CSCI567 Machine Learning (Spring 2021)

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University of Southern California

Feb 12, 2021

Outline

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Logistics

- Sign-up with your group members for the project!

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Linear Discriminant Analysis

The main bottleneck is *not knowing* $\mathcal{P}(X = \boldsymbol{x}|y = c)$

$$\mathcal{P}(y = c|X = \boldsymbol{x}) = \frac{\mathcal{P}(X = \boldsymbol{x}|y = c)\mathcal{P}(y = c)}{\mathcal{P}(X = \boldsymbol{x})}.$$

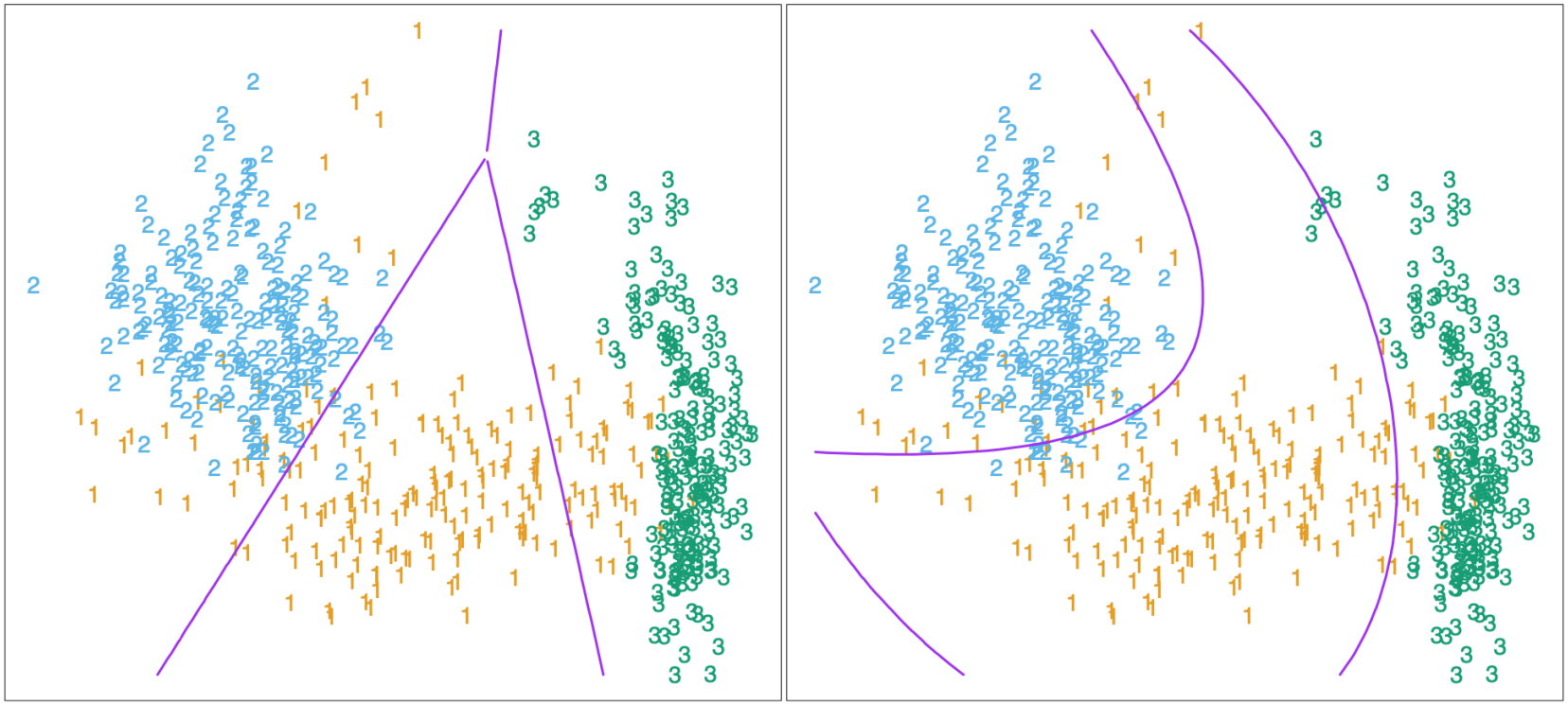
LDA makes two simplifying assumptions:

- Let $\mathcal{P}(X = \boldsymbol{x}|y = c) \sim \mathcal{N}(\boldsymbol{\mu}_c, \Sigma_c)$, and
- Let all class covariances be the same i.e. $\Sigma_c = \Sigma$ for all $c \in [C]$

If so, the decision boundary (for binary classification) is given by

$$\mathcal{P}(y = 0|X = \boldsymbol{x}) = \mathcal{P}(y = 1|X = \boldsymbol{x})$$
$$\mathcal{P}(X = \boldsymbol{x}|y = 0)\mathcal{P}(y = 0) = \mathcal{P}(X = \boldsymbol{x}|y = 1)\mathcal{P}(y = 1)$$

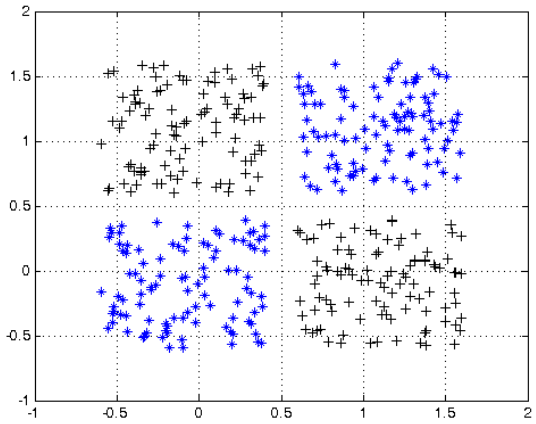
What do the decision boundaries look like?

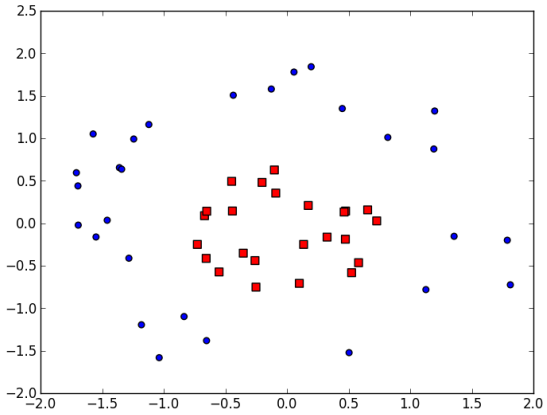


The decision boundaries are a quadratic when Σ's are not the same, this is known as *Quadratic Discriminant Analysis*!

Outline

Linear models are not always adequate





We can use a nonlinear mapping as discussed:

$$\boldsymbol{\phi}(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^{\mathsf{D}} \rightarrow \boldsymbol{z} \in \mathbb{R}^{\mathsf{M}}$$

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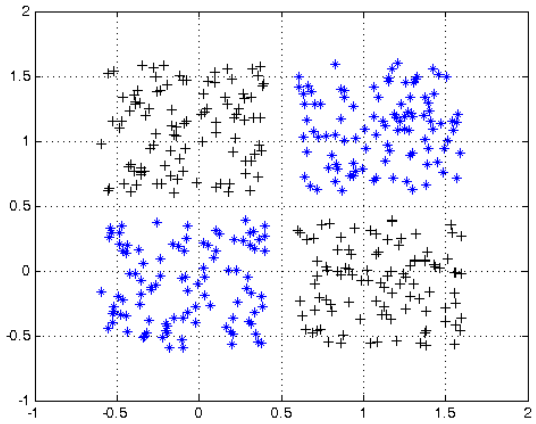

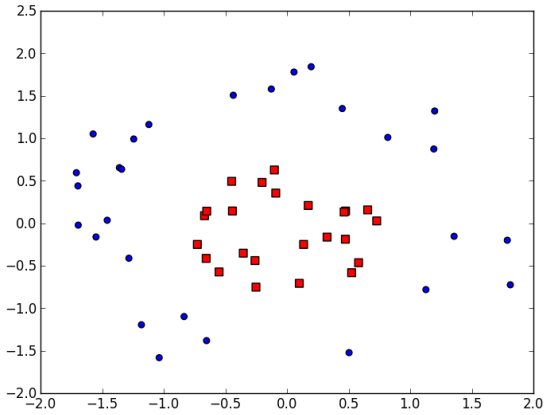

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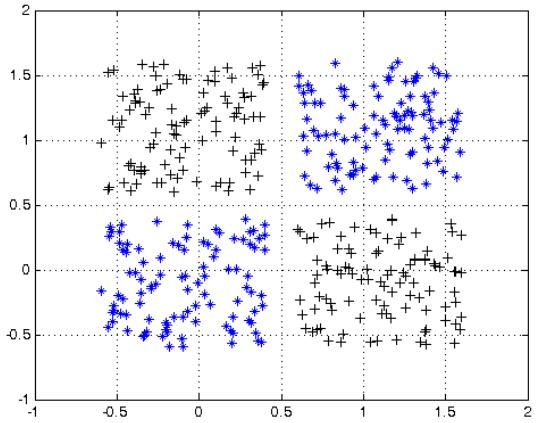

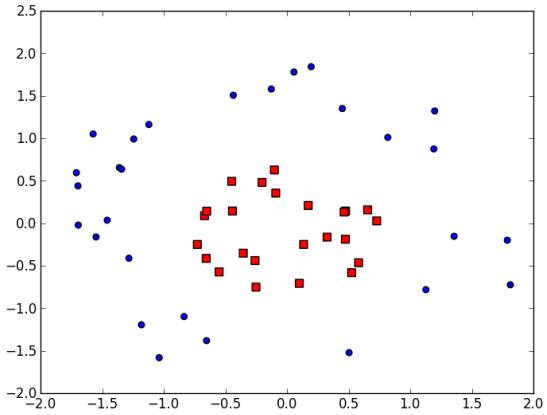

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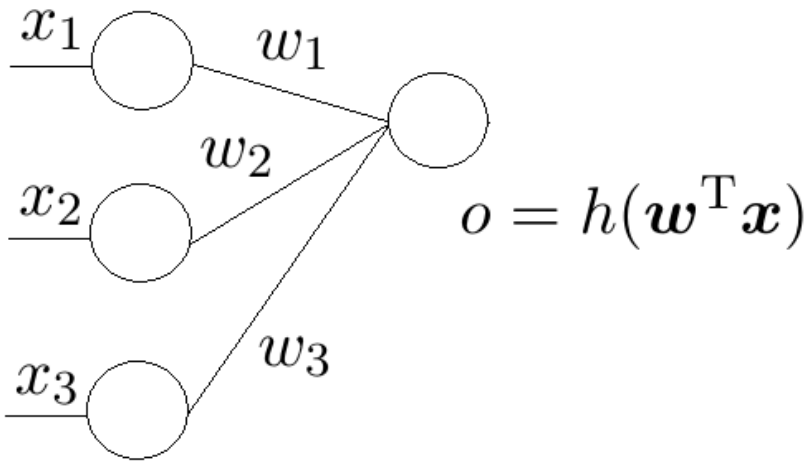
THE most popular nonlinear models nowadays: **neural nets**

Linear model as a one-layer neural net



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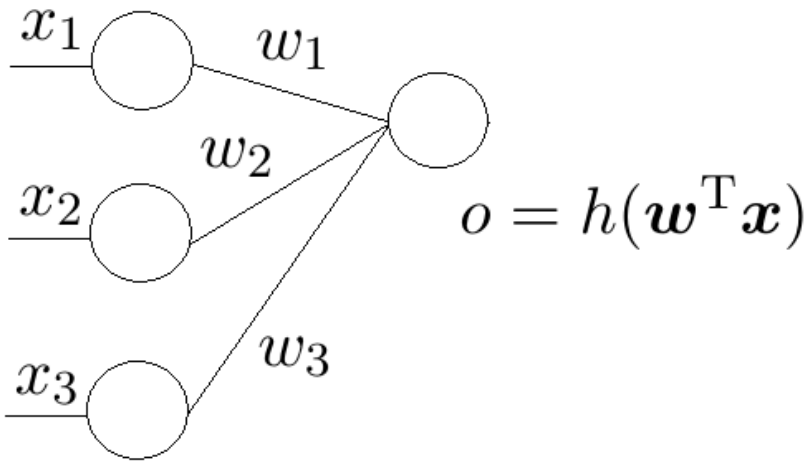

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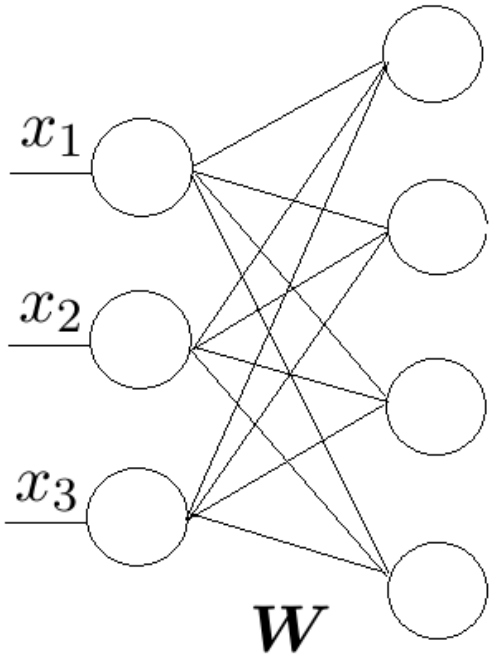
To create non-linearity, can use

- Rectified Linear Unit (**ReLU**): $h(a) = \max\{0, a\}$
- sigmoid function: $h(a) = \frac{1}{1+e^{-a}}$
- TanH: $h(a) = \frac{e^{a}-e^{-a}}{e^{a}+e^{-a}}$
- many more

More output nodes



$$\boldsymbol{o} = \boldsymbol{h}(\boldsymbol{W}\boldsymbol{x})$$

$\boldsymbol{W} \in \mathbb{R}^{4\times 3}$, $\boldsymbol{h} : \mathbb{R}^4 \to \mathbb{R}^4$ so $\boldsymbol{h}(\boldsymbol{a}) = (h_1(a_1), h_2(a_2), h_3(a_3), h_4(a_4))$

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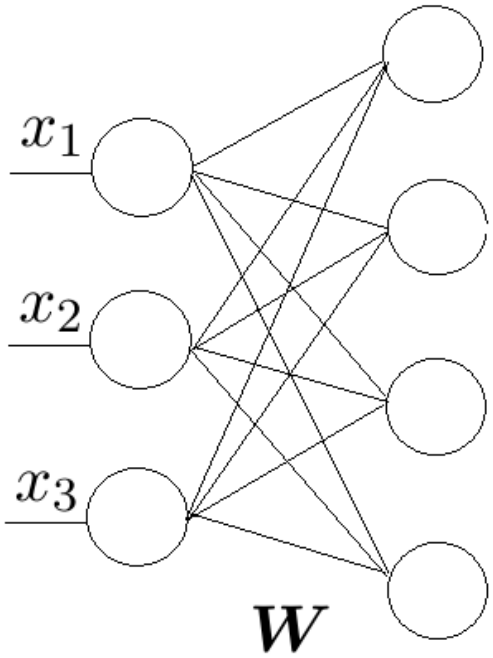

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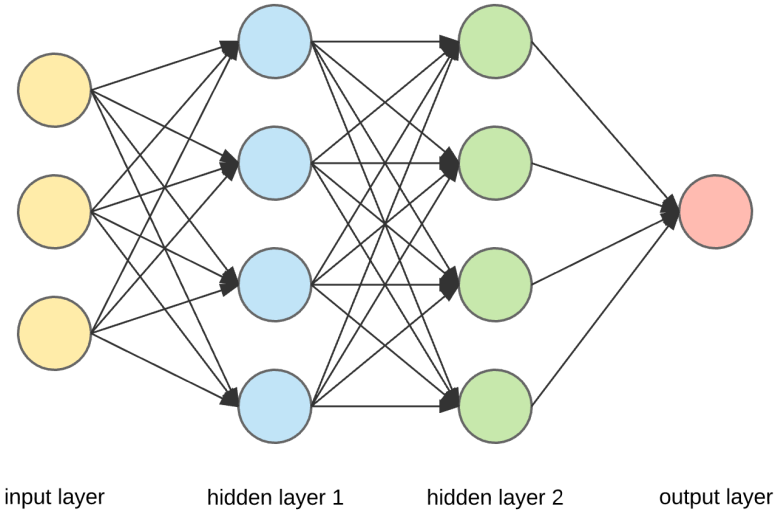
Can think of this as a nonlinear basis: $\boldsymbol{\Phi}(\boldsymbol{x}) = \boldsymbol{h}(\boldsymbol{W}\boldsymbol{x})$

More layers

Becomes a network:



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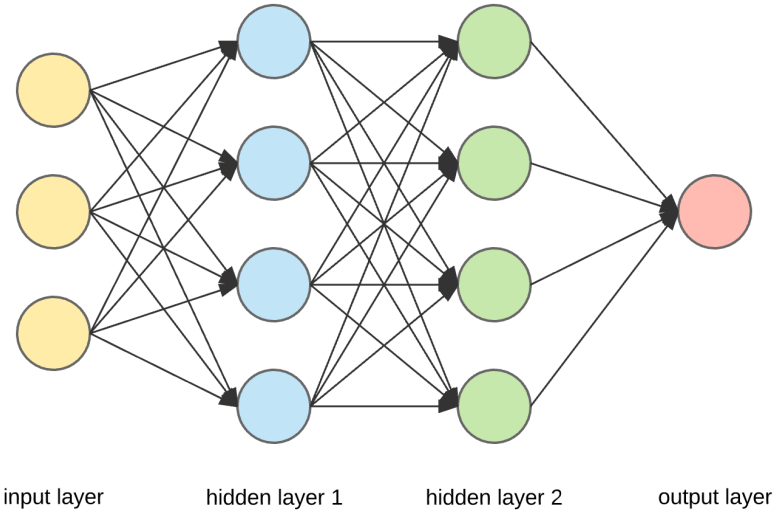

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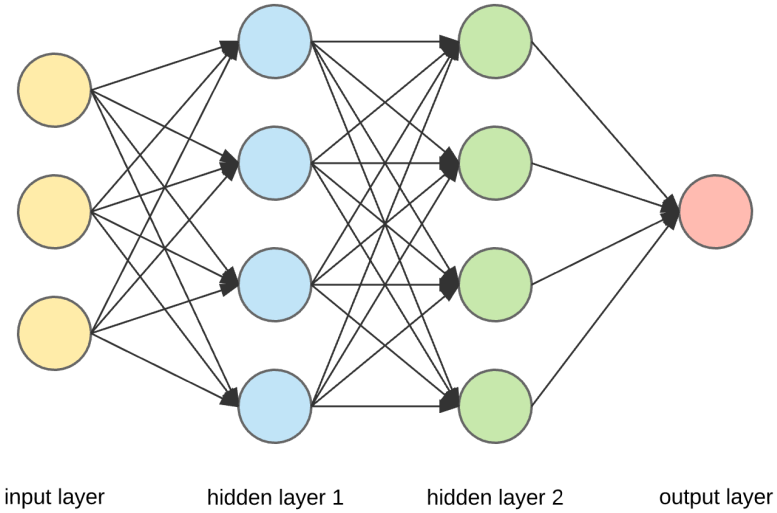

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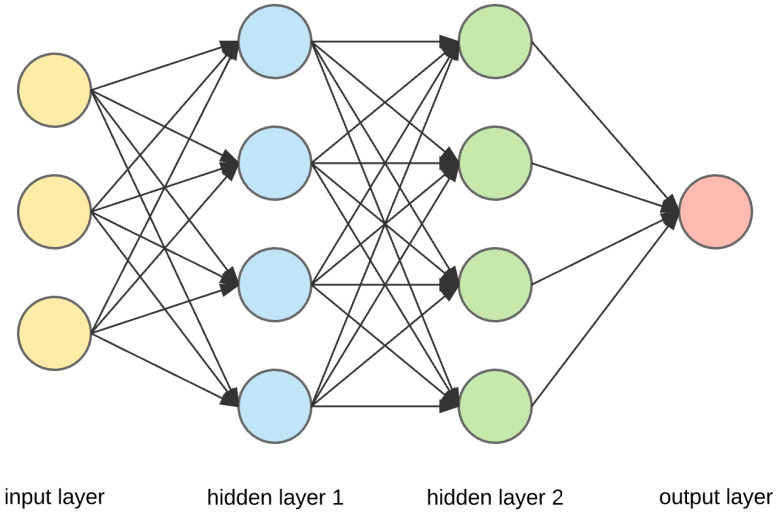

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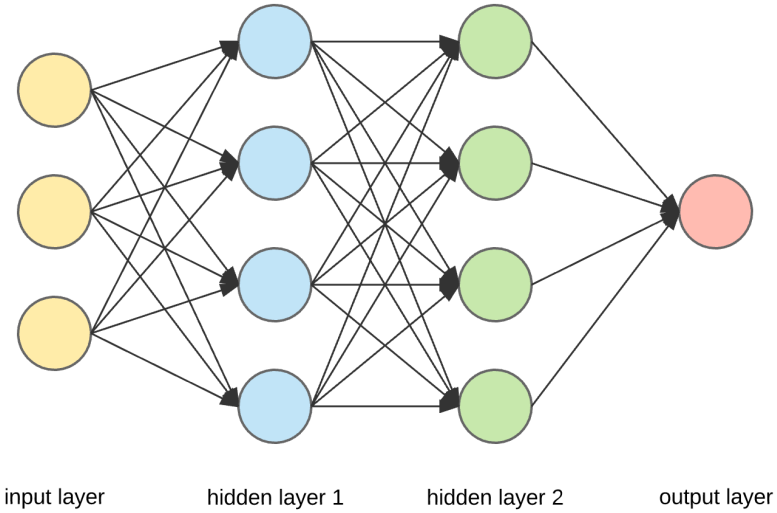

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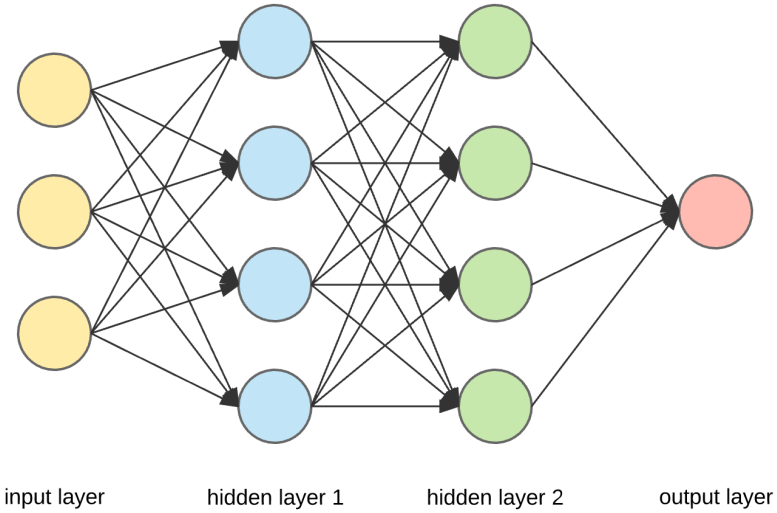

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- **deep** neural nets can have many layers and *millions* of parameters
- this is a **feedforward, fully connected** neural net, there are many variants

How powerful are neural nets?

Universal approximation theorem (Cybenko, 89; Hornik, 91):

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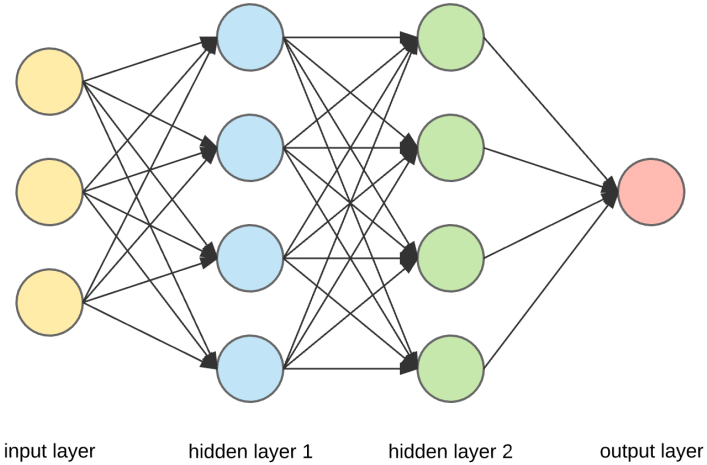
Designing network architecture is important and very complicated

- for feedforward network, need to decide number of hidden layers, number of neurons at each layer, activation functions, etc.

Math formulation

An L-layer neural net can be written as

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{h}_{\mathsf{L}}\left(\boldsymbol{W}_L \boldsymbol{h}_{\mathsf{L}-1}\left(\boldsymbol{W}_{L-1} \cdots \boldsymbol{h}_1\left(\boldsymbol{W}_1 \boldsymbol{x}\right)\right)\right)$$



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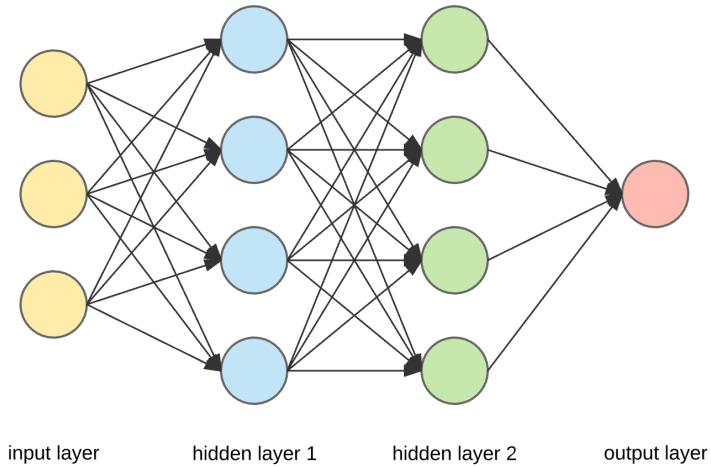

To ease notation, for a given input $\boldsymbol{x}$, define recursively

$$\boldsymbol{o}_0 = \boldsymbol{x}, \qquad \boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}, \qquad \boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell) \qquad (\ell = 1, \ldots, \mathsf{L})$$

where

- $\boldsymbol{W}_\ell \in \mathbb{R}^{\mathsf{D}_\ell \times \mathsf{D}_{\ell-1}}$ is the weights between layer $\ell - 1$ and ℓ
- $\mathsf{D}_0 = \mathsf{D}, \mathsf{D}_1, \ldots, \mathsf{D}_{\mathsf{L}}$ are numbers of neurons at each layer
- $\boldsymbol{a}_\ell \in \mathbb{R}^{\mathsf{D}_\ell}$ is input to layer ℓ
- $\boldsymbol{o}_\ell \in \mathbb{R}^{\mathsf{D}_\ell}$ is output to layer ℓ
- $\boldsymbol{h}_\ell : \mathbb{R}^{\mathsf{D}_\ell} \to \mathbb{R}^{\mathsf{D}_\ell}$ is activation functions at layer ℓ

Learning the model

No matter how complicated the model is, our goal is the same: minimize

$$\mathcal{E}(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_{\mathsf{L}}) = \frac{1}{N} \sum_{n=1}^{\mathsf{N}} \mathcal{E}_n(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_{\mathsf{L}})$$

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where

$$\mathcal{E}_n(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L}) = \begin{cases} \|\boldsymbol{f}(\boldsymbol{x}_n) - \boldsymbol{y}_n\|_2^2 & \text{for regression} \\ \ln\left(1 + \sum_{k \neq y_n} e^{f(\boldsymbol{x}_n)_k - f(\boldsymbol{x}_n)_{y_n}}\right) & \text{for classification} \end{cases}$$

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- for a composite function $f(g(w))$

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- for a composite function $f(g_1(w), \ldots, g_d(w))$

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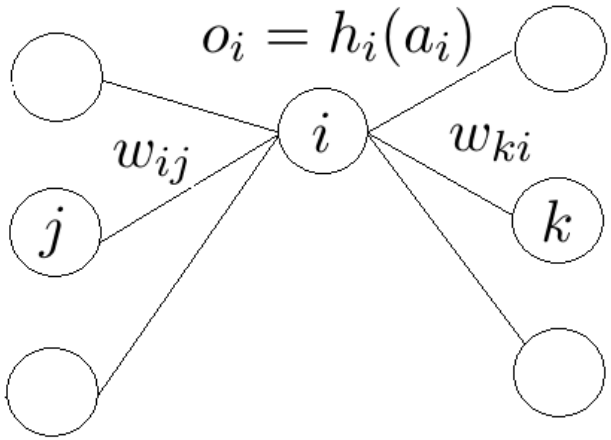
the simplest example $f(g_1(w), g_2(w)) = g_1(w)g_2(w)$

Computing the derivative

Drop the subscript ℓ for layer for simplicity.

Find the **derivative of $\mathcal{E}_n$ w.r.t. to w_{ij}**



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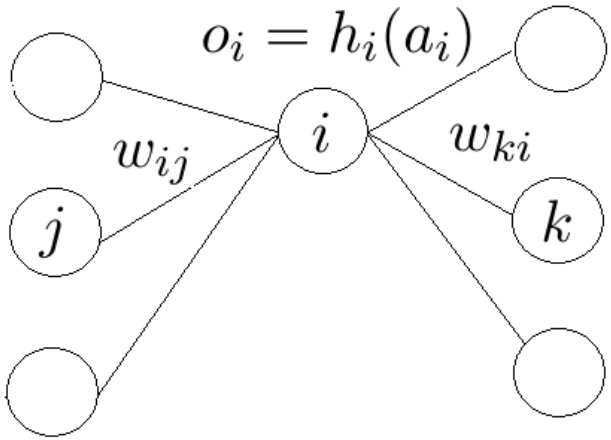

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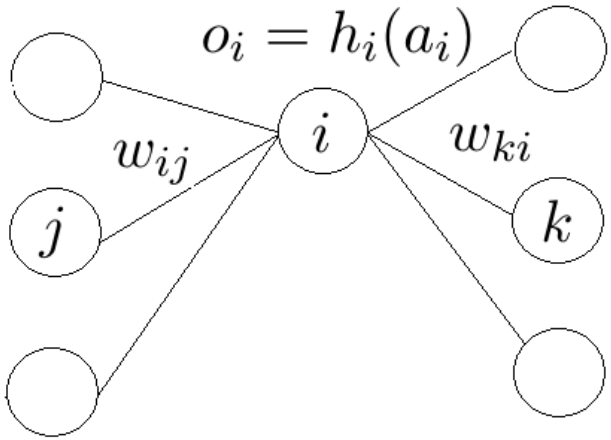

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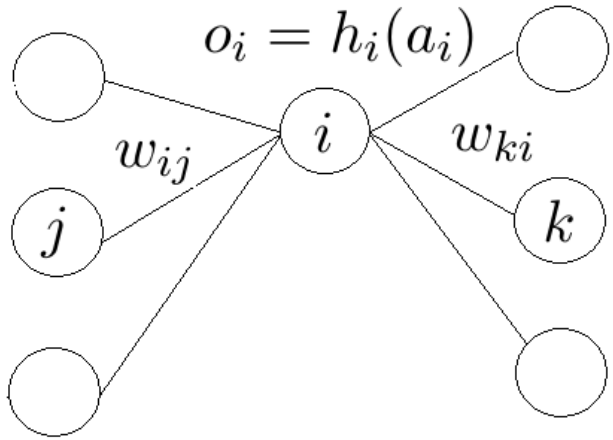

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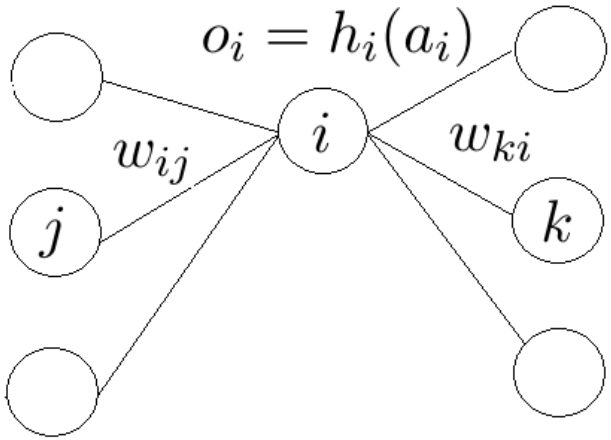

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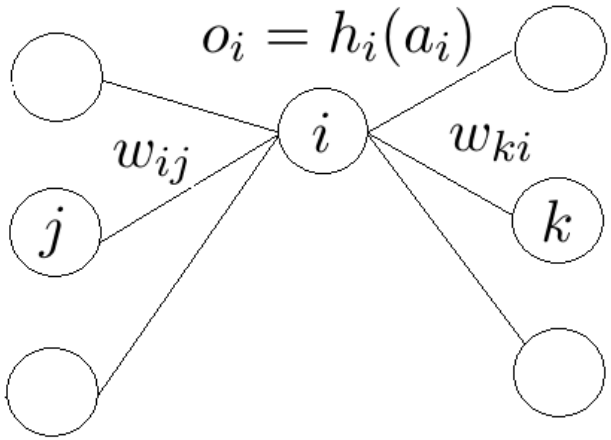

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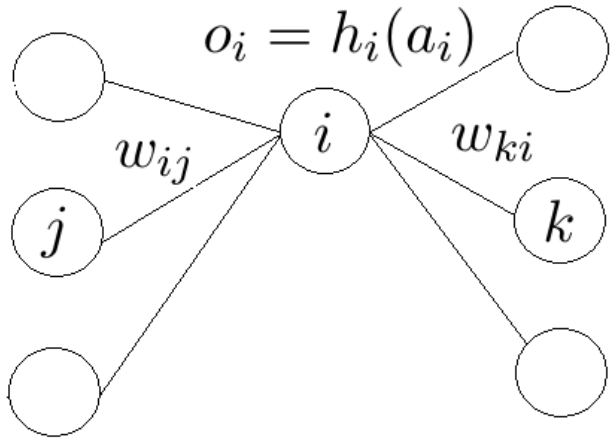

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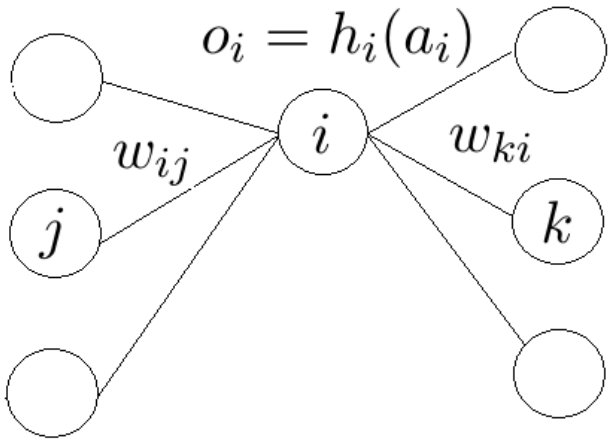
Computing the derivative

Adding the subscript for layer:

$$\frac{\partial \mathcal{E}_n}{\partial w_{\ell,ij}} = \frac{\partial \mathcal{E}_n}{\partial a_{\ell,i}} o_{\ell-1,j}$$

$$\frac{\partial \mathcal{E}_n}{\partial a_{\ell,i}} = \left(\sum_k \frac{\partial \mathcal{E}_n}{\partial a_{\ell+1,k}} w_{\ell+1,ki} \right) h'_{\ell,i}(a_{\ell,i})$$



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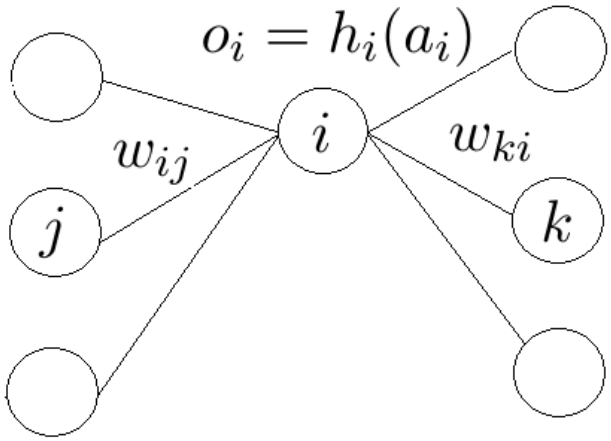


For the last layer, for square loss

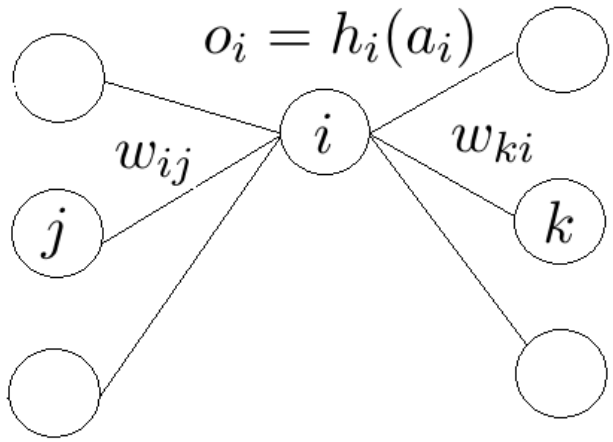
$$\frac{\partial \mathcal{E}_n}{\partial a_{\mathsf{L},i}} = \frac{\partial (h_{\mathsf{L},i}(a_{\mathsf{L},i}) - y_{n,i})^2}{\partial a_{\mathsf{L},i}}$$

Computing the derivative

Adding the subscript for layer:

$$\frac{\partial \mathcal{E}_n}{\partial w_{\ell,ij}} = \frac{\partial \mathcal{E}_n}{\partial a_{\ell,i}} o_{\ell-1,j}$$

$$\frac{\partial \mathcal{E}_n}{\partial a_{\ell,i}} = \left(\sum_k \frac{\partial \mathcal{E}_n}{\partial a_{\ell+1,k}} w_{\ell+1,ki} \right) h'_{\ell,i}(a_{\ell,i})$$



For the last layer, for square loss

$$\frac{\partial \mathcal{E}_n}{\partial a_{\mathsf{L},i}} = \frac{\partial (h_{\mathsf{L},i}(a_{\mathsf{L},i}) - y_{n,i})^2}{\partial a_{\mathsf{L},i}} = 2(h_{\mathsf{L},i}(a_{\mathsf{L},i}) - y_{n,i}) h'_{\mathsf{L},i}(a_{\mathsf{L},i})$$

Computing the derivative

Using **matrix notation** greatly simplifies presentation and implementation:

$$\frac{\partial \mathcal{E}_n}{\partial \boldsymbol{W}_\ell} = \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{a}_\ell} \boldsymbol{o}_{\ell-1}^{\mathrm{T}}$$

$$\frac{\partial \mathcal{E}_n}{\partial \boldsymbol{a}_\ell} = \begin{cases} \left(\boldsymbol{W}_{\ell+1}^{\mathrm{T}} \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{a}_{\ell+1}} \right) \circ \boldsymbol{h}'_\ell(\boldsymbol{a}_\ell) & \text{if } \ell < \mathsf{L} \\ 2(\boldsymbol{h}_\mathsf{L}(\boldsymbol{a}_\mathsf{L}) - \boldsymbol{y}_n) \circ \boldsymbol{h}'_\mathsf{L}(\boldsymbol{a}_\mathsf{L}) & \text{else} \end{cases}$$

where $\boldsymbol{v}_1 \circ \boldsymbol{v}_2 = (v_{11}v_{21}, \cdots, v_{1\mathsf{D}}v_{2\mathsf{D}})$ is the element-wise product (a.k.a. Hadamard product).

Verify yourself!

Putting everything into SGD

The **backpropagation** algorithm (**Backprop**)

Initialize $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_{\mathsf{L}}$. Repeat:

1. randomly pick one data point $n \in [\mathsf{N}]$

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   - update weights

$$\boldsymbol{W}_\ell \leftarrow \boldsymbol{W}_\ell - \eta \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{W}_\ell} = \boldsymbol{W}_\ell - \eta \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{a}_\ell} \boldsymbol{o}_{\ell-1}^{\mathrm{T}}$$

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Think about how to do the last two steps properly!

More tricks to optimize neural nets

Many variants based on backprop

- SGD with **minibatch**: randomly sample a batch of examples to form a stochastic gradient
- SGD with **momentum**
- ...

SGD with momentum

Initialize $\boldsymbol{w}_0$ and **velocity** $\boldsymbol{v} = \mathbf{0}$

For $t = 1, 2, \ldots$

- form a stochastic gradient $\boldsymbol{g}_t$
- update velocity $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \eta \boldsymbol{g}_t$ for some discount factor $\alpha \in (0, 1)$
- update weight $\boldsymbol{w}_t \leftarrow \boldsymbol{w}_{t-1} + \boldsymbol{v}$

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Updates for first few rounds:

- $\boldsymbol{w}_1 = \boldsymbol{w}_0 - \eta \boldsymbol{g}_1$
- $\boldsymbol{w}_2 = \boldsymbol{w}_1 - \alpha\eta \boldsymbol{g}_1 - \eta \boldsymbol{g}_2$
- $\boldsymbol{w}_3 = \boldsymbol{w}_2 - \alpha^2\eta \boldsymbol{g}_1 - \alpha\eta \boldsymbol{g}_2 - \eta \boldsymbol{g}_3$
- $\ldots$

Overfitting

Overfitting is very likely since the models are too powerful.

Methods to overcome overfitting:

- data augmentation
- regularization
- dropout
- early stopping
- ...

Data augmentation

Data: the more the better. How do we get more data?

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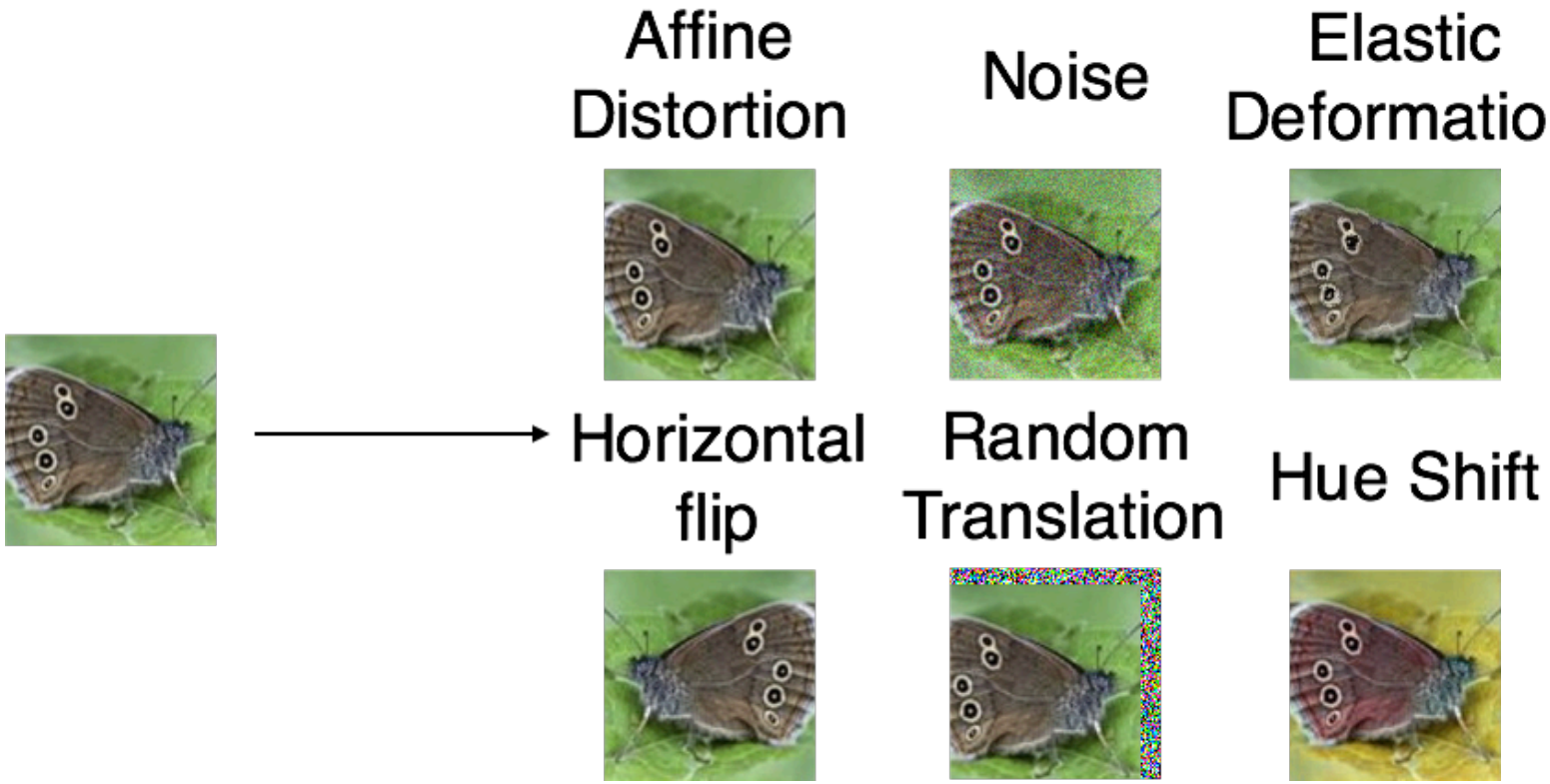
Exploit prior knowledge to add more training data



Regularization

L2 regularization: minimize

$$\mathcal{E}'(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_{\mathsf{L}}) = \mathcal{E}(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_{\mathsf{L}}) + \lambda \sum_{\ell=1}^{\mathsf{L}} \|\boldsymbol{W}_\ell\|_2^2$$

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$$\frac{\partial \mathcal{E}'}{\partial w_{ij}} = \frac{\partial \mathcal{E}}{\partial w_{ij}} + 2\lambda w_{ij}$$

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Simple change to the gradient:

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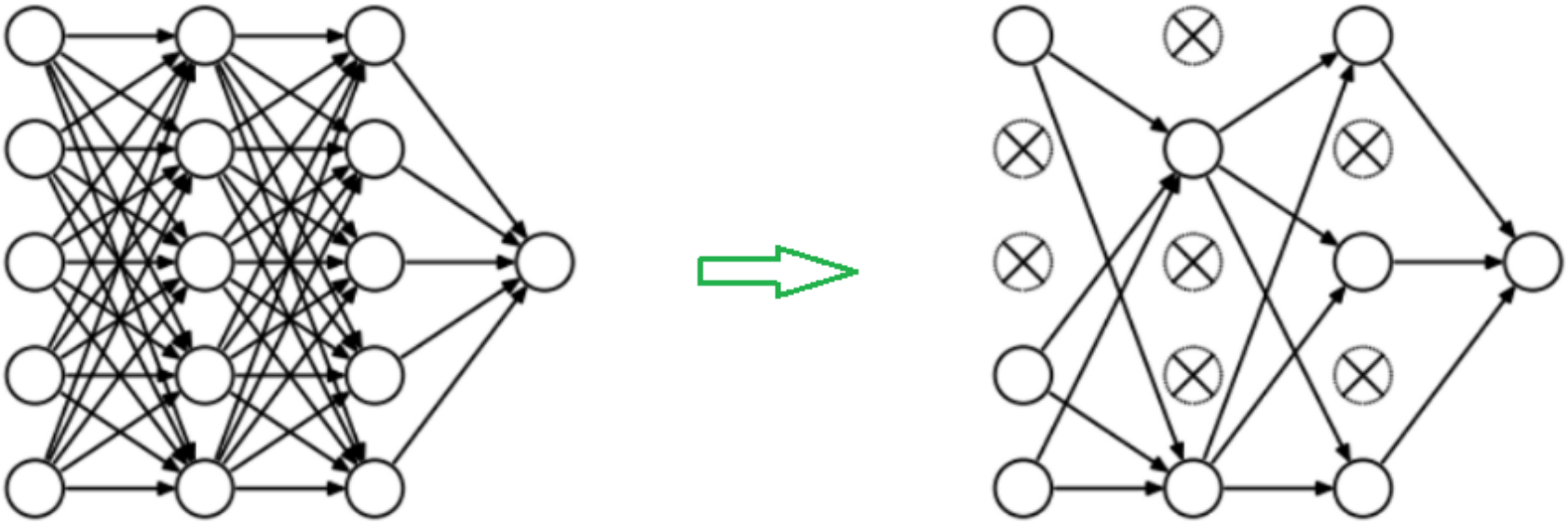
Introduce *weight decaying effect*

Dropout

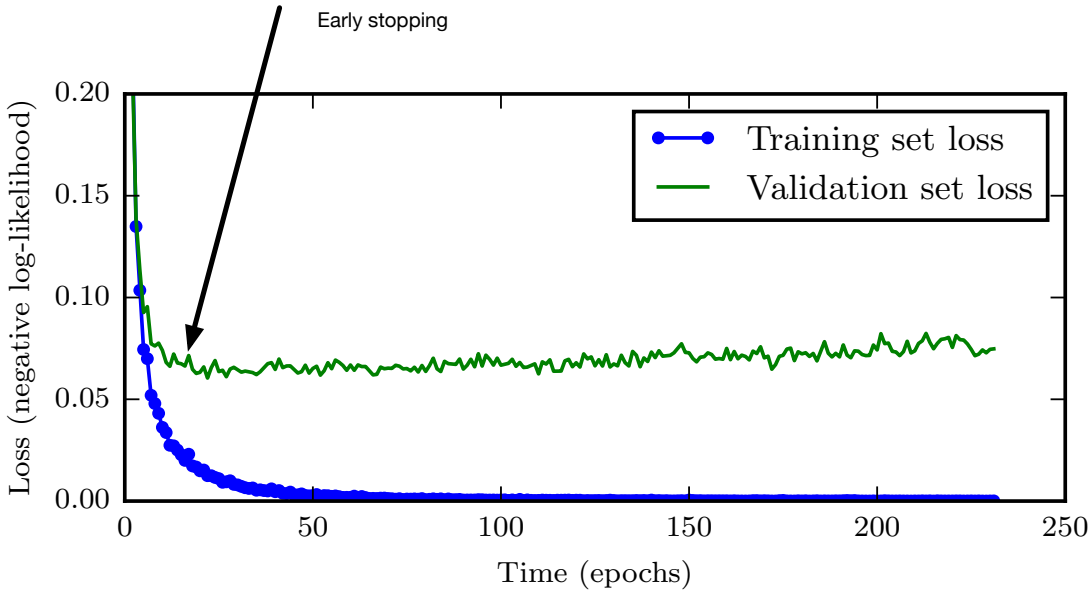
Randomly delete neurons during training



Very effective, makes training faster as well

Early stopping

Stop training when the performance on validation set stops improving



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- do need *a lot of data* to work well
- take *a lot of time* to train (need GPUs for massive parallel computing)
- take some work to select architecture and hyperparameters
- are still not well understood in theory