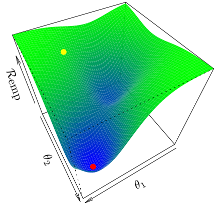
Introduction to Machine Learning

ML-Basics: Optimization

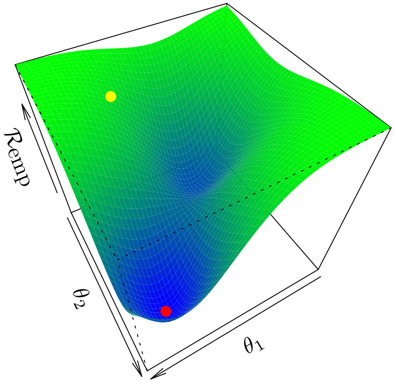


Learning goals

- 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 $\boldsymbol{\theta} \in \Theta$ with lowest empirical risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$.
- 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:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta} \in \Theta} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}).$$

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

$$\forall \boldsymbol{\theta} \in \Theta : \quad \mathcal{R}_{\text{emp}}(\hat{\boldsymbol{\theta}}) \leq \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}).$$

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

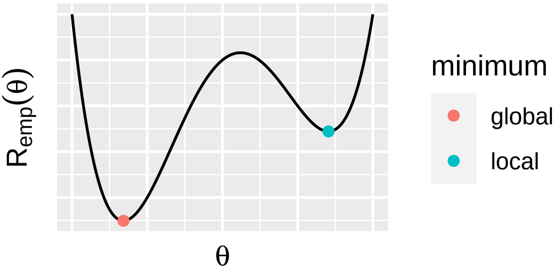
Which kind of numerical technique is reasonable for this problem strongly depends on model and parameter structure (continuous params? uni-modal $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$?). Here, we will only discuss very simple scenarios.

LOCAL MINIMA

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

$$\exists \epsilon > 0 \ \forall \boldsymbol{\theta} \text{ with } \left\| \hat{\boldsymbol{\theta}} - \boldsymbol{\theta} \right\| < \epsilon : \quad \mathcal{R}_{\text{emp}}(\hat{\boldsymbol{\theta}}) \leq \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}).$$

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

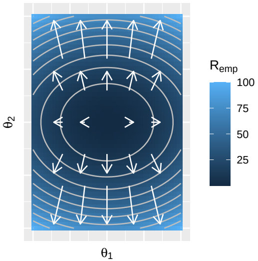


LOCAL MINIMA AND STATIONARY POINTS

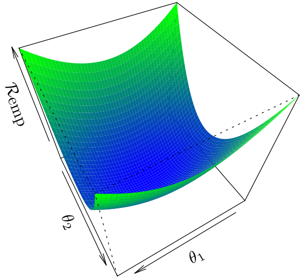
If $\mathcal{R}_{\text{emp}}$ is continuously differentiable in $\boldsymbol{\theta}$ then a **sufficient condition** for a local minimum is that $\hat{\boldsymbol{\theta}}$ is **stationary** with 0 gradient, so no local improvement is possible:

$$\frac{\partial}{\partial \boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\hat{\boldsymbol{\theta}}) = 0$$

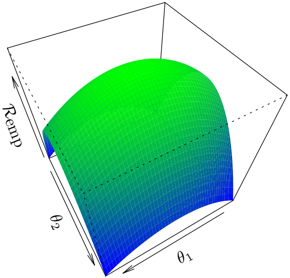
and the Hessian $\frac{\partial^2}{\partial \boldsymbol{\theta}^2} \mathcal{R}_{\text{emp}}(\hat{\boldsymbol{\theta}})$ is positive definite. While the neg. gradient points into the direction of fastest local decrease, the Hessian measures local curvature of $\mathcal{R}_{\text{emp}}$.



$\frac{\partial}{\partial \boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$



const. pos. def. Hessian



const. neg. def. Hessian

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.,

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \|\mathbf{X}\boldsymbol{\theta} - \mathbf{y}\|_2^2 = \sum_{i=1}^{n} (\boldsymbol{\theta}^\top \mathbf{x}^{(i)} - y^{(i)})^2 \ .$$

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

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

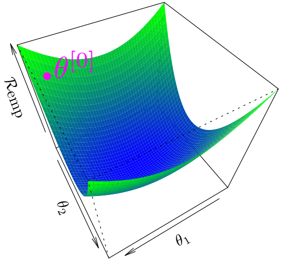
is a local minimum of $\mathcal{R}_{\text{emp}}$. If $\mathbf{X}$ is full-rank, $\mathcal{R}_{\text{emp}}$ is strictly convex and there is only one local minimum - which is also global.

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

GRADIENT DESCENT

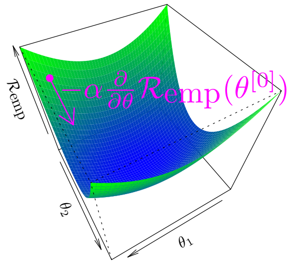
The simple idea of GD is to iteratively go from the current candidate $\boldsymbol{\theta}^{[t]}$ in the direction of the negative gradient, i.e., the direction of the steepest descent, with learning rate α to the next $\boldsymbol{\theta}^{[t+1]}$:

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

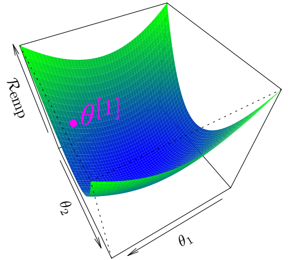


We choose a random start $\boldsymbol{\theta}^{[0]}$ with risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[0]}) = 76.25$.

GRADIENT DESCENT - EXAMPLE

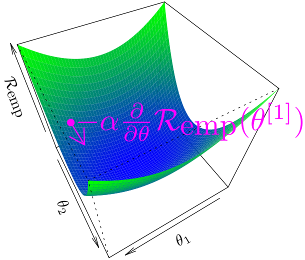


Now we follow in the direction of the negative gradient at $\boldsymbol{\theta}^{[0]}$.

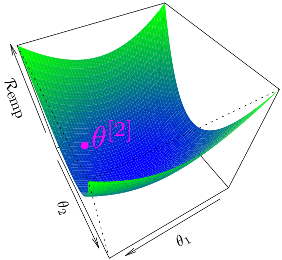


We arrive at $\boldsymbol{\theta}^{[1]}$ with risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[1]}) \approx 42.73$.
We improved: $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[1]}) < \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[0]})$.

GRADIENT DESCENT - EXAMPLE

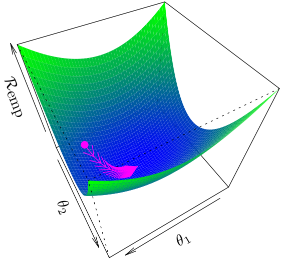


Again we follow in the direction of the negative gradient, but now at $\boldsymbol{\theta}^{[1]}$.

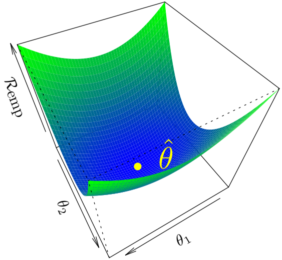


Now $\boldsymbol{\theta}^{[2]}$ has risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[2]}) \approx 25.08$.

GRADIENT DESCENT - EXAMPLE



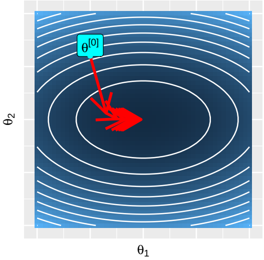
We iterate this until some form of convergence or termination.



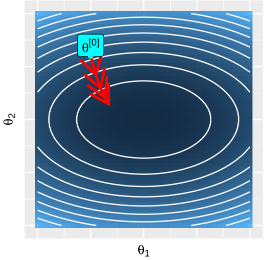
We arrive close to a stationary $\hat{\theta}$ which is hopefully at least a local minimum.

GRADIENT DESCENT - LEARNING RATE

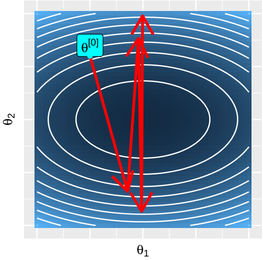
- The negative gradient is a direction that looks locally promising to reduce $\mathcal{R}_{\text{emp}}$.
- Hence it weights components higher in which $\mathcal{R}_{\text{emp}}$ decreases more.
- However, the length of $-\frac{\partial}{\partial \boldsymbol{\theta}}\mathcal{R}_{\text{emp}}$ measures only the local decrease rate, i.e., there are no guarantees that we will not go "too far".
- We use a learning rate α 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



good convergence for $\alpha 1$



poor convergence for $\alpha_2 (< \alpha_1)$



no convergence for $\alpha_3 (> \alpha_2)$

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.