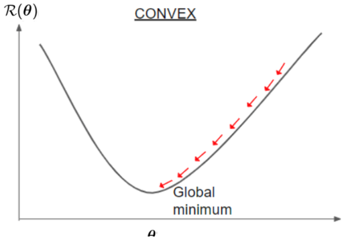
Optimization in Machine Learning

Deep dive

Gradient descent and optimality

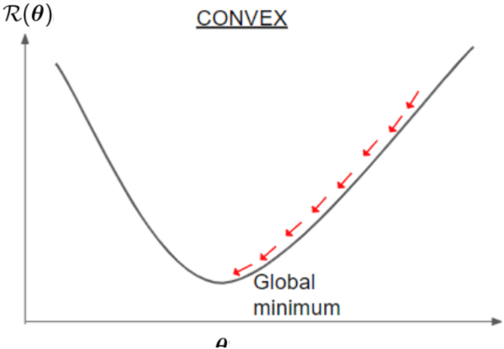


Learning goals

- Convergence of GD
- Proof strategy and tools
- Descent lemma

SETTING

- GD is **greedy**: **locally optimal** moves in each iteration
- If f is **convex**, **differentiable** and has a **Lipschitz gradient**, GD converges to global minimum for sufficiently small step sizes.



SETTING

- **Assumptions:**
  - f convex and differentiable
  - Global minimum $\boldsymbol{x}^*$ exists
  - f has Lipschitz gradient (∇f does not change too fast)

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

Theorem (Convergence of GD)**.** GD with step size $\alpha \leq 1/L$ yields

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

In other words: GD converges with rate $\mathcal{O}(1/k)$.

PROOF STRATEGY

1. Show that $f(\boldsymbol{x}^{[t]})$ **strictly decreases** with each iteration t

Descent lemma:

$$f(\boldsymbol{x}^{[t+1]}) \leq f(\boldsymbol{x}^{[t]}) - \frac{\alpha}{2} \|\nabla f(\boldsymbol{x}^{[t]})\|^2$$

2. Bound **error of one step**

$$f(\boldsymbol{x}^{[t+1]}) - f(\boldsymbol{x}^*) \leq \frac{1}{2\alpha} \left(\|\boldsymbol{x}^{[t]} - \boldsymbol{x}^*\|^2 - \|\boldsymbol{x}^{[t+1]} - \boldsymbol{x}^*\|^2 \right)$$

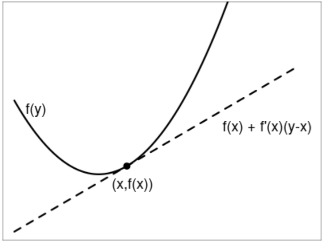
3. Finalize by **telescoping** argument

MAIN TOOL

- **Recall:** First order condition of convexity

Every tangent line of f is always below f.

$$f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^\top (\boldsymbol{y} - \boldsymbol{x})$$



DESCENT LEMMA

- **Recall:** ∇f Lipschitz $\implies \nabla^2 f(\mathbf{x}) \preccurlyeq L \cdot \mathbf{I}$ for all $\mathbf{x}$
- This gives convexity of $g(\mathbf{x}) := \frac{L}{2}\|\mathbf{x}\|^2 - f(\mathbf{x})$ since

$$\nabla^2 g(\mathbf{x}) = L \cdot \mathbf{I} - \nabla^2 f(\mathbf{x}) \succcurlyeq 0.$$

- First order condition of convexity of g yields

$$\begin{aligned}
& g(\mathbf{x}) \geq g(\mathbf{x}^{[t]}) + \nabla g(\mathbf{x}^{[t]})^\top (\mathbf{x} - \mathbf{x}^{[t]}) \\
\Leftrightarrow \quad & \frac{L}{2}\|\mathbf{x}\|^2 - f(\mathbf{x}) \geq \frac{L}{2}\|\mathbf{x}^{[t]}\|^2 - f(\mathbf{x}^{[t]}) + (L\mathbf{x}^{[t]} - \nabla f(\mathbf{x}^{[t]}))^\top (\mathbf{x} - \mathbf{x}^{[t]}) \\
\Leftrightarrow \quad & \vdots \\
\Leftrightarrow \quad & f(\mathbf{x}) \leq f(\mathbf{x}^{[t]}) + \nabla f(\mathbf{x}^{[t]})^\top (\mathbf{x} - \mathbf{x}^{[t]}) + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^{[t]}\|^2
\end{aligned}$$

- **Now:** One GD step with step size $\alpha \leq 1/L$:

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

DESCENT LEMMA

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

- **Note:** $\alpha \leq 1/L$ yields $L\alpha^2 \leq \alpha$
  - $\|\nabla f(\boldsymbol{x}^{[t]})\|^2 > 0$ unless $\nabla f(\boldsymbol{x}) = \mathbf{0}$
  - f **strictly decreases** with each GD iteration until optimum reached
  - Descent lemma yields bound on **guaranteed progress** if $\alpha \leq 1/L$ (explains why GD may diverge if step sizes too large)

ONE STEP ERROR BOUND

- Again, first order condition of convexity gives

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

- This and the descent lemma yields

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

- **Note:** Line 3 $\rightarrow$ 4 is hard to see (just expand line 4).

FINALIZATION

- Summing over iterations yields

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

- **Arguments:** Descent lemma (line 1).
  Telescoping sum (line 2 $\rightarrow$ 3).

$$
\boxed{f(\mathbf{x}^{[t+1]}) - f(\mathbf{x}^*) \leq \frac{\|\mathbf{x}^{[0]} - \mathbf{x}^*\|^2}{2\alpha k}}
$$