Statistical learning

1. Linear regression and stochastic gradient descent

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Notations

- \triangleright n sample size
- ▶ k number of features
- $ightharpoonup X \in \mathbf{R}^{n \times d}$ input data $(x_i)_{i=1,...,n}$
- $\hat{\beta} \in \mathbf{R}^d$ estimator of the weight parameters to build
- ▶ $y \in \mathbf{R}^n$ output data
- ▶ $\hat{y} \in \mathbb{R}^n$ predicted output

Least squares approximation

▶ The fit of a model to a data point is measured by its **residuals**

$$y_i - \hat{y_i}, i = 1, \ldots, n$$

► The least squared loss (or cost) function focuses in the **mean** squared error of this measure, that is

$$L(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \langle x_i, w \rangle)$$
 where $\ell(y, y') = \frac{1}{2} |y - y'|^2$

. We immediately note that

$$\nabla L(w) = \frac{1}{n} \sum_{i=1}^{n} \ell'(y_i, \langle x_i, w \rangle) x_i$$
 with $\ell'(y, y') = \partial_{y'} \ell(y, y')$

Least squares estimator

That leads us to the optimization problem :

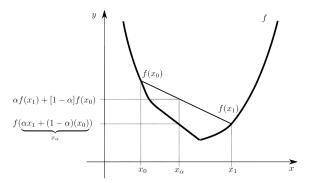
$$\hat{\beta} = \underset{w}{\operatorname{argmin}} L(w) \Leftrightarrow \nabla L(\hat{\beta}) = \vec{0} \tag{1}$$

- What are the conditions for uniqueness?
- ► Why is (1) true?
- We are looking for the estimators $\hat{y}_i = \langle x_i, \hat{\beta} \rangle$.

Convex functions

A function $f: \mathbf{R}^d \to \mathbf{R}$ is **convex** if for all $x, y \in \mathbf{R}^d$ and all $\alpha \in [0,1]$

$$f(\alpha x + (1 - \alpha)y) \le \alpha f(x) + (1 - \alpha)f(y)$$



Gradient Descent

Convergence of GD

One can show that this algorithm:

$$w_{t+1} = w_t - \gamma_t \cdot \nabla f(w_t) \tag{2}$$

converges to some $w_* \in \{\nabla f = 0\}$ for some **smooth functions** f with certain properties and some step size $\gamma_t := \gamma_t(f)$.

In our case, **convexity** is enough, but know that there is a more general class of functions that makes it still true.

Stochastic gradient descent (SGD)

If n is large, computing ∇L is expensive : it requires to explore the whole data set for just a step of the descent algorithm !

The idea of stochastic gradient is to build an **unbiased** estimator of ∇L : Choosing uniformly at random $N \in \{1, ..., n\}$, then

$$\partial_w \mathsf{E}[\ell(y_N,\langle x_N,w\rangle)] = \frac{1}{n} \sum_{i=1}^n \ell'(y_i,\langle x_i,w\rangle) x_i = \nabla L(w)$$

▶ Question : Can we use this estimator in (2) ?

Convergence of SGD

Theorem: Robbins-Monroe

Let ℓ be defined as previously, and $N_t, t \in \mathbf{N}$ a sequence of i.i.d. random variables uniformly distributed on $\{1, \ldots, n\}$. The algorithm

$$w_{t+1} = w_t - \gamma_t \cdot \partial_w \ell(y_{N_t}, \langle x_{N_t}, w_t \rangle)$$

converges to some $w_* \in \{\nabla L = 0\}$