Feed Forward Neural Networks

Machine Learning

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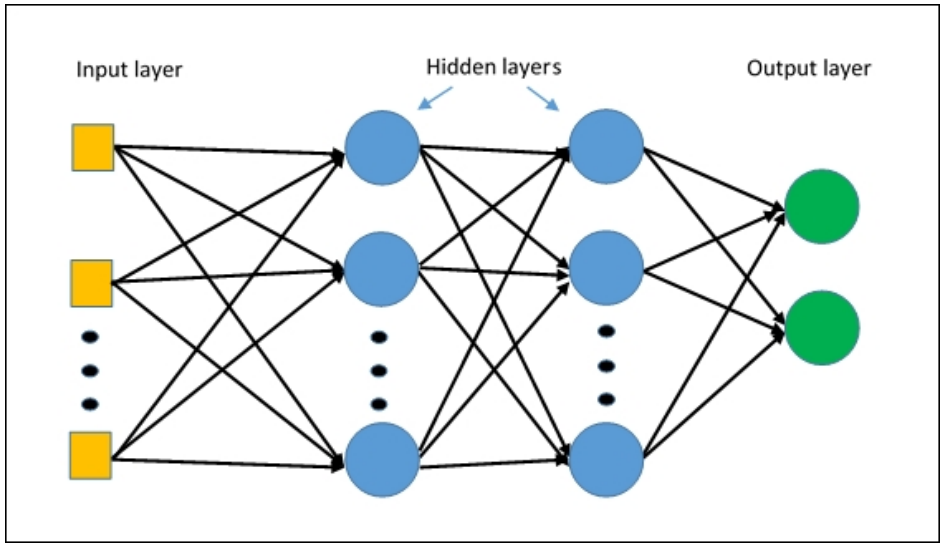
General Architecture

NN as a composition of functions

$$F(x) = f_{w_n} \circ f_{w_{n-1}} \circ ..f_{w_1}(x)$$



Composition of linear functions

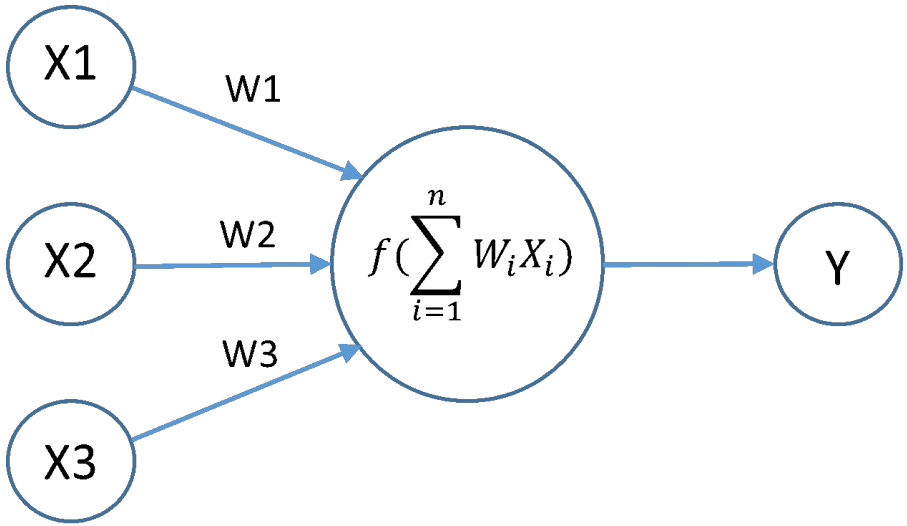
$$F(x) = XW_1W_2$$

where $X \in R^{NxD_1}$ - features
$W_1 \in R^{D_1xD_2}$, $W_2 \in R^{D_2xK}$ - weight matrices
K - number of classes

Neuron

$$y = \sum_{i=1}^{N} f(w_j i x_i + b)$$

where f - some non-linear activation function
w_i - learnable weights
b - learnable bias, usually incorporated into X
y - output of neuron
x - input of neuron

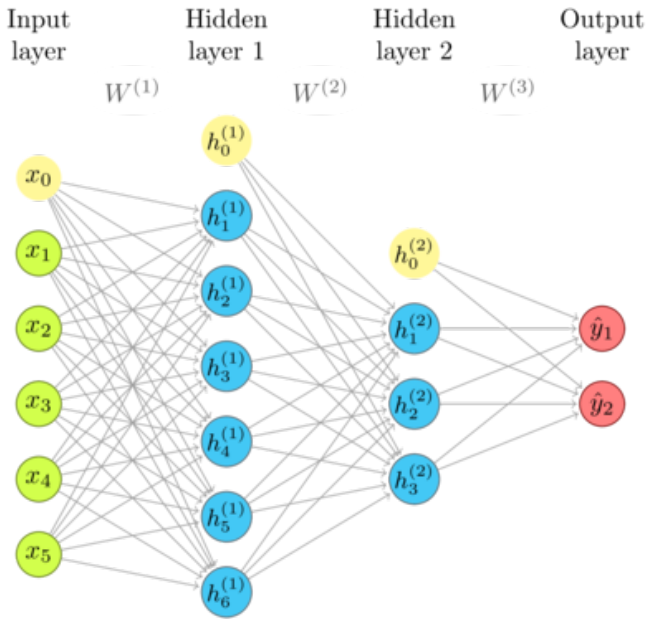


Dense Layers

It's more convenient to express the same thing in vector form

$$Y = f(XW)$$

where $X \in R^{NxD_1}$ - input of layer
$Y \in R^{NxD_2}$ - output of layer
$W \in R^{D_1 xD_2}$ - learnable weight matrix



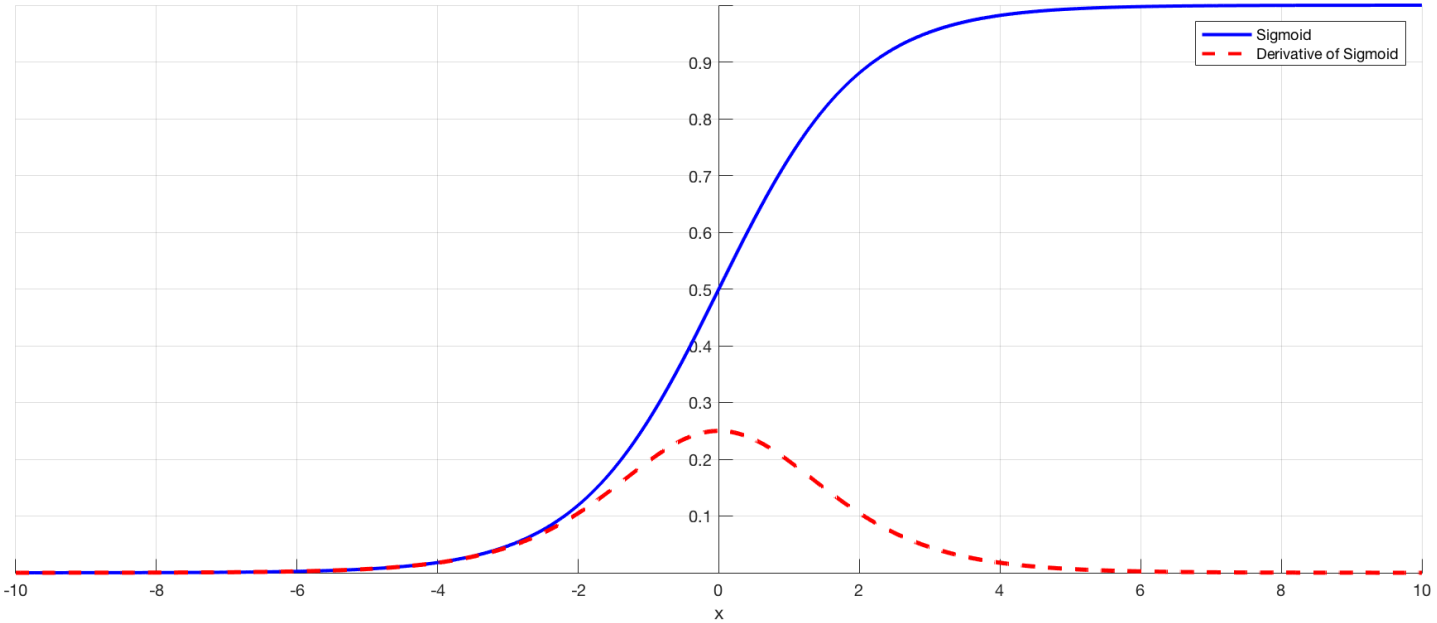
Activation Functions

Why we do not use linear activations?
Activation functions supposed to be nice in the sense of gradient properties.

Sigmoid

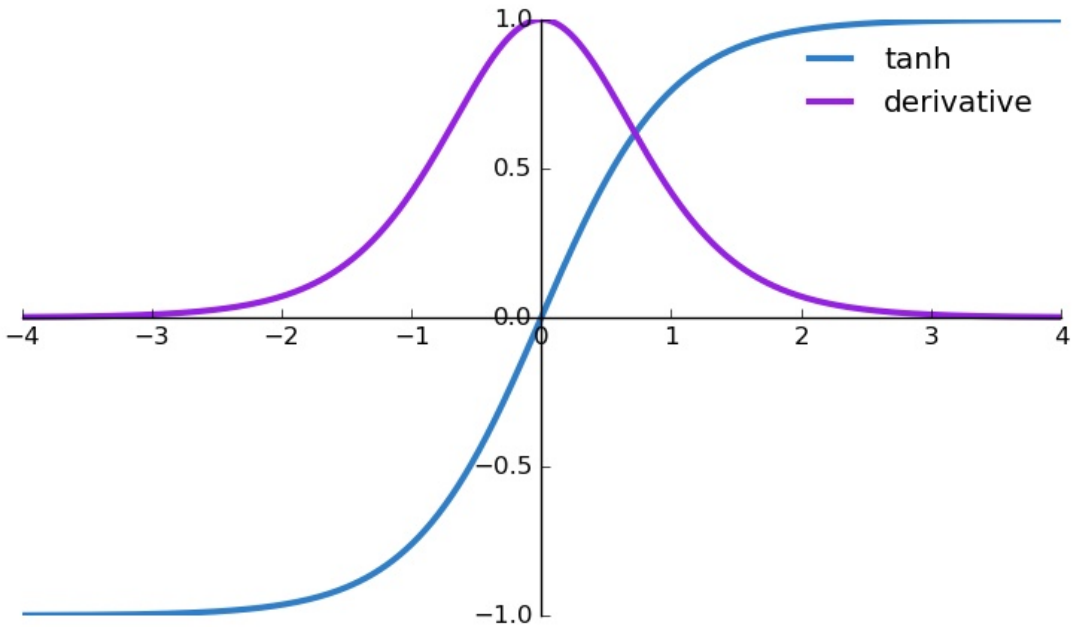
$$\sigma(z) = \frac{1}{1 + \exp^{-z}}$$

- vanishing gradient
- bad output distribution



Tanh

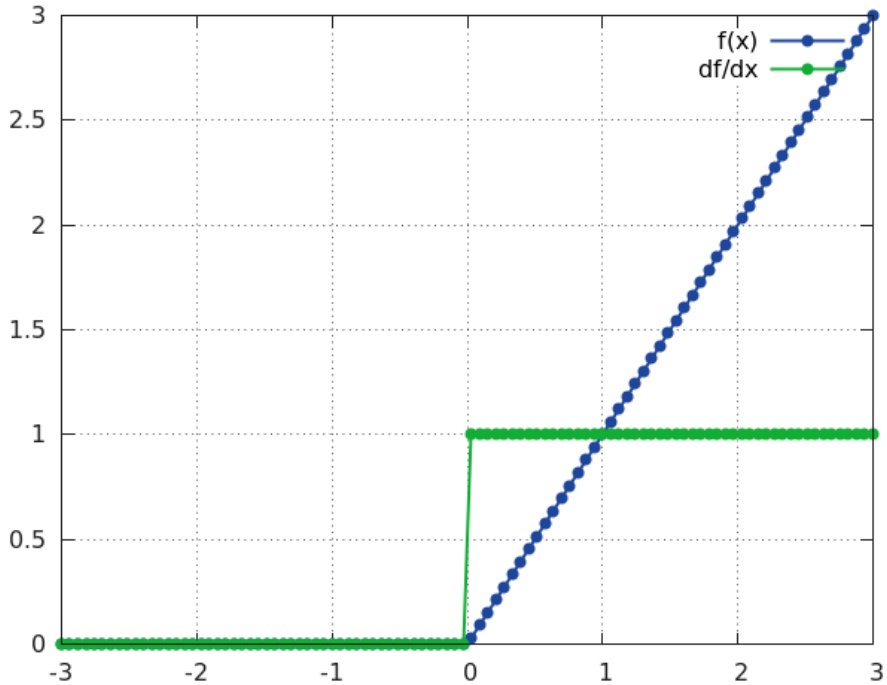
- vanishing gradient



RELU

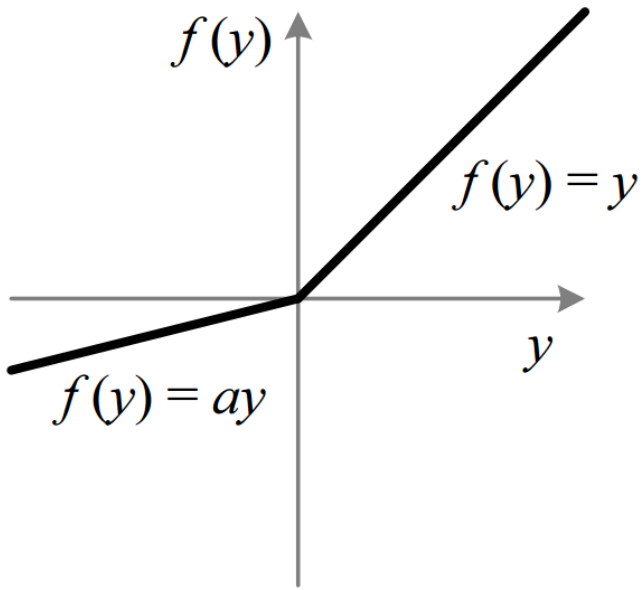
$$RELU(z) = \max(0, z)$$

- dead neurons if $z < 0$



PRELU

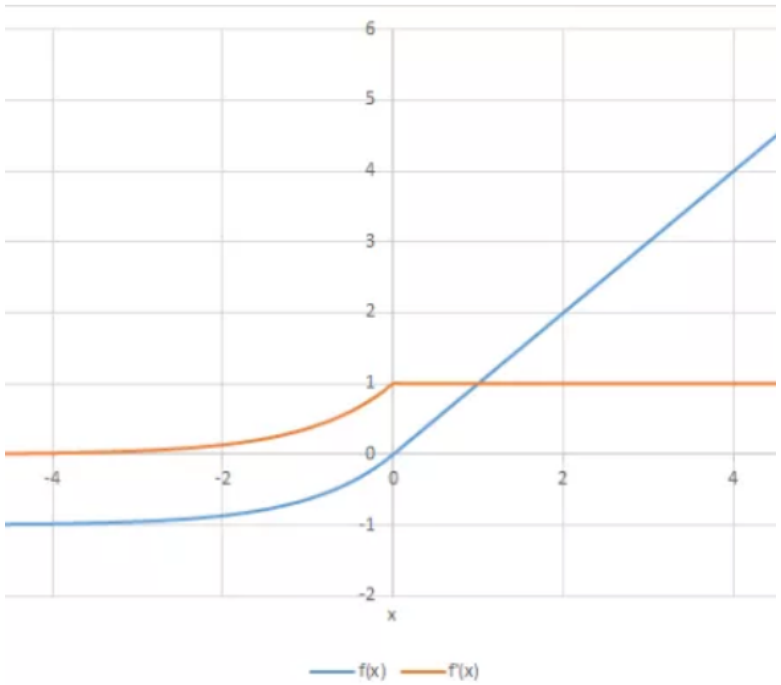
$$PRELU(z) = \begin{cases} z, & \text{if } z \geq 0 \\ \alpha z, & \text{if } z < 0 \end{cases} \tag{1}$$



ELU

$$ELU(z) = \begin{cases} z, & \text{if } z \geq 0 \\ \alpha(\exp^z - 1), & \text{if } z < 0 \end{cases} \tag{2}$$

- little longer computation than RELU



Weight initialization

As we train out neural network with gradient descent, it is important to have good initial point to start. Usually use use:

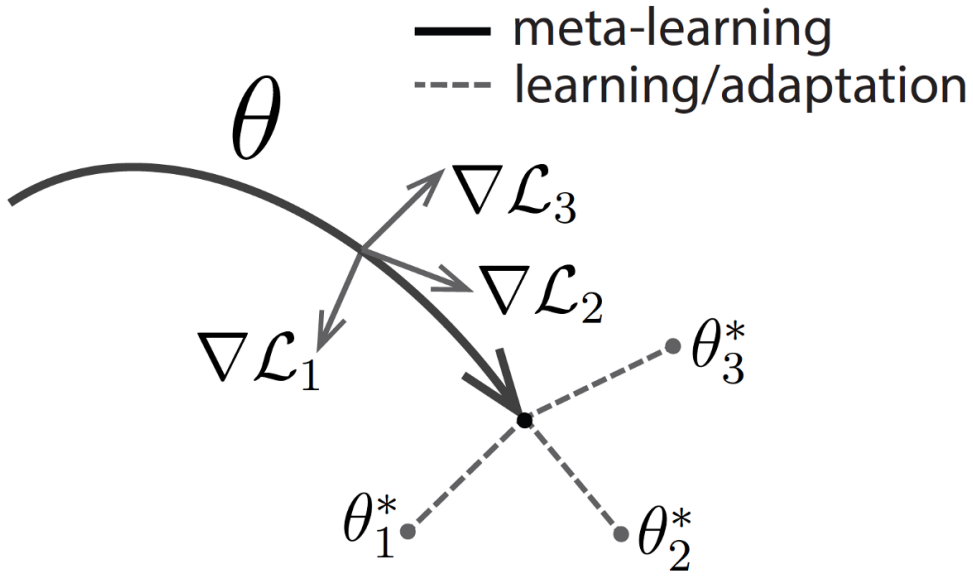
1. Uniform distribution in $[-d, d]$
2. Normal distribution $N(0, \sigma^2)$
3. Xavier initialization $N(0, \frac{2}{d_{in}+d_{out}})$

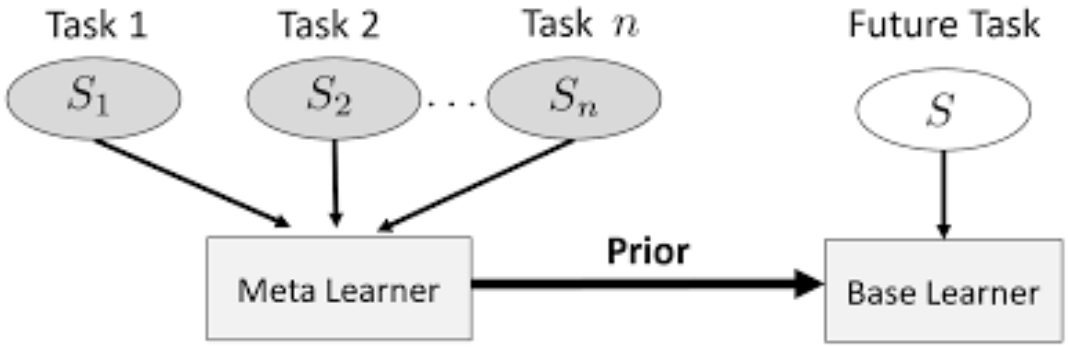
- Why we use distributions centered around zero?
- How it is connected with activation functions?
- shared weights

Transfer Learning

1. a big model is trained on a large dataset
2. learned weights from the model are used as a initialization for another, usually smaller, downstream task

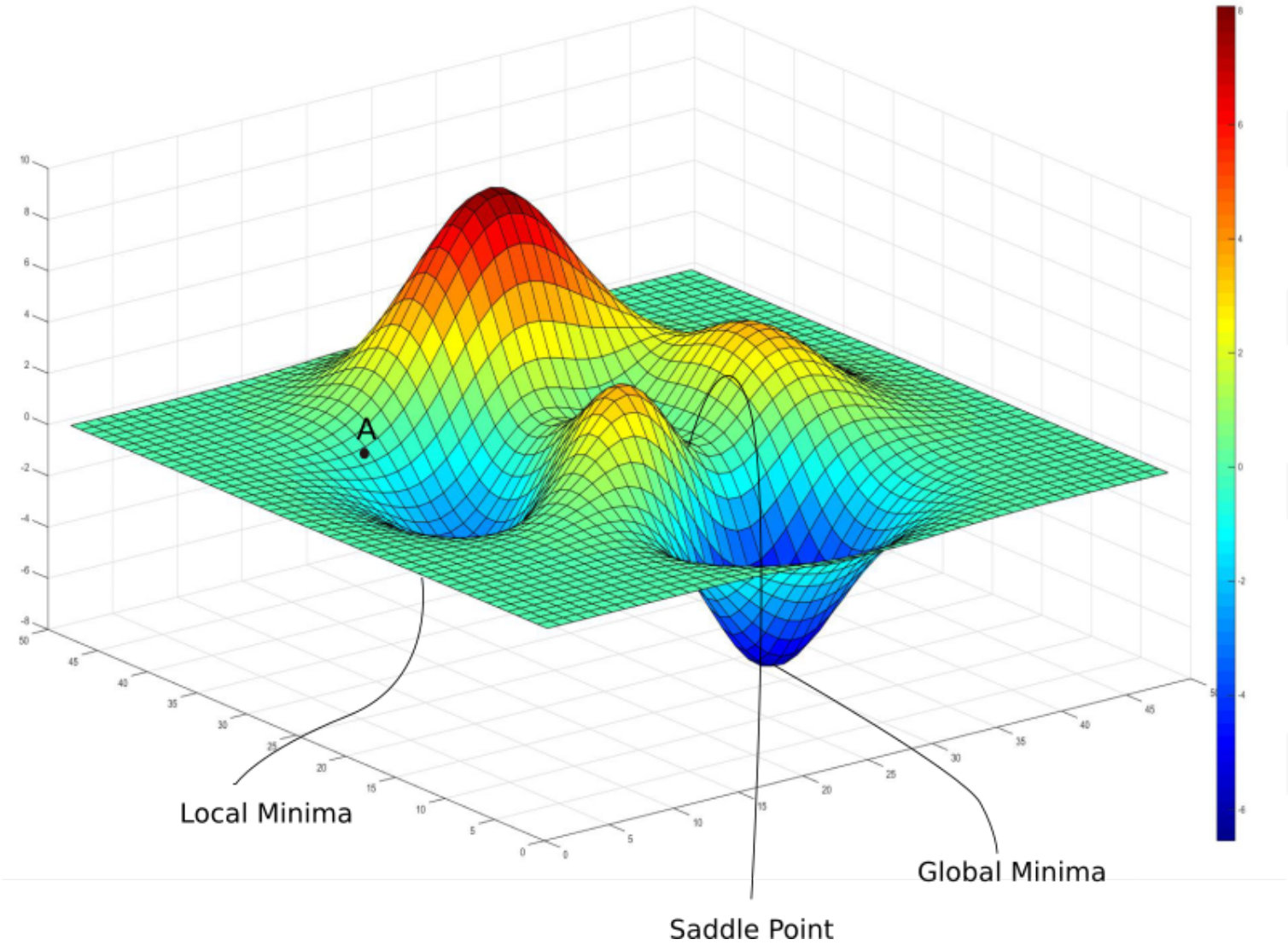
Meta Learning





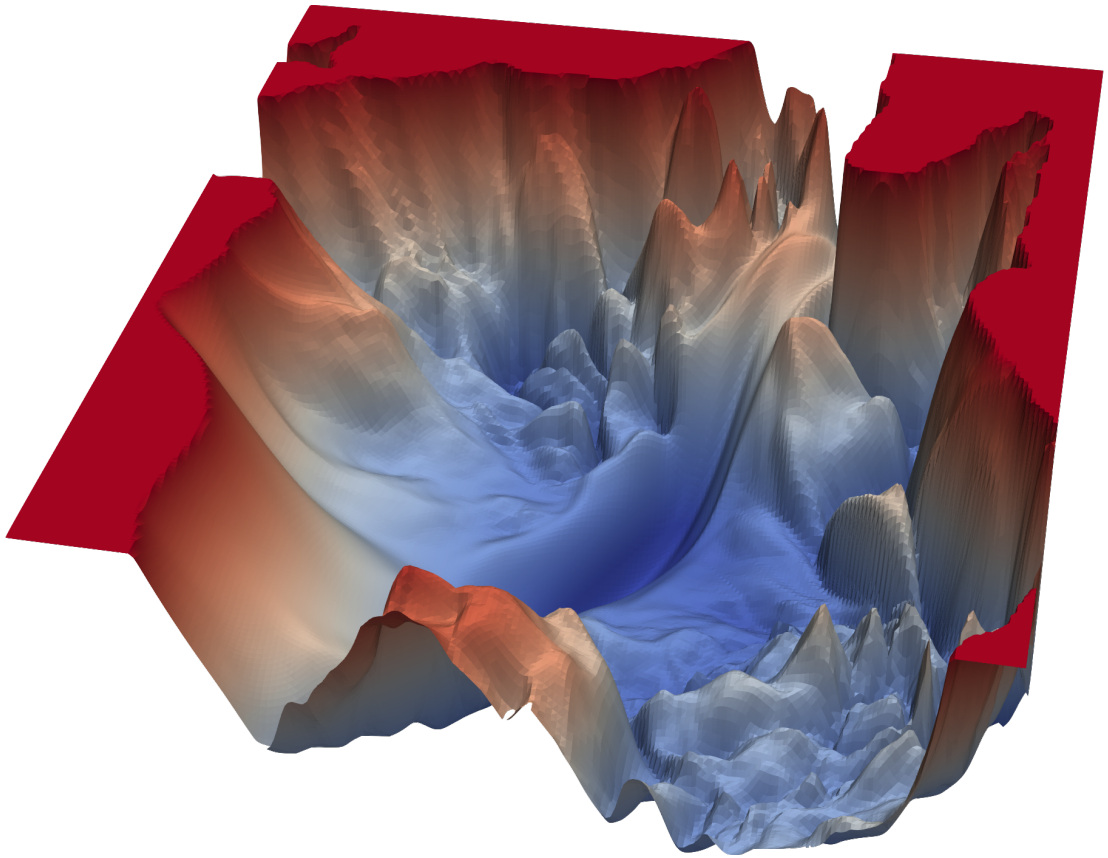
Loss surface

Many local minima



Loss surface

Wide local minimum



Vanilla SGD

$\theta_0 \leftarrow$ init
for **random** batch on step t = 1..max_iter:

$$\theta_t = \theta_{t-1} - \alpha \nabla_\theta J(\theta_{t-1})$$

J - loss function
θ_t - learnable parameters at step t
α - learning rate

- good theoretic properties
- slow convergence

SGD with momentum

$\theta_0 \leftarrow$ init
$m_0 \leftarrow 0$
for **random** batch on step t = 1..max_iter:

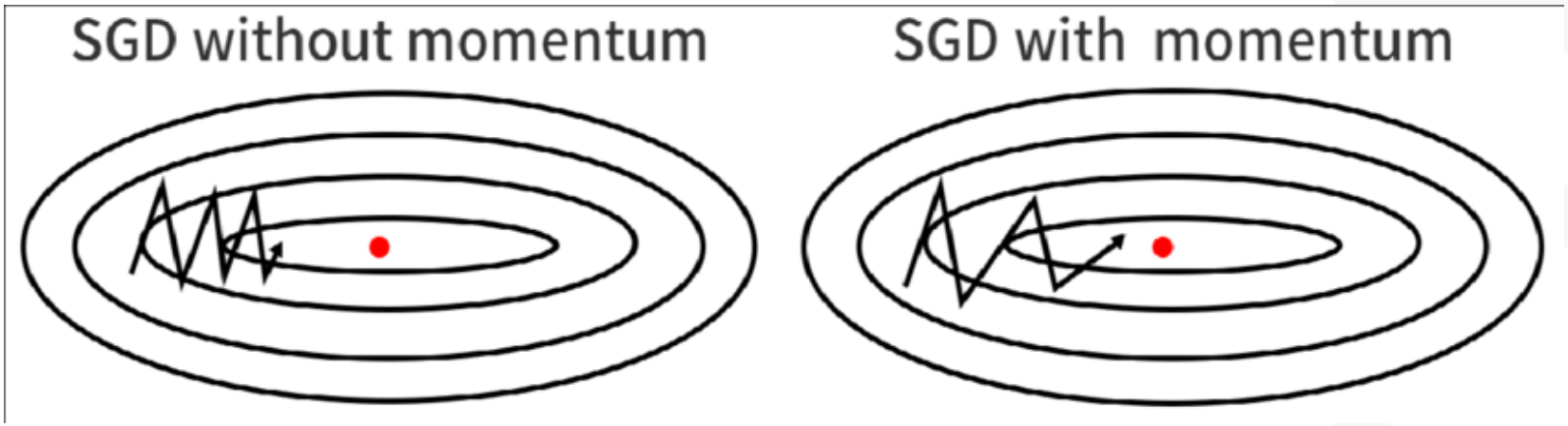
$$m_t = \beta m_{t-1} + (1 - \beta)\nabla_\theta J(\theta_{t-1})$$

$$\theta_t = \theta_{t-1} - \alpha m_t$$

where m_t - accumulated gradient at step t
β - momentum parameter

SGD with momentum

- Momentum cancels moves in "random" directions from stochastic nature of SGD
- Momentum inertia



RmsProp

$\theta_0 \leftarrow$ init $v_0 \leftarrow 0$
for random batch on step t = 1..max_iter:

$$g_t = \nabla_\theta J(\theta_{t-1})$$
$$v_t = \beta v_{t-1} + (1-\beta) g_t^2$$
$$\theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{v_t} + \epsilon} g_t$$

where v_t - accumulated squared components of gradient
β - parameter
$\epsilon << 1$ - to prevent division by zero

- gradient direction carries more information than its norm
- adjust gradient step size

Adam

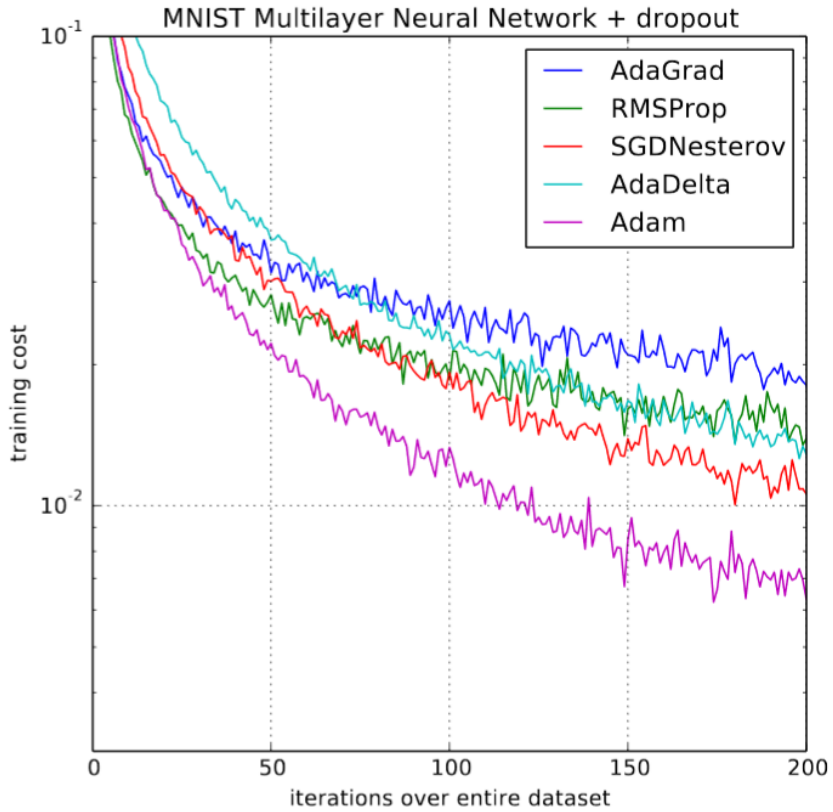
$\theta_0 \leftarrow$ init $v_0 \leftarrow 0$
$m_0 \leftarrow 0$
for random batch on step t = 1..max_iter:

$$g_t = \nabla_\theta J(\theta_{t-1})$$
$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$
$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$
$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$
$$\theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t$$

where m_t - accumulated momentum
v_t - accumulated squared components of gradient
β_1, β_2 - parameters
$\epsilon << 1$ - to prevent division by zero

Adam

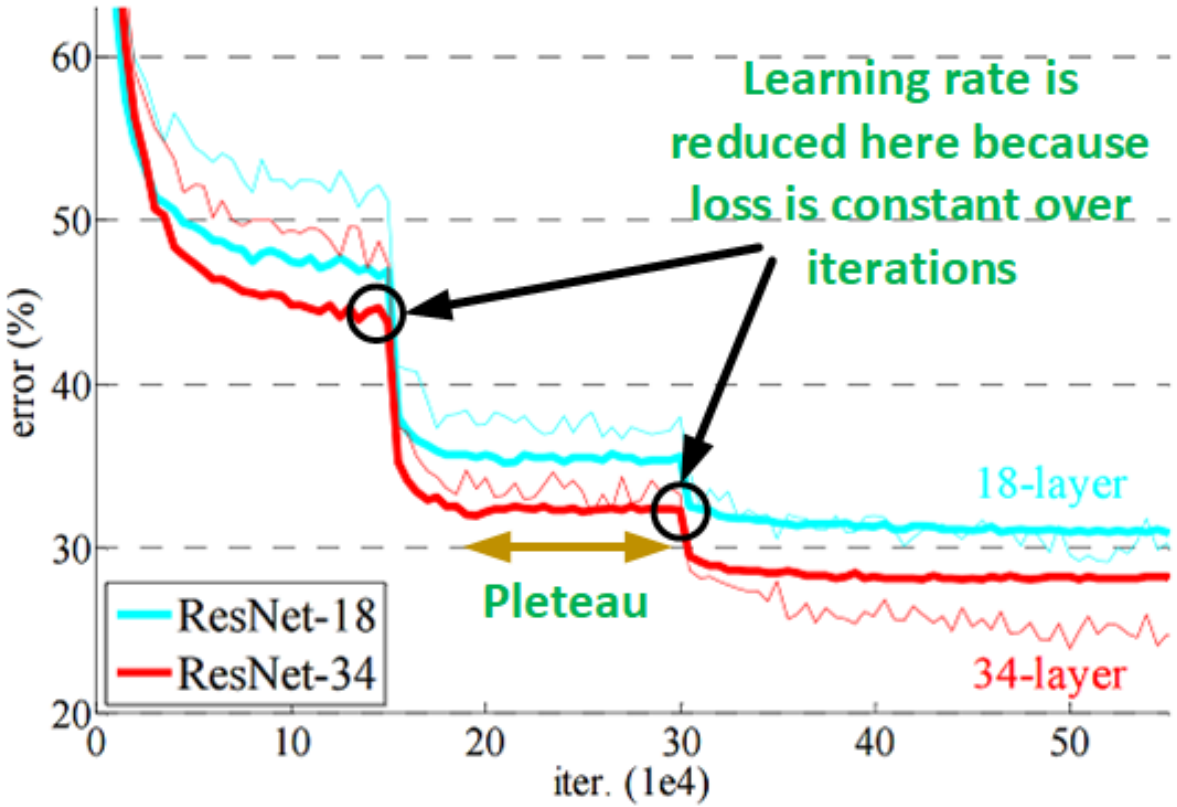
- essentially SGD with momentum + RmsProp
- corrections for $\hat{m}_t, \hat{v}_t$ are to make first optimization steps more stable. Because the calculation of m_t, v_t can be seen as geometric series



Reduce On Plateau

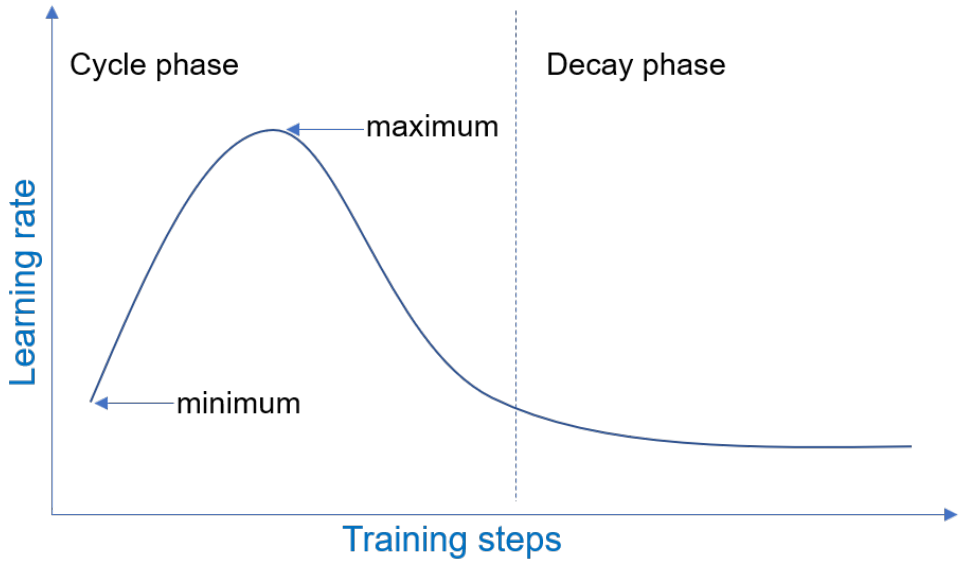
Reduce learning rate by some factor if loss is not decreasing enough.

- we can't converge to exact local minima
- unfortunately, we increase "sensitivity" to more narrow local minima.



Cycle LR

If weight initialization wasn't good enough, we try to increase learning rate at first few steps in a hope to jump into a better local minumum.



Regularization

Most popular:

1. L_2 norm regularization through weight decay
2. Early stopping
3. Data augmentation. Create new samples from the same domain to increase size of your dataset. Remember generalization bounds.
4. Dropout. Drop random nodes in a layer with probability p
5. Batch Normalization

Dropout

There are 2 interpretations for dropout:

- "Bagging" over neural networks
- Avoid feature coadaptation

Difference between bagging and dropout:

$$p(y|x) = \frac{1}{K}\sum_{i=1}^{K} p_i(y|x)$$

for bagging

$$p(y|x) = \sum_{\mu} p(\mu)p(y|x,\mu)$$

for dropout, where μ is mask on weights.
There is an exponential number of masks for fixed number of weights, that makes dropout more effective than explicit bagging.

Dropout

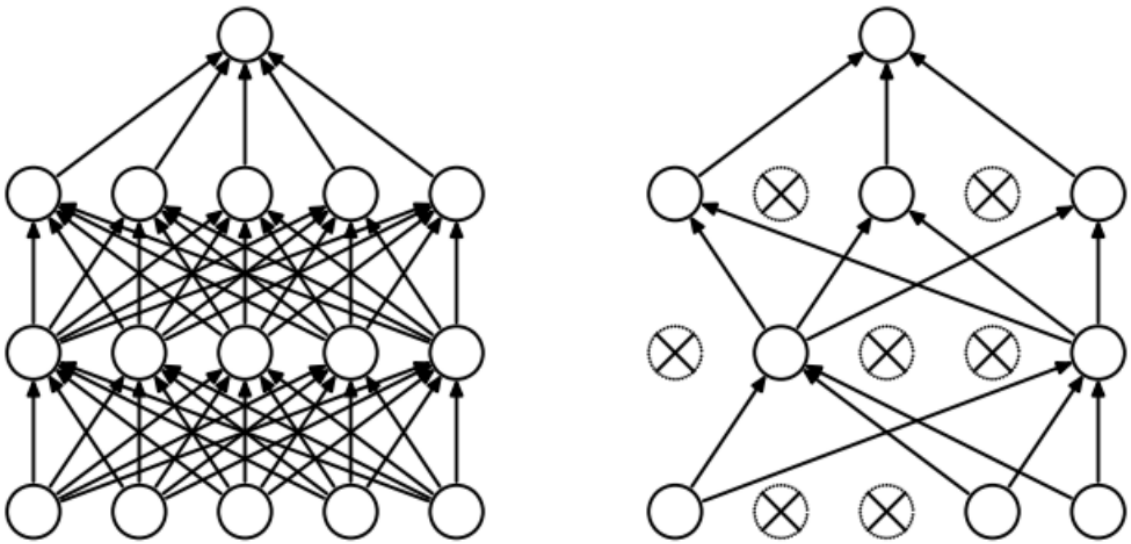
On training: On each batch randomly remove neurons in the previous layer with probability p.

On inference:

Ideally, sample all 2^n dropped-out networks and average predictions.

In practice, approximate by using the full network with each node's output weighted by a factor of $1 - p$, so the expected value of the output of any node is the same as in the training stages.

=> Although it effectively generates 2^n neural nets, but at test time only a single network needs to be tested.



(a) Standard Neural Net

(b) After applying dropout.

BatchNorm

On training:
on every batch t:

$$\mu_t = \frac{1}{m}\sum_{i=1}^{m} x_i$$

$$\sigma_t^2 = \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_t)$$

$$\hat{x}_i = \frac{x_i - \mu_t}{\sigma_t + \epsilon}$$

$$y_i = \gamma\hat{x}_i + \beta = BN_{\gamma,\beta}(x_i)$$

where μ_t - estimated batch mean
σ_t^2 - estimated batch variance
$\hat{x}_i$ - normalized input
γ - learnable scale parameter
β - learnable shift parameter

BatchNorm

On inference: we can't compute μ_t, σ_t^2. Instead, we use some running average over μ_t, σ_t^2 that were observed during training.

- NN in theory can learn γ, β to undo batch normalization. In practice, they usually don't
- BatchNorm stabilizes training by making surface of loss function more smooth