CSDS 440: Machine Learning

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Office hours T, Th 11:15-11:45 or by appointment

Training Phase

- Given Data:

x_1	x_2	y
0	0	-1
0	1	1

- Find (w, σ) so that the resulting perceptron matches y

Loss Function

- We will define a function called a "loss function"

$$L(\mathbf{w}, \sigma)$$

- This function will measure the difference between our *current estimates* of y ($\hat{\mathbf{y}}$) and the *true* y (which is known), over all training examples, with respect to $(\mathbf{w}, \sigma)$
- Then our goal will be to *minimize* the loss function with respect to $(\mathbf{w}, \sigma)$

Training Phase

- Given a training sample and their class labels

$$D = \begin{pmatrix} x_{11} & \dots & x_{1n} & -1 & y_1 \\ \vdots & & \vdots & \vdots & \vdots \\ x_{m1} & \cdots & x_{mn} & -1 & y_m \end{pmatrix}$$

- Find parameters

$$\mathbf{w} = \left(w_1, w_2, w_3, \ldots, w_n, \sigma\right)$$

- To **minimize** “loss” $L(\mathbf{w})$

$\hat{\mathbf{y}}$

Loss function

- A common loss function is "squared loss"

$$L(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \hat{y}_i)^2 = \frac{1}{2}\sum_{i=1}^{m}(y_i - sign(\mathbf{w}\bullet\mathbf{x}_i))^2$$

- Notice that $sign(1)=1$ and $sign(-1)=-1$, so if we can get $\mathbf{w}\cdot\mathbf{x}$ to equal $\mathbf{y}$ we can drop the *sign* function
  - This is easier to deal with (differentiable)

$$L(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \mathbf{w}\bullet\mathbf{x}_i)^2$$

Iterative parameter update

$$L(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{m}(y_i - \mathbf{w}\bullet\mathbf{x}_i)^2$$

- Calculate gradient with respect to parameters $\mathbf{w}$:

$$\frac{dL}{d\mathbf{w}} = \sum_{i=1}^{m}(y_i - \mathbf{w}\bullet\mathbf{x}_i)(-\mathbf{x}_i)$$

- Parameter Update:

$$\mathbf{w} \leftarrow \mathbf{w} - \eta\frac{dL}{d\mathbf{w}}$$

Learning rate
or
step size

Convergence

- This is gradient descent
- Notice that this loss function is everywhere differentiable and bounded below
  - A well defined (unique!) minimum exists for any D
  - This iterative procedure will find it

Stochastic G.D. vs Regular G.D.

Instead of summing the gradients across all examples, could perform update separately for each example (or a few examples)

Regular

$$\nabla_{\mathbf{w}} L = \sum_{i=1}^{m} (y_i - \mathbf{w} \bullet \mathbf{x}_i)(-\mathbf{x}_i)$$

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} L$$

Stochastic

$$\left.\begin{aligned} &\nabla_{\mathbf{w}} \tilde{L} = (y_i - \mathbf{w} \bullet \mathbf{x}_i)(-\mathbf{x}_i) \\ &\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \tilde{L} \end{aligned}\right\}_{i=1\ldots m}$$

Stochastic Gradient Descent

- Since the total gradient is a vector sum, this isn't the same as summing the gradient first

- But it is incremental, useful for online updates and can help with local minima (when it exists)

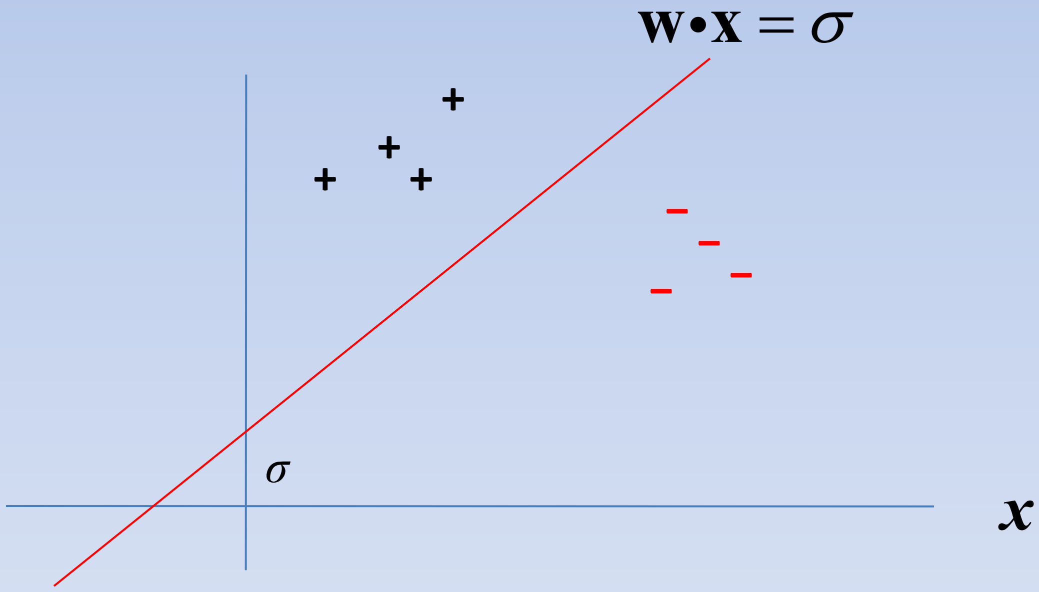
Stochastic G. D. Convergence

- If doing stochastic gradient descent, technically need η to go to zero and $\Sigma\eta^2$ to be bounded

- Since we'll usually perform finitely many parameter updates, often ignore this in practice

Geometry of the Perceptron

- A perceptron's separating surface defines a hyperplane in feature space



Linear Separability

- Since the perceptron defines a linear decision boundary, any dataset that it can separate with no error is said to be “linearly separable”
  - Such a dataset will have zero loss wrt our loss function

Logic with a perceptron

- Conjunctions

$$x_1 \wedge x_2 \wedge x_3 \Leftrightarrow y$$

$$1 \bullet x_1 + 1 \bullet x_2 + 1 \bullet x_3 \geq 3$$

- At least m-of-n

$$(x_1 \wedge x_2) \vee (x_1 \wedge x_3) \vee (x_2 \wedge x_3) \Leftrightarrow y$$

$$1 \bullet x_1 + 1 \bullet x_2 + 1 \bullet x_3 \geq 2$$

Things that can't be learned

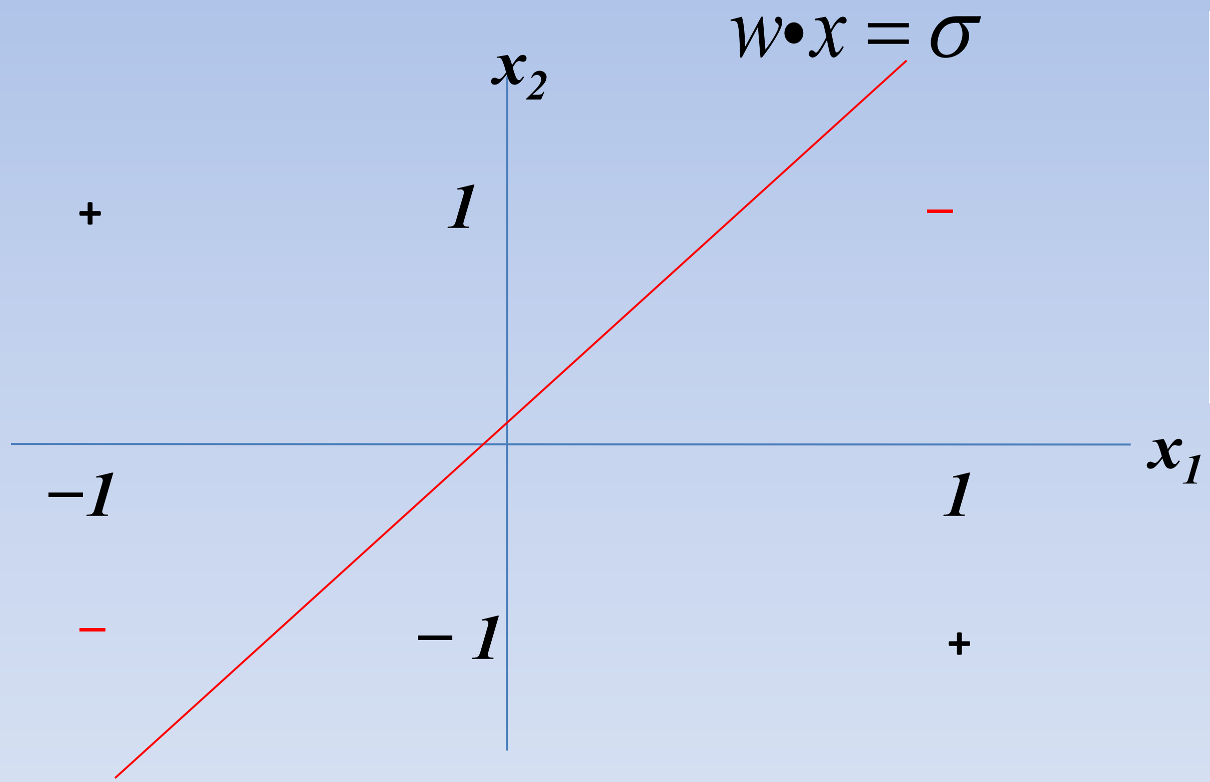
- Complex disjunctions

$$(x_1 \wedge x_2) \vee (x_3 \wedge x_4) \Leftrightarrow y$$

- Exclusive-OR

$$(x_1 \wedge \neg x_2) \vee (\neg x_1 \wedge x_2) \Leftrightarrow y$$

XOR and the Perceptron

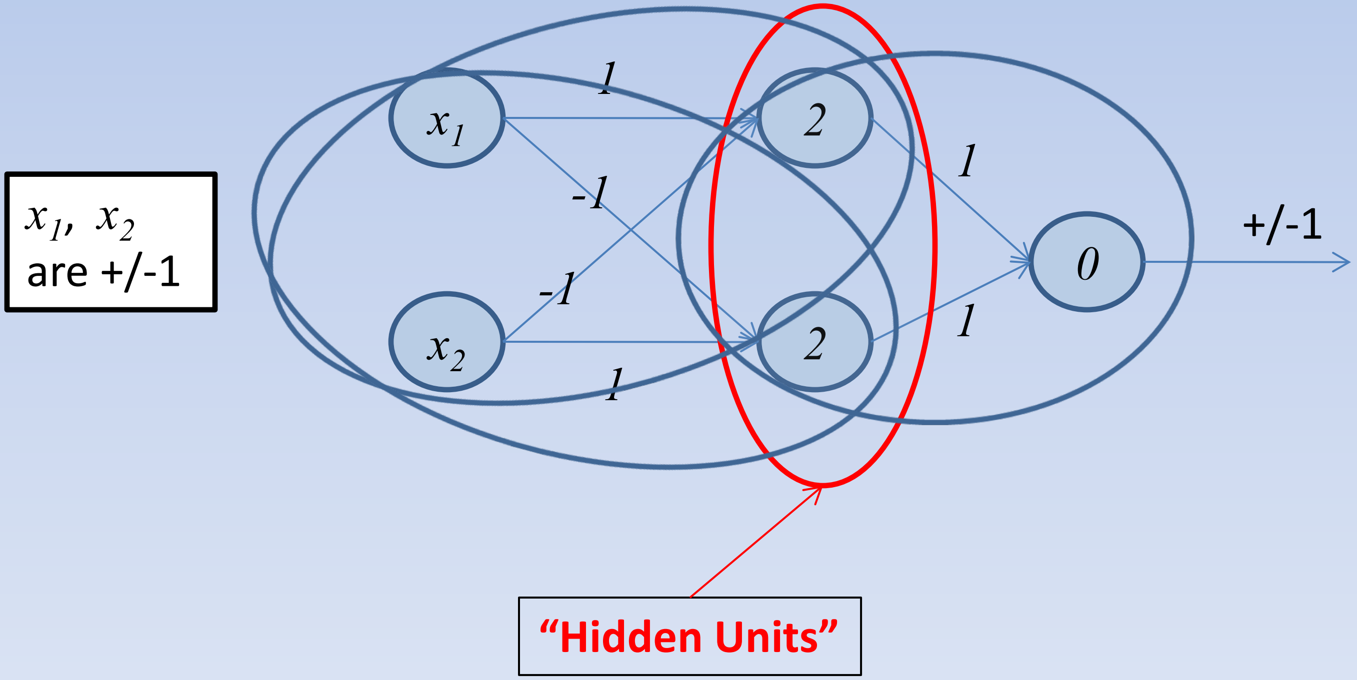


x_1	x_2	f
F	F	F
T	F	T
F	T	T
T	T	F

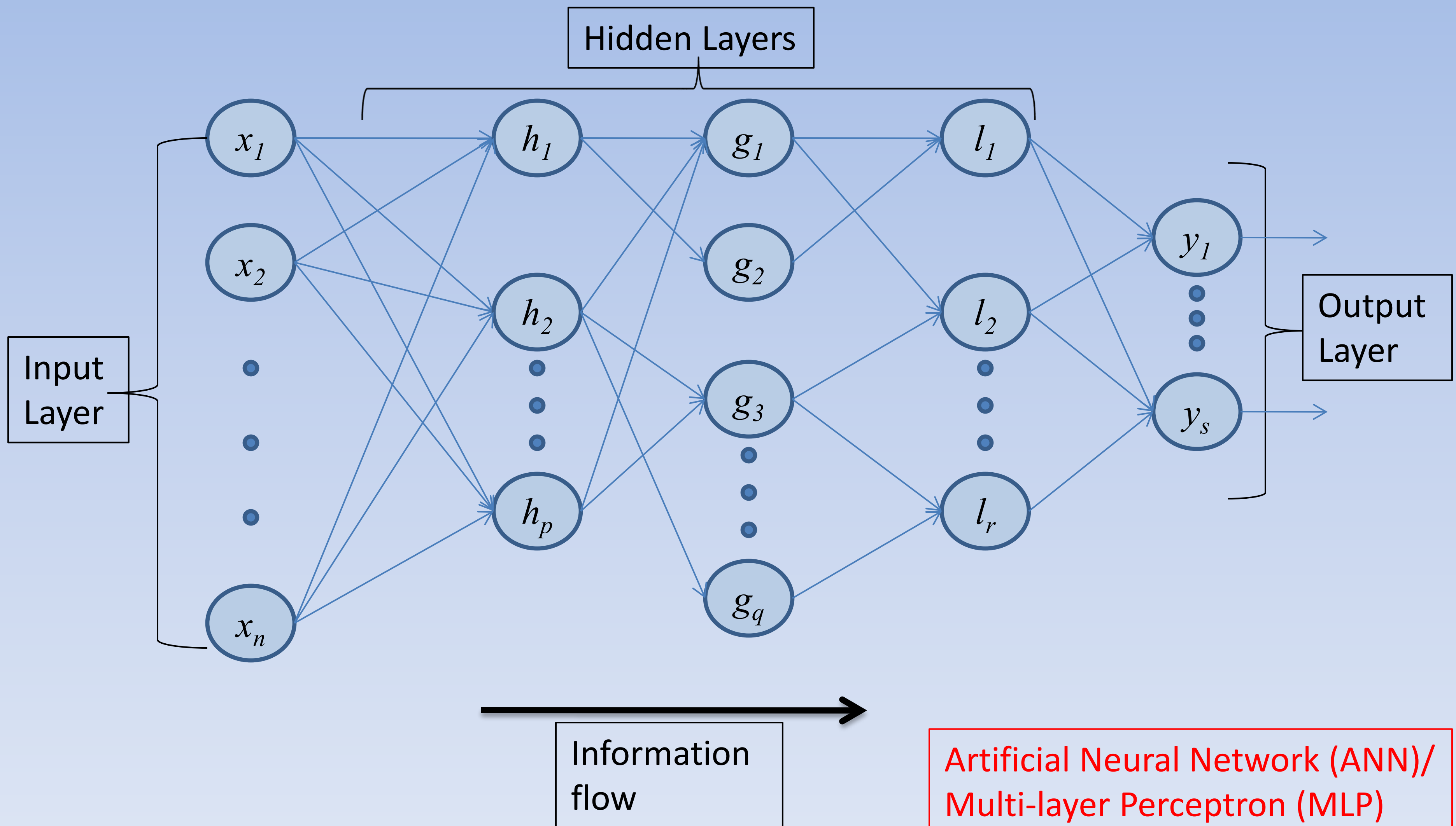
How to fix this?

Idea

- So far, single “neuron”
- Let’s connect them into a network



“Feedforward” Network Topology



Artificial Neural Network (ANN)/ Multi-layer Perceptron (MLP)

Representation Ability

- Every Boolean function can be represented by a network with one hidden layer of units (Minsky and Papert)
- Every bounded continuous function can be represented by a network with one hidden layer (Cybenko et al)*
- Every function on $\boldsymbol{R}^n$ can be represented by a network with two hidden layers! (Cybenko et al)*
  - *(with arbitrary numbers of hidden units)

Tradeoffs

- Very large number of degrees of freedom
  - Network topology
    - Number of layers, number of hidden units in each layer, edge configuration, even different activation functions
  - Network parameter values
- Power comes at a price
  - Very very easy to overfit if structure is complex
  - Very long time and large samples required to train
  - Structure and function relationship is opaque to people (and often uninterpretable even when not)

Training Phase (ANN)

- As before, given a training sample and their class labels

$$D = \begin{pmatrix} x_{11} & \cdots & x_{1n} & -1 & y_1 \\ \vdots & & \vdots & \vdots & \vdots \\ x_{m1} & \cdots & x_{mn} & -1 & y_m \end{pmatrix}$$

- Find parameters $\mathbf{w}$

- To minimize "loss" $L(\mathbf{w})$

Hidden Layer Activation Function

- For a perceptron, we used a *sign()* function as an activation function

- This function is problematic for optimization because it isn't differentiable
  - For perceptron this was OK, we were able to remove the *sign()* and handle this
  - But for a general ANN we need a smooth activation function

Activation Functions

- Sigmoid

$$h(\mathbf{x};\mathbf{w}) = (1+e^{-\mathbf{w}\bullet\mathbf{x}})^{-1}$$

- Radial Basis Function

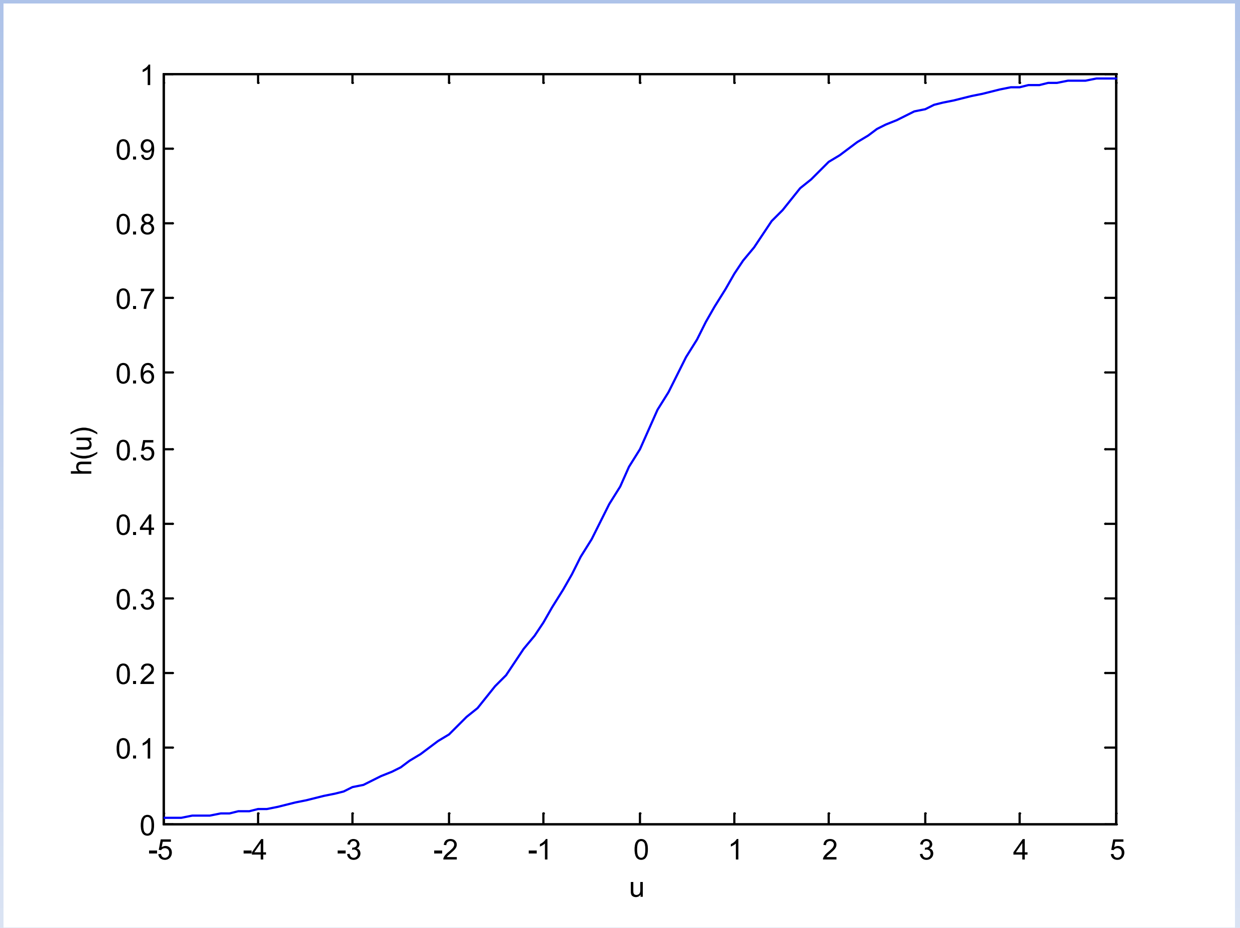
$$h(\mathbf{x};\mathbf{w},\mathbf{c},\beta) = e^{\beta\left\|\mathbf{w}\bullet\mathbf{x}-\mathbf{c}\right\|^2}$$

- Hyperbolic Tangent

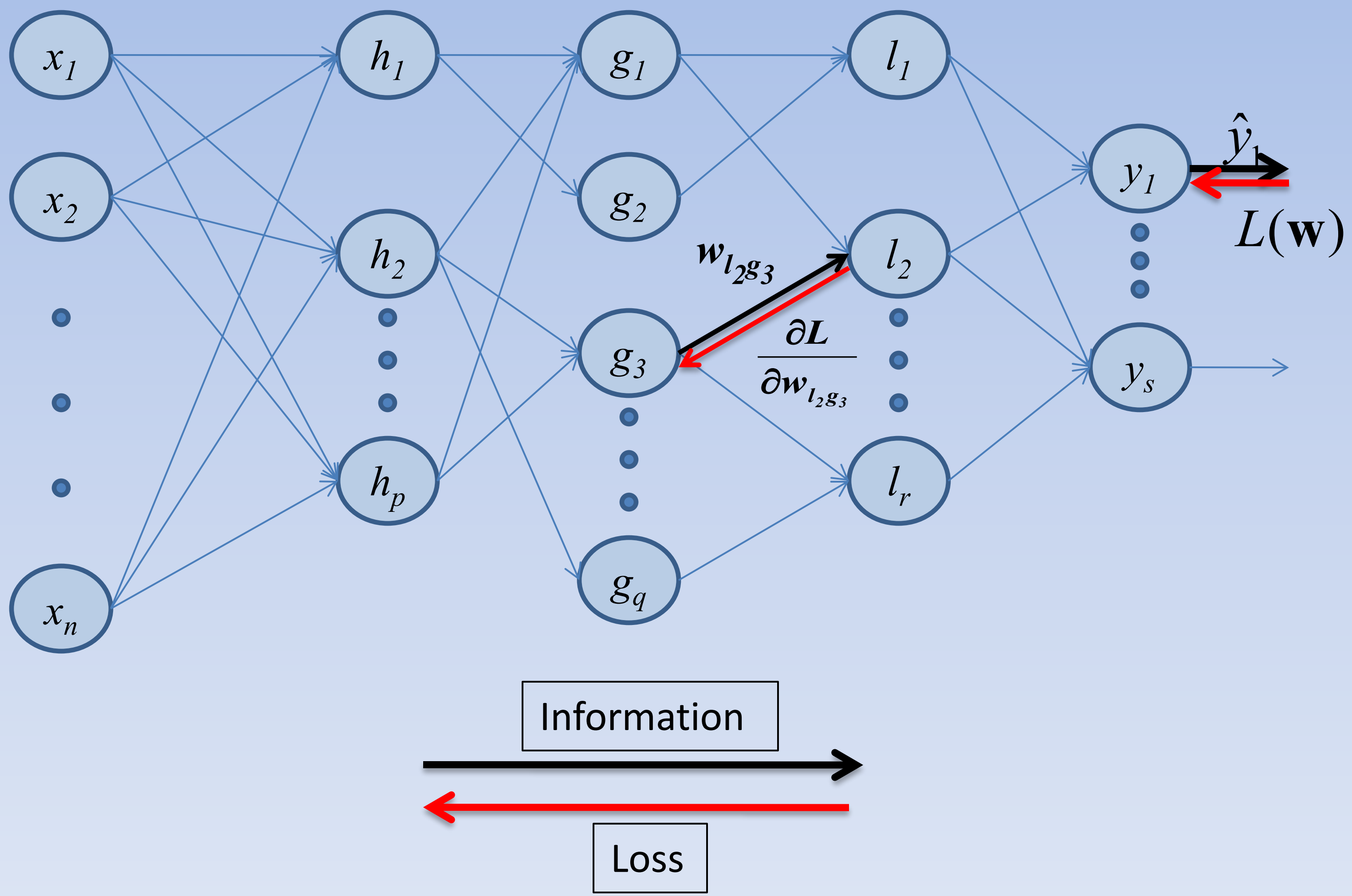
$$h(\mathbf{x};\mathbf{w},a,b) = a\,\frac{(e^{b\mathbf{w}\bullet\mathbf{x}} - e^{-b\mathbf{w}\bullet\mathbf{x}})}{(e^{b\mathbf{w}\bullet\mathbf{x}} + e^{-b\mathbf{w}\bullet\mathbf{x}})}$$

Activation Function: Sigmoid

$$h(u) = (1 + e^{-u})^{-1}$$



Backpropagation



Backpropagation

- Feed the examples forward through the network, observe the output and calculate the loss
- Perform “layer-wise” gradient descent on the loss function with respect to each weight, starting with output layer
  - For each weight in each layer, calculate its contribution to the overall loss using the chain rule
  - Update the weight in the negative gradient direction