Supplemental Training Procedures Deep Learning



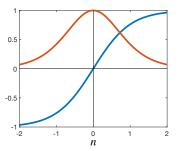
Objectives

- The basic training methods, like steepest descent and Adam, can be supplemented for improved performance.
- The supplements described in this chapter serve two purposes.
- Speed up the convergence of training.
- Ensure that the final trained network will perform as well on new data as it did on the training data.



Cause of slow training: vanishing gradient

- Two things sped up training of deep networks.
 - 1 The introduction of cuda for programming GPUs.
 - 2 Overcoming the vanishing gradient problem.
- For deep networks with sigmoid activation, gradient can become very small.

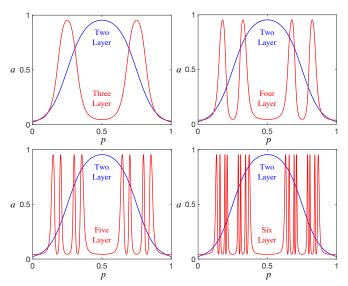


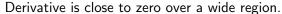
Tansig (tanh) activation function and its derivative





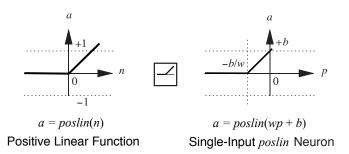
Cascading sigmoid layers







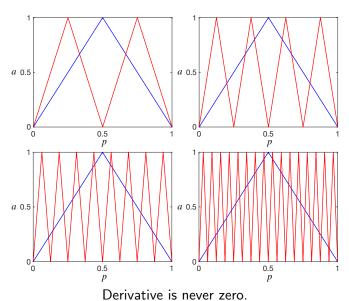
ReLU (or poslin) activation function







Cascading ReLU layers







Normalization at the input

- Sigmoid activations become saturated for n > 3 (exp(-3) $\simeq 0.05$).
- n = wp + b
- It is best to keep p in a standard range.

Normalize to [-1, 1]

$$\check{\mathbf{p}} = 2\left(\mathbf{p} - \mathbf{p}^{min}\right) \oslash \left(\mathbf{p}^{max} - \mathbf{p}^{min}\right) - 1$$

Normalize to zero mean and unity variance

$$\check{\mathbf{p}} = (\mathbf{p} - \mathbf{p}^{mean}) \oslash \mathbf{p}^{std}$$





Batch Normalization

- We want to perform normalization at each layer.
- However, the range of inputs to layers after layer 1 change during training.
- The normalization can be done using batches of data.

$$\begin{aligned} \mathbf{a}^{mean} &= \frac{1}{Q} \sum_{q=1}^{Q} \mathbf{a}_q \\ \mathbf{a}^{std} &= \sqrt{\frac{1}{Q} \sum_{q=1}^{Q} (\mathbf{a}_q - \mathbf{a}^{mean})^2 + \varepsilon} \\ \mathbf{\bar{a}}_q &= (\mathbf{a}_q - \mathbf{a}^{mean}) \oslash \mathbf{a}^{std} \\ \mathbf{\check{a}}_q &= \mathbf{w}^{bn} \circ \mathbf{\bar{a}}_q + \mathbf{b}^{bn} \end{aligned}$$





Backpropagating the batch

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_Q \end{bmatrix}$$

$$vec\left(\mathbf{A}\right) = \begin{bmatrix} \mathbf{a}_1^T & \mathbf{a}_2^T & \cdots & \mathbf{a}_Q^T \end{bmatrix}^T$$

$$\frac{\partial \left(vec\left(\mathbf{A}^1\right)\right)^T}{\partial vec\left(\mathbf{A}^1\right)} \xrightarrow{\partial \left(vec\left(\mathbf{A}^2\right)\right)^T} \frac{\partial \left(vec\left(\mathbf{A}^2\right)\right)^T}{\partial vec\left(\mathbf{N}^2\right)}$$

$$\mathbf{A}^1 \xrightarrow{\mathbf{A}^1} \mathbf{B}^1 \xrightarrow{\mathbf{A}^2} \mathbf{B}^2$$

$$\mathbf{B}^2 \times \mathbf{1}_{1,Q}$$

$$\mathbf{B}^2 \times \mathbf{1}_{1,Q}$$

$$\mathbf{B}^2 \times \mathbf{1}_{1,Q}$$





Backpropagating across the activation function and weight

The examples in the batch do not interact.

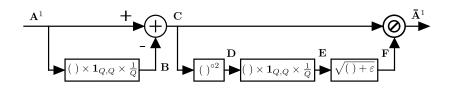
$$\frac{\partial \left(vec\left(\mathbf{N}^{2}\right)\right)^{T}}{\partial vec\left(\check{\mathbf{A}}^{1}\right)} = \begin{bmatrix} \left(\mathbf{W}^{2}\right)^{T} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \left(\mathbf{W}^{2}\right)^{T} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \cdots & \left(\mathbf{W}^{2}\right)^{T} \end{bmatrix}$$
$$\frac{\partial \left(vec\left(\mathbf{A}^{2}\right)\right)^{T}}{\partial vec\left(\mathbf{N}^{2}\right)} = \begin{bmatrix} \dot{\mathbf{F}}^{2}\left(\mathbf{n}_{1}^{2}\right) & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \dot{\mathbf{F}}^{2}\left(\mathbf{n}_{2}^{2}\right) & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \cdots & \dot{\mathbf{F}}^{2}\left(\mathbf{n}_{Q}^{2}\right) \end{bmatrix}$$





Backpropagating across the normalization

- The examples in each minibatch will interact with each other.
- Break up batch norm into simpler pieces and backpropagate.







Batch norm during inference

- The values for \mathbf{w}^{bn} and \mathbf{b}^{bn} at the end of training can be used for inference.
- During inference, we could have a batch of one, so standard deviation could not be computed.
- Batch norm must be operated with consistent mean and variance.
- One option is to use a smoothed version of the means and variances calculated during training.

$$\begin{split} \tilde{\mathbf{a}}_k^{mean} &= \delta \cdot \tilde{\mathbf{a}}_{k-1}^{mean} + (1 - \delta) \cdot \mathbf{a}_k^{mean} \\ \tilde{\mathbf{a}}_k^{std} &= \delta \cdot \tilde{\mathbf{a}}_{k-1}^{std} + (1 - \delta) \cdot \mathbf{a}_k^{std} \end{split}$$





Batch norm summary

- Batch norm was developed to prevent vanishing gradient when using sigmoid activations.
- Normalization keeps inputs from saturating sigmoid functions.
- In practice, it also improves training even for ReLU activations.
- Random changes in scaling from minibatch to minibatch may improve generalization.
- A related technique is layer normalization. More effective than batch norm in recurrent networks.



Weight initialization

- Proper initialization of weights can prevent activation saturation.
- If initial weights are too large, the sigmoid can be saturated.
- Zero initial weights occur at a saddle point of the performance surface.
- The backpropagation steps multiply by weights at each layer.
 If all weights are small, the gradient will be close to zero.
- We want to find a happy medium for the weight values.





Weight initialization

Approximate neuron output in linear region of sigmoid.

$$a_i^m \simeq \sum_{j=1}^{S^{m-1}} w_{i,j}^m a_j^{m-1} + b_i^m$$

- Set bias to zero, and assume activations from previous layer have mean zero and variance $\sigma_a^2(m-1)$.
- Assume initial weights are random values with mean zero and variance σ_w^2 .
- Assume activations and weights are independent.

$$var\left(a_{i}^{m}\right) \equiv \sigma_{a}^{2}(m) = S^{m-1}\sigma_{w}^{2}\sigma_{a}^{2}(m-1)$$

To maintain activation variance across layers:

$$\sigma_w^2 = \frac{1}{S^{m-1}}$$





Considering the backpropagation process

The standard backpropagation is:

$$\mathbf{s}^{m-1} = \dot{\mathbf{F}}^{m-1}(\mathbf{n}^{m-1})(\mathbf{W}^m)^T \mathbf{s}^m$$

If we are in the linear activation range:

$$s_i^{m-1} \simeq \sum_{j=1}^{S^m} w_{j,i}^m s_j^m$$

To maintain sensitivity variance across layers:

$$var\left(s_i^{m-1}\right) = \sigma_s^2(m-1) = S^m \sigma_w^2 \sigma_s^2(m)$$
$$\sigma_w^2 = \frac{1}{S^m}$$

Trying to maintain forward and backward variance constant:

$$\sigma_w^2 = \frac{2}{S^{m-1} + S^m}, \text{ Xavier Initialization}$$



Gradient clipping

- In deep networks,
 - Small weights can produce small gradients (vanishing gradient).
 - Large weights can produce large gradients (exploding gradient).
- Exploding gradient usually occurs in recurrent networks.
- Solution: scale the gradient to limit the norm.
- This is gradient clipping.





Improving generalization

- A network generalizes well if it performs as well on unseen data as on the training data.
- When a network overfits the training data, it will not generalize well.
- In early stopping, a validation set is removing from training.
 When validation error goes up, training stops.
- In regularization, a penalty term (usually sum of squared weights) is added to the performance function.
- In dropout a percentage of neurons in a selected layer are randomly deactivated at each iteration.
- Dropout is never used with batch normalization.



