ECE521 Lecture9

Neural Networks
Deep Learning

UNIVERSITY OF TORONTO

Outline

- **Multi-class classification**
- Learning multi-layer neural networks
- Bag-of-tricks for deep neural networks
    - Local minimums and initialization
    - Early stopping and regularization
    - Dataset normalization

Measuring distance in probability space

- We learnt that the squared L2 distance is an important concept that captures the natural distance measure between the two points in Euclidean space. The Kullback-Leibler divergence is an equally important concept that is an appropriate distance measure between two probability distributions:

$$KL(Q\|P) = \sum_x Q(x) \log \frac{Q(x)}{P(x)}$$

  - KL divergence is an asymmetric distance function: $KL(Q\|P) \neq KL(P\|Q)$
  - KL divergence is also nonnegative for any two distributions

Binary cross-entropy loss

- Consider the *Q* distribution to be the discrete probability distribution of the observed binary labels $t \in \{0, 1\}$ in the training dataset
  - $Q(t = 1|\mathbf{x}) = t$ is either zero or one depending on the training example. (The dataset is observed, so there is no randomness)
- Choose the *P* distribution to be the model's prediction: $P(t = 1|\mathbf{x}) = \hat{y}(\mathbf{x})$. The KL divergence between *Q* and *P* is in fact the cross-entropy loss:

$$\begin{aligned} KL(Q\|P) &= \sum_t Q(t|\mathbf{x}) \log \frac{Q(t|\mathbf{x})}{P(t|\mathbf{x})} = -\sum_t Q(t|\mathbf{x}) \log P(t|\mathbf{x}) + \boxed{\sum_t Q(t|\mathbf{x}) \log Q(t|\mathbf{x})} \\ &= -Q(t=1|\mathbf{x}) \log P(t=1|\mathbf{x}) - Q(t=0|\mathbf{x}) \log P(t=0|\mathbf{x}) \\ &= \underbrace{-t \log \hat{y} - (1-t) \log(1-\hat{y})}_{\text{cross entropy}} \end{aligned}$$

this is zero
0*log(0)→0

  - The cross-entropy loss function measure the distance between the empirical data distribution and the model predictive distribution

Multi-class cross-entropy loss and softmax

- It is easy to use the KL divergence interpretation to generalize the cross-entropy loss to a multi-class scenario:
  - Let there be *K* classes, with class labels $t \in \{1, \cdots, K\}$
  - The multi-class cross entropy loss is therefore:

$$KL(Q\|P) = \sum_t Q(t|\mathbf{x}) \log \frac{Q(t|\mathbf{x})}{P(t|\mathbf{x})} = -\sum_{k=1}^{K} k \log P(t=k|\mathbf{x})$$

  - Similarly, the multi-class generalization of the sigmoid function is the *softmax function*. The multi-class predictive distribution becomes:

$$P(t=k|\mathbf{x}) = \frac{e^{z_k}}{\sum_j e^{z_j}}$$

Here z_k are the outputs of a neural network or linear regression

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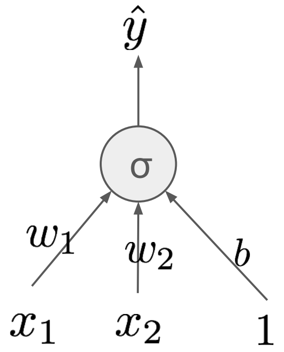
Example 1: representing digital circuits with neural networks

- Let us look at a simple example of a soft OR gate simulated by a neural network:
    - Use a single sigmoid neuron with two inputs and a bias unit.

	x2=0	x2=1
x1=0	0	1
x1=1	1	1



Example 1: representing digital circuits with neural networks

- Let us look at a simple example of a soft OR gate simulated by a neural network:
  - Use a single sigmoid neuron with two inputs and a bias unit.
  - One possible solution is to use the bias as a threshold while setting w_1 and w_2 to be large positive values. When either of the inputs is non-zero, the sigmoid neuron will be turned on and the output will be 1.

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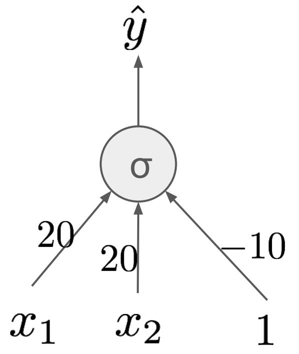
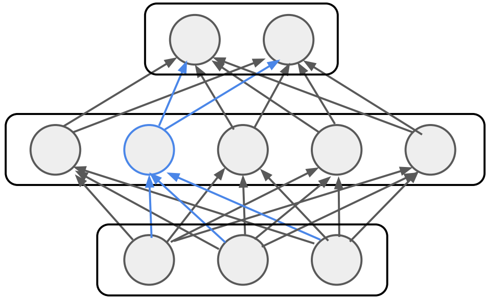
x1=0	0	1
x1=1	1	1



Learning fully connected multi-layer neural networks

- There are many choices when “crafting” the architecture of a neural network. The fully connected multi-layer NN is the most general multi-layer NN:
    - Each neuron has its incoming weights connected to *all* the neurons from the previous layer and its outgoing weights connected to *all* the neurons in the next layer.
- Fully connected network is the go-to architecture choice if we do not have any additional information about the dataset.
    - After choosing the network architecture, there are a few more engineering choices: #hidden units, #layers, the type of activation function.
    - The output units type: linear, logistic or softmax are determined by output tasks, i.e. regression or classification task



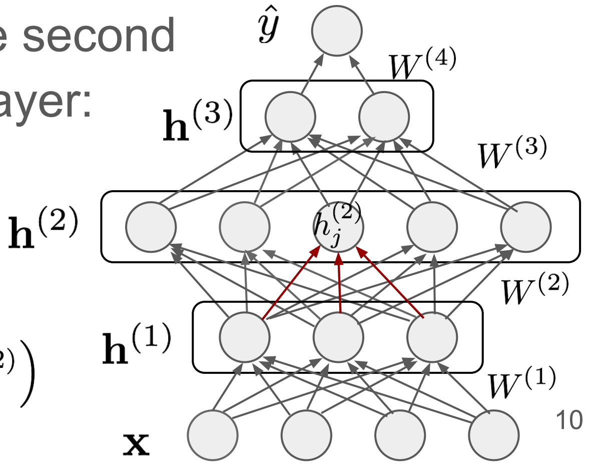
Learning fully connected multi-layer neural networks

- Consider a fully connected neural network with 3 hidden layers:
  - The input to the neural network is an *N*-dimensional vector $\mathbf{x}$. There are *H1, H2,* and *H3* hidden units in the three hidden layers. We use superscript to index the layers.
  - There are four weight matrices among the hidden layers, e.g. $W^{(2)} \in \mathbb{R}^{H_2 \times H_1}, b^{(2)} \in \mathbb{R}^{H_2}$
  - The *j*th row of the weight matrix $W^{(2)}$ is denoted as $W_j^{(2)} \in \mathbb{R}^{H_1}$
- The hidden activation of the *j*th hidden unit $h_j^{(2)}$ in the second hidden layer is the weighted sum of the first hidden layer:

$$h_j^{(2)} = \phi\left(z_j^{(2)}\right) = \phi\left(\sum_i w_{ij}^{(2)} h_i^{(1)} + b_j^{(2)}\right) = \phi\left({W_j^{(2)}}^T \mathbf{h}^{(1)} + b_j^{(2)}\right)$$

  - We can use vector notation to express the hidden vector:

$$\mathbf{h}^{(2)} = \begin{bmatrix} h_1^{(2)} \\ \vdots \\ h_{H_2}^{(2)} \end{bmatrix} = \begin{bmatrix} \phi\left(z_1^{(2)}\right) \\ \vdots \\ \phi\left(z_{H_2}^{(2)}\right) \end{bmatrix} = \phi\left(\begin{bmatrix} {W_1^{(2)}}^T \\ \vdots \\ {W_{H_2}^{(2)}}^T \end{bmatrix} \mathbf{h}^{(1)} + b^{(2)}\right) = \phi\left(W^{(2)}\mathbf{h}^{(1)} + b^{(2)}\right)$$



Learning fully connected multi-layer neural networks

- For a single data point, we can write the the hidden activations of the fully connected neural network as a recursive computation using the vector notation:

$$\mathbf{z}^{(1)} = W^{(1)}\mathbf{x} + b^{(1)}, \quad \mathbf{h}^{(1)} = \left(\mathbf{z}^{(1)}\right)$$

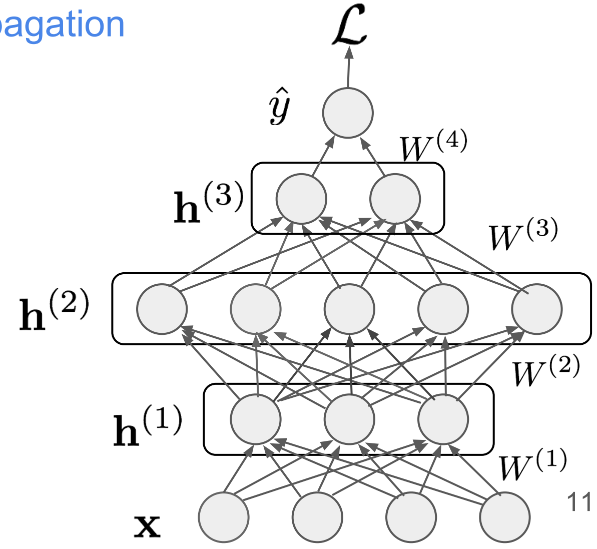
$$\mathbf{z}^{(2)} = W^{(2)}\mathbf{h}^{(1)} + b^{(2)}, \quad \mathbf{h}^{(2)} = \phi\left(\mathbf{z}^{(2)}\right)$$

$$\mathbf{z}^{(3)} = W^{(3)}\mathbf{h}^{(2)} + b^{(3)}, \quad \mathbf{h}^{(3)} = \phi\left(\mathbf{z}^{(3)}\right)$$

$$\mathbf{z}^{(4)} = W^{(4)}\mathbf{h}^{(3)} + b^{(4)}, \quad \hat{y} = f\left(\mathbf{z}^{(4)}\right)$$

  - *f()* is the output activation function
  - The output of the network is then used to compute the loss function on the training data

forward propagation



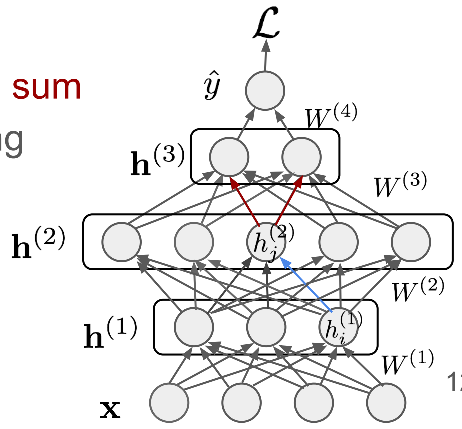
Learning fully connected multi-layer neural networks

- Learning neural networks using stochastic gradient descent requires the gradient of the weight matrices from each hidden layer.
  - Let us consider the gradient of the loss for a single training example. The gradient w.r.t. the incoming weights $w_{ij}^{(2)}$ of the *j*th hidden units in the second layer is the *product* of the hidden activation from layer one *and* the partial derivative of z_j. Remember: $h_j^{(2)} = \phi\left(z_j^{(2)}\right) = \phi\left(\sum_i w_{ij}^{(2)} h_i^{(1)} + b_j^{(2)}\right)$

$$\frac{\partial \mathcal{L}}{\partial w_{ij}^{(2)}} = \frac{\partial \mathcal{L}}{\partial z_j^{(2)}} \frac{\partial z_j^{(2)}}{\partial w_{ij}^{(2)}} = \frac{\partial \mathcal{L}}{\partial z_j^{(2)}} h_i^{(1)}$$

  - The partial derivative of z_j in the second hidden layer is the weighted sum of the partial derivatives from the third layer, weighted by the outgoing weights of the *j*th hidden units

$$\frac{\partial \mathcal{L}}{\partial z_j^{(2)}} = \frac{\partial \mathcal{L}}{\partial h_j^{(2)}} \frac{\partial h_j^{(2)}}{\partial z_j^{(2)}} = \left(\sum_i \frac{\partial \mathcal{L}}{\partial z_i^{(3)}} \frac{\partial z_i^{(3)}}{\partial h_j^{(2)}}\right) \frac{\partial h_j^{(2)}}{\partial z_j^{(2)}} = \boxed{\left(\sum_i \frac{\partial \mathcal{L}}{\partial z_i^{(3)}} w_{ji}^{(3)}\right)} \frac{\partial h_j^{(2)}}{\partial z_j^{(2)}}$$



Learning fully connected multi-layer neural networks

- Similar to the hidden-activation computation, the weighted sum of the partial derivatives can be rewritten using vector notation:

$$\frac{\partial \mathcal{L}}{\partial z_j^{(2)}} = \left(\sum_i \frac{\partial \mathcal{L}}{\partial z_i^{(3)}} w_{ji}^{(3)} \right) \frac{\partial h_j^{(2)}}{\partial z_j^{(2)}} = \left(\mathcal{W}_{j\cdot}{}^{(3)T} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(3)}} \right) \frac{\partial h_j^{(2)}}{\partial z_j^{(2)}}$$

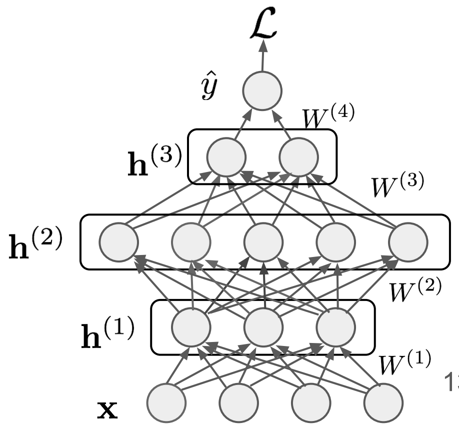
$$\frac{\partial \mathbf{h}^{(2)}}{\partial \mathbf{z}^{(2)}} = \begin{bmatrix} \frac{\partial h_1^{(2)}}{\partial z_1^{(2)}} 0 & \cdots & 0 \\ \vdots & \frac{\partial h_j^{(2)}}{\partial z_j^{(2)}} & \vdots \\ 0 & \cdots & \frac{\partial h_{H_2}^{(2)}}{\partial z_{H_2}^{(2)}} \end{bmatrix} = \operatorname{diag}\left\{ \begin{bmatrix} \frac{\partial h_1^{(2)}}{\partial z_1^{(2)}} \\ \vdots \\ \frac{\partial h_{H_2}^{(2)}}{\partial z_{H_2}^{(2)}} \end{bmatrix} \right\}$$

  - Here, $\mathcal{W}_{j\cdot}^{(3)}$ is the *j*th column of the weight matrix $W^{(3)}$

$$\frac{\partial \mathcal{L}}{\partial z_j^{(2)}} = \left(\sum_i \frac{\partial \mathcal{L}}{\partial z_i^{(3)}} w_{ji}^{(3)} \right) \frac{\partial h_j^{(2)}}{\partial z_j^{(2)}} = \left(\mathcal{W}_{j\cdot}^{(3)T} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(3)}} \right) \frac{\partial h_j^{(2)}}{\partial z_j^{(2)}}$$

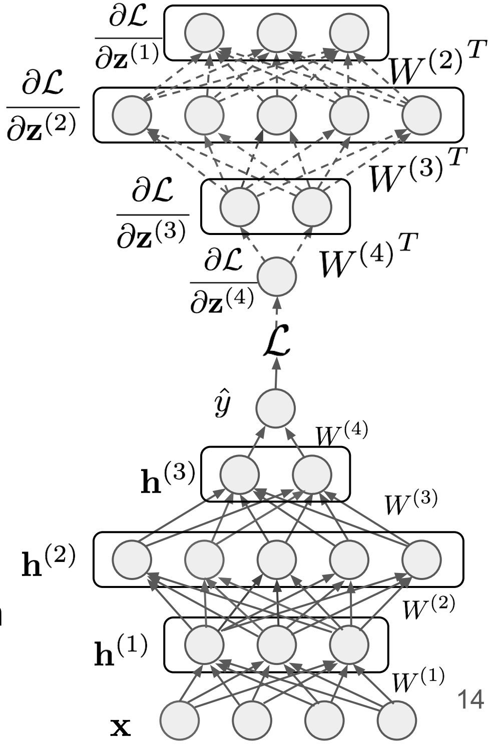
  - Use a matrix vector product to express the partial derivatives of *z* for the second hidden layer:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(2)}} = \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial z_1^{(2)}} \\ \vdots \\ \frac{\partial \mathcal{L}}{\partial z_{H_2}^{(2)}} \end{bmatrix} = \frac{\partial \mathbf{h}^{(2)}}{\partial \mathbf{z}^{(2)}} \left(\begin{bmatrix} \mathcal{W}_{1\cdot}^{(3)T} \\ \vdots \\ \mathcal{W}_{H_2\cdot}^{(3)T} \end{bmatrix} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(3)}} \right) = \frac{\partial \mathbf{h}^{(2)}}{\partial \mathbf{z}^{(2)}} \left(W^{(3)T} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(3)}} \right)$$



Learning fully connected multi-layer neural networks

- For a single training data, computing the gradient w.r.t. the weight matrices is also a recursive procedure:
  - Remember: $\mathbf{z}^{(4)} = W^{(4)}\mathbf{h}^{(3)} + b^{(4)}, \quad \hat{y} = f\left(\mathbf{z}^{(4)}\right)$
  - Back-propagation is similar to running the neural network backwards using the transpose of the weight matrices



$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(1)}}$
$W^{(2)^T}$
$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(2)}}$
$W^{(3)^T}$
$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(3)}}$
$W^{(4)^T}$
$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(4)}}$
$\mathcal{L}$
$\hat{y}$
$W^{(4)}$
$\mathbf{h}^{(3)}$
$W^{(3)}$
$\mathbf{h}^{(2)}$
$W^{(2)}$
$\mathbf{h}^{(1)}$
$W^{(1)}$
$\mathbf{x}$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(4)}} = \frac{\partial \hat{y}}{\partial \mathbf{z}^{(4)}} \frac{\partial \mathcal{L}}{\partial \hat{y}}, \qquad \frac{\partial \mathcal{L}}{\partial W^{(4)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(4)}} \mathbf{h}^{(3)^T}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(3)}} = \frac{\partial \mathbf{h}^{(3)}}{\partial \mathbf{z}^{(3)}} \left(W^{(4)^T} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(4)}} \right), \qquad \frac{\partial \mathcal{L}}{\partial W^{(3)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(3)}} \mathbf{h}^{(2)^T}$$

back-propagation

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(2)}} = \frac{\partial \mathbf{h}^{(2)}}{\partial \mathbf{z}^{(2)}} \left(W^{(3)^T} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(3)}} \right), \qquad \frac{\partial \mathcal{L}}{\partial W^{(2)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(2)}} \mathbf{h}^{(1)^T}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(1)}} = \frac{\partial \mathbf{h}^{(1)}}{\partial \mathbf{z}^{(1)}} \left(W^{(2)^T} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(2)}} \right), \qquad \frac{\partial \mathcal{L}}{\partial W^{(1)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{(1)}} \mathbf{x}^T$$

What about the expression for the bias units?

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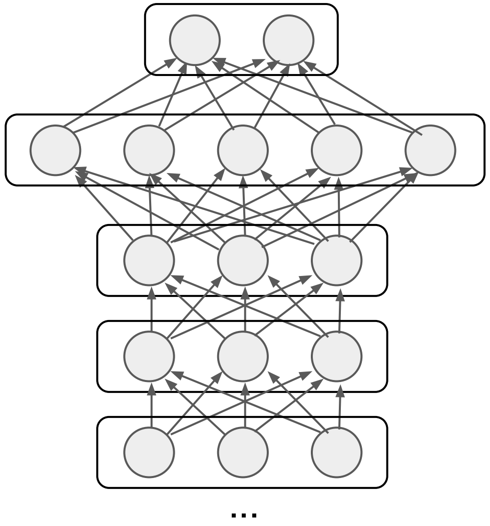
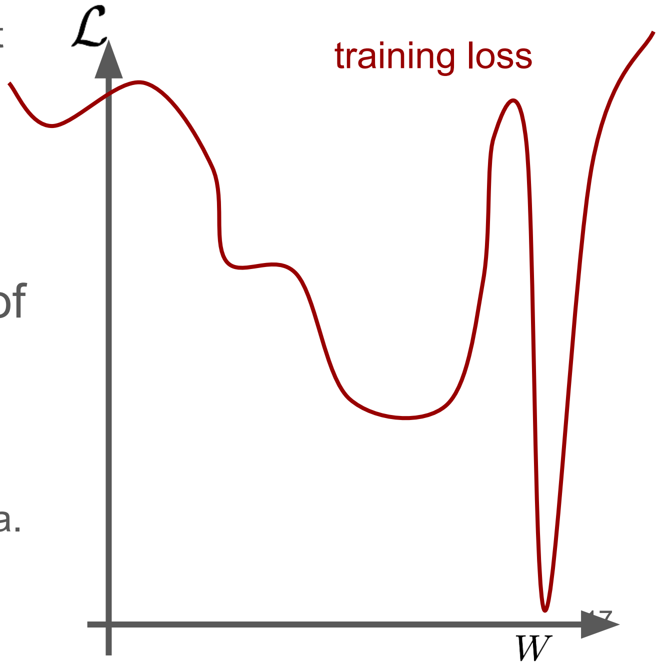
Hyper-parameters

- At the beginning, there were the choices:
  - How many hidden units to use in each hidden layer?
  - How many layers in total?
  - Which hidden activation function?
- Good answer: decide these hyper-parameters using validation set.
- Best practical answer:
  - Around 500-2000 hidden units
  - 2-3 layers
  - Choosing ReLU often leads to fast convergence



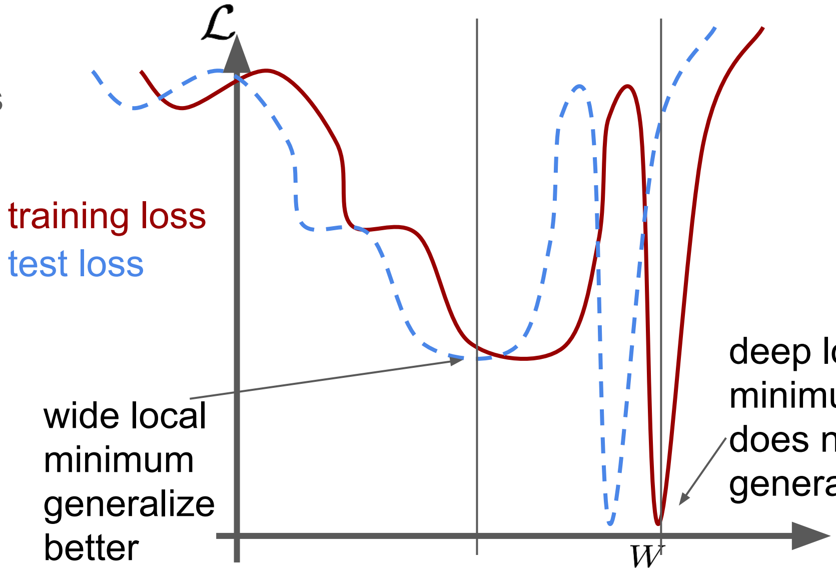
Parameter initialization

- The loss functions for neural networks w.r.t. the weight matrices in general are non-convex.
    - Different weight initialization schemes can lead to significant differences in final performance.
    - Use random initialization (e.g. Gaussian with std. 0.01) and avoid constant initialization
- Non-convex optimization is not a crazy idea. Most of the local minima in a neural network loss function are not bad.
    - As long as the model has enough capacity to model the data.
    - Stochastic gradient descent can usually find local minima that are “good”.



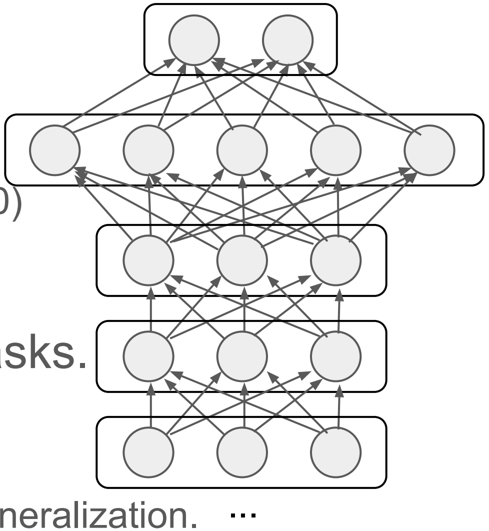
Some local optima generalize better than others

- Between the two neural networks that both get very low training loss during learning, we prefer the model that learns the underlying statistical patterns of the data and can generalize to unseen examples during test time.
    - The test loss function and the training loss are almost always slightly different.
    - Wide shallow basins can typically generalize better than deep narrow local minima.
    - The subsampling noise from SGD helps to find shallow basins.


$\mathcal{L}$
training loss
test loss
wide local minimum generalize better
deep local minimum does not generalize
W

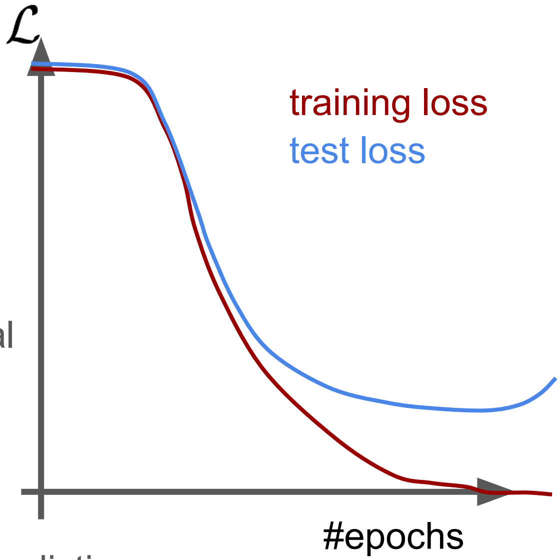
Careful initialization

- For really deep neural networks (> 5 layers), random initialization from a constant-variance Gaussian noise will not work well. The back-propagated partial derivatives will likely be too small to learn anything useful.
    - Simple fix: initialize the weight matrices to identity matrices if you can. (Le, Jaitly and Hinton, 2015)
    - More elaborate fix: adapt the std. of the zero-mean Gaussian initialization to be 1/sqrt{#inputs x #outputs} aka *Xavier initialization* (Xavier Glorot and Yoshua Bengio, 2010)
- Oftentimes it is beneficial to initialize the weights from another model that was "pre-trained" on some other tasks.
    - Initialize the model from an auto-encoder or ImageNet models.
    - Weight matrices in the early layers are transferable and help generalization.



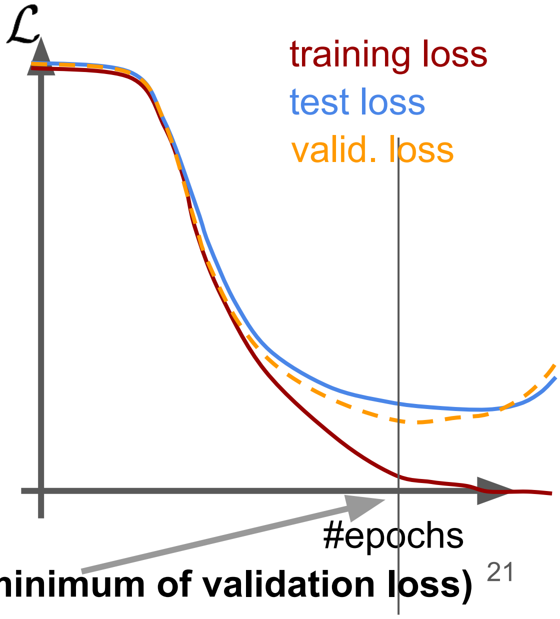
Regularize the capacity of deep neural networks

- Given enough hidden units, neural networks can overfit to any arbitrary training dataset. Regularizing a neural network is equivalent to restricting its capacity.
    - Reducing the number of hidden units to limit the model capacity has a sound statistical justification: you need more training examples than the number of weights to have enough *statistical power* when estimating the unknown model parameter.
    - Alternatively, one can have an over-parameterized model and deal with overfitting through a very strong regularizer such that most of the weights are close to zero, e.g. using weight decay.
    - In deep learning applications, strong-regularizer approaches often work much better. A good heuristic is to prefer a globally simple prediction function with some irregular local behaviour.



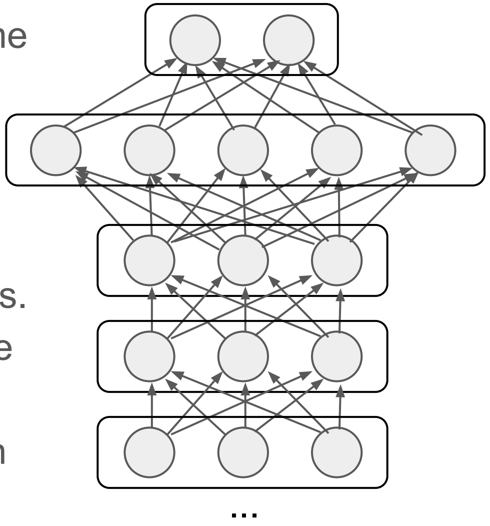
Early stopping

- A very simple trick to ensure that most of the weights are as close to zero as possible involves monitoring the *validation loss.* You stop learning at the minimum of the validation loss curve (aka “early stopping”) before attaining the minimum training loss.
    - The goal of machine learning is to generalize well on test data instead of finding the minimum training loss.
    - The weights are typically initialized around zero. “Early stopping” terminates the learning process prematurely before the weights grow too large and thus limit the capacity of the model.
    - It is by far the most commonly used regularization technique.



Dropout

- Another simple trick to effectively regularize deep NNs is to remove hidden units randomly during training. Dropout prevents “co-adaptation” of the hidden units and encourage independence among the neurons.
    - Dropout can be understood as stochastic training on all the permutations of neural network architectures that share the same weight matrices.
    - Efficiently shares the statistical power among an ensemble of neural networks.
    - During test time, the “mean” network is used to make predictions. If each hidden unit is dropped out 50% of the time in training, we need to compensate during test time by *reducing* the weight matrix by a factor of 2, such that the expected activation of each hidden unit stays the same for both training and testing.



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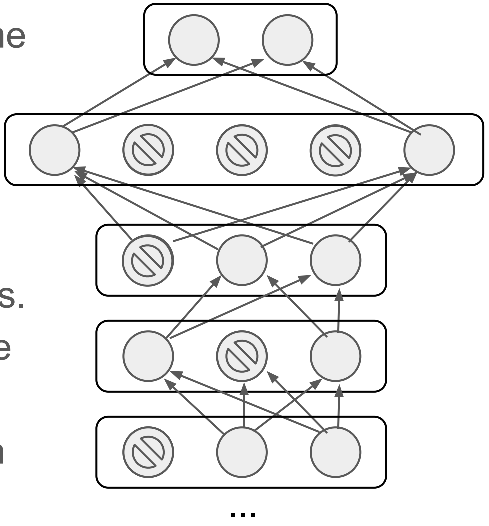

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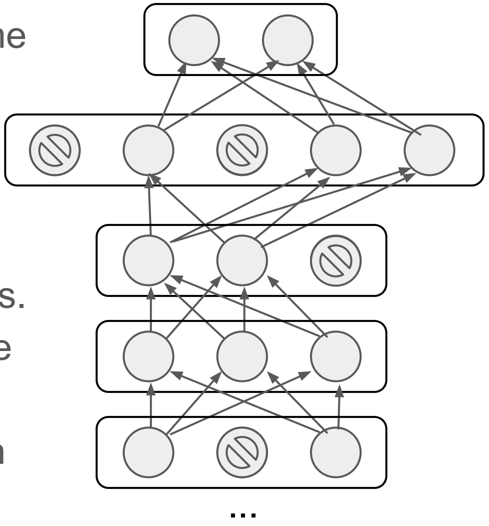

Dataset normalization

- Learning can often be made easier by pre-processing the training dataset before performing any training.
  - The simplest normalization scheme is to centre the input $\mathbf{x}$ and remove its variance for each input dimension. It fixes the scaling discrepancy among the input dimensions (e.g. removes the units of measurement).
  - For each of the *N* input dimensions, estimate its mean and variance from the training data and transform the *m*th training example by:

$$\bar{x}_n^{(m)} = (x_n^{(m)} - \mu_n)/\sigma_n$$

$$\mu_n = \frac{1}{M}\sum_{m=1}^{M} x_n^{(m)} \qquad \sigma_n = \sqrt{\frac{1}{M-1}\sum_{m=1}^{M}(x_n^{(m)} - \mu_n)^2}$$

  - We can further remove the covariance among the input dimensions, i.e. whitening the data using Principal Component Analysis (PCA): next lecture