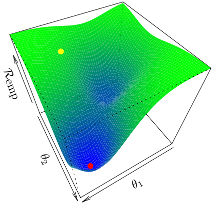
# Introduction to Machine Learning

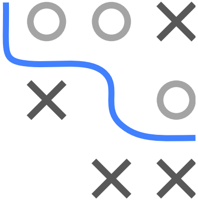
# ML-Basics
# Optimization



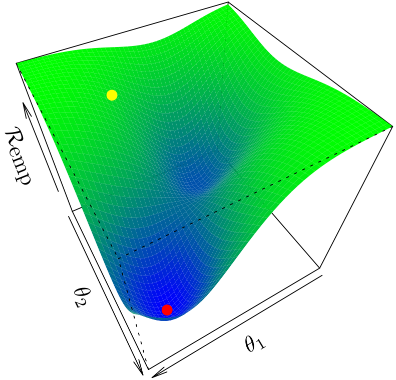

**Learning goals**

- 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

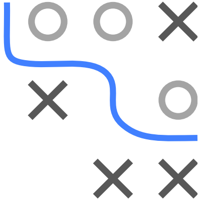
# LEARNING AS PARAMETER OPTIMIZATION



- Operationalize search for model $f$ that matches training data best by looking for parametrization $\boldsymbol{\theta} \in \Theta$ with lowest risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$
- Traverse error surface downwards; often local search from some start point to minimum (hopefully)



# LEARNING AS PARAMETER OPTIMIZATION



ERM optimization problem:

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

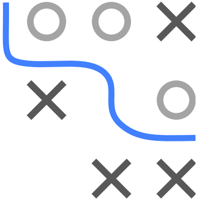
For **(global) minimum** $\hat{\boldsymbol{\theta}}$:

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

Does not imply that $\hat{\boldsymbol{\theta}}$ is unique

- Best numerical optimizer depends on problem structure
- Continuous params? Uni-modal $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$?
- Numerical optimization not our focus here, now

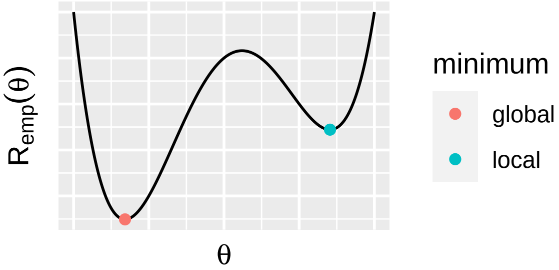
# LOCAL MINIMA



- Definition of **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 local minimum is easier than global one

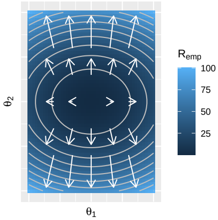


# LOCAL MINIMA AND STATIONARY POINTS

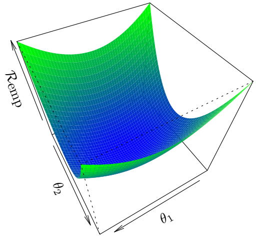
If $\mathcal{R}_{\text{emp}}$ continuously differentiable, **sufficient condition** for local minimum:
$\hat{\boldsymbol{\theta}}$ is **stationary**, so 0 gradient, so no local improvement possible:

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

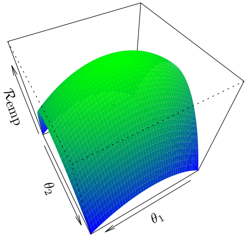
**and** Hessian at $\hat{\boldsymbol{\theta}}$ is positive definite.
Neg. gradient points into direction of fastest local decrease;
Hessian measures local curvature.




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




const. pos. def. Hessian

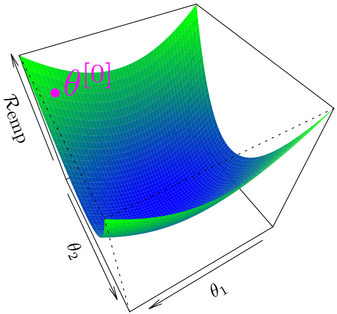



const. neg. def. Hessian

# GRADIENT DESCENT

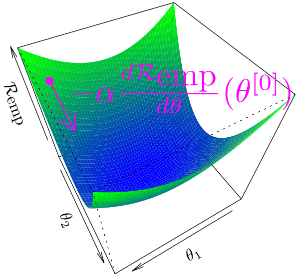
- Iteratively improve current candidate $\boldsymbol{\theta}^{[t]}$
- Move in direction of neg. gradient, so direction of steepest descent
- Use step size / learning rate $\alpha$

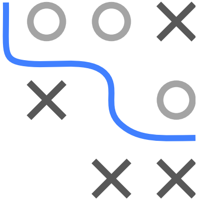
$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \alpha \frac{d\mathcal{R}_{\text{emp}}}{d\boldsymbol{\theta}}(\boldsymbol{\theta}^{[t]})$$



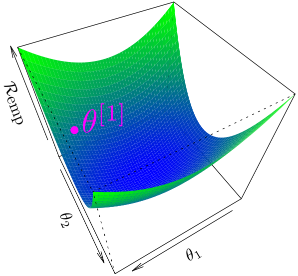

Random start $\boldsymbol{\theta}^{[0]}$ with $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[0]}) = 76.25$.

# GRADIENT DESCENT - EXAMPLE



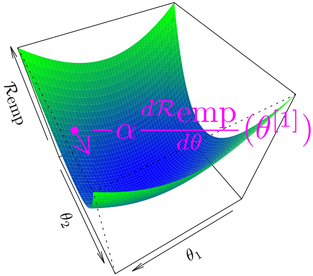



Direction of the neg. gradient at $\boldsymbol{\theta}^{[0]}$

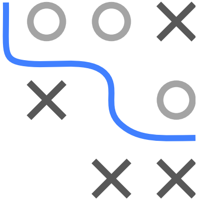


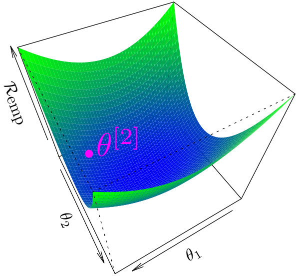

Arrive at $\boldsymbol{\theta}^{[1]}$ with $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[1]}) \approx 42.73$
We improved: $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[1]}) < \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[0]})$

# GRADIENT DESCENT - EXAMPLE



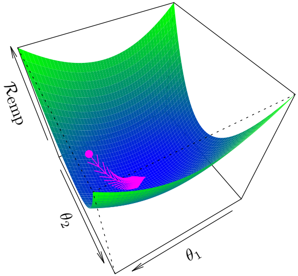

Now iterate, do the same at $\boldsymbol{\theta}^{[1]}$



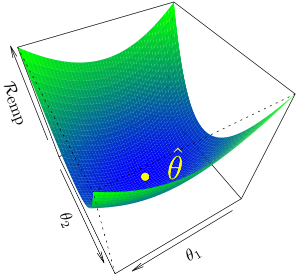



Now $\boldsymbol{\theta}^{[2]}$ has risk $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}^{[2]}) \approx 25.08$

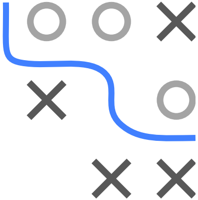
# GRADIENT DESCENT - EXAMPLE




We iterate this until some form of convergence or termination

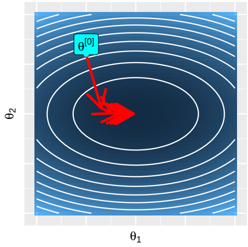



We arrive close to a stationary $\hat{\theta}$ which is hopefully at least a local minimum

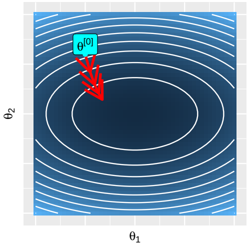


# GRADIENT DESCENT - LEARNING RATE

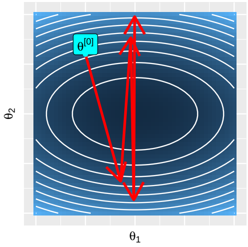
- Neg. gradient is direction that looks locally promising to reduce $\mathcal{R}_{\text{emp}}$
- Hence weights components higher in which $\mathcal{R}_{\text{emp}}$ decreases more
- However, the length of $-\frac{d}{d\boldsymbol{\theta}}\mathcal{R}_{\text{emp}}$ measures only the local decrease rate,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




good convergence for $\alpha_1$




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




no convergence for $\alpha_3(>\alpha_1)$

# FURTHER TOPICS

- Few models, e.g. linear regression, can be optimized analytically.
- GD is a so-called first-order method. Second-order methods (like Newton-Raphson) use the Hessian to refine the search direction for faster convergence.
- There exist many improvements of GD (momentum, ADAM), e.g., to smartly control the learn rate, to escape saddle points, to mimic second order behavior without computing the Hessian.
- If the gradient is not computed on the complete data, but instead on small, random batches, this is **stochastic gradient descent** (SGD). For large-scale problems, this is usually more efficient.