Optimization

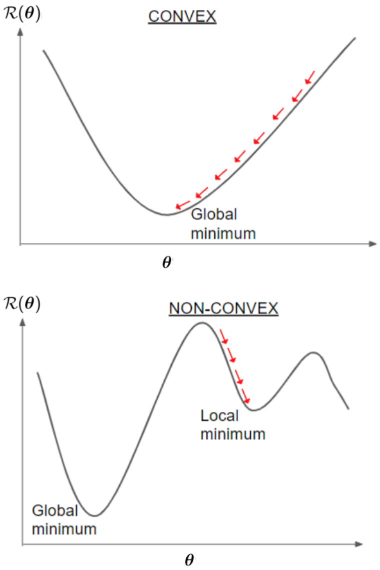
Deep Dive: Gradient Descent & Optimality

Learning goals

- LEARNING GOAL 1
- LEARNING GOAL 2

GRADIENT DESCENT AND OPTIMALITY

- GD is a greedy algorithm: In every iteration, it makes locally optimal moves.
- If $\mathcal{R}(\boldsymbol{\theta})$ is **convex** and **differentiable**, and its gradient is Lipschitz continuous, GD is guaranteed to converge to the global minimum (for small enough step-size).
- However, if $\mathcal{R}(\boldsymbol{\theta})$ has multiple local optima and/or saddle points, GD might only converge to a stationary point (other than the global optimum), depending on the starting point.



GRADIENT DESCENT AND OPTIMALITY

We assume that the gradient of the convex and differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ is Lipschitz continuous with $L > 0$:

$$||\nabla f(\boldsymbol{x}) - \nabla f(\boldsymbol{y})|| \leq L||\boldsymbol{x} - \boldsymbol{y}|| \quad \text{for all } x, y$$

This means that the gradient can't change arbitrarily fast.

Now we have a look at the convergence of gradient descent with a fixed step size $\alpha \leq 1/L$.
Convergence: Let $f : \mathbb{R}^n \to \mathbb{R}$ be convex and have L-Lipschitz continuous gradients and assuming that the global minimum x^* exists. Then gradient descent with k iterations with a fixed step-size $\alpha \leq 1/L$ will yield a solution $f(x^k)$, which satisfies

$$f(x^k) - f(x^*) \leq \frac{||x^0 - x^*||^2}{2\alpha k}$$

This means, that GD converges with rate $\mathcal{O}(1/k)$.

GRADIENT DESCENT AND OPTIMALITY

Proof: The assumption that ∇f is Lipschitz continuous implies that $\nabla^2 f(x) \preccurlyeq LI$ for all x. The generalized inequality $\nabla^2 f(x) \preccurlyeq LI$ means that $LI - \nabla^2 f(x)$ is positive semidefinite. This means that $v^\top \nabla^2 f(u) v \leq L||v||^2$ for any u and v.

Therefore, we can perform a quadratic expansion of f around $\tilde{x}$ obtaining the following inequality:

$$\begin{aligned} f(x) &\approx f(\tilde{x}) + \nabla f(\tilde{x})^\top (x - \tilde{x}) + 0.5(x - \tilde{x})^\top \nabla^2 f(\tilde{x})(x - \tilde{x}) \\ &\leq f(\tilde{x}) + \nabla f(\tilde{x})^\top (\tilde{x}) + 0.5L||x - \tilde{x}||^2, \end{aligned}$$

as the blue term is at most $0.5L||x - \tilde{x}||^2$. This is called the descent lemma.

Now, we are doing one update via gradient descent with a step size $\alpha \leq 1/L$:

$$\tilde{x} = x^{t+1} = x^t - \alpha \nabla f(x^t)$$

and plug this in the descent lemma.

GRADIENT DESCENT AND OPTIMALITY

We get

$$
\begin{aligned}
f(x^{t+1}) &\leq f(x^t) - \nabla f(x^t)^\top (x^{t+1} - x^t) + \frac{1}{2} L ||x^{t+1} - x^t||^2 \\
&= f(x^t) + \nabla f(x^t)^\top (x^t - \alpha \nabla f(x^t) - x^t) + \frac{1}{2} L ||x^t - \alpha \nabla f(x^t) - x^t||^2 \\
&= f(x^t) - \nabla f(x^t)^\top \alpha \nabla f(x^t) + \frac{1}{2} L ||\alpha \nabla f(x^t)||^2 \\
&= f(x^t) - \alpha ||\nabla f(x^t)||^2 + \frac{1}{2} L \alpha^2 ||\nabla f(x^t)||^2 \\
&= f(x^t) - (1 - \frac{1}{2} L \alpha) \alpha ||\nabla f(x^t)||^2 \\
&\leq f(x^t) - \frac{1}{2} \alpha ||\nabla f(x^t)||^2,
\end{aligned}
$$

where we used $\alpha \leq 1/L$ and therefore $-(1 - \frac{1}{2} L\alpha) \leq \frac{1}{2} L \frac{1}{L} - 1 = -\frac{1}{2}$.
Since $\frac{1}{2}\alpha||\nabla f(x^t)||^2$ is always positive unless $\nabla f(x) = 0$, it implies that f strictly decreases with each iteration of GD until the optimal value is reached. So, it is a bound on guaranteed progress, when $\alpha \leq 1/L$.

GRADIENT DESCENT AND OPTIMALITY

Now, we bound $f(x)$ in terms of $f(x^*)$ and use that f is convex:

$$f(x) \leq f(x^*) + \nabla f(x)^T(x - x^*)$$

When we combine this and the bound derived before, we get

$$\begin{aligned} f(x^{t+1}) - f(x^*) &\leq \nabla f(x)^\top (x - x^*) - \frac{\alpha}{2}||\nabla f(x)||^2 \\ &= \frac{1}{2\alpha}\left(||x - x^*||^2 - ||x - x^* - \alpha\nabla f(x)||^2\right) \\ &= \frac{1}{2\alpha}\left(||x - x^*||^2 - ||x^{t+1} - x^*||^2\right) \end{aligned}$$

This holds for every iteration of GD.

GRADIENT DESCENT AND OPTIMALITY

Summing over iterations, we get:

$$\begin{aligned}
\sum_{t=0}^{k} f(x^{t+1}) - f(x^*) &\leq \sum_{t=0}^{k} \frac{1}{2\alpha} \left(||x^t - x^*||^2 - ||x^{t+1} - x^*||^2 \right) \\
&= \frac{1}{2\alpha} \left(||x^0 - x^*||^2 - ||x^k - x^*||^2 \right) \\
&\leq \frac{1}{2\alpha} \left(||x^0 - x^*||^2 \right),
\end{aligned}$$

where we used that the LHS is a telescoping sum. In addition, we know that f decreases on every iteration, so we can conclude that

$$f(x^k) - f(x^*) \leq \frac{||x^0 - x^*||^2}{2\alpha k}$$