On the Training of Neural Networks

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Mathematical Introduction to Machine Learning

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The problem for computing gradients

- Consider a general network defined by the **forward propagation**:

$$\begin{aligned} x^0 &= x \\ x^\ell &= h(x^{\ell-1}; \theta^\ell) \text{ for } \ell = 1, 2, \ldots, L, \\ f(x; \Theta) &= x^L. \end{aligned}$$

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- **Why is this problem not trivial?**

The back-propagation algorithm

- By the chain rule,

$$\frac{\partial E}{\partial \theta^\ell} = \frac{\partial x^\ell}{\partial \theta^\ell}\frac{\partial E}{\partial x^\ell} = \frac{\partial h(x^{\ell-1};\theta^\ell)}{\partial \theta^\ell}\frac{\partial E}{\partial x^\ell}.$$

Let gradient signal $\delta^\ell := \frac{\partial E}{\partial x^\ell}$. Then, it can be recursively computed via the chain rule:

$$\delta_{\ell-1} = \frac{\partial x^\ell}{\partial x^{\ell-1}}\frac{\partial E}{\partial x^\ell} = \frac{\partial h(x^{\ell-1};\theta^l)}{\partial x^{\ell-1}}\delta_\ell$$
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- **Note:** Compute the red parts need to access the hidden states $\{x^\ell\}_{\ell=0}^L$, which are computed **during the forward propagation**.

A visualization of back-prop algorithm

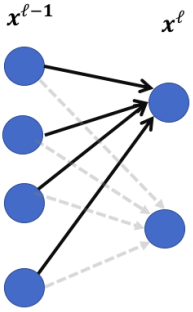
When $h(z;\theta^\ell) = A^\ell \sigma_\ell(z) + b^\ell$, we have $\frac{\partial E}{\partial b^\ell} = \frac{\partial E}{\partial x^\ell}$ and $\delta^\ell = \frac{\partial E}{\partial A^\ell}$ satisfies

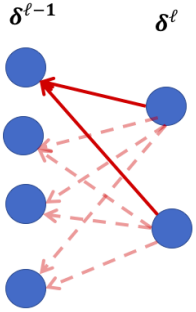
Forward Propagation

$$x^0 = x$$
$$x^\ell = A^\ell \sigma(x^{\ell-1}) + b^\ell$$

Back Propagation

$$\delta^L = l'(f, y)$$
$$\delta^{\ell-1} = \sigma'(x^{\ell-1}) \odot (A^\ell)^T \delta^\ell$$





Computational and memory cost analysis

Backprop algorithm is a **smart** way to implement the chain rule.

Consider a network of depth L, width m, and the batch size B.

- The **computational cost** is $O(Bm^2L)$.
  - Reducing the dependence on B and m is not difficult via parallelization. **GPUs are great!! Nvidia Tesla A100 has 6912 cores! RTX 4090 has 16384 cores!**
  - Reducing the dependence on L is challenging as the computation is essentially serial when do forward and backward propagations.

Computational and memory cost analysis

Backprop algorithm is a **smart** way to implement the chain rule.

Consider a network of depth L, width m, and the batch size B.

- The **memory cost** is $O(BmL + m^2L)$. The blue part is due to we need to store the hidden state for computing gradient.
  - Big memory is necessary for training large models. **A100 has 80G memory while RTX 4090 has only 24G.**

  For training large models, we can
  - Buy A100 and H100 if you are rich.
  - Reduce the batch size.
  - Try zero-order algorithms?

Gradient Vanishing and Exploding

- **Gradient Vanishing:**

$$\delta^{\ell} = [\sigma'(x^{\ell}) \odot (A^{\ell+1})^T][\sigma'(x^{\ell+1}) \odot (A^{\ell+2})^T] \cdots [\sigma'(x^{L-1}) \odot (A^{L})^T \delta^{L}]$$

The value is approximately the multiplication of $L - l$ term. If $\sigma'(z^{\ell}) < 1$ or $\|A^{\ell}\|_2 < 1$, then δ^{ℓ} will be exponentially small.

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- Roughly, $\delta^\ell \approx (\sigma'(x)\|A\|_2)^{L-\ell}$. This implies that **deep networks are harder to train than shallow networks**.
- More precisely, it is the not the small/large gradient causes the difficulty of training. It is due to the disparity of gradient scales among different layers. Hence, it is impossible to choose an appropriate learning rate for all the layers.

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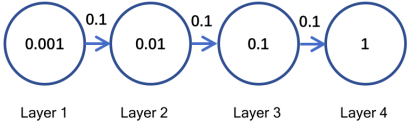

Observation

The **vanishing/exploding gradient** is the major obstacle in training deep nets.

Alleviate gradient vanishing: activation function

- **Saturating activation:** For saturating activation function, when $|z| > O(1)$, we have $\sigma'(z) \approx 0$. This is extremely bad for deep networks.
- **Non-saturating activation:** Use ReLU and its variants as the nonlinear activation function.

Alleviate gradient vanishing: Initialization

Avoid the gradient vanishing at the initialization.

- Consider the commonly random initialization $W_{i,j}^{\ell} \in \mathcal{N}(0, t_w^2), b_j^{\ell} = 0$ (we will discuss why Gaussian is preferred later) and the standard Gaussian input: $\boldsymbol{x} \sim \mathcal{N}(0, I_d)$.

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- Denote by $\boldsymbol{x}^{\ell}$ the output of ℓ-th layer: $\boldsymbol{x}^{\ell+1} = \sigma(W^{\ell}\boldsymbol{x}^{l} + b^{l})$. We would like to find initializations such that

$$\mathbb{E}[|x_i^{\ell}|^2] = 1, \quad \ell \in [L], i \in [m^{\ell}]$$

where x_i^{ℓ} is the output of the i-th neuron of ℓ-th layer.

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- Consider ReLU activation and at initialization, we have

$$\begin{aligned}
\mathbb{E}[|x_i^{\ell+1}|^2] &= \mathbb{E}[\sigma^2(\sum_{j=1}^{m_\ell} W_{i,j}^{\ell} x_j^{\ell})] \\
&= \mathbb{E}_{\boldsymbol{x}^{\ell}} \mathbb{E}_{\xi_{i,j}\sim\mathcal{N}(0,1)}[\|\boldsymbol{x}^{\ell}\|^2 t_w^2 \sigma^2(\sum_{j=1}^{m_\ell} \xi_{i,j}^{\ell} \hat{x}_j^{\ell})|\boldsymbol{x}^{\ell}] \\
&= \mathbb{E}_{\boldsymbol{x}^{\ell}} \mathbb{E}_{\xi\sim\mathcal{N}(0,1)}[\|\boldsymbol{x}^{\ell}\|^2 t_w^2 \sigma^2(\xi)|\boldsymbol{x}^{\ell}] \\
&= t_w^2 \mathbb{E}_{\xi\sim\mathcal{N}(0,1)}[\sigma^2(\xi)] m^{\ell}. \qquad \text{Assume } \mathbb{E}[|x_i^{\ell}|^2] = 1. \qquad (1)
\end{aligned}$$

Initialization

Note that $\mathbb{E}_{\xi\sim\mathcal{N}(0,1)}[\sigma^2(\xi)] = \frac{1}{\sqrt{2\pi}}\int_0^\infty z^2 e^{-z^2/2} = 1/2$. Hence, $\mathbb{E}[|x_i^{\ell+1}|^2] = 1$ leads to

$$t_w^2 = \frac{2}{m_\ell}.$$

- The initialization $W_{i,j}^\ell \sim \mathcal{N}(0, \frac{2}{m_\ell}), b_j = 0$ is called **Kaiming-He initialization**, which has become the default initialization for all the ReLU-like activation functions.

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- Similarly, we can get $t_w^2 = \frac{1}{m^\ell}$ if $\sigma(z) = z$. This corresponds to the LeCun initialization. LeCun initialization works pretty well for the $\tanh$ activation function, since $\tanh \approx x$ when x is close to the origin.

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- Similar argument can be used to derive the initialization for other activation functions.
- It is also common to use the uniform initialization: $W_{i,j}^\ell \sim \text{Unif}[-t, t]$, where the specific value of t can be derived similarly.

Numerical illustration

In the following figure, we see that with the right initialization, we can avoid the vanishing/exploding for both the forward and backward propogation **at the initialization**.

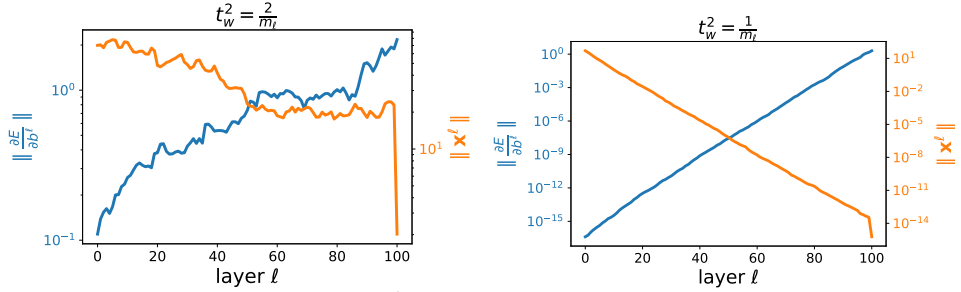

Figure 1: ReLU networks with $L = 100, m^\ell = 200, l = 1, \ldots, L-1$. **Left:** The case of $t_w^2 = 2/m_l$ (Kaiming-He initialization); **Right:** The case of $t_w^2 = 1/m_l$ (LeCun initialization).

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    1. Consider a two-layer neural network

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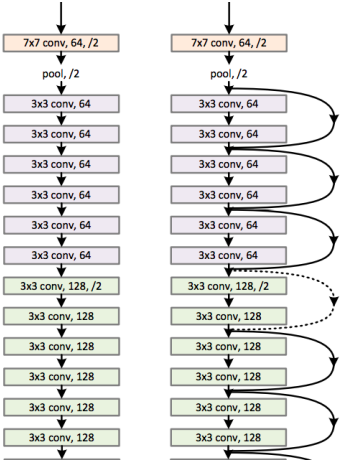
3. We can explore other forms of initialization, e.g., **the orthogonal initialization**: choosing W^ℓ to be the multiple of an orthogonal matrix (if $m_{\ell+1} = m_\ell$). Whether these initializations overperform or underperform random Gaussians seems to be problem dependent and is not fully understood.

Alleviate the gradient vanishing: Skip connections



- Intuitively speaking, **skip connections** build highways for the information propagation, such that information does not need to go through the convolutional, fully-connected, and activation layers.

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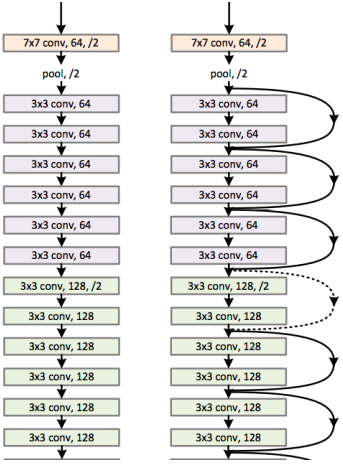

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- Mathematically,
  - $x^{\ell+1} = x^{\ell} + h_{\ell}(x^{\ell})$
  - $x^{L} = x^{\ell} + \sum_{i=\ell}^{L-1} h_i(x^i)$
  - $\frac{\partial E}{\partial x^{\ell}} = \frac{\partial E}{\partial x^{L}} \left(1 + \sum_{i=\ell}^{L-1} \frac{\partial h_i(x^i)}{\partial x^{\ell}}\right)$.

  If the residual blocks $\{h_i\}$ are small, one can see that the gradients are almost independent of the depth. So the gradient is well-controlled.
- History: **LSTM** $\rightarrow$ **Highway network** $\rightarrow$ **ResNet**.

Numerical evidence

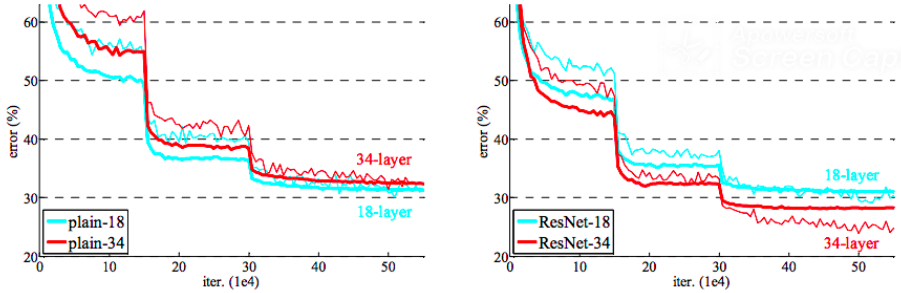

Figure 4. Training on **ImageNet**. Thin curves denote training error, and bold curves denote validation error of the center crops. Left: plain networks of 18 and 34 layers. Right: ResNets of 18 and 34 layers. In this plot, the residual networks have no extra parameter compared to their plain counterparts.

The above figure is taken from the original paper by Kaiming He et al.
https://arxiv.org/abs/1512.03385.

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- A batch normalization layer define a map: $\mathrm{BN}_{\gamma,\beta} : \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\} \to \{\tilde{\boldsymbol{x}}_1, \ldots \tilde{\boldsymbol{x}}_m\}$ through

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} \boldsymbol{x}_i$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (\boldsymbol{x}_i - \mu_{\mathcal{B}})^2$$

$$\widehat{\boldsymbol{x}}_i \leftarrow \frac{\boldsymbol{x}_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$$

$$\tilde{\boldsymbol{x}}_i \leftarrow \gamma \widehat{\boldsymbol{x}}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(\boldsymbol{x}_i)$$

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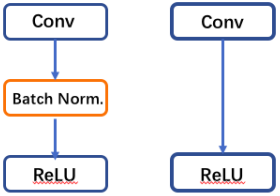

Figure 2: **Left:** Convolutional nets with BN; **Right:** Convolutional without BN.

Performance of BN

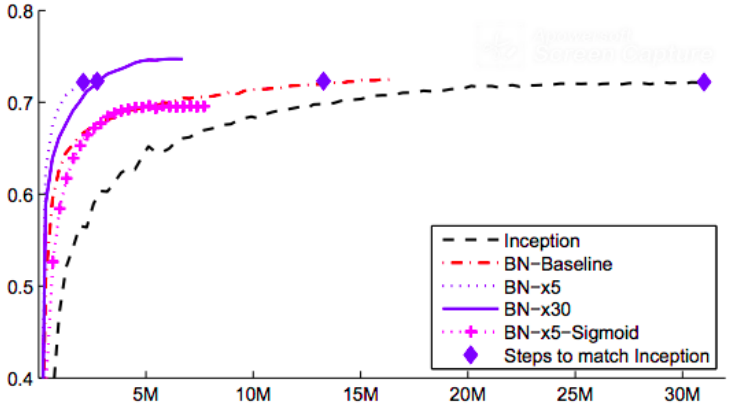

Figure 3: Validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps. BN-baseline: same as inception with BN layers added before each nonlinearity. BN-x5: inception with batch normalization and the learning rate is increased by a factor 5, compared to the baseline. BN-x30 is similar. This figure is taken from https://arxiv.org/pdf/1502.03167.pdf.

Black magics: Batch normalization

BN is VERY useful for training very deep nets. But it also causes several strange issues.

- For networks with BN layers, **we cannot use too small batch size**, e.g. $B = 1$, where the σ_B and μ_B are far away from the σ and μ, the ones over the whole dataset.)

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- For networks with BN layers, **we cannot use too small batch size**, e.g. $B = 1$, where the σ_B and μ_B are far away from the σ and μ, the ones over the whole dataset.)
- How do we compute σ_B and μ_B during the inference, where we may only have one sample?
  Use the following ones obtained from the moving average during the training:

$$\sigma^{\text{inf}} \leftarrow (1-\alpha)\sigma^{\text{inf}} + \alpha\sigma_B^t \tag{2}$$

$$\mu^{\text{inf}} \leftarrow (1-\alpha)\mu^{\text{inf}} + \alpha\mu_B^t, \tag{3}$$

  where σ_B^t, μ_B^t are the statistics calculated at the t-th step of training.

Black magics: Batch normalization

- **Training and test disparity:**
  - At the training time, $\{\sigma_B, \mu_B\}$ are computed over the samples at the current batch.
  - At the inference/testing time, $\{\sigma^{\text{inf}}, \mu^{\text{inf}}\}$ are fixed, which are approximations of the statistics of whole dataset obtained by the moving average during the training.

Layer normalization

- Let $Z = (\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N)^T \in \mathbb{R}^{N \times H}$ be our feature map. The first and second dimension are the bach and feature dimension, respectively.
- A layer normalization (LN) layer define a map $\mathrm{LN}_{\boldsymbol{\gamma},\boldsymbol{\beta}} : \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N\} \to \{\tilde{\boldsymbol{z}}_1, \ldots \tilde{\boldsymbol{z}}_N\}$ through

$$\mu_i = \frac{1}{H}\sum_{j=1}^{H} z_{i,j}, \quad \sigma_i = \sqrt{\frac{1}{H}\sum_{j=1}^{H}(z_{i,j} - \mu_i)^2} \quad \text{for } i = 1, \ldots, N, \tag{4}$$

$$\hat{\boldsymbol{z}}_i \leftarrow \boldsymbol{\gamma} \odot \frac{\boldsymbol{z}_i - \mu_i}{\sigma_i} + \boldsymbol{\beta}, \tag{5}$$

  where the learnable rescaling factors $\boldsymbol{\gamma}, \boldsymbol{\beta} \in \mathbb{R}^H$.
- Different from BN, 1) LN normalizes data along the feature dimension; 2) LN does rescaling in an element-wise manner.
- **Question: Is element-wise rescaling necessary?**

A visual comparison between BN and LN

- BN are often used in MLP and CNN. LN are more popular in training RNN and Transformer.
- LN can be applied even the batch size is 1.

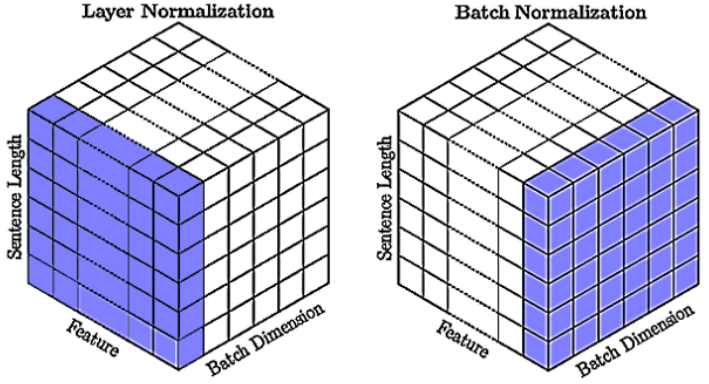

Figure 4: Taken from https://www.kaggle.com/code/halflingwizard/how-does-layer-normalization-work.

Gradient clipping

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- Gradient clipping is widely used in training recurrent neural networks (RNNs) and Transformer models. One potential mechanism behind clipping is to mitigate the impact of heavy-tailed noise. Recall that in the convergence analysis of SGD, convergence requires

$$\mathbb{E}[|\xi_t|^2] < \infty.$$

What happens if the above condition is not met? Read: Why are adaptive methods good for attention models?

Adaptive learning rate optimizers

Motivation

- Gradients of different layers are at different scales. Recall that the convergence depends on the condition number.
- Layer-wise learning rates! A great idea but hard to implement.
- Adaptive learning rates:

  Automatically tune learning rates according to the size of each coordinate.

Adagrad

- Consider to minimize $\min_{x \in \mathbb{R}^p} f(x)$. Let g_t be the t-th step (stochastic) gradient.
- SGD updates as follows

$$x_{t+1} = x_t - \eta g_t.$$

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- The adaptive gradient (Adagrad) method updates as follows

$$\begin{aligned} G_{t+1} &= G_t + g_t^2 \\ x_{t+1} &= x_t - \eta \frac{g_t}{\sqrt{G_{t+1} + \varepsilon}}, \end{aligned}$$

where $\varepsilon \sim 10^{-7}$ prevents the division by zero. All multiplication and division should be understood in an elemenwise way.

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- Note that where $G_t = \sum_{s=0}^{t} g_t^2$ stores the maginitude of each coordinate.
- **Issue:** G_t is increasing monotonically. Thus, the effective learning rate is decreasing in time.

RMSProp

- RMSProp (Tieleman & Hinton, 2012) iterates as follows

$$v_{t+1} = \beta v_t + (1-\beta) g_t^2$$
$$x_{t+1} = x_t - \eta \frac{g_t}{\sqrt{v_{t+1} + \varepsilon}}.$$

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- If $\beta = 0, g_t = \nabla f(x_t)$ (i.e., the full-batch case), it becomes

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- RMSProp is originally proposed as a stochastic version of rProp. [**Q: Why is it non-trivial?**]

ADAM [2] Optimizer

1. Compute the (stochastic) gradient g_t.
2. Estimate the first-order and second-order moment:

$$m_{t+1} = \beta_1 m_t + (1 - \beta_1) g_t$$
$$v_{t+1} = \beta_2 v_t + (1 - \beta_2) g_t^2.$$

[2] Adaptive momentum: https://arxiv.org/pdf/1412.6980.pdf

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4. Update parameters:

$$x_{t+1} = x_t - \eta \frac{m_{t+1}}{\sqrt{v_{t+1}+\varepsilon}}.$$

   Again, the square root and division are computed in coordinate-wise manner.

In a summary,

ADAM=RMSProp + momentum

[2] Adaptive momentum: https://arxiv.org/pdf/1412.6980.pdf

ADAM: Explanation

1. Common initialization: $m_0 = 0, v_0 = 0$. This causes m_t and g_t to be small for small t. Let $\mathbb{E}[g_t^2] = g^2$

$$\mathbb{E}[v_t] = (1 - \beta_2) \sum_{s=0}^{t} \beta_2^s \mathbb{E}[g_{t-s}^2] \approx g^2 (1 - \beta_2^t).$$

   The bias-correction step is used to correct this initialization bias.

2. We can also initialize $m_0 = g_0, v_0 = g_0^2$, for which the bias-correction step is not necessary.

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2. We can also initialize $m_0 = g_0, v_0 = g_0^2$, for which the bias-correction step is not necessary.
3. Default parameters are $\beta_1 = 0.9, \beta_2 = 0.999, \varepsilon = 10^{-8}$. The learning rate should be tunned experimentally in each problem.
4. There are (very recent) convergence results for ADAM both in the convex and non-convex case. However, all these theoretical results are not interesting since they cannot explain why ADAM converges faster than SGD.

Continuous-time limits of ADAM

Let $\beta_1 = 1 - \eta\gamma_1, \beta_2 = 1 - \eta\gamma_2$. Then, taking $\eta \to 0$, the limit becomes

$$\begin{aligned} \dot{m}_t &= \gamma_1(\nabla f(x_t) - m_t) \\ \dot{v}_t &= \gamma_2(|\nabla f(x_t)|^2 - v_t) \\ \dot{x}_t &= -\frac{m_t}{\sqrt{v_t + \varepsilon}} \end{aligned}$$

Taking $\gamma_1, \gamma_2 \to \infty$, we obtain the signGD flow:

$$\dot{x}_t = -\frac{\nabla f(x_t)}{\sqrt{|\nabla f(x_t)|^2 + \varepsilon}}.$$

Caution: Different scalings may lead to different continous-time limits.

A comparison of different optimizers

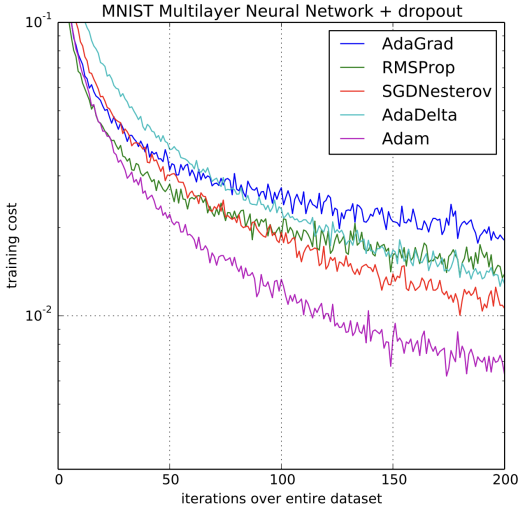


Figure 5: Taken from the original Adam paper https://arxiv.org/pdf/1412.6980.pdf.

A short summary

- All first order optimizers are based on gradient descent.
- Both stochastic and non-stochastic gradient descent can be augmented by momentum (Nesterov or heavy-ball) to more easily escape flat regions.
- Coordinate-wise adaptive learning rates can be used to improve GD/SGD (with or without momentum) if the energy landscape is flat in some directions and steep in others.
- Continuous time limits can give insight into the behavior of different optimizers for small learning rates.
- The most popular optimizers in practice are SGD and (stochastic) ADAM.
- There are many similar algorithms (Adadelta, AMSgrad, Adamax, Nadam, ...) and tricks for specific cases (e.g. deep learning)

Regularization

Over-parameterization in deep learning

- Neural networks often work in the over-parameterized regime, i.e., the number of samples are much larger than data size.

CIFAR-10	# train: 50,000
Inception	1,649,402
Alexnet	1,387,786
MLP 1x512	1,209,866
ImageNet	**# train: ~1,200,000**
Inception V4	42,681,353
Alexnet	61,100,840
Resnet-{18;152}	11,689,512; 60,192,808
VGG-{11;19}	132,863,336; 143,667,240

Weight decay and squared ℓ_2 regularization

- Let $\theta_{t+1} = \theta_t - \eta h_t$ be the update of our algorithm. The +weight decay is given by

$$\theta_{t+1} = \theta_t - \eta(h_t + \lambda\theta_t) = (1 - \lambda\eta)\theta_t - \eta h_t.$$

- When optimizer is SGD, it is equivalent to the squared ℓ^2 regularization as

$$\nabla\left(\hat{\mathcal{R}}(\theta) + \frac{\lambda}{2}\|\theta\|^2\right) = \nabla\hat{\mathcal{R}}(\theta) + \lambda\theta.$$

- **For other optimizers like ADAM, they are not equivalent**. This issue was first pointed out in https://openreview.net/pdf?id=rk6qdGgCZ and currently, Adam + weight decay (AdamW) has become the default optimizers in training large language models (LLMs), e.g., ChatGPT.
- **Why weight decay is so useful in training LLMs is still unclear !!! [A research topic!!]**

You should always try it due to the simplicity.

Batch normalization

- BN is originally proposed to improve the training.
- In practice, it is found that BN can also improve the generalization significantly.
- Always try it, since it improves both convergence and generalization.
- Why BN has regularization effect is still unclear now.
- **Unfortunately,** BN is never used in RNNs/LSTMs and Transformers. In these architectures, instead **layer normalization** is used.

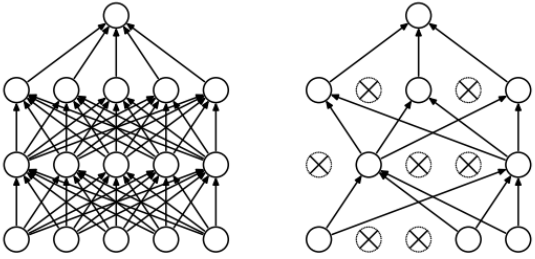
Dropout: Basic Definition

Normal Forward-prop

$$z_i^\ell = \boldsymbol{w}_i^\ell x^{\ell-1} + b_i^\ell$$
$$x_i^\ell = \sigma(z_i^\ell)$$

Dropout Forward-prop

$$r_i^{\ell-1} \sim \text{Bernoulli}(p)$$
$$\tilde{\boldsymbol{x}}^{\ell-1} = \boldsymbol{r}^{\ell-1} \odot \boldsymbol{x}^{\ell-1} \quad \text{(masked)}$$
$$z_i^\ell = \boldsymbol{w}_i^\ell x^{\ell-1} + b_i^\ell$$
$$x_i^\ell = \sigma(z_i^\ell)$$



(a) Standard Neural Net

(b) After applying dropout.

- In each step, the dropping mask is randomly sampled. Hence, the masks are different in different steps.
- The drop ratio is given by $1 - p$.

Dropout: A stochastic approximation explanation

- Dropout defines a stochastic network $f(x;\xi,\theta)$, where ξ denotes the dropping mask. Note that in fact $f(x;\xi,\theta) = f(x;\xi \odot \theta)$.
- Denote by π the distribution of the mask ξ. Then the training of Dropout goes as follows,

$$\begin{aligned} \xi_t &\sim \pi \\ \theta_{t+1} &= \theta_t - \eta \nabla_\theta \hat{\mathcal{R}}(f(\cdot;\xi_t,\theta_t)), \end{aligned} \tag{6}$$

  which is exactly SGD of batch size 1 for minimizing

$$\hat{\mathcal{R}}_{\text{drop}}(\theta) = \mathbb{E}_{\xi\sim\pi}[\hat{\mathcal{R}}(f(\cdot;\xi,\theta))]. \tag{7}$$

The regularization effect of dropout

- Let $\hat{\mathcal{R}}(f) = \frac{1}{n}\sum_{i=1}^{n}(f(x_i) - y_i)^2$. Let $F_\theta(x) = \mathbb{E}_\xi[f(x;\xi,\theta)]$ be the effective model.
- Then,

$$\begin{aligned}\hat{\mathcal{R}}_{\text{drop}}(\theta) &= \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_\xi(f(x_i;\xi,\theta) - y_i)^2 \\ &= \frac{1}{n}\sum_{i=1}^{n}(F_\theta(x_i) - y_i)^2 + \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_\xi(f(x_i;\xi,\theta) - F(x_i;\theta))^2 \\ &= \hat{\mathcal{R}}(F_\theta) + Q_p(\theta),\end{aligned}$$

where the $Q_p(\cdot)$ term plays the role of regularization. Moreover,

$$Q_p(\theta) \to 0 \text{ as } p \to 1.$$

Mean-field approximation

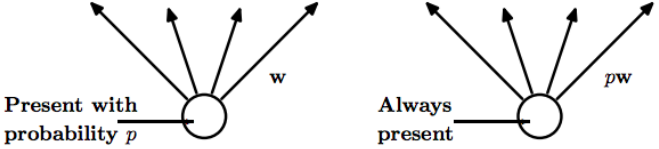
- The model is given by $F_\theta(x) = \mathbb{E}_\xi[f(x;\xi,\theta)]$, which means that the effective model is an average/ensemble of sparse subnetworks.
- At training, stochastic approximation is applied. At testing, we can use Monte-Carlo approximation:

$$F_\theta(x) \approx \frac{1}{m}\sum_{j=1}^{m} f(x;\xi_j,\theta).$$

- MC approximation is reliable but computationaly expensive. A more effecient way is the mean-field approximation:

$$\mathbb{E}_\xi[f(x;\xi,\theta)] \approx f(x;\mathbb{E}[\xi],\theta]) = f(x;p\theta),$$

where the last step is due to $f(x;\xi,\theta) = f(x;\xi\odot\theta)$.



(a) At training time (b) At test time

The error of mean-field approximation

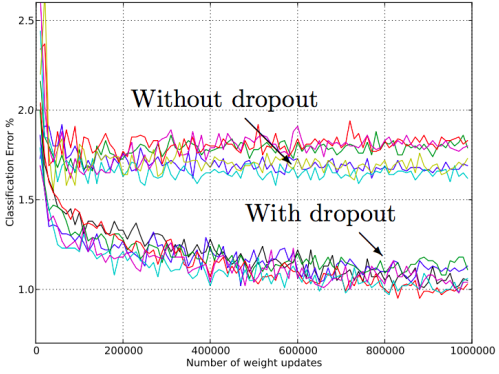
- Let $\mu = \mathbb{E}_\xi[\xi]$. For general $h \in C^2$, we have

$$\mathbb{E}_\xi[h(\xi)] = \mathbb{E}_\xi[h(\mu) + h'(\mu)(\xi - \mu) + O(|\xi - \mu|^2)] \tag{8}$$
$$= h(\mathbb{E}[\xi]) + O(\mathrm{Var}[\xi]). \tag{9}$$

- The error of mean-field approximation is constant. But why it is small enough is unclear.

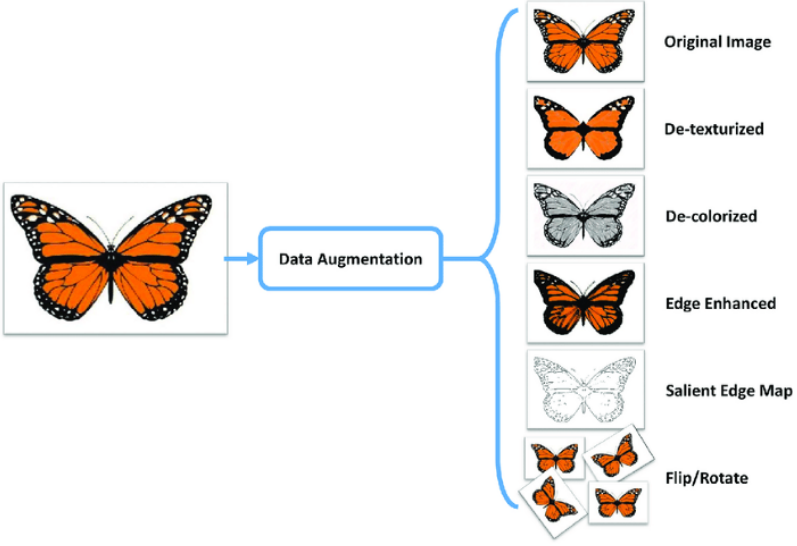
Dropout performance

- Usually, dropout is only applied to fully connected layer.
- Improvement depends on the problem.
- Training is much slower.



Data argumentation

- Increase the amount of data by adding slightly modified copies.
- Typically, most image transformations do not change the label, such as cropping, rotation, translation, resize, adding noise, Gaussian blurring.



Regularization in Modern ML

- **Traditional viewpoint:** Add *explicit regulatizations*, e.g., Weight decay, batch/layer normalization, dropout, data argumentation.

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Regularization in Modern ML

- **Traditional viewpoint:** Add *explicit regulatizations*, e.g., Weight decay, batch/layer normalization, dropout, data argumentation.
- **Modern ML:** A specific algorithm (with a specific initialization) only converges to certain solution, which is called implicit regularization/bias.

- For convex problem, GD with small initialization nearly converges to minimum ℓ_2-norm solution.
- For neural networks, the mechasim of implicit regularization is still puzlled due to the non-convexity.

Implicit regularization

model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78

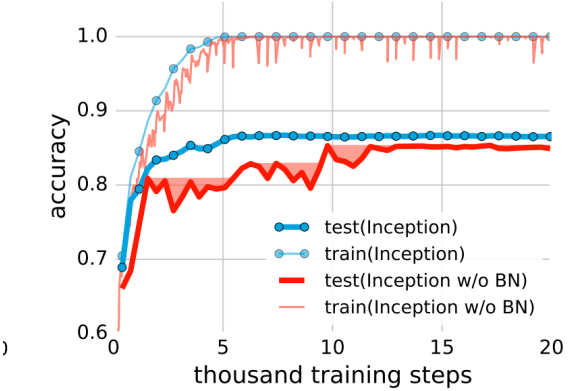

Figure 6: Taken from [Chiyuan Zhang, et al, ICLR2017]

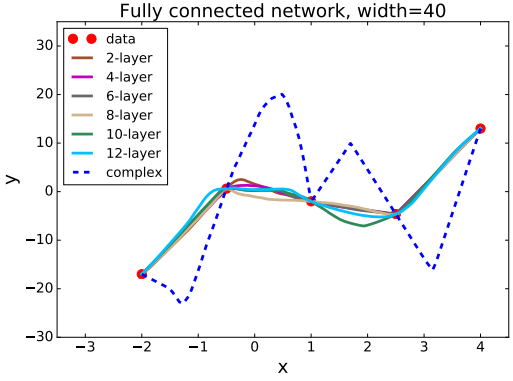

Figure 7: The algorithm is gradient descent (GD). Taken from (Wu, Zhu and E, 2017)

SGD noise

The following table is taken from https://arxiv.org/pdf/2109.14119.pdf.

Experiment	Mini-batching	Epochs	Steps	Modifications	Val. Accuracy %
Baseline SGD	✓	300	117,000	-	95.70(±0.11)
Baseline FB	✗	300	300	-	75.42(±0.13)
FB train longer	✗	3000	3000	-	87.36(±1.23)
FB clipped	✗	3000	3000	clip	93.85(±0.10)
FB regularized	✗	3000	3000	clip+reg	95.36(±0.07)
FB strong reg.	✗	3000	3000	clip+reg+bs32	95.67(±0.08)
FB in practice	✗	3000	3000	clip+reg+bs32+shuffle	95.91(±0.14)

Table 2: Summary of validation accuracies in percent on the CIFAR-10 validation dataset for each of the experiments with data augmentations considered in Section 3. All validation accuracies are averaged over 5 runs.

- We can conclude that

$$\text{SGD} > \text{GD}$$

$$\text{SGD} \geq \text{GD} + (\text{sophisticated explicit regularization.})$$

- The SGD noise must impose certain implicit regularization effects. SGD with large LR and small batch size is always preferred.

Flat minima hypothesis (FMP)

The famous **flat minima hypothesis** (Hochreiter and Schmidhuber, 1995; Keskar et al., 2016):

- SGD converges to flatter minima.
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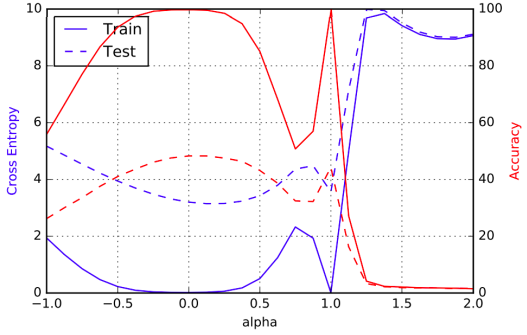

Figure 8: The landscape for for $\theta(\alpha) := (1-\alpha)\theta_{SGD} + \alpha\theta_{GD}$. Taken from (Keskar et al., 2016).

Some remarks

- For neural network models, SGD can always pick up solutions generalizing quite well.
- Explicit regularizations, such as weight decay, dropout, etc. only marginally improve the generalization performance, compared to implicit regularizations.
- Explicit regularizations are critically important in some scenarios, such as highly noisy data, unsupervised learning (GAN), etc.

Summary

- BackProp algorithm, Gradient vanishing/exploding phenomenon.
  - Initialization, skip connections, batch normalization.
  - Layer-wise learning rates, Adaptive learning rate methods.
- Explict regularization: Weight decay, batch normalization, dropout, data augmentation.
- Implicit regularization: SGD and SGD noise.

Reading

- https://www.deeplearningbook.org/contents/regularization.html
- https://www.deeplearningbook.org/contents/optimization.html