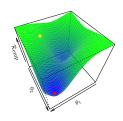
# Introduction to Machine Learning

# **ML-Basics: Optimization**

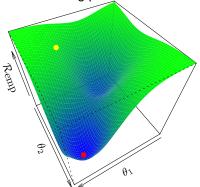


#### Learning goals

- Understand how the risk function is optimized to learn the optimal parameters of a model
- Understand the idea of gradient descent as a basic risk optimizer

#### LEARNING AS PARAMETER OPTIMIZATION

- We have seen, we can operationalize the search for a model f that matches training data best, by looking for its parametrization  $\theta \in \Theta$  with lowest empirical risk  $\mathcal{R}_{emp}(\theta)$ .
- Therefore, we usually traverse the error surface downwards; often by local search from a starting point to its minimum.



### LEARNING AS PARAMETER OPTIMIZATION

The ERM optimization problem is:

$$\hat{oldsymbol{ heta}} = \mathop{\mathsf{arg\,min}}_{oldsymbol{ heta} \in \Theta} \mathcal{R}_{\mathsf{emp}}(oldsymbol{ heta}).$$

For a **(global) minimum**  $\hat{\theta}$  it obviously holds that

$$orall oldsymbol{ heta} \in \Theta: \quad \mathcal{R}_{\mathsf{emp}}(oldsymbol{\hat{ heta}}) \leq \mathcal{R}_{\mathsf{emp}}(oldsymbol{ heta}).$$

This does not imply that  $\hat{\theta}$  is unique.

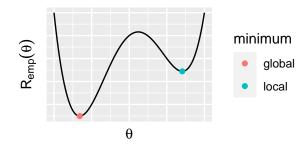
Which kind of numerical technique is reasonable for this problem strongly depends on model and parameter structure (continuous params? uni-modal  $\mathcal{R}_{\text{emp}}(\theta)$ ?). Here, we will only discuss very simple scenarios.

#### LOCAL MINIMA

If  $\mathcal{R}_{emp}$  is continuous in  $\theta$  we can define a **local minimum**  $\hat{\theta}$ :

$$\exists \epsilon > 0 \; orall oldsymbol{ heta} \; ext{ with } \left\| \hat{oldsymbol{ heta}} - oldsymbol{ heta} 
ight\| < \epsilon : \quad \mathcal{R}_{\mathsf{emp}}(oldsymbol{\hat{ heta}}) \leq \mathcal{R}_{\mathsf{emp}}(oldsymbol{ heta}).$$

Clearly every global minimum is also a local minimum. Finding a local minimum is easier than finding a global minimum.

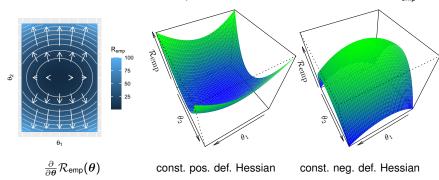


#### LOCAL MINIMA AND STATIONARY POINTS

If  $\mathcal{R}_{emp}$  is continuously differentiable in  $\theta$  then a **sufficient condition** for a local minimum is that  $\hat{\theta}$  is **stationary** with 0 gradient, so no local improvement is possible:

$$rac{\partial}{\partial oldsymbol{ heta}} \mathcal{R}_{emp}(oldsymbol{\hat{ heta}}) = 0$$

and the Hessian  $\frac{\partial^2}{\partial \theta^2} \mathcal{R}_{emp}(\hat{\theta})$  is positive definite. While the neg. gradient points into the direction of fastest local decrease, the Hessian measures local curvature of  $\mathcal{R}_{emp}$ .



#### **LEAST SQUARES ESTIMATOR**

Now, for given features  $\mathbf{X} \in \mathbb{R}^{n \times p}$  and target  $\mathbf{y} \in \mathbb{R}^n$ , we want to find the best linear model regarding the squared error loss, i.e.,

$$\mathcal{R}_{\mathsf{emp}}(oldsymbol{ heta}) = \|\mathbf{X}oldsymbol{ heta} - \mathbf{y}\|_2^2 = \sum_{i=1}^n (oldsymbol{ heta}^ op \mathbf{x}^{(i)} - y^{(i)})^2 \;.$$

With the sufficient condition for continously differentiable functions it can be shown that the **least squares estimator** 

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}.$$

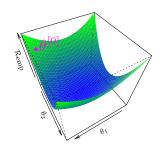
is a local minimum of  $\mathcal{R}_{emp}$ . If **X** is full-rank,  $\mathcal{R}_{emp}$  is strictly convex and there is only one local minimum - which is also global.

**Note:** Often such analytical solutions in ML are not possible, and we rather have to use iterative numerical optimization.

#### **GRADIENT DESCENT**

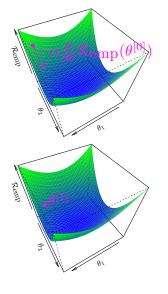
The simple idea of GD is to iteratively go from the current candidate  $\theta^{[t]}$  in the direction of the negative gradient, i.e., the direction of the steepest descent, with learning rate  $\alpha$  to the next  $\theta^{[t+1]}$ :

$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \alpha \frac{\partial}{\partial \boldsymbol{\theta}} \mathcal{R}_{emp}(\boldsymbol{\theta}^{[t]}).$$



We choose a random start  $heta^{[0]}$  with risk  $\mathcal{R}_{\sf emp}( heta^{[0]}) = 76.25$ .

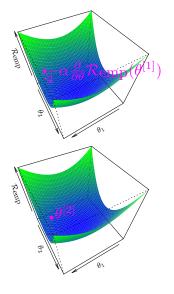
### **GRADIENT DESCENT - EXAMPLE**



Now we follow in the direction of the negative gradient at  $\theta^{[0]}$ .

We arrive at  $heta^{[1]}$  with risk  $\mathcal{R}_{emp}( heta^{[1]}) pprox 42.73$ . We improved:  $\mathcal{R}_{emp}( heta^{[1]}) < \mathcal{R}_{emp}( heta^{[0]})$ .

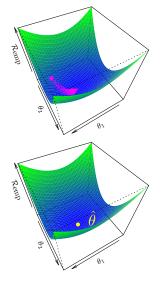
# **GRADIENT DESCENT - EXAMPLE**



Again we follow in the direction of the negative gradient, but now at  $\theta^{[1]}$ .

Now  $heta^{[2]}$  has risk  $\mathcal{R}_{\mathsf{emp}}( heta^{[2]}) pprox 25.08$ .

## **GRADIENT DESCENT - EXAMPLE**

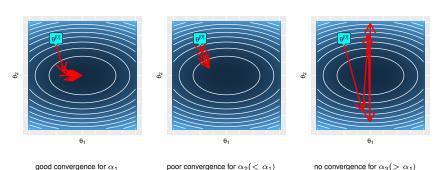


We iterate this until some form of convergence or termination.

We arrive close to a stationary  $\hat{\theta}$  which is hopefully at least a local minimum.

#### **GRADIENT DESCENT - LEARNING RATE**

- The negative gradient is a direction that looks locally promising to reduce  $\mathcal{R}_{\text{emp}}$ .
- $\bullet$  Hence it weights components higher in which  $\mathcal{R}_{\text{emp}}$  decreases more.
- However, the length of  $-\frac{\partial}{\partial \theta}\mathcal{R}_{\text{emp}}$  measures only the local decrease rate, i.e., there are no guarantees that we will not go "too far".
- We use a learning rate  $\alpha$  to scale the step length in each iteration. Too much can lead to overstepping and no converge, too low leads to slow convergence.
- Usually, a simple constant rate or rate-decrease mechanisms to enforce local convergence are used



#### **FURTHER TOPICS**

- GD is a so-called first-order method. Second-order methods use the Hessian to refine the search direction for faster convergence.
- There exist many improvements of GD, e.g., to smartly control the learn rate, to escape saddle points, to mimic second order behavior without computing the expensive Hessian.
- If the gradient of GD is not derived from the empirical risk of the whole data set, but instead from a randomly selected subset, we call this **stochastic gradient descent** (SGD). For large-scale problems this can lead to higher computational efficiency.