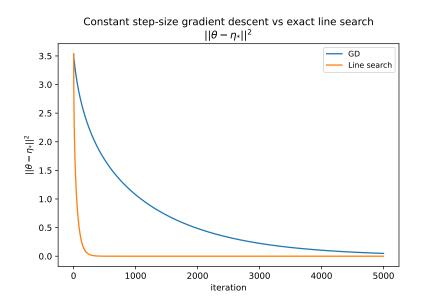
## FTML practical session 5



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# 1 GRADIENT DESCENT AND LINE SEARCH FOR A LEAST SQUARES PROBLEM

We come back to a least squares problem. We recall the setting here:

- $\chi = \mathbb{R}^d$
- $-y = \mathbb{R}$
- $\theta = \mathbb{R}^d$  defines the estimator, which is the function  $x \to x^T \theta$ .
- design matrix :  $X \in \mathbb{R}^{n,d}$
- vector of outputs (labels) :  $y \in \mathbb{R}^n$ .

We want to minimize the function f representing the empirical risk:

$$f(\theta) = \frac{1}{2n} ||X\theta - y||^2 \tag{1}$$

#### 1.1 Gradient descent

We recall that the gradient and the Hessian write:

$$\begin{split} \nabla_{\theta} f(\theta) &= \frac{1}{n} X^{T} (X\theta - y) \\ &= H\theta - \frac{1}{n} X^{T} y \end{split} \tag{2}$$

$$H = \frac{1}{n} X^{\mathsf{T}} X \tag{3}$$

An iteration of the gradient algorithm writes:

$$\theta_{t+1} = \theta_t - \gamma \nabla_{\theta} f(\theta_t) \tag{4}$$

#### 1.2 Global minimizers

We consider the global minimizers of f, noted  $\eta^*$ . They all necessary verify

$$\nabla_{\theta} f(\eta^*) = 0 \tag{5}$$

Which means that

$$H\eta * = \frac{1}{n} X^{\mathsf{T}} y \tag{6}$$

As  $\theta \to f(\theta)$  is convex, we know that this condition is also sufficient : any vector that cancels the gradient is a global minimum.

If H is not invertible, there might be several minimizes. However, if f is strongly convex, then H is invertible and  $\eta^*$  is unique. We will consider such a case here. In general, H is a positive semi-definite matrix, and here we hence consider the case where it is definite positive.

#### 1.3 Line search: A nested optimization problem

Considering a fixed iteration step  $\theta_t$ , we note

$$\alpha(\gamma) = \theta_{t} - \gamma \nabla_{\theta} f(\theta_{t}) \tag{7}$$

The **exact line seach** method attempts to find the optimal step  $\gamma^*$ , at each iteration. This means, given the position  $\theta_t$ , the parameter  $\gamma$  that minimizes the function defined by

$$g(\gamma) = f(\theta_{t} - \gamma \nabla_{\theta} f(\theta_{t}))$$

$$= f(\alpha(\gamma))$$
(8)

Is  $g : \mathbb{R} \to \mathbb{R}$  a convex function?

Find the value  $\gamma^*$  that minimizes  $\gamma \to g(\gamma)$  for a given  $\theta_t$ , and implement both a constant step GD and a GD where  $\gamma$  is set optimally thanks to this method (exact line search). Compare the convergence speeds by measuring the distance between the iterate and the OLS estimator  $\eta^*$  at each iteration.

You should observe a result like figures 1 and 2. Some template files can be found in exercice\_1\_line\_search/

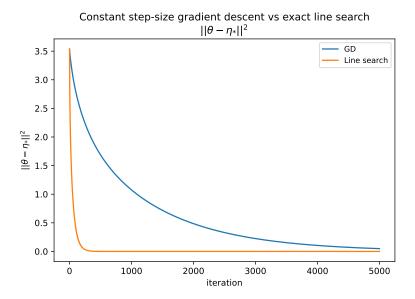


FIGURE 1 – Convergence to the global minimizer.

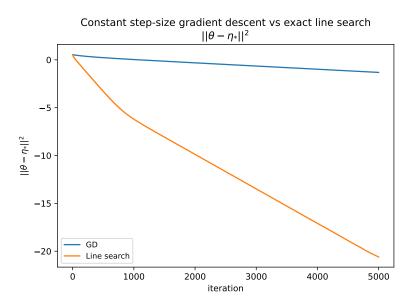


FIGURE 2 – Convergence to the global minimizer in log scale.