

Introduction to Deep Learning

Chapter 7: Basic Regularization

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Winter term 2021



TRAINING NEURAL NETWORKS

Training of neural nets is composed of two iterative steps:

- ➊ **Forward pass:** The information of the inputs flows through the model to produce a prediction. Based on this prediction, the empirical loss is computed.
- ➋ **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 $L(y, f(x, \theta))$, where y and $f(x, \theta)$ 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:

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

TRAINING NEURAL NETWORKS

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

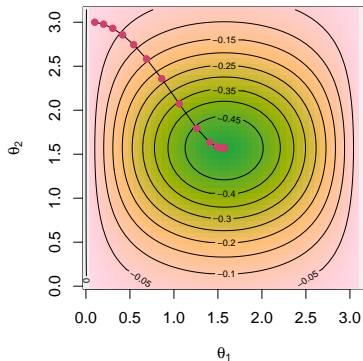
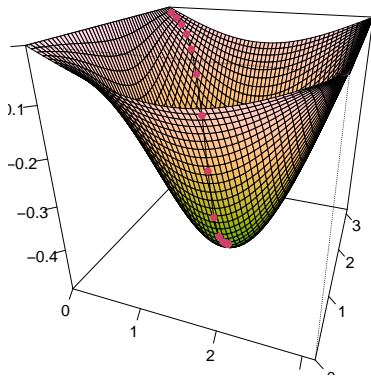
- First, we calculate the gradient $\nabla \mathcal{R}$ at a point $\theta^{[t]}$.
- “Standing” at $\theta^{[t]}$, we then improve the minimization by performing the following update:

$$\theta^{[t+1]} = \theta^{[t]} - \alpha \nabla \mathcal{R} \left(\theta^{[t]} \right).$$

- 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:

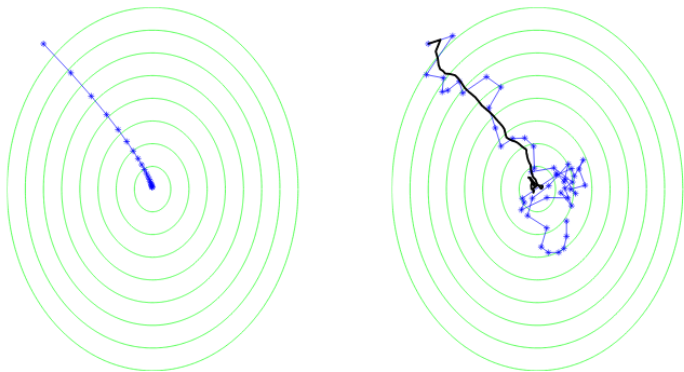
$$\theta^{[t+1]} = \theta^{[t]} - \alpha \cdot \frac{1}{n} \cdot \sum_{i=1}^n \nabla_{\theta} L \left(y^{(i)}, f(\mathbf{x}^{(i)} \mid \theta^{[t]}) \right)$$

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

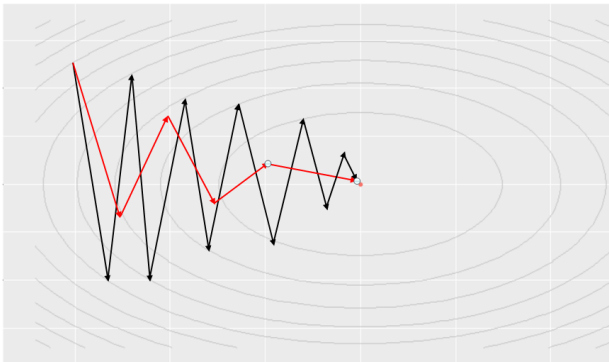
- 1: Initialize parameter vector $\theta^{[0]}$
- 2: $t \leftarrow 0$
- 3: **while** stopping criterion not met **do**
- 4: Randomly shuffle data and partition into minibatches J_1, \dots, J_K of size m
- 5: **for** $k \in \{1, \dots, K\}$ **do**
- 6: $t \leftarrow t + 1$
- 7: Compute gradient estimate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

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

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

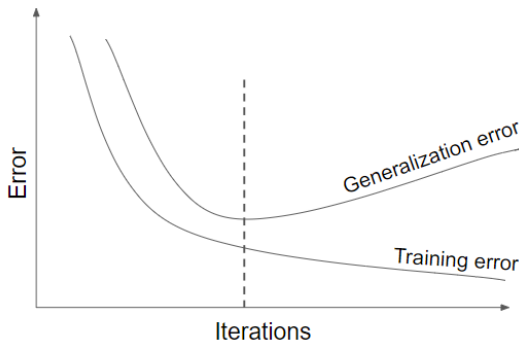
- While SGD remains a popular optimization strategy, learning with it can sometimes be slow.
- Momentum is designed to accelerate learning, by accumulating an exponentially decaying moving average of past gradients.



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

EARLY STOPPING

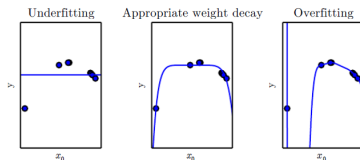
- When training with an iterative optimizer, it is commonly the case that after a certain number of iterations, generalization error begins to increase even though training error continues to decrease.
- **Early stopping** refers to stopping the algorithm, before the generalization error increases, i.e., before the algorithm begins to overfit.



FURTHER REGULARIZATION STRATEGIES

Parameter penalties

- Same as Ridge Regression/L2-Regularization
- Often referred to as *weight decay* since weights are pulled to zero if they are not updated by large enough values.



FURTHER REGULARIZATION STRATEGIES

Dropout

- Force the network to generalize by reducing its capacity to memorize data.
- Each neuron has a fixed probability to be deactivated at each training step.

