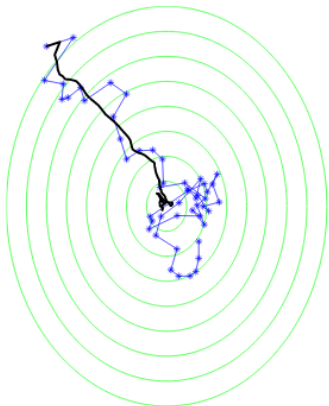


# Optimization in Machine Learning

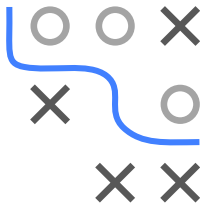
## First order methods

### SGD



#### Learning goals

- SGD
- Stochasticity
- Convergence
- Batch size

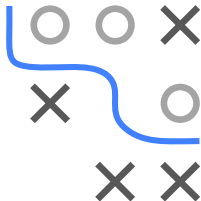




# STOCHASTIC GRADIENT DESCENT / 2

## Algorithm Basic SGD pseudo code

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

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

- for a data set

$$\mathcal{D} = \left( \left( \mathbf{x}^{(1)}, y^{(1)} \right), \dots, \left( \mathbf{x}^{(n)}, y^{(n)} \right) \right)$$

- a loss function  $L(y, f(\mathbf{x}))$ , e.g., L2 loss  $L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$ ,
- and a model class  $f$ , e.g., the linear model  $f(\mathbf{x}^{(i)} \mid \theta) = \theta^\top \mathbf{x}$ .



## SGD IN ML / 2

For large data sets, computing the exact gradient

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

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

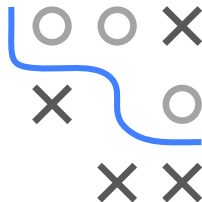
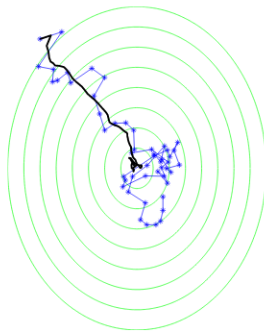
$$\hat{\mathbf{d}} = \frac{1}{m} \sum_{i \in J} \nabla_{\theta} L \left( y^{(i)}, f \left( \mathbf{x}^{(i)} \mid \theta \right) \right),$$

for  $J \subset 1, 2, \dots, n$  random subset.

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



# STOCHASTICITY OF SGD



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.

(Source: Shalev-Shwartz et al., Understanding Machine Learning, 2014.)

# STOCHASTICITY OF SGD / 2

Assume batch size  $m = 1$  (statements also apply for larger batches).

- **(Possibly) suboptimal direction:** Approximate gradient  $\hat{\mathbf{d}} = \nabla_{\mathbf{x}} g_i(\mathbf{x})$  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  $\mathbf{d} = \nabla_{\mathbf{x}} g(\mathbf{x}) = \sum_{i=1}^n \nabla_{\mathbf{x}} g_i(\mathbf{x})$ :

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

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



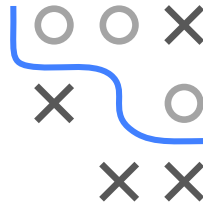
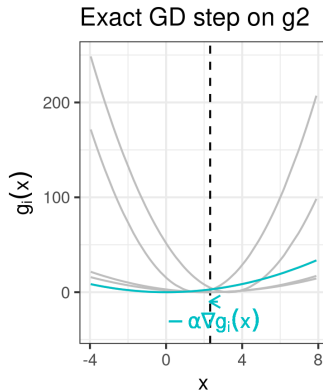
**Example:**  $g(\mathbf{x}) = \sum_{i=1}^5 g_i(\mathbf{x})$ ,  $g_i$  quadratic. Batch size  $m = 1$ .

[illegible]

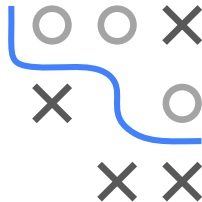
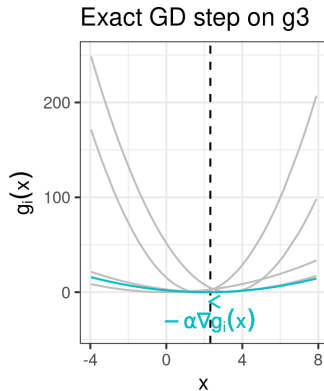
The plot shows a convex function  $g_l(x)$  on a grid. The x-axis ranges from -4 to 8, and the y-axis ranges from 0 to 200. A dashed vertical line is drawn at  $x=2$ , representing the minimum of the function. A red arrow labeled  $-\alpha \nabla g_l(x)$  points from the minimum towards the left, indicating the direction of the subgradient.



**Example:**  $g(\mathbf{x}) = \sum_{i=1}^5 g_i(\mathbf{x})$ ,  $g_i$  quadratic. Batch size  $m = 1$ .

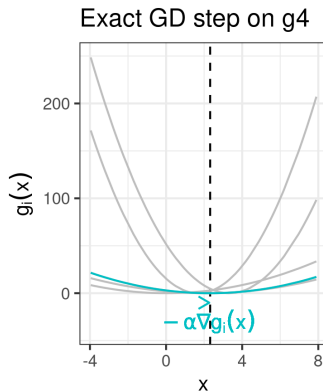
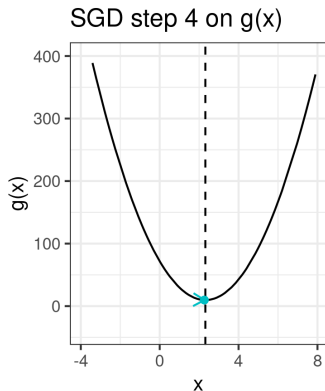


**Example:**  $g(\mathbf{x}) = \sum_{i=1}^5 g_i(\mathbf{x})$ ,  $g_i$  quadratic. Batch size  $m = 1$ .



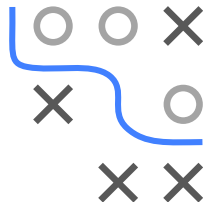
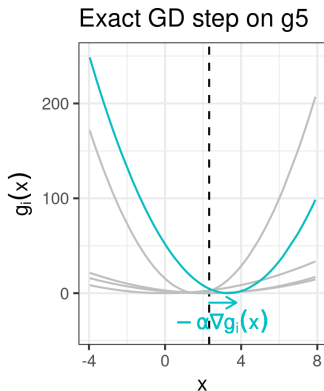
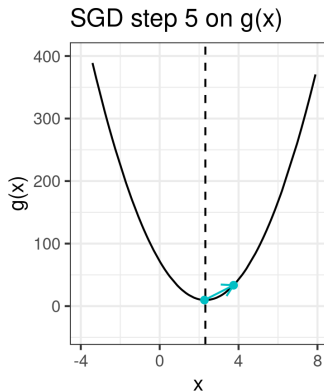
# ERRATIC BEHAVIOR OF SGD

**Example:**  $g(\mathbf{x}) = \sum_{i=1}^5 g_i(\mathbf{x})$ ,  $g_i$  quadratic. Batch size  $m = 1$ .



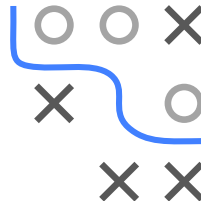
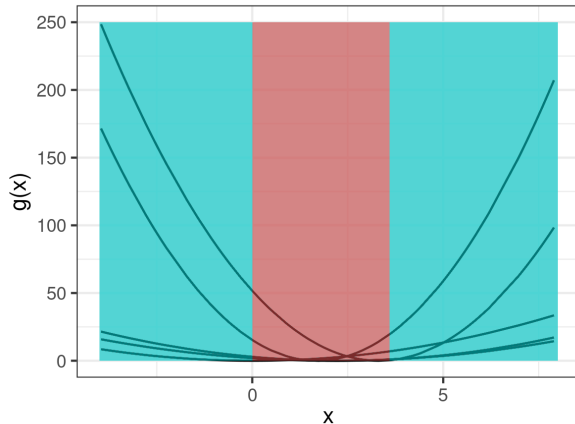
# ERRATIC BEHAVIOR OF SGD

**Example:**  $g(\mathbf{x}) = \sum_{i=1}^5 g_i(\mathbf{x})$ ,  $g_i$  quadratic. Batch size  $m = 1$ .



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

# ERRATIC BEHAVIOR OF SGD



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

**Red area** (“confusion area”):  $-\nabla g_i(\mathbf{x})$  might point away from minimum and perform a suboptimal move.



# CONVERGENCE OF SGD

As a consequence, SGD has worse convergence properties than GD.

**But:** Can be controlled via **increasing batches** or **reducing step size**.

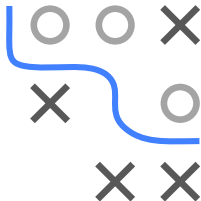
**The larger the batch size  $m$**

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

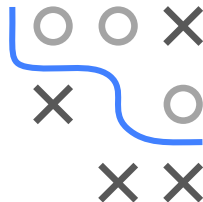
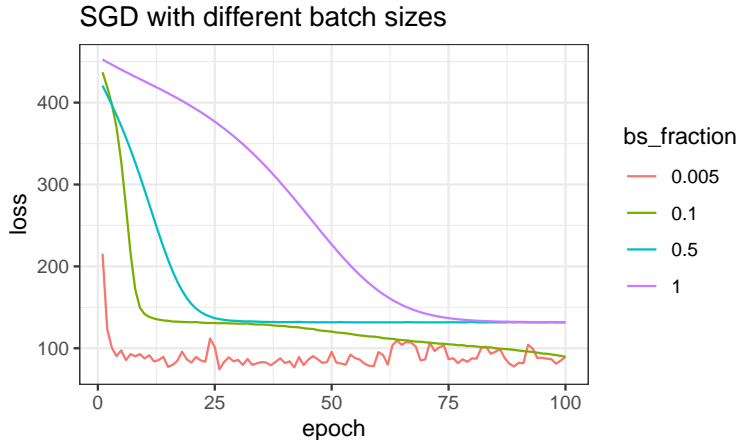
**The smaller the step size  $\alpha$**

- 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.