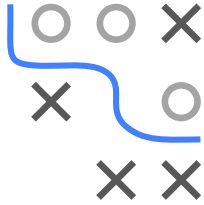
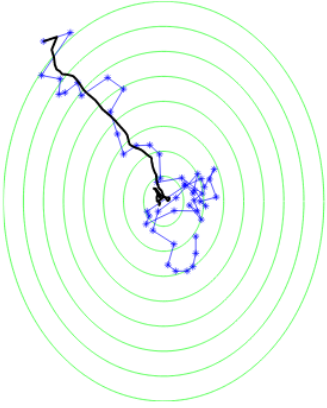
Optimization in Machine Learning



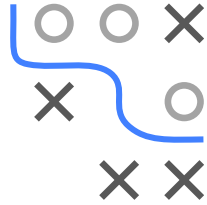
First order methods
SGD



Learning goals

- Understand stochastic gradient descent
- Understand stochasticity and variance of SGD
- Know convergence properties of SGD
- Understand effect of batch size

STOCHASTIC GRADIENT DESCENT



- NB: We use g instead of f as objective, because f is used as model in ML
- $g : \mathbb{R}^d \to \mathbb{R}$ objective, g is **average over functions**:

$$g(\boldsymbol{x}) = \frac{1}{n} \sum_{i=1}^{n} g_i(\boldsymbol{x}), \qquad g \text{ and } g_i \text{ smooth}$$

- Stochastic gradient descent (SGD) approximates the gradient

$$\begin{aligned} \nabla_{\boldsymbol{x}} g(\boldsymbol{x}) = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\boldsymbol{x}} g_i(\boldsymbol{x}) &:= \mathbf{d} \quad \text{by} \\ \frac{1}{|J|} \sum_{i \in J} \nabla_{\boldsymbol{x}} g_i(\boldsymbol{x}) &:= \hat{\mathbf{d}}, \end{aligned}$$

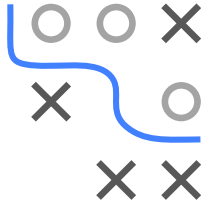
  with random subset $J \subset \{1, 2, \ldots, n\}$ of gradients called **mini-batch**

- This is done e.g. when computing the true gradient is **expensive**

SGD ALGORITHM

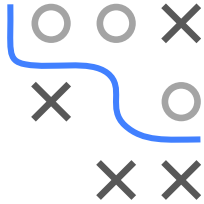
Algorithm Basic SGD pseudo code

1: Initialize $\boldsymbol{x}^{[0]}$, $t = 0$
2: **while** stopping criterion not met **do**
3: Randomly shuffle indices and partition into minibatches $J_1, \ldots, J_K$ of size m
4: **for** $k \in \{1, \ldots, K\}$ **do**
5: $t \leftarrow t + 1$
6: Compute gradient estimate with J_k: $\hat{\mathbf{d}}^{[t]} \leftarrow \frac{1}{m} \sum_{i \in J_k} \nabla_{\boldsymbol{x}} g_i(\boldsymbol{x}^{[t-1]})$
7: Apply update: $\boldsymbol{x}^{[t]} \leftarrow \boldsymbol{x}^{[t-1]} - \alpha \cdot \hat{\mathbf{d}}^{[t]}$
8: **end for**
9: **end while**



- Instead of drawing batches randomly we might want to go through the g_i sequentially (unless g_i are sorted in any way)
- Updates are computed faster, but also more stochastic:
  - In the simplest case, batch-size $m := |J_k|$ is set to $m = 1$
  - If n is a billion, computation of update is a billion times faster
  - **But** (later): Convergence rates suffer from stochasticity!

SGD IN ML

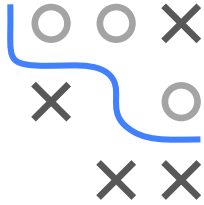


- In ML, we perform ERM:

$$\mathcal{R}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \underbrace{L\left(y^{(i)}, f\left(\boldsymbol{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)}_{g_i(\boldsymbol{\theta})}$$

- for a data set $\mathcal{D} = \left(\left(\boldsymbol{x}^{(1)}, y^{(1)}\right), \ldots, \left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right)$
- a loss function $L\left(y, f(\boldsymbol{x})\right)$, e.g., L2 loss $L\left(y, f(\boldsymbol{x})\right) = (y - f(\boldsymbol{x}))^2$
- and a model class f, e.g., the linear model $f\left(\boldsymbol{x}^{(i)} \mid \boldsymbol{\theta}\right) = \boldsymbol{\theta}^\top \boldsymbol{x}$

SGD IN ML



- For large data sets, computing the exact gradient

$$\mathbf{d} = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\boldsymbol{\theta}} L \left(y^{(i)}, f\left(\boldsymbol{x}^{(i)} \mid \boldsymbol{\theta}\right) \right)$$

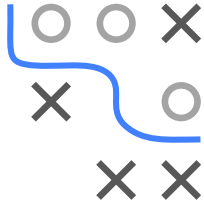
  may be expensive or even infeasible to compute and is approximated by

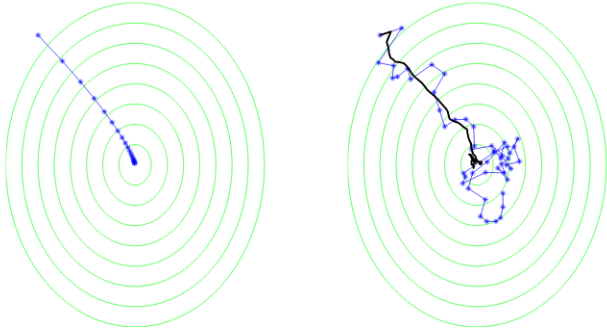
$$\hat{\mathbf{d}} = \frac{1}{m} \sum_{i \in J} \nabla_{\boldsymbol{\theta}} L \left(y^{(i)}, f\left(\boldsymbol{x}^{(i)} \mid \boldsymbol{\theta}\right) \right),$$

  for $J \subset \{1, 2, \ldots, n\}$ random subset

- **NB:** Often, maximum size of J technically limited by memory size

STOCHASTICITY OF SGD





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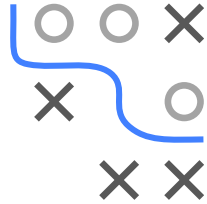
Minimize $g(x_1, x_2) = 1.25(x_1 + 6)^2 + (x_2 - 8)^2$ **Left:** GD, **Right:** SGD
Black line shows average value across multiple runs

STOCHASTICITY OF SGD



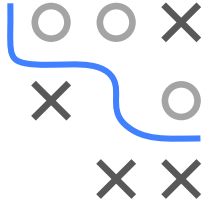
- Assume batch size $m = 1$ (statements also apply for larger batches)
- **(Possibly) suboptimal direction:** Approximate gradient $\hat{\mathbf{d}} = \nabla_{\boldsymbol{x}} g_i(\boldsymbol{x})$ might point in suboptimal (possibly not even a descent!) direction
- **Unbiased estimate:** If J drawn i.i.d., approximate gradient $\hat{\mathbf{d}}$ is an unbiased estimate of gradient $\mathbf{d} = \nabla_{\boldsymbol{x}} g(\boldsymbol{x}) = \sum_{i=1}^{n} \nabla_{\boldsymbol{x}} g_i(\boldsymbol{x})$:

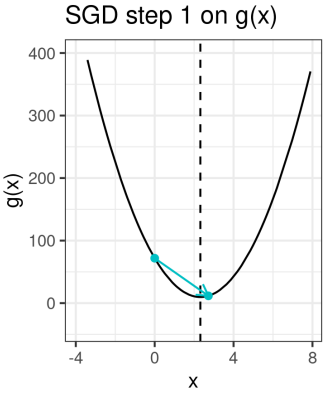
$$\begin{aligned} \mathbb{E}_i \left[\nabla_{\boldsymbol{x}} g_i(\boldsymbol{x}) \right] &= \sum_{i=1}^{n} \nabla_{\boldsymbol{x}} g_i(\boldsymbol{x}) \cdot \mathbb{P}(i = i) \\ &= \sum_{i=1}^{n} \nabla_{\boldsymbol{x}} g_i(\boldsymbol{x}) \cdot \frac{1}{n} = \nabla_{\boldsymbol{x}} g(\boldsymbol{x}). \end{aligned}$$

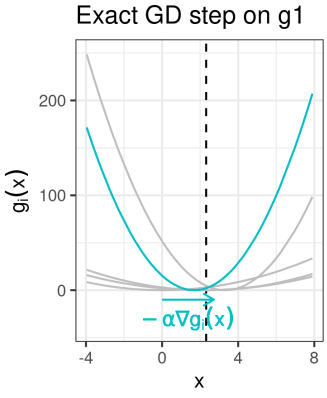
- **Conclusion:** SGD might perform single suboptimal moves, but moves in “right direction” **on average**

ERRATIC BEHAVIOR OF SGD

Example: $g(\boldsymbol{x}) = \sum_{i=1}^{5} g_i(\boldsymbol{x})$, g_i quadratic, batch size $m = 1$







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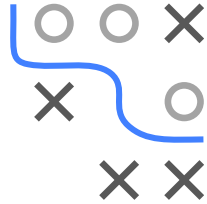

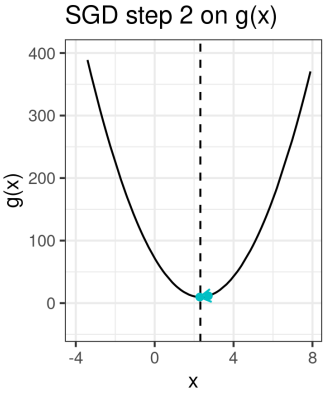

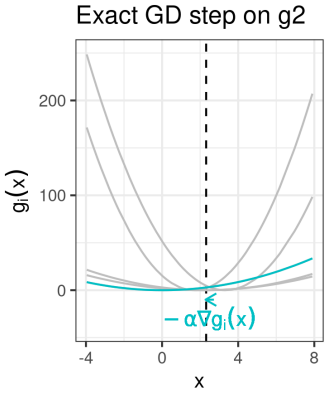

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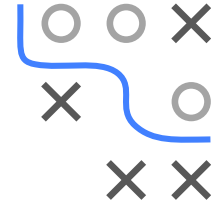

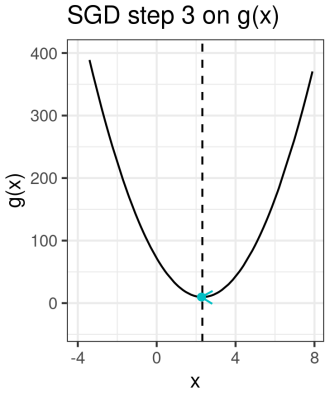

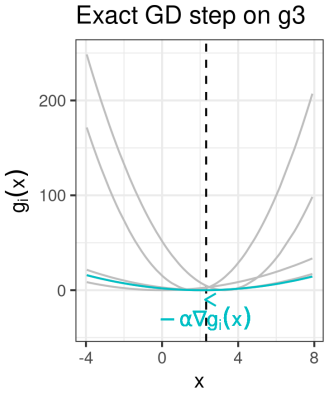

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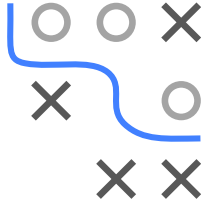

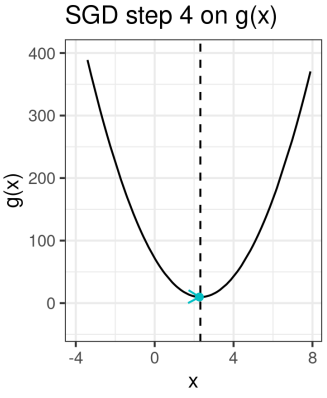

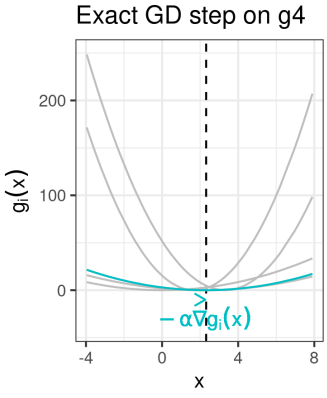

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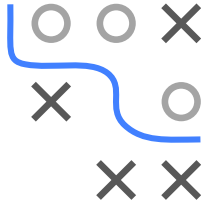
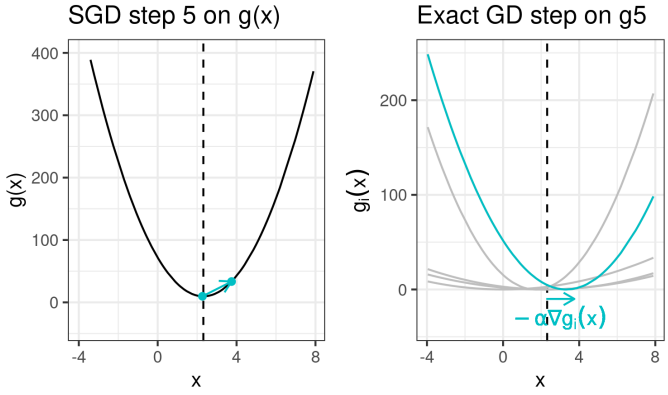
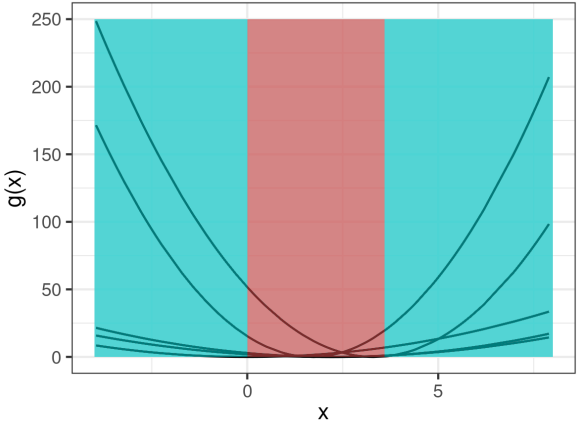
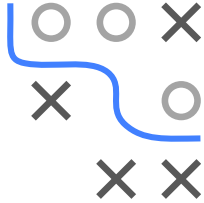




In iteration 5, SGD performs a suboptimal move away from the minimum.

ERRATIC BEHAVIOR OF SGD

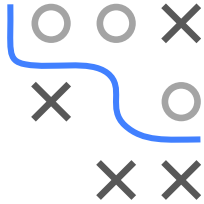




Blue area: Each $-\nabla g_i(\boldsymbol{x})$ points towards minimum

Red area ("confusion area"): $-\nabla g_i(\boldsymbol{x})$ might point away from minimum and perform a suboptimal move

ERRATIC BEHAVIOR OF SGD



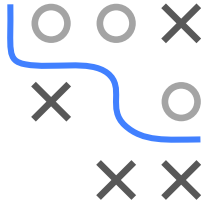
- At location $\boldsymbol{x}$, "confusion" is captured by variance of gradients

$$\frac{1}{n}\sum_{i=1}^{n} \|\nabla_{\boldsymbol{x}} g_i(\boldsymbol{x}) - \nabla_{\boldsymbol{x}} g(\boldsymbol{x})\|^2$$

- If term is 0, next step goes in gradient direction (for each i)
- If term is small, next step *likely* goes in gradient direction
- If term is large, next step likely goes in direction different than gradient

CONVERGENCE OF SGD

- As a consequence, SGD has worse convergence properties than GD
- **But:** Can be controlled via **increasing batches** or **reducing step size**



The larger the batch size m

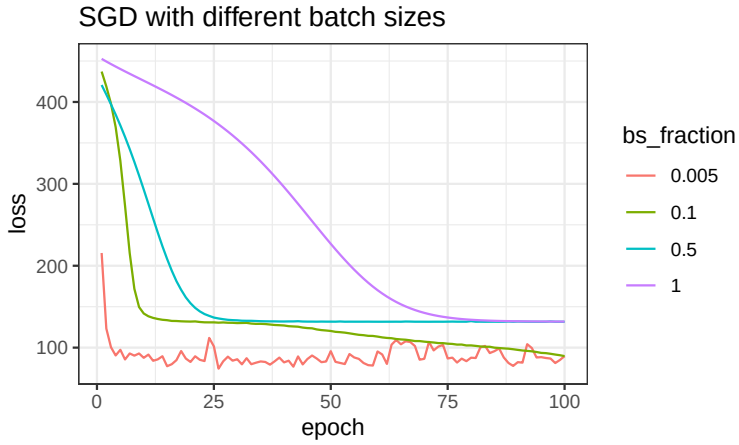
- the better the approximation to $\nabla_{\boldsymbol{x}} g(\boldsymbol{x})$
- the lower the variance
- the lower the risk of performing steps in the wrong direction

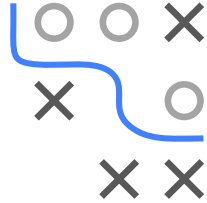
The smaller the step size α

- the smaller a step in a potentially wrong direction
- the lower the effect of high variance

As maximum batch size is usually limited by computational resources (memory), choosing the step size is crucial

EFFECT OF BATCH SIZE





SGD for a NN with batch size $\in \{0.5\%, 10\%, 50\%\}$ of the training data

The higher the batch size, the lower the variance