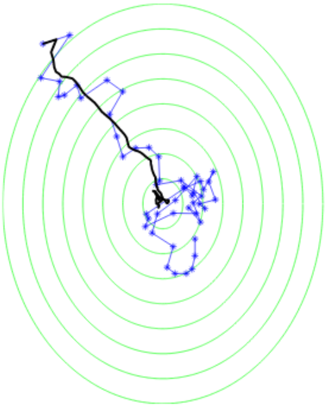
Optimization in Machine Learning

First order methods
SGD Further Details

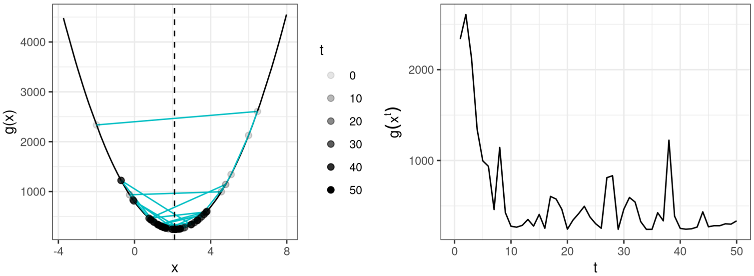


Learning goals

- Decreasing step size for SGD
- Stopping rules
- SGD with momentum

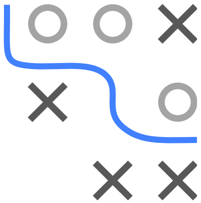
SGD WITH CONSTANT STEP SIZE

Example: SGD with constant step size.



Fast convergence of SGD initially. Erratic behavior later (variance too big).

SGD WITH DECREASING STEP SIZE



- **Idea:** Decrease step size to reduce magnitude of erratic steps.
- **Trade-off:**
  - if step size $\alpha^{[t]}$ decreases slowly, large erratic steps
  - if step size decreases too fast, performance is impaired
- SGD converges for sufficiently smooth functions if

$$\frac{\sum_{t=1}^{\infty}\left(\alpha^{[t]}\right)^2}{\sum_{t=1}^{\infty}\alpha^{[t]}} = 0$$

("how much noise affects you" by "how far you can get").

ADVANCED STEP SIZE CONTROL

Why not Armijo-based step size control?

- Backtracking line search or other approaches based on Armijo rule usually not suitable: Armijo condition

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

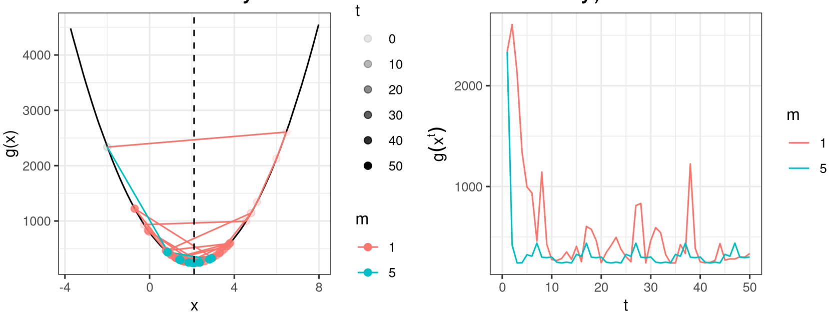
  requires evaluating full gradient.
- But SGD is used to *avoid* expensive gradient computations.
- Research aims at finding inexact line search methods that provide better convergence behaviour, e.g., Vaswani et al., *Painless Stochastic Gradient: Interpolation, Line-Search, and Convergence Rates*. NeurIPS, 2019.

MINI-BATCHES

- Reduce noise by increasing batch size m for better approximation

$$\hat{\mathbf{d}} = \frac{1}{m} \sum_{i \in J} \nabla_{\mathbf{x}} g_i(\mathbf{x}) \approx \frac{1}{n} \sum_{i=1}^{n} \nabla_{\mathbf{x}} g_i(\mathbf{x}) = \mathbf{d}$$

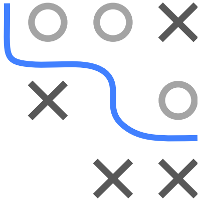
- Usually, the batch size is limited by computational resources (e.g., how much data you can load into the memory)



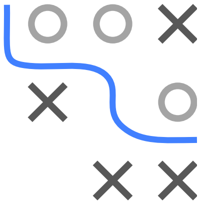
Example continued. Batch size $m = 1$ vs. $m = 5$.

STOPPING RULES FOR SGD

- **For GD**: We usually stop when gradient is close to 0 (i.e., we are close to a stationary point)
- **For SGD**: individual gradients do not necessarily go to zero, and we cannot access full gradient.
- Practicable solution for ML:
  - Measure the validation set error after T iterations
  - Stop if validation set error is not improving



SGD AND ML



General remarks:

- SGD is a variant of GD
- SGD particularly suitable for large-scale ML when evaluating gradient is too expensive / restricted by computational resources
- SGD and variants are the most commonly used methods in modern ML, for example:
  - Linear models

    Note that even for the linear model and quadratic loss, where a closed form solution is available, SGD might be used if the size n of the dataset is too large and the design matrix does not fit into memory.
  - Neural networks
  - Support vector machines
  - ...

SGD WITH MOMENTUM

SGD is usually used with momentum due to reasons mentioned in previous chapters.

Algorithm Stochastic gradient descent with momentum

require step size α and momentum φ
require initial parameter $\boldsymbol{x}$ and initial velocity $\boldsymbol{\nu}$
while stopping criterion not met **do**
    Sample mini-batch of m examples
    Compute gradient estimate $\nabla \hat{g}(\mathbf{x})$ using mini-batch
    Compute velocity update: $\boldsymbol{\nu} \leftarrow \varphi \boldsymbol{\nu} - \alpha \nabla \hat{g}(\mathbf{x})$
    Apply update: $\boldsymbol{x} \leftarrow \boldsymbol{x} + \boldsymbol{\nu}$
end while