Intro to Deep Neural Networks: Multi-layer Perceptrons

CS771: Introduction to Machine Learning

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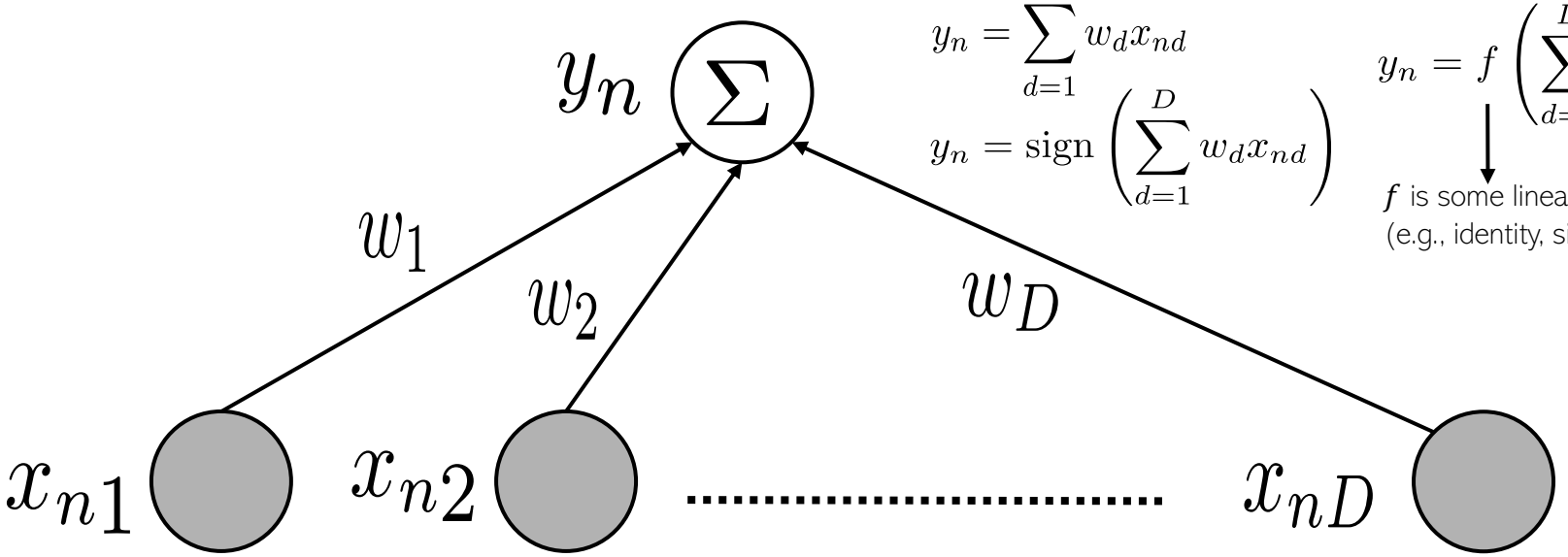
Limitation of Linear Models

- Linear models: Output produced by taking a linear combination of input features



$$y_n = \sum_{d=1}^{D} w_d x_{nd}$$

$$y_n = \text{sign}\left(\sum_{d=1}^{D} w_d x_{nd}\right)$$

$$y_n = f\left(\sum_{d=1}^{D} w_d x_{nd}\right)$$

f is some linear/nonlinear function (e.g., identity, sign, or sigmoid)

Linear regression, logistic regression, SVM, etc

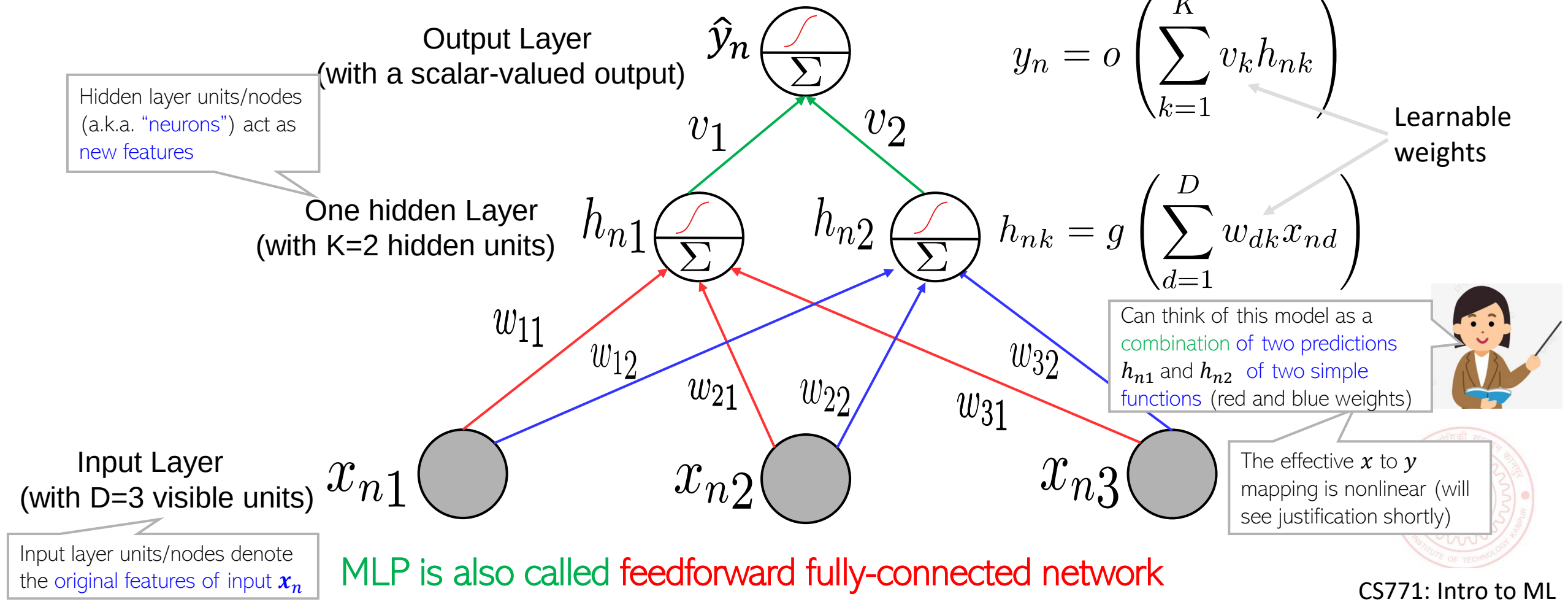
- A basic unit of the form $\boldsymbol{y = f(w^\top x)}$ is known as the "Perceptron" (not to be confused with the Perceptron "algorithm", which learns a linear classification model)

- This can't however learn nonlinear functions or nonlinear decision boundaries

Although can kernelize to make them nonlinear

Neural Networks: Multi-layer Perceptron (MLP)

- An MLP is a network containing several Perceptron units across many layers
- An MLP consists of an input layer, an output layer, and one or more hidden layers



MLP is also called feedforward fully-connected network

Illustration: Neural Net with Single Hidden Layer

- Compute K pre-activations for each input $\boldsymbol{x}_n$

A linear model with learnable weight vec $\boldsymbol{w}_k$

$$z_{nk} = \boldsymbol{w}_k^\top \boldsymbol{x}_n = \sum_{d=1}^{D} w_{dk} x_{nd} \quad (k = 1,2,\dots,K)$$

- Apply nonlinear activation on each pre-act

Called a hidden unit

$$h_{nk} = g(z_{nk}) \quad (k = 1,2,\dots,K)$$

- Apply a linear model with $\boldsymbol{h}_n$ acting as features

A linear model with learnable weight vec $\boldsymbol{v}$

Score of the input

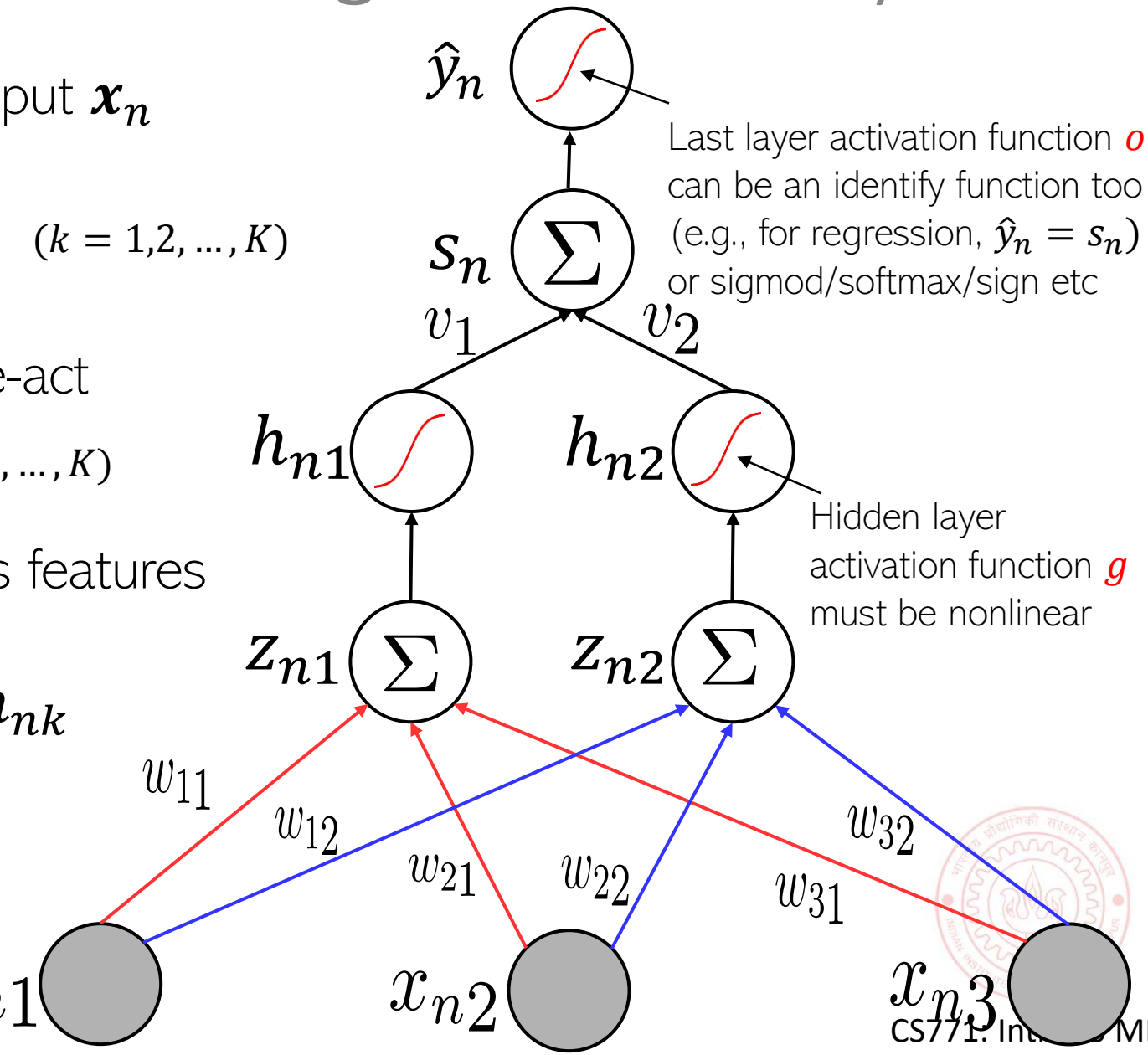
$$s_n = \boldsymbol{v}^\top \boldsymbol{h}_n = \sum_{k=1}^{K} v_k h_{nk}$$

- Finally, output is produced as

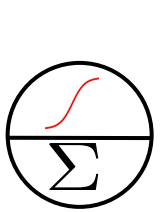
Score converted to the actual prediction

$$\hat{y}_n = o(s_n)$$

- Loss: $\mathcal{L}(\boldsymbol{W}, \boldsymbol{v}) = \sum_{n=1}^{N} \ell(y_n, \hat{y}_n)$

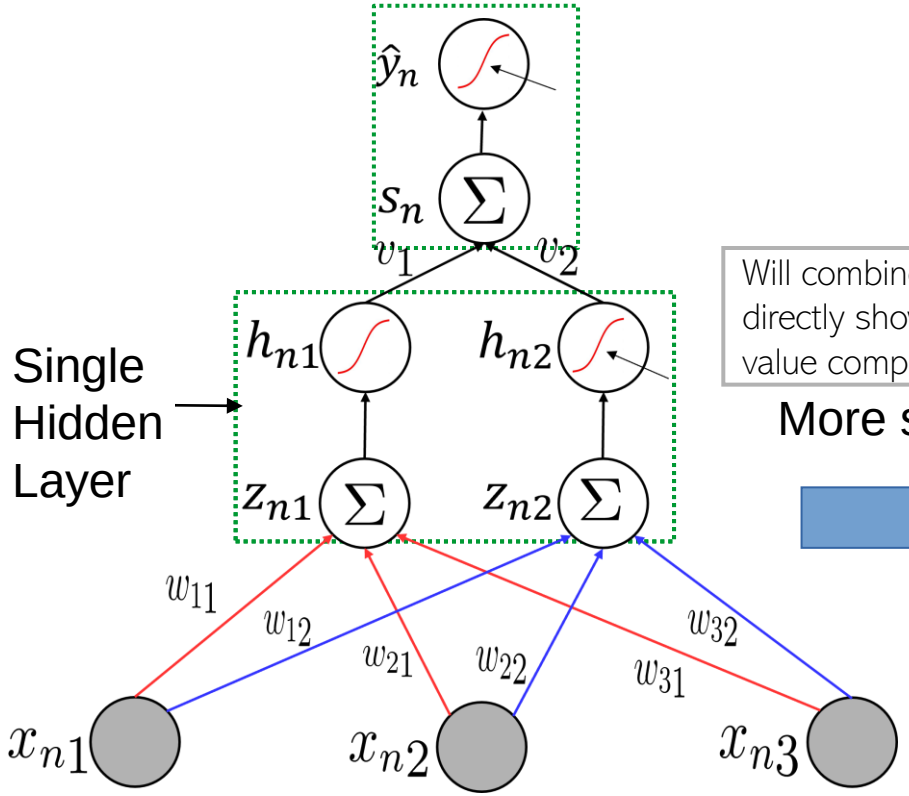


Neural Nets: A Compact Illustration



Will denote a linear combination of inputs followed by a nonlinear operation on the result

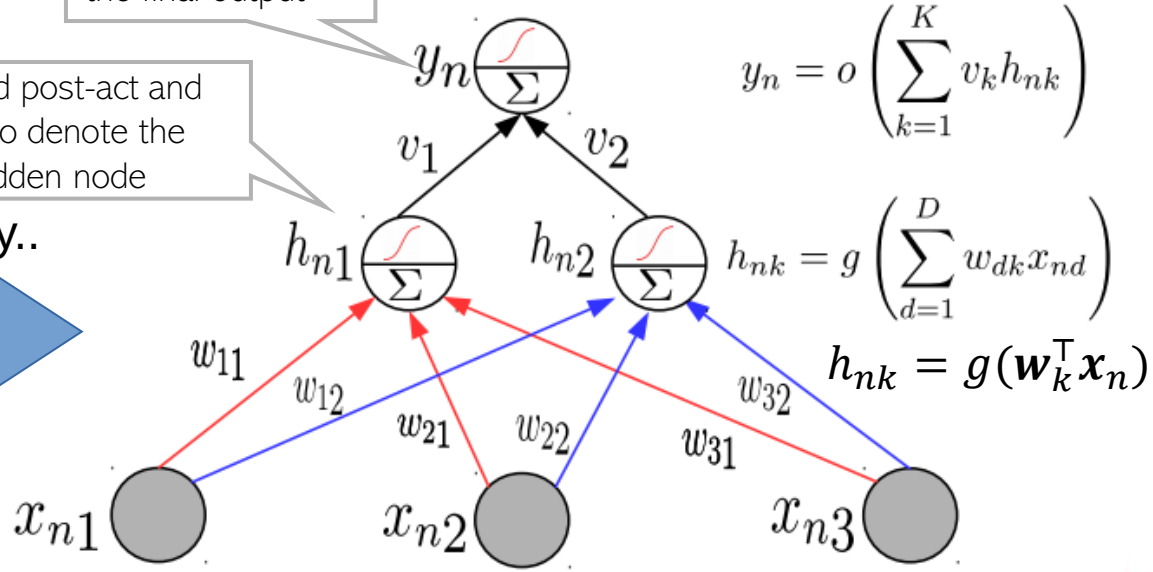
- Note: Hidden layer pre-act z_{nk} and post-act h_{nk} will be shown together for brevity



Will combine pre-act and post-act and directly show only h_{nk} to denote the value computed by a hidden node

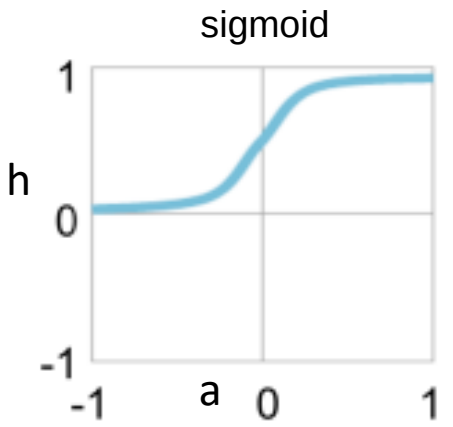
More succinctly..

Will directly show the final output

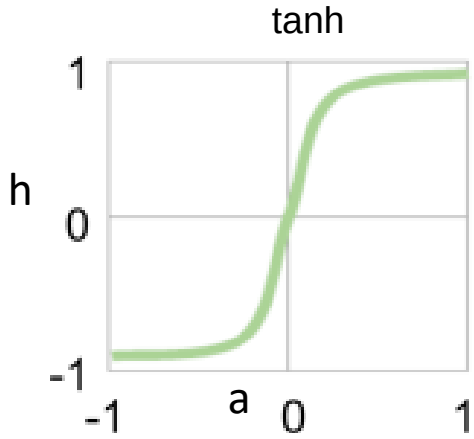


- Denoting $\boldsymbol{W} = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_K]$, $\boldsymbol{w}_k \in \mathbb{R}^D$, $\boldsymbol{h}_n = g(\boldsymbol{W}^\top \boldsymbol{x}_n) \in \mathbb{R}^K$ ($K = 2, D = 3$ above). Note: g applied elementwise on pre-activation vector $\boldsymbol{z}_n = \boldsymbol{W}^\top \boldsymbol{x}_n$

Activation Functions: Some Common Choices



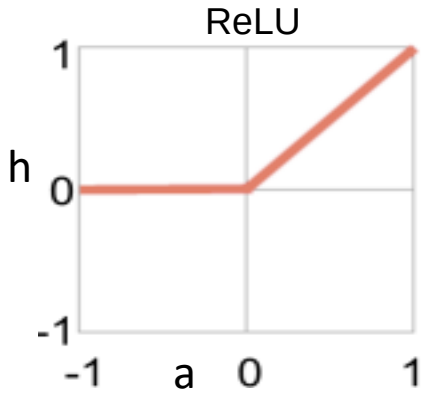
For sigmoid as well as tanh, gradients saturate (become close to zero as the function tends to its extreme values)



Preferred more than sigmoid. Helps keep the mean of the next layer's inputs close to zero (with sigmoid, it is close to 0.5)

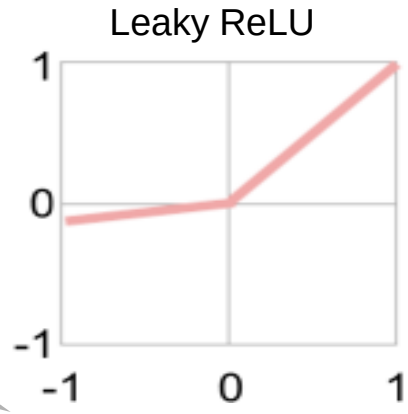
Sigmoid: $h = \sigma(a) = \frac{1}{1+\exp(-a)}$

tanh (tan hyperbolic): $h = \frac{\exp(a)-\exp(-a)}{\exp(a)+\exp(-a)} = 2\sigma(2a) - 1$



ReLU and Leaky ReLU are among the most popular ones (also efficient to compute)

Helps fix the dead neuron problem of ReLU when a is a negative number



$y = \boldsymbol{v}^\top(g(\boldsymbol{W}^\top x)) = \boldsymbol{v}^\top \boldsymbol{W}^\top x$

Still linear

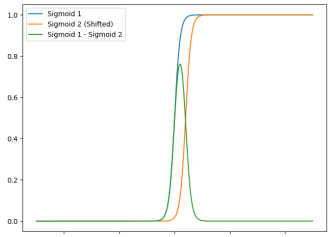
Imp: Without nonlinear activation, a deep neural network is equivalent to a linear model no matter how many layers we use

Most activation functions are monotonic but there exist some non-monotonic activation functions as well (e.g., Swish: $a \times \sigma(\beta a)$)

ReLU (Rectified Linear Unit): $h = \max(0, a)$

Leaky ReLU: $h = \max(\beta a, a)$ where β is a small postive number

MLP Can Learn Any Nonlinear Function

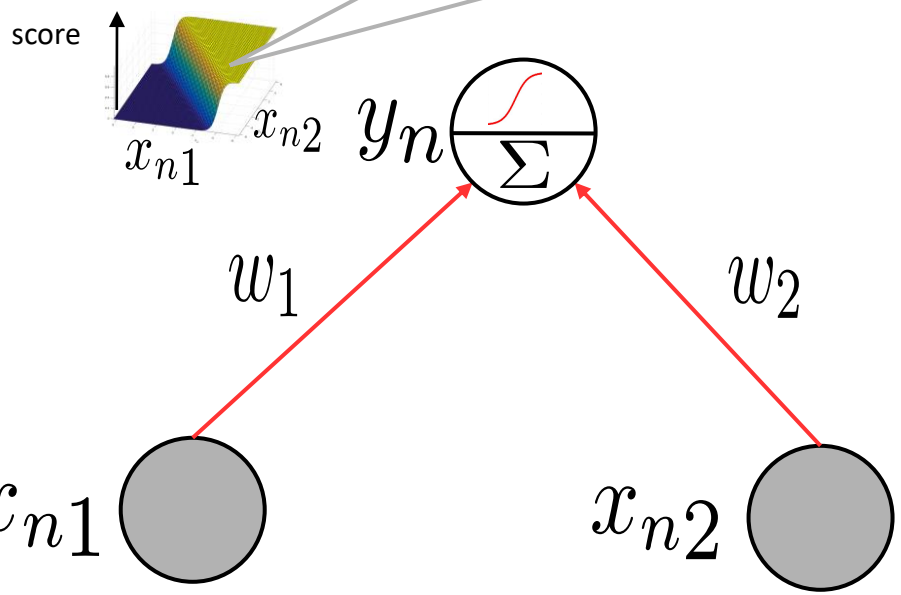


- An MLP can be seen as a composition of multiple linear models combined nonlinearly

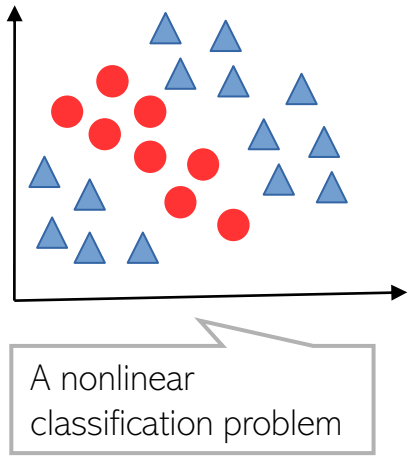
Score monotonically increases. One-sided increase (not ideal for learning nonlinear decision boundaries). Just a linear model

Obtained by composing the two one-sided increasing score functions (using learnable weights v_1 and v_2 to "add" them). This can now learn the nonlinear decision boundary (high score in the middle)

High-score in the middle and low-score on either of the two sides of it. Exactly what we want for the given classification problem

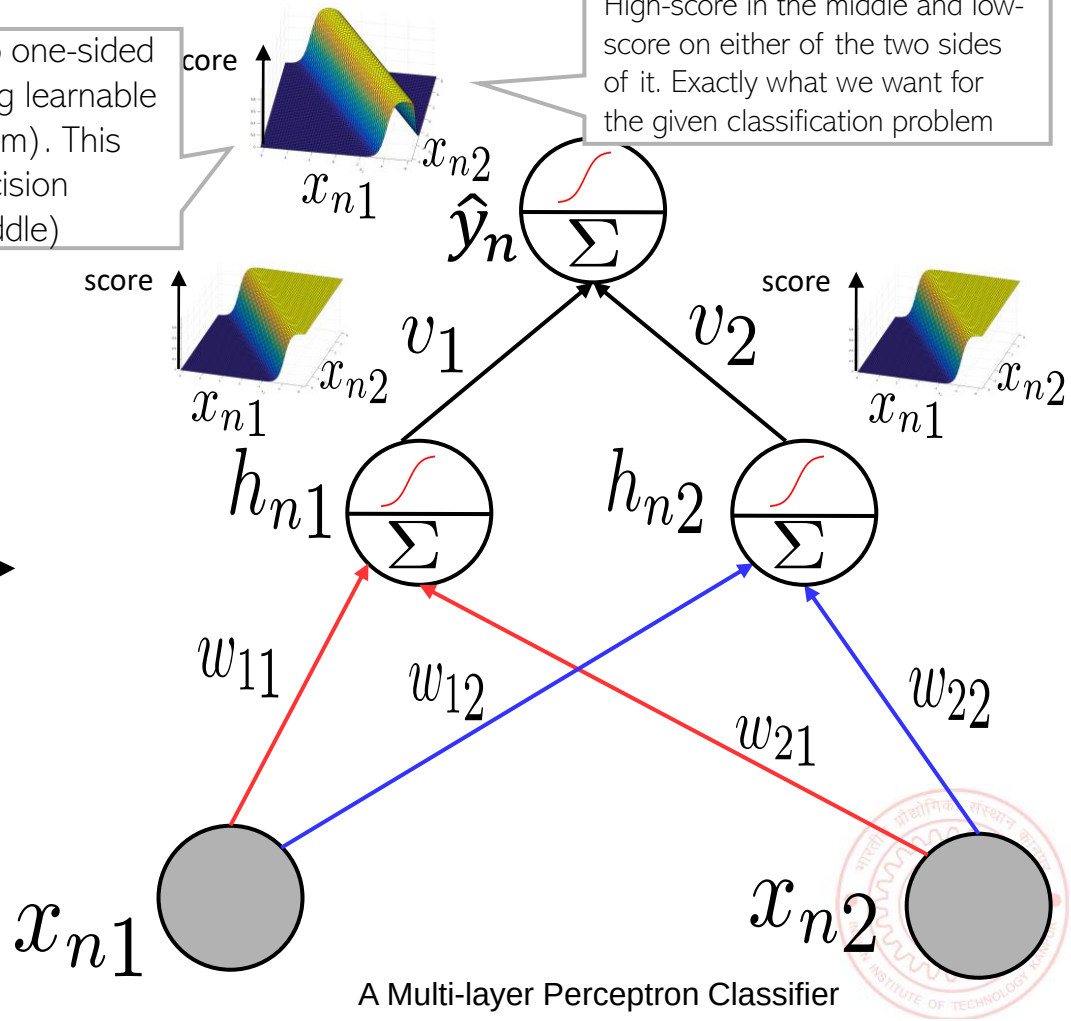


Standard Single "Perceptron" Classifier (no hidden units)



A nonlinear classification problem

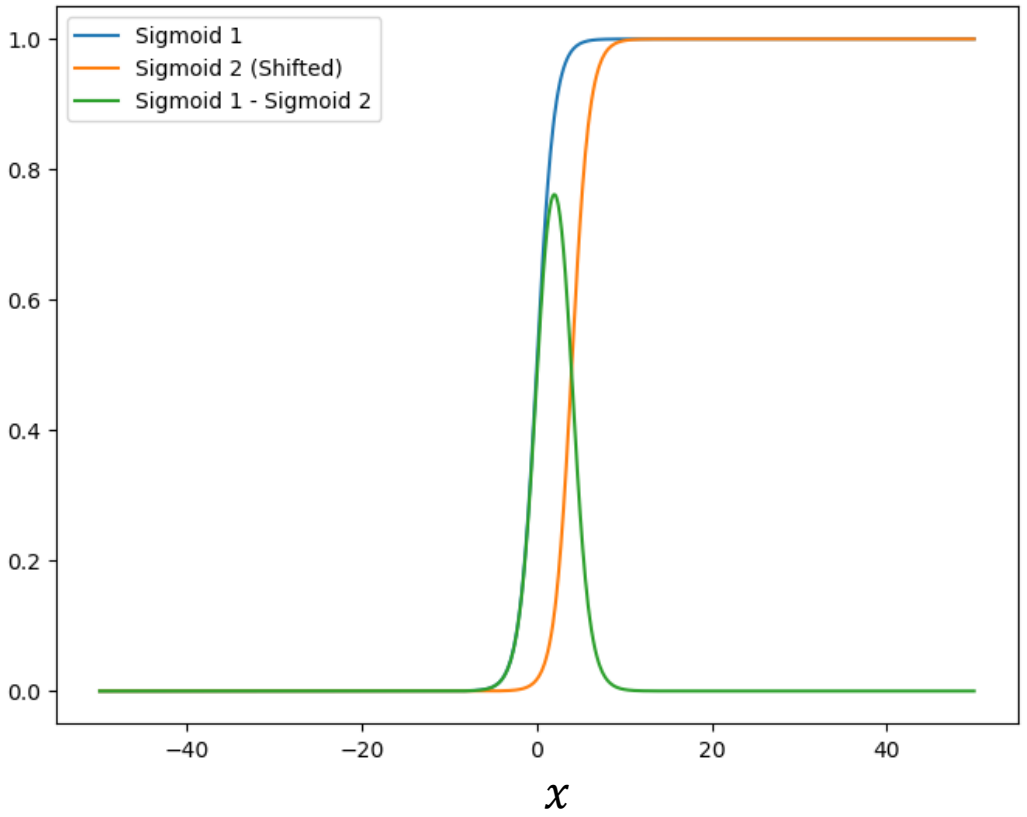
A single hidden layer MLP with sufficiently large number of hidden units can approximate any function (Hornik, 1991)



A Multi-layer Perceptron Classifier (one hidden layer with 2 units)
Capable of learning nonlinear boundaries

Superposition of two linear models = Nonlinear model

$p(y = \text{red}|x)$



Two sigmoids (blue and orange) can be combined via a shift and a subtraction operation to result in a nonlinear separation boundary

Likewise, more than two sigmoids can be combined to learn even more sophisticated separation boundaries

Nonlinear separation boundary

Examples of some basic NN/MLP architectures

Single Hidden Layer and Single Output

- One hidden layer with K nodes and a single output (e.g., scalar-valued regression or binary classification)

$\hat{y}_n = o(\boldsymbol{v}^\top \boldsymbol{h}_n)$

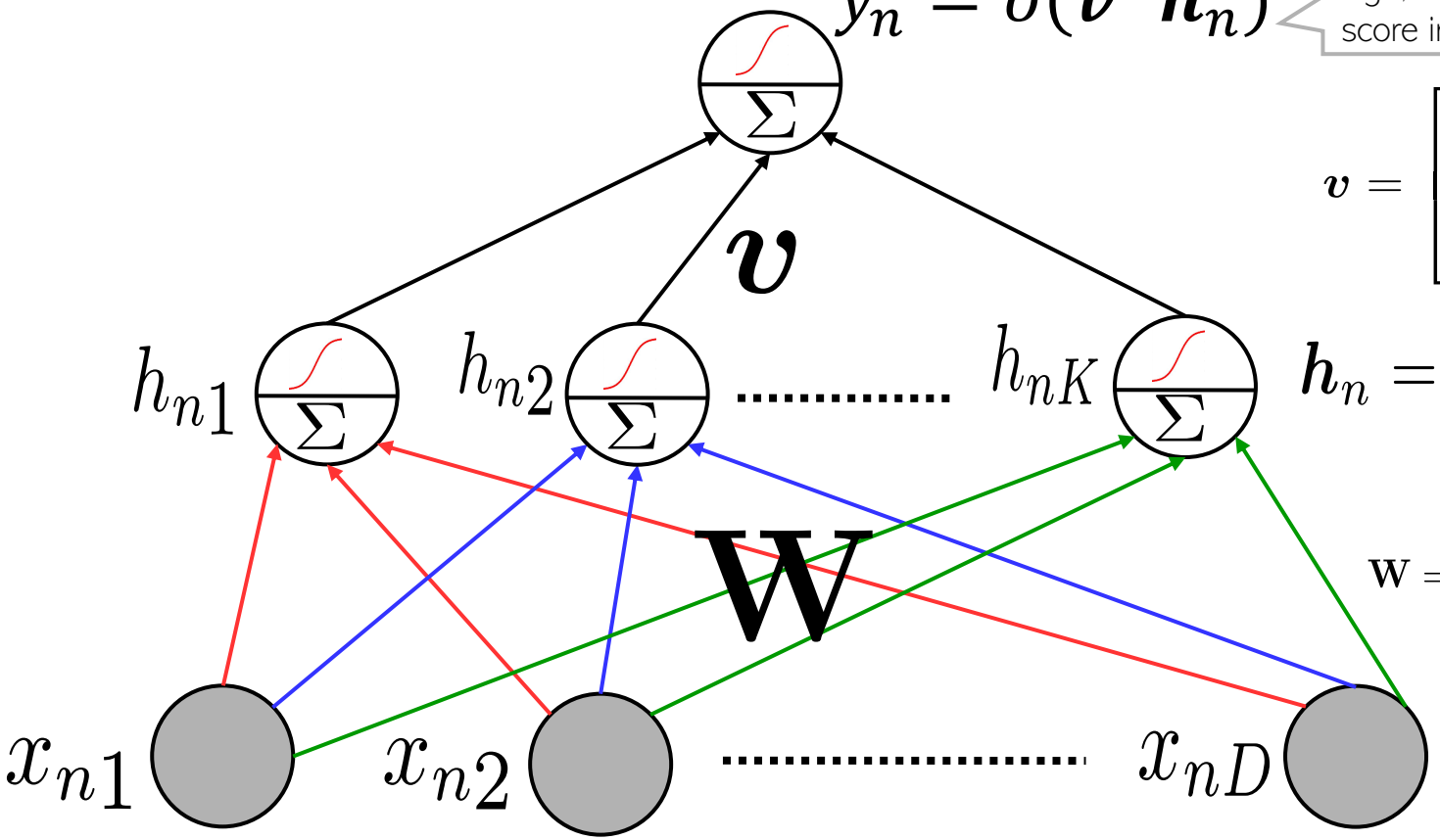
o is a suitable function (e.g., identity, sign, or sigmoid, etc) to convert the score into the actual response

$$\boldsymbol{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_K \end{bmatrix}$$

$\boldsymbol{h}_n = g(\mathbf{W}^\top \boldsymbol{x}_n)$

g is a nonlinear activation function

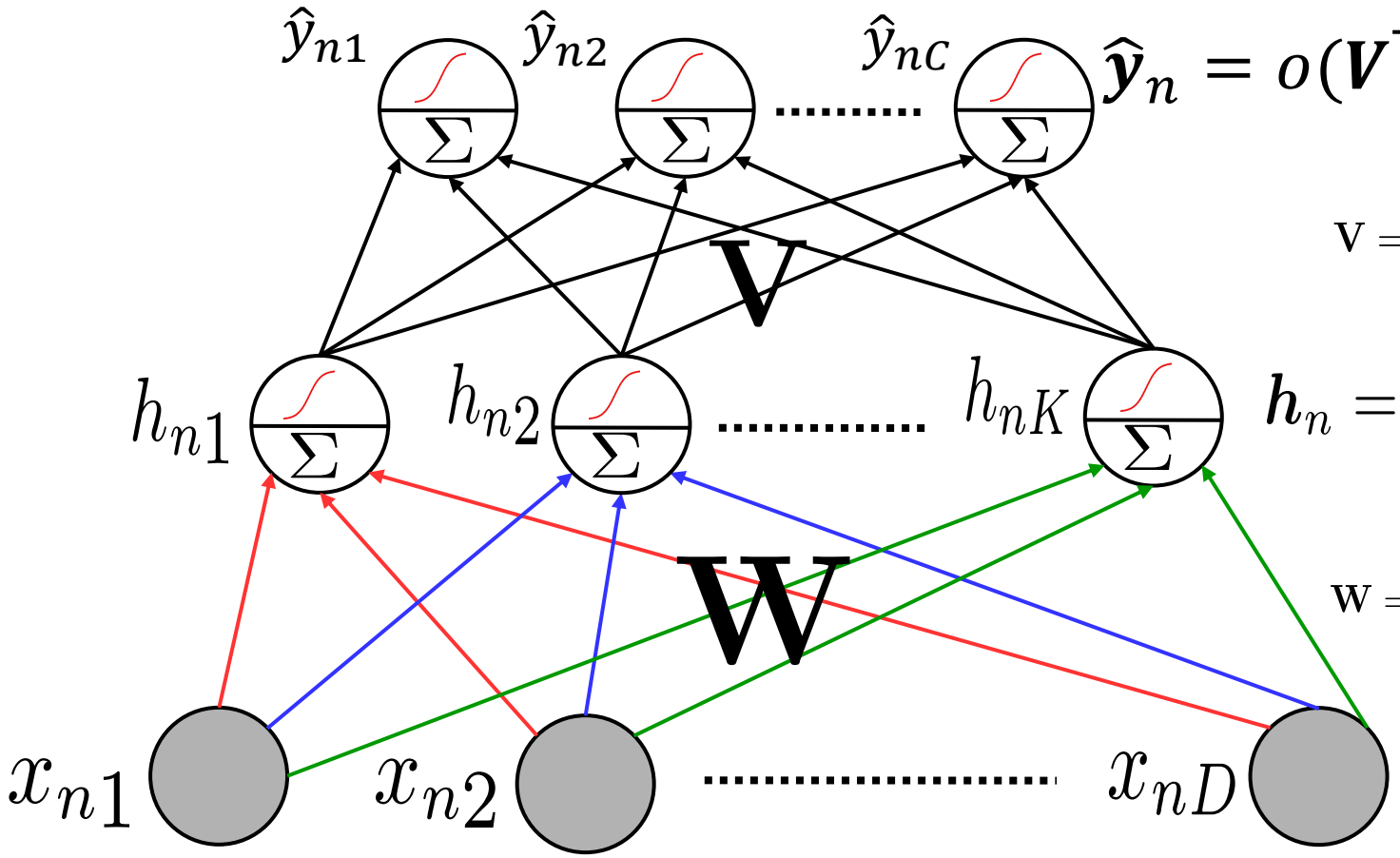
$$\mathbf{W} = \begin{bmatrix} w_{11} & \cdots & w_{1K} \\ \vdots & \ddots & \vdots \\ w_{D1} & \cdots & w_{DK} \end{bmatrix}$$



Single Hidden Layer and Multiple Outputs

- One hidden layer with K nodes and a vector of C outputs (e.g., vector-valued regression or multi-class classification or multi-label classification)

o is a suitable function (e.g., identity, sign, or softmax, etc) to convert the score into the actual response vector for x_n



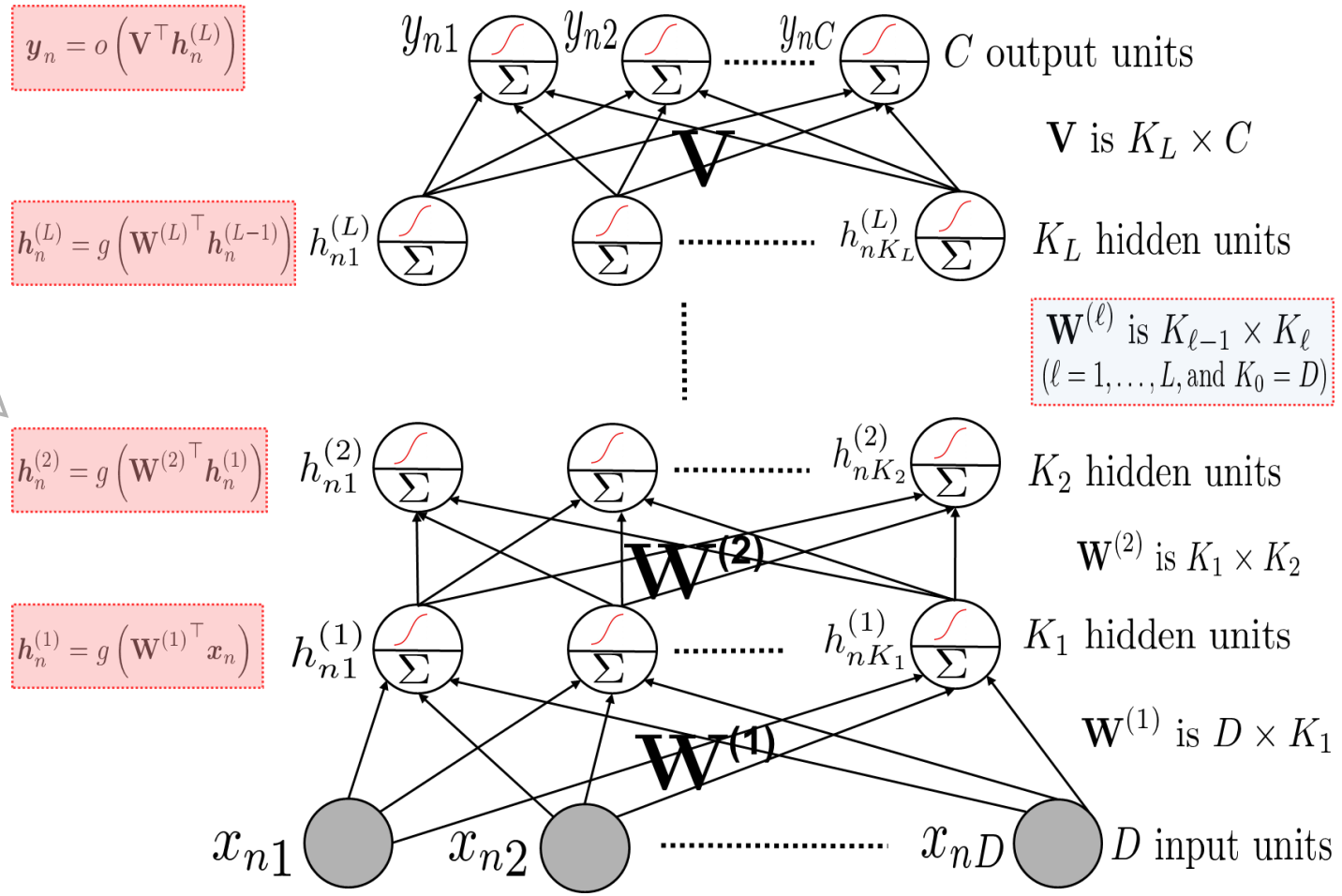
$$\mathbf{V} = \begin{bmatrix} v_{11} & \cdots & v_{1C} \\ \vdots & \ddots & \vdots \\ v_{K1} & \cdots & v_{KC} \end{bmatrix}$$

g is a nonlinear activation function

$$\mathbf{W} = \begin{bmatrix} w_{11} & \cdots & w_{1K} \\ \vdots & \ddots & \vdots \\ w_{D1} & \cdots & w_{DK} \end{bmatrix}$$

Multiple Hidden Layers (One/Multiple Outputs)

- Most general case: Multiple hidden layers with (with same or different number of hidden nodes in each) and a scalar or vector-valued output



Each hidden layer uses a nonlinear activation function g (essential, otherwise the network can't learn nonlinear functions and reduces to a linear model)

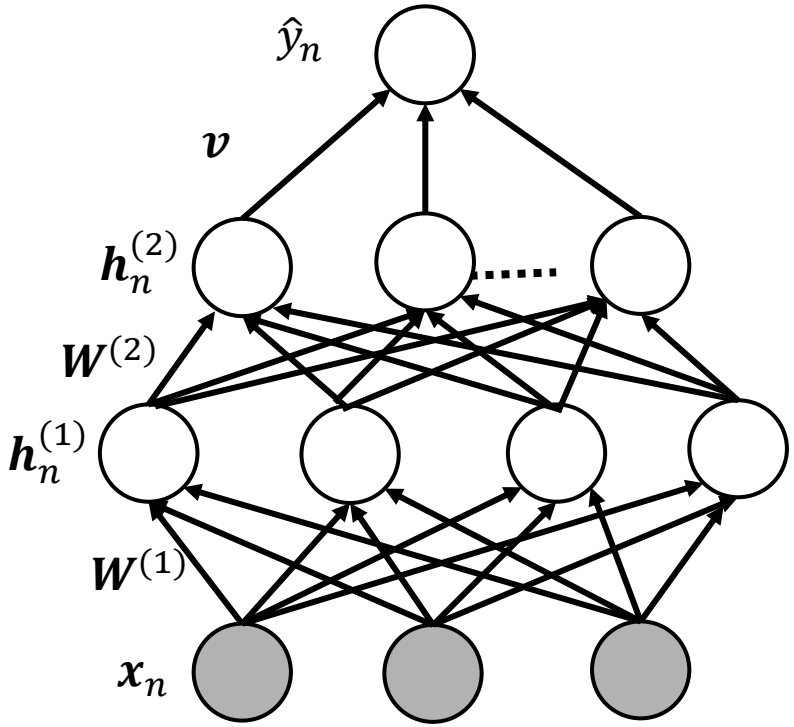
Note: Nonlinearity g is applied element-wise on its inputs so $h_n^{(\ell)}$ has the same size as vector $W^{(\ell)} h_n^{(\ell-1)}$

The Bias Term

- Each layer's pre-activations $\boldsymbol{z}_n^{(\ell)}$ have a an add bias term $\boldsymbol{b}^{(\ell)}$ (has the same size as $\boldsymbol{z}_n^{(\ell)}$ and $\boldsymbol{h}_n^{(\ell)}$) as well

$$\boldsymbol{z}_n^{(\ell)} = \boldsymbol{W}^{(\ell)\top} \boldsymbol{h}_n^{(\ell-1)} + \boldsymbol{b}^{(\ell)}$$

$$\boldsymbol{h}_n^{(\ell)} = g(\boldsymbol{z}_n^{(\ell)})$$



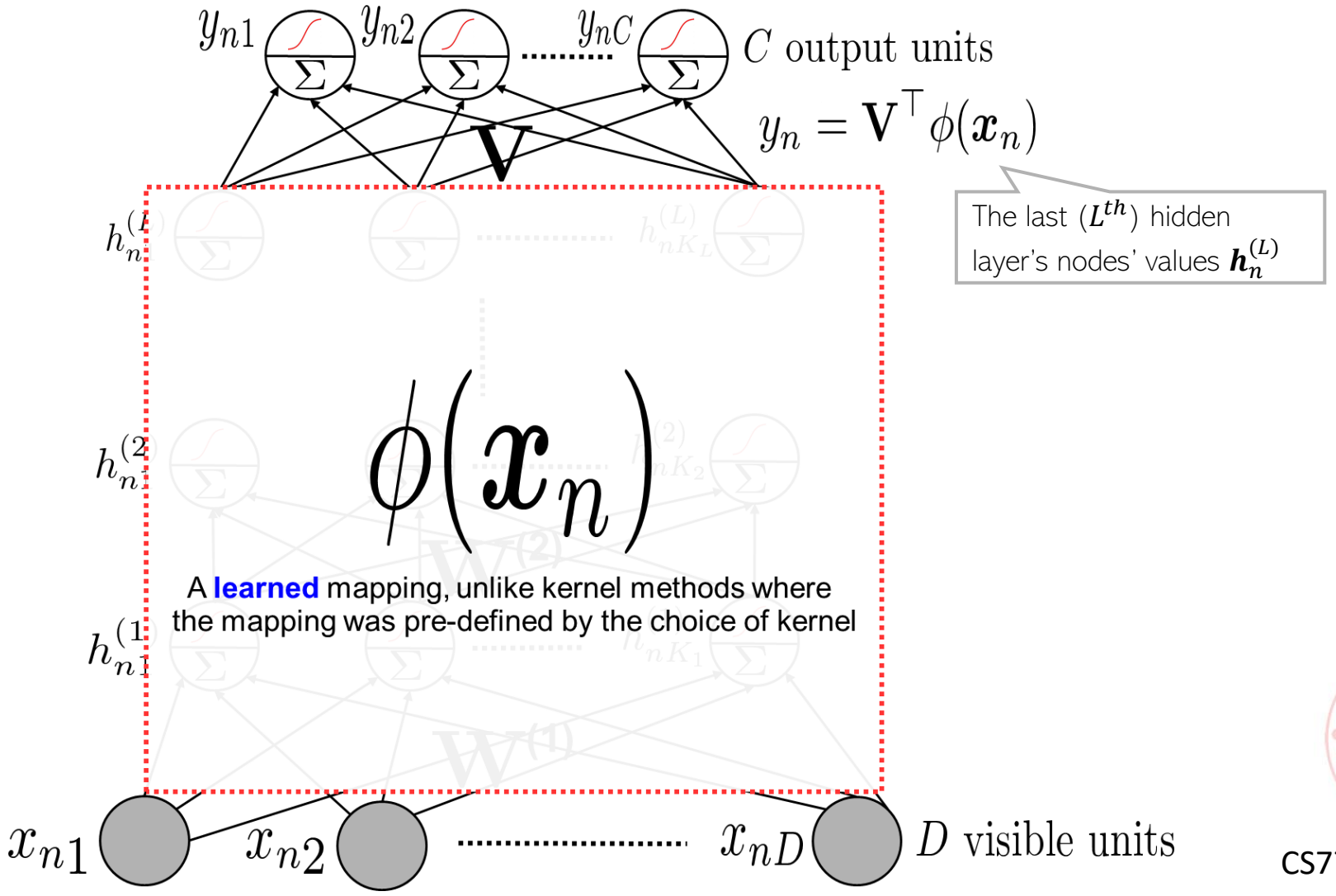
- Bias term increases the expressiveness of the network and ensures that we have nonzero activations/pre-activations even if this layer's input is a vector of all zeros

- Note that the bias term is the same for all inputs (does not depend on $\boldsymbol{n}$)

- The bias term $\boldsymbol{b}^{(\ell)}$ is also learnable

Neural Nets are Feature Learners

- Hidden layers can be seen as learning a feature rep. $\boldsymbol{\phi}(\boldsymbol{x}_n)$ for each input $\boldsymbol{x}_n$



Kernel Methods vs Neural Nets

Also note that neural nets are faster than kernel methods at test time since kernel methods need to store the training examples at test time whereas neural nets do not

- Recall the prediction rule for a kernel method (e.g., kernel SVM)

$$y_n = \boldsymbol{w}^\top \boldsymbol{\phi}(\boldsymbol{x}_n) \quad \text{OR} \quad y_n = \sum_{i=1}^{N} \alpha_n k(\boldsymbol{x}_i, \boldsymbol{x}_n)$$

- It's like a one hidden layer NN with
  - Pre-defined N features $\{k(\boldsymbol{x}_i, \boldsymbol{x}_n)\}_{i=1}^N$ acting as feature vector $\boldsymbol{h}_n$
  - $\{\alpha_i\}_{n=1}^N$ are learnable output layer weights

- It's also like a one hidden layer NN with
  - Pre-defined M features $\boldsymbol{\phi}(\boldsymbol{x}_n)$ (M being size of feature mapping $\boldsymbol{\phi}$) acting as feature vector $\boldsymbol{h}_n$
  - $\boldsymbol{w} \in \mathbb{R}^M$ are learnable output layer weights

- Both kernel methods and deep neural networks extract new features from the inputs
  - For kernel methods, the features are pre-defined via the kernel function
  - For deep NN, the features are learned by the network

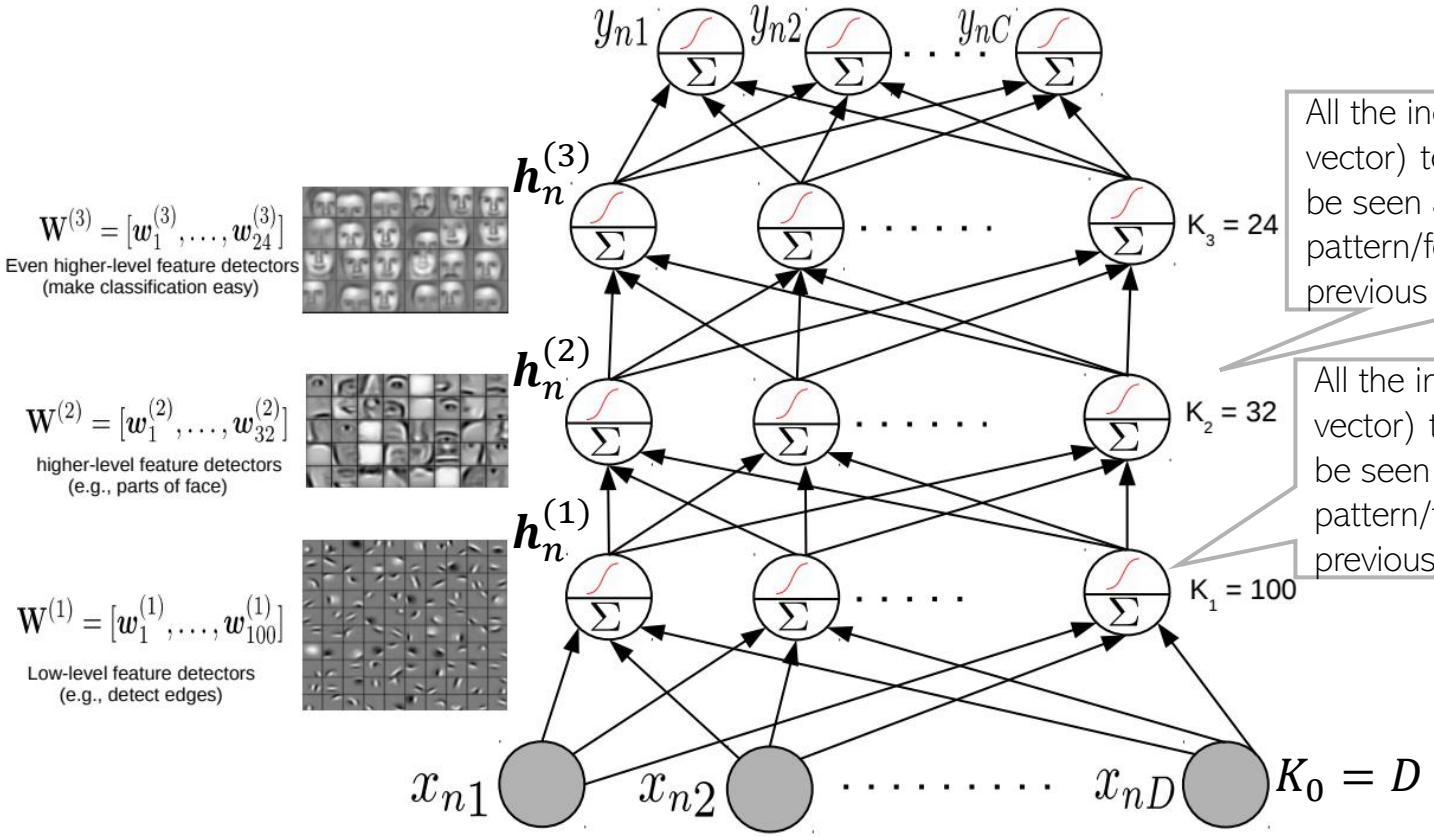
- Note: Kernels can also be learned from data ("kernel learning") in which case kernel methods and deep neural nets become even more similar in spirit ☺

Features Learned by a Neural Network

$\boldsymbol{W}^{(\ell)} = [\boldsymbol{w}_1^{(\ell)}, \boldsymbol{w}_2^{(\ell)}, \ldots, \boldsymbol{w}_{K_\ell}^{(\ell)}]$ is $K_{\ell-1} \times K_\ell$ matrix of weights between layer $\ell - 1$ and ℓ

$\boldsymbol{W}^{(\ell)}$ collectively represents the K_ℓ feature detectors for layer ℓ

- $\boldsymbol{w}_k^{(\ell)} \in \mathbb{R}^{K_{\ell-1}}$ denotes "feature detector" for feature k of layer ℓ
- For input $\boldsymbol{x}_n$, $h_{nk}^{(\ell)} = g(\boldsymbol{w}_k^{(\ell)\top} \boldsymbol{h}_n^{(\ell-1)})$ is the value of feature k in layer ℓ



All the incoming weights (a vector) to a hidden node can be seen as representing a pattern/feature-detector of previous layer's inputs

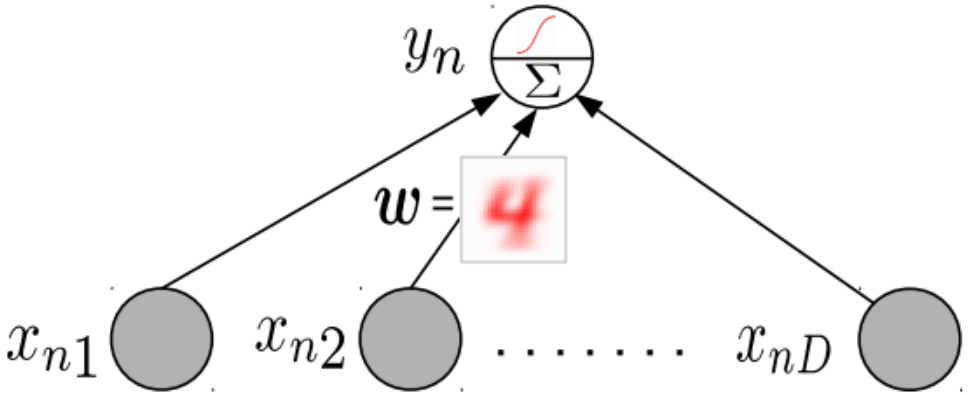
E.g., $\boldsymbol{w}_{32}^{(2)}$ denotes a feature detector

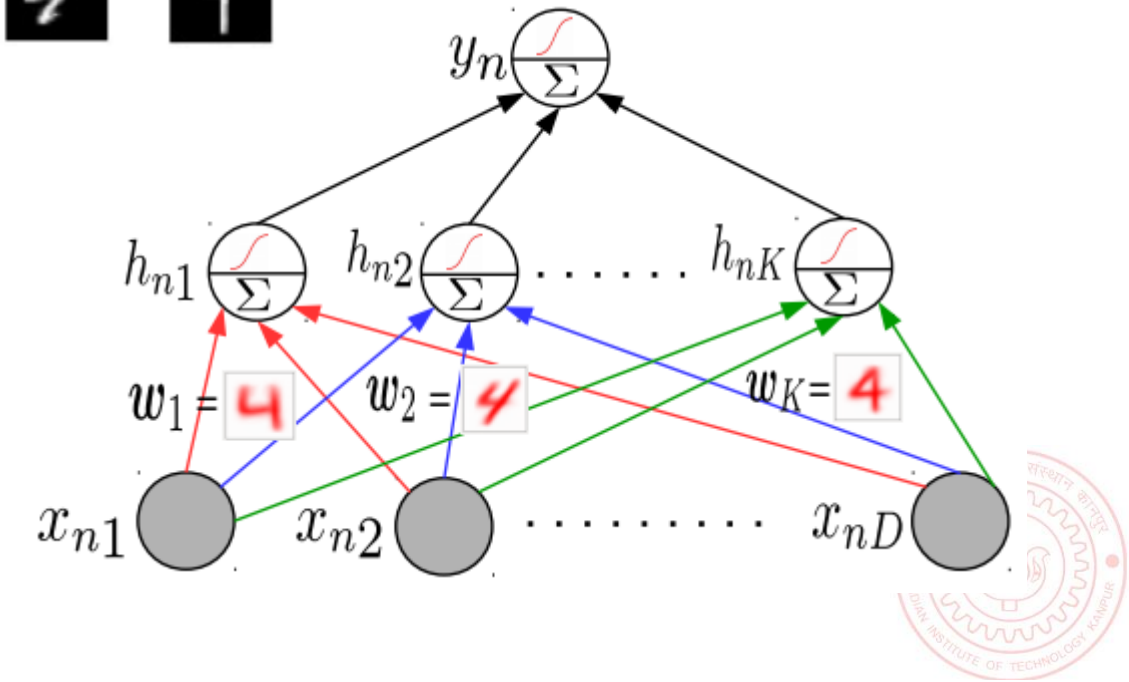
All the incoming weights (a vector) to a hidden node can be seen as representing a pattern/feature-detector of previous layer's inputs

E.g., $\boldsymbol{w}_{100}^{(1)}$ denotes a feature detector

Why Neural Networks Work Better: Another View

- Linear models tend to only learn the "average" pattern
  - E.g., Weight vector of a linear classification model represent average pattern of a class
- Deep models can learn multiple patterns (each hidden node can learn one pattern)
  - Thus deep models can learn to capture more subtle variations that a simpler linear model

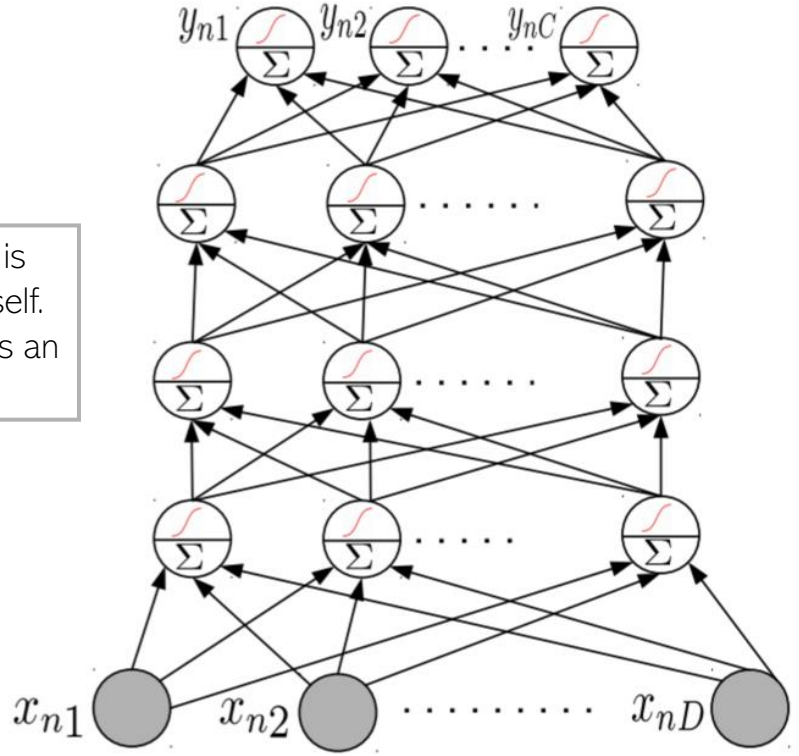




Neural Nets: Some Aspects

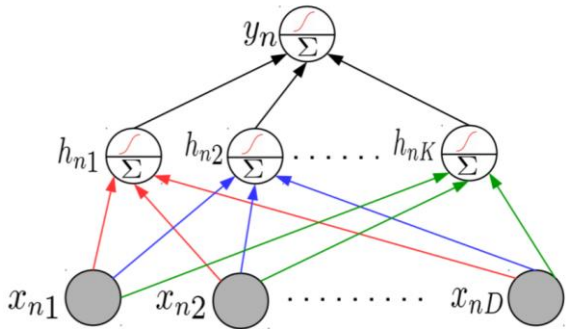
- Much of the magic lies in the hidden layers
- Hidden layers learn and detect good features
- Need to consider a few aspects
  - Number of hidden layers, number of units in each hidden layer
  - Why bother about many hidden layers and not use a single very wide hidden layer (recall Hornik's universal function approximator theorem)?
  - Complex networks (several, very wide hidden layers) or simpler networks (few, moderately wide hidden layers)?
  - Aren't deep neural network prone to overfitting (since they contain a huge number of parameters)?

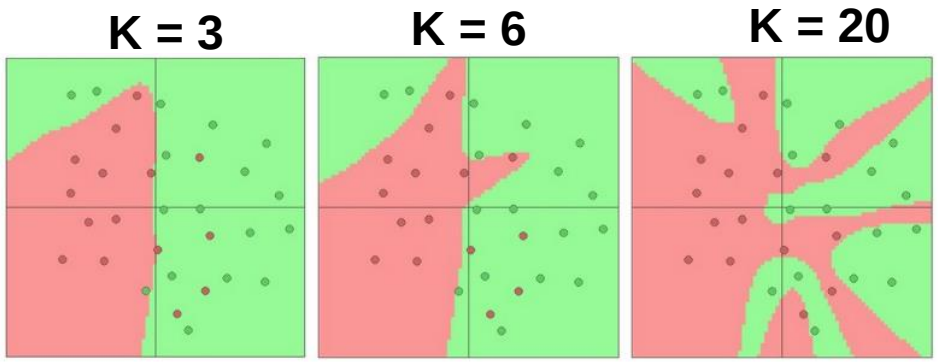
Choosing the right NN architecture is important and a research area in itself. Neural Architecture Search (NAS) is an automated technique to do this



Representational Power of Neural Nets

- Consider a single hidden layer neural net with K hidden nodes

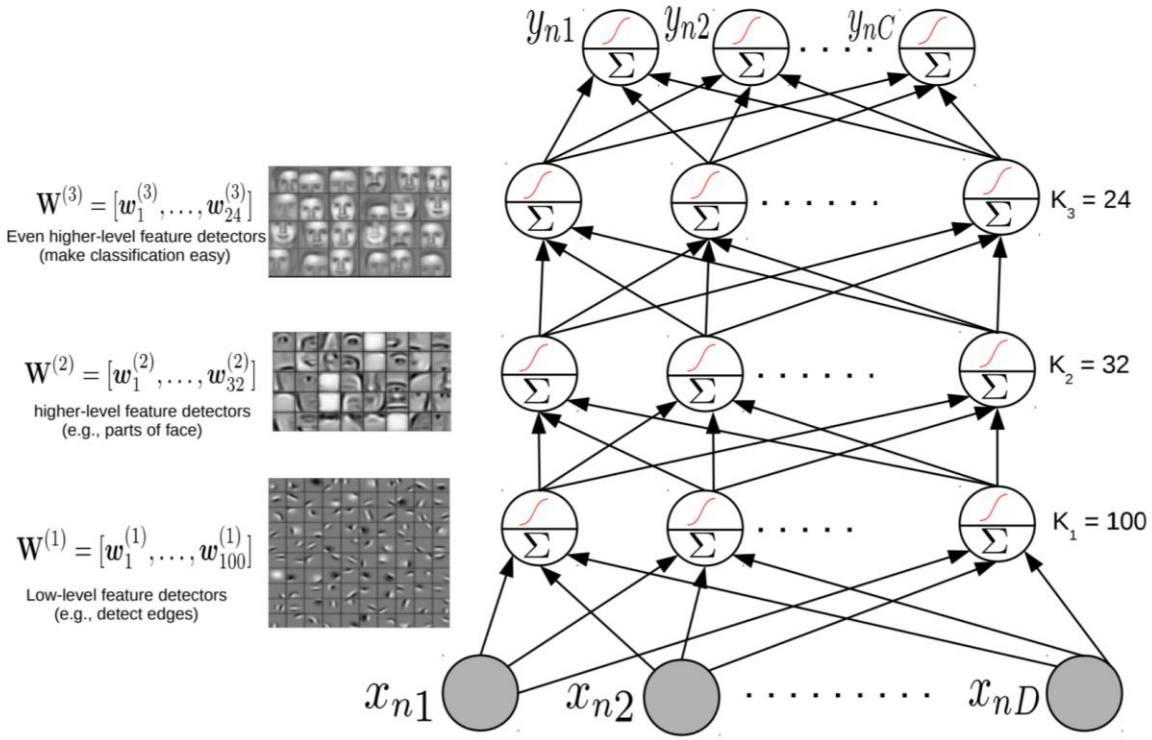




- Recall that each hidden unit "adds" a simple function to the overall function
- Increasing K (number of hidden units) will result in a more complex function
- Very large K seems to overfit (see above fig). Should we instead prefer small K?
- No! It is better to use large K and regularize well. Reason/justification:
  - Simple NN with small K will have a few local optima, some of which may be bad
  - Complex NN with large K will have many local optimal, all equally good (theoretical results on this)
- We can also use multiple hidden layers (each sufficiently large) and regularize well

Wide or Deep?

- While very wide single hidden layer can approx. any function, often we prefer many, less wide, hidden layers



- Higher layers help learn more directly useful/interpretable features (also useful for compressing data using a small number of features)