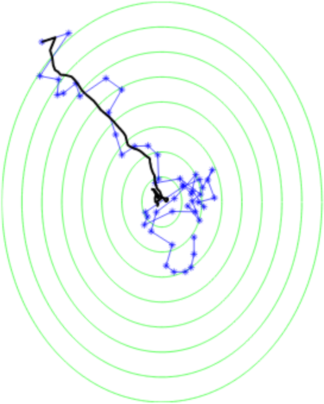
# Optimization in Machine Learning

# First order methods: SGD Further Details

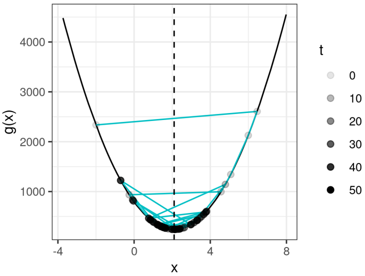


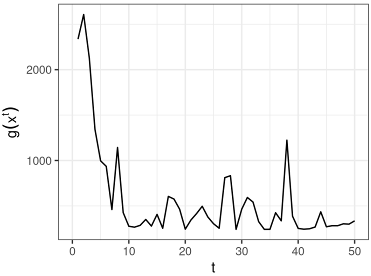
**Learning goals**

- 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

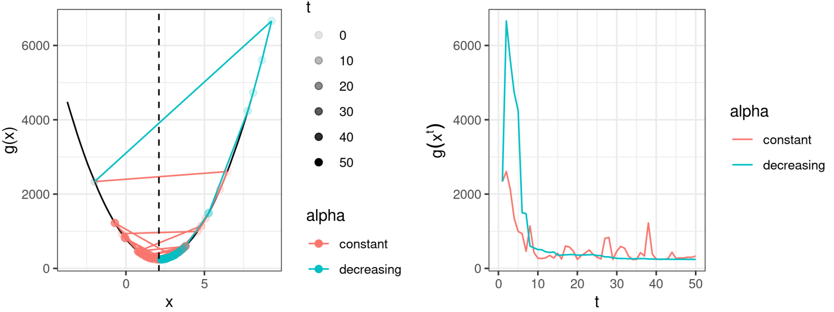
- **Idea:** Decrease step size to reduce magnitude of erratic steps.
- **Trade-off:**
  - if step size $\alpha^{[t]}$ decreases slowly, variance of $\nabla_{\mathbf{x}} g_i(\mathbf{x})$ also decreases slowly
  - if step size decreases too fast, performance is impaired
- SGD converges for sufficiently 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").

# SGD WITH DECREASING STEP SIZE

- Popular solution: step size fulfilling $\alpha^{[t]} \in \mathcal{O}(1/t)$.




Example continued. Step size $\alpha^{[t]} = 0.2/t$.

- Often not working well in practice: step size gets small quite fast.
- Alternative: $\alpha^{[t]} \in \mathcal{O}(1/\sqrt{t})$

# 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

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

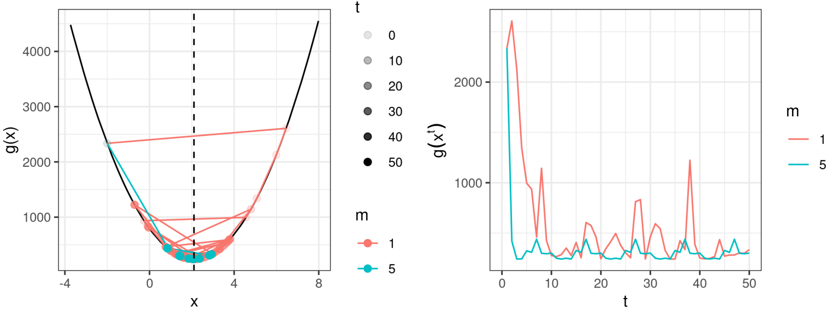
  requires evaluating full gradient.
- But SGD is used to *avoid* expensive gradient computations.
- Research aims at finding inexact line search methods that provide better convergence behaviour, e.g., Vaswani et al., *Painless Stochastic Gradient: Interpolation, Line-Search, and Convergence Rates*. NeurIPS,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