# **Training DNNs: Tricks**

#### Ju Sun

Computer Science & Engineering University of Minnesota, Twin Cities

March 5, 2020

### Recap: last lecture

#### Training DNNs

$$\min_{\boldsymbol{W}} \frac{1}{m} \sum_{i=1}^{m} \ell\left(\boldsymbol{y}_{i}, \frac{\text{DNN}_{\boldsymbol{W}}}{\boldsymbol{W}}\left(\boldsymbol{x}_{i}\right)\right) + \frac{\Omega\left(\boldsymbol{W}\right)}{2}$$

- What methods? Mini-batch stochastic optimization due to large m
  - \* SGD (with momentum), Adagrad, RMSprop, Adam
  - \* diminishing LR (1/t, exp delay, staircase delay)
- Where to start?
  - \* Xavier init., Kaiming init., orthogonal init.
- When to stop?
  - \* early stopping: stop when validation error doesn't improve

#### This lecture: additional tricks/heuristics that improve

- convergence speed
- task-specific (e.g., classification, regression, generation) performance

### **Outline**

#### **Data Normalization**

Regularization

Hyperparameter search, data augmentation

Suggested reading

# Why scaling matters?

Consider a ML objective:  $\min_{\boldsymbol{w}} f(\boldsymbol{w}) \doteq \frac{1}{m} \sum_{i=1}^{m} \ell\left(\boldsymbol{w}^{\intercal} \boldsymbol{x}_{i}; y_{i}\right)$ , e.g.,

- Least-squares (LS):  $\min_{\boldsymbol{w}} \frac{1}{m} \sum_{i=1}^{m} \|y_i \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_i\|_2^2$
- Logistic regression:  $\min_{\boldsymbol{w}} \ -\frac{1}{m} \sum_{i=1}^{m} \left[ y_i \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_i \log \left( 1 + e^{\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_i} \right) \right]$
- Shallow NN prediction:  $\min_{m{w}} \ \frac{1}{m} \sum_{i=1}^{m} \|y_i \sigma\left(m{w}^\intercal m{x}_i\right)\|_2^2$

Gradient:  $\nabla_{\boldsymbol{w}} f = \frac{1}{m} \sum_{i=1}^{m} \ell' \left( \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_i; y_i \right) \boldsymbol{x}_i$ .

- What happens when coordinates (i.e., features) of  $x_i$  have different orders of magnitude? Partial derivatives have different orders of magnitudes  $\Longrightarrow$  slow convergence of vanilla GD (recall why adaptive grad methods)

Hessian:  $\nabla_{\boldsymbol{w}}^2 f = \frac{1}{m} \sum_{i=1}^m \ell'' \left( \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_i; y_i \right) \boldsymbol{x}_i \boldsymbol{x}_i^{\mathsf{T}}.$ 

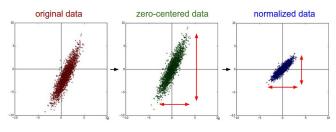
- Suppose the off-diagonal elements of  $x_i x_i^{\mathsf{T}}$  are relatively small (e.g., when features are "independent").
- What happens when coordinates (i.e., features) of  $x_i$  have different orders of magnitude? Conditioning of  $\nabla^2_{w} f$  is bad, i.e., f is elongated

#### Fix the scaling: first idea

Normalization: make each feature zero-mean and unit variance, i.e., make each row of  $X=[x_1,\ldots,x_m]$  zero-mean and unit variance, i.e.

$$X' = rac{X - \mu}{\sigma} \quad (\mu$$
—row means,  $\sigma$ —row std, broadcasting applies)

$$X = (X - X.mean(axis=1))/X.std(axis=1)$$



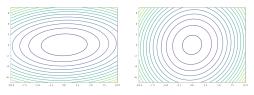
Credit: Stanford CS231N

NB: for data matrices, we often assume each column is a data point, and each row is a feature. This convention is different from that assumed in Tensorflow and PyTorch.

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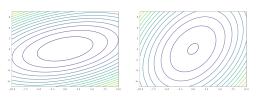
## Fix the scaling: first idea

For LS, works well when features are approximately independent



before vs. after the normalization

For LS, works not so well when features are highly dependent.



before vs. after the normalization

## Fix the scaling: second idea

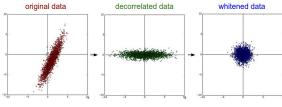
#### PCA and whitening

**PCA**, i.e., zero-center and rotate the data to align principal directions to coordinate directions

X -= X.mean(axis=1) #centering
U, S, VT = np.linalg.svd(X, full\_matrices=False)
Xrot = U.T@X #rotate/decorrelate the data
$$(math: X = USV^{\mathsf{T}}, then U^{\mathsf{T}}X = SV)$$

**Whitening**: PCA + normalize the coordinates by singular values

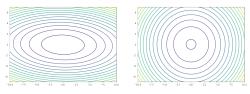
Xwhite =1/(S+eps)\*Xrot 
$$\#$$
 (math:  $X_{
m white} = V$ ) original data decorrelated data whitened data



Credit: Stanford CS231N

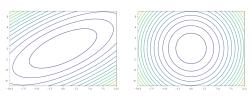
### Fix the scaling: second idea

For LS, works well when features are approximately independent



before vs. after the whitening

For LS, also works well when features are highly dependent.



before vs. after the whitening

### In DNNs practice

fixing the feature scaling makes the landscape "nicer"—derivatives and curvatures in all directions are roughly even in magnitudes. So for DNNs,

- Preprocess the input data
  - \* zero-center
  - \* normalization
  - \* PCA or whitening (less common)
- But recall our model objective  $\min_{\boldsymbol{w}} f(\boldsymbol{w}) \doteq \frac{1}{m} \sum_{i=1}^{m} \ell(\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_i; y_i)$  vs. DL objective

$$\min_{\boldsymbol{W}} \ \tfrac{1}{m} \sum_{i=1}^{m} \ell\left(\boldsymbol{y}_{i}, \sigma\left(\boldsymbol{W}_{k} \sigma\left(\boldsymbol{W}_{k-1} \ldots \sigma\left(\boldsymbol{W}_{1} \boldsymbol{x}_{i}\right)\right)\right)\right) + \Omega\left(\boldsymbol{W}\right)$$

- \* DL objective is much more complex
- \* But  $\sigma(\mathbf{W}_k \sigma(\mathbf{W}_{k-1} \dots \sigma(\mathbf{W}_1 \mathbf{x}_i)))$  is a composite version of  $\mathbf{w}^\intercal \mathbf{x}_i$ :

$$W_1x_i$$
,  $W_2\sigma(W_1x_i)$ ,  $W_3\sigma(W_2\sigma(W_1x_i))$ , ...

Idea: also process the input data to some/all hidden layers

#### **Batch normalization**

#### Apply normalization to the input data to some/all hidden layers

-  $\sigma\left(\boldsymbol{W}_{k}\sigma\left(\boldsymbol{W}_{k-1}\ldots\sigma\left(\boldsymbol{W}_{1}\boldsymbol{x}_{i}\right)\right)\right)$  is a composite version of  $\boldsymbol{w}^{\intercal}\boldsymbol{x}_{i}$ :

$$oldsymbol{W}_1oldsymbol{x}_i,\ oldsymbol{W}_2oldsymbol{\sigma}\left(oldsymbol{W}_1oldsymbol{x}_i
ight),\ oldsymbol{W}_3oldsymbol{\sigma}\left(oldsymbol{W}_2oldsymbol{\sigma}\left(oldsymbol{W}_1oldsymbol{x}_i
ight)
ight),\ \ldots$$

- Apply **normalization** to the outputs of the colored parts based on the statistics of a **mini-batch** of  $x_i$ 's, e.g.,

$$W_2 \underbrace{\sigma(W_1x_i)}_{\doteq z_i} \longrightarrow W_2 \underbrace{\operatorname{BN}(\sigma(W_1x_i))}_{\operatorname{BN}(z_i)}$$

– Let  $oldsymbol{z}_i$ 's be generated from a mini-batch of  $oldsymbol{x}_i$ 's and  $oldsymbol{Z} = [oldsymbol{z}_1 \dots oldsymbol{z}_{|B|}]$ ,

$$\mathrm{BN}\left(z^{j}\right)=rac{z^{j}-\mu_{oldsymbol{z}^{j}}}{\sigma_{oldsymbol{z}^{j}}}\quad ext{for each row }z^{j} ext{ of }oldsymbol{Z}.$$

Flexibity restored by optional scaling  $\gamma_j$ 's and shifting  $\beta_j$ 's:

$$\mathrm{BN}_{\gamma_j,oldsymbol{eta}_j}\left(oldsymbol{z}^j
ight) = \gamma_j rac{oldsymbol{z}^j - \mu_{oldsymbol{z}^j}}{\sigma_{oldsymbol{z}^j}} + eta_j \quad ext{for each row } oldsymbol{z}^j ext{ of } oldsymbol{Z}.$$

Here,  $\gamma_j$ 's and  $\beta$ 's are trainable (optimization) variables!

### Batch normalization: implementation details

$$W_{2} \underbrace{\underbrace{\sigma\left(W_{1}x_{i}\right)}_{\doteq z_{i}} \longrightarrow W_{2} \underbrace{\operatorname{BN}\left(\sigma\left(W_{1}x_{i}\right)\right)}_{\operatorname{BN}\left(z_{i}\right)} \qquad \operatorname{BN}_{\gamma_{j},\beta_{j}}\left(z^{j}\right) = \gamma_{j} \frac{z^{j} - \mu_{z^{j}}}{\sigma_{z^{j}}} + \beta_{j} \ \forall \ j$$

Question: how to perform training after plugging in the BN operations?

$$\min_{\boldsymbol{W}} \ \frac{1}{m} \sum_{i=1}^{m} \ell\left(\boldsymbol{y}_{i}, \sigma\left(\boldsymbol{W}_{k} \underline{\mathsf{BN}}\left(\sigma\left(\boldsymbol{W}_{k-1} \dots \underline{\mathsf{BN}}\left(\sigma\left(\boldsymbol{W}_{1} \boldsymbol{x}_{i}\right)\right)\right)\right)\right)\right) + \Omega\left(\boldsymbol{W}\right)$$

Answer: for all j,  $\mathrm{BN}_{\gamma_j,\boldsymbol{\beta}_j}\left(\boldsymbol{z}^j\right)$  is nothing but a differentiable function of  $\boldsymbol{z}^j$ ,  $\gamma_j$ , and  $\beta_j$  — chain rule applies!

- $\mu_{z^j}$  and  $\sigma_{z^j}$  are differentiable functions of  $z^j$ , and  $(z^j, \gamma_j, \beta_j) \mapsto \text{BN}_{\gamma_i, \beta_i}(z^j)$  is a vector-to-vector mapping
- Any row  $\pmb{z}^j$  depends on all  $\pmb{x}_k$ 's in the current mini-batch B as  $\pmb{Z} = [\pmb{z}_1 \dots \pmb{z}_{|B|}] \longleftarrow [\pmb{x}_1 \dots \pmb{x}_{|B|}]$
- Without BN:

$$\begin{array}{l} \nabla_{\boldsymbol{W}} \frac{1}{|B|} \sum_{k=1}^{|B|} \ell\left(\boldsymbol{W}; \boldsymbol{x}_k, \boldsymbol{y}_k\right) = \frac{1}{|B|} \sum_{k=1}^{|B|} \nabla_{\boldsymbol{W}} \ell\left(\boldsymbol{W}; \boldsymbol{x}_k, \boldsymbol{y}_k\right) \text{, the} \\ \text{summands can be computed in parallel and then aggregated} \\ \text{With BN: } \nabla_{\boldsymbol{W}} \frac{1}{|B|} \sum_{k=1}^{|B|} \ell\left(\boldsymbol{W}; \boldsymbol{x}_k, \boldsymbol{y}_k\right) \text{ has to be computed altogether,} \\ \text{due to the inter-dependency across the summands} \end{array}$$

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#### Batch normalization: implementation details

$$\mathrm{BN}_{\gamma_j, \boldsymbol{\beta}_j}\left(\boldsymbol{z}^j\right) = \gamma_j \frac{\boldsymbol{z}^j - \mu_{\boldsymbol{z}^j}}{\sigma_{\boldsymbol{z}^j}} + \beta_j \ \forall \ j$$

What about validation/test, where only a single sample is seen each time?

idea: use the average  $\mu_{z^j}$ 's and  $\sigma_{z^j}$ 's over the training data  $(\gamma_j)$ 's and  $\beta_j$ 's are learned)

In practice, collect the momentum-weighted running averages: e.g., for each hidden node with BN,

$$\overline{\mu} = (1 - \eta) \, \overline{\mu}_{old} + \eta \mu_{new}$$

$$\overline{\sigma} = (1 - \eta) \, \overline{\sigma}_{old} + \eta \sigma_{new}$$

with e.g.,  $\eta=0.1.$  In PyTorch, torch.nn.BatchNorm1d, torch.nn.BatchNorm2d, torch.nn.BatchNorm3d depending on the input shapes

#### Batch normalization: implementation details

Question: BN before or after the activation?

```
egin{aligned} oldsymbol{W}_2\sigma(oldsymbol{W}_1oldsymbol{x}_i) &\longrightarrow oldsymbol{W}_2rac{	ext{BN}}{	ext{BN}}(\sigma(oldsymbol{W}_1oldsymbol{x}_i)) & 	ext{(after)} \ oldsymbol{W}_2\sigma(oldsymbol{W}_1oldsymbol{x}_i) &\longrightarrow oldsymbol{W}_2(\sigma(egin{aligned} 	ext{BN}}{	ext{(W}_1oldsymbol{x}_i)})) & 	ext{(before)} \end{aligned}
```

- The original paper [loffe and Szegedy, 2015] proposed the "before" version (most of the original intuition has since proved wrong)
- But the "after" version is more intuitive as we have seen
- Both are used in practice and debatable which one is more effective
  - \* https://www.reddit.com/r/MachineLearning/comments/ 67gonq/d\_batch\_normalization\_before\_or\_after\_relu/
  - \* https://blog.paperspace.com/ busting-the-myths-about-batch-normalization/
  - \* https://github.com/gcr/torch-residual-networks/issues/5
  - \* [Chen et al., 2019]

# Why BN works?

Short answer: we don't know yet

#### Long answer:

- Originally proposed to deal with internal covariate shift [loffe and Szegedy, 2015]
- The original intuition later proved wrong and BN is shown to make the optimization problem "nicer" (or "smoother")
   [Santurkar et al., 2018, Lipton and Steinhardt, 2019]
- Yet another explanation from optimization perspective [Kohler et al., 2019]
- A good research topic

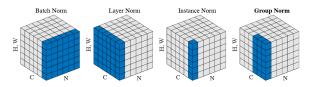
# **Batch PCA/whitening?**

fixing the feature scaling makes the landscape "nicer"—derivatives and curvatures in all directions are roughly even in magnitudes. So for DNNs,

- Add (pre-)processing to input data
  - \* zero-center
  - \* normalization
  - \* PCA or whitening (less common)
- Add batch-processing steps to some/all hidden layers
  - \* Batch normalization
  - \* Batch PCA or whitening? Doable but requires a lot of work [Huangi et al., 2018, Huang et al., 2019, Wang et al., 2019]

normalization is most popular due to the simplicity

#### Zoo of normalization



Normalization methods. Each subplot shows a feature map tensor, with N as the batch axis, C as the channel axis, and (H, W) as the spatial axes. The pixels in blue are normalized by the same mean and variance, computed by aggregating the values of these pixels.

Credit: [Wu and He, 2018]

normalization in different directions/groups of the data tensors

weight normalization: decompose the weight as magnitude and direction  $m{w} = g \frac{m{v}}{\| m{v} \|_2}$  and perform optimization in  $(g, m{v})$  space

An Overview of Normalization Methods in Deep Learning

https://mlexplained.com/2018/11/30/

an-overview-of-normalization-methods-in-deep-learning/

Check out PyTorch normalization layers

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### **Outline**

Data Normalization

### Regularization

Hyperparameter search, data augmentation

Suggested reading

# Regularization to avoid overfitting

Training DNNs  $\min_{\boldsymbol{W}} \frac{1}{m} \sum_{i=1}^{m} \ell\left(\boldsymbol{y}_{i}, \text{DNN}_{\boldsymbol{W}}\left(\boldsymbol{x}_{i}\right)\right) + \lambda \Omega\left(\boldsymbol{W}\right)$  with **explicit** regularization  $\Omega$ . But which  $\Omega$ ?

- $\Omega\left(\boldsymbol{W}\right) = \sum_{k} \left\|\boldsymbol{W}_{k}\right\|_{F}^{2}$  where k indexes the layers penalizes large values in  $\boldsymbol{W}$  and hence avoids steep changes (set weight\_decay as  $\lambda$  in torch.optim.xxxx)
- $\Omega\left(m{W}\right) = \sum_{k} \left\|m{W}_{k}\right\|_{1}$  promotes sparse  $m{W}_{k}$ 's (i.e., many entries in  $m{W}_{k}$ 's to be near zero; good for feature selection)

- $\begin{array}{l} \ \Omega \left( \boldsymbol{W} \right) = \left\| \boldsymbol{J}_{\mathrm{DNN}_{\boldsymbol{W}}} \left( \boldsymbol{x} \right) \right\|_F^2 \text{promotes smoothness of the function} \\ \text{represented by } \mathrm{DNN}_{\boldsymbol{W}} \\ \text{[Varga et al., 2017, Hoffman et al., 2019, Chan et al., 2019]} \end{array}$
- Constraints,  $\delta_{C}\left(\boldsymbol{W}\right) \doteq \begin{cases} 0 & \boldsymbol{W} \in C \\ \infty & \boldsymbol{W} \notin C \end{cases}$ , e.g., binary, norm bound
- many others!

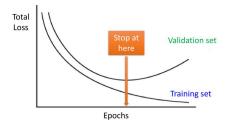
# Implicit regularization

Training DNNs  $\min_{\boldsymbol{W}} \frac{1}{m} \sum_{i=1}^{m} \ell\left(\boldsymbol{y}_{i}, \text{DNN}_{\boldsymbol{W}}\left(\boldsymbol{x}_{i}\right)\right) + \lambda \Omega\left(\boldsymbol{W}\right)$  with implicit regularization — operation that is not built into the objective but avoids overfitting

- early stopping
- batch normalization
- dropout
- ..

## **Early stopping**

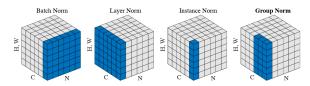
A practical/pragmatic stopping strategy: early stopping



... periodically check the validation error and stop when it doesn't improve

Intuition: avoid the model to be too specialized/perfect for the training data More concrete math examples: [Bishop, 1995, Sjöberg and Ljung, 1995]

## Batch/general normalization



Normalization methods. Each subplot shows a feature map tensor, with N as the batch axis, C as the channel axis, and (H, W) as the spatial axes. The pixels in blue are normalized by the same mean and variance, computed by aggregating the values of these pixels.

Credit: [Wu and He, 2018]

normalization in different directions/groups of the data tensors

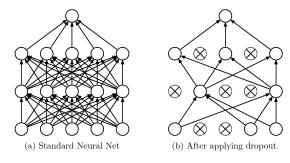
weight normalization: decompose the weight as magnitude and direction  $w=g\frac{v}{\|v\|_2}$  and perform optimization in (g,v) space

An Overview of Normalization Methods in Deep Learning

https://mlexplained.com/2018/11/30/

an-overview-of-normalization-methods-in-deep-learning/

# **Dropout**



Credit: [Srivastava et al., 2014]

#### Idea: kill each non-output neuron with probability 1-p, called Dropout

- perform Dropout independently for each training sample and each iteration
- for each neuron, if the original output is x, then the expected output with Dropout: px. So rescale the actual output by 1/p
- no Dropout at test time!

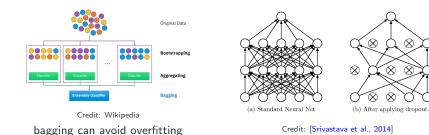
### **Dropout: implementation details**

```
p = 0.5 # probability of keeping a unit active, higher = less dropout
def train step(X):
 # forward pass for example 3-layer neural network
 H1 = np.maximum(0, np.dot(W1, X) + b1)
 U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
 H1 *= U1 # drop!
 H2 = np.maximum(0. np.dot(W2. H1) + b2)
 U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask, Notice /p!
 H2 *= U2 # drop!
 out = np.dot(W3, H2) + b3
 # backward pass: compute gradients... (not shown)
 # perform parameter update... (not shown)
def predict(X):
 # ensembled forward pass
 H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
 H2 = np.maximum(0, np.dot(W2, H1) + b2)
 out = np.dot(W3, H2) + b3
```

Credit: Stanford CS231N

What about derivatives? Back-propagation for each sample and then aggregate PyTorch: torch.nn.Dropout, torch.nn.Dropout2d, torch.nn.Dropout3d

# Why Dropout?



For an n-node network,  $2^n$  possible sub-networks.

Consider the average/ensemble prediction  $\mathbb{E}_{SN}\left[SN\left(oldsymbol{x}
ight)\right]$  over  $2^{n}$  of sub-networks and the new objective

$$F(\boldsymbol{W}) \doteq \frac{1}{m} \sum_{i=1}^{m} \ell(\boldsymbol{y}_{i}, \mathbb{E}_{SN}[SN_{\boldsymbol{W}}(\boldsymbol{x}_{i})])$$

Mini-batch SGD with Dropout samples data point and model simultaneously (stochastic composite optimization [Wang et al., 2016, Wang et al., 2017] )

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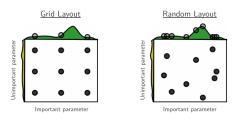
Suggested reading

## Hyperparameter search

...tunable parameters (vs. learnable parameters, or optimization variables)

- Network architecture (depth, width, activation, loss, etc)
- Optimization methods
- Initialization schemes
- Initial LR and LR schedule/parameters
- regularization methods and parameters
- etc

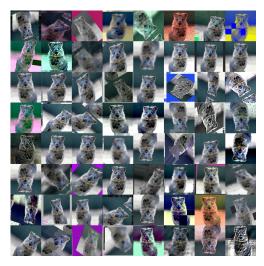
https://cs231n.github.io/neural-networks-3/#hyper



Credit: [Bergstra and Bengio, 2012]

### **Data augmentation**

- More relevant data always help!
- Fetch more external data
- Generate more internal data: generate based on whatever you want to be robust to
  - vision: translation, rotation, background, noise, deformation, flipping, blurring, occlusion, etc



Credit: https://github.com/aleju/imgaug

See one example here https:

#### **Outline**

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Suggested reading

### Suggested reading

- Chap 7, Deep Learning (Goodfellow et al)
- Stanford CS231n course notes: Neural Networks Part 2: Setting up the Data and the Loss https://cs231n.github.io/neural-networks-2/
- Stanford CS231n course notes: Neural Networks Part 3: Learning and Evaluation https://cs231n.github.io/neural-networks-3/
- http://neuralnetworksanddeeplearning.com/chap3.html

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