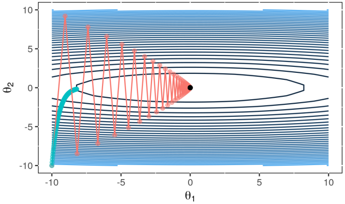
Optimization in Machine Learning

First order methods
Step size and optimality

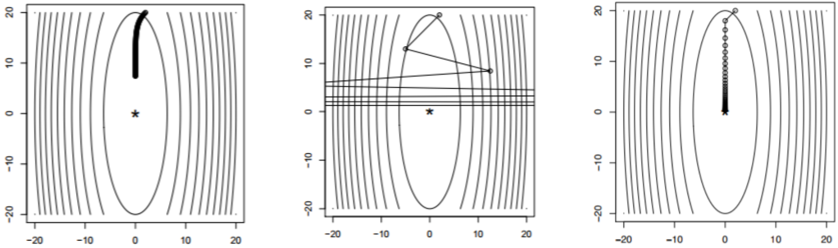


Learning goals

- Impact of step size
- Fixed vs. adaptive step size
- Exact line search
- Armijo rule & Backtracking
- Bracketing & Pinpointing

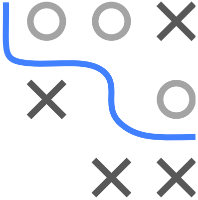
CONTROLLING STEP SIZE: FIXED & ADAPTIVE

- Iteration t: Choose not only descent direction $\mathbf{d}^{[t]}$, but also step size $\alpha^{[t]}$
- First approach: **Fixed** step size $\alpha^{[t]} = \alpha > 0$
  - If α too small, procedure may converge very slowly (left)
  - If α too large, procedure may not converge $\rightarrow$ "jumps" around optimum (middle)
- **Adaptive** step size $\alpha^{[t]}$ can provide better convergence (right)



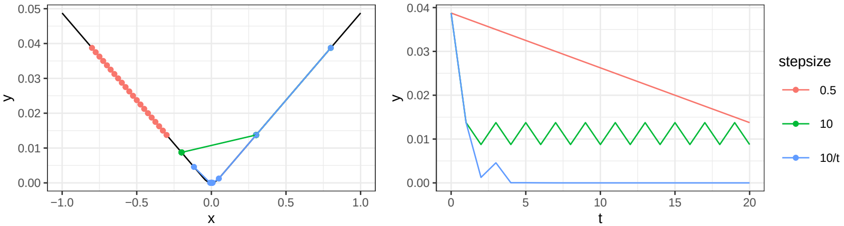
Steps of line searches for $f(\mathbf{x}) = 10x_1^2 + x_2^2/2$

STEP SIZE CONTROL: DIMINISHING STEP SIZE



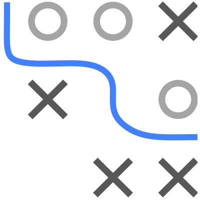
- How can we adaptively control step size?
- A natural way of selecting $\alpha^{[t]}$ is to decrease its value over time
- **Example:** GD on

$$f(x) = \begin{cases} \frac{1}{2}x^2 & \text{if } |x| \leq \delta, \\ \delta \cdot (|x| - 1/2 \cdot \delta) & \text{otherwise.} \end{cases}$$



GD with small constant (**red**), large constant (**green**), and diminishing (**blue**) step size

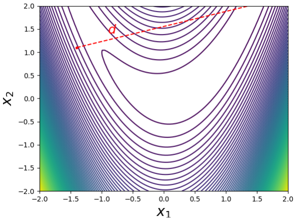
STEP SIZE CONTROL: EXACT LINE SEARCH

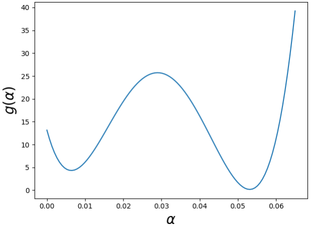


- Use **optimal** step size in each iteration:

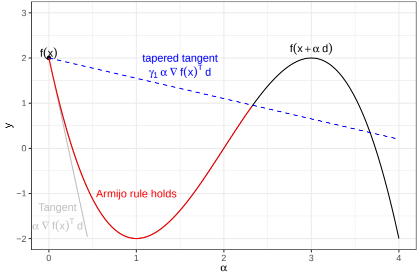
$$\alpha^{[t]} = \arg\min_{\alpha \in \mathbb{R}_{\geq 0}} g(\alpha) = \arg\min_{\alpha \in \mathbb{R}_{\geq 0}} f(\mathbf{x}^{[t]} + \alpha \mathbf{d}^{[t]})$$

- Need to solve a **univariate** optimization problem in each iteration ⇒ univariate optimization methods
- **Problem:** Expensive, prone to poorly conditioned problems
- **But:** No need for *optimal* step size. Only need a step size that is "good enough".
- **Reason:** Effort may not pay off, but in some cases slows down performance.



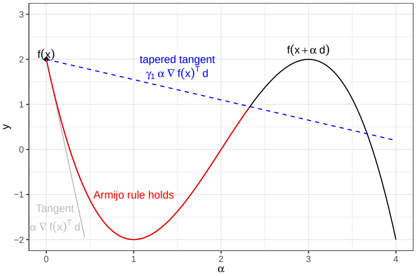


ARMIJO RULE



- **Inexact line search:** Minimize objective "sufficiently" without computing optimal step size exactly
- Common condition to guarantee "sufficient" decrease: **Armijo rule**

ARMIJO RULE

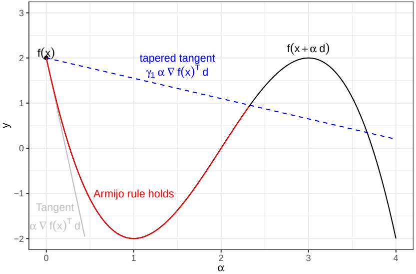


- Fix $\gamma_1 \in (0, 1)$. α satisfies **Armijo rule** in $\mathbf{x}$ for descent direction $\mathbf{d}$ if

$$f(\mathbf{x} + \alpha\mathbf{d}) \leq f(\mathbf{x}) + \gamma_1 \alpha \nabla f(\mathbf{x})^\top \mathbf{d}.$$

- **Note:** $\nabla f(\mathbf{x})^\top \mathbf{d} < 0$ ($\mathbf{d}$ *descent* dir.) $\implies f(\mathbf{x} + \alpha\mathbf{d}) < f(\mathbf{x})$.

ARMIJO RULE



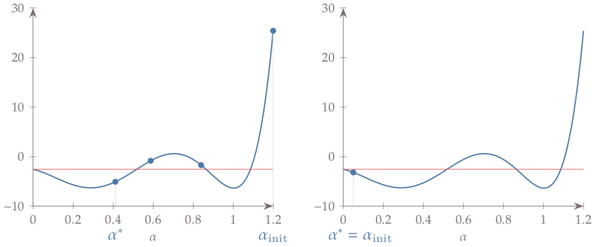
- **Feasibility:** For descent direction **d** and $\gamma_1 \in (0, 1)$, there exists $\alpha > 0$ fulfilling Armijo rule.In many cases, Armijo rule guarantees local convergence of GD and is therefore frequently used.

BACKTRACKING LINE SEARCH

- Procedure to meet the Armijo rule: **Backtracking** line search
- **Idea:** Decrease α until Armijo rule is met

Algorithm Backtracking line search

Choose initial step size $\alpha = \alpha_{\text{init}}$, $0 < \gamma_1 < 1$ and $0 < \tau < 1$
while $f(\mathbf{x} + \alpha \mathbf{d}) > f(\mathbf{x}) + \gamma_1 \alpha \nabla f(\mathbf{x})^\top \mathbf{d}$ **do**
    Decrease α: $\alpha \leftarrow \tau \cdot \alpha$
end while



(Source: Martins and Ning. *Engineering Design Optimization*, 2021.)

WOLFE CONDITIONS

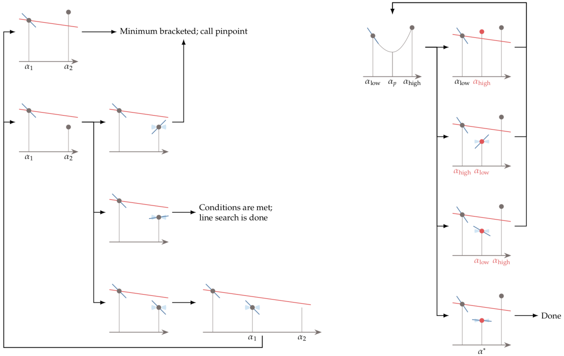
- Backtracking is simple and shows good performance in practice
- **But:** Two undesirable scenarios
  1. Initial step size α_{init} is too large $\Rightarrow$ need multiple evaluations of f
  2. Step size is too small with highly negative slopes
- **Solution** for small step sizes:
  - Fix γ_2 with $0 < \gamma_1 < \gamma_2 < 1$.
  - α satisfies **sufficient curvature condition** in $\mathbf{x}$ for $\mathbf{d}$ if

$$|\nabla f(\mathbf{x} + \alpha \mathbf{d})^\top \mathbf{d}| \leq \gamma_2 |\nabla f(\mathbf{x})^\top \mathbf{d}|.$$

Armijo rule + sufficient curvature condition = **Wolfe conditions**

WOLFE CONDITIONS

- **Algorithm** for finding a Wolfe point (point satisfying Wolfe conditions):
  1. **Bracketing:** Find interval containing Wolfe point
  2. **Pinpointing:** Find Wolfe point in interval from bracketing

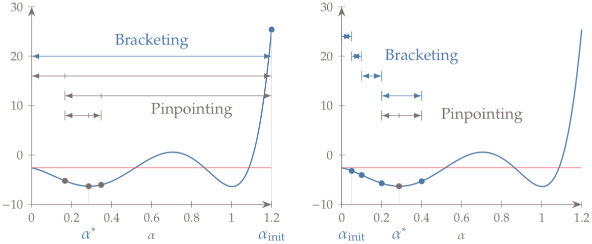


Left: Bracketing.**Right:** Pinpointing.

(Source: Martins and Ning. *EDO*, 2021.)

BRACKETING & PINPOINTING

- **Example:**
  - Large initial step size results in quick bracketing but multiple pinpointing steps (**left**).
  - Small initial step size results in multiple bracketing steps but quick pinpointing (**right**).



Source: Martins and Ning. *EDO*, 2021.