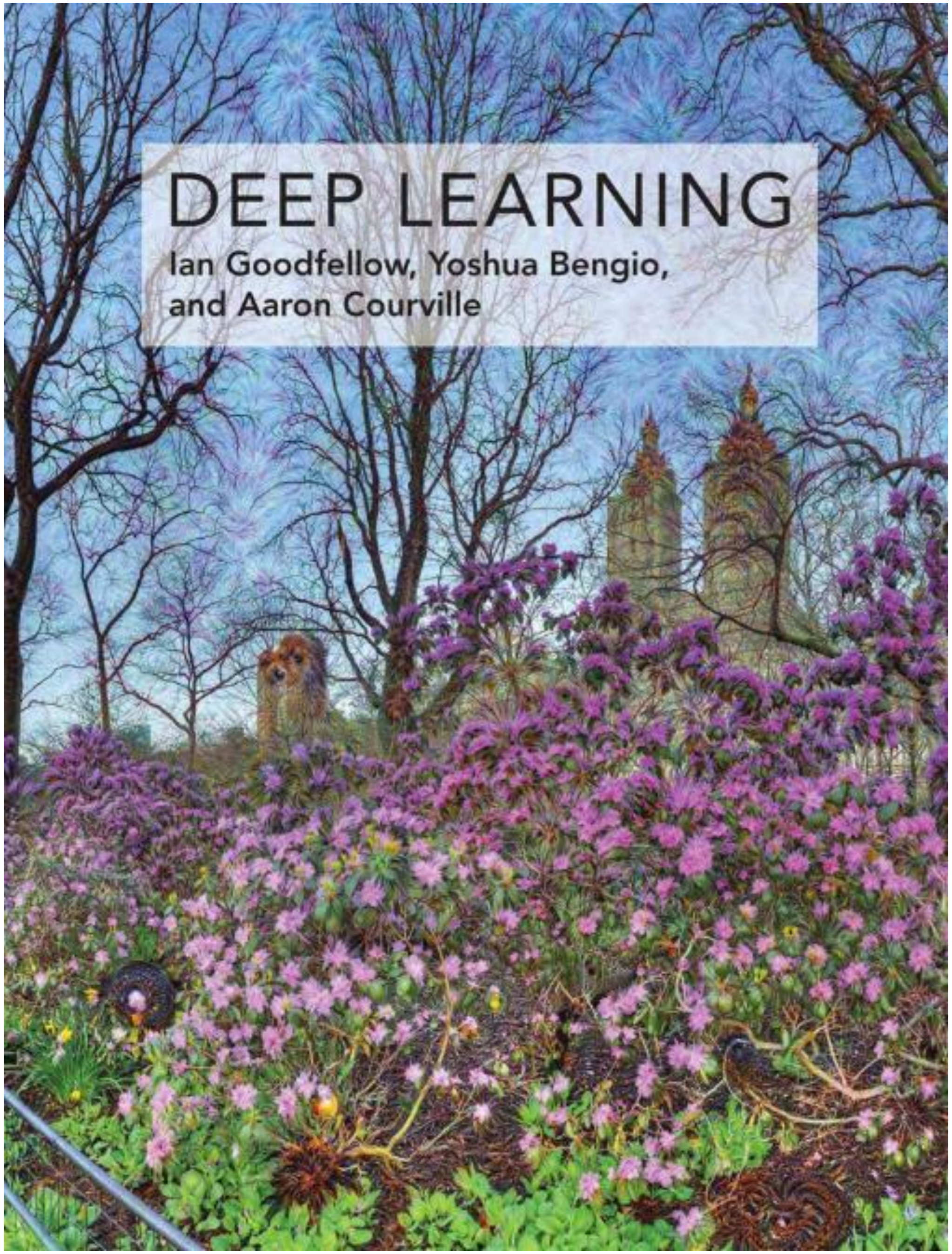
Optimization for Training Deep Models

Fundamentals of Media Processing (Machine Learning Part)

Lecturer:
佐藤　真一（Prof. SATO　Shinichi）
池畑　諭（Prof. IKEHATA　Satoshi）10/27, 11/10, 11/17, 11/21, 12/1, 12/8
山岸　順一（Prof. Junichi Yamagishi）
児玉　和也（Prof. KODAMA　Kazuya）
孟　洋（Prof. MO　Hiroshi）



Chapter 1-9 (out of 20)

An introduction to a broad range of topics in deep learning, covering mathematical and conceptual background, deep learning techniques used in industry, and research perspectives.

- Due to my background, I will mainly talk about "image"
- I will introduce some applications beyond this book

Deep Learning

An MIT Press book in preparation

Ian Goodfellow, Yoshua Bengio and Aaron Courville

Book Exercises External Links

Lectures

We plan to offer lecture slides accompanying all chapters of this book. We currently offer slides for only some chapters. If you are a course instructor and have your own lecture slides that are relevant, feel free to contact us if you would like to have your slides linked or mirrored from this site.

1. Introduction
   - Presentation of Chapter 1, based on figures from the book [.key] [.pdf]
   - **Video** of lecture by Ian and discussion of Chapter 1 at a reading group in San Francisco organized by Alena Kruchkova
2. Linear Algebra [.key][.pdf]
3. Probability and Information Theory [.key][.pdf]
4. Numerical Computation [.key] [.pdf] [youtube]
5. Machine Learning Basics [.key] [.pdf]
6. Deep Feedforward Networks [.key] [.pdf]
   - Video (.flv) of a presentation by Ian and a group discussion at a reading group at Google organized by Chintan Kaur.
7. Regularization for Deep Learning [.pdf] [.key]
8. Optimization for Training Deep Models
   - **Gradient Descent and Structure of Neural Network Cost Functions** [.key] [.pdf] These slides describe how gradient descent behaves on different kinds of cost function surfaces. Intuition for the structure of the cost function can be built by examining a second-order Taylor series approximation of the cost function. This quadratic function can give rise to issues such as poor conditioning and saddle points. Visualization of neural network cost functions shows how these and some other geometric features of neural

Free copy of the book and useful materials are available at

https://www.deeplearningbook.org/lecture_slides.html

Schedule

10/27 (Today)	Introduction	Chap. 1
	probability, information theory, numerical computation	Chap. 2,3,4
11/10	Machine Learning Basics	Chap. 5
11/17, 11/24, 12/1	Deep Feedforward Networks	Chap. 6
	Regularization and Deep Learning	Chap. 7
	Optimization for Training Deep Models	Chap. 8
12/8	Convolutional Neural Networks	Chap. 9 and more

Review: How Deep Learning Differs from Pure Optimization

- Empirical Risk Minimization: We do not need the true distribution p_{data} but empirical distribution $\hat{p}_{\text{data}}$ defined by the training set. The training process based on minimizing the averaging training error is known as ***empirical risk minimization***

- Exactly minimizing 0-1 loss is typically intractable in classification problem. We typically optimizes a ***surrogate loss function*** such as thee ***negative log-likelihood*** of the correct class. Training halts when a convergence criterion (e.g., ***early stopping)*** is satisfied (not at local minima), which avoids over-fitting

- The objective function usually decomposes as a sum over training examples with ***minibatch*** in ***stochastic descent algorithm***

How to Define Minibatch Size?

- Larger batches provide a more accurate estimate of the gradient, but the improvement is less than linear returns
- Multicore architectures are usually underutilized by extremely small batches, which motivates using some absolute minimum batch size, below which there is no reduction in the time to process a minibatch
- If all examples in the batch are to be processed in parallel, then the amount of memory scales with the batch size. For many hardware setups this is the limiting factor in batch size
- When using GPUs, it is common for power of 2 batch size to offer better runtime (e.g., 16 to 256)
- Small batches can offer a regularizing effect, perhaps due to the noise they add to the learning process. Generalization error is often best for a batch size of 1 though the total runtime can be very high.

Other Tips for Minibatch Algorithm

- The minibatches must be selected randomly to compute an unbiased estimate of the expected gradient from a set of samples

- Many datasets are arranged that two successive examples are highly correlated, therefore the ***shuffle of data*** is necessary

- An interesting motivation for minibatch stochastic gradient descent is that it follows the gradient of the true generalization error as long as no examples are repeated. Nevertheless, most implementations of minibatch stochastic gradient descent shuffle the dataset once and then pass through it multiple times (***epochs***) (i.e., the second path is unbiased) to reduce the training loss

- With extremely large training datasets, it is becoming more common to use each training example *only once*

Challenges in Neural Network Optimization (1)

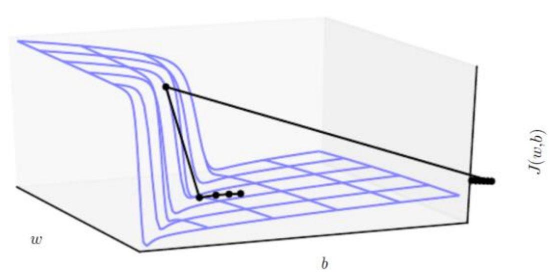
- Ill-Conditioning:
  - Ill-conditioning of Hessian matrix H can manifest by causing SGD to get stuck in the sense that even very small steps increase the cost function (i.e., $-\epsilon \boldsymbol{g}^T \boldsymbol{g} + \frac{1}{2}\epsilon^2 \boldsymbol{g}^T H \boldsymbol{g} > \mathbf{0}$):

$$f(\boldsymbol{x}^0 - \epsilon \boldsymbol{g}) \approx f(\boldsymbol{x}^0) - \epsilon \boldsymbol{g}^T \boldsymbol{g} + \frac{1}{2}\epsilon^2 \boldsymbol{g}^T H \boldsymbol{g}$$

- Local Minima:
  - Neural networks and any models with multiple equivalently parametrized latent variables all have multiple local minima because of the ***model identifiability*** problem (e.g, swapping model weights may cause the same output (***weight space symmetry***)). Today, it is not considered problematic for sufficiently large neural networks with early stopping

Challenges in Neural Network Optimization (2)

- Saddle Points:
  - Saddle points are more common than local minima in neural networks
  - The Eigen values of Hessian matrix at a saddle point has both positive negative value, which makes the optimization unstable. Fortunately, Goodfellow(2015) showed that gradient descent trajectory rapidly escaped this region unlike Newton's method
- Cliffs and Exploding Gradients:
  - Neural networks with many layers often have extremely steep regions resembling cliff which may move the parameters quite rapidly (especially in recurrent neural network). We can avoid this by applying the ***gradient clipping*** in section 10



Challenges in Neural Network Optimization (3)

- Long-Term Dependencies:
  - When we need to repeatedly multiplying *the same weights* in extremely deep graph (e.g., recurrent neural networks), the vanishing and exploding gradient problem may occur. On the other hand the feedforward network does not have this issue since the weights are different (See details in section 10.7)
- Theoretical limits of Optimization
  - Some theoretical results show that there exist problem classes that are intractable by neural networks, but it can be difficult to tell whether a particular problem falls into that class. It is also difficult to tell whether an optimization algorithm gave the solution we needed
  - Developing more realistic bounds on the performance of optimization algorithms therefore an important goal for machine learning research

About Stochastic Gradient Descent

- It is common to decay the learning rate linearly until iteration τ:
  - $\epsilon_k = (1-\alpha)\epsilon_0 + \alpha\epsilon_\tau$ with $\alpha = k/\tau$
  - Usually τ is set to the number of iterations required to make a few hundred passes through the training set. ϵ_τ should be set to roughly 1 percent the value of ϵ_0. ϵ_0 is generally decided by monitoring the first few iterations and using a learning rate that is higher than the best-performing learning rate at this time

- The convergence rate of the SGD for the convex problem is $O(1/k)$ or $O(1/\sqrt{k})$. Bousquet(2008) mentioned that it may not be worthwhile to pursue an optimization algorithm that converges faster than $O(1/k)$ for machine learning tasks (faster convergence corresponds to overfitting)

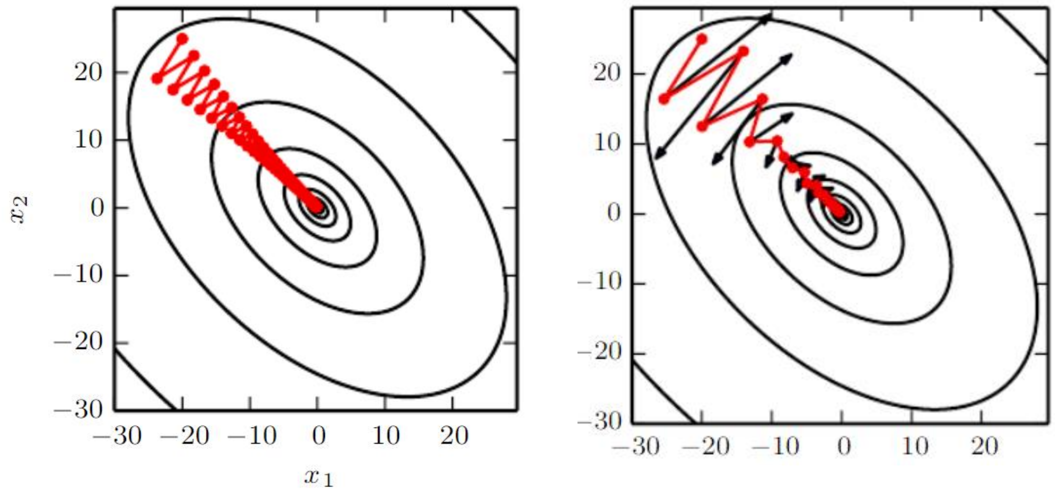
Momentum (1)

- Unfortunately, SGD can be slow. The ***momentum*** is designed to accelerate learning, especially in the face of high curvature, small but consistent gradient, or noisy gradients
- The momentum algorithm accumulates an exponentially decaying moving average of past gradients and continues to move in their direction
- The momentum algorithm introduces the velocity $\boldsymbol{v}$**,** which is the direction and speed at which the parameters move through parameter space

$$\boldsymbol{v}^t \leftarrow -\epsilon \boldsymbol{g}^t + \alpha \boldsymbol{v}^{t-1} = \alpha \boldsymbol{v}^{t-1} - \epsilon \nabla_\theta \left(\frac{1}{m} \sum_{i=1}^{m} L\left(f\left(x^i; \theta\right), y^i\right) \right)$$

$$\boldsymbol{\theta}^t \leftarrow \boldsymbol{\theta}^{t-1} + \boldsymbol{v}^t = \boldsymbol{\theta}^{t-1} - \epsilon \boldsymbol{g}^t + \alpha \boldsymbol{v}^{t-1}$$

Momentum (2)



Algorithm 8.2 Stochastic gradient descent (SGD) with momentum

---

Require: Learning rate ϵ, momentum parameter α

Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$

while stopping criterion not met **do**

Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.

Compute gradient estimate: $\boldsymbol{g} \leftarrow \frac{1}{m}\nabla_{\boldsymbol{\theta}}\sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), \boldsymbol{y}^{(i)})$.

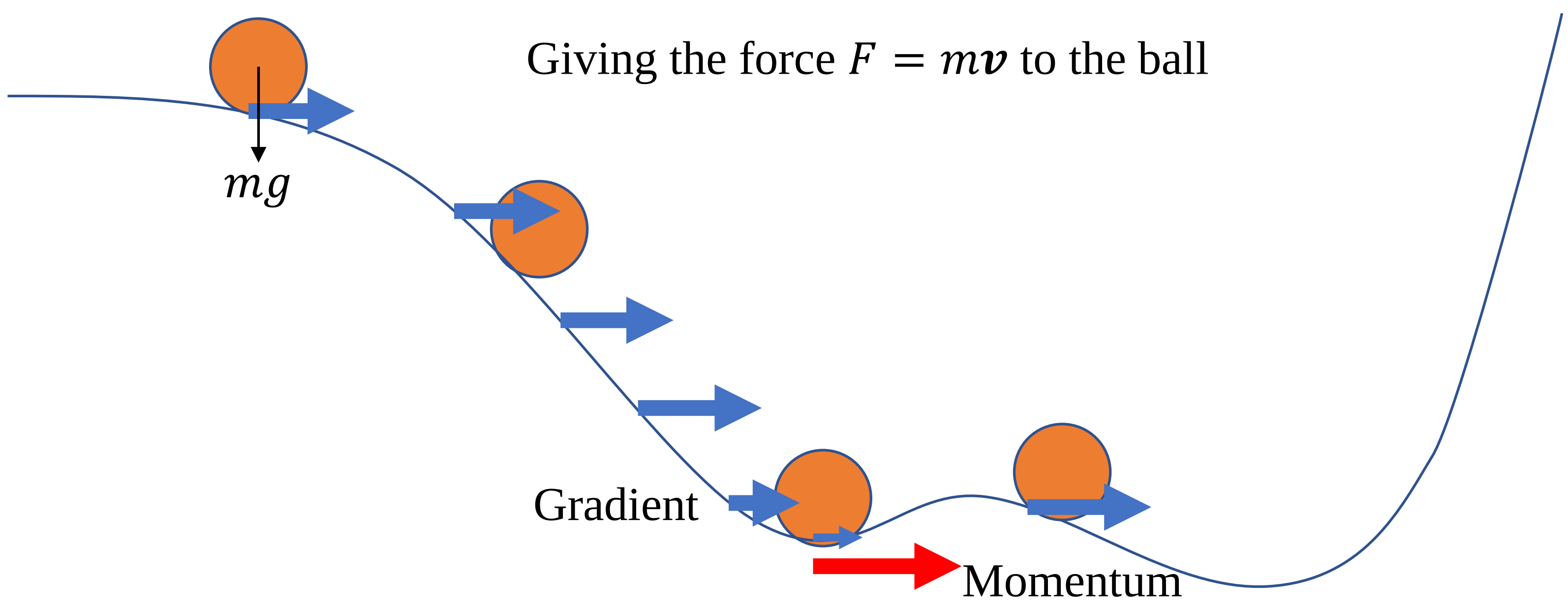
Compute velocity update: $\boldsymbol{v} \leftarrow \alpha\boldsymbol{v} - \epsilon\boldsymbol{g}$.

Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$.

end while

Momentum (3)

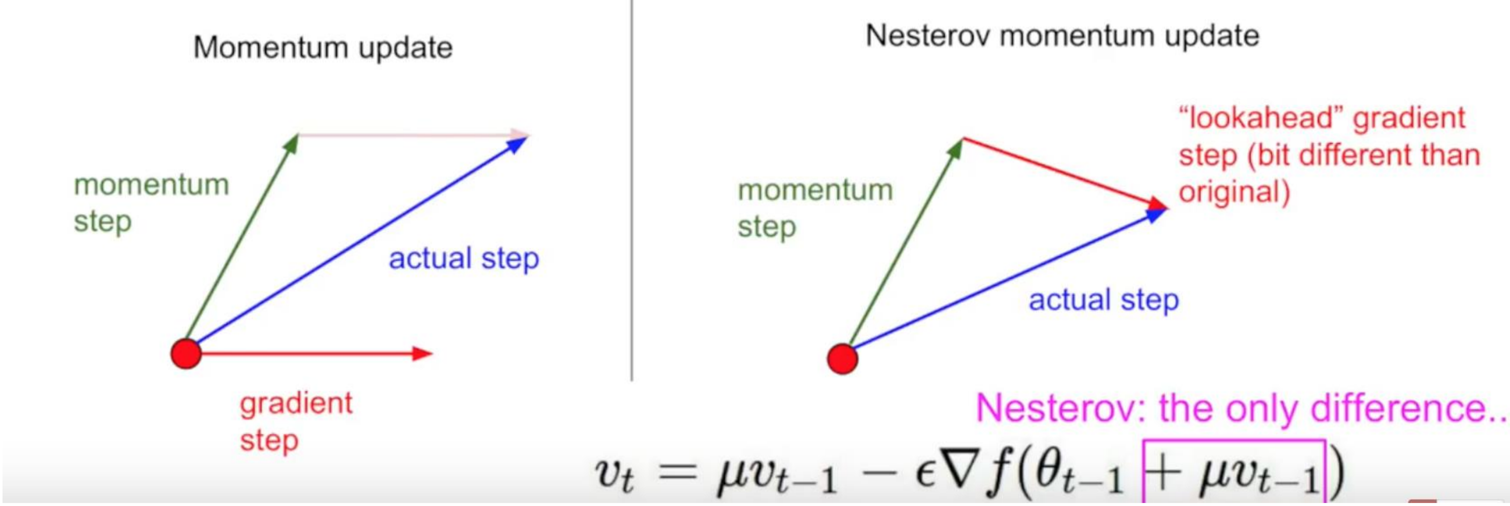
- If the momentum algorithm always observes gradient $\boldsymbol{g}$, then it will accelerate in the direction of $-\boldsymbol{g}$, until reaching a terminal velocity where the size of each step is $\epsilon\|\boldsymbol{g}\|/(1-\alpha)$
- Common values of α used in practice include 0.5, 0.9, 0.99. For example 0.9 corresponds to multiplying the maximum speed by 10 relative to the gradient descent method. α may also be adaptive starting from the small value and is later raised.



Momentum (4)

- ***Nesterov Momentum*** (Sutskever2013)
  - A variance of the momentum algorithm that was inspired by Nesterov's accelerated gradient method (Nesterov1983). The gradient is evaluated after the current velocity is applied. Nesterov Momemtum does not improve the rate of convergence in the stochastic gradient

$$\boldsymbol{v}^t \leftarrow \alpha \boldsymbol{v}^{t-1} - \epsilon \nabla_\theta \left(\frac{1}{m} \sum_{i=1}^{m} L\left(f\left(x^i; \theta^{t-1} + \alpha \boldsymbol{v}\right), y^i\right) \right)$$



https://medium.com/@ramrajchandradevan/the-evolution-of-gradient-descend-optimization-algorithm-4106a6702d39

Parameter Initialization (Weight)

- Some heuristics are available for choosing the initial scale of the weights:
  - Initialize the weights of a fully connected layer with m inputs and n outputs by sampling each weight from the uniform distribution of $U(-\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}})$,
  - Glorot(2010) suggest using the normalized initialization $W_{i,j} \sim U\left(-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right)$
  - Saxe(2013) recommend initializing to random orthogonal matrices, with a carefully chosen scaling or gain factor g that accounts for the nonlinearity applied at each layer
  - Martens(2010) introduced an alternative initialization scheme called sparse initialization, in which each unit is initialized to have exactly k nonzero weights to avoid the weights being too small
  - It is also good idea to treat the initial scale of the weights as a hyper parameter if computational resources allows it

Implementation in Keras Library

Ones [source]

```
keras.initializers.Ones()
```

Initializer that generates tensors initialized to 1.

Constant [source]

```
keras.initializers.Constant(value=0)
```

Initializer that generates tensors initialized to a constant value.

Arguments

value: float; the value of the generator tensors.

RandomNormal [source]

```
keras.initializers.RandomNormal(mean=0.0, stddev=0.05, seed=None)
```

Initializer that generates tensors with a normal distribution.

Arguments

mean: a python scalar or a scalar tensor. Mean of the random values to generate. stddev: a python scalar or a scalar tensor. Standard deviation of the random values to generate. seed: A Python integer. Used to seed the random generator.

RandomUniform [source]

```
keras.initializers.RandomUniform(minval=-0.05, maxval=0.05, seed=None)
```

Initializer that generates tensors with a uniform distribution.

Arguments

minval: A python scalar or a scalar tensor. Lower bound of the range of random values to generate. maxval: A python scalar or a scalar tensor. Upper bound of the range of random values to generate. Defaults to 1 for float types. seed: A Python integer. Used to seed the random generator.

TruncatedNormal [source]

```
keras.initializers.TruncatedNormal(mean=0.0, stddev=0.05, seed=None)
```

Initializer that generates a truncated normal distribution.

These values are similar to values from a `RandomNormal` except that values more than two standard deviations from the mean are discarded and re-drawn. This is the recommended initializer for neural network weights and filters.

Arguments

mean: a python scalar or a scalar tensor. Mean of the random values to generate. stddev: a python scalar or a scalar tensor. Standard deviation of the random values to generate. seed: A Python integer. Used to seed the random generator.

VarianceScaling [source]

```
keras.initializers.VarianceScaling(scale=1.0, mode='fan_in', distribution='normal', seed=None)
```

Initializer capable of adapting its scale to the shape of weights.

glorot_uniform

```
keras.initializers.glorot_uniform(seed=None)
```

Glorot uniform initializer, also called Xavier uniform initializer.

It draws samples from a uniform distribution within [-limit, limit] where `limit` is `sqrt(6 / (fan_in + fan_out))` where `fan_in` is the number of input units in the weight tensor and `fan_out` is the number of output units in the weight tensor.

Arguments

- seed: A Python integer. Used to seed the random generator.

Returns

An initializer.

References

- Understanding the difficulty of training deep feedforward neural networks

he_normal

```
keras.initializers.he_normal(seed=None)
```

He normal initializer.

It draws samples from a truncated normal distribution centered on 0 with `stddev = sqrt(2 / fan_in)` where `fan_in` is the number of input units in the weight tensor.

Arguments

- seed: A Python integer. Used to seed the random generator.

Returns

An initializer.

References

- Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification

lecun_normal

```
keras.initializers.lecun_normal(seed=None)
```

LeCun normal initializer.

It draws samples from a truncated normal distribution centered on 0 with `stddev = sqrt(1 / fan_in)` where `fan_in` is the number of input units in the weight tensor.

Arguments

- seed: A Python integer. Used to seed the random generator.

Returns

An initializer.

References

- Self-Normalizing Neural Networks

Orthogonal [source]

```
keras.initializers.Orthogonal(gain=1.0, seed=None)
```

Initializer that generates a random orthogonal matrix.

Arguments

- gain: Multiplicative factor to apply to the orthogonal matrix.
- seed: A Python integer. Used to seed the random generator.

References

- Exact solutions to the nonlinear dynamics of learning in deep linear neural networks

Identity [source]

```
keras.initializers.Identity(gain=1.0)
```

Initializer that generates the identity matrix.

Only use for 2D matrices. If the long side of the matrix is a multiple of the short side, multiple identity matrices are concatenated along the long side.

Arguments

gain: Multiplicative factor to apply to the identity matrix.

lecun_uniform

```
keras.initializers.lecun_uniform(seed=None)
```

LeCun uniform initializer.

It draws samples from a uniform distribution within [-limit, limit] where `limit` is `sqrt(3 / fan_in)` where `fan_in` is the number of input units in the weight tensor.

Arguments

- seed: A Python integer. Used to seed the random generator.

Returns

An initializer.

References

- Efficient BackProp

glorot_normal

```
keras.initializers.glorot_normal(seed=None)
```

Glorot normal initializer, also called Xavier normal initializer.

It draws samples from a truncated normal distribution centered on 0 with `stddev = sqrt(2 / (fan_in + fan_out))` where `fan_in` is the number of input units in the weight tensor and `fan_out` is the number of output units in the weight tensor.

Arguments

- seed: A Python integer. Used to seed the random generator.

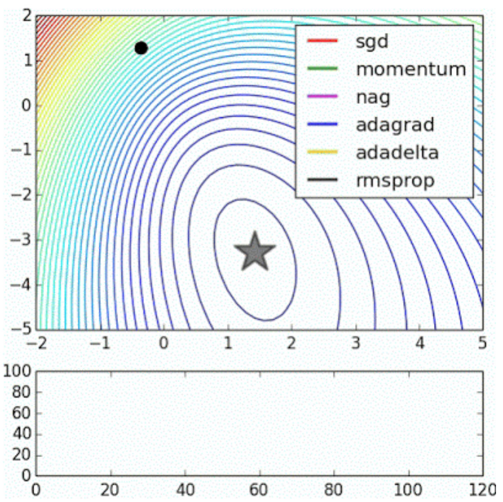
Parameter Initialization (Bias)

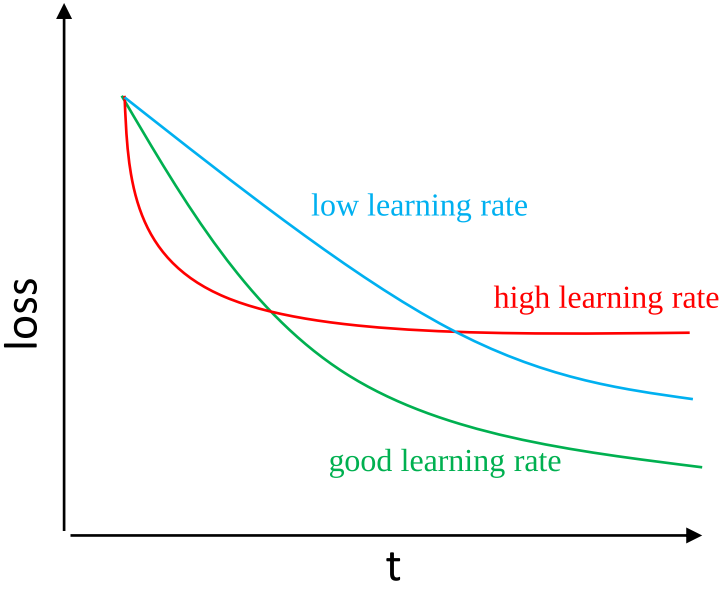
- There are a few situations where we may set some biases to nonzero values:
  - If a bias is for an output unit, then it is often beneficial to initialize the bias to obtain the right marginal statistics of the output (e.g., $\mathrm{softmax}(\mathbf{b}) = \mathbf{c}$ (output distribution))
  - Sometimes we may want to choose the bias to avoid causing too much saturation at initialization. For example, we may set the bias of a ReLU hidden unit to 0.1
  - If we have a gate unit (decide if a unit is participate or not), then we firstly want to choose the output of the unit is one by adding the bias (e.g., LSTM model in chapter 10)
- Besides these random methods of initialization, it is possible to initialize model parameters using machine learning. A common strategy is to initialize the supervised model using unsupervised model trained on the same inputs (See Part III)

Algorithms with Adaptive Learning Rate

- The learning rate is reliably one of the most difficult to set hyperparameters because it significantly affects model performance

- Here we introduce some important algorithms
  - AdaGrad
  - RMSProp
  - Adam





http://www.denizyuret.com/2015/03/alec-radfords-animations-for.html

AdaGrad (Duchi2011)

- ***AdaGrad*** individually adapts the learning rates of all parameters by scaling them inversely proportional to the square root of the sum of all the historical squared values of the gradient. Empirically, the accumulation of squared gradients from the beginning of training can result in excessive decrease in learning rate (e.g., passing points whose gradient is large at early steps)

Algorithm 8.4 The AdaGrad algorithm

Require: Global learning rate ϵ
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant δ, perhaps 10^{-7}, for numerical stability
  Initialize gradient accumulation variable $\boldsymbol{r} = \boldsymbol{0}$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$.
    Accumulate squared gradient: $\boldsymbol{r} \leftarrow \boldsymbol{r} + \boldsymbol{g} \odot \boldsymbol{g}$.
    Compute update: $\Delta \boldsymbol{\theta} \leftarrow -\frac{\epsilon}{\delta + \sqrt{\boldsymbol{r}}} \odot \boldsymbol{g}$. (Division and square root applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta \boldsymbol{\theta}$.
  end while

RMSProp (Hinton2012)

- ***RMSProp*** modifies AdaGrad to perform better in the nonconvex setting by using exponentially decaying average to discard history from the extreme past to avoid the gradient decreases too rapidly

Algorithm 8.5 The RMSProp algorithm

Require: Global learning rate ϵ, decay rate ρ (e.g., 0.9)
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant δ, usually 10^{-6}, used to stabilize division by small numbers
Initialize accumulation variables $\boldsymbol{r} = 0$
while stopping criterion not met **do**
Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$.
Accumulate squared gradient: $\boldsymbol{r} \leftarrow \rho \boldsymbol{r} + (1-\rho) \boldsymbol{g} \odot \boldsymbol{g}$.
Compute parameter update: $\Delta \boldsymbol{\theta} = -\frac{\epsilon}{\sqrt{\delta + \boldsymbol{r}}} \odot \boldsymbol{g}$. ($\frac{1}{\sqrt{\delta+\boldsymbol{r}}}$ applied element-wise)
$\epsilon = 0.01$
Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta \boldsymbol{\theta}$.
end while

Adam (Kingma2014)

- ***Adam*** is a combination of RMSProp and momentum. In Adam, momentum is incorporated directly as an estimate of the first-order moment of the gradient. Adam includes bias corrections to the estimates for both the first-order moments and the second-order moments to account for their initialization at the origin

Algorithm 8.7 The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)
Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1)$. (Suggested defaults: 0.9 and 0.999 respectively)
Require: Small constant δ used for numerical stabilization (Suggested default: 10^{-8})
Require: Initial parameters $\boldsymbol{\theta}$
  Initialize 1st and 2nd moment variables $\boldsymbol{s} = \mathbf{0}$, $\boldsymbol{r} = \mathbf{0}$
  Initialize time step $t = 0$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    $t \leftarrow t + 1$
    Update biased first moment estimate: $\boldsymbol{s} \leftarrow \rho_1 \boldsymbol{s} + (1 - \rho_1)\boldsymbol{g}$ ←Momentum
    Update biased second moment estimate: $\boldsymbol{r} \leftarrow \rho_2 \boldsymbol{r} + (1 - \rho_2)\boldsymbol{g} \odot \boldsymbol{g}$ ←RMSProp (with decay rate)
    Correct bias in first moment: $\hat{\boldsymbol{s}} \leftarrow \frac{\boldsymbol{s}}{1-\rho_1^t}$
    Correct bias in second moment: $\hat{\boldsymbol{r}} \leftarrow \frac{\boldsymbol{r}}{1-\rho_2^t}$
    Compute update: $\Delta\boldsymbol{\theta} = -\epsilon \frac{\hat{\boldsymbol{s}}}{\sqrt{\hat{\boldsymbol{r}}}+\delta}$ (operations applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
  end while

$$s_1 = 0.9 * s_0 + 0.1 * g = 0.1g$$

$$r_1 = 0.999 * r_0 + 0.001 * g^2 = 0.001g^2$$

$$\frac{s}{\sqrt{r} + \delta} = \frac{0.1g}{\sqrt{0.001g^2} + \delta}$$

$$\frac{\hat{s}}{\sqrt{\hat{r}} + \delta} = \frac{0.1/0.9g}{\sqrt{0.001g^2/0.009} + \delta}$$

Approximate Second-Order Methods (1)

- ***Newton's method***
  - In deep learning, the surface of the objective function typically nonconvex, where eigenvalues of Hessian are not all positive (i.e., local minima and saddle points). To avoid this, we can regularize Hessian by adding a constant value along the diagonal of the Hessian. However, only networks with a very small number of parameters can be practically trained via Newton's method due to the significant computational burden.

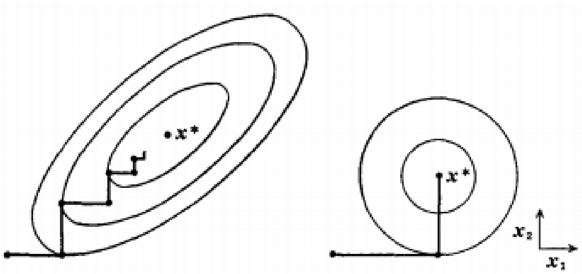
Algorithm 8.8 Newton's method with objective $J(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), y^{(i)})$

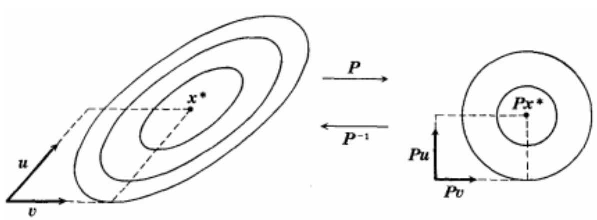
Require: Initial parameter $\boldsymbol{\theta}_0$
Require: Training set of m examples
while stopping criterion not met **do**
  Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m}\nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
  Compute Hessian: $\boldsymbol{H} \leftarrow \frac{1}{m}\nabla^2_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
  Compute Hessian inverse: $\boldsymbol{H}^{-1}$
  Compute update: $\Delta\boldsymbol{\theta} = -\boldsymbol{H}^{-1}\boldsymbol{g}$
  Apply update: $\boldsymbol{\theta} = \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
end while

$$\Delta\theta = -[H + \alpha I]^{-1}\boldsymbol{g}$$

Approximate Second-Order Methods (2)

- ***Conjugate Gradient***
  - Efficiently avoids the calculation of the inverse Hessian by iteratively descending conjugate directions (When $\boldsymbol{\rho}_t^T H \boldsymbol{\rho}_{t-1} = 0$, $\boldsymbol{\rho}_t$ and $\boldsymbol{\rho}_{t-1}$ are ***conjugate*** w.r.t H).





conjugate orthogonal

Algorithm 8.9 The conjugate gradient method

Require: Initial parameters $\boldsymbol{\theta}_0$
Require: Training set of m examples
  Initialize $\boldsymbol{\rho}_0 = \mathbf{0}$
  Initialize $g_0 = 0$
  Initialize $t = 1$
  while stopping criterion not met **do**
    Initialize the gradient $\boldsymbol{g}_t = \mathbf{0}$
    Compute gradient: $\boldsymbol{g}_t \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Compute $\beta_t = \frac{(\boldsymbol{g}_t - \boldsymbol{g}_{t-1})^\top \boldsymbol{g}_t}{\boldsymbol{g}_{t-1}^\top \boldsymbol{g}_{t-1}}$ (Polak-Ribière)
    (Nonlinear conjugate gradient: optionally reset β_t to zero, for example if t is a multiple of some constant k, such as $k = 5$)
    Compute search direction: $\boldsymbol{\rho}_t = -\boldsymbol{g}_t + \beta_t \boldsymbol{\rho}_{t-1}$
    Perform line search to find: $\epsilon^* = \text{argmin}_\epsilon \frac{1}{m} \sum_{i=1}^{m} L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}_t + \epsilon \boldsymbol{\rho}_t), \boldsymbol{y}^{(i)})$
    (On a truly quadratic cost function, analytically solve for ϵ^* rather than explicitly searching for it)
    Apply update: $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \epsilon^* \boldsymbol{\rho}_t$
    $t \leftarrow t + 1$
  end while

Approximate Second-Order Methods (3)

- ***BFGS (Broyden-Fletcher-Goldfarb-Shanno algorithm)***
  - Attempts to bring some of the advantages of Newton's method without the computational burden by approximating Hessian
  - The memory costs of the BFGS algorithm can be significantly decreased (L-BFGS) by avoiding storing the complete inverse Hessian approximation B_k by assuming that B_0 is a identity matrix (sparse)

From an initial guess $\mathbf{x}_0$ and an approximate Hessian matrix B_0 the following steps are repeated as $\mathbf{x}_k$ converges to the solution:

1. Obtain a direction $\mathbf{p}_k$ by solving $B_k \mathbf{p}_k = -\nabla f(\mathbf{x}_k)$.
2. Perform a one-dimensional optimization (line search) to find an acceptable stepsize α_k in the direction found in the first step, so $\alpha_k = \arg\min f(\mathbf{x}_k + \alpha \mathbf{p}_k)$.
3. Set $\mathbf{s}_k = \alpha_k \mathbf{p}_k$ and update $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k$.
4. $\mathbf{y}_k = \nabla f(\mathbf{x}_{k+1}) - \nabla f(\mathbf{x}_k)$.
5. $B_{k+1} = B_k + \dfrac{\mathbf{y}_k \mathbf{y}_k^{\mathrm{T}}}{\mathbf{y}_k^{\mathrm{T}} \mathbf{s}_k} - \dfrac{B_k \mathbf{s}_k \mathbf{s}_k^{\mathrm{T}} B_k}{\mathbf{s}_k^{\mathrm{T}} B_k \mathbf{s}_k}$.

$$\boldsymbol{H}_{k+1} = \left[\boldsymbol{I} - \frac{\boldsymbol{s}_k \boldsymbol{y}_k^T}{\boldsymbol{y}_k^T \boldsymbol{s}_k}\right] \boldsymbol{H}_k \left[\boldsymbol{I} - \frac{\boldsymbol{y}_k \boldsymbol{s}_k^T}{\boldsymbol{y}_k^T \boldsymbol{s}_k}\right] + \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{y}_k^T \boldsymbol{s}_k}$$

$$\boldsymbol{V}_k = \boldsymbol{I} - \rho_k \boldsymbol{y}_k \boldsymbol{s}_k^T, \rho_k = 1/\boldsymbol{y}_k^T \boldsymbol{s}_k$$

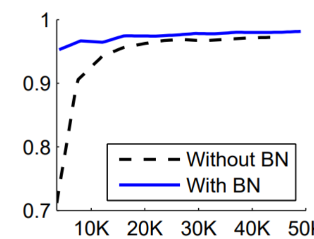
$$\boldsymbol{H}_{k+1} = \boldsymbol{V}_k^T \boldsymbol{H}_k \boldsymbol{V}_k + \rho_k \boldsymbol{s}_k \boldsymbol{s}_k^T$$

$$\begin{aligned} \boldsymbol{H}_{k+1} = & \left(\boldsymbol{V}_k^T \cdots \boldsymbol{V}_{k-m}^T\right) \boldsymbol{H}_0 \left(\boldsymbol{V}_{k-m} \cdots \boldsymbol{V}_k\right) \\ & + \rho_0 \left(\boldsymbol{V}_k^T \cdots \boldsymbol{V}_{k-m+1}^T\right) \boldsymbol{s}_0 \boldsymbol{s}_0^T \left(\boldsymbol{V}_{k-m+1} \cdots \boldsymbol{V}_k\right) \\ & + \rho_1 \left(\boldsymbol{V}_k^T \cdots \boldsymbol{V}_{k-m+2}^T\right) \boldsymbol{s}_1 \boldsymbol{s}_1^T \left(\boldsymbol{V}_{k-m+2} \cdots \boldsymbol{V}_k\right) \\ & \vdots \\ & + \rho_k \boldsymbol{s}_k \boldsymbol{s}_k^T \end{aligned}$$

https://en.wikipedia.org/wiki/Broyden%E2%80%93Fletcher%E2%80%93Goldfarb%E2%80%93Shanno_algorithm

Batch Normalization

- ***Internal Covariate Shift*** (Shimodaira2000): Training deep neural networks changes the distribution of each layer's inputs during training, even when the parameters of the previous layers slightly change, which slows down the training by requiring lower learning rates and careful parameter initialization
- ***Batch Normalization*** (BN, Loffe2015) is applied after the activation to reparametrize the model to make units normalized by a *unit Gaussian* ($\mu = 0,\ \sigma^2 = 1$). For a layer with d-channel input $x = \left(x^{(1)}, \dots, x^{(d)}\right)$, we will normalize each dimension



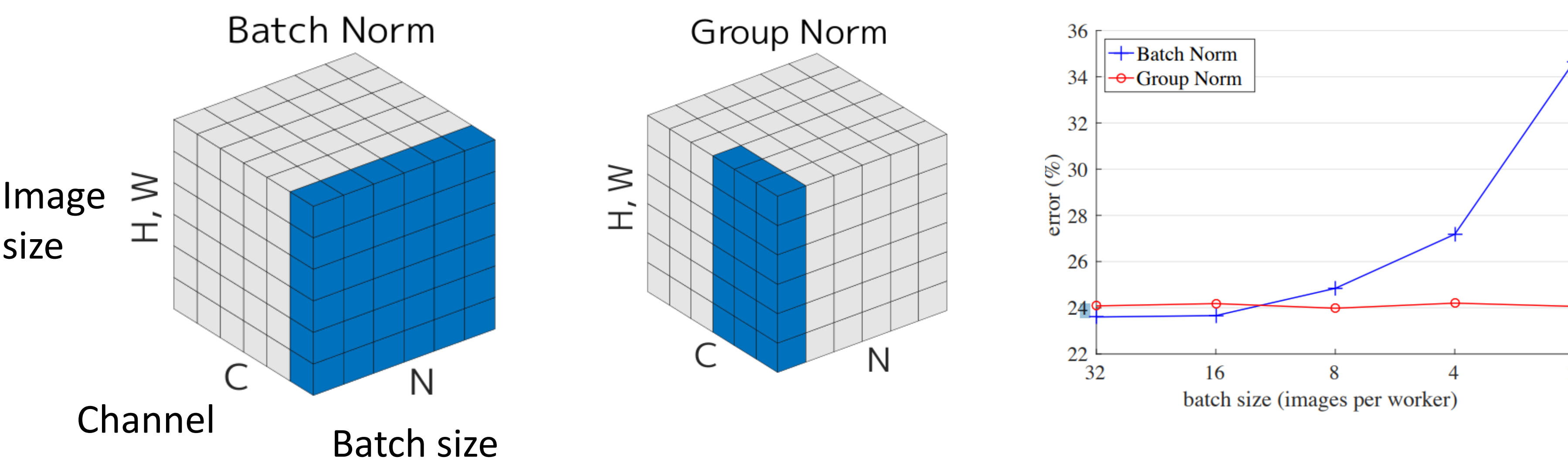
$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

- The expectation and variance are computed over the mini-batch (e.g., $x_1^{(k)}, \dots, x_{256}^{(k)}$). To maintain the expressive power, it is common to use $\alpha\hat{x}^{(k)} + \beta$ (α, β are learnable parameters)

Group Normalization

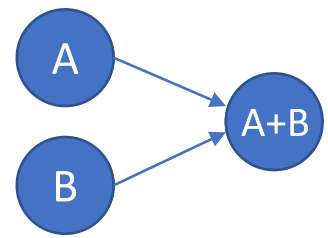
- In BN, a small batch leads to inaccurate estimation of the batch statistics, and reducing BN's batch size increases the model error dramatically

- ***Group Normalization*** (GN, Wu2018) divides channels into groups and normalizes the features within each group. GN does not exploit the batch dimension, and its computation is independent of batch sizes

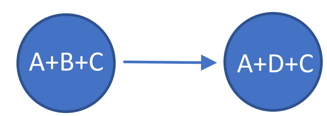


Supervised Pretraining

- ***Greedy algorithms***
  - break a problem into many components, then combine individually optimized component (the global optima is not guaranteed)
  - Often followed by the ***fine-tuning***



- ***Greedy supervised algorithms***
  - break a problem into many supervised learning problem
  - Instead of pretraining one layer at a time, we can train a deep convolutional network and then use the first and last few layers to initialize even deeper networks



- ***FitNets*** (Romero2015)
  - Firstly, train a teacher network and then train the student network (deeper and thinner) with a supervision by the teacher network (using a intermediate representations learned by a teacher)

Coordinate Descent

- It may be possible to solve an optimization problem quickly by minimizing a multivariate function w.r.t a single variable x_i while fixing x_j. This practice is known as ***(block) coordinate descent***

- For example, consider a cost function:

$$J(H,W) = \sum_{i,j} |H_{i,j}| + \sum_{i,j} (X - W^T H)^2_{i,j}$$

- The entire problem is nonconvex, but a subproblem w.r.t a single variable (W, H) is convex

- Coordinate Descent is not a good strategy when variables are strongly related e.g., $f = (x_1 - x_2)^2 + \alpha(x_1^2 - x_2^2)$

Polyak Averaging

- ***Polyak Averaging*** (Polyak1992) consists of averaging several points in the trajectory through parameter space visited by an optimization algorithm:

$$\hat{\theta}^t = \frac{1}{\mathrm{t}} \sum_i \theta^i$$

θ^i are points where gradient descent visited

- The basic idea is that the optimization algorithm may leap back and forth across a valley several times without ever visiting a point near the bottom of the valley. The average of all the locations on either side should be close to the bottom of the valley though

- In nonconvex problems, it is typical to use an exponentially decaying running average:

$$\hat{\theta}^t = \alpha \hat{\theta}^{t-1} + (1 - \alpha)\theta^t$$

Continuation Methods

- ***Continuation Methods***
  - Starting from solving the easiest problem and then refine the solution to solve incrementally harder problems until we arrive at a solution to the true underlying problem
  - Traditional continuation method is based on smoothing (blurring) the object function
  - Intuitively, some nonconvex functions become approximately convex by being blurred to avoid the local minima

- ***Curriculum learning***
  - the idea of planning a learning process to begin by learning simple concepts and progress to learning more complex concepts (e.g., animal training, natural languages)