

Introduction to Deep Learning

Chapter 2: Basic Training

Bernd Bischl

Department of Statistics – LMU Munich WS 2021/2022



TRAINING NEURAL NETWORKS

Training of neural nets is composed of two iterative steps:

- Forward pass: The information of the inputs flows through the model to produce a prediction. Based on this prediction, the empirical loss is computed.
- Backward pass: The information of the prediction error flows backward through the network to update the weights in a way that the error reduces.

Recall: The error is calculated via a loss function $L(y, f(\mathbf{x}, \theta))$, where y and $f(\mathbf{x}, \theta)$ are the true target and the network outcome respectively.

TRAINING NEURAL NETWORKS

• For regression, the L2 loss is typically used:

$$L(y, f(\mathbf{x})) = \frac{1}{2}(y - f(\mathbf{x}))^2$$

• For classification, the binary/categorical cross entropy:

$$L(y, f(\mathbf{x})) = y \log f(\mathbf{x}) + (1 - y) \log(1 - f(\mathbf{x}))$$

Note: Evaluated the loss on the data, the risk function is computed:

$$\mathcal{R}_{\mathsf{emp}} = \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)}\right)\right)$$

TRAINING NEURAL NETWORKS

To minimize the risk, the **gradient descent** (GD) method can be used.

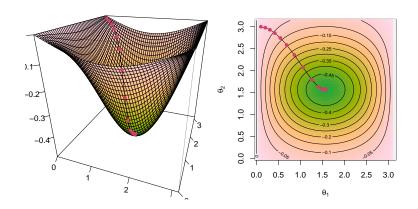
- First, we calculate the gradient $\nabla \mathcal{R}$ at a point $\theta^{[t]}$.
- "Standing" at $\theta^{[t]}$, we then improve the minimization by performing the following update:

$$oldsymbol{ heta}^{[t+1]} = oldsymbol{ heta}^{[t]} - lpha
abla \mathcal{R}\left(oldsymbol{ heta}^{[t]}
ight)$$
 .

ullet α determines the length of the step and is called the **learning rate**.

Note: Since $\nabla \mathcal{R}$ always points in the direction of the steepest ascent, $-\nabla \mathcal{R}$ always points in the direction of the steepest descent!

EXAMPLE: GRADIENT DESCENT



"Walking down the hill, towards the valley."

WEIGHT UPDATES WITH BACKPROPAGATION

• To update each weight $w \in \theta$ in the network, we need their gradients with regards to the risk.

 Since weights are stacked in layers inside the network, we need to repeatedly apply the "chain rule of calculus". This process is called backpropagation.

• After obtaining the gradients, the weights can be updated by GD:

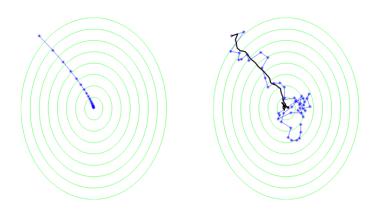
$$\boldsymbol{\theta}^{[t+1]} = \boldsymbol{\theta}^{[t]} - \alpha \cdot \frac{1}{n} \cdot \sum_{i=1}^{n} \nabla_{\theta} L\left(y^{(i)}, f(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}^{[t]})\right)$$

STOCHASTIC GRADIENT DESCENT

- Optimization algorithms that use the entire training set to compute updates in one huge step are called **batch** or **deterministic**. This is computationally very costly or often impossible.
- Instead of running the sum over the whole dataset (batch mode),
 one can run over small subsets (minibatches) of size m.
- With minibatches of size m, a full pass over the training set (called an **epoch**) consists of $\frac{n}{m}$ gradient updates.
- This stochastic version of the batch gradient is known as Stochastic Gradient Descent (SGD).

STOCHASTIC GRADIENT DESCENT

An illustration of the SGD algorithm: on the left is GD and on the right is SGD. The black line depicts the averaged value of θ .



source : Shalev-Shwartz and Ben-David. Understanding machine learning: From theory to algorithms. Cambridge University
Press. 2014.

STOCHASTIC GRADIENT DESCENT

Algorithm Basic SGD pseudo code

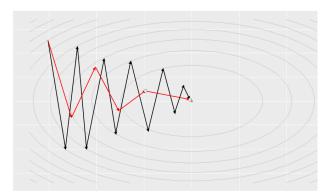
- 1: Initialize parameter vector $\theta^{[0]}$
- 2: $t \leftarrow 0$
- 3: while stopping criterion not met do
- 4: Randomly shuffle data and partition into minibatches $J_1, ..., J_K$ of size m
- 5: for $k \in \{1, ..., K\}$ do
- 6: $t \leftarrow t + 1$
- 7: Compute gradient estimate with J_k :

$$\hat{g}^{[t]} \leftarrow \frac{1}{m} \sum_{i \in J_k} \nabla_{\theta} L(y^{(i)}, f(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}^{[t-1]}))$$

- 8: Apply update: $\theta^{[t]} \leftarrow \theta^{[t-1]} \alpha \hat{g}^{[t]}$
- 9: end for
- 10: end while

SGD WITH MOMENTUM

- While SGD remains a popular optimization strategy, learning with it can sometimes be slow.
- Momentum is designed to accelerate learning, by accumulating an exponentially decaying moving average of past gradients.



GD (black) versus momentum (red) when dealing with ravines