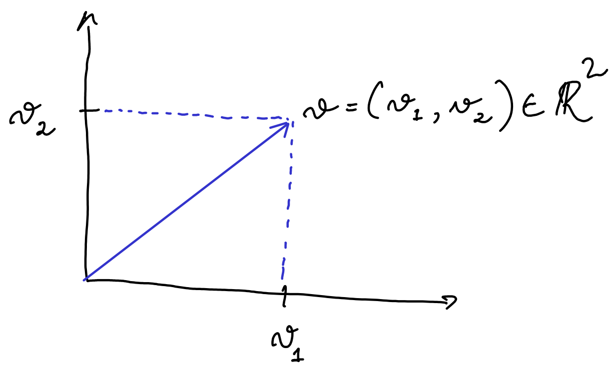


Vectors

Vectors are "arrays" of numbers, e.g.

$$v = (v_1, \dots, v_m) \in \mathbb{R}^m$$

We can consider a vector as a point in space, where each element v_i giving the coordinate along the i-th axis, e.g.



Norms assigns "lengths" to vectors.

The L^p-norm of a vector $v \in \mathbb{R}^m$ is

$$\|v\|_p = \left(\sum_i |v_i|^p \right)^{1/p}$$

with $p \in \mathbb{R}$ and $p \geq 1$.

The special case L^2 is the Euclidian norm, denoted $\|v\| = \|v\|_2$.

Operations on vectors

For all $a \in \mathbb{R}$, $u = (u_1, \dots, u_m) \in \mathbb{R}^m$, and $v = (v_1, \dots, v_m) \in \mathbb{R}^m$,

$$a u = (a u_1, \dots, a u_m) \qquad \text{scalar multiplication}$$

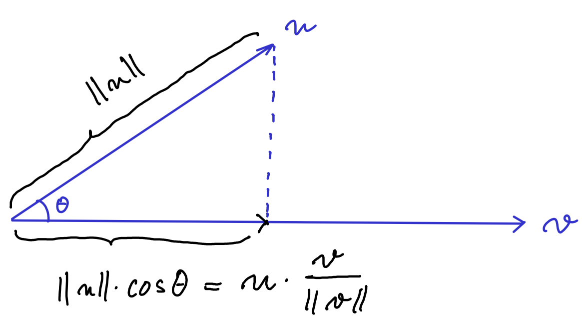
$$u + v = (u_1 + v_1, \dots, u_m + v_m) \qquad \text{vector addition}$$

$$u \cdot v = \sum_{i=1}^{m} u_i v_i \qquad \text{dot product}$$

Theorem (Geometric Interpretation of Dot Product)

If the angle between two vectors $u, v \in \mathbb{R}^m$ is θ, then

$$u \cdot v = \|u\| \cdot \|v\| \cdot \cos\theta$$



Partial Derivative

The partial derivative of a function

$$f(x_1, \dots, x_m)$$

in the direction of variable x_i at the point $u = (u_1, \dots, u_m)$ is

$$\frac{\partial f}{\partial x_i}(u_1, \dots, u_m) = \lim_{h \to 0} \frac{f(u_1, \dots, u_i + h, \dots, u_m) - f(u_1, \dots, u_m)}{h}$$

Intuitively the derivative of a function $g(x_i) = f(x_1, \dots, x_n)$, where all variables except x_i are fixed as constants.

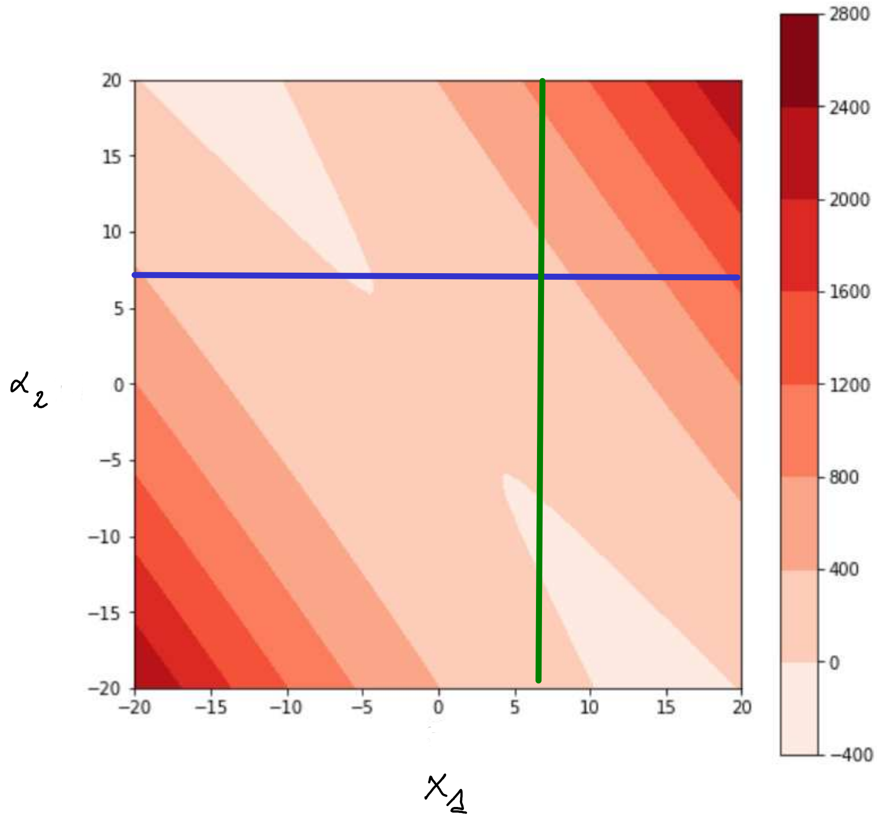
Example

$$f(x_1, x_2) = 2x_1^2 + x_2^2 + 3x_1x_2 + 4$$

$$\frac{\partial f}{\partial x_1} = 4x_1 + 3x_2$$

$$\frac{\partial f}{\partial x_2} = 2x_2 + 3x_1$$

Partial Derivatives : Geometric Interpretation



$\frac{\partial f}{\partial x_1}$ is the rate of change of f along dimension x_1 (i.e., blue line)

$\frac{\partial f}{\partial x_2}$ is the rate of change of f along dimension x_2 (i.e., green line)

Gradient

Definition

The gradient of a function $f(x_1, \dots, x_m)$ is

$$\nabla f := \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_m} \right)$$

Example

$$f(x_1, x_2) = 2x_1^2 + x_2^2 + 3x_1x_2 + 4$$

$$\nabla f(x_1, x_2) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2} \right)$$

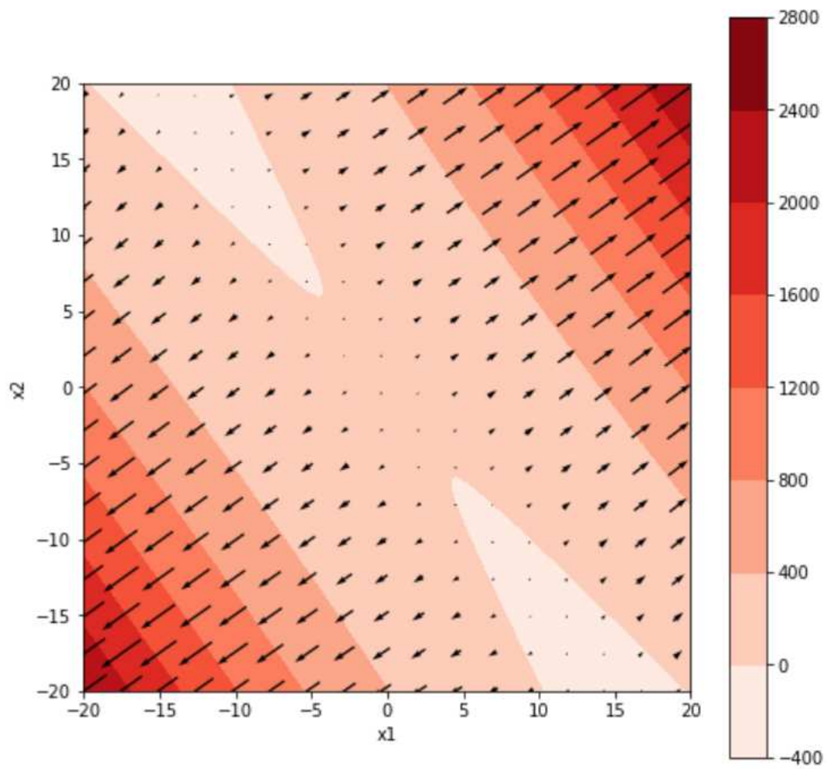
$$= \left(4x_1 + 3x_2, 2x_2 + 3x_1 \right)$$

Visualisation of the Gradient

Remark

If $f : \mathbb{R}^m \to \mathbb{R}$, then $\nabla f : \mathbb{R}^m \to \mathbb{R}^m$,

i.e., the gradient is a vector-valued function that maps vectors to vectors



Chain Rule (special case)

For one-dimensional functions

If $y = f(u)$ and

$u = g(x)$

then

$$\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx}$$

For higher dimensional functions

If $y = f(u_1, \dots, u_m)$ and

$u_i = g_i(x_1, \dots, x_n)$ for $i \in \{1, \dots, m\}$

then

$$\frac{\partial y}{\partial x_i} = \sum_{j=1}^{m} \frac{\partial y}{\partial u_j} \cdot \frac{\partial u_j}{\partial x_i}$$

Chain Rule (Example)

$$h(x_1, x_2) = (ax_1 + bx_2)^2 \; x_1 x_2$$

We can express h by defining

$$y = f(u_1, u_2) := u_1^2 \cdot u_2$$

$$u_1 = g_1(x_1, x_2) := ax_1 + bx_2$$

$$u_2 = g_2(x_1, x_2) := x_1 x_2$$

Applying the chain rule gives

$$\frac{\partial h}{\partial x_1} = \frac{\partial y}{\partial x_1} = \frac{\partial f}{\partial u_1} \cdot \frac{\partial u_1}{\partial x_1} + \frac{\partial f}{\partial u_2} \cdot \frac{\partial u_2}{\partial x_1}$$

$$= 2u_1 u_2 \cdot a + u_1^2 \cdot x_2$$

$$= u_1 (2au_2 + u_1 x_2)$$

$$= (ax_1 + bx_2)(2a \; x_1 x_2 + (ax_1 + bx_2) x_2)$$

$$= (ax_1 + bx_2) \, x_2 \, (3ax_1 + bx_2)$$

Similarly, the chain rule gives

$$\frac{\partial h}{\partial x_2} = \frac{\partial y}{\partial x_2} = \frac{\partial f}{\partial u_1} \frac{\partial u_1}{\partial x_2} + \frac{\partial f}{\partial u_2} \cdot \frac{\partial u_2}{\partial x_2}$$

$$= 2u_1 u_2 b + u_1^2 \, x_1$$

$$= u_1 (2bu_2 + u_1 x_1)$$

$$= (ax_1 + bx_2)(2bx_1 x_2 + (ax_1 + bx_2) x_1)$$

$$= (ax_1 + bx_2) \, x_1 \, (3bx_2 + ax_1)$$

Directional Derivative

Definition

Given a function

$$f : \mathbb{R}^m \to \mathbb{R}$$

and a vector

$\boldsymbol{v} = (v_1, \dots, v_m)$, with $\|\boldsymbol{v}\| = 1$

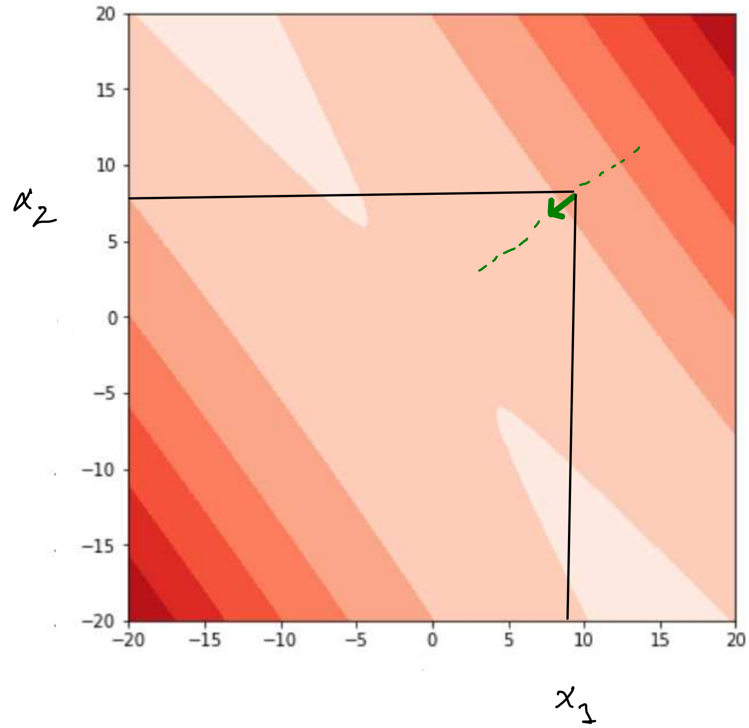
the directional derivative of f in

$\boldsymbol{x} = (x_1, \dots, x_m)$

along the vector $\boldsymbol{v}$ is

$$\nabla_{\boldsymbol{v}} f(\boldsymbol{x}) := \lim_{\alpha \to 0} \frac{f(\boldsymbol{x} + \alpha \boldsymbol{v}) - f(\boldsymbol{x})}{\alpha}$$

$$= \lim_{\alpha \to 0} \frac{f(x_1 + \alpha v_1, \dots, x_m + \alpha v_m) - f(x_1, \dots, x_m)}{\alpha}$$



Computing Directional Derivative

The following theorem implies that if we know the gradient ∇f, then we can compute the derivative in any direction v.

Theorem

gradient

$$\nabla_v f(x) = \nabla f(x) \cdot v$$

directional derivative

dot product

Proof

Define the function

$$h(\alpha) := f(u_1, \dots, u_m)$$

where

$$u_i := x_i + \alpha v_i \quad \text{for all } i \in \{1, \dots, m\}.$$

Note that $h : \mathbb{R} \to \mathbb{R}$, i.e., h is a one-dimensional real-valued function.

$$\nabla_v f(x) = \lim_{\alpha \to 0} \frac{f(x + \alpha v) - f(x)}{\alpha} \quad \text{by def. of } \nabla_u f$$

$$= \lim_{\alpha \to 0} \frac{h(0+\alpha) - h(0)}{\alpha} \quad \text{by def. of } g$$

(1) $$= h'(0) \quad \text{by def. of derivative}$$

Using the chain rule, we have

(2) $$h'(\alpha) = \frac{dh}{d\alpha} = \sum_{i=1}^{m} \frac{\partial f}{\partial u_i} \cdot \frac{\partial u_i}{\partial \alpha} = \sum_{i=1}^{m} \frac{\partial f}{\partial u_i} \cdot v_i$$

Note that for $\alpha = 0$, we have

(3) $$u_i = x_i + 0 \cdot v_i = x_i$$

Using (1), (2), and (3), we get

$$\nabla_v f(x) = h'(0) = \sum_{i=1}^{m} \frac{\partial f}{\partial x_i} \cdot v_i = \nabla f(x) \cdot v$$

$\square$

The Gradient Points towards Steepest Ascent

The vector v along which f has steepest ascent is

$$\underset{v,\,\|v\|=1}{\operatorname{argmax}} \; \nabla_v f(x)$$

$$= \underset{v,\,\|v\|=1}{\operatorname{argmax}} \; \nabla f(x) \cdot v$$

angle between v and $\nabla f(x)$

$$= \underset{v,\,\|v\|=1}{\operatorname{argmax}} \; \|\nabla f(x)\| \, \|v\| \cdot \cos\theta$$

$$= \underset{v,\,\|v\|=1}{\operatorname{argmax}} \; \|\nabla f(x)\| \cdot \cos\theta$$

$\Longrightarrow$ The vector v which gives the steepest ascent is the vector that has angle $\theta = 0$ to ∇f, i.e., the vector v which points in the same direction as ∇f.

Method of Gradient Descent

NB! This is the most important slide in this module!

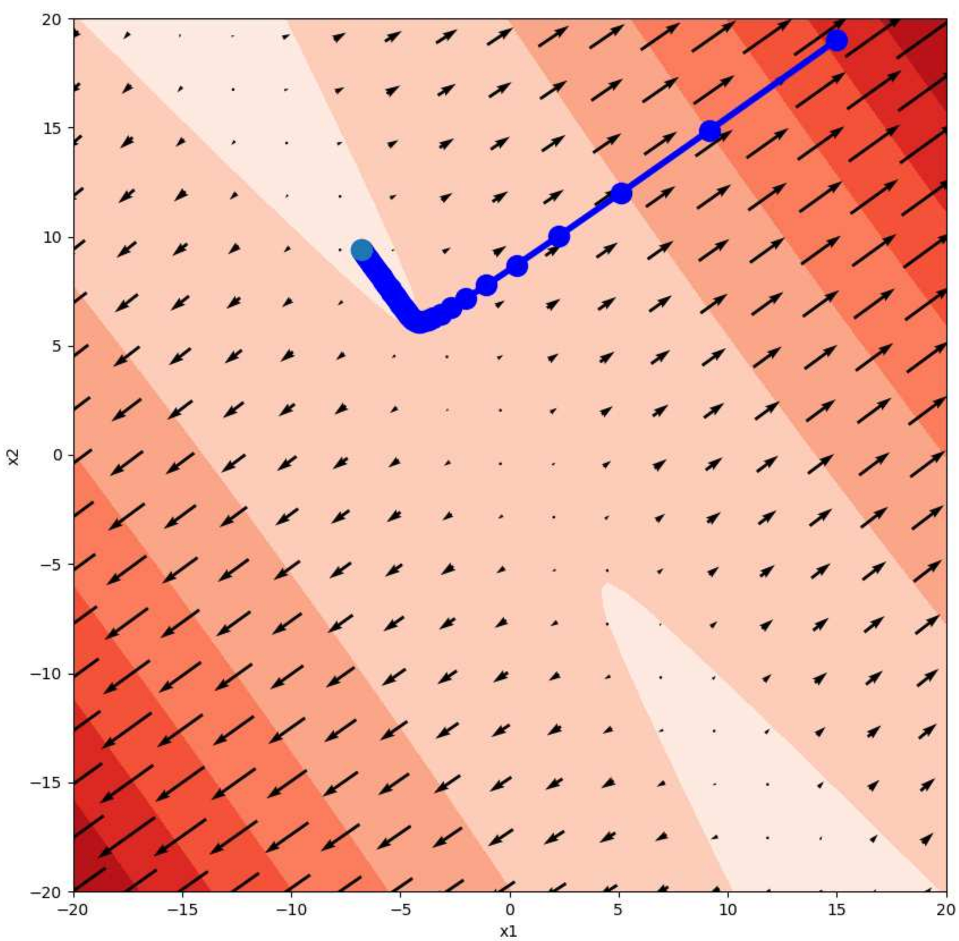
Input: cost function $J : \mathbb{R}^m \to \mathbb{R}$
learning rate $\varepsilon \in \mathbb{R}, \varepsilon > 0$

$x \leftarrow$ some initial point in $\mathbb{R}^m$
while termination condition not met {

$$x \leftarrow x - \varepsilon \cdot \nabla J(x)$$

}

A. Cauchy (1789-1857)



Summary

- Functions of multiple variables
- Partial derivatives and the chain rule
- Gradients
  - Direction of steepest ascent
- Gradient descent

Next time

- Feed forward neural networks
- The backpropagation algorithm