IFT6390
Fondements de l'apprentissage machine

Optimization
Basic principles and techniques

Professor: Ioannis Mitliagkas
Slides: Pascal Vincent

Optimization?

- The training phase of a learning algorithm often involves optimization
- That is, finding the values of the parameters θ of the function f_θ that minimize (or maximize) some objective $J(\theta)$
- Objective example: empirical risk (or «mean error») on the training data:

$$J(\theta) = \hat{R}(f_\theta, D_n)$$

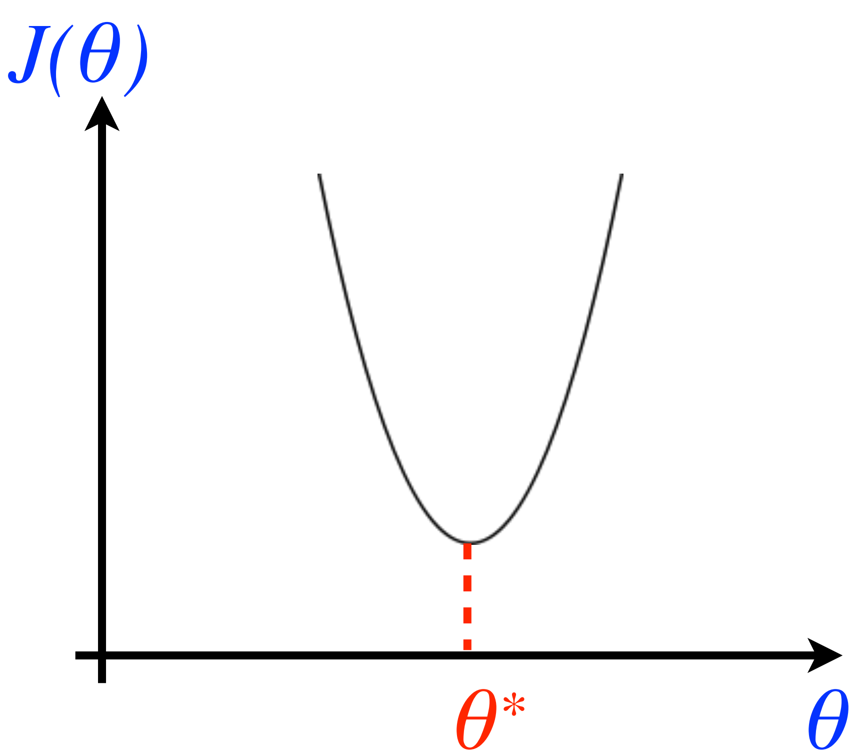
The optimization problem

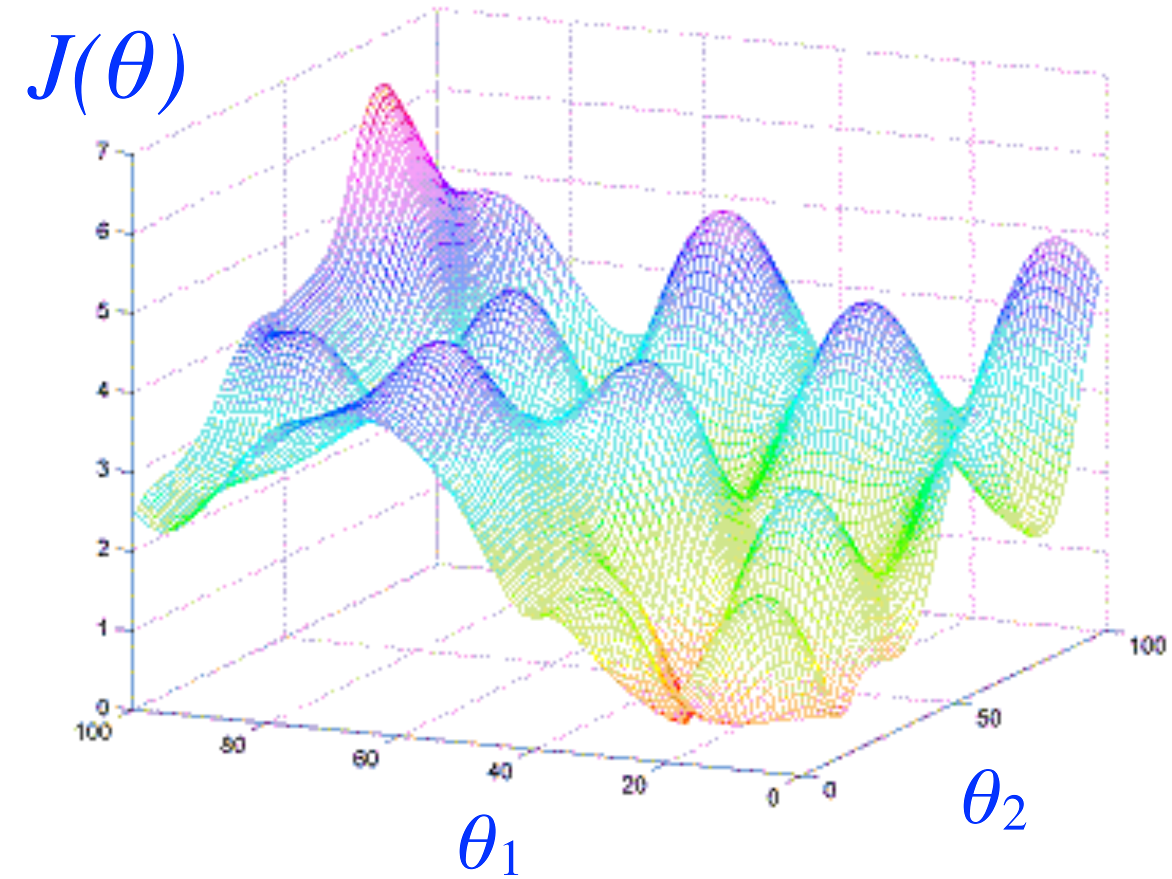
$$\theta^* = \arg\min_{\theta} J(\theta)$$

Optimal value of the parameters

How to find it ???

Landscape of the loss function:





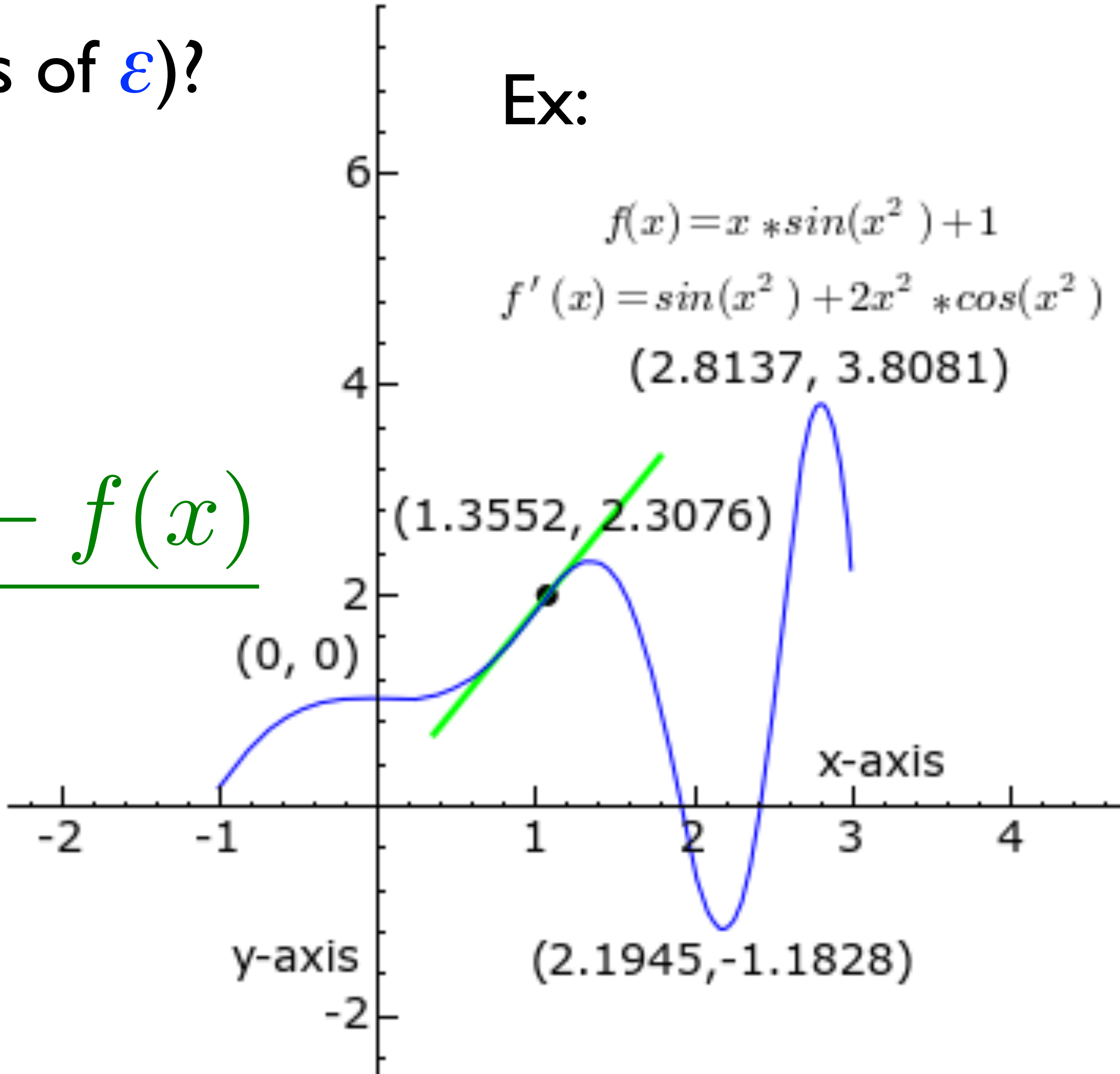
Reminder: derivative

- Measures the **sensitivity** of a function f to a change of its input (at a point x).

- Let $f : \mathbb{R} \to \mathbb{R}$. At a point x, if we add a small ε to x, how much will $f(x)$ move (in multiples of ε)?

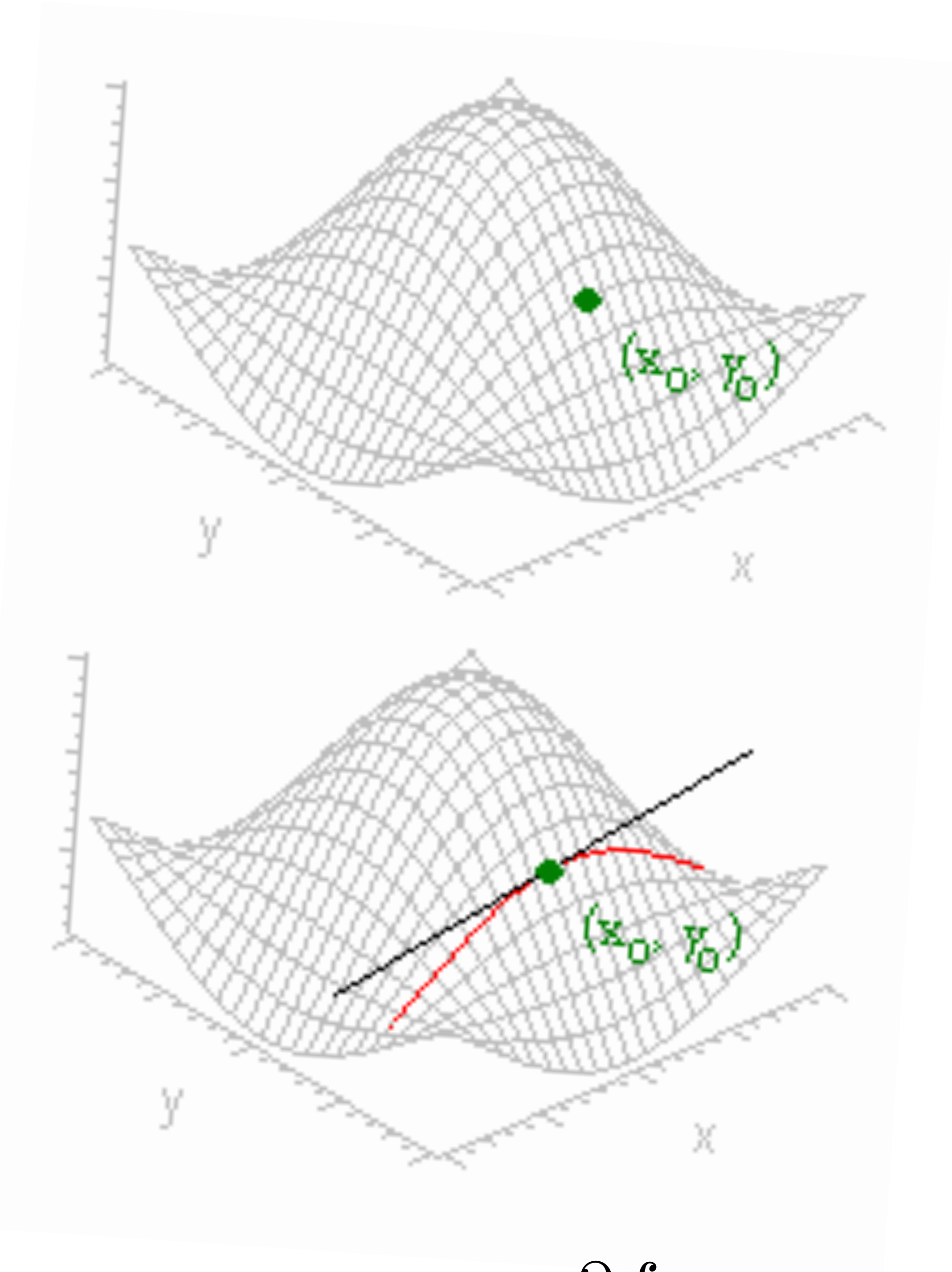
$$
\begin{aligned}
f'(x) &= \frac{\partial f}{\partial x}(x) \\
&= \lim_{\epsilon \to 0} \frac{f(x+\epsilon) - f(x)}{\epsilon}
\end{aligned}
$$

Ex:



- Geometrically: this is the **slope** of the curve at each point.

Partial derivative



- For a function taking vectors (i.e. several parameters) as input.

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

- We can evaluate it at x:
  $f(x) = f(x_1, \ldots, x_m)$

- And measure how **sensitive** it is to each of its input separately (assuming the others fixed)

$$f'_{x_k}(x) = \frac{\partial f}{\partial x_k}(x)$$

partial derivative of f with respect to x_k, evaluated at x

$$= \lim_{\epsilon \to 0} \frac{f(x_1, \ldots, x_k + \epsilon, \ldots, x_m) - f(x_1, \ldots, x_k, \ldots, x_m)}{\epsilon}$$

Gradient

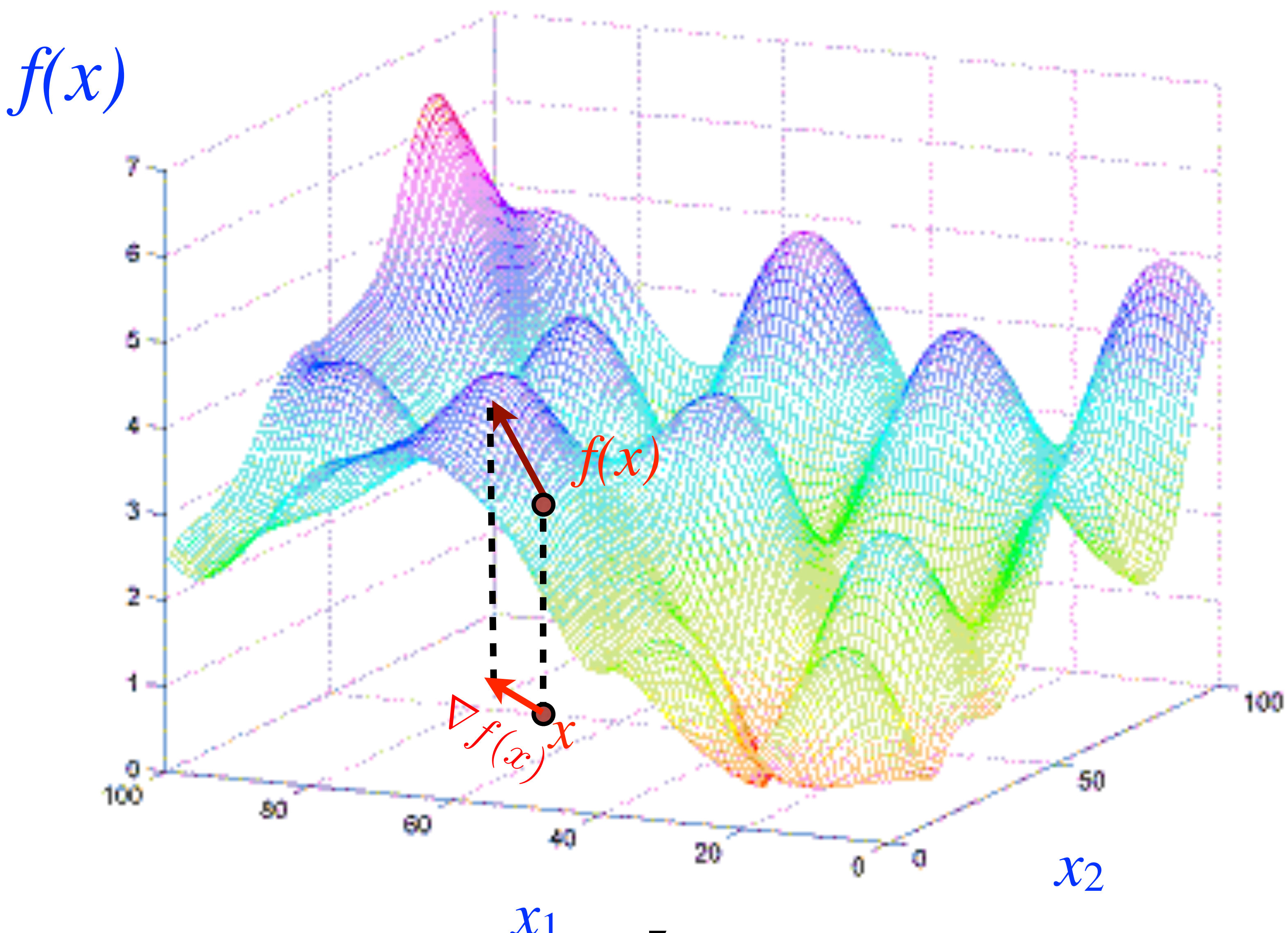
- The gradient is the vector of partial derivatives:

$$\nabla f(x) = \frac{\partial f}{\partial x}(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_m} \end{pmatrix}(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(x) \\ \frac{\partial f}{\partial x_2}(x) \\ \vdots \\ \frac{\partial f}{\partial x_m}(x) \end{pmatrix}$$

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

Gradient: geometry

- The gradient points in the direction of the steepest slope (uphill/ascending)



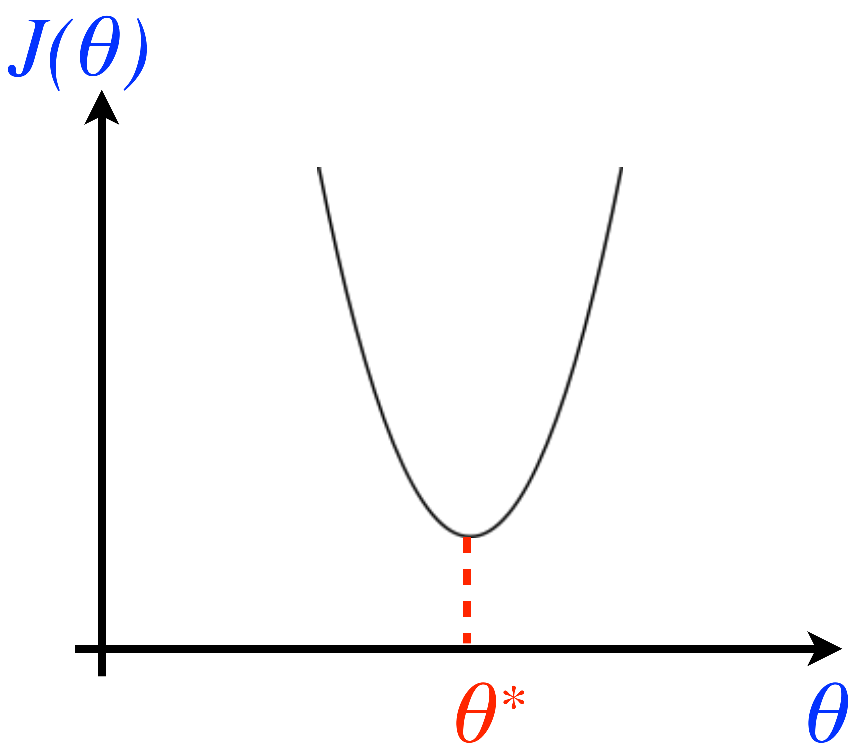
The optimization problem

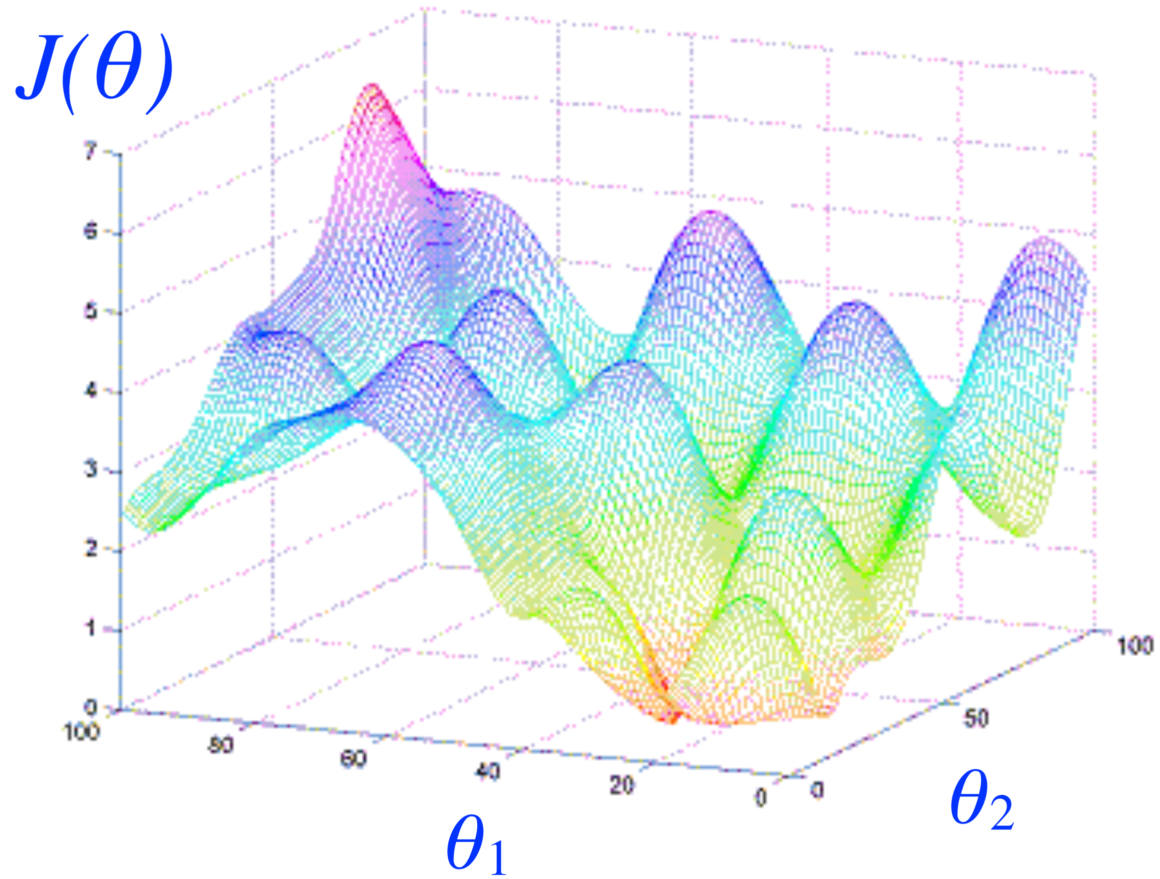
$$\theta^* = \arg\min_{\theta} J(\theta)$$

Optimal value of the parameters

How to find it ???

Landscape of the loss function:



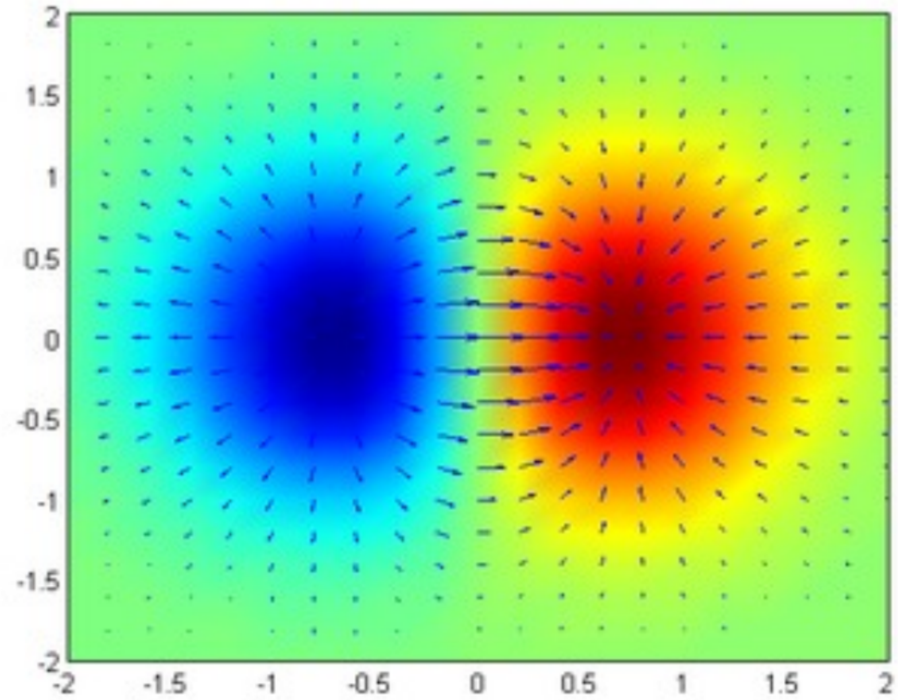


Gradient

- Let $\theta=(\theta_1, \ldots, \theta_m)$ be a vector of parameters.
- Let $J(\theta)$ be a scalar function: the objective function to minimize.
- The gradient is the vector of the partial derivatives:

$$\nabla J(\theta) = \frac{\partial J}{\partial \theta}(\theta) = \begin{pmatrix} \frac{\partial J}{\partial \theta_1} \\ \frac{\partial J}{\partial \theta_2} \\ \vdots \\ \frac{\partial J}{\partial \theta_m} \end{pmatrix}(\theta) = \begin{pmatrix} \frac{\partial J}{\partial \theta_1}(\theta) \\ \frac{\partial J}{\partial \theta_2}(\theta) \\ \vdots \\ \frac{\partial J}{\partial \theta_m}(\theta) \end{pmatrix}$$

Properties of the gradient



- The inner product $\langle \nabla f(\mathbf{x}), \mathbf{v} \rangle$ between the gradient of f at $\mathbf{x}$ and any unit vector $\mathbf{v} \in \mathbb{R}^n$ is the *directional derivative* of f in the direction of $\mathbf{v}$ (i.e. the rate at which f changes at $\mathbf{x}$ in the direction $\mathbf{v}$).

$\rightarrow$ $\nabla f(\mathbf{x})$ points towards the direction of greatest increase of f at $\mathbf{x}$.

$\rightarrow$ Points such that $\nabla f(\mathbf{x}) = \mathbf{0}$ are called stationary points.

$\rightarrow$ The gradient $\nabla f(\mathbf{x})$ is orthogonal to the contour line passing through $\mathbf{x}$.

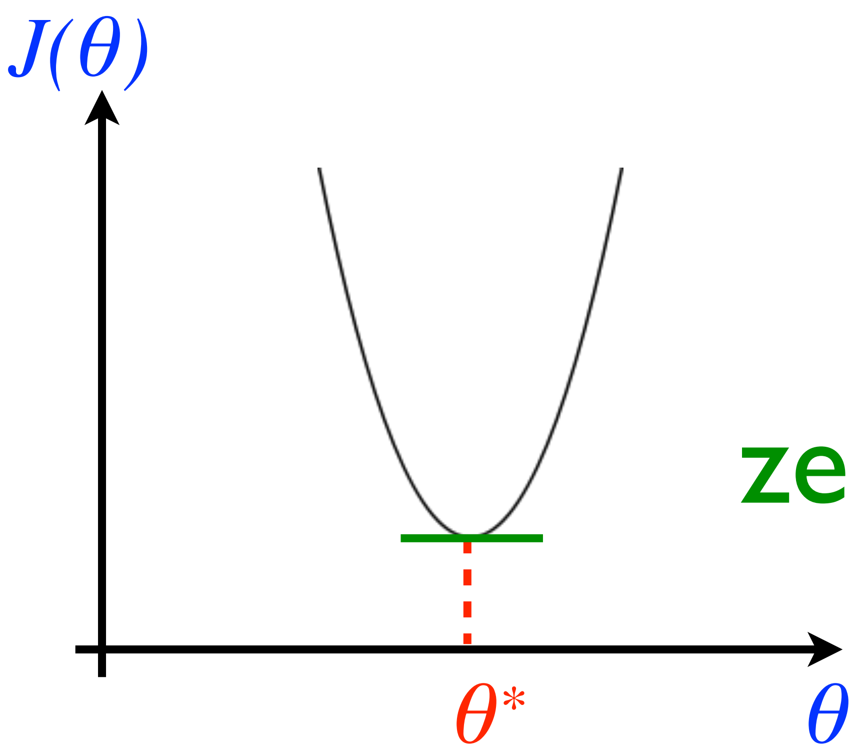
The main property

At the optimum, the **gradient** is zero:

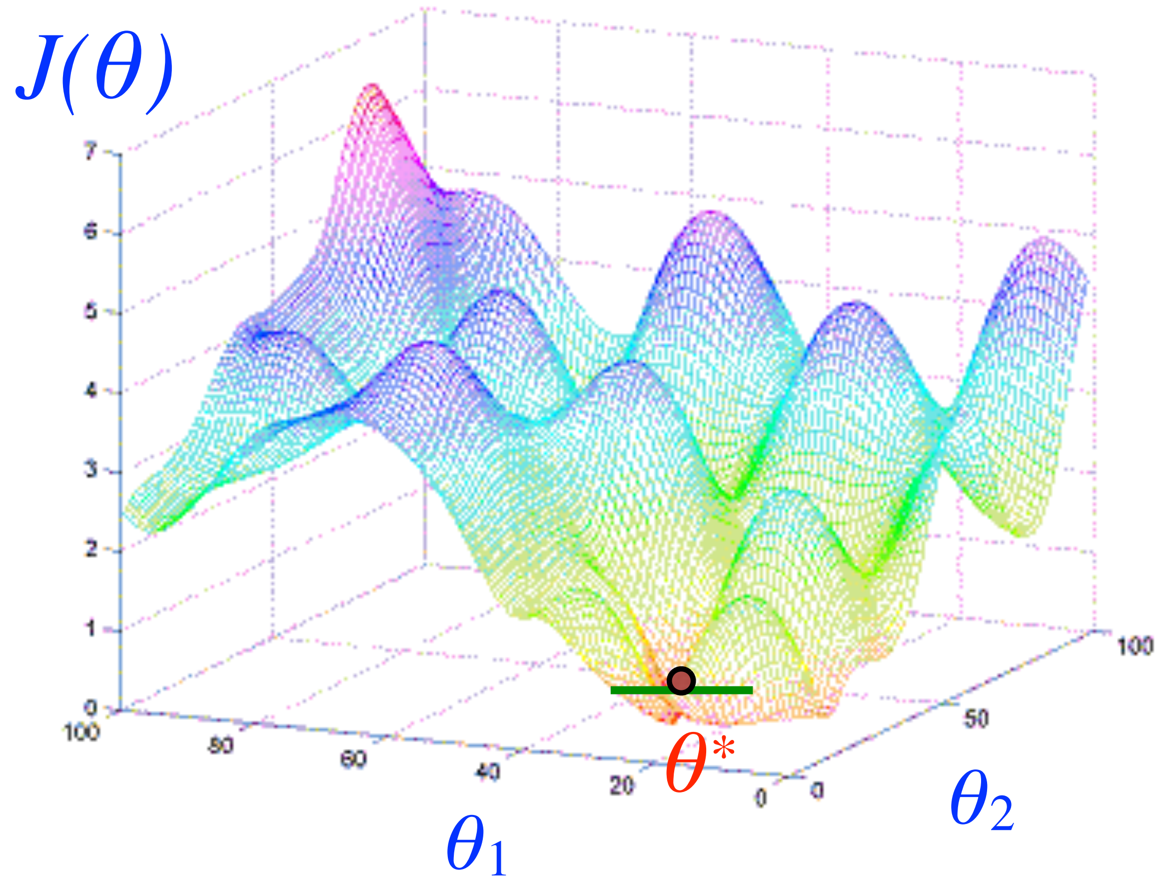
the «slope»

$$\frac{\partial J}{\partial \theta}(\theta^*) = 0$$

Landscape of the loss function:



zero slope



Analytical solution

- **Sometimes** we can solve the equation (system) analytically to find the optimal θ:

$$\frac{\partial J}{\partial \theta} = 0 \qquad \begin{cases} \frac{\partial J}{\partial \theta_1} = 0 \\ \frac{\partial J}{\partial \theta_2} = 0 \\ \qquad \vdots \\ \frac{\partial J}{\partial \theta_m} = 0 \end{cases}$$

...

$$\theta = \ldots$$

- Examples of problem with analytical solutions:
  - Maximum likelihood to estimate the parameters of a Gaussian
  - Linear regression / Ridge regression

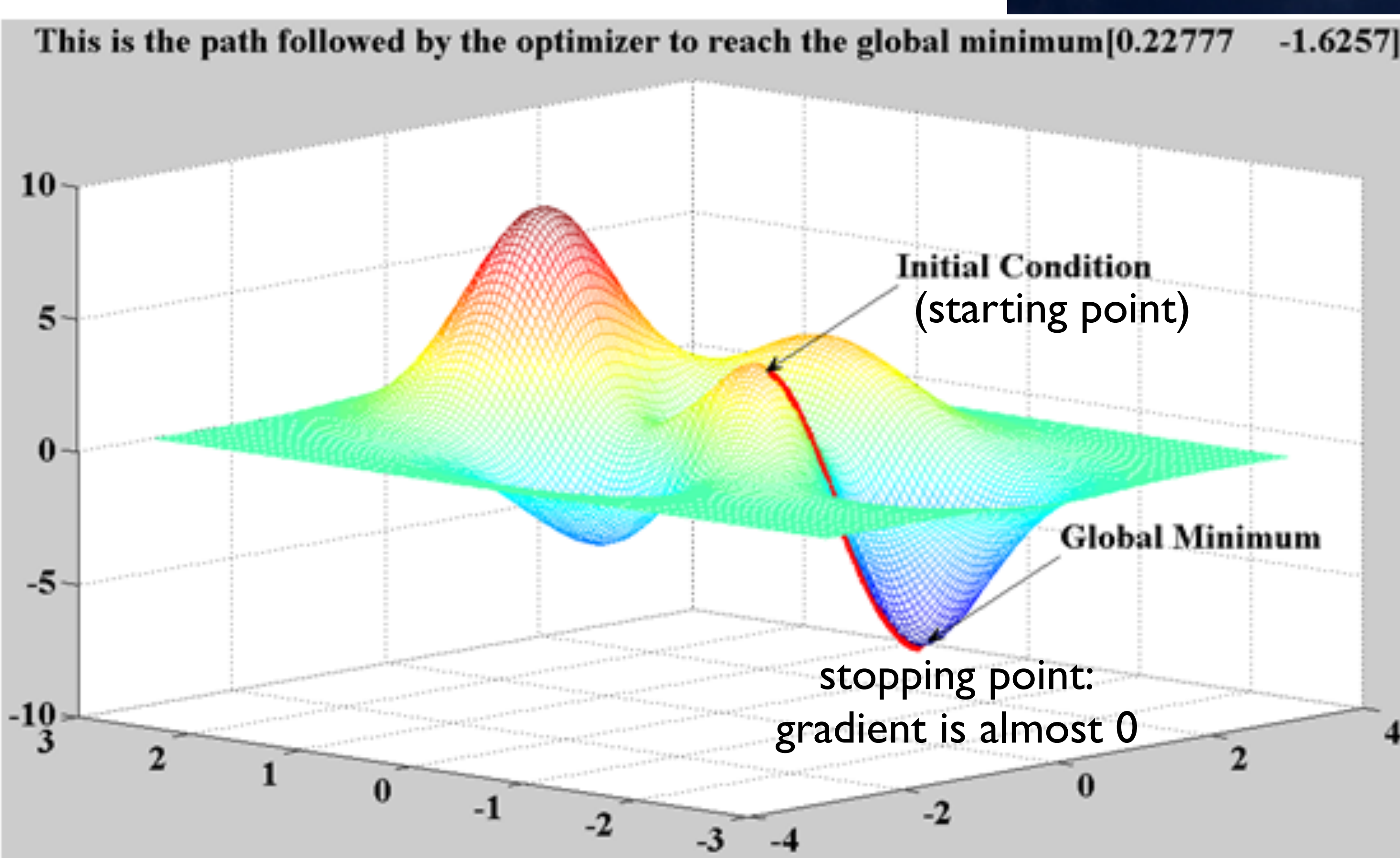
Search algorithm

- **In most cases,** there is no analytical solution to the equation $\frac{\partial J}{\partial \theta} = 0$
- In this case we can use an **iterative algorithm** to search for an optimal solution.
- Method 1: **exhaustive search!**
  try all possible values of θ (or fine grid search) and keep the best one...
  => NOT POSSIBLE FOR HIGH-DIMENSIONAL θ (m>4).
- Method 2: **gradient descent!**

Gradient descent

- Initialize θ randomly (using an appropriate heuristic)
- Until convergence, repeat $\theta \leftarrow \theta - \eta \frac{\partial J}{\partial \theta}(\theta)$

We update θ by taking a step in the direction opposite to the gradient (direction of the steepest descent).



Gradient descent

learning rate

$$\theta \leftarrow \theta - \eta \frac{\partial J}{\partial \theta}(\theta)$$

- η is a positive real number called the *«learning rate»* or *«step size»*.
  It controls the size of the steps in parameter space (how much we update θ).

- This is a *crucial* hyper-parameter for the optimization procedure (needs to be chosen carefully).

- Often, we slightly decrease the learning rate at each iteration.
  Ex.: at iteration t, we set the learning rate to $\eta(t) = \dfrac{\lambda}{t_0 + t}$

  Here t_0 and λ are hyper-parameters (to be carefully chosen...).

Gradient descent
stopping criteria

$$\theta \leftarrow \theta - \eta \frac{\partial J}{\partial \theta}(\theta)$$

- We stop the gradient descent iterations when the updates leave θ almost unchanged.
- That is, when the norm of the gradient gets smaller than some small threshold: $$\left\| \frac{\partial J}{\partial \theta}(\theta) \right\| < \epsilon$$
- We may even want to stop earlier, before reaching the optimal point (for example to prevent overfitting and generalize better) => early stopping *(use an other criterion to decide when to stop, for example using a validation set; more on that later...)*

Gradient descent
what solution do we get in the end?

Gradient descent converges to a point where the **gradient** is (almost) zero:

$$\frac{\partial J}{\partial \theta}(\theta) \approx 0$$

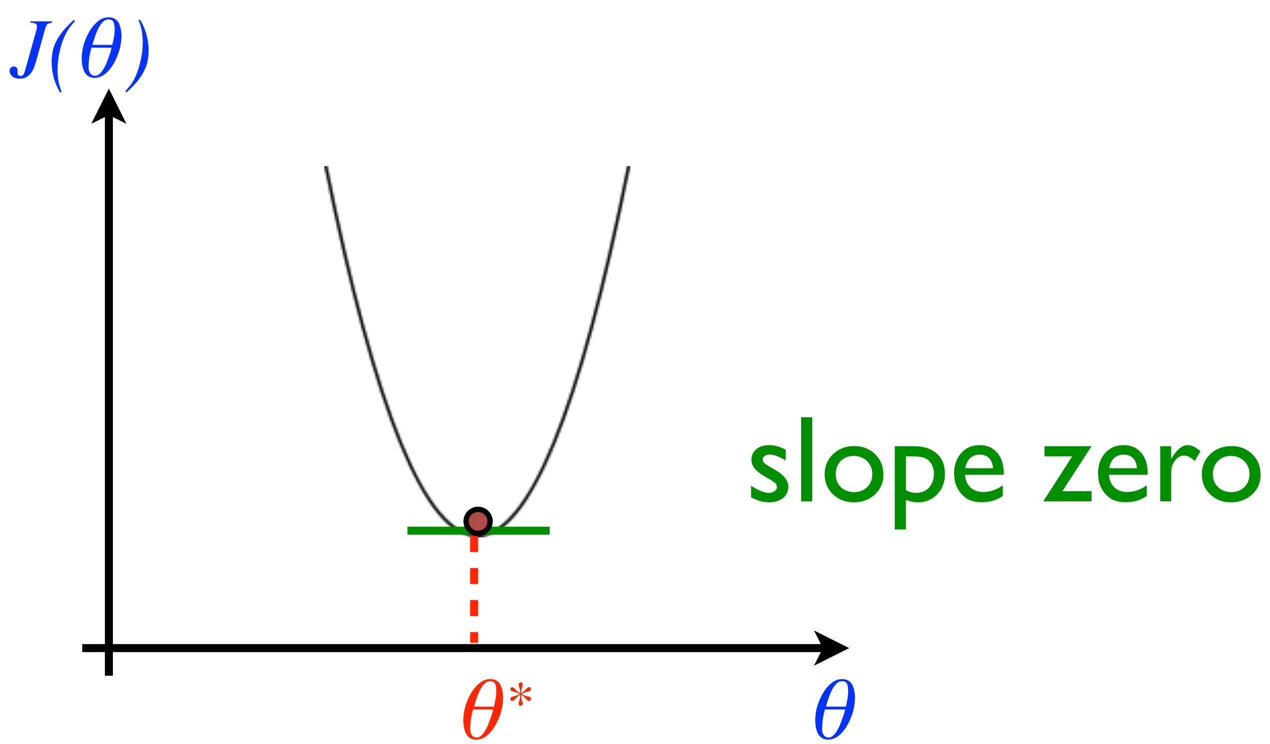
Gradient descent

Convex objective

Gradient descent converges to a point where the **gradient** is (almost) zero:

$$\frac{\partial J}{\partial \theta}(\theta) \approx 0$$

Landscape of the loss function:



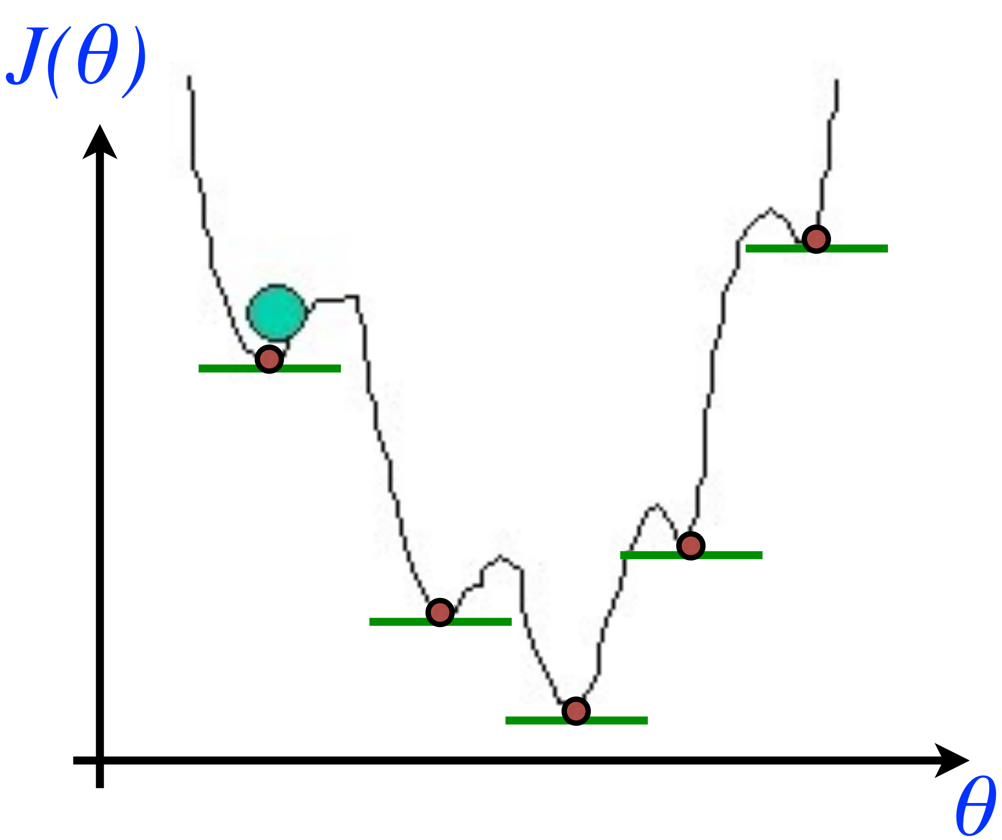
For a convex objective, we reach the **global minimum**

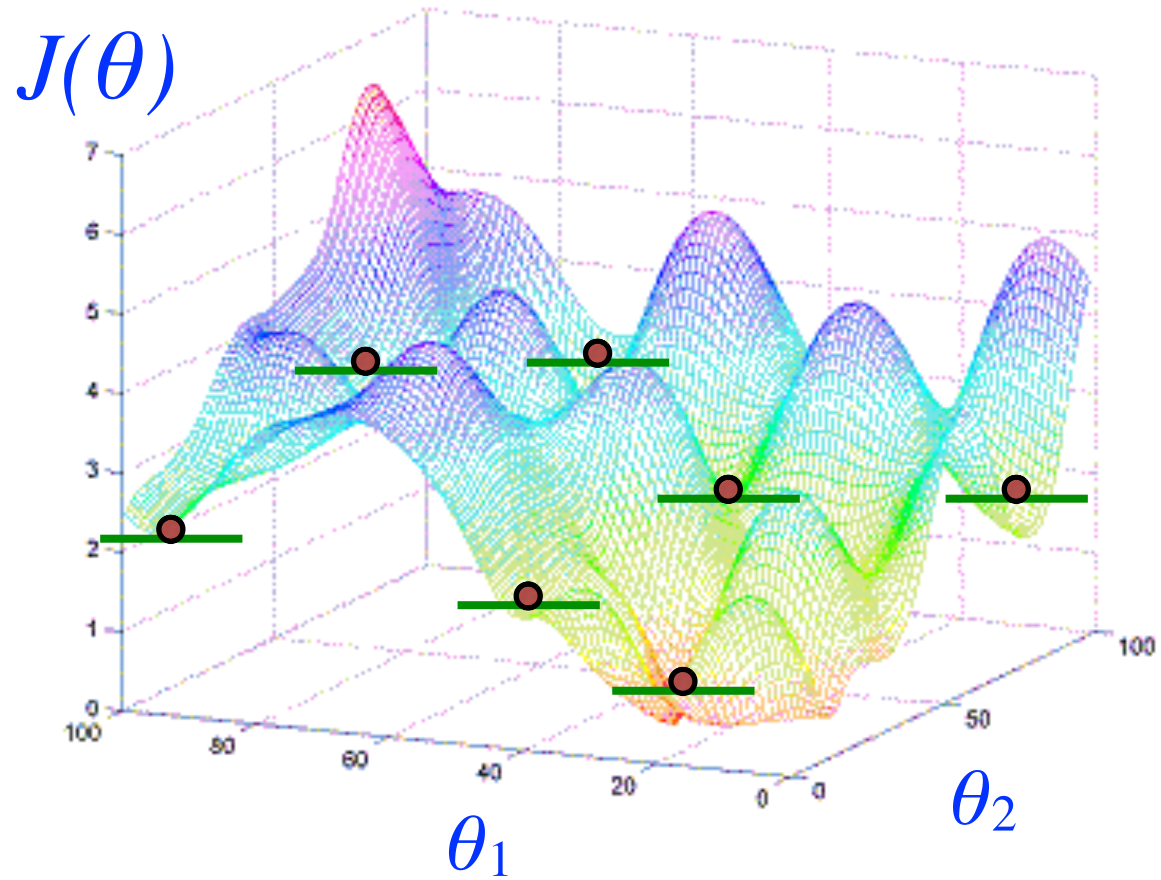
Gradient descent

objective is non-convex

Gradient descent converges to a point where the **gradient** is (almost) zero: $$\frac{\partial J}{\partial \theta}(\theta) \approx 0$$

For a non convex objective function there can be *many* such points: all *local* extrema (minima, maxima saddle points).





➠ In practice, we converge to a **local minimum** (rather than a global one) which depends on the starting point.

Typical minimization objective for learning tasks

- In machine learning, the objective function to minimize is often a sum or a mean over the *n* examples of the training set $D_n = \{z^{(1)}, \ldots, z^{(n)}\}$

  of a loss/cost function *L (empirical risk):*

$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} L(z^{(i)}; \theta)$$

- Remark: minimizing the sum or the mean are equivalent (they have the same minima).

Typical gradient
for learning tasks

- Gradient of the mean = mean of the gradients:

$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} L(z^{(i)}; \boldsymbol{\theta})$$

$$\begin{aligned}
\frac{\partial J}{\partial \theta}(\theta) &= \frac{\partial}{\partial \theta}\left(\frac{1}{n}\sum_{i=1}^{n} L(z^{(i)}; \theta)\right) \\
&= \frac{1}{n}\sum_{i=1}^{n} \frac{\partial}{\partial \theta} L(z^{(i)}; \theta)
\end{aligned}$$

Gradient descent

batch, mini-batch

- In «batch» gradient descent, we compute the mean of the gradients over all n examples in D_n

$$\nabla(\theta) = \frac{\partial J}{\partial \theta}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \frac{\partial}{\partial \theta} L(z^{(i)};\theta) = \underset{z \in D_n}{\text{mean}} \left[\frac{\partial}{\partial \theta} L(z \quad ;\theta) \right]$$

before each update of the parameters: $\theta \leftarrow \theta - \eta \nabla(\theta)$

- In «mini-batch» gradient descent with batch size n', approximate the mean of the gradients by computing the mean over only $n' < n$ examples in D_n

$$\nabla(\theta) = \underset{z \in \text{minibatch}}{\text{mean}} \left[\frac{\partial}{\partial \theta} L(z \quad ;\theta) \right] \approx \frac{\partial J}{\partial \theta}(\theta)$$

(these n' examples, different each time, are called a *mini batch*)

Gradient descent

batch, mini-batch, stochastic/online

Algo:

$$\nabla(\theta) = \operatorname*{mean}_{z \in \text{minibatch}} \left[\frac{\partial}{\partial \theta} L(z^{(i)}; \theta) \right] \approx \frac{\partial J}{\partial \theta}(\theta)$$ *Gradient computation*

$$\theta \leftarrow \theta - \eta \nabla(\theta)$$ *Parameter update*

- Before each computation of ∇ the n' examples of the mini-batch should ideally be drawn randomly from D_n.
- But for efficiency, we often take examples *sequentially* in D_n to construct the mini-batches (starting with the first n' examples, then the following n', etc., and we repeat).
- Remark: with $n'=n$ we fall back onto the *batch gradient descent.*
- The case $\boldsymbol{n'=1}$ (we use only one examples for each gradient computation) is called online/stochastic gradient descent.

Gradient descent variants

There exist a lot of optimization algorithms based on gradient descent:

- *Momentum* technique
- Conjugate gradient
- Second-order methods. (use information about the «curvature» of the objective by taking second-order derivatives into account: the Hessian)
  Ex: Newton's method.
- ...

All these are for continuous parameters and assume we can efficiently compute a «gradient».

Newton's method

Gradient: vector of first-order derivatives

$$\nabla_J = \frac{\partial J}{\partial \theta} = \begin{pmatrix} \frac{\partial J}{\partial \theta_1} \\ \frac{\partial J}{\partial \theta_2} \\ \vdots \\ \frac{\partial J}{\partial \theta_m} \end{pmatrix}$$

Simple (batch) gradient descent:

$$\theta \leftarrow \theta - \eta \nabla_J(\theta)$$

Newton's method (batch):

$$\theta \leftarrow \theta - \eta H(\theta)^{-1} \nabla_J(\theta)$$

Hessian: matrix of second-order derivatives

$$H = \frac{\partial^2 J}{\partial \theta^2} = \begin{pmatrix} \frac{\partial^2 J}{\partial \theta_1^2} & \frac{\partial^2 J}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2 J}{\partial \theta_1 \partial \theta_m} \\ \frac{\partial^2 J}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 J}{\partial \theta_2^2} & \cdots & \frac{\partial^2 J}{\partial \theta_2 \partial \theta_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 J}{\partial \theta_m \partial \theta_1} & \frac{\partial^2 J}{\partial \theta_m \partial \theta_2} & \cdots & \frac{\partial^2 J}{\partial \theta_m^2} \end{pmatrix}$$

Not straight-forward for mini-batch

H^{-1}: difficult and costly to compute

Constrained optimization

- In what we saw, there were no constraints on the parameters
- Sometimes, we also want the parameters to satisfy one or more constraints
(ex: positive, sum to1, ...)
- Constrained optimization => more complex algorithms.
Ex: linear/quadratic 'programming', ...