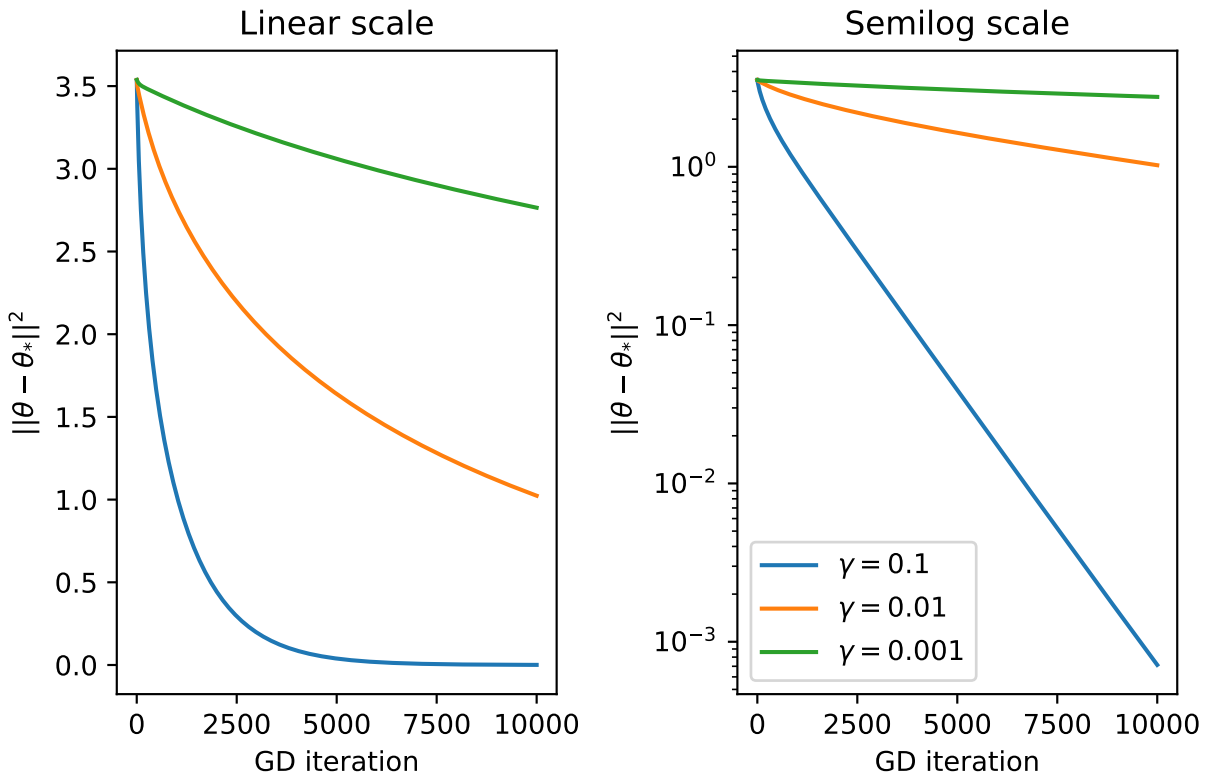
Machine learning I, supervised learning: gradient algorithms

Gradient descent: squared distance to the OLS estimator
$||\theta - \theta^*||^2$



Minimization of functions

In machine learning, we face **function minimization problems**. Typically, the function to minimize if the empirical risk on the train set, that will typically depend on a parameter $\theta \in \mathbb{R}^d$.

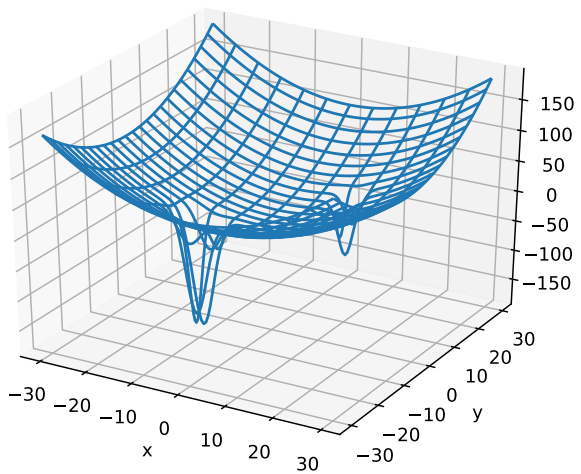


Figure – Example of a function to minimize

Analytic minimum

What is the minimum of the function

$$f : x \to (x - 1)^2 + 3.5 \tag{1}$$

And for what value x is it obtained ?

Context

In machine learning, we often encounter problems in high dimension, where closed-form solutions to the **empirical risk minimization** problem are **not** available (e.g. for logistic regression), or where even if they are available, the necessary computation time is too large (OLS).

Context

In machine learning, we often encounter problems in high dimension, where closed-form solutions are not avaible, or where even if they are available, the necessary computation time is too large.

Example 1 : Computing the OLS estimator requires a matrix inversion, which is $\mathcal{O}(d^3)$.

$$\hat{\theta} = (X^T X)^{-1} X^T y \tag{2}$$

Context

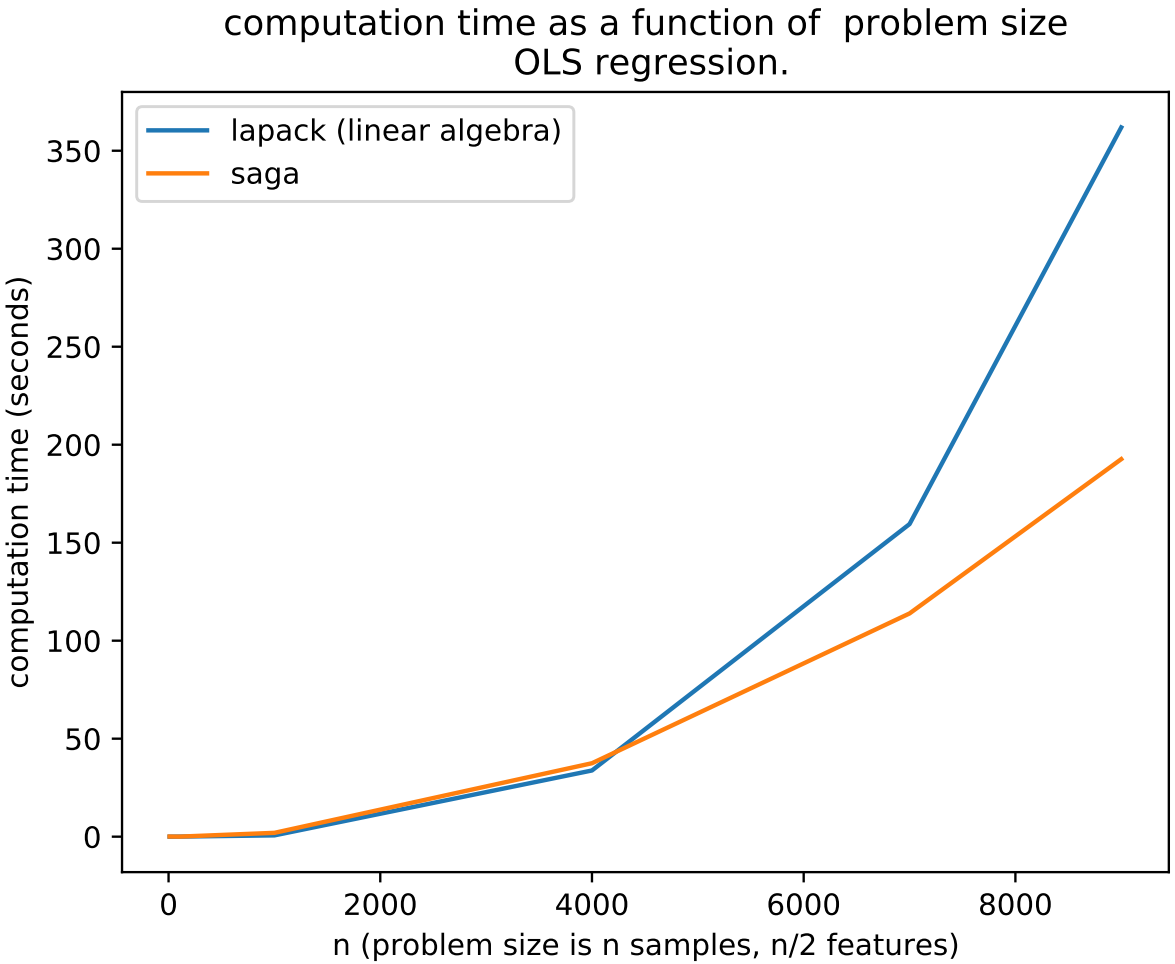
In machine learning, we often encounter problems in high dimension, where closed-form solutions are not avaible, or where even if they are available, the necessary computation time is too large.

Example 2 : The cancellation of the gradient of the objective function with logistic loss has no closed-form solution.

Context

Instead, we often use **iterative** algorithm such as Gradient descent (GD) or Stochastic gradient descent (SGD). SGD is the standard optimization algorithm for large-scale machine learning.

SGD vs Lapack



Derivation and variation

- In the case a function $f : \mathbb{R} \to \mathbb{R}$, we can study its variations by computing its derivative f', **if it exists**
- If $f'(x) > 0$, the function grows around x.
- If $f'(x) < 0$, the function decreases around x.
- If x is a local extremum, $f'(x) = 0$
- Is the reciprocal true ?

One dimensional functions

If $f : \mathbb{R} \mapsto \mathbb{R}$ is differentiable (dérivable) :
(Landau notation)

$$f(a+h) = f(a) + hf'(a) + o(h) \tag{3}$$

Physicist notation :

$$f(a+h) \simeq f(a) + hf'(a) \tag{4}$$

Gradient update

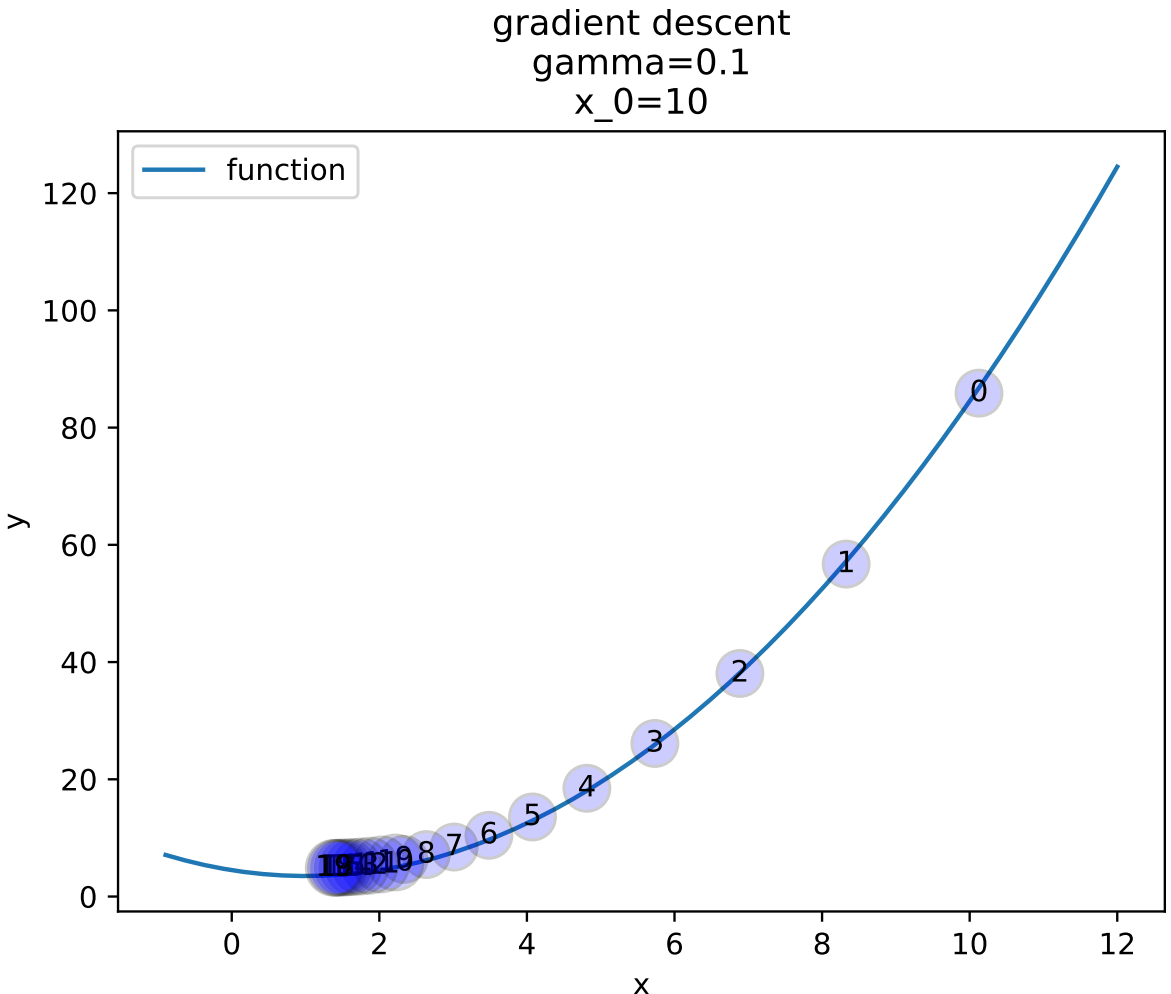
In one dimension (the function depends on $x \in \mathbb{R}$) :

$$x \leftarrow x - \gamma f'(x) \tag{5}$$

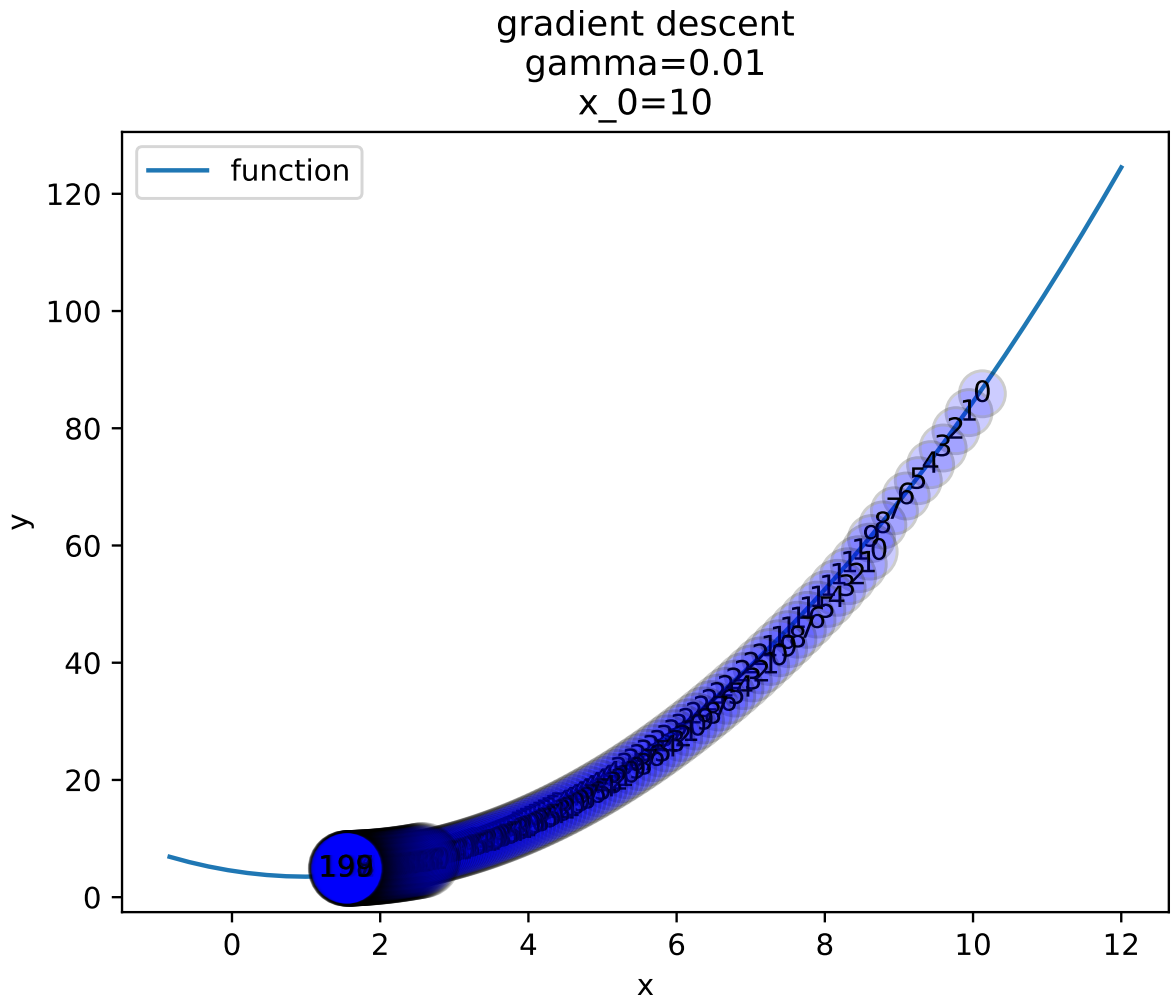
- $\leftarrow$ means "is substituted by".
- $\gamma > 0$ is a real number called the **learning rate** (hyperparameter of the algorithm).

Examples in 1 dimension

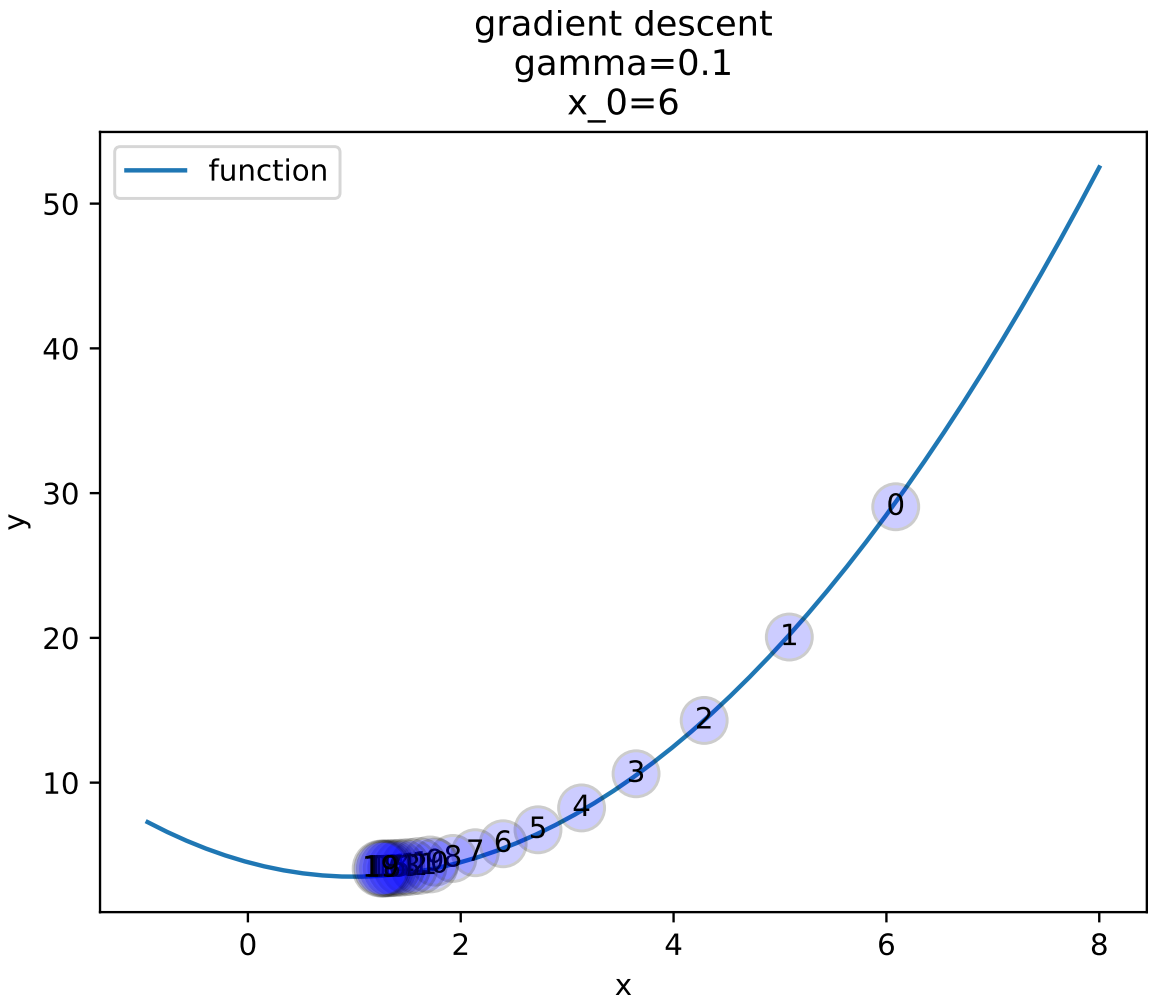
In the following examples, we use the script **gradients/1d_function.py**



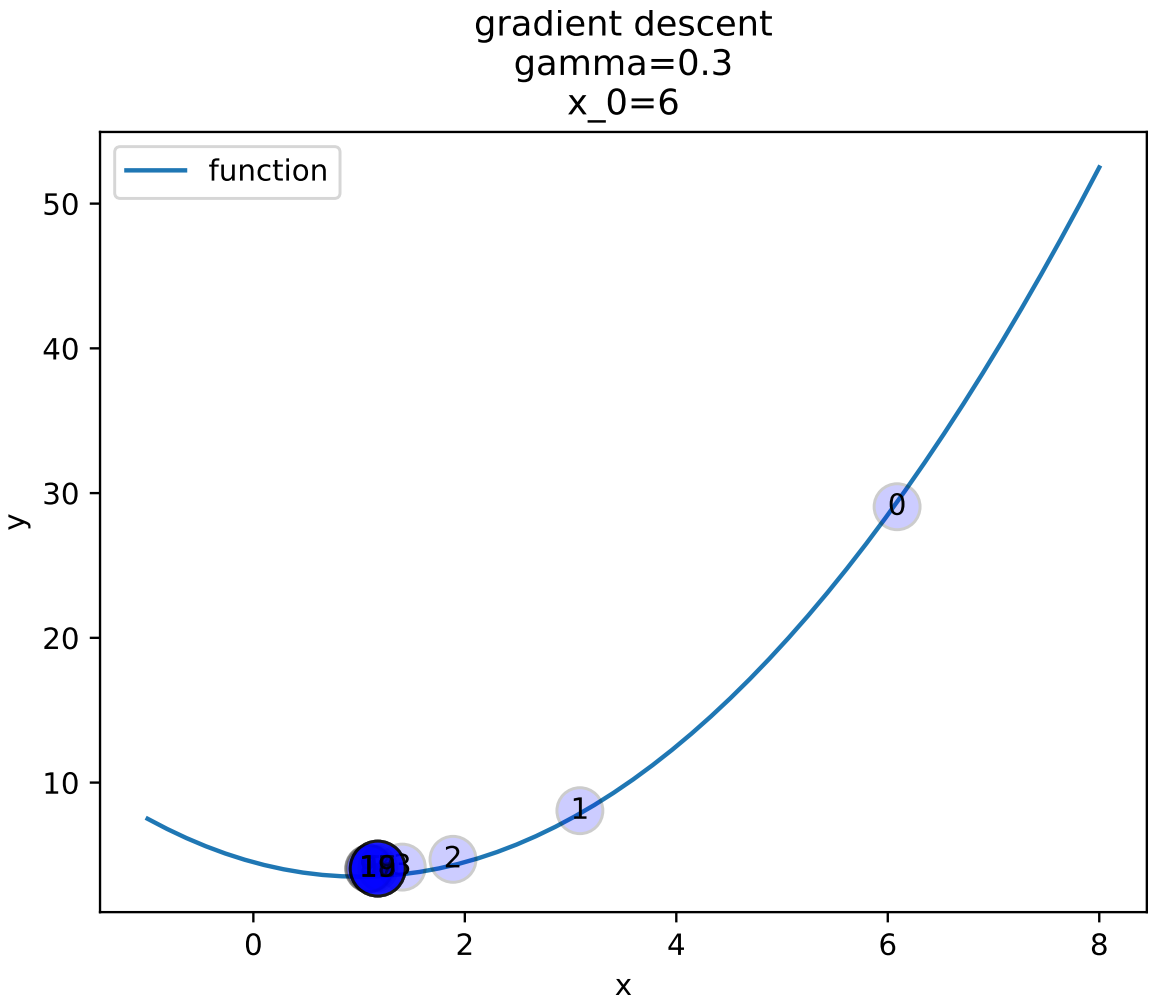
Examples in 1 dimension



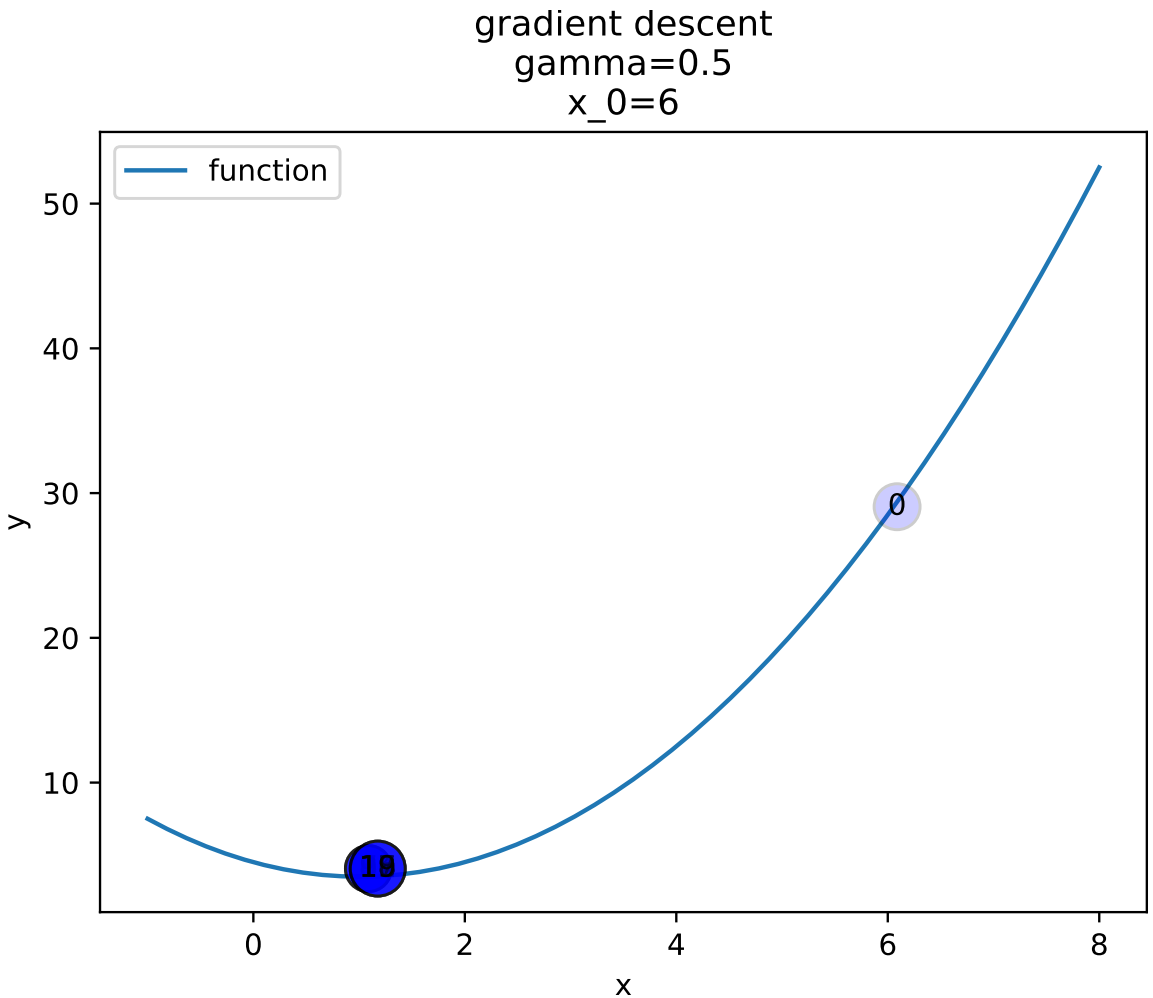
Examples in 1 dimension



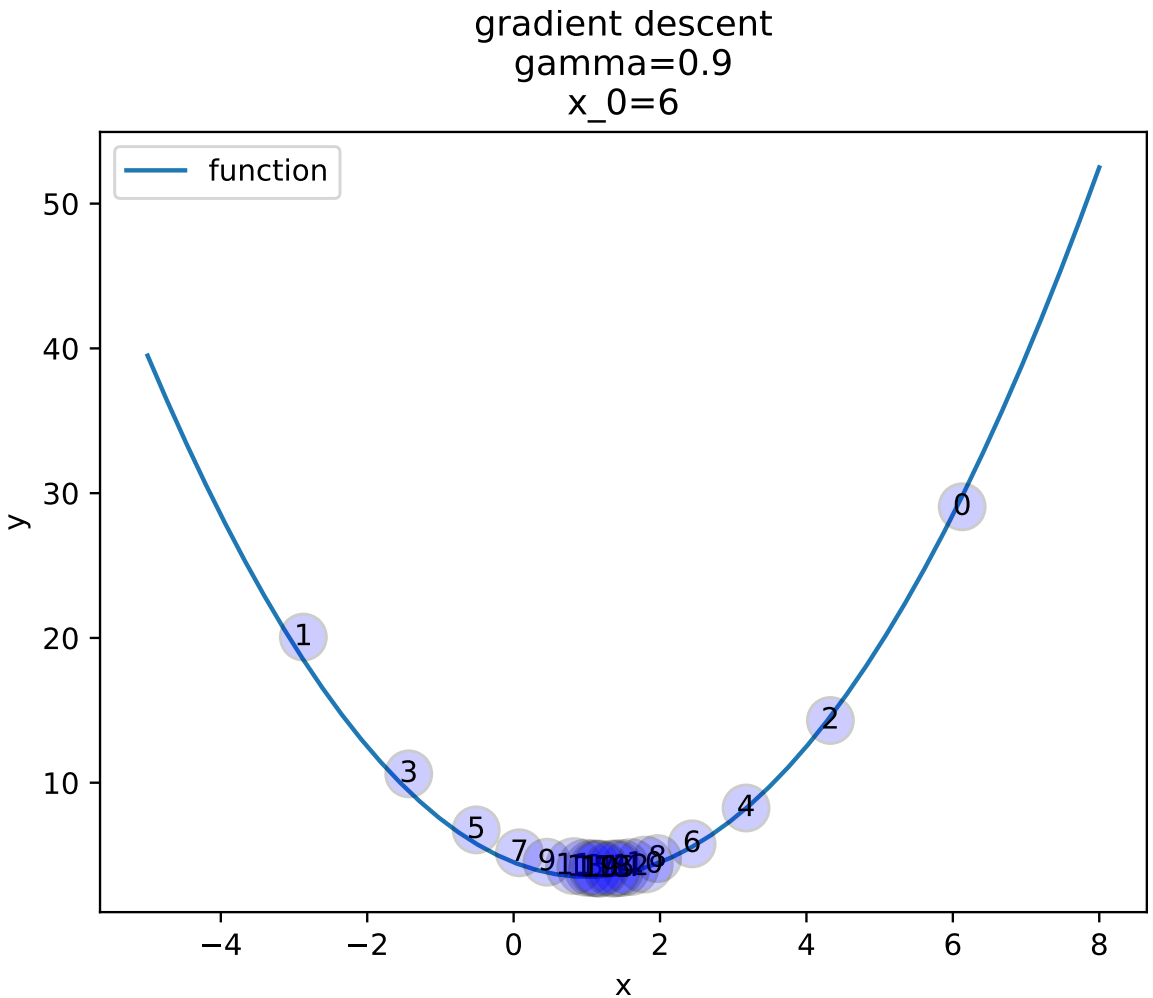
Examples in 1 dimension



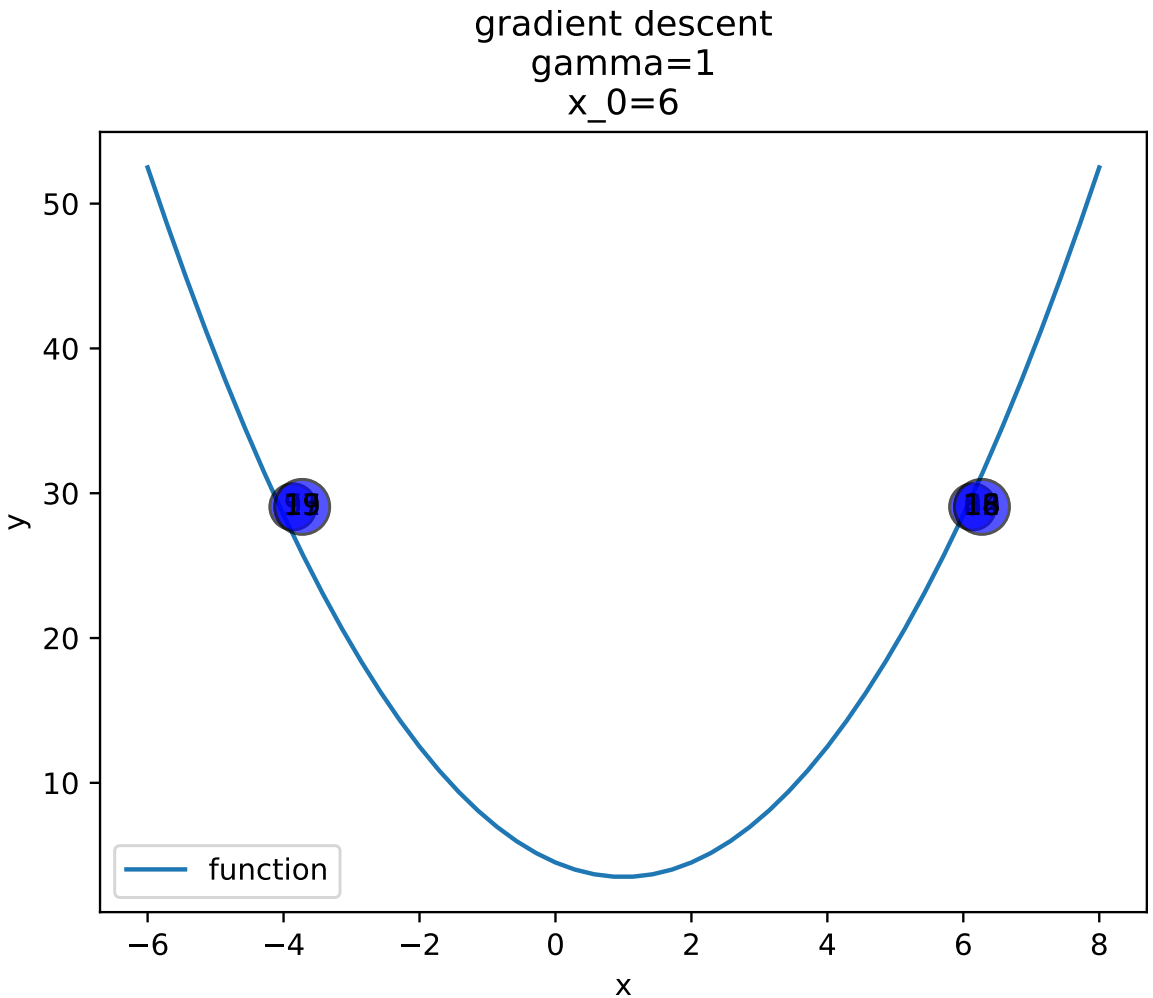
Examples in 1 dimension



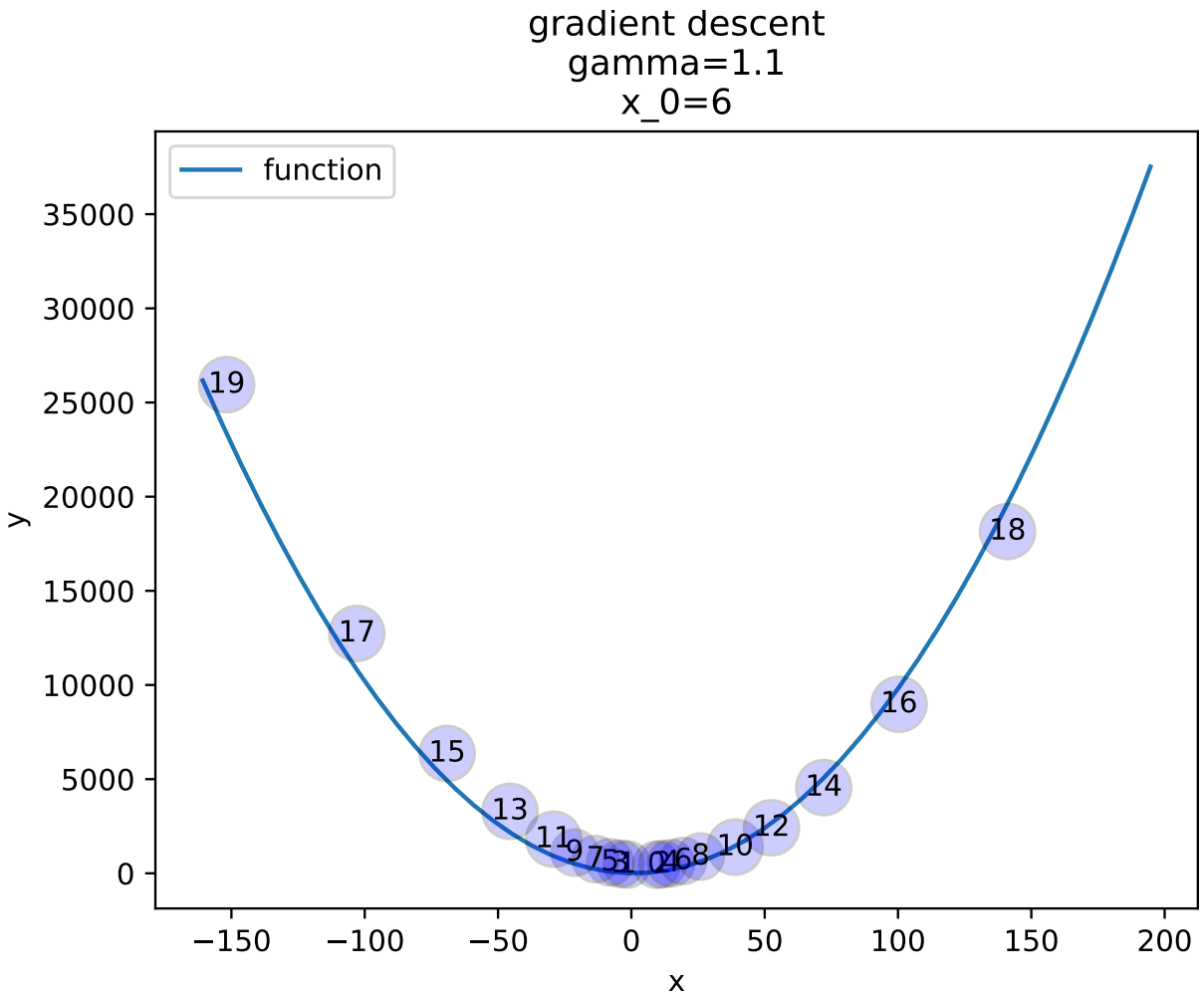
Examples in 1 dimension



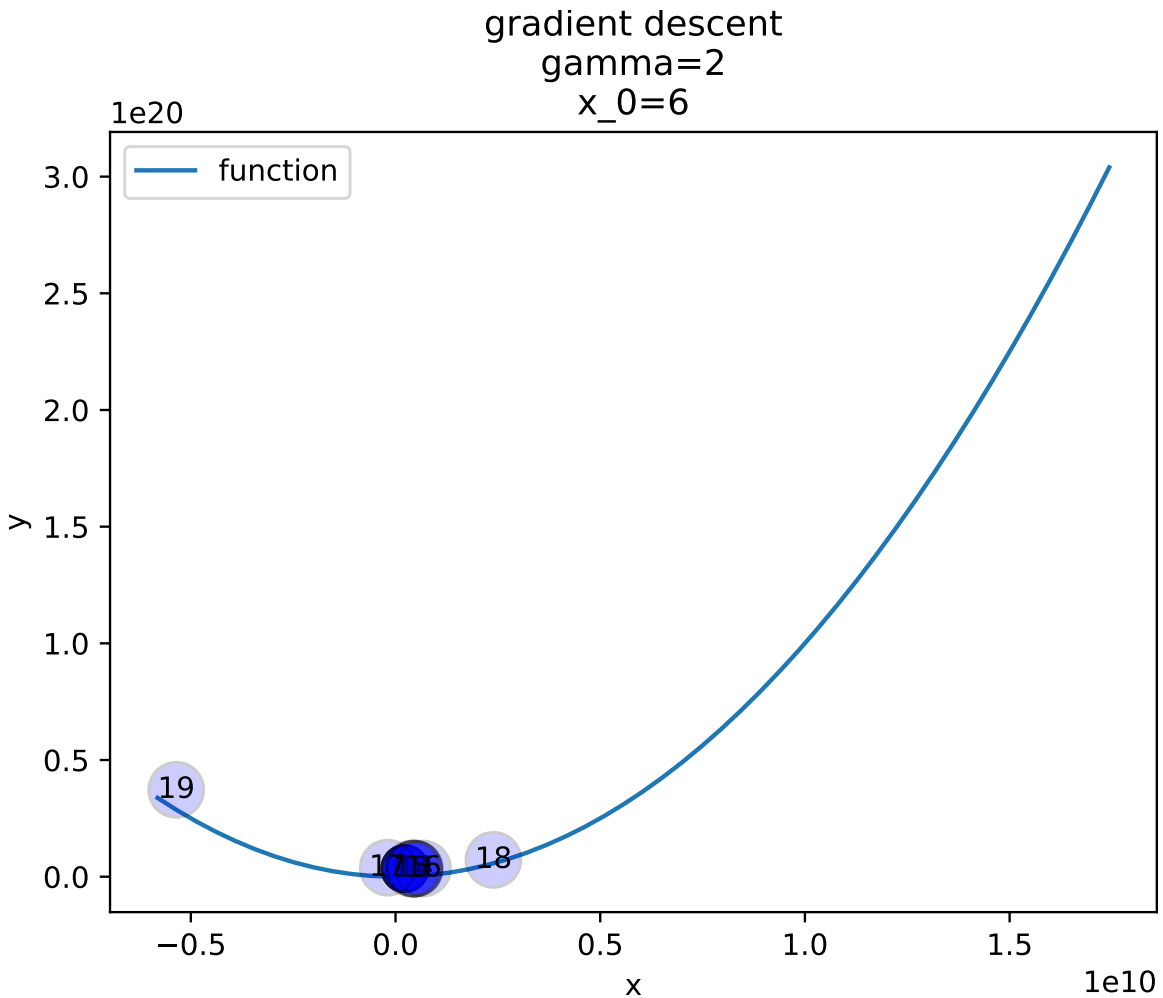
Examples in 1 dimension



Examples in 1 dimension



Examples in 1 dimension



Gradients

The **gradient** is the generalization of the derivative to functions with more than 1 input variable.
Example : consider a function f that has 2 parameters as inputs. If f is differentiable, the gradient writes :

$$\nabla f(x, y) = (\frac{\delta f}{\delta x}(x, y), \frac{\delta f}{\delta y}(x, y)) \tag{6}$$

$\frac{\delta f}{\delta x}(x, y)$ is the **partial derivative** with respect to x, commputed in (x, y).

Example gradient

If

$$f(x, y) = x^2 + 3xy + 1 \tag{7}$$

Then

$$\forall (x, y) \in \mathbb{R}^2, \nabla f(x, y) = (2x + 3y, 3x) \tag{8}$$

Multiple-variable functions

If $f : \mathbb{R}^d \mapsto \mathbb{R}$ is differentiable (dérivable) :
(Landau notation)

$$f(\theta + h) = f(\theta) + \langle \nabla f(\theta) | h \rangle + o(h) \tag{9}$$

Physicist notation :

$$f(\theta + h) \simeq f(\theta) + \langle \nabla f(\theta) | h \rangle \tag{10}$$

Gradient descent

$$\theta \leftarrow \theta - \gamma \nabla f(\theta) \tag{11}$$

γ must be carefully chosen.

- too large γ : the minimization might not work
- too small γ : the minimization will be too slow

Gradient descent algorithm summary :

- In one dimension (the function depends on $x \in \mathbb{R}$) :

$$x \leftarrow x - \gamma f'(x) \tag{12}$$

- In $d > 1$ dimensions (the function depends on $\theta \in \mathbb{R}^d$) :

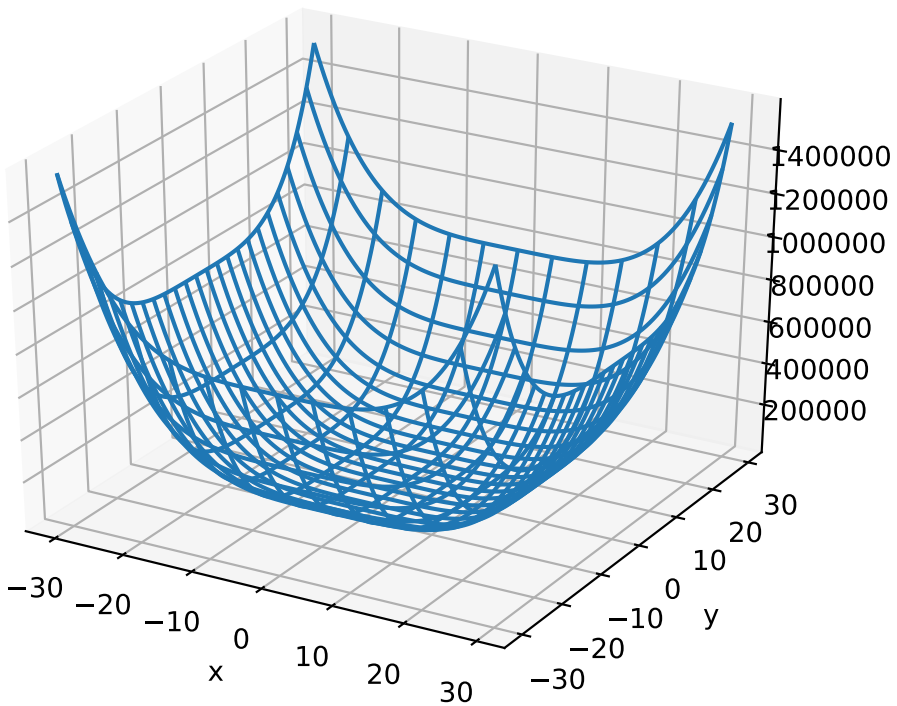
$$\theta \leftarrow \theta - \gamma \nabla f(\theta) \tag{13}$$

- $\leftarrow$ means "is substituted by".
- $\gamma > 0$ is a the **learning rate**.

Gradient

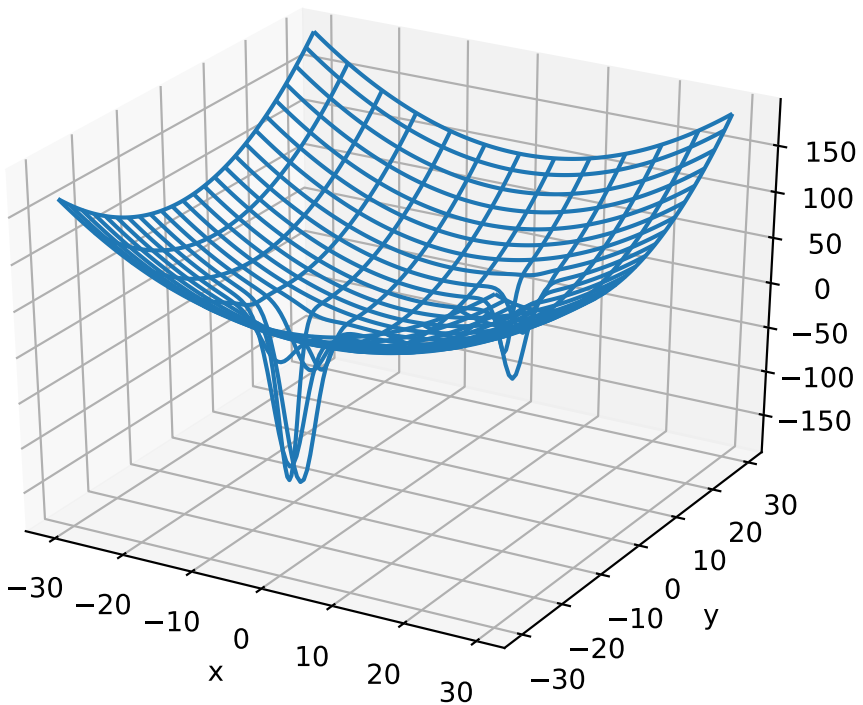
Exercice 1 : **Implementing the gradient algorithm in $\mathbb{R}^2$**

We will use the algorithm on two functions defined over $\mathbb{R}^2$.



Gradient

Exercice 1 : **Implementing the gradient algorithm in $\mathbb{R}^2$** We will use the algorithm on two functions defined over $\mathbb{R}^2$.

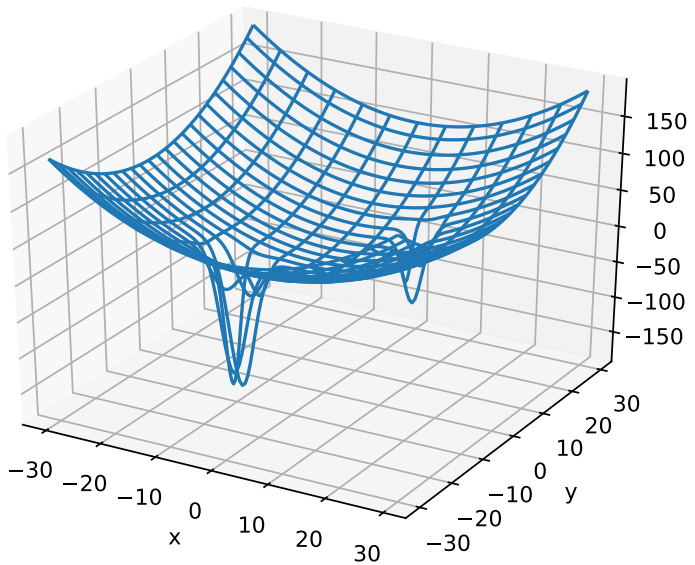


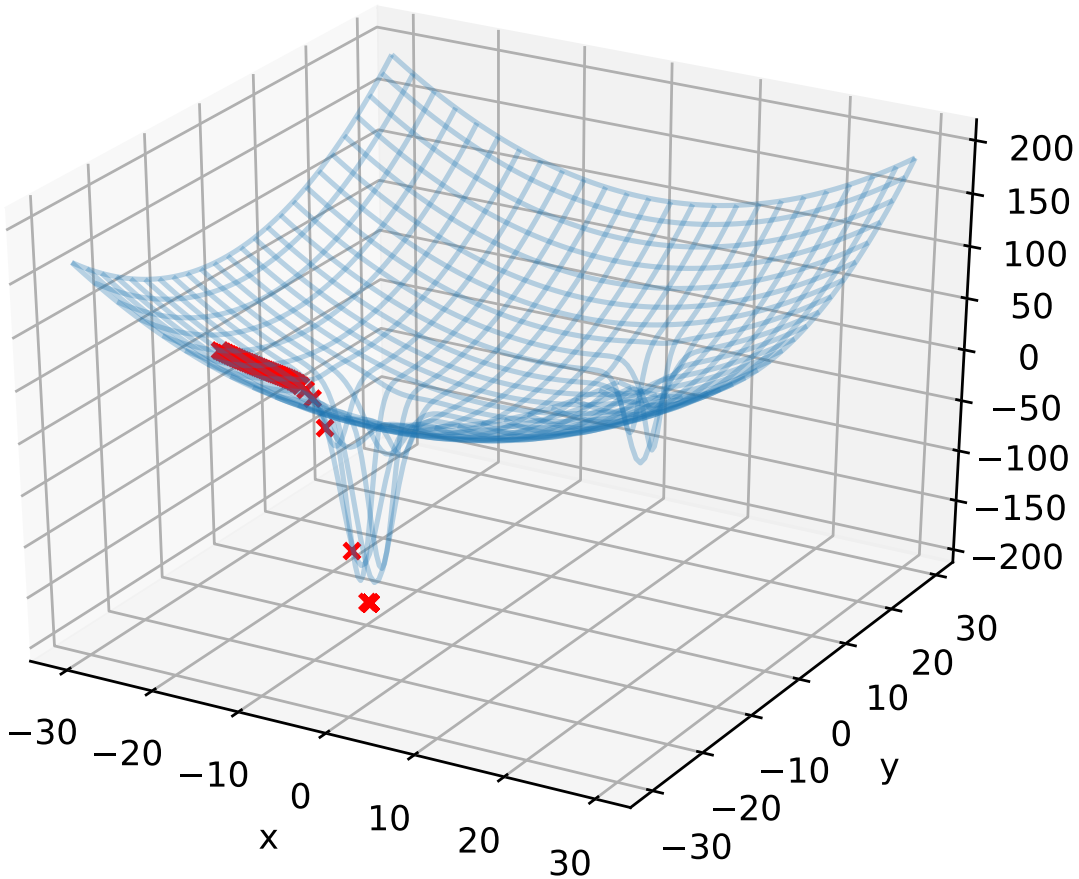
Gradient

Exercice 1 : **Implementing the gradient algorithm**

cd ./gradient and use the files **gradient_algo_1.py** and **gradient_algo_2.py** in order to implement the algorithm to find **minima**.

Experiment with all the parameters that you consider relevant (several are) to assess their impact on the algorithm.




200
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0
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−100
−150
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x
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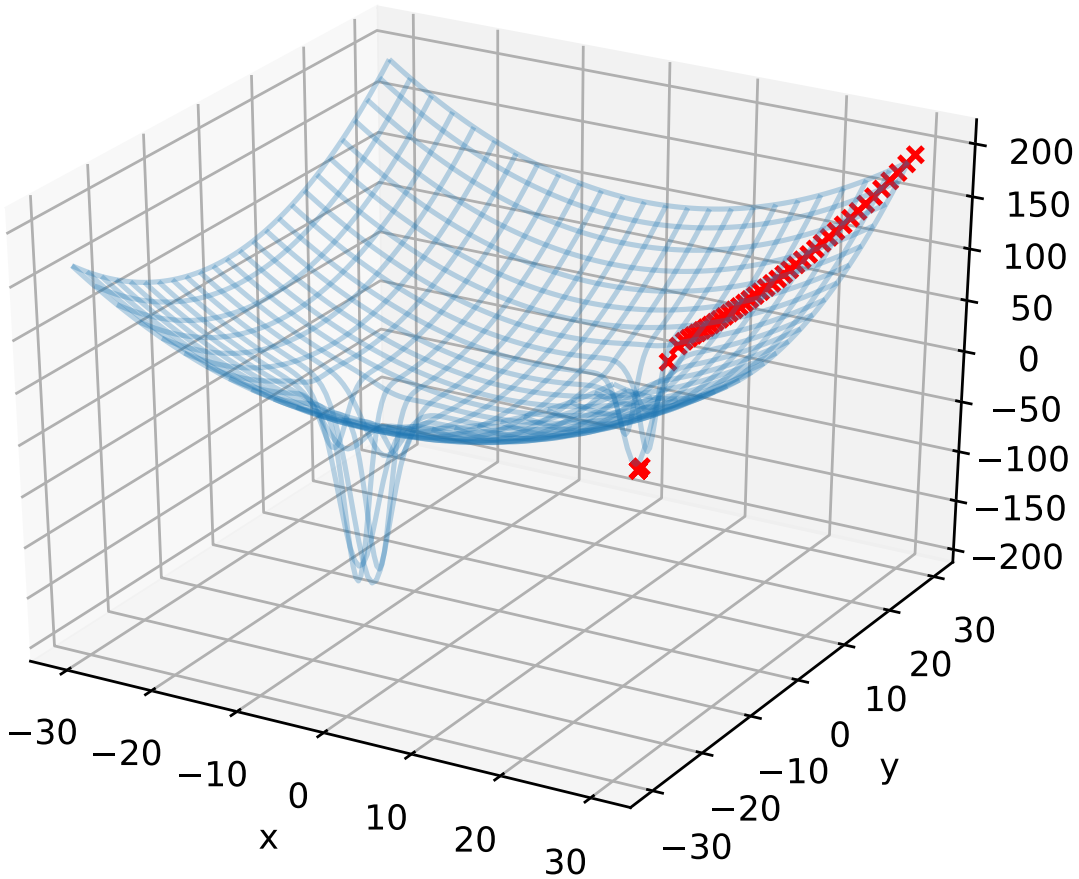
y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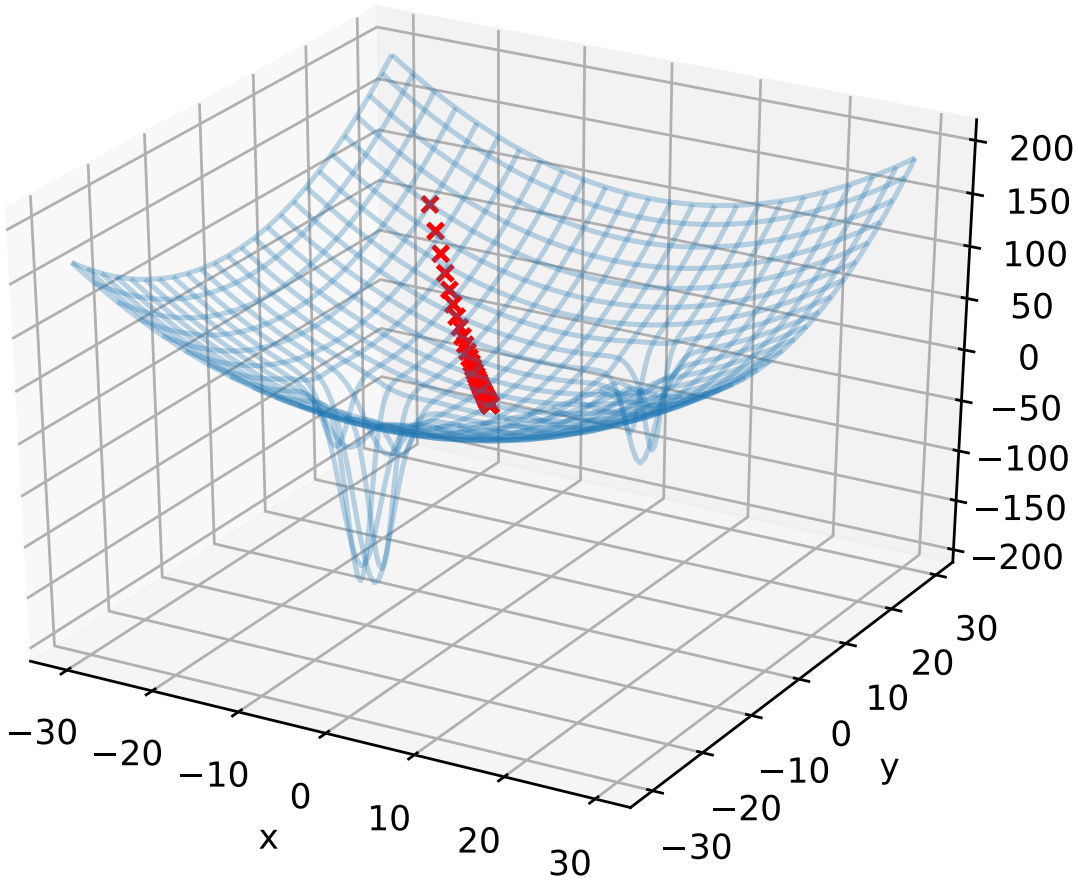
−10
−20
−30
y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−100
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−200
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−20
−10
0
10
20
30
x
30
20
10
0
−10
−20
−30
y

Convergence speed

For some problems, it is possible to have garantees on the convergence speed of gradient descent. The results will depend on the following properties of the objective function :

- convexity or strong convexity
- smoothness (Lipshitz-continuous gradients) or non-smoothness
- condition number

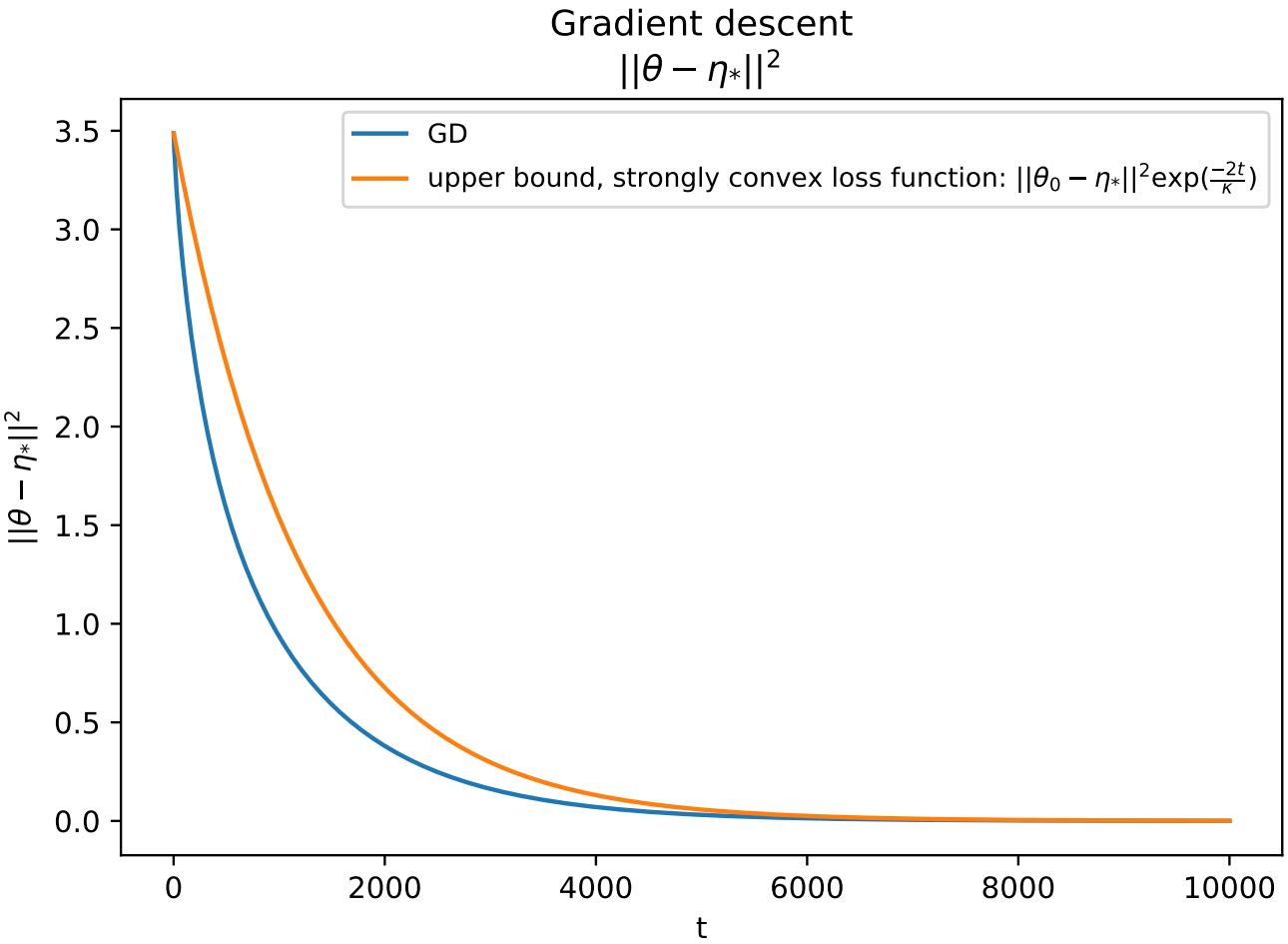
Smoothness (Example of theoretical criterion)

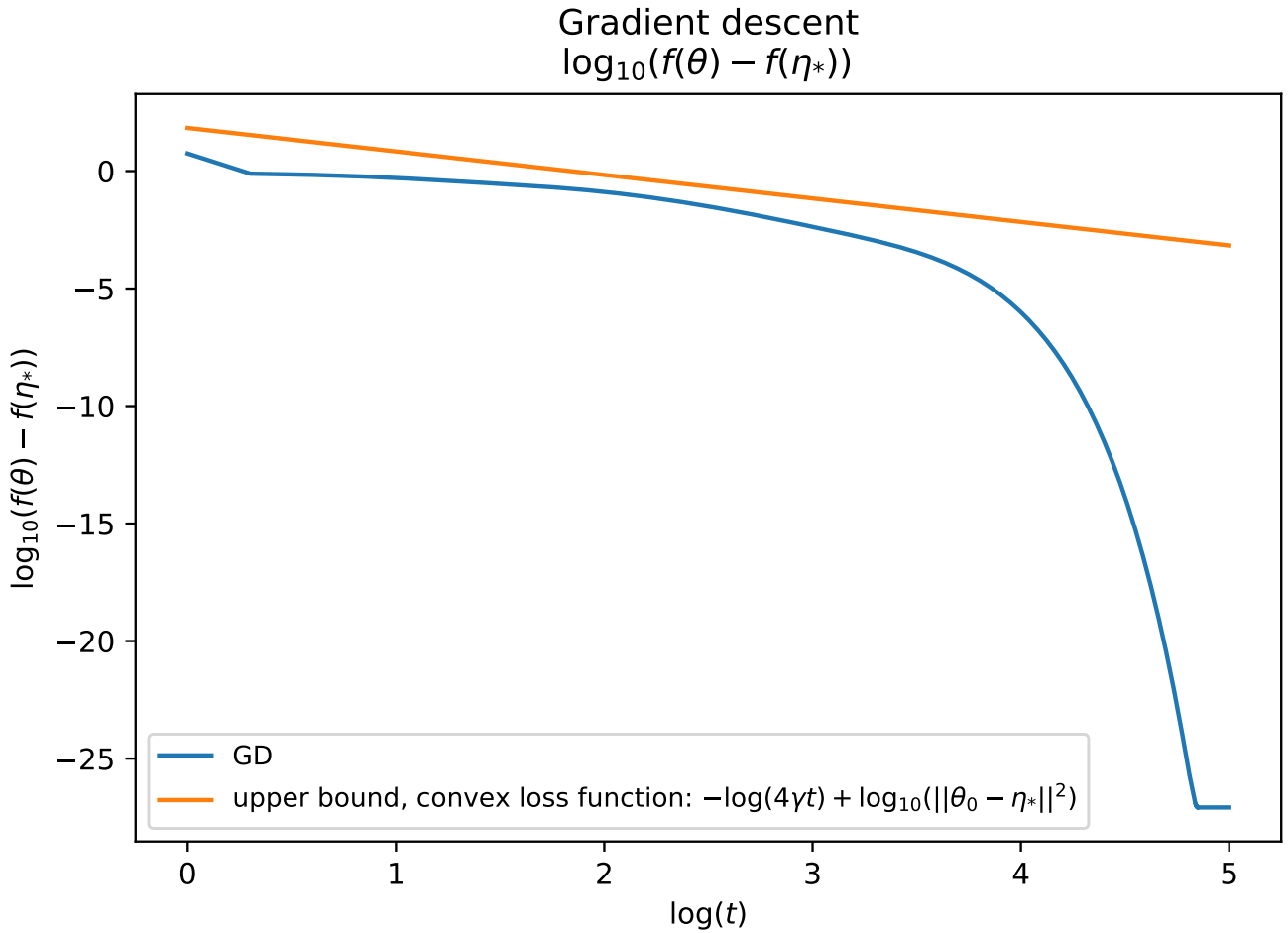
Définition

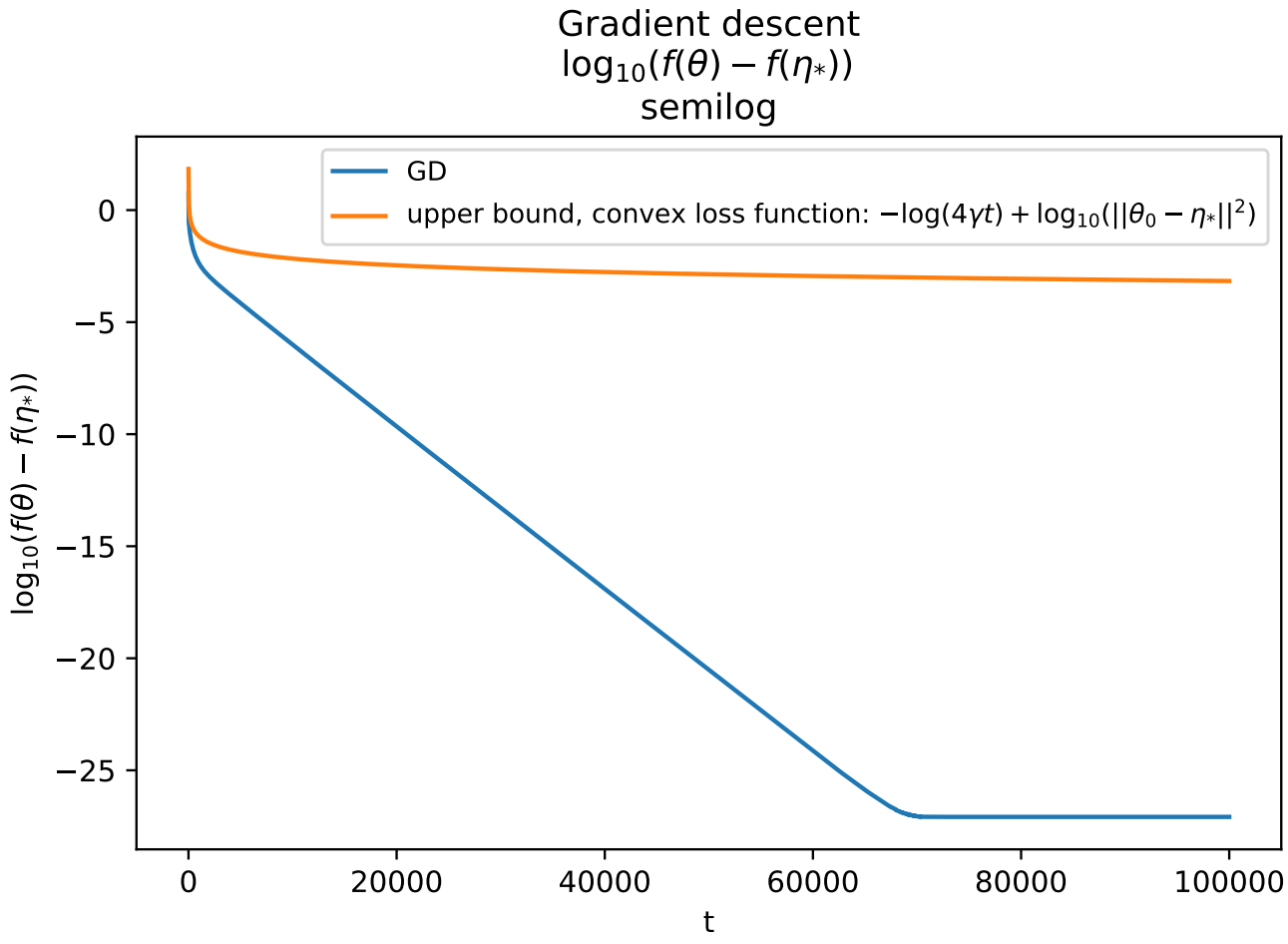
Smoothness

A differentiable function f with real values is said L-smooth if and only if

$$\forall x, y \in \mathbb{R}^d, |f(y) - f(x) - \nabla_x f(y - x)| \leq \frac{L}{2}||y - x||^2$$


Gradient descent
$||\theta - \eta_*||^2$
GD
upper bound, strongly convex loss function: $||\theta_0 - \eta_*||^2 \exp(\frac{-2t}{\kappa})$
$||\theta - \eta_*||^2$
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
2000
4000
6000
8000
10000
t

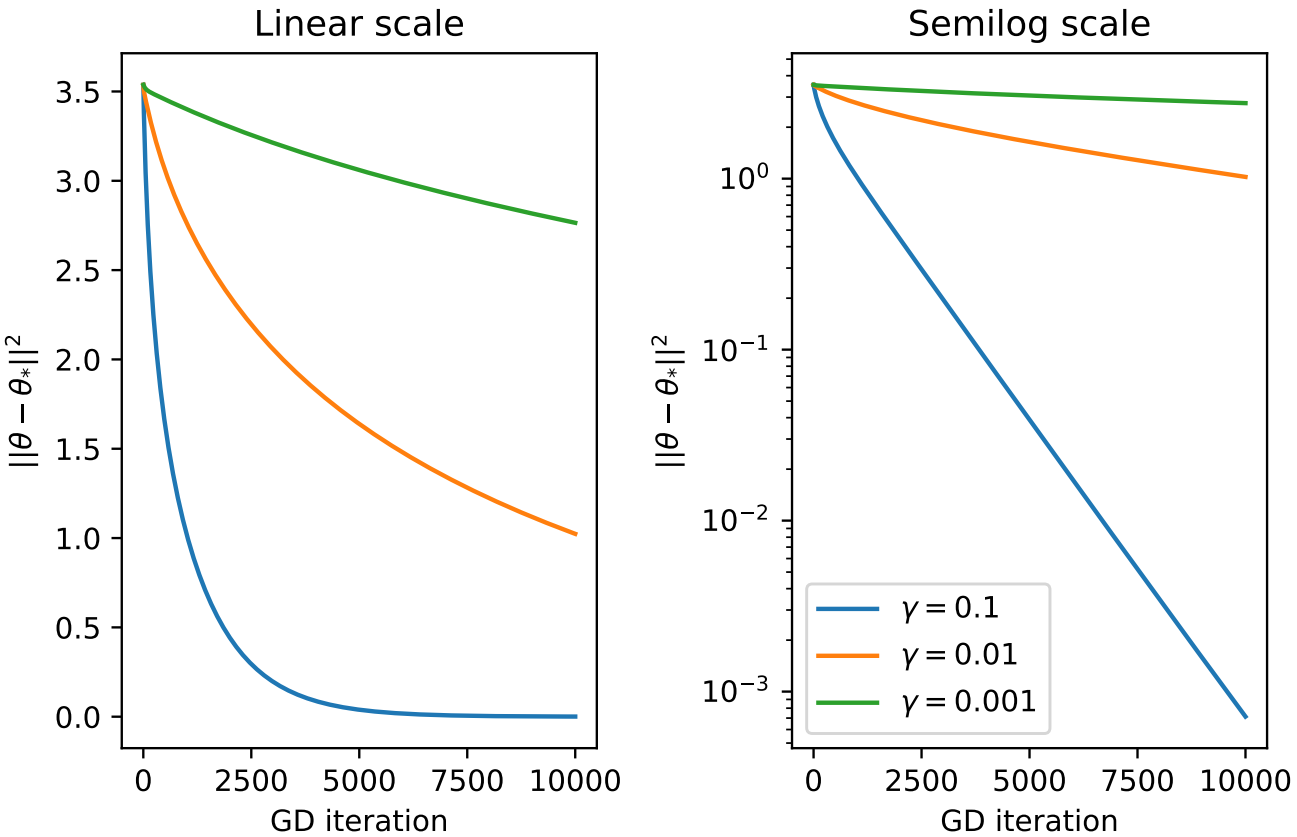

Gradient descent
$\log_{10}(f(\theta) - f(\eta_*))$
0
−5
−10
−15
−20
−25
$\log_{10}(f(\theta) - f(\eta_*))$
0
1
2
3
4
5
$\log(t)$
GD
upper bound, convex loss function: $-\log(4\gamma t) + \log_{10}(||\theta_0 - \eta_*||^2)$


Gradient descent
$\log_{10}(f(\theta) - f(\eta_*))$
semilog
GD
upper bound, convex loss function: $-\log(4\gamma t) + \log_{10}(||\theta_0 - \eta_*||^2)$
0
−5
−10
−15
−20
−25
$\log_{10}(f(\theta) - f(\eta_*))$
0
20000
40000
60000
80000
100000
t

Extensions

- Line search
- Nesterov accleration (optimal rates among algorithms that linearly combine gradients)

Gradient descent: squared distance to the OLS estimator
$||\theta - \theta^*||^2$



Stochastic gradient descent

In machine learning, we often consider an objective function of the form

$$f(\theta) = \frac{1}{n} \sum_{i=1}^{n} l(y_i, f_\theta(x_i)) + \Omega(\theta) \tag{14}$$

Example with Ridge regression :

$$f(\theta) = \frac{1}{n} \sum_{i=1}^{n} ((\theta|x_i) - y_i)^2 + \lambda ||\theta||^2 \tag{15}$$

- $f_\theta(x_i) = (\theta|x_i)$ (dot product)
- $l(z, z') = (z - z')^2$

Batch gradient

In machine learning, we often consider an objective function of the form

$$f(\theta) = \frac{1}{n} \sum_{i=1}^{n} l(y_i, f_\theta(x_i)) + \Omega(\theta) \tag{16}$$

Computing the gradient of f requires at least n calculations, and each calculation also has a complexity that depends on the dimension d. When n and d are large, this can be quite slow.

Stochastic gradient descent

We consider an objective function of the form

$$f(\theta) = \frac{1}{n} \sum_{i=1}^{n} l(y_i, f_\theta(x_i)) + \Omega(\theta) \tag{17}$$

Instead of computing the **batch gradient** $\nabla f(\theta)$, we will compute :

$$u(i, \theta) = \nabla_\theta [l(y_i, f_\theta(x_i)) + \Omega(\theta)] \tag{18}$$

for a randomly sampled $i \in [1, n]$. $u(i, \theta)$ is an **estimation** of the full (batch) gradient $\nabla_\theta f$.
Example with Ridge regression :

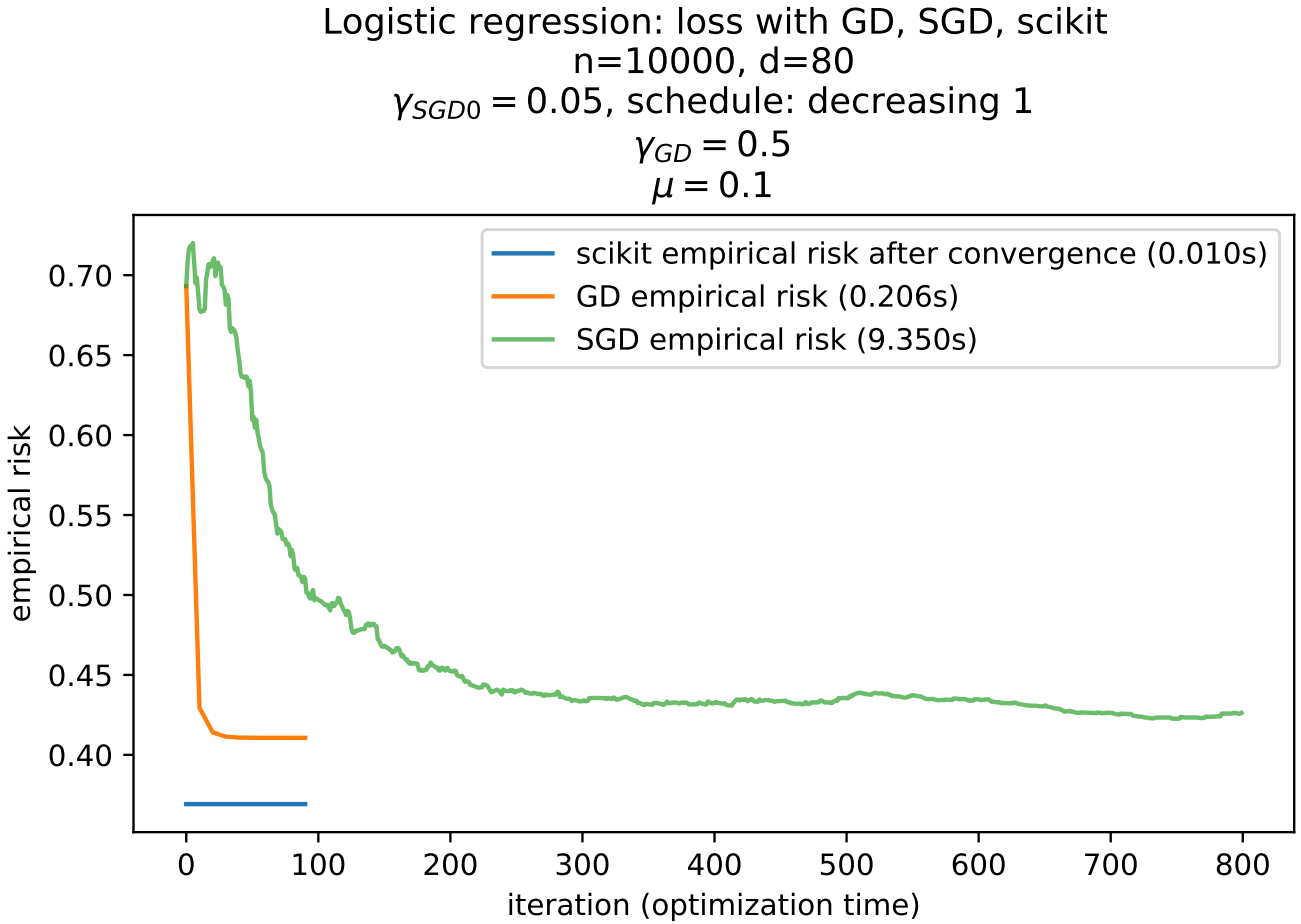
$$\begin{aligned} u(i, \theta) &= \nabla_\theta [((\theta | x_i) - y_i)^2 + \lambda ||\theta||^2] \\ &= 2((\theta | x_i) - y_i) x_i + 2\lambda\theta \end{aligned} \tag{19}$$

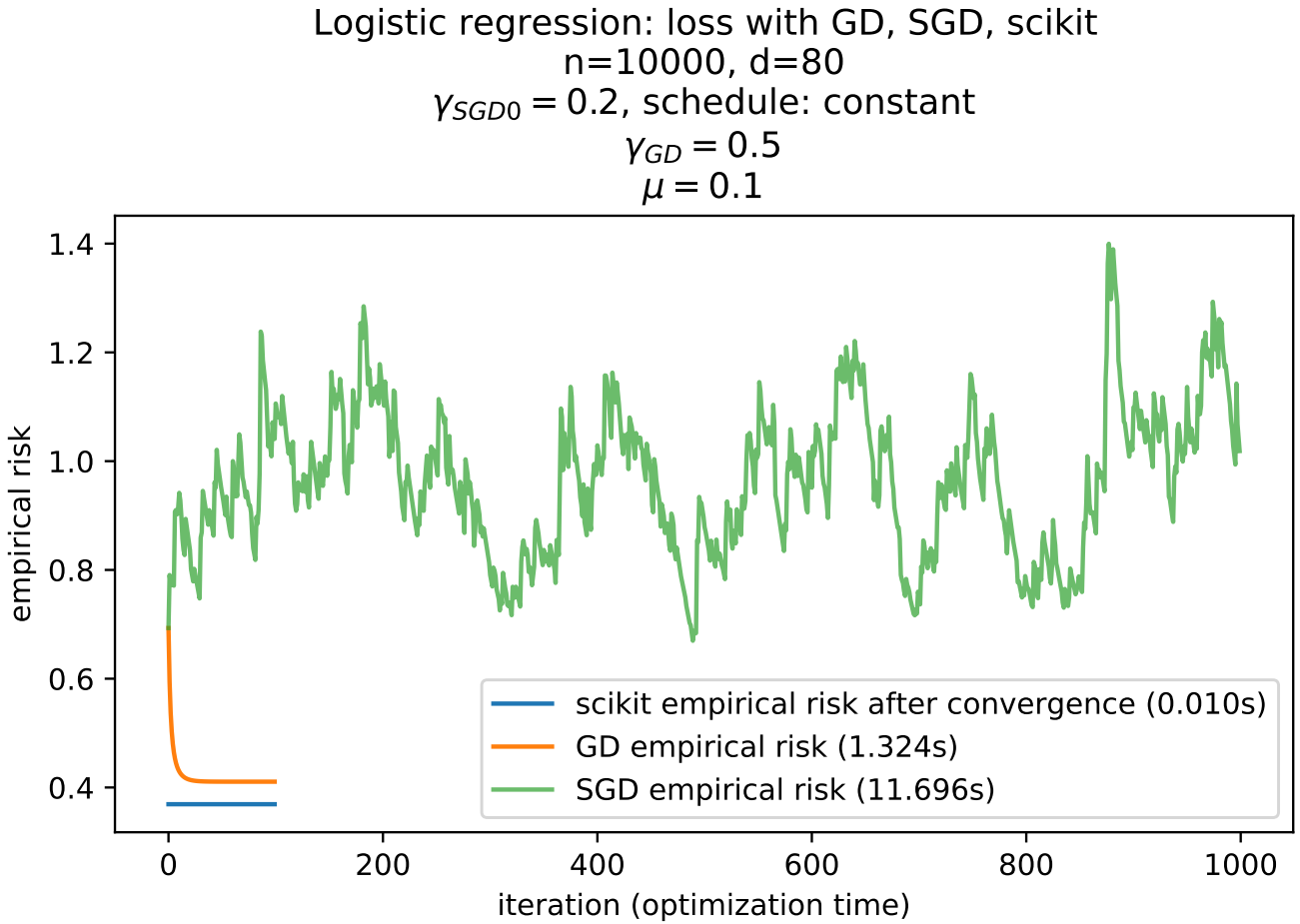
Tradeoff

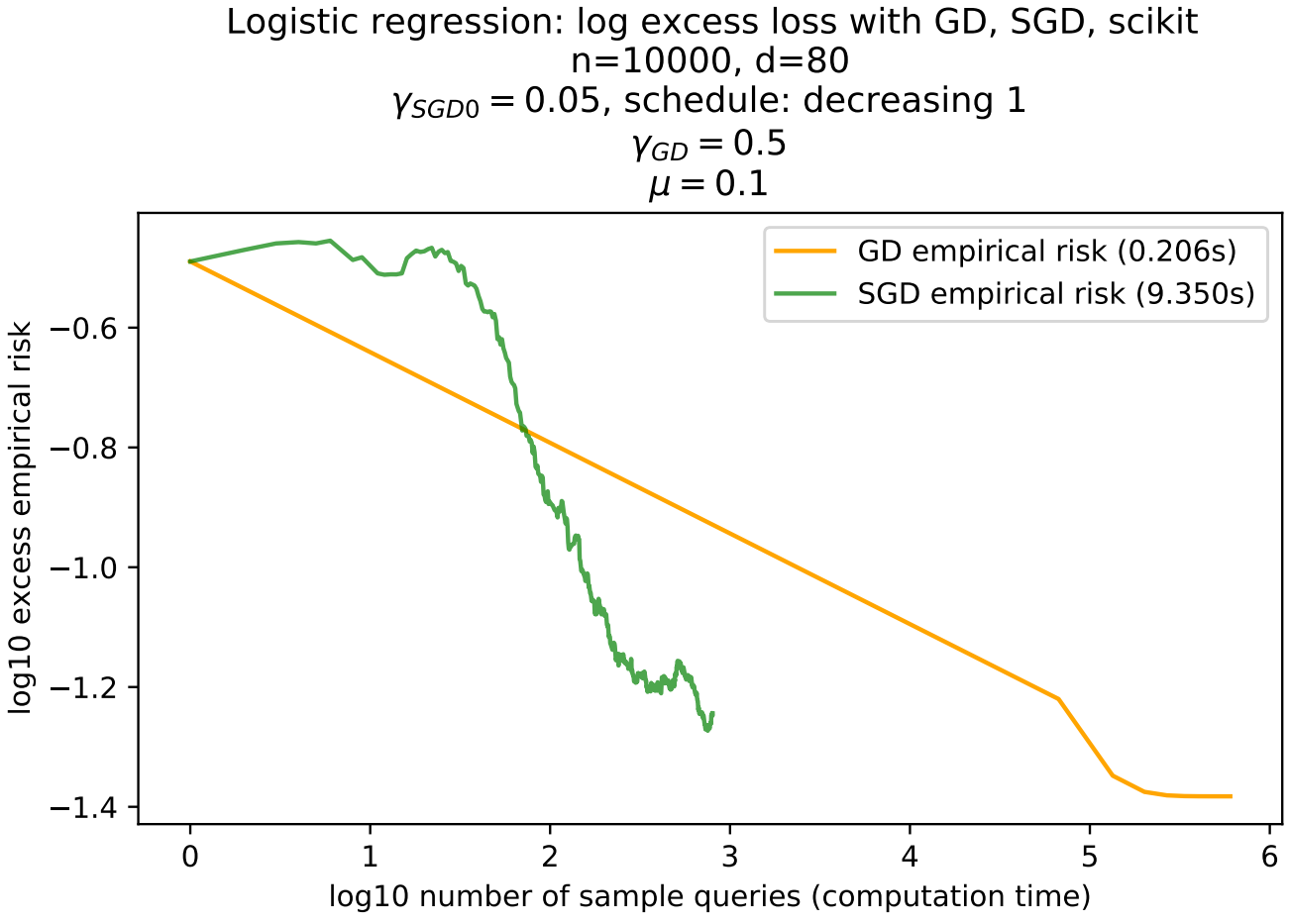
By replacing the computation of the full gradient (GD) by this estimation (SGD) :

- we reduce the computation time (divide it by n)
- but reduce precision of the optimization

To summarize : if n is really large, SGD is often better.


Logistic regression: loss with GD, SGD, scikit
n=10000, d=80
$\gamma_{SGD0} = 0.05$, schedule: decreasing 1
$\gamma_{GD} = 0.5$
$\mu = 0.1$
scikit empirical risk after convergence (0.010s)
GD empirical risk (0.206s)
SGD empirical risk (9.350s)
empirical risk
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0
100
200
300
400
500
600
700
800
iteration (optimization time)


Logistic regression: loss with GD, SGD, scikit
n=10000, d=80
$\gamma_{SGD0} = 0.2$, schedule: constant
$\gamma_{GD} = 0.5$
$\mu = 0.1$
empirical risk
1.4
1.2
1.0
0.8
0.6
0.4
0
200
400
600
800
1000
iteration (optimization time)
scikit empirical risk after convergence (0.010s)
GD empirical risk (1.324s)
SGD empirical risk (11.696s)


Logistic regression: log excess loss with GD, SGD, scikit
n=10000, d=80
$\gamma_{SGD0} = 0.05$, schedule: decreasing 1
$\gamma_{GD} = 0.5$
$\mu = 0.1$
GD empirical risk (0.206s)
SGD empirical risk (9.350s)
log10 excess empirical risk
−0.6
−0.8
−1.0
−1.2
−1.4
0
1
2
3
4
5
6
log10 number of sample queries (computation time)

Comparison (advanced)

The ridge regression problem is smooth and strongly convex.

- GD has a convergence rate of $\mathcal{O}(\exp(-\frac{t}{\kappa}))$. To get an error of ϵ, we must have $t = \mathcal{O}(\kappa \log \frac{1}{\epsilon})$. Since each iteration requires $\mathcal{O}(nd)$ computations, the computation time will be $\mathcal{O}(\kappa nd \log \frac{1}{\epsilon})$.
- SGD has a convergence rate of $\mathcal{O}(\frac{\kappa}{t})$. To get an error of ϵ, we must have $t = \mathcal{O}(\frac{\kappa}{\epsilon})$. Since each iteration is $\mathcal{O}(d)$, we have a computation time of $\mathcal{O}(\frac{\kappa d}{\epsilon})$.

Comparison (advanced)

As a consequence :

- When n is large and ϵ not too small, GD will need more computation time to reach error ϵ. An order of magnitude can be obtained by studying the value ϵ^* such that

$$\kappa n d \log \frac{1}{\epsilon^*} = \frac{\kappa d}{\epsilon^*}$$

Which translates to

$$\epsilon^* \log \epsilon^* = -\frac{1}{n}$$

- When $\epsilon \to 0$, GD becomes faster than SGD to reach this precision.

Conclusion

For lower precision and large n, SGD is a preferable.
In machine learning, due to the estimation error that is $\mathcal{O}(\frac{1}{\sqrt{n}})$, a very high precision is often not needed

Extensions of SGD

See also :

- Variance reduction methods (SAG, SAGA)