Optimization and Training Techniques

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Outline

- Optimization Algorithms

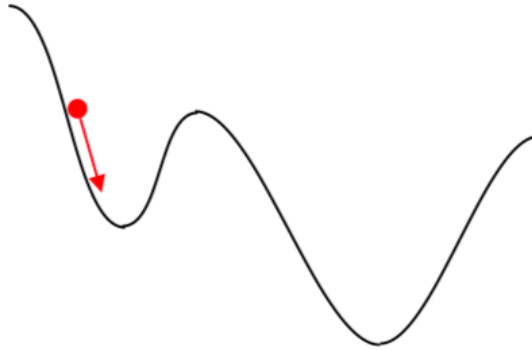- Training Techniques

Stochastic Gradient Descent (SGD)

- Suppose $\boldsymbol{w}$ is the parameter to optimize. The updating in SGD is

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - lr * \nabla f(\boldsymbol{w}_t)$$
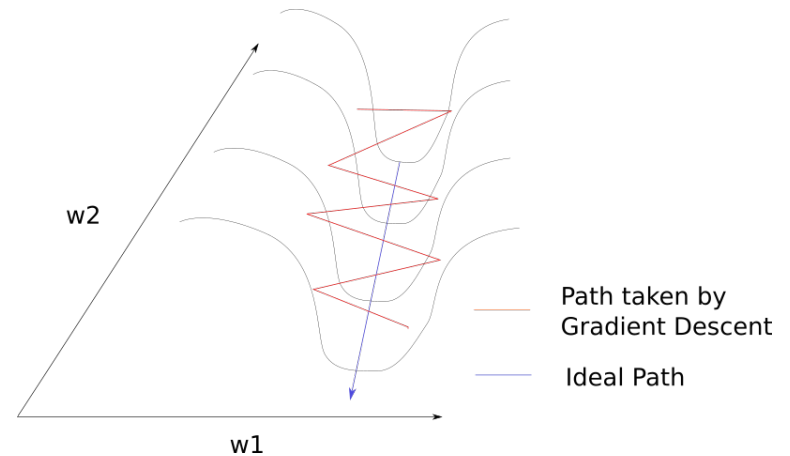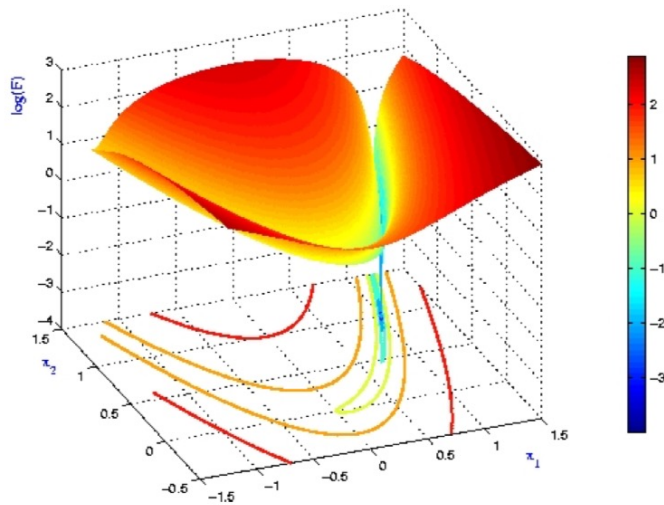
- $\nabla f(\boldsymbol{w})$ is the stochastic gradient of the loss $\mathcal{L}$, estimated with only partial training data

- lr is the learning rate

- Problems with SGD

  ➢ Very easy to get stuck at local optima

  ➢ Slow convergence due to the pathological curvature in NNs
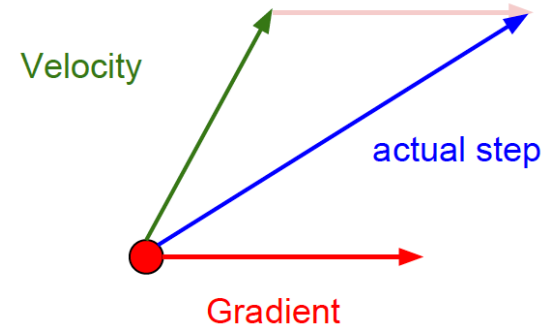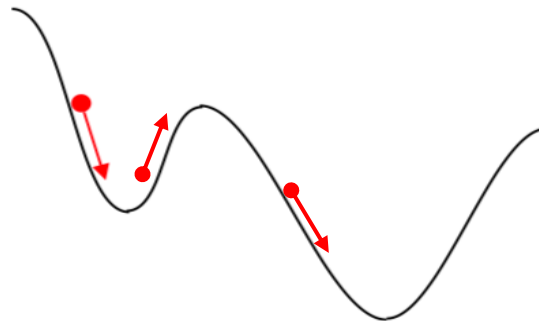
SGD + Momentum

- Updating equation

$$\boldsymbol{v}_t = \rho \boldsymbol{v}_{t-1} + \nabla f(\boldsymbol{w}_t)$$

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - lr \cdot \boldsymbol{v}_t$$

Velocity

actual step

Gradient

where $\rho \in (0,1)$ is the decay rate, often chosen as 0.9, 0.95, 0.99

The updating process can be *understood as a ball falling down from a rugged hillside*, with the friction strength proportional to ρ
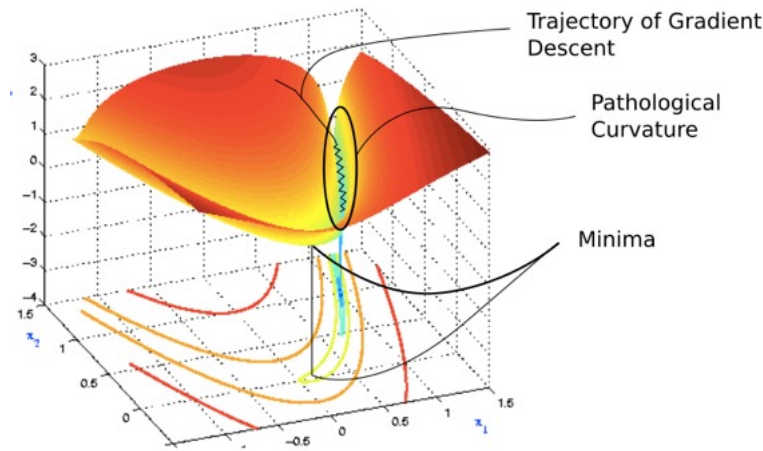
RMSProp

- Updating equation

$$s_t = \rho \cdot s_{t-1} + (1-\rho)\big(\nabla f(w_t)\big)^2$$

$$w_{t+1} = w_t - lr \cdot \nabla f(w_t) \oslash \sqrt{s_t}$$

where s_t is the weighted average of squared gradients until the current time step; $\oslash$ denotes elementwise division

It *rescales the gradients of different dimensions to the same level*, alleviating the pathological curvature problem

Supplement: Moving average

$$s_1 = \rho \cdot s_0 + (1 - \rho)\big(\nabla f(\boldsymbol{w}_1)\big)^2$$

$$s_2 = \rho^2 \cdot s_0 + \rho(1 - \rho)\big(\nabla f(\boldsymbol{w}_1)\big)^2 + (1 - \rho)\big(\nabla f(\boldsymbol{w}_2)\big)^2$$

Weighting

$$s_3 = \rho^3 \cdot s_0 + \rho^2(1 - \rho)\big(\nabla f(\boldsymbol{w}_1)\big)^2 + \rho(1 - \rho)\big(\nabla f(\boldsymbol{w}_2)\big)^2 + (1 - \rho)\big(\nabla f(\boldsymbol{w}_3)\big)^2$$

$$\vdots$$

The weights are decaying for earlier records

It can be verified that all weights are summed to be 1, that is

$$(1 - \rho) + \rho(1 - \rho) + \rho^2(1 - \rho) + \rho^3(1 - \rho) + \cdots$$

$$= \frac{1 - \rho^n}{1 - \rho}(1 - \rho) \rightarrow 1$$

Adam

- Updating equation

$$\boldsymbol{m}_t = \beta_1 \cdot \boldsymbol{m}_{t-1} + (1 - \beta_1)\nabla f(\boldsymbol{w}_t)$$

$$\boldsymbol{s}_t = \beta_2 \cdot \boldsymbol{s}_{t-1} + (1 - \beta_2)\big(\nabla f(\boldsymbol{w}_t)\big)^2$$

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - lr \cdot \boldsymbol{m}_t \oslash \sqrt{\boldsymbol{s}_t}$$

Same as RMSProp, except the $\boldsymbol{m}_t$

where $\boldsymbol{m}_t$ is the moving average of the past gradients

A modified version of RMSProp, with *the the exact gradient $\nabla f(\boldsymbol{w}_t)$ replaced by its moving average $\boldsymbol{m}_t$*

- Default settings: $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $lr = 10^{-3}$
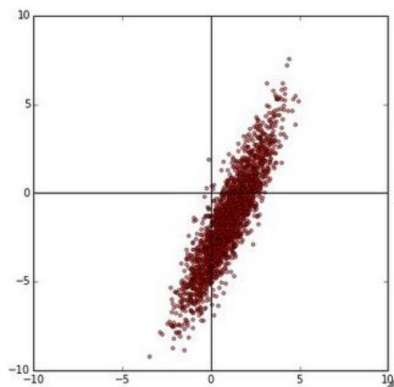
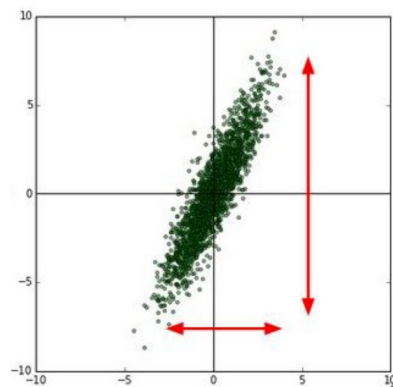- By setting $\beta_1 = 0$, Adam is degenerated to RMSProp

Outline

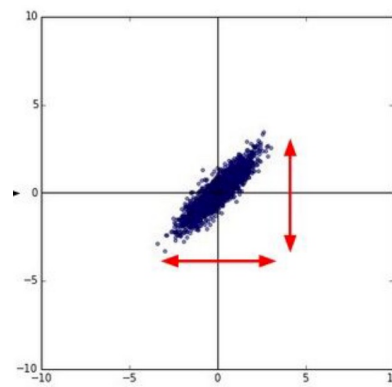- Optimization Algorithms

- Training Techniques

Preprocessing

- Commonly used data preprocessing methods:

  1) Centering the data, *i.e.* subtracting the data mean

  2) Normalizing the variance for each dimension
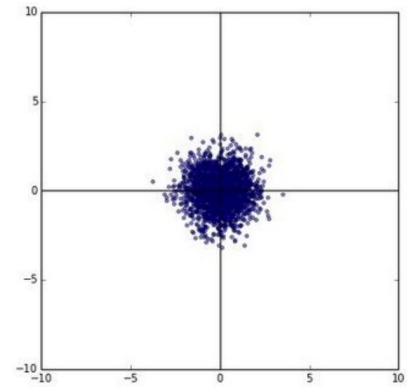
  3) Whitening the data

| Original | Centered | Variance Normalized | Whitened |

- Up to the characteristics of data, we may use one or several

  methods above to preprocess the data

- Why centering and normalizing operations are helpful?

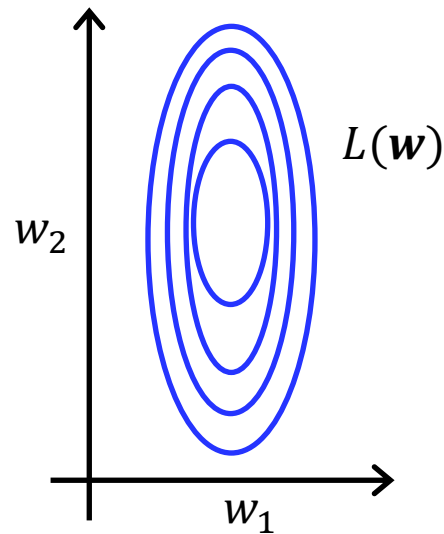 Let's take the linear regression problem as the example

  ➢ The features in original data have very different scales

Size (feet) x_1	# bedrooms x_2	# floors x_3	# years (Ages) x_4	Price ($ 1000) y
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178

  ➢ Under the case, the loss function is

$$L(\boldsymbol{w}) = \frac{1}{n} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2$$

➤ Obviously, the cost function $L(\boldsymbol{w})$ decreases at different rates for different dimensions

This results in the *slow convergence* of gradient descent. *Why??*

➤ If the features are preprocessed to similar scales, then the loss function looks like
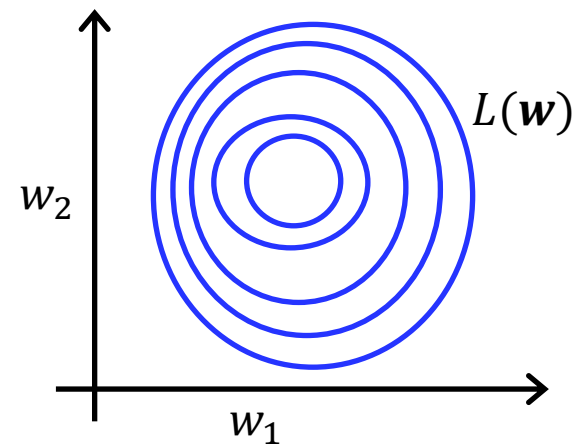
Initialization

1) Initializing the weights of all layers by the random samples drawn from fixed Gaussian distribution, *e.g.*

$$W \sim \mathcal{N}(0, 0.01^2)$$

➢ It works well for neural networks that are not too deep (*e.g.* layer $\# < 8$)

➢ If ReLU is used as the activation function, some people also suggest to use the truncated Gaussian distribution, *i.e.*

$$W \sim \mathcal{N}_T(0, 0.01^2)$$

2) When the network goes deeper, it can then be initialized by a Gaussian $W \sim \mathcal{N}(0, \sigma_i^2)$ with the variance of each layer *inversely proportional to the number of neurons* in the previous layer, *i.e.*

$$\sigma_i = \frac{1}{\sqrt{\# \, neurons \, in \, (i-1)\text{th} \, layer}}$$

Hyper-parameter Tuning

- There are a lot of parameters that need to be set before starting the training, such as the learning rate, decay parameters in RMSprop and Aadm, dropout rate *etc*

- To set appropriate values for these hyper-parameters, we need to split the whole dataset into three parts, *i.e.* training set, validation set, and test set


Training set   Validation set   Test set
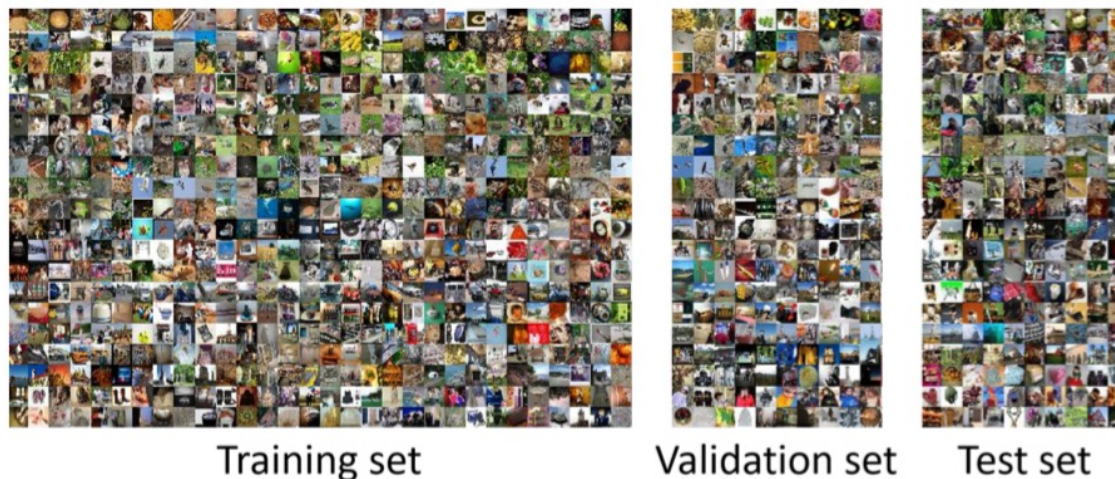
- Train the model on the training set

- Tune the hyper-parameters according to the performance on the validation set

- Test the performance on the test set, and report it as the final performance

- The hyper-parameters are not tuned blindly, but instead can be chosen according to some guidelines

  1) First try some default values that perform well on many tasks

  2) Choose values based on phenomenon observed during training
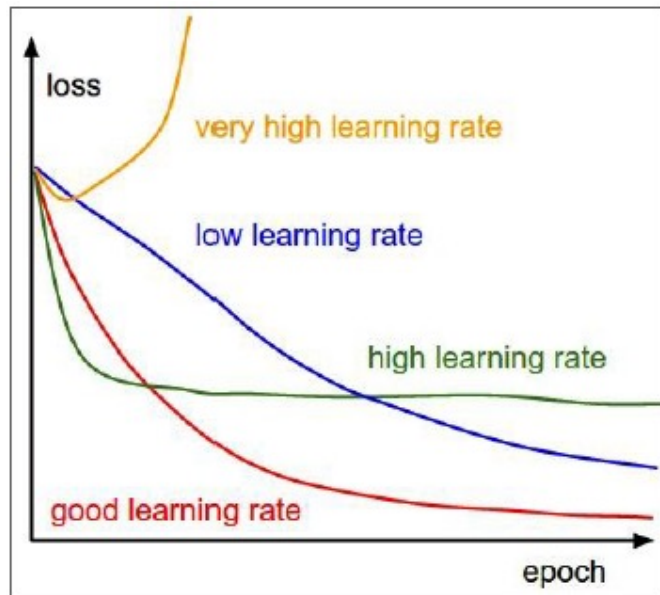
The training loss curve implies the possible range of good learning rate
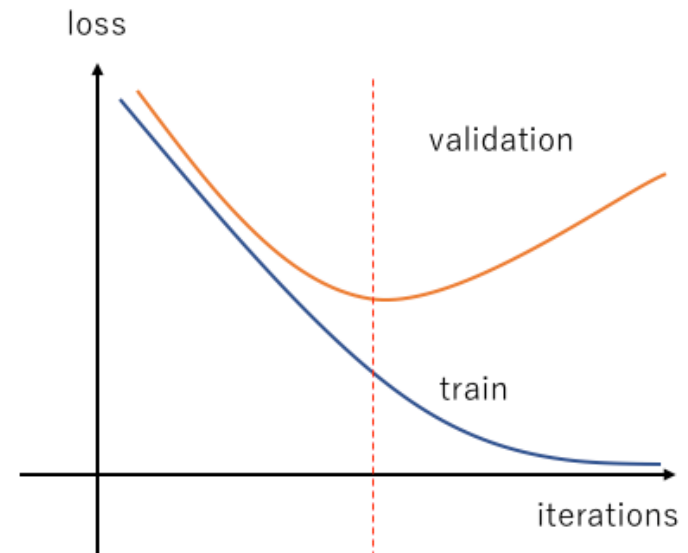
The relation between performance on training and validation sets indicates the model is too flexible