Lecture 8 vol 1 and vol 2

Advanced optimization

Information Systems
(Machine Learning)

Andrey Filchenkov

08.11.2018 and 22.11.2018

Lecture plan

- Second derivative tests
- Rethinking logistic regression
- Vanishing/exploding gradients
- Activation functions for DNNs
- Data preprocessing for DNNs
- Improving descent for DNNs
- Batch normalization

- The presentation is prepared with materials of
  - K.V. Vorontsov's course "Machine Leaning",
  - D. Polykovsky and K. Khrabrov "Neural networks in machine learning".
- Slides are available online: **goo.gl/BspjhF**

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Stochastic gradient descent (reminder)

Stochastic gradient descent:

$w^{[0]}$ is **an initial guess values**;

$x_{(1)}, \dots, x_{(\ell)}$ is **an objects order**;

$$w^{(k+1)} = w^{(k)} - \mu L'\big(\langle w^{(k)}, x_{(k)}\rangle y_{(k)}\big) x_{(k)} y_{(k)},$$

$$Q^{(k+1)} = (1-\alpha) Q^{(k)} + \alpha L\big(\langle w^{(k)}, x_{(k)}\rangle y_{(k)}\big).$$

Stop when values of Q and/or w do not change much.

Newton-Raphson method

$$Q(a, T^{\ell}) = \sum_{i=1}^{\ell} (f(x_i, w) - y_i)^2 \to \min_{\theta \in \mathbb{R}^p}.$$

1. Choose an initial guess $w^{(0)} = \left(w_1^{(0)}, \dots, w_p^{(0)}\right)$.
2. Repeat iteratively:

$$w^{(t+1)} = w^{(t)} - \eta_t \left(Q''\left(w^{(t)}\right)\right)^{-1} Q'\left(w^{(t)}\right),$$

where $Q'\left(w^{(t)}\right)$ is gradient of Q in $w^{(t)}$;

$Q''\left(w^{(t)}\right)$ is a hessian Q in $w^{(t)}$;

η_t is step (usually $\eta_t = 1$).

Gradient and hessian

jth element of gradient:

$$\frac{\partial Q(w)}{\partial w_j} = 2\sum_{i=1}^{\ell}(f(x_i, w) - y_i)\frac{\partial f(x_i, w)}{\partial w_j}.$$

(j, k)th element of hessian:

$$\frac{\partial^2 Q(w)}{\partial w_j \delta w_k} = 2\sum_{i=1}^{\ell}\frac{\partial f(x_i, w)}{\partial w_j}\frac{\partial f(x_i, w)}{\partial \theta_k} -$$

$$-2\sum_{i=1}^{\ell}(f(x_i, w) - y_i)\frac{\partial^2 f(x_i, w)}{\partial w_j \partial w_k}.$$

Problem

It is very inconvenient to compute hessian each time in each point (cubic complexity).

To avoid this, **quasi-netwon methods** are used to use approximate estimation of hessian.

Newton-Gauss method

Main idea is **linearization**:

$$f(x_i, w) \approx f\left(x_i, w^{(t)}\right) + \sum_{j=1}^{p} \left(w_j - w_j^{(t)}\right) \frac{\partial f\left(x_i, w_j^{(t)}\right)}{\partial w_j} +$$

$$+o\left(w_j - w_j^{(t)}\right).$$

$F_t = F_t = \left(\frac{\partial f_i}{\partial \theta_j}(x_i, w^{(t)})\right)_{j=1..\ell}^{j=1..p}$ is matrix of first derivatives.

$f_t = \left(f\left(x_i, w^{(t)}\right)\right)_{i=1..\ell}$ is vector of f values.

Newton-Gauss as linear regression series

$$w^{(t+1)} = w^{(t)} - h_t \left(F_t^\top F_t\right)^{-1} F_t \left(f^{(t)} - y\right),$$

$\beta = \left(F_t^\top F_t\right)^{-1} F_t \left(f^{(t)} - y\right)$ is a solution for the problem

$$\left\|F_t \beta - \left(f^{(t)} - y\right)\right\|^2 \to \min_{\beta}.$$

This is a series of linear regression problems.

It converges with the same speed as Netwon-Raphson method.

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Logistic regression

Constraint: $Y = \{-1, +1\} = \{y_{-1}, y_{+1}\}$

Linear classifier:

$$a_w(x, T^\ell) = \operatorname{sign}\left(\sum_{i=1}^{n} w_i f_i(x) - w_0\right).$$

where $w_1, \dots, w_n \in \mathbb{R}$ are features weights.

$$a_w(x, T^\ell) = \operatorname{sign}(\langle w, x \rangle).$$

$$\Pr(y|x) = \sigma(\langle w, x \rangle y),$$

where $\sigma(s) = \frac{1}{1+e^{-s}}$, which is **logistic (sigmoid) function**

Logarithmic loss function

$$\widetilde{Q_w}\left(a,T^{\ell}\right) = \sum_{i}^{\ell} \ln(1+\exp(-\langle w,x\rangle y)) \to \min_w.$$

We can apply Newton-Raphson method:

$$w^{(t+1)} = w^{(t)} - \eta_t \left(Q''\left(w^{(t)}\right)\right)^{-1} Q'\left(w^{(t)}\right).$$

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Newton-Raphson application

jth element of gradient:

$$\frac{\partial Q(w)}{\partial w_j} = -\sum_{i=1}^{\ell} (1 - \sigma_i) y_i f_j(x_i)\,,$$

(j, k)th element of hessian:

$$\frac{\partial^2 Q(w)}{\partial w_j \delta w_k} = \sum_{i=1}^{\ell} (1 - \sigma_i) \sigma_i f_j(x_i) f_k(x_i)\,,$$

where $\sigma_i = \sigma(y_i w^\top x_i)$.

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Newton-Raphson application

$F_{\ell\times n} = (f_i(x_i))$ is features-objects matrix;

$\Gamma_{\ell\times\ell} = \mathrm{diag}\left(\sqrt{(1-\sigma_i)\sigma_i}\right)$;

$\tilde{F} = \Gamma F$ is a weighted feature-object matrix;

$\tilde{y}_i = y_i\sqrt{(1-\sigma_i)\sigma_i}$, $(\tilde{y}_i)_{i=1}^{\ell}$ is a weighted answer vector.

$$\left(Q''(w)\right)^{-1}Q'(w) = -\left(F^\top\Gamma^2F\right)^{-1}F^\top\Gamma\tilde{y} =$$
$$= -\left(\tilde{F}^\top\tilde{F}\right)^{-1}\tilde{F}^\top\tilde{y} = -\tilde{F}^{+}\tilde{y}.$$

Logistic regression solution

$$Q(w) = \|\tilde{F}w - \tilde{y}\|^2 =$$

$$= \sum_{i=1}^{\ell} (1 - \sigma_i)\sigma_i \left(w^\top x - \frac{y_i}{\sigma_i} \right)^2 \to \min_w .$$

σ_i is a probability of true classification.

$(1 - \sigma_i)\sigma_i$ is degree of “sureness” of object classification, which is margin.

This solution is performed in a way if we apply regression to solve classification.

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Example

- Imagine we have a deep feedforward network with d layers
- Each derivative on each level will result into

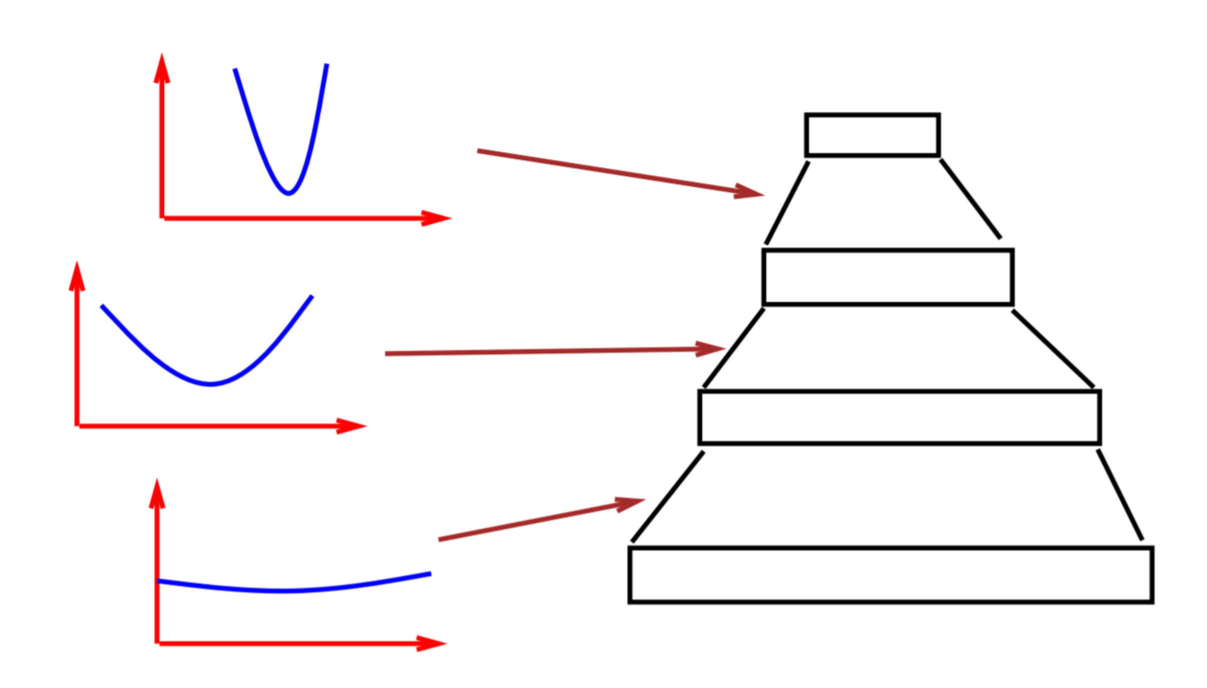
$$\frac{\partial L(w)}{\partial u_d} = \frac{\partial L(w)}{\partial a} \cdot \frac{\partial a}{\partial u_d} = (y - a)\sigma'(w_d u_d) w_d \leq 2 \cdot \frac{1}{4} w_d$$

$$\frac{\partial L(w)}{\partial u_{d-1}} = \frac{\partial L(w)}{\partial u_d} \cdot \frac{\partial u_d}{\partial u_{d-1}} \leq 2 \cdot \left(\frac{1}{4}\right)^2 w_d w_{d-1}$$

It either vanishes or explodes.

Second order methods?

- Second derivative is smaller on lower layers



- There are some improvements

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Tanh

- Activation function $a = \tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$
- Gradient with respect to the input

$$\frac{\partial a}{\partial x} = 1 - \tanh^{2}(x)$$

- Similar to sigmoid, but with different output range $[-1, +1]$
- Stronger gradients, because data is centered around 0 (not 0.5)
- Less bias to hidden layer neurons as now outputs can be both positive and negative (more likely to have zero mean in the end)

ReLU

- Activation function a $= h(x) = \max(0, x)$
- Gradient with respect to the input

$$\frac{\partial a}{\partial x} = \begin{cases} 1, \text{if } x > 0, \\ 0, \text{otherwise.} \end{cases}$$

- Very popular in computer vision and speech recognition

ReLU analysis

- Much faster computations, gradients
- No vanishing or exploding problems, only comparison, addition, multiplication
- People claim biological plausibility
- Sparse activations
- No saturation

- Non-symmetric
- Non-differentiable at 0
- A large gradient during training can cause a neuron to "die". Higher learning rates mitigate the problem

Softplus

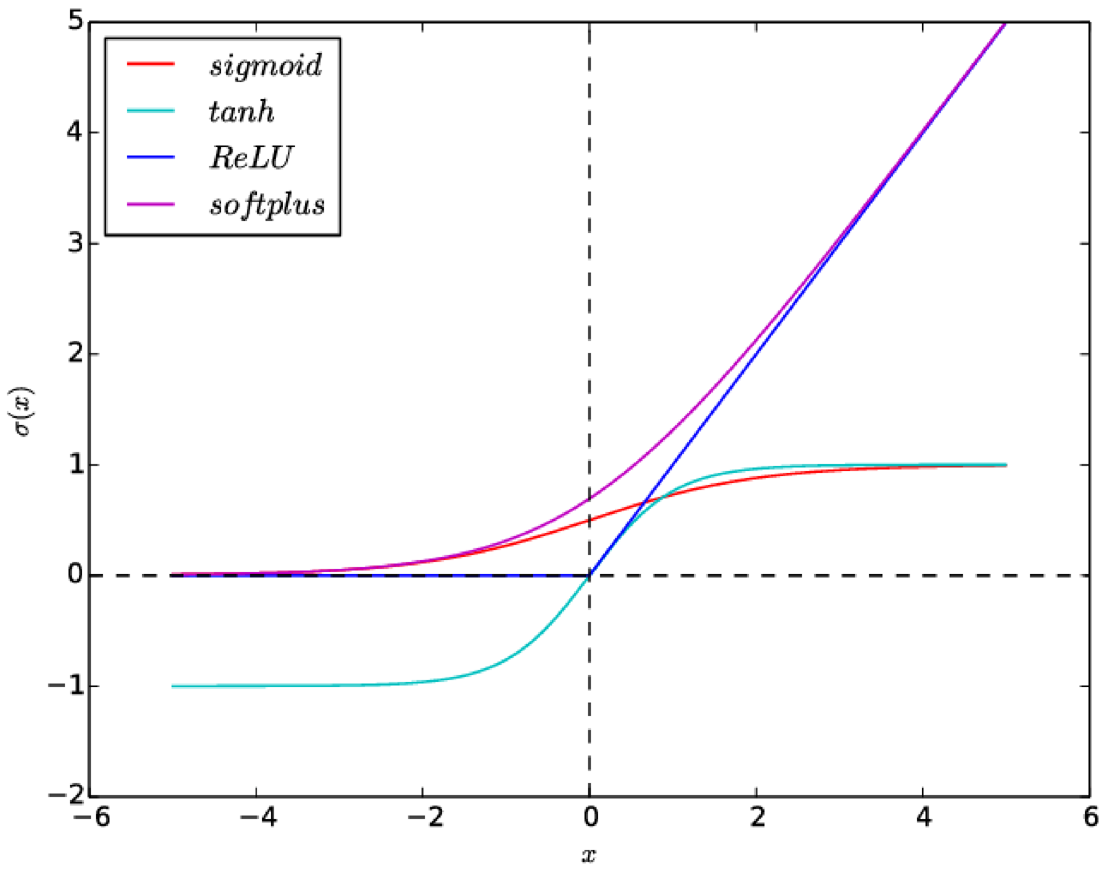
Soft approximation (softplus):

$$a = h(x) = \ln(1 + e^{x})$$

- Differentiable at 0

- Slower
- Empirically, do not outperforms ReLU

Activation functions in one plot



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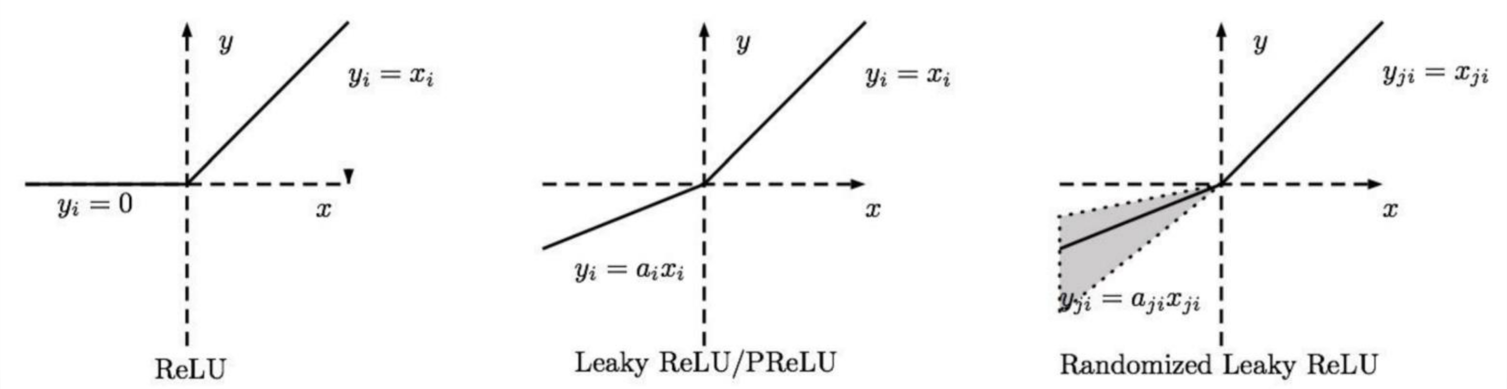
Other ReLUs

Noisy ReLU: $h(x) = \max(0, x + \varepsilon), \varepsilon \sim N(0, \sigma(x))$

Leaky ReLU: $h(x) \begin{cases} x, \text{if } x > 0, \\ 0.01x, \text{otherwise.} \end{cases}$

Parametric ReLu: $h(x) = \begin{cases} x, \text{if } x > 0 \\ \beta x, \text{otherwise} \end{cases}$

(parameter β is trainable)



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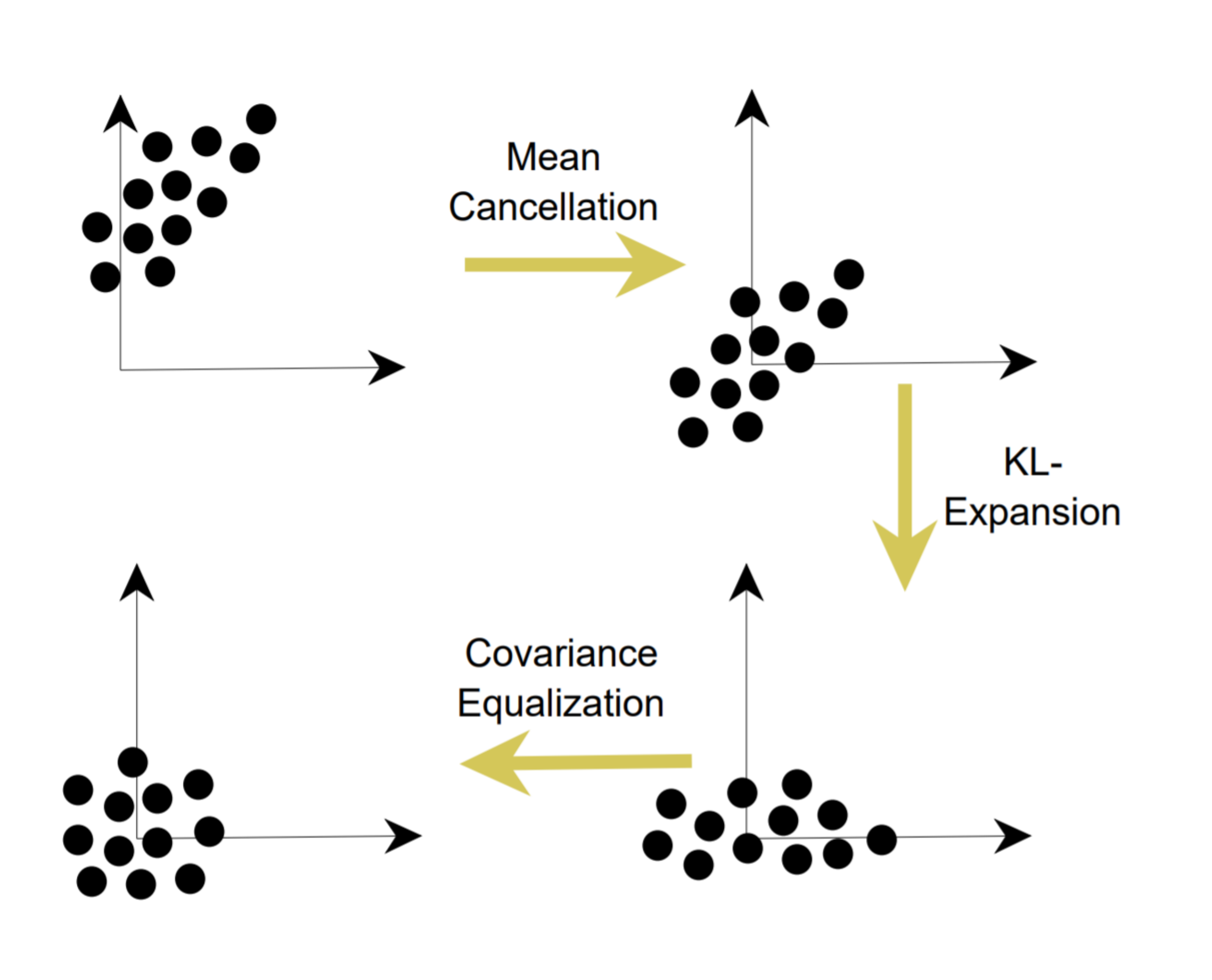
Data preprocessing

Data preprocessing is useful in general and is very important for deep learning optimization. Three main steps:

Types of data augmentation:

- Mean cancellation (centers data)
- Decorrelation [Karhunen-Loeve expansion]
- Scaling

Data preprocessing



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Decorrelation

Covariance matrix: $\mathrm{Cov}(X) = \frac{1}{N} X X^{\mathrm{T}}$

Decorrelation: $\hat{X} = \mathrm{Cov}^{-1/2}(X) \cdot X$

$\mathrm{Cov}(\hat{X}) = I$

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Initial weights selection

- Selection of weights is important to the quality of solution and even convergence of descent.
- Typical scenario is to initialize weights with something small random

Xavier motivation

- Assume we have activation function f, which is linear nearby 0:
$$f(x) = x$$
- tanh is an example of such function

Main idea is to put weights in such linear region and maintain variance to be constant

Evaluating variance (1/2)

$$u_{d+1} = f(u_d w_d) \approx u_d w_d$$

$$\mathrm{D}(u_{d+1,k}) = \mathrm{D}\left(\sum_{i=1}^{n_d} u_{d,i} w_{d,i,k}\right) = \sum_{i=1}^{n_d} \mathrm{D}(u_{d,i} w_{d,i,k})$$

n_d is a number of neurons at dth layer

We can assume that they are independent

$$\mathrm{D}(u_{d+1,k}) = n_i \mathrm{D}(u_{d,i} w_{d,i,k}) =$$
$$= n_i \left(\mathrm{E}(u_{d,i}^2)\mathrm{E}(w_{d,i,k}^2) - \mathrm{E}^2(u_{d,i})\mathrm{E}^2(w_{d,i,k})\right) =$$
$$n_i \mathrm{D}(u_{d,i})\mathrm{D}(w_{d,i,k})$$

Evaluating variance (2/2)

$$\mathrm{D}(u_{d+1}) = \mathrm{D}(x)\prod_{j=1}^{d} n_j\,\mathrm{D}(w_j)$$

$$\mathrm{D}\left(\frac{\partial L}{\partial u_d}\right) = \mathrm{D}\left(\frac{\partial L}{\partial u_N}\right)\prod_{j=d}^{N} n_{j+1}\,\mathrm{D}(w_j)$$

Our requirements $\forall d, h \leq N$:

$$\mathrm{D}(u_d) = \mathrm{D}(u_h)$$

$$\mathrm{D}\left(\frac{\partial L}{\partial u_d}\right) = \mathrm{D}\left(\frac{\partial L}{\partial u_h}\right)$$

Xavier

$\mathrm{D}(u_d) = \mathrm{D}(u_h), \mathrm{D}\left(\frac{\partial L}{\partial u_d}\right) = \mathrm{D}\left(\frac{\partial L}{\partial u_h}\right)$ is equivalent to

$$\forall d \begin{cases} n_d D(w_d) = 1 \\ n_{d+1} D(w_d) = 1 \end{cases}$$

Trade off: $D(w_d) = \frac{2}{n_d + n_{d+1}}$

$$w_d \sim U\left[\frac{-\sqrt{6}}{n_d + n_{d+1}}, \frac{\sqrt{6}}{n_d + n_{d+1}}\right].$$

What to do with ReLU? He

$$\mathrm{D}(u_{d+1}) = \mathrm{D}(x)\prod_{j=1}^{d}\frac{1}{2}n_j\,\mathrm{D}(w_j)$$

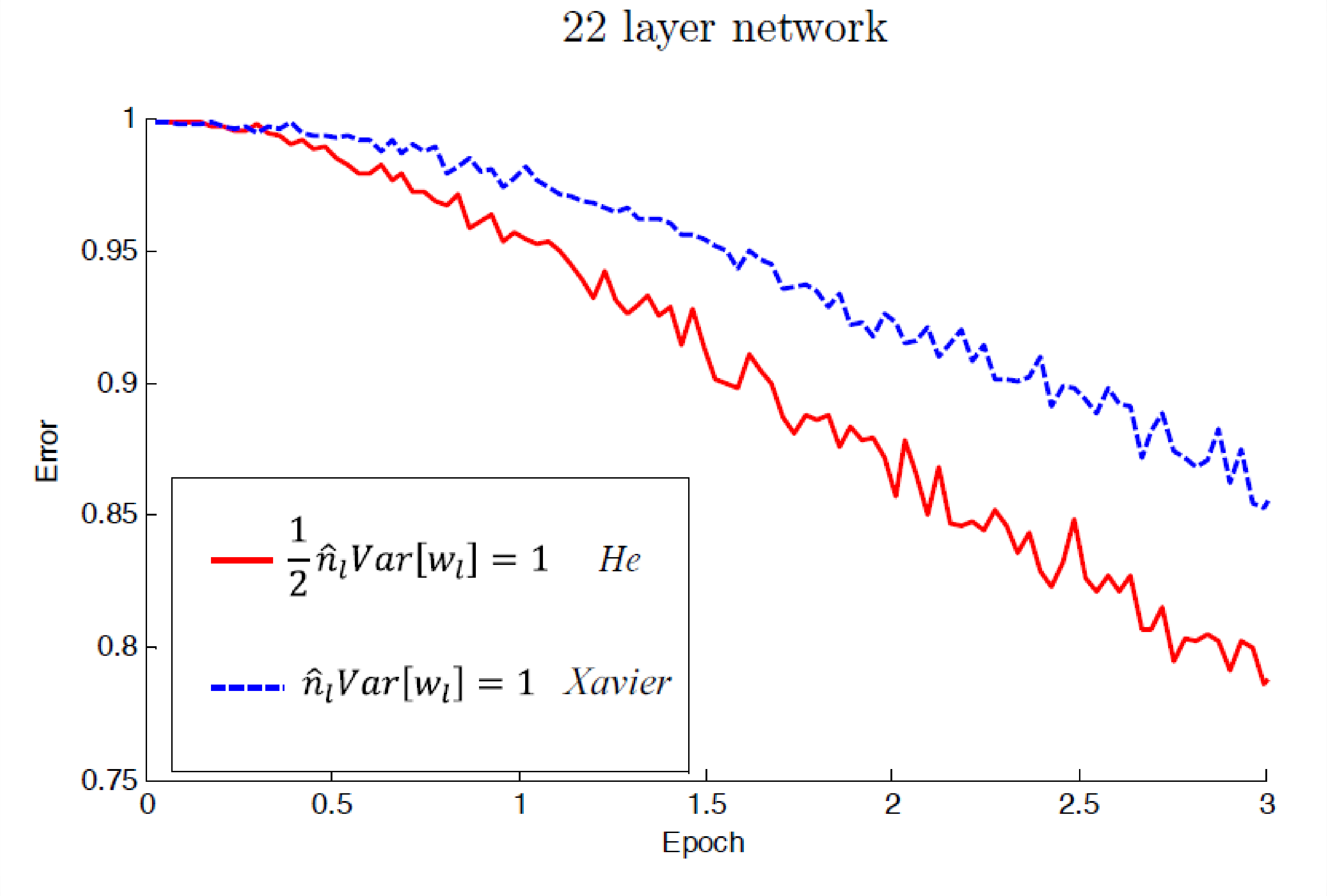
$$\mathrm{D}\left(\frac{\partial L}{\partial u_d}\right) = \mathrm{D}\left(\frac{\partial L}{\partial u_N}\right)\prod_{j=d}^{N}\frac{1}{2}n_{j+1}\,\mathrm{D}(w_j)$$

$$\forall d\ \begin{cases} n_d D(w_d) = 1/2 \\ n_{d+1} D(w_d) = 1/2 \end{cases}$$

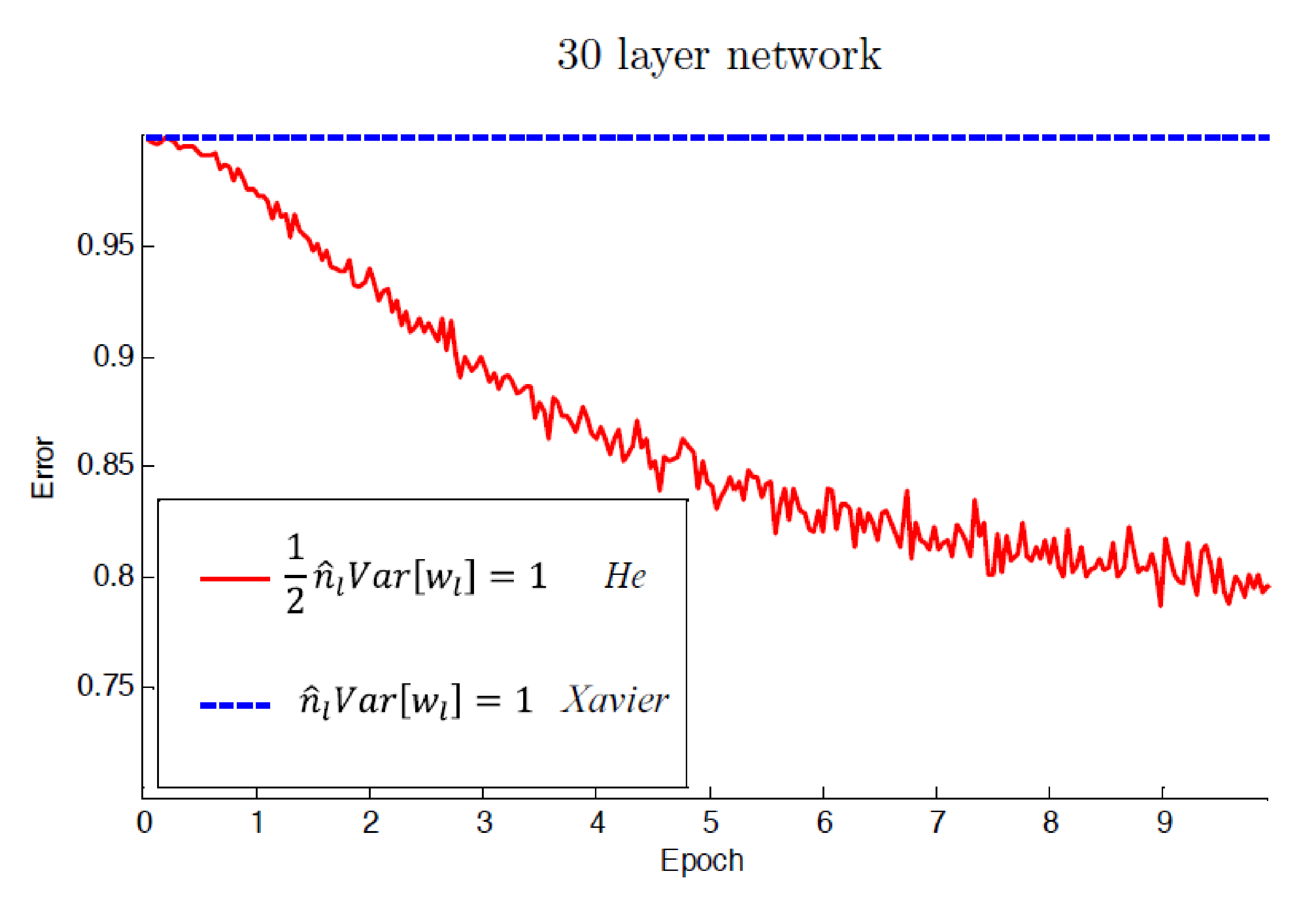
Gaussian is often used:

$w_d \sim N\left[0, \frac{2}{n_d}\right]$ or $w_d \sim N\left[0, \frac{2}{n_{d+1}}\right]$

Xavier vs He (1/2)



Xavier vs He (2/2)



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Stochastic gradient descent (2nd reminder)

Stochastic gradient descent:

$w^{(0)}$ is an initial guess values

$$w^{(k+1)} = w^{(k)} - \mu \frac{\partial L(w^{(k)})}{\partial w}$$

Momentum

Momentum:

$w^{(0)}$ is an initial guess values;

v are updates:

$$w^{(k+1)} = w^{(k+1)} - v^{(k+1)}$$

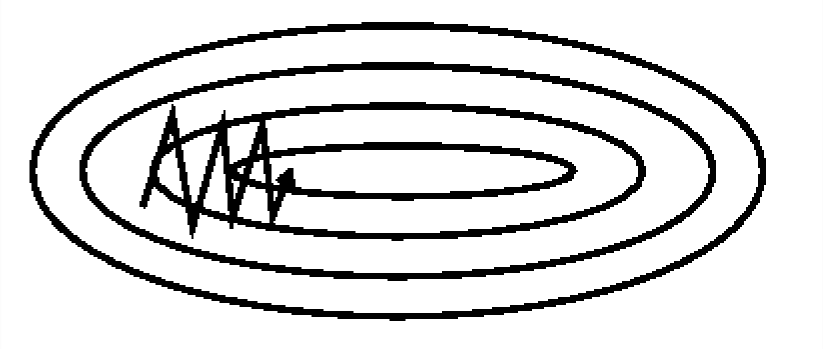
$$v^{(k+1)} = \gamma v^{(k)} + \mu \frac{\partial L(w^{(k)})}{\partial w},$$

γ is momentum, usually set to 0.9

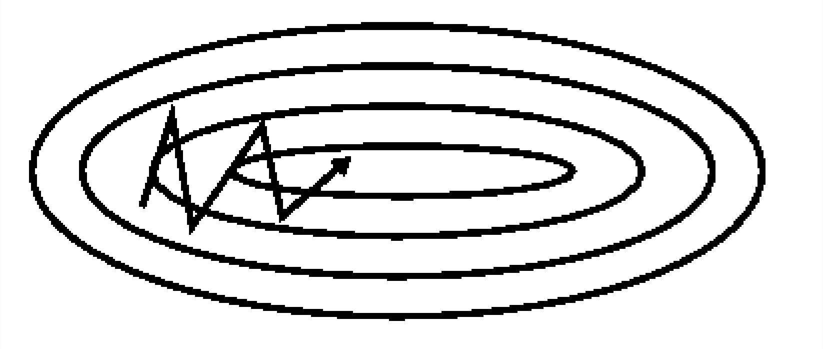
Momentum discussion

Advantages:

- in general is faster in complex terrain when moving in right direction



without Momentum



with Momentum

Disadvantages:

- may fly over minima

Nesterov accelerated gradient

NAG:

$w^{(0)}$ is an initial guess values;

ν are updates:

$$w^{(k+1)} = w^{(k+1)} - \nu^{(k+1)}$$

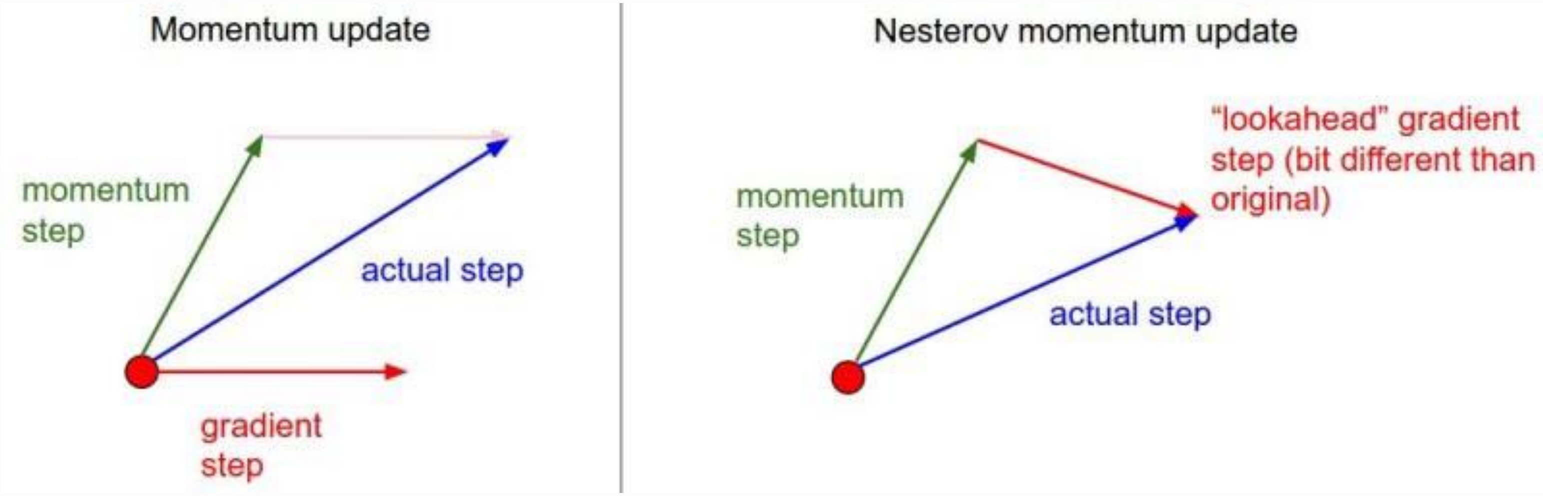
$$\nu^{(k+1)} = \gamma\nu^{(k)} + \mu\frac{\partial L\left(w^{(k)} - \nu^{(k)}\right)}{\partial w},$$

γ is momentum, usually set to 0.9

NAG discussion

Advantages:

- In general, works better
- Convergence proven in certain conditions



- How to choose learning rate?

Adagrad

$$g_{i,(k)} = \frac{\partial L\left(w_i^{(k)}\right)}{\partial w_i}.$$

Adagrade:

$w^{(0)}$ is an initial guess values;

for each i

$$w_i^{(k+1)} = w_i^{(k)} - \frac{\mu}{\sqrt{G_{i,i}^{(k)} + \varepsilon}} g_{i,(k)},$$

where G is a diagonal matrix where each diagonal element i, i is the sum of the squares of the gradients $g_{i,(k)}$up to time step k and

ε is a smoothing term that avoids division by zero.

Adagrade discussion

Advantages:

- Eliminates the need to manually tune the learning rate. Most implementations use a default value of 0.01 and leave it at that.

Disadvantages:

- Accumulation of the squared gradients in the denominator leads to the sum keeping growing during training. Eventually, algorithm stops to learn anything.

RMSProp

$$E^{(k)}[g_i^2] \; = \gamma E^{(k-1)}[g_i^2] + (1-\gamma) g_{i,(k)}^2$$

RMSProp:

$w^{(0)}$ is an initial guess values;

for each i

$$w_i^{(k+1)} = w_i^{(k)} - \frac{\mu}{\sqrt{E^{(k)}[g_i^2] + \varepsilon}} g_{i,(k)},$$

where ε is a smoothing term that avoids division by zero.

Set γ to be 0.9

Adadelta (1/3)

$$w^{(k+1)} = w^{(k)} - \mu\left(Q''\left(w^{(k)}\right)\right)^{-1} Q'\left(w^{(k)}\right)$$

$$w^{(k+1)} = w^{(k)} + \Delta w^{(k)}$$

$\left(Q''\left(w^{(k)}\right)\right)^{-1}$ is hard to evaluate, so let think it is diagonal

$$\left(Q''\left(w^{(k)}\right)\right) \approx \operatorname{diag}\left(\frac{\partial Q^2\left(w_i^{(k)}\right)}{\partial w_i^2}\right)$$

$$\Delta w_i^{(k)} \approx \left(\frac{\partial Q^2\left(w_i^{(k)}\right)}{\partial w_i^2}\right)^{-1}\left(\frac{\partial Q\left(w_i^{(k)}\right)}{\partial w_i}\right)$$

$$\frac{\partial Q^2\left(w_i^{(k)}\right)}{\partial w_i^2} \approx \frac{\left(\frac{\partial Q\left(w_i^{(k)}\right)}{\partial w_i}\right)}{\Delta w_i^{(k)}}$$

Adadelta (2/3)

$$E^{(k)}[g_i^2] \;= \gamma E^{(k-1)}[g_i^2] + (1-\gamma) g_{i,(k)}^2$$

$$RMS^{(k)}[g_i] = \sqrt{E^{(k)}[g_i^2] + \varepsilon}$$

$$RMS^{(k)}[\Delta w_i] = \sqrt{E^{(k)}\left[\Delta w_i^2\right] + \varepsilon}$$

$$\frac{\partial Q^2\left(w_i^{(k)}\right)}{\partial w_i^2} \approx \frac{\left(\frac{\partial Q\left(w_i^{(k)}\right)}{\partial w_i}\right)}{\Delta w_i^{(k)}} \approx \frac{g_i^{(k)}}{\Delta w_i^{(k-1)}} = \frac{RMS^{(k)}[g_i]}{RMS^{(k-1)}[\Delta w_i]}.$$

Adadelta (3/3)

Adadelta:

$w^{(0)}$ is an initial guess values;

for each i

$$w_i^{(k+1)} = w_i^{(k)} - \frac{RMS^{(k-1)}[\Delta w_i]}{RMS^{(k)}[g_i]} g_i^{(k)}$$

No learning rate is required!

In practice, learning rate is still added to improve performance.

Adam (Adaptive Moment Estimation)

$$m_{(k)} = E^{(k)}[g_i] = \gamma_1 E^{(k-1)}[g_i] + (1-\gamma_1)g_{i,(k)}$$
$$b_{(k)} = E^{(k)}[g_i^2] = \gamma_2 E^{(k-1)}[g_i^2] + (1-\gamma_2)g_{i,(k)}^2$$

We want them to be unbiased:

$$\mathrm{E}\left(m_{(k)}\right) = \mathrm{E}\left(g_{(k)}\right), \mathrm{E}\left(b_{(k)}\right) = \mathrm{E}\left(g_{(k)}^2\right)$$

To satisfy it, we need amendment:

$$\begin{cases} \widehat{m}_{(k)} = \dfrac{m_{(k)}}{1-\gamma_1^k} \\ \hat{b}_{(k)} = \dfrac{b_{(k)}}{1-\gamma_2^k} \end{cases}$$

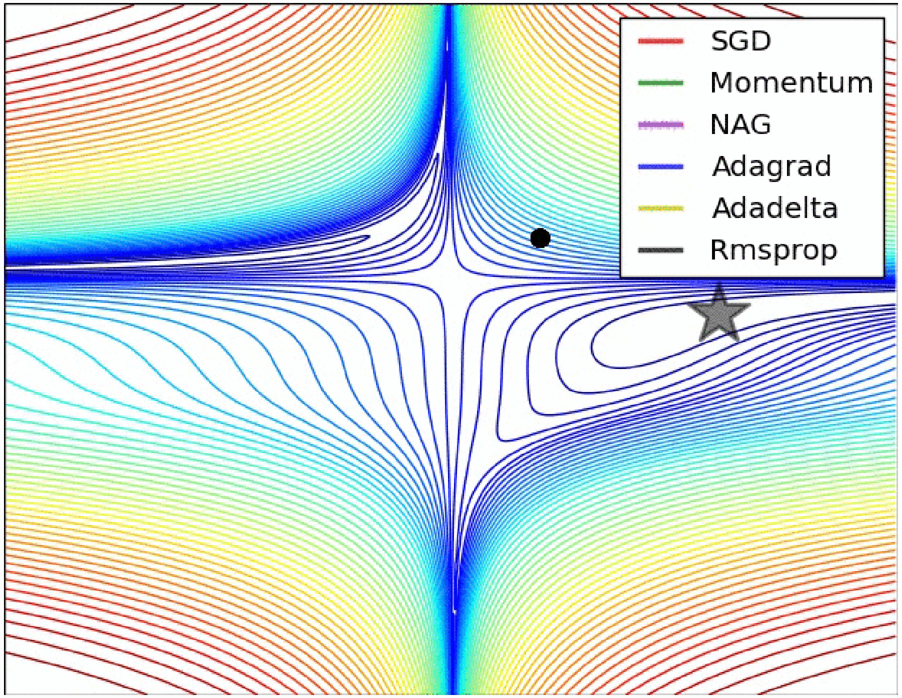
Adam (Adaptive Moment Estimation)

Adam:

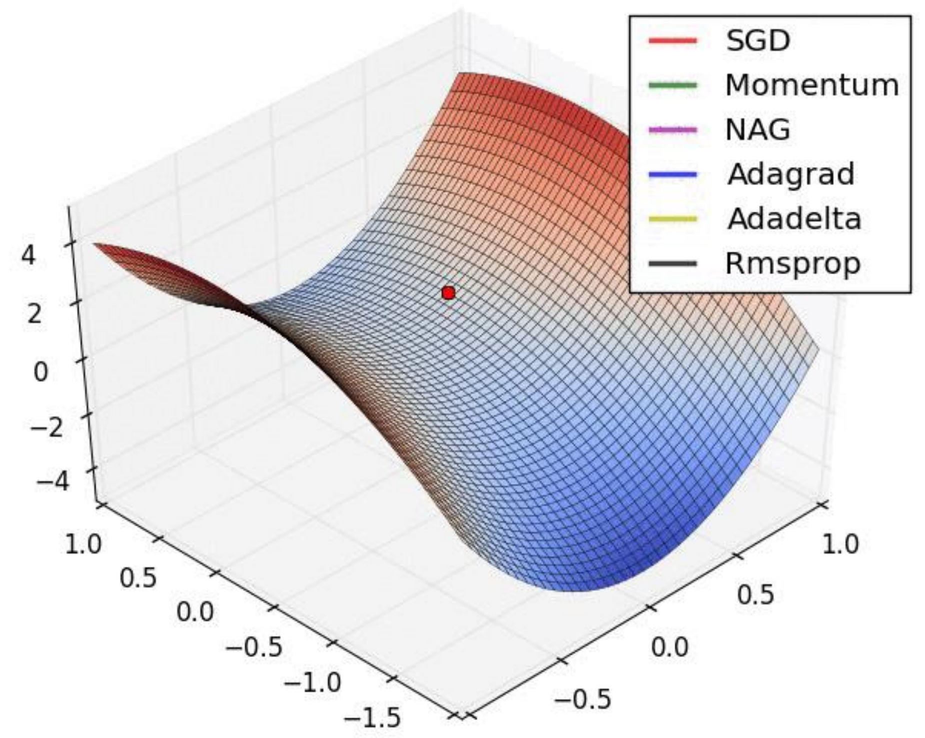
$w^{(0)}$ is an initial guess values

$$w^{(k)} = w^{(k)} - \frac{\mu}{\sqrt{\hat{b}_{(k)}^{2} + \varepsilon}} \widehat{m}_{(k)}$$

Comparison



SGD
Momentum
NAG
Adagrad
Adadelta
Rmsprop



SGD
Momentum
NAG
Adagrad
Adadelta
Rmsprop
4
2
0
−2
−4
1.0
0.5
0.0
−0.5
−1.0
−1.5
1.0
0.5
0.0
−0.5

Additional steps

- Shuffling and Curriculum Learning
- Early stopping
- Gradient noise
- Batch normalization

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Layer-wise SGD problem

After updating weights, domains are updates

Main idea: maintain covariance constant for each layer input:

$$\hat{x}_d = \frac{x_d - \mathrm{E}(x_i)}{\sqrt{\mathrm{D}(x_d) + \varepsilon}}$$

E and D should be evaluated on each mini-batch

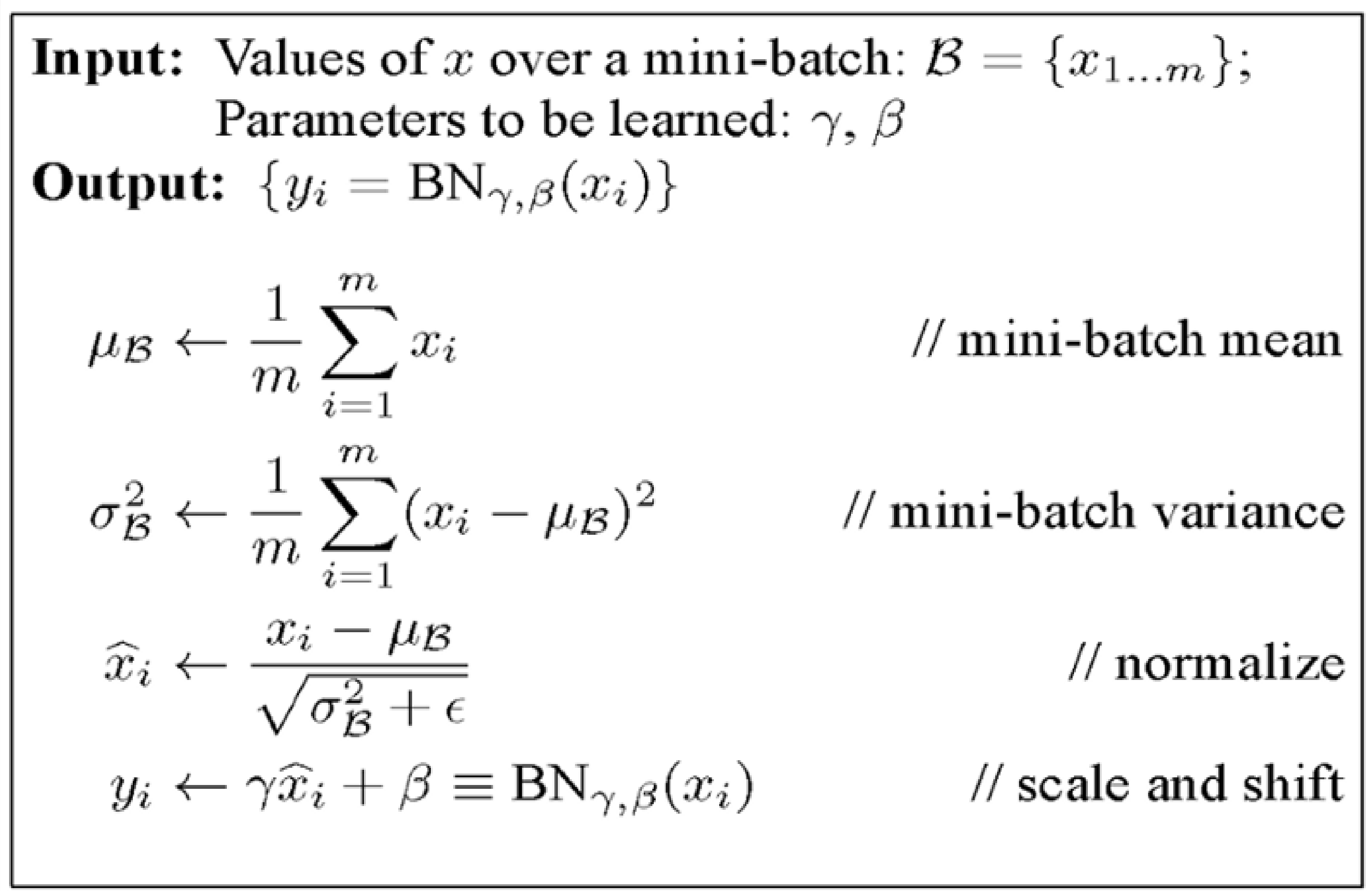
Parametric layer for batch normalization

Add a parametric layer with rescaling:

$$\hat{y}_d = \gamma_d \hat{x}_d + \beta_d$$

γ and β can be learned

Batch normalization algorithm

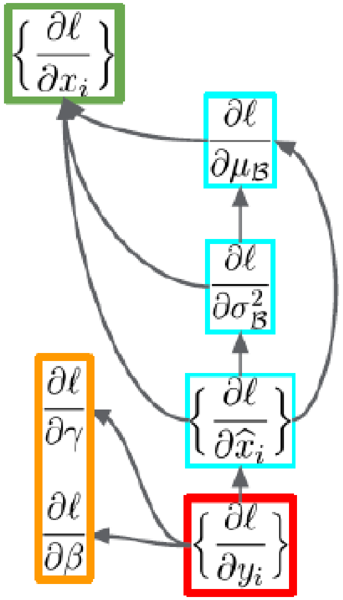


```
Input: Values of $x$ over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
       Parameters to be learned: $\gamma$, $\beta$
Output: $\{y_i = \text{BN}_{\gamma,\beta}(x_i)\}$

    $\mu_\mathcal{B} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i$                          // mini-batch mean
    $\sigma_\mathcal{B}^2 \leftarrow \frac{1}{m} \sum_{i=1}^{m} (x_i - \mu_\mathcal{B})^2$     // mini-batch variance
    $\widehat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}}$                      // normalize
    $y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \text{BN}_{\gamma,\beta}(x_i)$         // scale and shift
```

Gradient descent for BN

We will learn BN layer as a layer



$\left\{\frac{\partial \ell}{\partial x_i}\right\}$
$\frac{\partial \ell}{\partial \mu_{\mathcal{B}}}$
$\frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2}$
$\frac{\partial \ell}{\partial \gamma}$
$\frac{\partial \ell}{\partial \beta}$
$\left\{\frac{\partial \ell}{\partial \widehat{x}_i}\right\}$
$\left\{\frac{\partial \ell}{\partial y_i}\right\}$

$$\frac{\partial \ell}{\partial \widehat{x}_i} = \frac{\partial \ell}{\partial y_i} \cdot \gamma$$

$$\frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot (x_i - \mu_{\mathcal{B}}) \cdot \frac{-1}{2}(\sigma_{\mathcal{B}}^2 + \epsilon)^{-3/2}$$

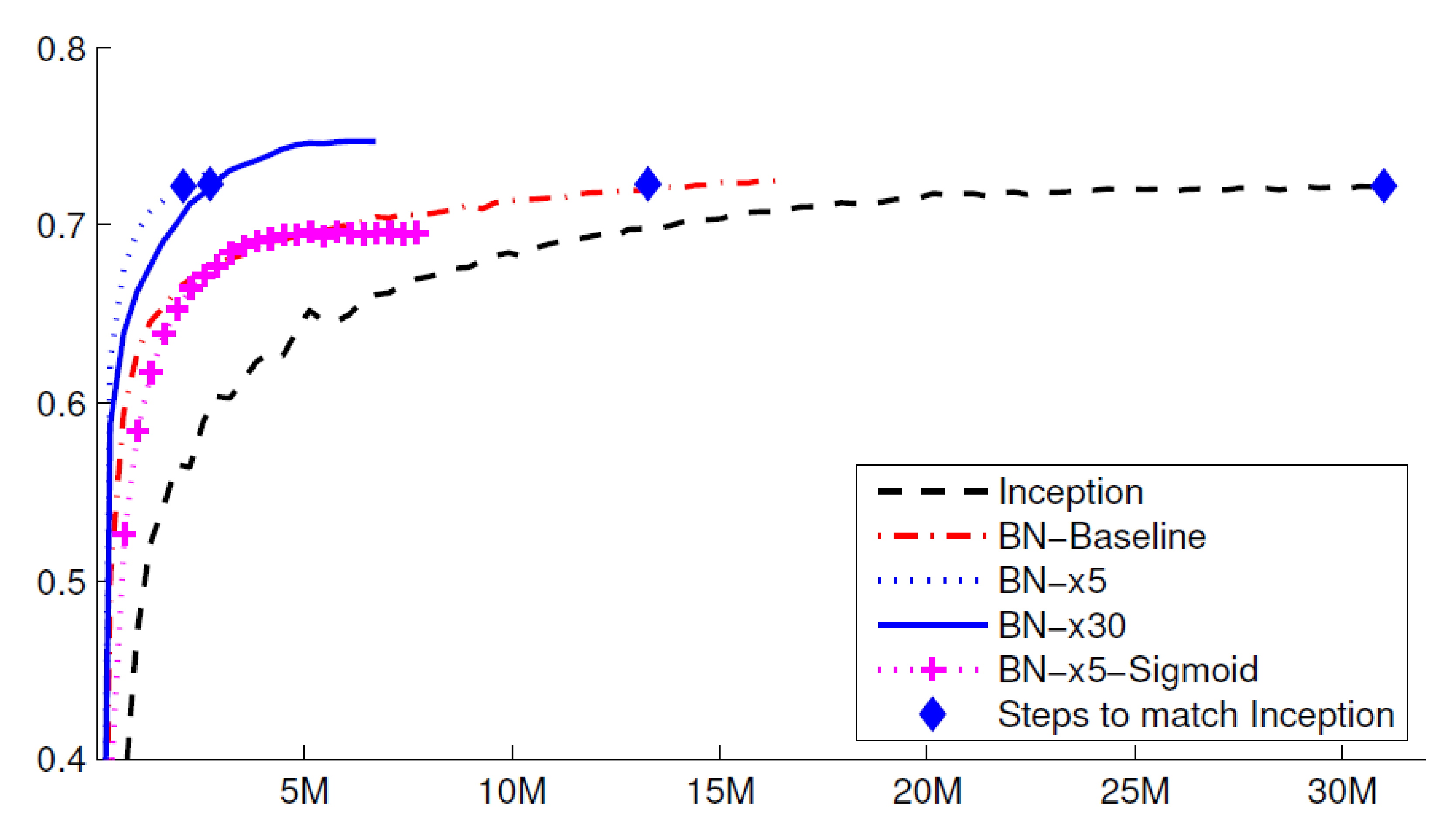
$$\frac{\partial \ell}{\partial \mu_{\mathcal{B}}} = \left(\sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \right) + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{\sum_{i=1}^{m} -2(x_i - \mu_{\mathcal{B}})}{m-1}$$

$$\frac{\partial \ell}{\partial x_i} = \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{1}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{2(x_i - \mu_{\mathcal{B}})}{m-1} + \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} \cdot \frac{1}{m}$$

$$\frac{\partial \ell}{\partial \gamma} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i} \cdot \widehat{x}_i$$

$$\frac{\partial \ell}{\partial \beta} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i}$$

Batch-normalization comparison



Batch normalization analysis

- Works fast
- Converge fast
- Make other regularization not so useful