Optimization Methods for Deep Learning

Gradient descent for non-convex optimization

Decsent Lemma: Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be twice differentiable, and $\|\nabla^2 f\|_2 \leq \beta$. Then setting the learning rate $\eta = 1/\beta$, and applying gradient descent, $x_{t+1} = x_t - \eta \nabla f(x_t)$, we have:

$$f(x_t) - f(x_{t+1}) \geq \frac{1}{2\beta} \|\nabla f(x_t)\|_2^2.$$

Converging to stationary points

Theorem: In $T = O(\frac{\beta}{\epsilon^2})$ iterations, we have $\|\nabla f(x)\|_2 \leq \epsilon$.

Gradient Descent for Quadratic Functions

Problem: $\min_x \frac{1}{2} x^\top A x$ with $A \in \mathbb{R}^{d \times d}$ being positive-definite.

Theorem: Let $\lambda_{\max}$ and $\lambda_{\min}$ be the largest and the smallest eigenvalues of A. If we set $\eta \leq \frac{1}{\lambda_{\max}}$, we have

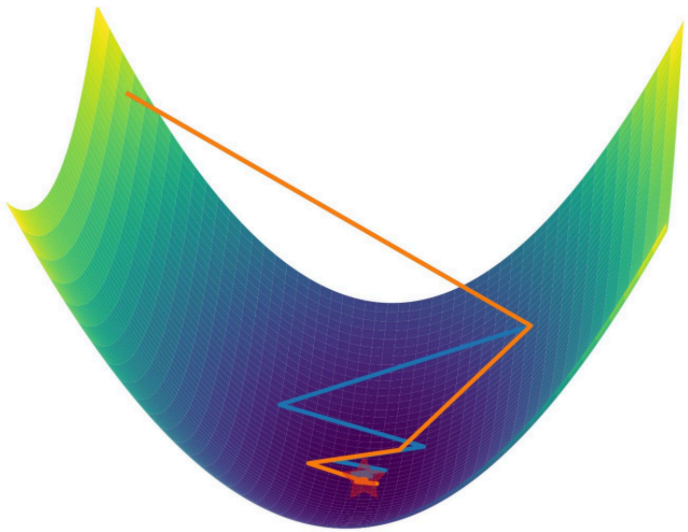
$$\|x_t\|_2 \leq \left(1 - \eta \lambda_{\min}\right)^t \|x_0\|_2$$

Momentum: Heavy-Ball Method (Polyak '64)

Problem: $\min_x f(x)$

Method: $v_{t+1} = -\nabla f(x_t) + \beta v_t$

$$x_{t+1} = x_t + \eta v_{t+1}$$



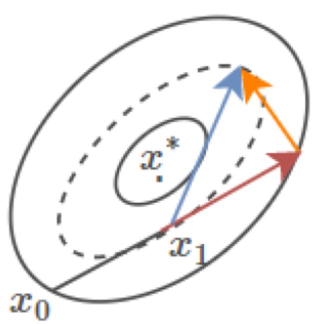
Momentum: Nesterov Acceleration (Nesterov '89)

Problem: $\min_x f(x)$

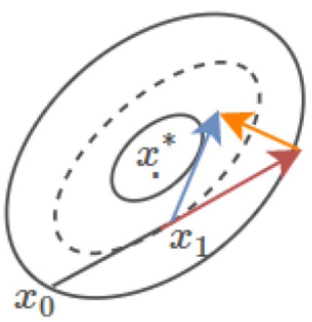
Method: $v_{t+1} = -\nabla f(x_t + \beta v_t) + \beta v_t$

$$x_{t+1} = x_t + \eta v_{t+1}$$

Polyak's Momentum

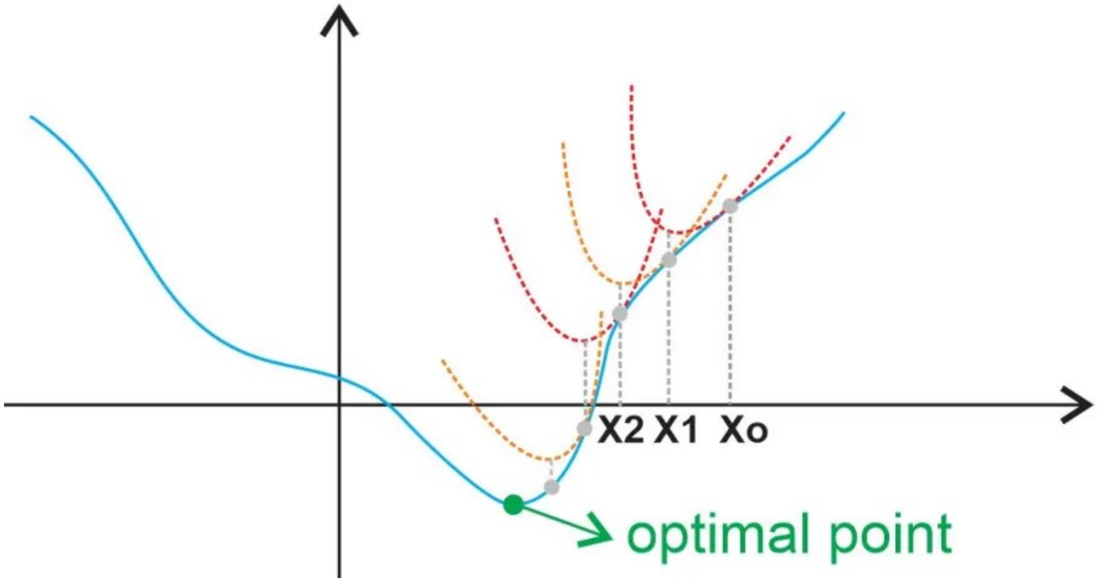


Nesterov Momentum



Newton's Method

Newton's Method: $x_{t+1} = x_t - \eta(\nabla^2 f(x_t))^{-1} \nabla f(x_t)$



AdaGrad (Duchi et al. '11)

Newton Method: $x_{t+1} = x_t - \eta(\nabla^2 f(x_t))^{-1} \nabla f(x_t)$

AdaGrad: separate learning rate for every parameter

$$x_{t+1} = x_t - \eta(G_{t+1} + \epsilon I)^{-1} \nabla f(x_t),\ (G_t)_{ii} = \sqrt{\sum_{j=1}^{t-1} \left(\nabla f(x_t)_i\right)^2}$$

RMSProp (Hinton et al. ’12)

AdaGrad: separate learning rate for every parameter

$$x_{t+1} = x_t - \eta(G_{t+1} + \epsilon I)^{-1} \nabla f(x_t), \ (G_t)_{ii} = \sqrt{\sum_{j=1}^{t-1} \left(\nabla f(x_t)_i \right)^2}$$

RMSProp: exponential weighting of gradient norms

$$x_{t+1} = x_t - \eta(G_{t+1} + \epsilon I)^{-1/2} \nabla f(x_t),$$
$$(G_{t+1})_{ii} = \beta(G_t)_{ii} + (1 - \beta)(\nabla f(x_t)_i)^2$$

AdaDelta (Zeiler '12)

RMSProp:

$$x_{t+1} = x_t - \eta(G_{t+1} + \epsilon I)^{-1/2} \nabla f(x_t),$$
$$(G_{t+1})_{ii} = \beta(G_t)_{ii} + (1 - \beta)(\nabla f(x_t)_i)^2$$

AdaDelta:

$$x_{t+1} = x_t - \eta \Delta x_t,$$
$$\Delta x_t = \sqrt{u_t + \epsilon} \cdot (G_{t+1} + \epsilon I)^{-1/2} \nabla f(x_t)$$
$$(G_{t+1})_{ii} = \rho(G_t)_{ii} + (1 - \rho)(\nabla f(x_t)_i)^2,$$
$$u_{t+1} = \rho u_t + (1 - \rho)\|\Delta x_t\|_2^2$$

Adam (Kingma & Ba '14)

Momentum:

$v_{t+1} = -\nabla f(x_t) + \beta v_t, x_{t+1} = x_t + \eta v_{t+1}$

RMSProp: exponential weighting of gradient norms

$x_{t+1} = x_t - \eta (G_{t+1} + \epsilon I)^{-1} \nabla f(x_t),$

$(G_t)_{ii} = \beta (G_t)_{ii} + (1 - \beta)(\nabla f(x_t)_i)^2$

Adam

$v_{t+1} = \beta_1 v_t + (1 - \beta_1) \nabla f(x_t)$

$(G_{t+1})_{ii} = \beta_2 (G_t)_{ii} + (1 - \beta_2)(\nabla f(x_t)_i)^2$

$x_{t+1} = x_t - \eta (G_{t+1} + \epsilon I)^{-1/2} v_{t+1}$

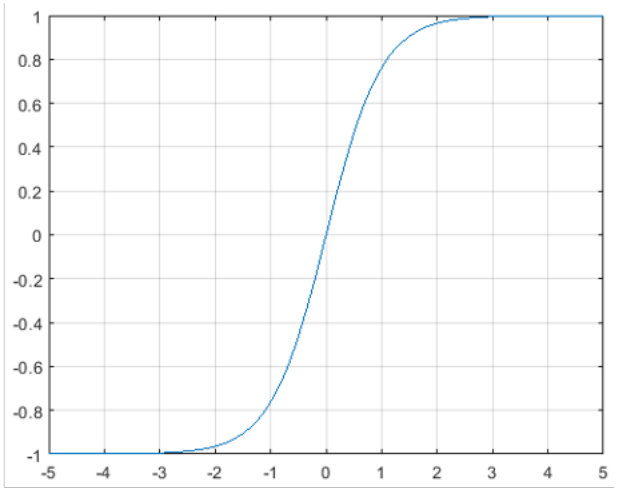
Default choice nowadays.

Important Techniques in Neural Network Training

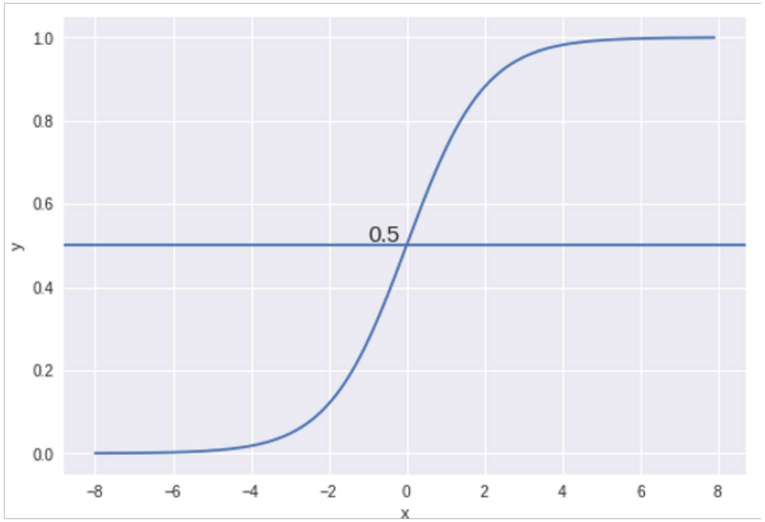
Gradient Explosion / Vanishing

- Deeper networks are harder to train:
  - Intuition: gradients are products over layers
  - Hard to control the learning rate

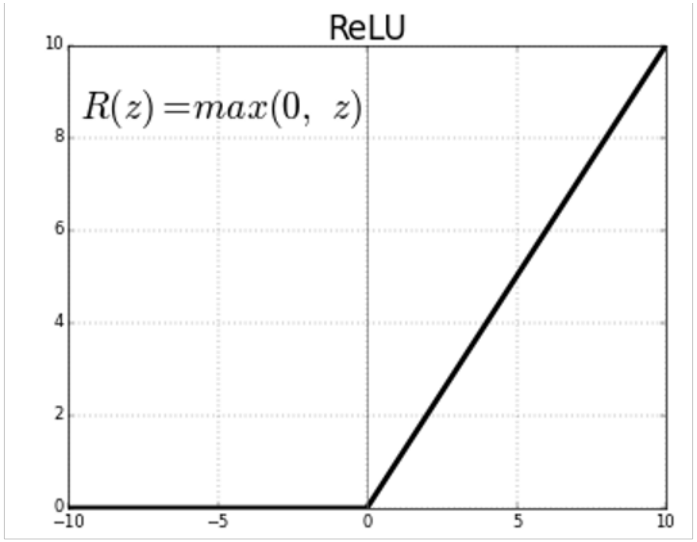
Activation Functions



tanh

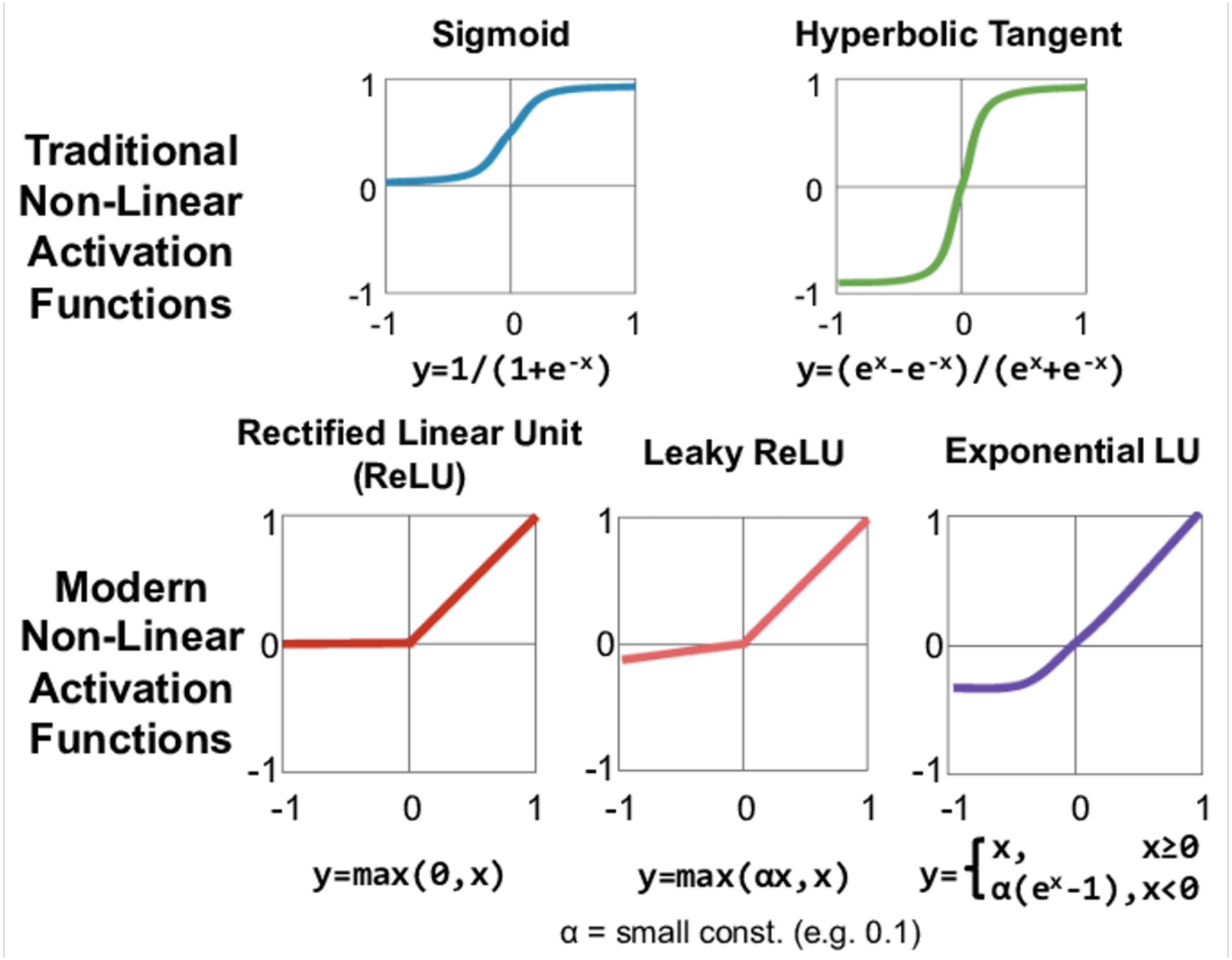


sigmoid



Rectified Linear United

Activation Function



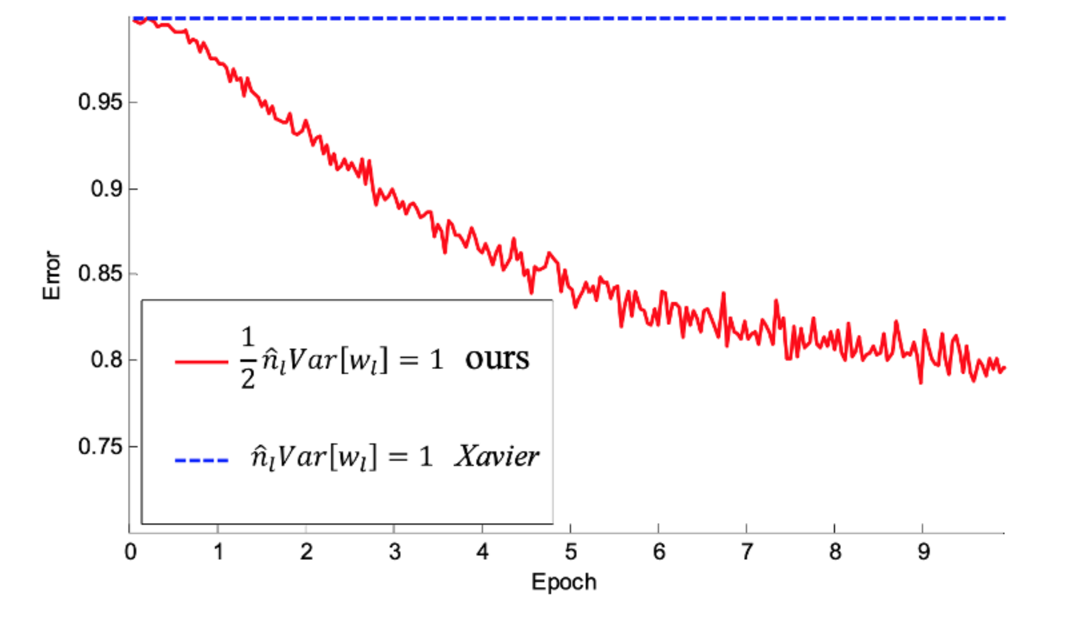
Initialization

- Zero-initialization
- Large initialization
- Small initialization

- Design principles:
  - Zero activation mean
  - Activation variance remains same across layers

Kaiming Initialization (He et al. '15)

- $W_{ij}^{(h)} \sim \mathcal{N}\left(0, \frac{2}{d_h}\right)$.
- $b^{(h)} = 0$
- Designed for ReLU activation
- 30-layer neural network



Kaiming Initialization (He et al. '15)

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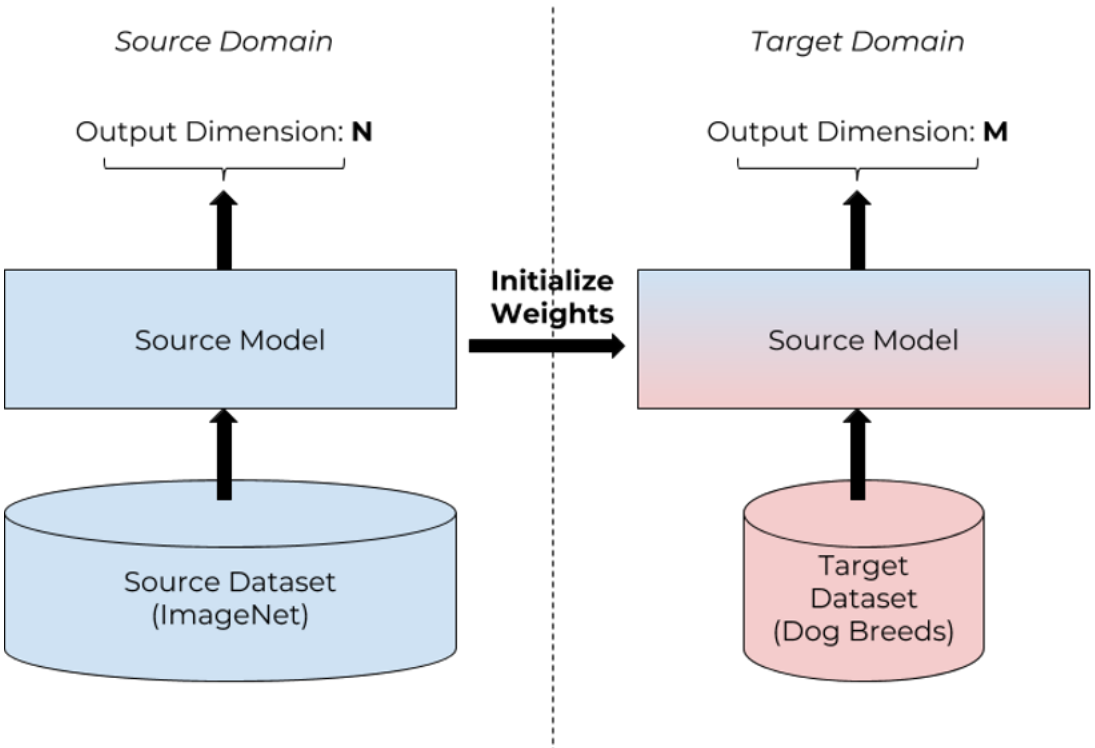
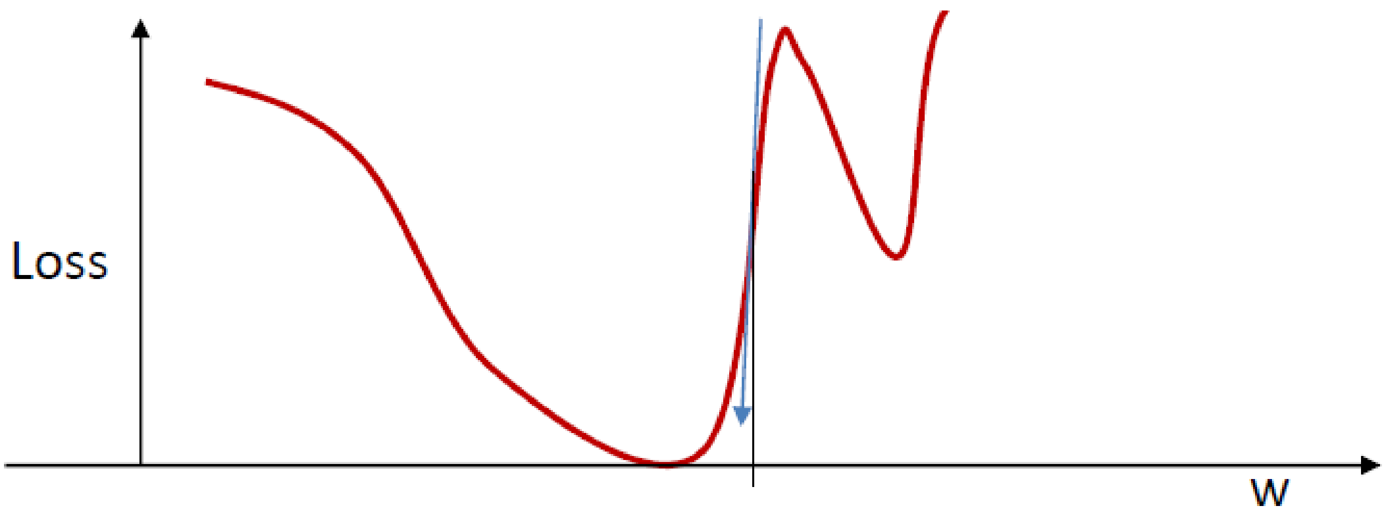
Initialization by Pre-training

- Use a pre-trained network as initialization
- And then fine-tuning



Gradient Clipping

- The loss can occasionally lead to a steep descent
- This result in immediate instability
- If gradient norm bigger than a threshold, set the gradient to the threshold.



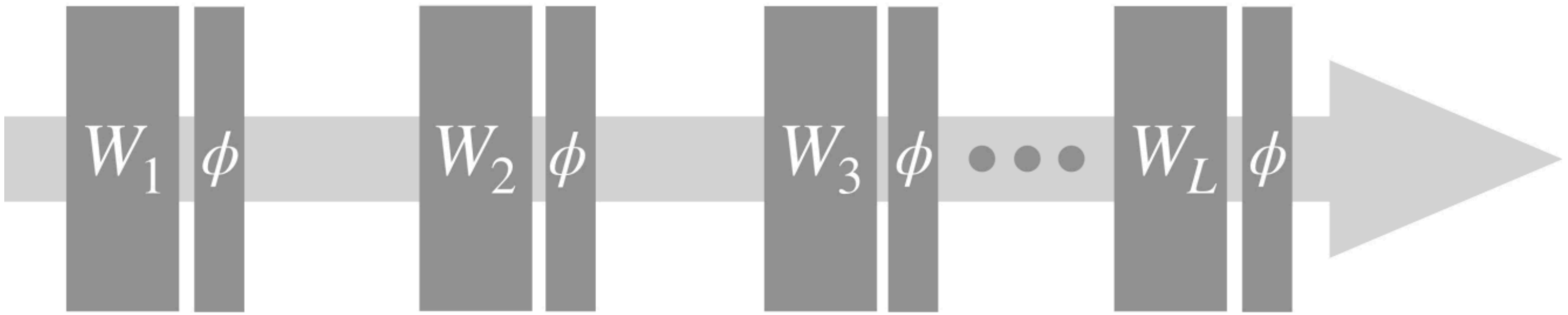
Batch Normalization (Ioffe & Szegedy, '14)

- Normalizing/whitening (mean = 0, variance = 1) the inputs is generally useful in machine learning.
  - Could normalization be useful at the level of hidden layers?
  - **Internal covariate shift**: the calculations of the neural networks change the distribution in hidden layers even if the inputs are normalized

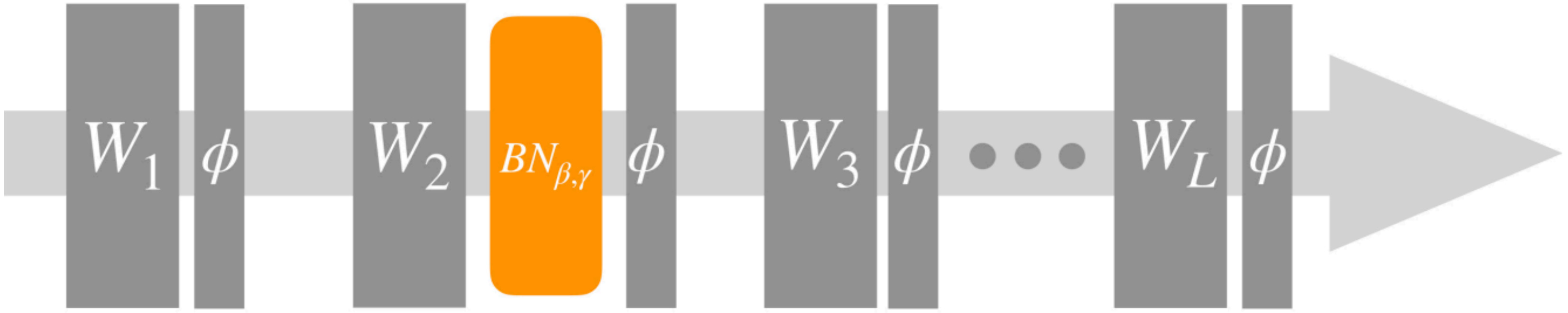
- **Batch normalization** is an attempt to do that：
  - Each unit's **pre-activation** is normalized (mean subtraction, std division)
  - During training, mean and std is computed for each minibatch (can be backproped!

Batch Normalization (Ioffe & Szegedy, '14)

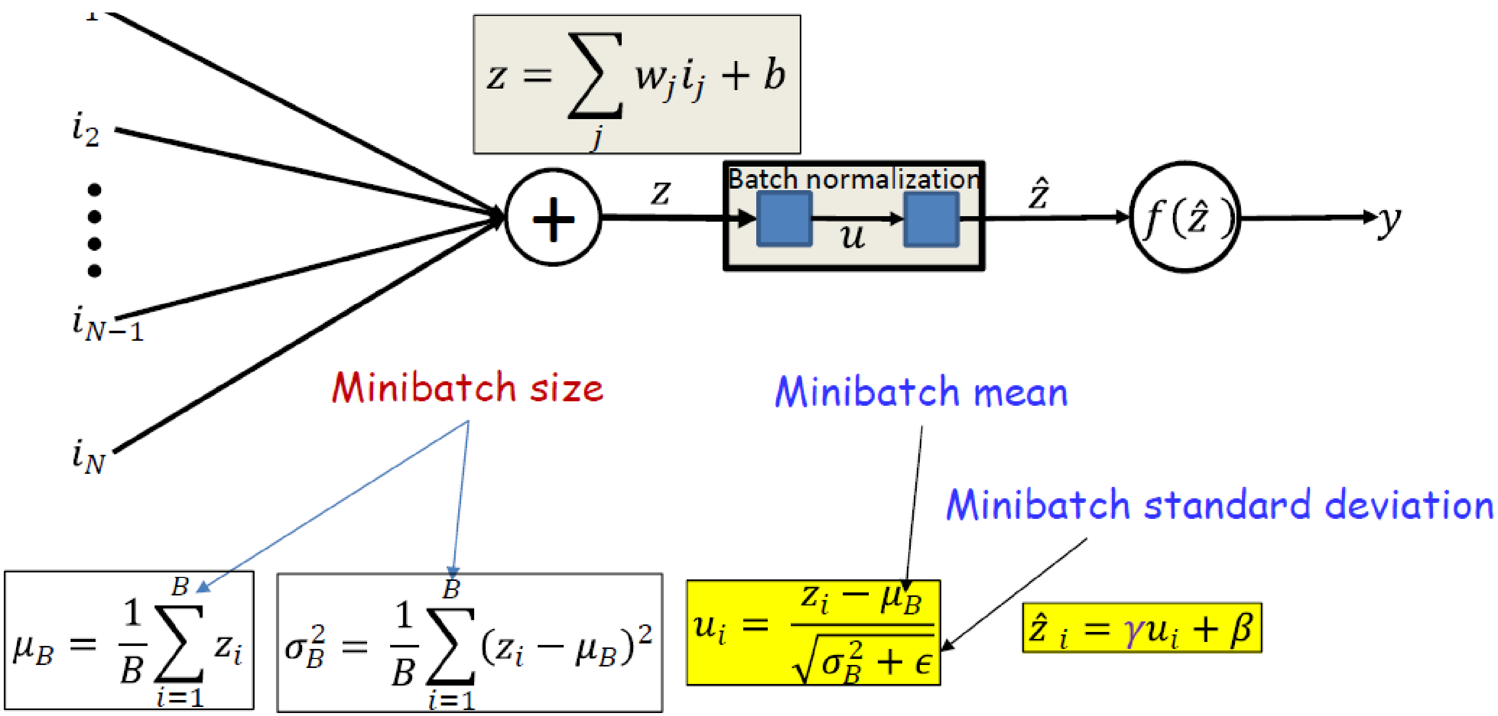
Standard Network



Adding a BatchNorm layer (between weights and activation function)



Batch Normalization (Ioffe & Szegedy, '14)



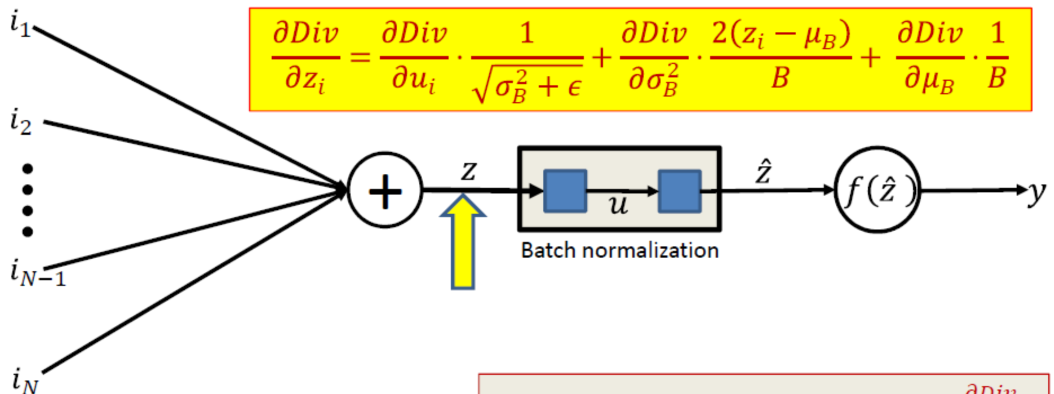
Batch Normalization (Ioffe & Szegedy, '14)

- BatchNorm at training time
  - Standard backprop performed for each single training data
  - Now backprop is performed over entire batch.

$$\frac{\partial Div}{\partial \sigma_B^2} = \frac{-1}{2}(\sigma_B^2 + \epsilon)^{-3/2} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}$$

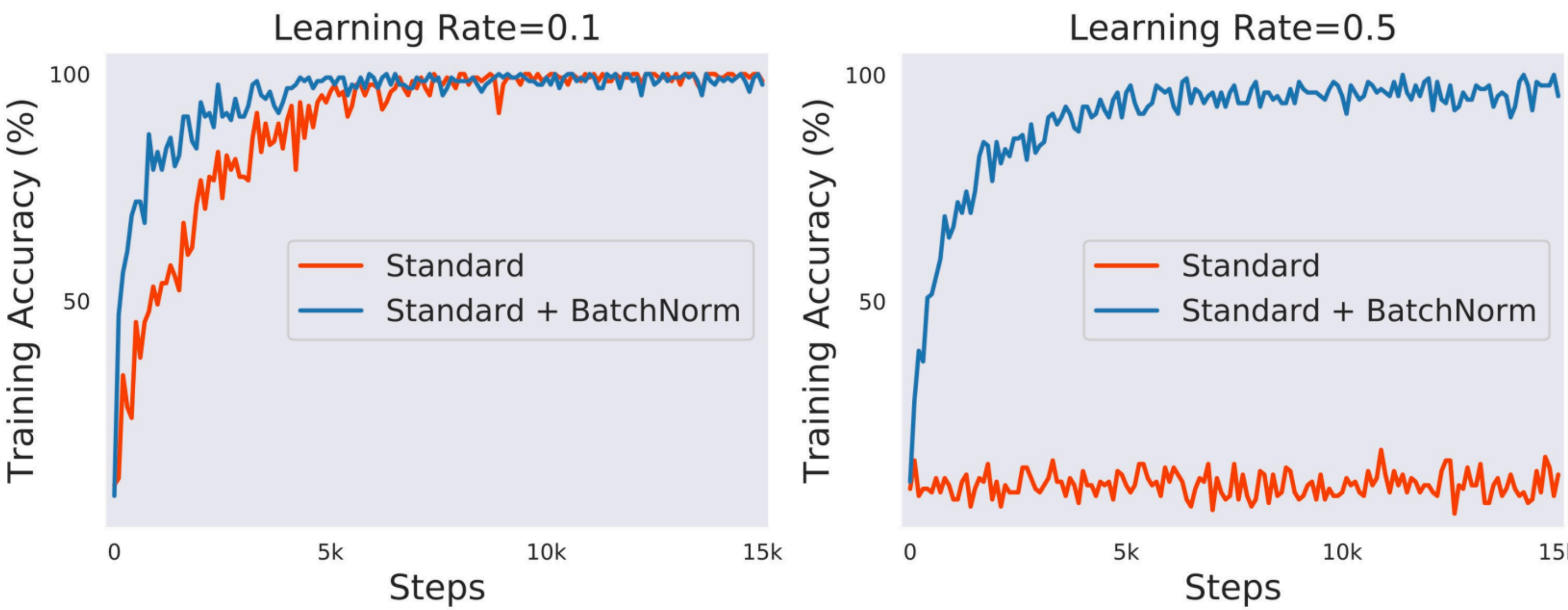
$$\frac{\partial Div}{\partial \mu_B} = \frac{-1}{\sqrt{\sigma_B^2 + \epsilon}} \sum_{i=1}^{B} \frac{\partial Div}{\partial u_i}$$

$$\frac{\partial Div}{\partial z_i} = \frac{\partial Div}{\partial u_i} \cdot \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} + \frac{\partial Div}{\partial \sigma_B^2} \cdot \frac{2(z_i - \mu_B)}{B} + \frac{\partial Div}{\partial \mu_B} \cdot \frac{1}{B}$$



The rest of backprop continues from $\frac{\partial Div}{\partial z_i}$

Batch Normalization (Ioffe & Szegedy, '14)



What is BatchNorm actually doing?

- May not due to covariate shift (Santurkar et al. ‘18):
  - Inject non-zero mean, non-standard covariance Gaussian noise after BN layer: removes the whitening effect
  - Still performs well.

- Only training β, γ with random convolution kernels gives non-trivial performance (Frankle et al. ’20)

- BN can use exponentially increasing learning rate! (Li & Arora ’19)

More normalizations

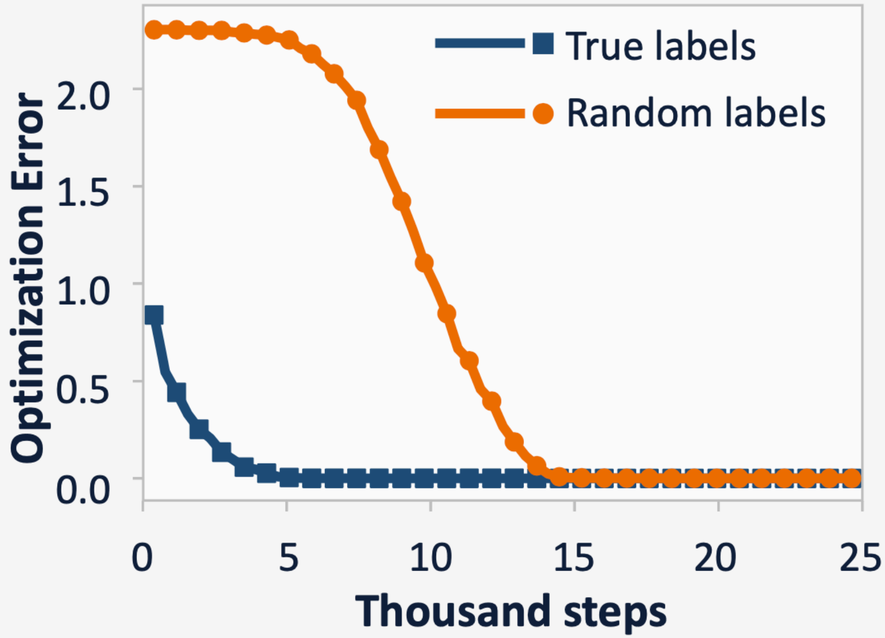
- Layer normalization (Ba, Kiros, Hinton, ’16)
  - Batch-independent
  - Suitable for RNN, MLP
- Weight normalization (Salimans, Kingma, ’16)
  - Suitable for meta-learning (higher order gradients are needed)
- Instance normalization (Ulyanov, Vedaldi, Lempitsky, ’16)
  - Batch-independent, suitable for generation tasks
- Group normalization (Wu & He, ‘18)
  - Batch-independent, improve BatchNorm for small batch size

Non-convex Optimization Landscape

Gradient descent finds global minima

Practice: gradient descent

$$\theta(t+1) \leftarrow \theta(t) - \eta \frac{\partial L(\theta(t))}{\partial \theta(t)}$$



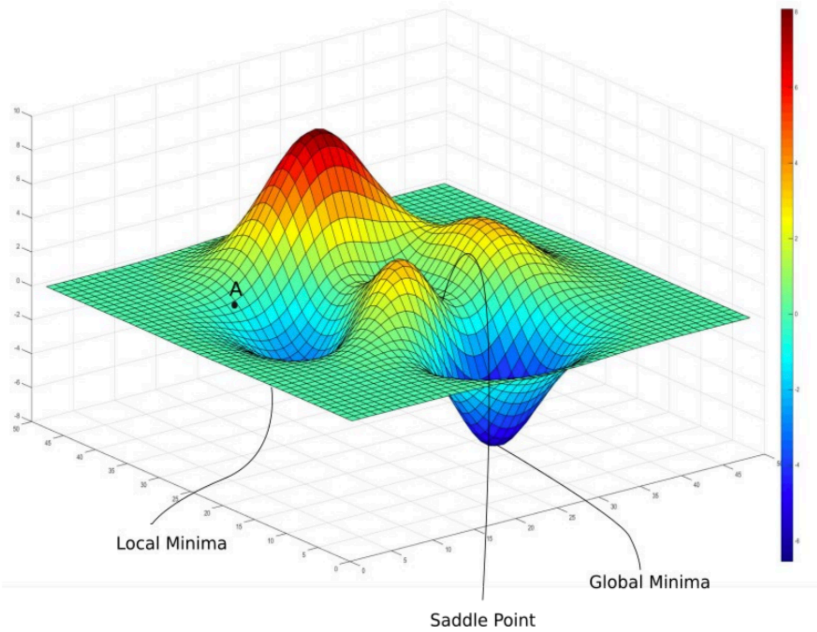
Optimization error **-> 0** for both ***true labels*** and ***random labels*** !

Zhang Bengio Hardt Recht Vinyals 2017

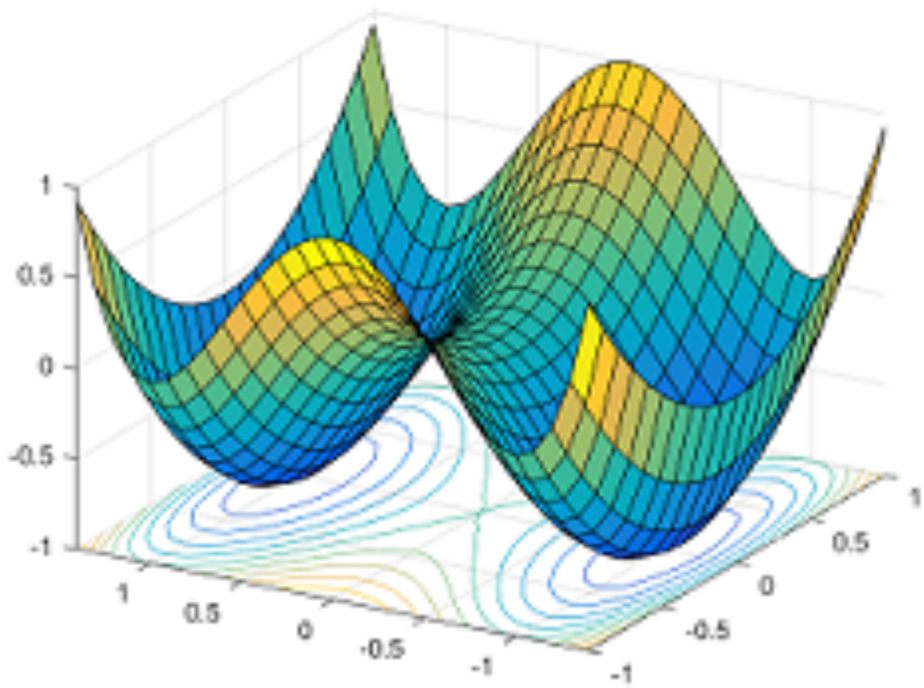
Understanding DL Requires Rethinking Generalization

Types of stationary points

- Stationary points: $x : \nabla f(x) = 0$
- Global minimum:
  $x : f(x) \leq f(x') \forall x' \in \mathbb{R}^d$
- Local minimum:
  $x : f(x) \leq f(x') \forall x' : \|x - x'\| \leq \epsilon$
- Local maximum:
  $x : f(x) \geq f(x') \forall x' : \|x - x'\| \leq \epsilon$
- Saddle points: stationary points that are not a local min/max

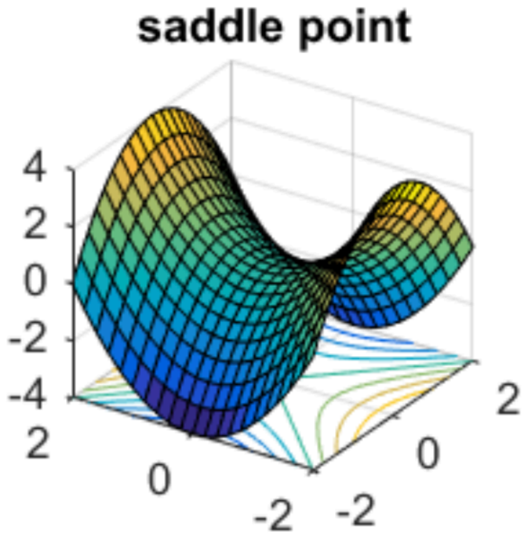


Landscape Analysis



- All local minima are global!
- Gradient descent can escape saddle points.

Strict Saddle Points (Ge et al. '15, Sun et al. '15)

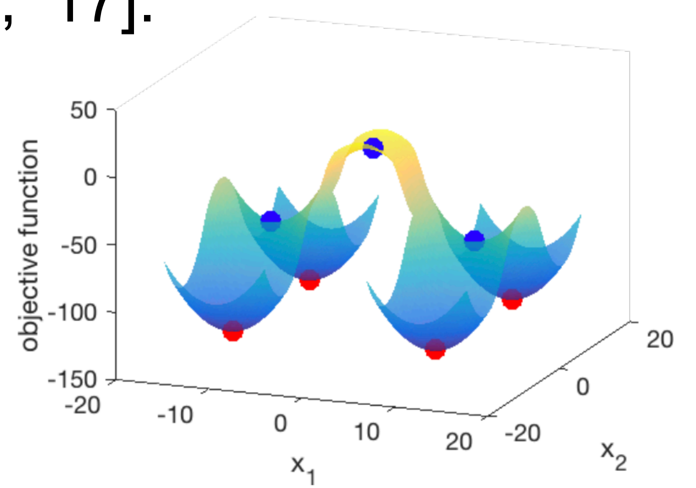


- Strict saddle point: a saddle point and $\lambda_{\min}(\nabla^2 f(x)) < 0$

Escaping Strict Saddle Points

- Noise-injected gradient descent can escape strict saddle points in polynomial time [Ge et al., ’15, Jin et al., ’17].
- Randomly initialized gradient descent can escape all strict saddle points asymptotically [Lee et al., ’15].
  - Stable manifold theorem.
- Randomly initialized gradient descent can take exponential time to escape strict saddle points [Du et al., ’17].

If 1) all local minima are global, and 2) are saddle points are strict, then noise-injected (stochastic) gradient descent finds a global minimum in polynomial time



What problems satisfy these two conditions

- Matrix factorization
- Matrix sensing
- Matrix completion
- Tensor factorization
- Two-layer neural network with quadratic activation

What about neural networks?

- Linear networks (neural networks with linear activations functions): all local minima are global, but there exists saddle points that are not strict [Kawaguchi ’16].

- Non-linear neural networks with:
  - Virtually any non-linearity,
  - Even with Gaussian inputs,
  - Labels are generated by a neural network of the same architecture,

There are many bad local minima [Safran-Shamir ’18, Yun-Sra-Jadbaie ’19].