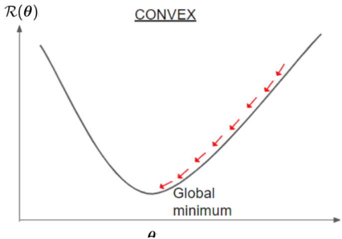
Optimization in Machine Learning

Deep dive: Gradient descent and optimality

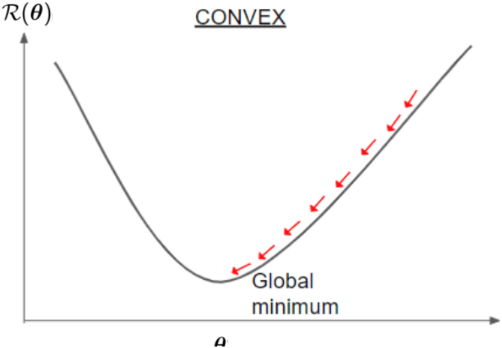


Learning goals

- Convergence of GD

GRADIENT DESCENT AND OPTIMALITY

- GD is a greedy algorithm: In every iteration, it makes locally optimal moves.
- If $f(\mathbf{x})$ is **convex** and **differentiable**, and its gradient is Lipschitz continuous, GD is guaranteed to converge to the global minimum for small enough step-size.



GRADIENT DESCENT AND OPTIMALITY

Assume $f : \mathbb{R}^d \to \mathbb{R}$ convex and differentiable and assume that global minimum $\mathbf{x}^*$ exists. Assume ∇f is Lipschitz continuous with $L > 0$:

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

(i.e., gradient can't change arbitrarily fast).

Convergence of GD: GD with k iterations with starting point $\mathbf{x}^{[0]}$ and fixed step-size $\alpha \leq 1/L$ will yield a solution $f(\mathbf{x}^{[k]})$, which satisfies

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

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

GRADIENT DESCENT AND OPTIMALITY

Proof: From ∇f Lipschitz it follows that $\nabla^2 f(\mathbf{x}) \preccurlyeq L \cdot \mathbf{I}$ for all $\mathbf{x}$.

NB: The generalized inequality $\nabla^2 f(\mathbf{x}) \preccurlyeq LI$ means that $L \cdot \mathbf{I} - \nabla^2 f(\mathbf{x})$ is positive semidefinite. This means that $\boldsymbol{v}^\top \nabla^2 f(\boldsymbol{u})\boldsymbol{v} \leq L||\boldsymbol{v}||^2$ for any $\boldsymbol{u}$ and $\boldsymbol{v}$.

We perform a quadratic expansion of f around $\tilde{\mathbf{x}}$:

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

as the blue term is at most $0.5 \cdot L \cdot ||\mathbf{x} - \tilde{\mathbf{x}}||^2$.

Now, do one GD update with step size $\alpha \leq 1/L$:

$$
\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} - \alpha \nabla f\left(\mathbf{x}^{[t]}\right)
$$

and plug this in the descent lemma.

GRADIENT DESCENT AND OPTIMALITY

We get

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

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 $\frac{1}{2}\alpha||\nabla f(\mathbf{x}^{[t]})||^2$ is always positive unless $\nabla f(\mathbf{x}) = 0$, 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 if $\alpha \leq 1/L$. The sequence is also bounded from below, as we assume the existence of a global min, hence it convergences.

GRADIENT DESCENT AND OPTIMALITY

Now, we bound $f(\mathbf{x}^{[t]})$ in terms of $f(\mathbf{x}^*)$ using that f is convex. By 1st-order condition of convexity: Every tangent / 1st order Taylor is always below f (develop at $\mathbf{x}^{[t]}$, var of linear function is $\mathbf{x}$):

$$f(\mathbf{x}^{[t]}) + \nabla f(\mathbf{x}^{[t]})^\top (\mathbf{x} - \mathbf{x}^{[t]}) \leq f(\mathbf{x})$$

So this holds also for $\mathbf{x} = \mathbf{x}^*$

$$f(\mathbf{x}^{[t]}) - f(\mathbf{x}^*) \leq \nabla f(\mathbf{x}^{[t]})^\top (\mathbf{x}^{[t]} - \mathbf{x}^*)$$

GRADIENT DESCENT AND OPTIMALITY

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

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

3rd to 4th line might be harder to see, simply multiply-out 4th line.
This holds for every iteration of GD.

GRADIENT DESCENT AND OPTIMALITY

Summing over iterations, we get:

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

where we used that f decreases in every iter, and the 2nd line is a telescoping sum. Hence

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