

L02: CNN Training

Bei Yu

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CNN Intialization

Gradient Descent Methods

Learning rate annealing

Normalization

Overview



CNN Intialization

Gradient Descent Methods

Learning rate annealing

Normalization

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CNN Initialization



- Constant initialization or Random initialization
- Orthogonal initialization
- Xaiver initialization
- Kaiming initialization

Initialization methods contain/adapt materials developed by

- Kaiming He et al. (Dec. 2015). "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification". In: Proceedings of the IEEE International Conference on Computer Vision (ICCV)
- Andrew M. Saxe, James L. McClelland, and Surya Ganguli (2013). Exact solutions to the nonlinear dynamics of learning in deep linear neural networks. eprint: arXiv:1312.6120
- Xavier Glorot and Yoshua Bengio (13–15 May 2010). "Understanding the difficulty of training deep feedforward neural networks". In: ed. by Yee Whye Teh and Mike Titterington. Vol. 9. Proceedings of Machine Learning Research. Chia Laguna Resort, Sardinia, Italy: JMLR Workshop and Conference Proceedings, pp. 249–256. URL: http://proceedings.mlr.press/v9/glorot10a.html

Constant initialization or Random initialization



Constant Initialization

Constant Initialization

All weights are initialized by a constant This will reduce the learning efficiency and generalization ability of a neural network

Random initialization

Uniform distribution intialization¹

 $W \sim U[a,b]$

Gaussian initialization

 $W \sim Normal(\mu, \sigma^2)$

¹https://www.ucd.ie/msc/t4media/Uniform%20Distribution.pdf

Xaiver Initialization



Definition

 z^i is the input vector of layer *i*, and s^i is the feature vector of the activation function at layer *i*, we have $s^i = z^i \cdot W^i + b^i$ and $z^{i+1} = f(s^i)$ where *f* is the symmetric activation function with unit derivative at 0 (i.e., f'(0) = 1)

Insight

For the stable mapping from the input domain to the target domain, we want to make the standard derivation of the input domain and the target domain are as equal as possible (i.e., keep the information flowing better in the neural networks)

Forward propagation

$$Var(z^{i}) = Var(x) \cdot \prod_{i'=0}^{i-1} n_{i'} Var(W^{i'})$$

Backward propagation

$$Var(\frac{\partial Cost}{\partial s^i}) = Var(\frac{\partial Cost}{\partial s^d}) \cdot \prod_{i'=i}^d n_{i'+1} Var(W^{i'})$$

Xaiver Initialization



Forward propagation

 $\forall (i), n_i Var(W^i) = 1$

Backward propagation

$$\forall (i), n_{i+1} Var(W^i) = 1$$

As a compromise between two constraints

$$\forall (i), Var(W^i) = \frac{2}{n_i + n_{i+1}}$$

Assume we use a Uniform distribution

$$W \sim U[-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}]$$

Xaiver inititialization

$$W \sim U[-rac{\sqrt{6}}{\sqrt{n_i+n_{i+1}}},rac{\sqrt{6}}{\sqrt{n_i+n_{i+1}}}]$$

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Kaiming Initialization



Insight

W has a symmetric distribution around zero and E[b] = 0

Follow the same rule with Xaiver initialization

We have

$$Var(z^i) = \frac{1}{2}Var(x^i)$$

Kaiming initialization

$$W \sim U[-\sqrt{rac{6}{n_i}},\sqrt{rac{6}{n_{i+1}}}]$$

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Insight

Solve the problem of gradient varnishing and exloding in Recurrent Neural Networks

Assume that we are taking a RNN as a form below

A form of a RNN

 $y_t = W^t \cdot y_0$

We apply orthogonal decomposition to W

We have

 $y_t = Q\Lambda^t Q \cdot y_0$

Since an orthogonal matrix has the eigenvalue of one, so the gradients would not varnish or explode during the training phase





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Basic gradient descent methods



Batch gradient descent

- Stochastic gradient descent
- Mini-batch gradient descent

Reference

Sebastian Ruder (2016). An overview of gradient descent optimization algorithms. eprint: arXiv:1609.04747

Batch gradient descent



The gradient of the cost function w.r.t. the parameters θ

$$\theta = \theta - \eta \cdot \bigtriangledown_{\theta} J(\theta)$$

Features

- The algorithm performs slowly
- The algorithm cannot update the model online (i.e., with new examples on-the-fly)
- The datasets cannot fit in memory possibly

Tips

Batch gradient descent is guaranteed to converge to the global minimum for convex error surfaces and to a local minimum for non-convex surfaces

Stochastic gradient descent



The gradient of the cost function w.r.t. the parameters θ

 $\theta = \theta - \eta \cdot \nabla_{\theta} J(\theta; x^i, y^i)$

Features

- The algorithm usually much faster
- The algorithm can be used to learn online
- SGD cause the objective function to fluctuate heavily since it performs frequent updates with a high variance

Tips

The fluctuation can help to jump to new and potentially better local minima

Stochastic graident descent²





²By Joe pharos at the English language Wikipedia, CC BY-SA 3.0

Mini-batch gradient descent



The gradient of the cost function w.r.t. the parameters θ

$$heta = heta - \eta \cdot \bigtriangledown_{ heta} J(heta; x^{(i:i+n)}, y^{(i:i+n)})$$

Features

- Reduce the variance of the parameter updates, which can lead to more stable convergence
- Make use of highly optmized matrix optmizations libraries to accelerate the gradient (i.e., very efficient)

Tips

Most of training methods utilize mini-batch gradient descent method

Challenges



Challenges

- It is difficult to decide a proper learning rate
- It is difficult to decide a proper learning rate schedule
- It is not reasonable to update all parameters using the same learning rate
- It is difficult to jump out of local minima and also saddle points

Gradient descent optimization methods



Gradient descent optmization methods contain/adapt materials developed by

- Ning Qian (1999). "On the momentum term in gradient descent learning algorithms". In: Neural networks 12.1, pp. 145–151
- Yurii E Nesterov (1983). "A method for solving the convex programming problem with convergence rate O (1/k²)". In: *Dokl. akad. nauk Sssr.* Vol. 269, pp. 543–547
- Matthew D Zeiler (2012). "Adadelta: an adaptive learning rate method". In: arXiv preprint arXiv:1212.5701
- John Duchi, Elad Hazan, and Yoram Singer (2011). "Adaptive subgradient methods for online learning and stochastic optimization.". In: *Journal of machine learning research* 12.7
- Diederik P Kingma and Jimmy Ba (2014). "Adam: A method for stochastic optimization". In: arXiv preprint arXiv:1412.6980

Momentum



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$$v_t = \gamma v_{t-1} + \eta \bigtriangledown_{\theta} J(\theta)$$
$$\theta = \theta - v_t$$

Features

The momentum increases for dimensions whose gradients point in the same directions

The momentum reduces updates for dimensions whose gradients change directions

Tips

The momentum term γ is usually set to 0.9 or a similar value

³Genevieve B. Orr, Willamette University cs449.

Nesterov



$$v_t = \gamma v_{t-1} + \eta \bigtriangledown_{\theta} J(\theta - \gamma v_{t-1})$$

$$\theta = \theta - v_t$$

Features

- NAG uses predicted update to prevent us from going too fast compared with Momentum
- It increases the performance of RNNs on a number of tasks

Adagrad



$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,ii} + \epsilon}} \cdot g_{t,i}$$
$$g_{t,i} = \bigtriangledown_{\theta_t} J(\theta_{t,i})$$

where $G_t \in \mathbb{R}^{d \times d}$ is a diagonal matrix where each diagonal elment $G_{t,ii}$ is the sum of squares of the gradients w.r.t. θ_i up to time step t, ϵ is a smoothing term which avoids division by zero (e.g., 1e - 8)

Features

- The learning rate η for different parameters can be varied based on the past gradients
- The accumulated sum of the denominator keeps growing during training, which may cause gradient varnishing

Tips

The initial learing rate η of most applications uses 0.01 as a default value

Adadelta



$$\theta_{t+1,i} = \theta_{t,i} + \Delta \theta_{t,i}$$
$$\Delta \theta_{t,i} = -\frac{RMS[\Delta \theta]_{t-1,i}}{RMS[g]_{t,i}}g_{t,i}$$

where

$$RMS[\Delta\theta]_{t,i} = \sqrt{E[\Delta\theta^2]_{t,i} + \epsilon}$$
$$E[\Delta\theta^2]_{t,i} = \gamma E[\Delta\theta^2]_{t-1,i} + (1-\gamma)\Delta\theta_{t,i}^2$$

Tips

With Adadelta, we do not need to set a default learning rate, since it has benn eliminated from the update rule

RMSprop



$$E[g^2]_t = \gamma E[g^2]_{t-1} + (1-\gamma)g_t^2$$
$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}}g_t$$

Tips

Hinton suggests γ to be set to 0.9 and a good default value for the learning rate η is 0.001 4

Adam



where

$$\begin{aligned}
\hat{\theta}_{t+1} &= \theta_t - \frac{\eta}{\sqrt{\hat{v} + \epsilon}} \hat{m}_t \\
\hat{m}_t &= \frac{m_t}{1 - \beta_1^t} \\
\hat{v}_t &= \frac{v_t}{1 - \beta_2^t} \\
m_t &= \beta_1 m_{t-1} + (1 - \beta_1) g_t \\
v_t &= \beta_2 v_{t-1} + (1 - \beta_2) g_t^2
\end{aligned}$$

Tips

The authors propse the default value of eta_1 to be 0.9, 0.999 for eta_2 and 10^{-8} for ϵ



- Choose one of the adaptive learning-rate optimization methods usually obtain better performance and you will not need to tune the learning rate with the default value
- Adam might be the best overall choice
- Vanilla SGD is robust to different initialization methods and learning rate annealing schedulers

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Different annealing methods





Cosine

Cyclical

Learning rate annealing methods contain/adapt materials developed by

- Leslie N Smith (2017). "Cyclical learning rates for training neural networks". In: 2017 IEEE Winter Conference on Applications of Computer Vision (WACV). IEEE, pp. 464–472
- Ilya Loshchilov and Frank Hutter (2016). "Sgdr: Stochastic gradient descent with warm restarts". In: arXiv preprint arXiv:1608.03983





Step learning rate scheduler

Decay the learning rate by a pre-defined step size exponentially characterized by γ

Cosine learning rate scheduler



Cosine annealing method / SGDR (i.e., Stochastic Gradient Descent with warm Restarts)

$$\eta_t = \eta_{min}^t + \frac{1}{2}(\eta_{max}^i - \eta_{min}^i)(1 + \cos(\frac{T_{cur}}{T_i}\pi))$$

Where T_i represents the total epoch numbers



Top-1 and Top-5 test errors obtained by SGD with momentum (i.e., Default) and SGDR on WRN-28-10 trained on a version of ImageNet

Cyclical learning rate scheduler



Insight

The essence of this learning rate policy comes from the observation that increasing the learning rate might have a short term negtive effect and yet achieve a longer term beneficial effect



Triangular learning rate policy

Cyclical learning rate scheduler





Classification accuracy while training CIFAR-10

Tips

- Experiments show that it often is good to set stepsize equal to 2-10 times the number of iterations in an epoch (e.g., stepsize = 8 · epoch)
- Use LR range test to estimate reasonable minimum and maximum boundary values

Cyclical learning rate scheduler





Classification accuracy as a function of increasing learning rate for 8 epochs

The figure shows that the model starts to converge from the beginning, so it is reasonable to set the baseline learning rate to 0.001. Furthermore, when the learning rate is above 0.006, the accuracy rise gets rough and eventually begins to drop so it is reasonable to set the maximum learning rate to 0.006

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Normalization



Reduce Internal Covariate Shift, accelerate the training and improve the performance of a neural network

- Batch normalization
- Layer normalization
- Instance normalization
- Weight normalization

Normalization methods contain/adapt materials developed by

- Sergey loffe and Christian Szegedy (2015). "Batch normalization: Accelerating deep network training by reducing internal covariate shift". In: arXiv preprint arXiv:1502.03167
- Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton (2016). "Layer normalization". In: arXiv preprint arXiv:1607.06450
- Dmitry Ulyanov, Andrea Vedaldi, and Victor Lempitsky (2016). "Instance normalization: The missing ingredient for fast stylization". In: arXiv preprint arXiv:1607.08022
- Tim Salimans and Durk P Kingma (2016). "Weight normalization: A simple reparameterization to accelerate training of deep neural networks". In: Advances in neural information processing systems, pp. 901–909

Batch normalization



Internal Covariate Shift

Internal Covariate Shift is as the change in the distribution of network activations due to the change in network parameters during training

Algorithm 1 Batch Normalization Transform

Input: Values of *x* over a mini-batch: $\mathcal{B} = x_{1,2,...,m}$;

- 1: Parameters to be learned: γ,β
- **Output:** $y_i = BN_{\gamma,\beta}(x_i)$
- 2: // mini-batch mean
- 3: $\mu_{\mathcal{B}} = \frac{1}{m} \sum_{i=1}^{m} x_i$ 4: // mini-batch variance
- 5: $\sigma_{\mathcal{B}}^2 = \frac{1}{m} \sum_{i=1}^{m} (x_i \mu_{\mathcal{B}})^2$
- 6: // normalize

7:
$$\hat{x}_i = \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

8: // scale and shift

9:
$$y_i = \gamma \hat{x_i} + \beta \equiv BN_{\gamma,\beta}(x_i)$$

Batch normalization

Back propagation with Batch Normalization

• Use chain rules to optmize γ and β :

$$\begin{split} \frac{\partial \ell}{\partial \hat{x}_{i}} &= \frac{\partial \ell}{\partial y_{i}} \cdot \gamma \\ \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^{2}} &= \sum_{i=1}^{m} \frac{\partial \ell}{\partial \hat{x}_{i}} \cdot (x_{i} - \mu_{\mathcal{B}}) \cdot \frac{-1}{2} (\sigma_{\mathcal{B}}^{2} + \epsilon)^{\frac{-3}{2}} \\ \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} &= \sum_{i=1}^{m} \frac{\partial \ell}{\partial \hat{x}_{i}} \cdot \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^{2} + \epsilon}} \\ &= \frac{\partial \ell}{\partial \hat{x}_{i}} \cdot \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^{2} + \epsilon}} + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^{2}} \cdot \frac{2(x_{i} - \mu_{\mathcal{B}})}{m} + \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} \cdot \frac{1}{m} \\ \frac{\partial \ell}{\partial \gamma} &= \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_{i}} \cdot \hat{x}_{i} \\ \frac{\partial \ell}{\partial \beta} &= \sum_{i=1}^{m} \frac{\partial \ell}{\partial i} \end{split}$$



Batch normalization



Algorithm 2 Training a Batch Normalization Network

Input: Network N with trainable parameters Θ ;

1: subset of activations $x_{k=1}^{kK}$

Output: Batch-normalized network for inference, N_{BN}^{inf}

- 2: $N_{BN}^{tr} \leftarrow N \; / /$ Training BN network
- 3: for k = 1 to K do
- 4: Add transformation $y^{(k)} = BN_{\gamma^k,\beta^{(k)}}(x^{(k)})$ to N_{BN}^{tr} (i.e., Algorithm of Batch Normalization Transform)
- 5: Modify each layer in N_{BN}^{tr} with input $x^{(k)}$ to take $y^{(k)}$ instead

6: end for

- 7: Train N_{BN}^{tr} to optimize the parameters $\Theta \bigcup \gamma^k, \beta_{k=1}^{kK}$
- 8: $N_{BN}^{inf} \leftarrow N_{BN}^{tr}$ // Inference BN network with frozen parameters
- 9: for k = 1 to *K* do

10: // For clarity,
$$x\equiv x^{(k)}, \gamma\equiv\gamma^{(k)}, \mu_{\mathcal{B}}\equiv\mu_{\mathcal{B}}^{(k)}$$

- 11: Process multiple training mini-batches \mathcal{B} , each of size *m*, and average over them: 12: $E[x] \leftarrow E_{\mathcal{B}}[\mu_{\mathcal{B}}]$ 13: $VAR[x] \leftarrow \frac{m}{m-1}E_{\mathcal{B}}[\sigma_{\mathcal{B}}^2]$
- 14: In N_{BN}^{inf} , replace the transform $y = BN_{\gamma,\beta}(x)$ with $y = \frac{\gamma}{\sqrt{VAR[x] + \epsilon}} \cdot x + (\beta \frac{\gamma E[x]}{\sqrt{VAR[x] + \epsilon}})$ 15: end for

Weight normalization



$$w = \frac{g}{\|v\|}v$$

where the gradients of g and v:

$$\nabla_{g}L = \frac{\nabla_{w}L \cdot v}{\|v\|}$$
$$\nabla_{v}L = \frac{g}{\|v\|} \nabla_{w}L - \frac{g \nabla_{w}L}{\|v\|^{2}}v$$

The relationship between Batch normalization

The pre-activation t for each mini-batch in the Batch normalization

$$t' = \frac{t - \mu[t]}{\sigma[t]}$$

 $t = v \cdot x$

and

For the special case of a single layer with the input features x that has been whitened (i.e., $\mu[x] = 0$ and $\sigma[x] = 1$) Weight normalization is given by $\mu[t] = 0$ and $\sigma[t] = ||v||$

Weight normalization





Training error for CIFAR-10 using different network parameterizations

Layer normalization



$$a^{t} = W_{hhh}h^{t-1} + W_{xh}x^{t}$$

$$h^{t} = f[\frac{g}{\sigma^{t}} \bigodot (a^{t} - \mu^{t}) + b]$$

$$\mu^{t} = \frac{1}{H} \sum_{i=1}^{H} a^{t}_{i}$$

$$\sigma^{t} = \sqrt{\frac{1}{H} \sum_{i=1}^{H} (a^{t}_{i} - \mu^{t})^{2}}$$

where x^t is the current input, h^{t-1} is the previous vector of hidden states. W_{hh} is the recurrent hidden to hidden weights, W_{xh} is the bottom up input to hidden weights, \bigcirc is the element-wise multiplication between two vectors, b and g are defined as the bias and gain parameters of the same dimension as h^t

Features

- Layer normalization does not calculate the mean and standard derivation based on the mini-batch, which can be utilized in RNN rather than Batch normalization
- All the hidden units share the same normalization terms μ and σ
- Layer normalization does not impose any constraint on the size of a mini-batch and it can be used in the pure online regime with batch size 1

Instance normalization



Let $x \in \mathbb{R}^{T \times C \times W \times H}$ and x_{tijk} denote its *tijk*-th element where *j* and *k* span spatial dimensions, *i* is the feature channel (color channel if the input is an RGB image), and *t* is the index of the image in the batch. The instance normalization is formulated as:

$$y_{tijk} = \frac{x_{tijk} - \mu_{ti}}{\sqrt{\sigma_{ti}^2 + \epsilon}}$$
$$\mu_{ti} = \frac{1}{HW} \sum_{l=1}^{W} \sum_{m=1}^{W} m = 1^H x_{tilm}$$
$$\sigma_{ti}^2 = \frac{1}{HW} \sum_{l=1}^{W} \sum_{m=1}^{H} (x_{tilm} - \mu_{ti})^2$$

Features

Instance normalization is used in the style transfer task (i.e., task-specific technique)

It is based on Batch normalization

Instance normalization





Stylization examples using instance normalization. First row: style images, second row: original images and its stylized versions