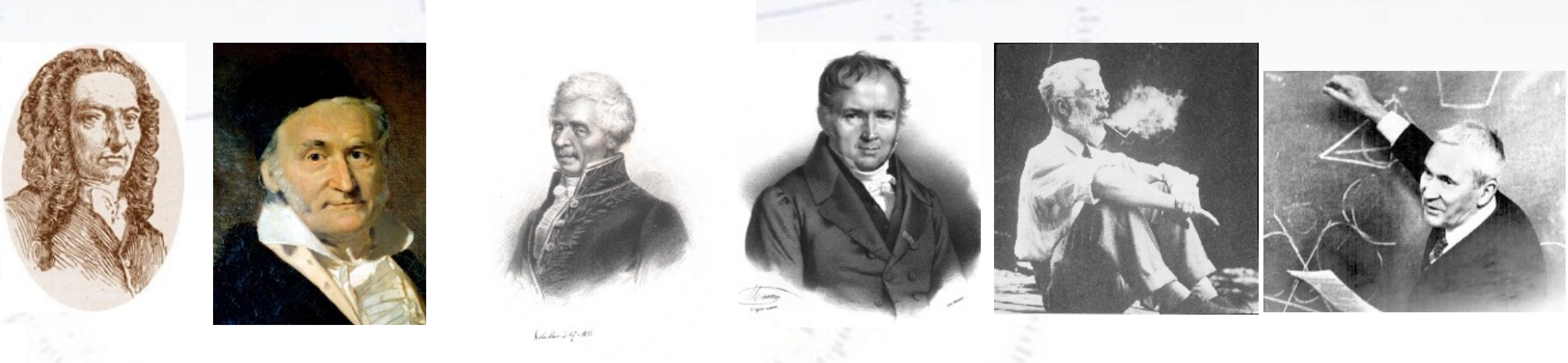
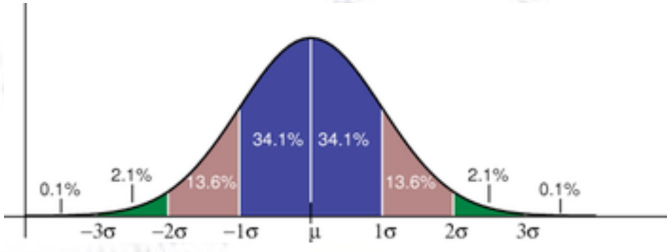
Applied ML

Stochastic Gradient Descent



Troels C. Petersen (NBI)



"Statistics is merely a quantisation of common sense - Machine Learning is a sharpening of it!"

(Normal) Gradient Descent

The choice of loss function, L, depends on the problem at hand, and in particular what you find important! You want to minimise this with respect to the model parameters θ:

$$L(\theta) = \frac{1}{N} \sum_{i}^{N} L_i(\theta)$$

In order to find the optimal solution, one can use Gradient Descent, typically **based on the whole dataset**:

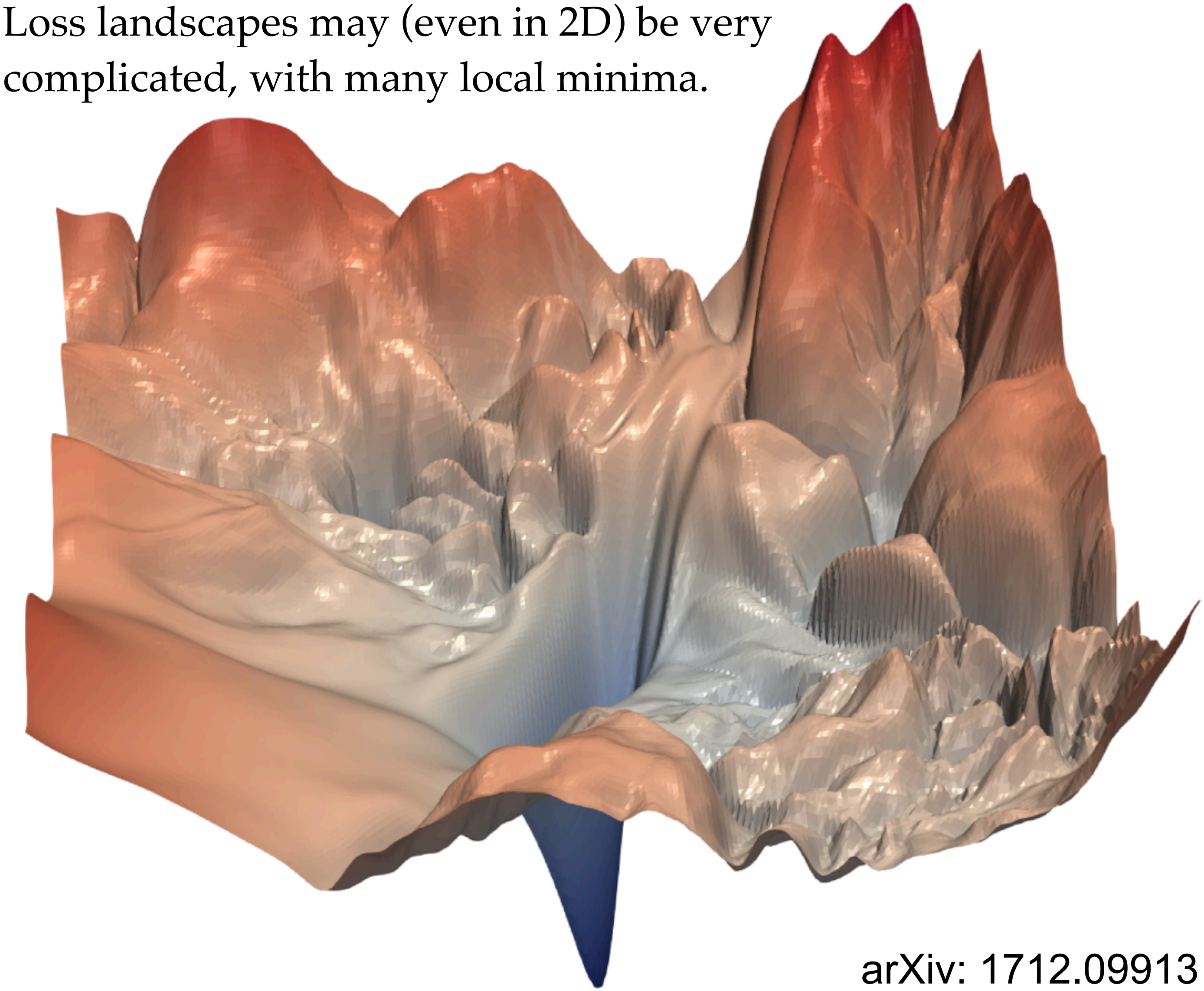
$$\theta_{j+1} = \theta_j - \eta \nabla L(\theta) = \theta_j - \frac{\eta}{N} \sum_{i}^{N} \nabla L_i(\theta)$$

This is the procedure used by e.g. Minuit and other minimisation routines.

Note the very important parameter: **Learning rate η**.

(Nasty) Loss Landscapes

Loss landscapes may (even in 2D) be very complicated, with many local minima.



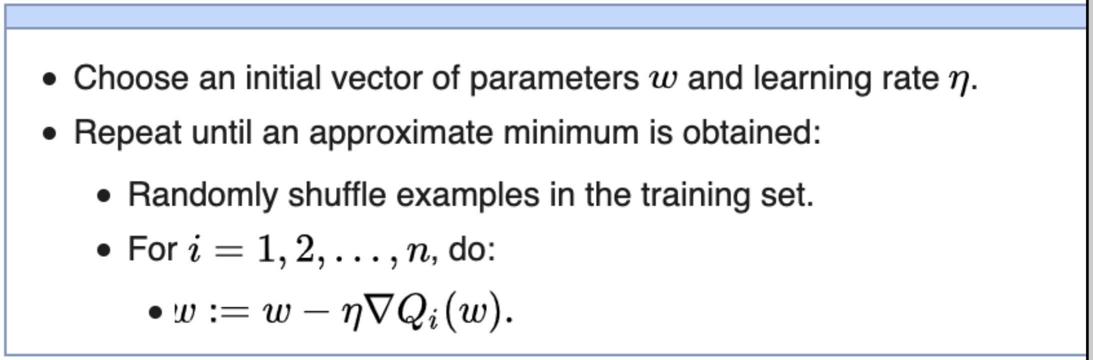
arXiv: 1712.09913

Stochastic Gradient Descent

In order to give the gradient descent some degree of “randomness” (stochastic), one evaluates the below function **for small batches** instead of the full dataset.

$$\theta_{j+1} = \theta_j - \eta \nabla L(\theta) = \theta_j - \frac{\eta}{N} \sum_i^N \nabla L_i(\theta)$$

The algorithm thus becomes:



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• Choose an initial vector of parameters $w$ and learning rate $\eta$.
• Repeat until an approximate minimum is obtained:
    • Randomly shuffle examples in the training set.
    • For $i = 1, 2, \ldots, n$, do:
        • $w := w - \eta \nabla Q_i(w)$.
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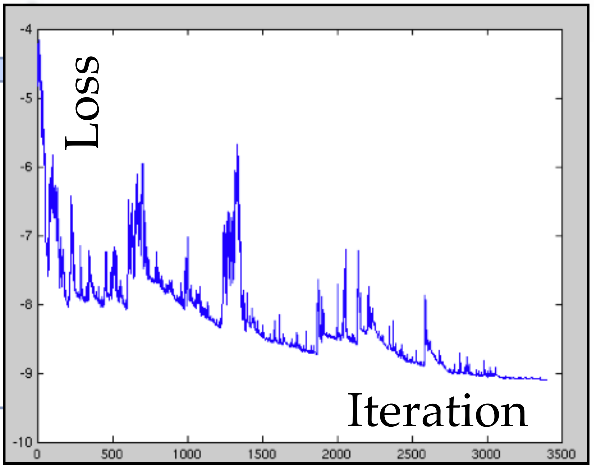


Not only does this vectorise well and gives smoother descents, but with decreasing learning rate, **it “almost surely” finds the global minimum** (Robbins-Siegmund theorem).

Example

Consider fitting a straight line $y_{hat} = \theta_1 + \theta_2$ x, given features (x_1, x_2, …, x_n) and estimated responses (y_1, y_2, …, y_n) using least squares. The Loss function is then:

$$L(\theta) = \sum_i^N L_i(\theta) = \sum_i^N (\hat{y}_i - y_i)^2 = \sum_i^N (\theta_1 + \theta_2 x_i - y_i)^2$$

To minimise this, we could consider stochastic gradient descent, where for each iteration, we only evaluate the gradient in a small batch (or single point):

$$\left[\begin{array}{c}\theta_1\\ \theta_2\end{array}\right]_{j+1} = \left[\begin{array}{c}\theta_1\\ \theta_2\end{array}\right]_j - \eta \left[\begin{array}{c}\frac{\partial}{\partial\theta_1}(\theta_1 + \theta_2 x_i^2 - y_i)^2\\ \frac{\partial}{\partial\theta_2}(\theta_1 + \theta_2 x_i^2 - y_i)^2\end{array}\right]_j$$

The learning rate and batch size are the two Hyper Parameters, where it is the learning rate, that is the most important.

https://en.wikipedia.org/wiki/Stochastic_gradient_descent

Choosing Learning Rate

Too low learning rate: Convergence very (too) slow.
Too high learning rate: Random jumps and no convergence.
You want to increase it until it fails and then just below…

Ristet brød er let at lave
blot man vil erindre:
når det oser, skal det have
to minutter mindre.

Piet Hein

There's an art of knowing when.// Never try to guess.// Toast until it smokes and then// twenty seconds less.

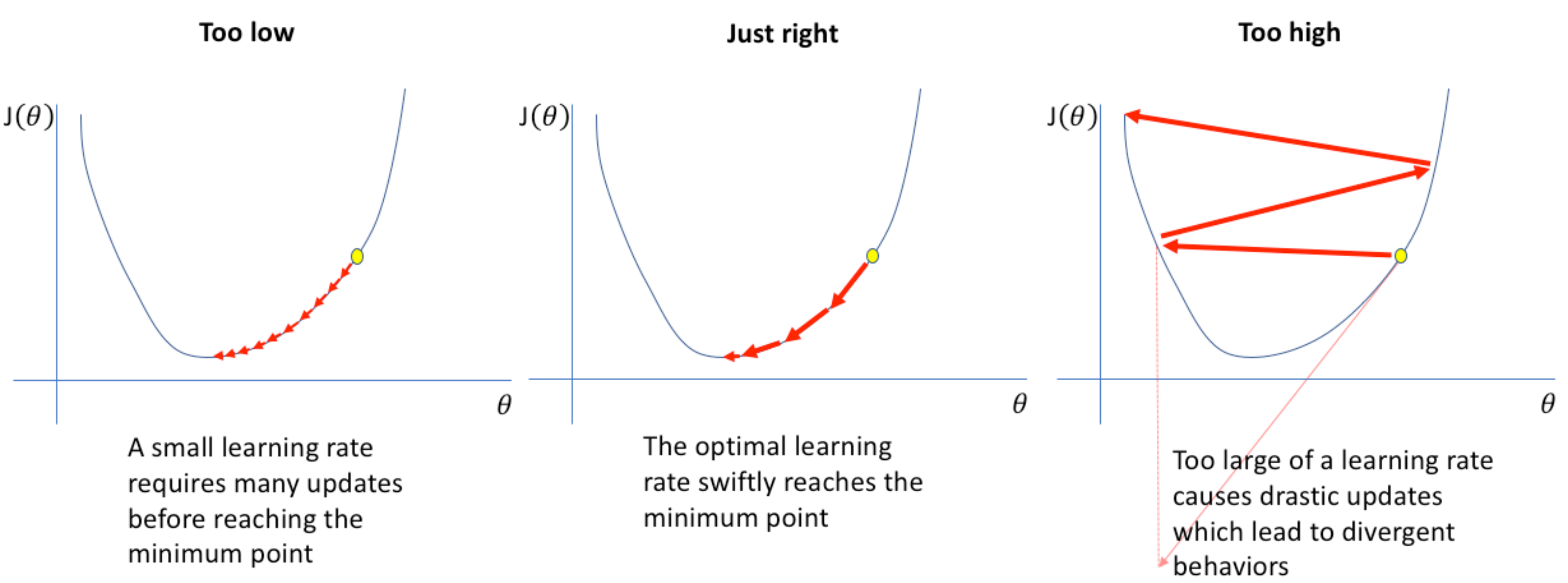
Learning Rate Schedulers

But, there is **no reason to consider a fixed value for the learning rate**!

More practically, one would typically adapt the learning rate to the situation:

- When exploring: Use larger learning rate.
- When exploiting: Use lower learning rate (when converging).

Below is illustrated what happens, when the learning rate is right/wrong.



A small learning rate requires many updates before reaching the minimum point

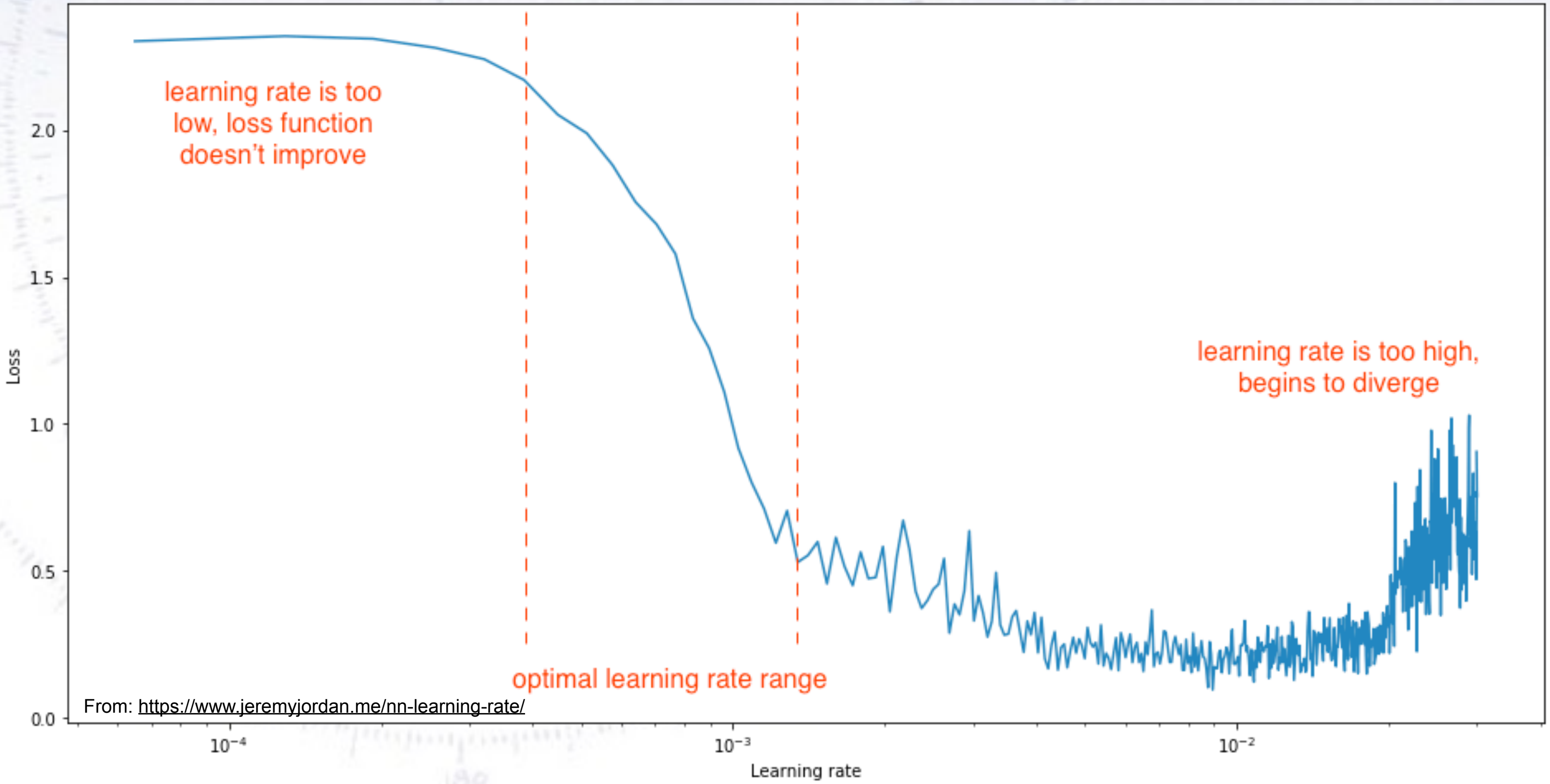
The optimal learning rate swiftly reaches the minimum point

Too large of a learning rate causes drastic updates which lead to divergent behaviors

From: https://www.jeremyjordan.me/nn-learning-rate/

Learning Rate Schedulers

First, we want to investigate, which learning rates are relevant (and best) for our problem. **The best learning rate is when the loss decreases the fastest**. Thus we look for the greatest slope of the loss as a function of learning rate:



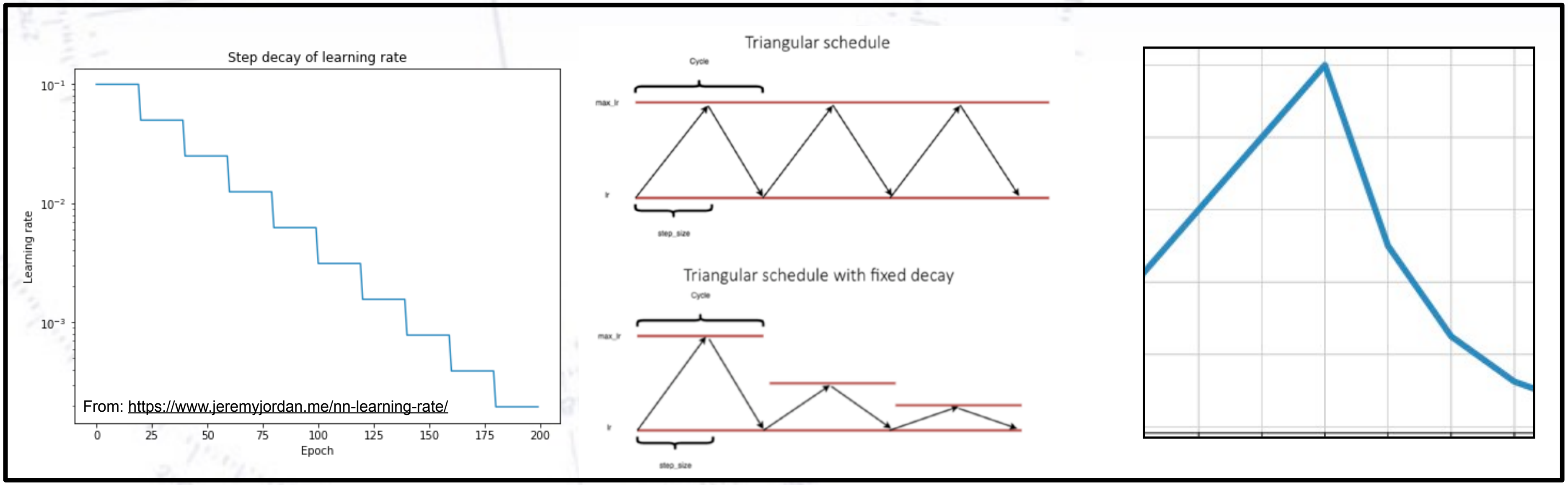
From: https://www.jeremyjordan.me/nn-learning-rate/

Learning Rate Schedulers

For this reason, Learning Rate Schedulers have been “invented”.

There are MANY different types, and as usual, there is no “right answer”.

However, it is fair to say, that the learning rate is (especially for NNs) the most important Hyper Parameter, and thus it **requires attention**.



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