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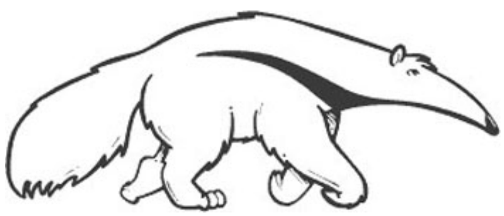
Machine Learning and Data Mining

Multi-layer Perceptrons & Neural Networks: Basics

Prof. Alexander Ihler



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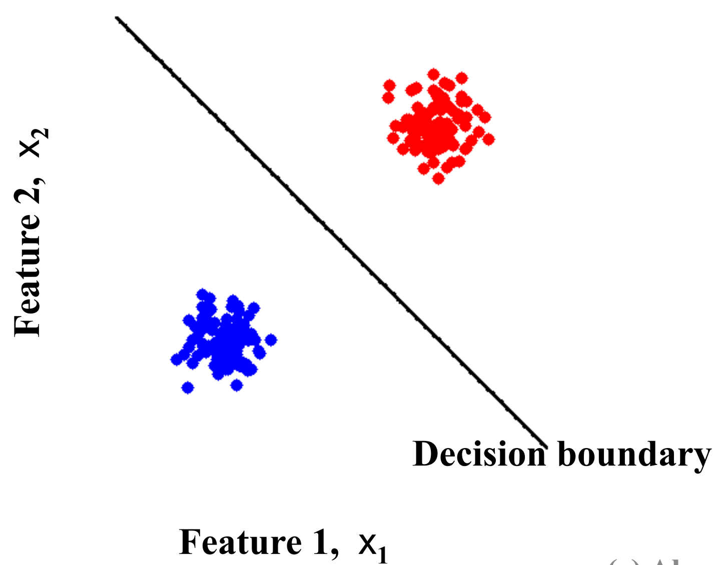
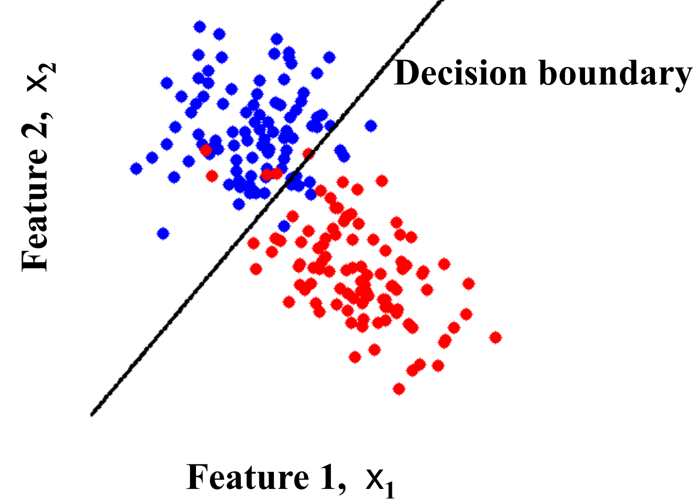
Linear Classifiers (Perceptrons)

- Linear Classifiers
  - a linear classifier is a mapping which partitions feature space using a linear function (a straight line, or a hyperplane)
  - separates the two classes using a straight line in feature space
  - in 2 dimensions the decision boundary is a straight line

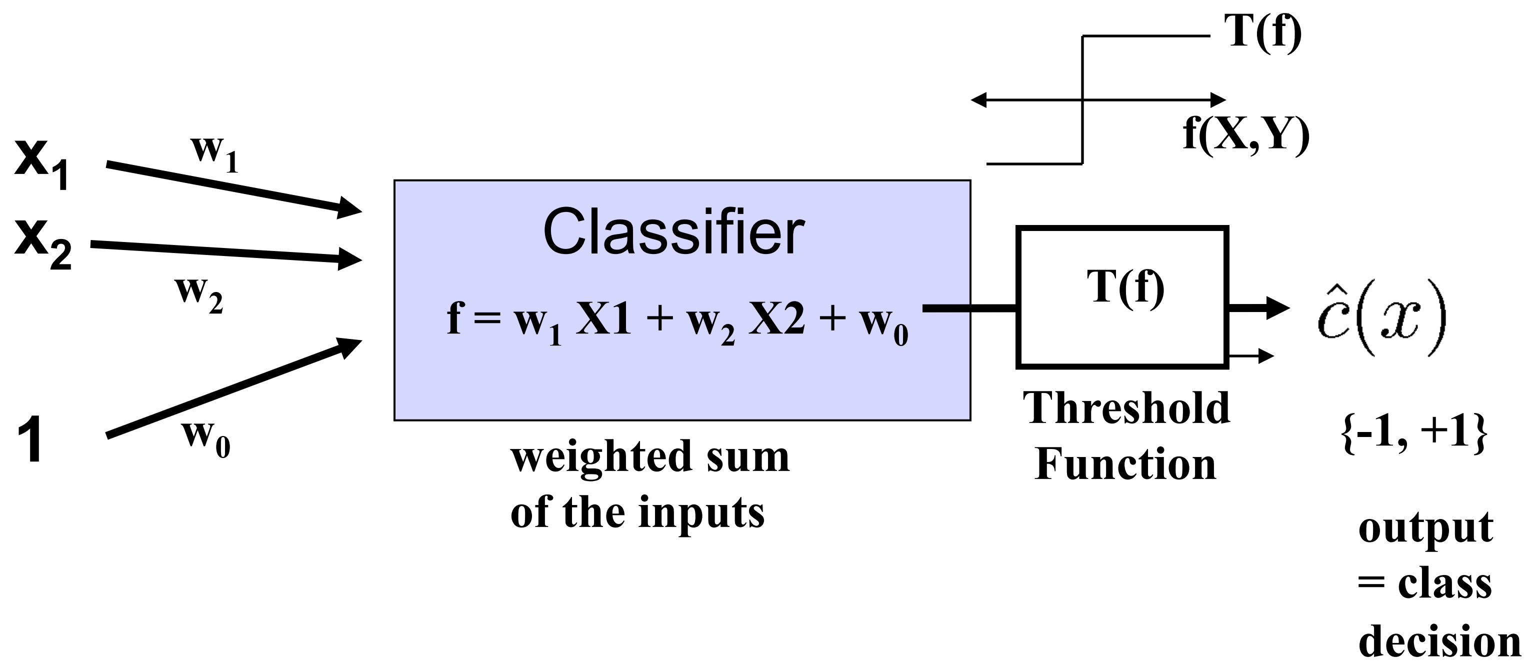
Linearly separable data



Linearly non-separable data



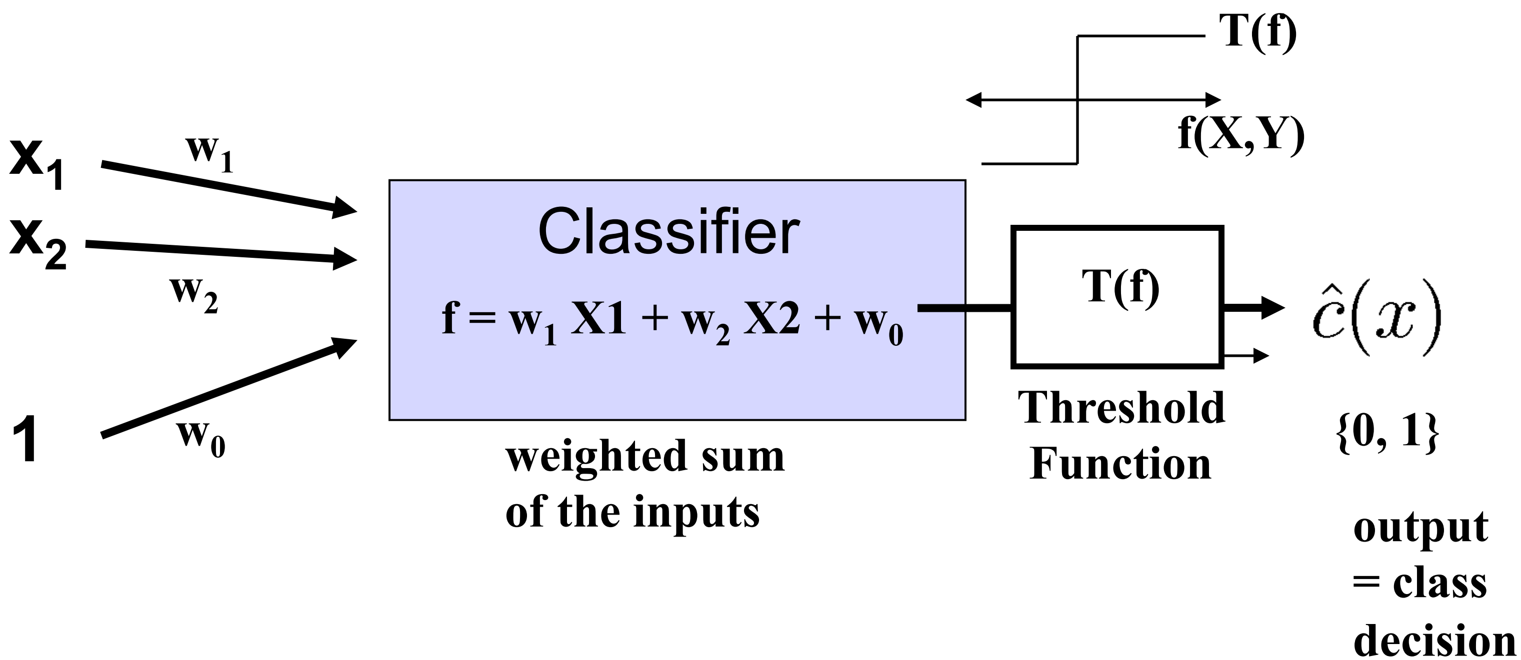
Perceptron Classifier (2 features)



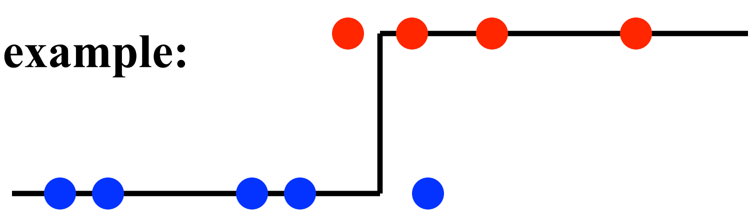
Decision Boundary at $f(x) = 0$

Solve: $X_2 = -w_1/w_2\, X_1 - w_0/w_2$ (Line)

Perceptron (Linear classifier)



1D example:

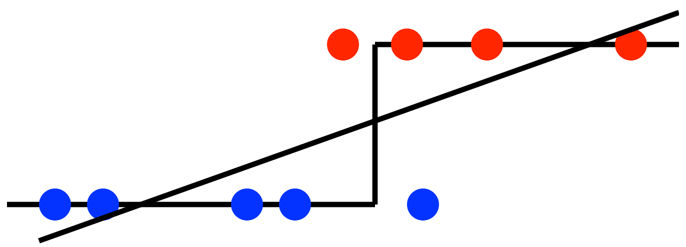


$T(f) = 0$ if $f < 0$
$T(f) = 1$ if $f > 0$

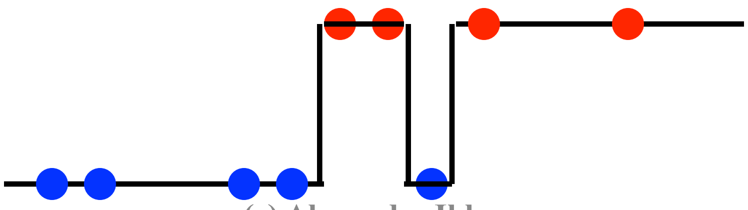
Decision boundary = "x such that T(w_1 x + w_0) transitions"

Features and perceptrons

- Recall the role of features
  - We can create extra features that allow more complex decision boundaries
  - Linear classifiers
  - Features [1,x]
    - Decision rule: T(ax+b) = ax + b >/< 0
    - Boundary ax+b =0 => point
  - Features [1,x,x^2]
    - Decision rule T(ax^2+bx+c)
    - Boundary ax^2+bx+c = 0 = ?



  - What features can produce this decision rule?

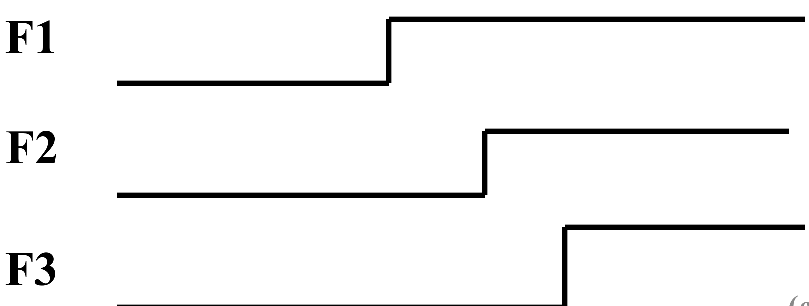


Features and perceptrons

- Recall the role of features
  - We can create extra features that allow more complex decision boundaries
  - For example, polynomial features

    $\Phi(x) = [1 \;\; x \;\; x^2 \;\; x^3 \; \ldots]$

- What other kinds of features could we choose?
  - Step functions?

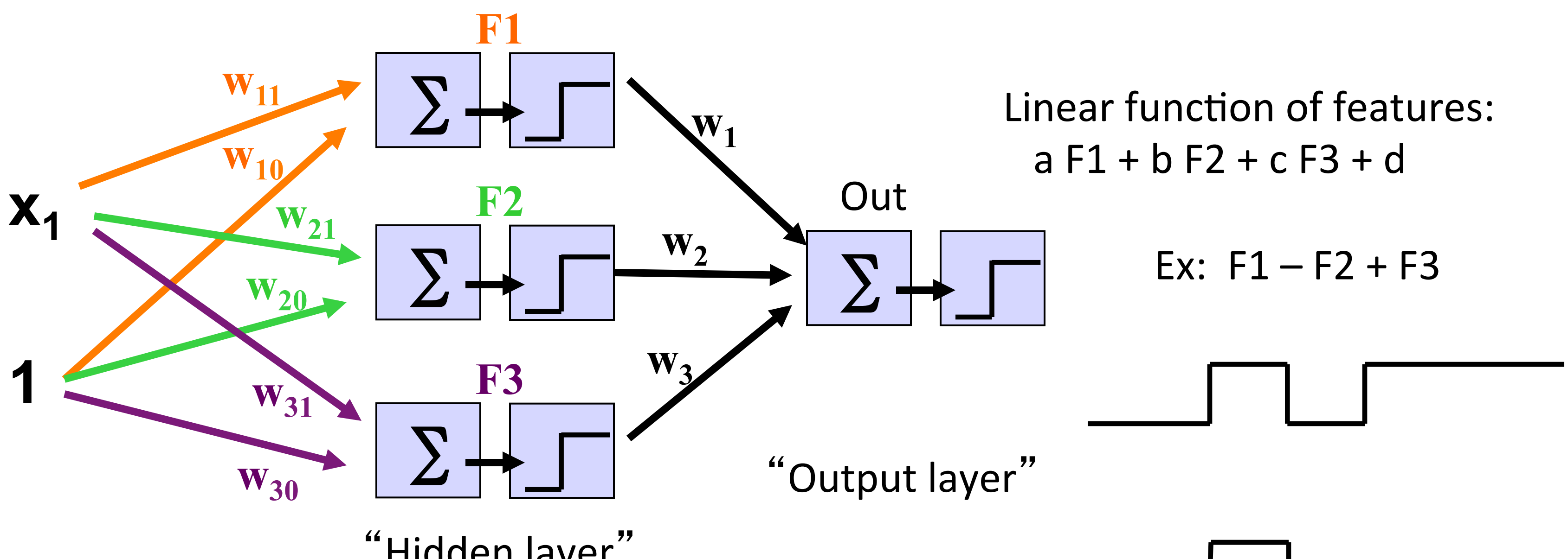


Linear function of features
a F1 + b F2 + c F3 + d

Ex: F1 – F2 + F3

Multi-layer perceptron model

- Step functions are just perceptrons!
  - "Features" are outputs of a perceptron
  - Combination of features output of another



$$W^1 = \begin{matrix} w_{10} & w_{11} \\ w_{20} & w_{21} \\ w_{30} & w_{31} \end{matrix} \qquad W^2 = \begin{matrix} w_1 \\ w_2 \\ w_3 \end{matrix}$$

Multi-layer perceptron model

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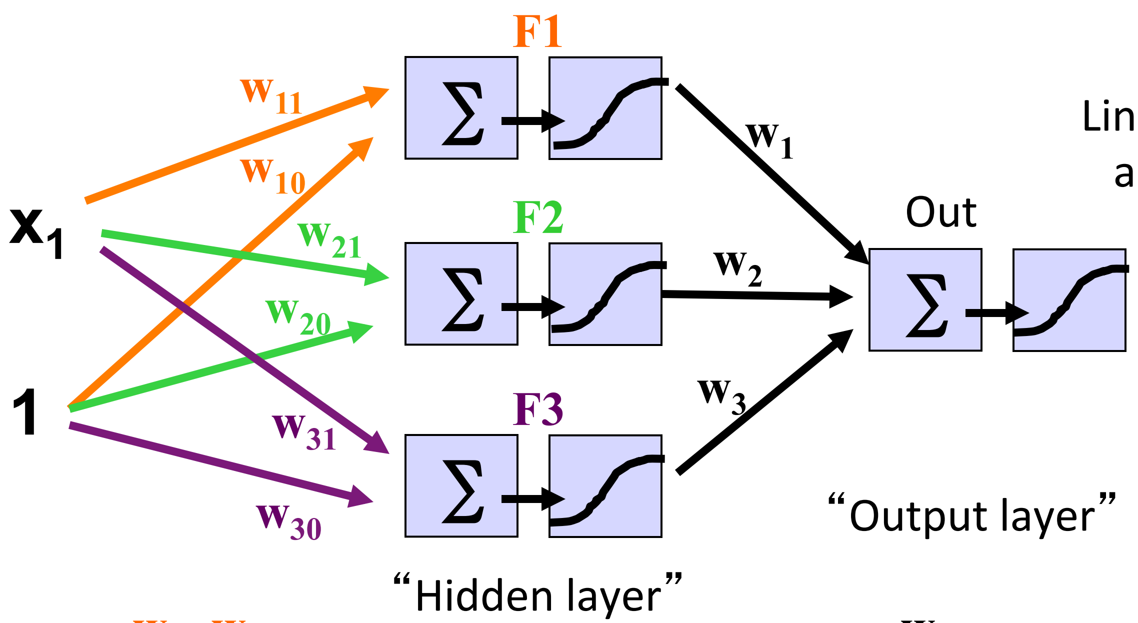
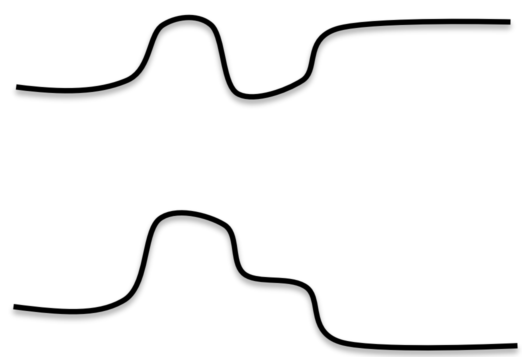
Regression version: Remove activation function from output



Linear function of features:
a F1 + b F2 + c F3 + d

Ex: F1 – F2 + F3



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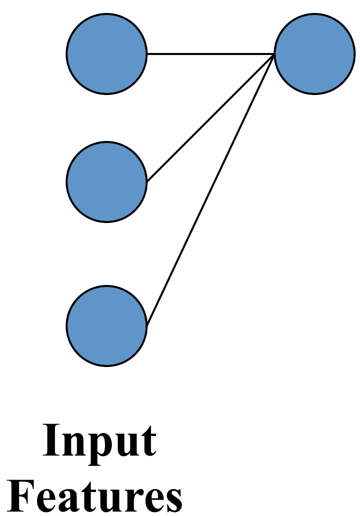
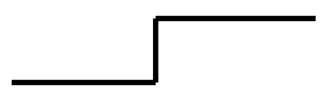
Features of MLPs

- Simple building blocks
  - Each element is just a perceptron f'n

- Can build upwards





Perceptron:
Step function /
Linear partition

Features of MLPs

- Simple building blocks
  - Each element is just a perceptron f’n

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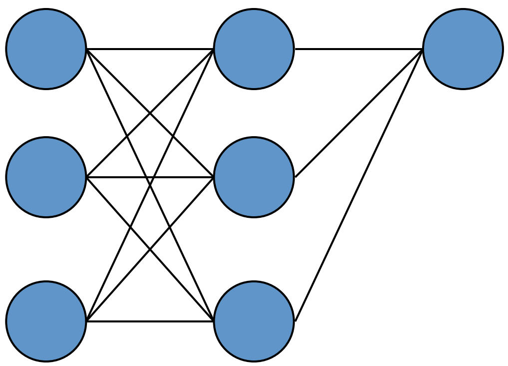
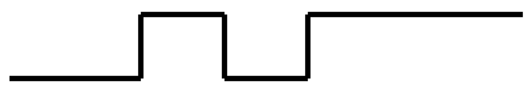


Input Features **Layer 1**

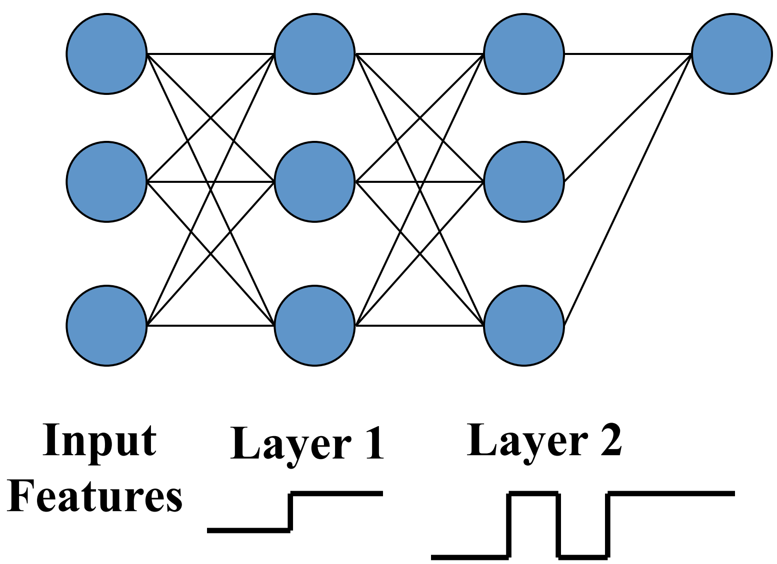


2-layer:
“Features” are now partitions
All linear combinations of those partitions

Features of MLPs

- Simple building blocks
  - Each element is just a perceptron f'n

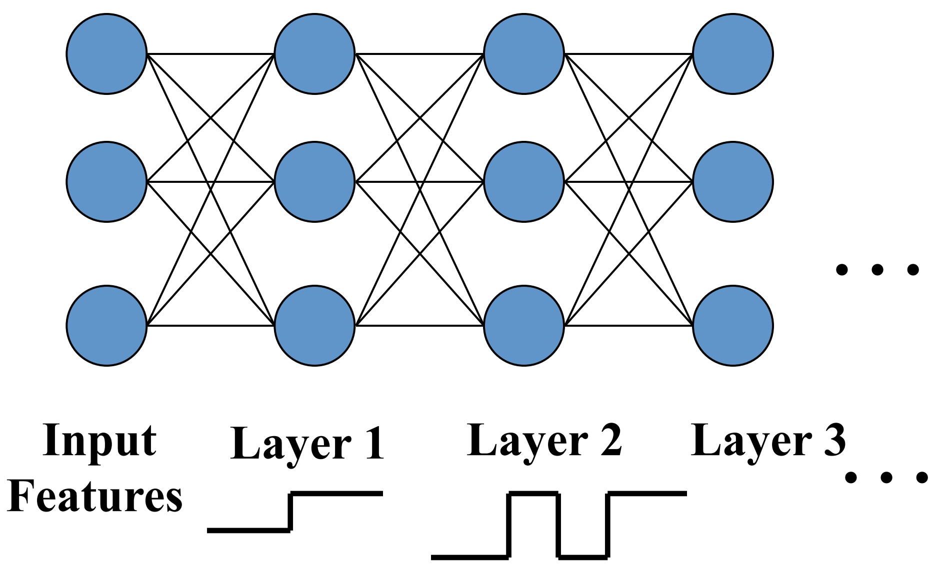
- Can build upwards



3-layer:
"Features" are now complex functions
Output any linear combination of those

Features of MLPs

- Simple building blocks
  - Each element is just a perceptron f' n
- Can build upwards



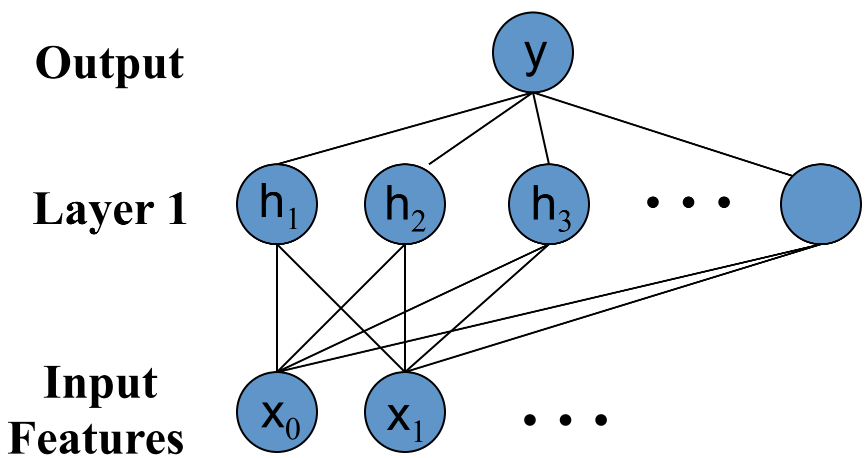
Current research:
"Deep" architectures
(many layers)

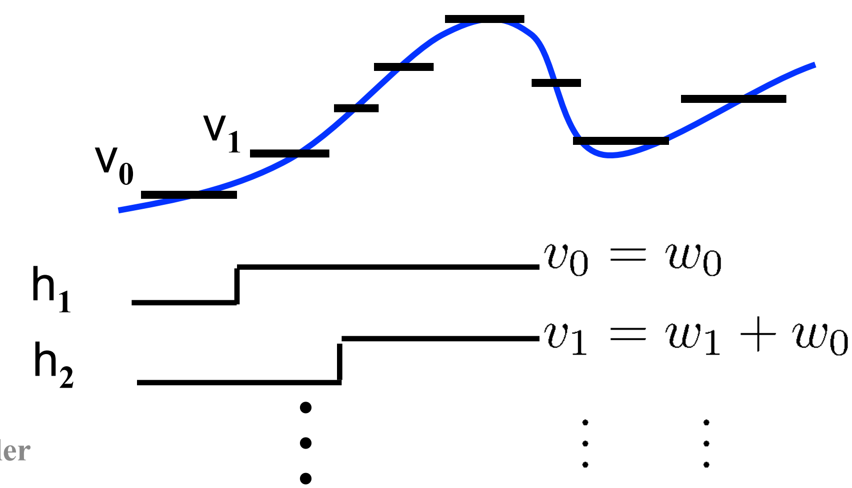
Features of MLPs

- Simple building blocks
  - Each element is just a perceptron function

- Can build upwards

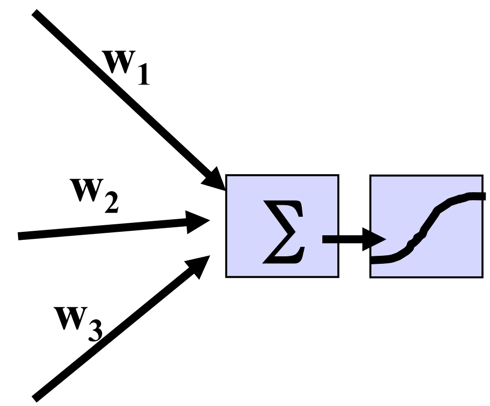
- Flexible function approximation
  - Approximate arbitrary functions with enough hidden nodes



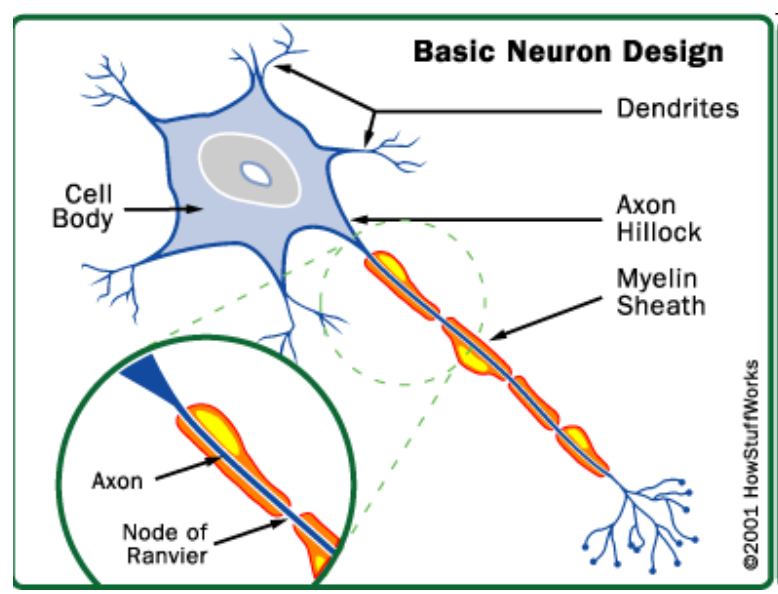


Neural networks

- Another term for MLPs
- Biological motivation

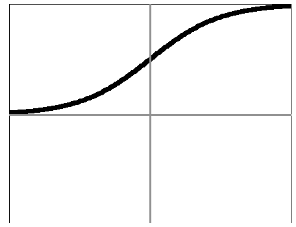
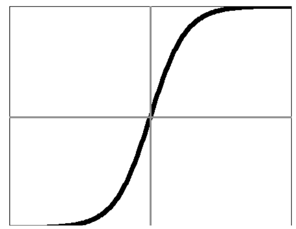
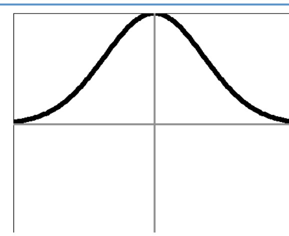
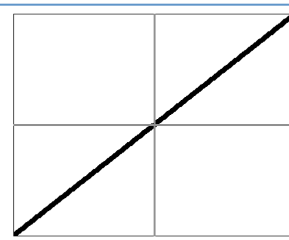


- Neurons
  - "Simple" cells
  - Dendrites sense charge
  - Cell weighs inputs
  - "Fires" axon



"How stuff works: the brain"

Activation functions

Logistic	$\sigma(z) = \frac{1}{1+\exp(-z)}$		$\frac{\partial\sigma}{\partial z}(z) = \sigma(z)(1-\sigma(z))$
Hyperbolic Tangent	$\sigma(z) = \frac{1-\exp(-2z)}{1+\exp(-2z)}$		$\frac{\partial\sigma}{\partial z}(z) = 1-(\sigma(z))^2$
Gaussian	$\sigma(z) = \exp(-z^2/2)$		$\frac{\partial\sigma}{\partial z}(z) = -z\sigma(z)$
Linear	$\sigma(z) = z$		$\frac{\partial\sigma}{\partial z}(z) = 1$

And others…

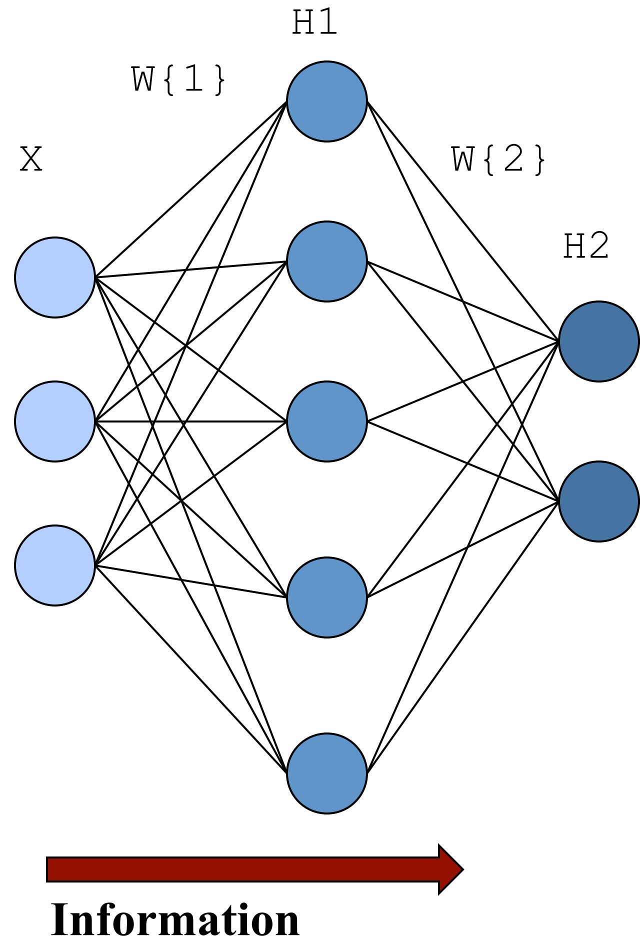
Feed-forward networks

- Information flows left-to-right
  - Input observed features
  - Compute hidden nodes (parallel)
  - Compute next layer…

```
X1 = [ones(m,1) X];   % constant feature
T  = W1 * X1;         % linear response
H  = Sig( T );        % activation f'n

H1 = [ones(m,1) H];   % constant feature
S  = W2 * H1;         % linear response
H2 = Sig( S );        % activation f'n

% ...
```

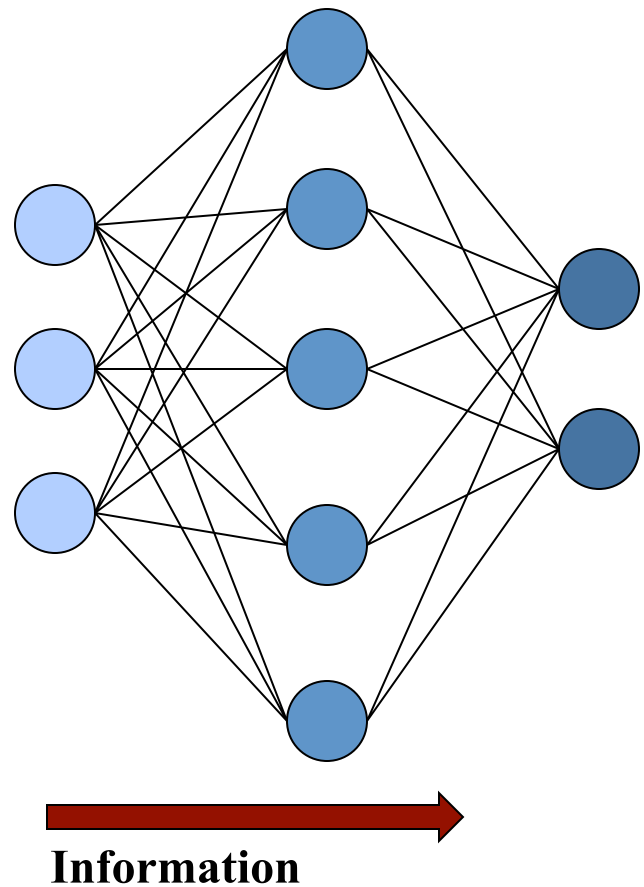


- Alternative: recurrent NNs…

Feed-forward networks

A note on multiple outputs:

- Regression:
  - Predict multi-dimensional y
  - "Shared" representation
    = fewer parameters
- Classification
  - Predict binary vector
  - Multi-class classification
    y = 2 = [0 0 1 0 …]
  - Multiple, joint binary predictions
    (image tagging, etc.)
  - Often trained as regression (MSE),
    with saturating activation



Machine Learning and Data Mining

Multi-layer Perceptrons & Neural Networks: Backpropagation

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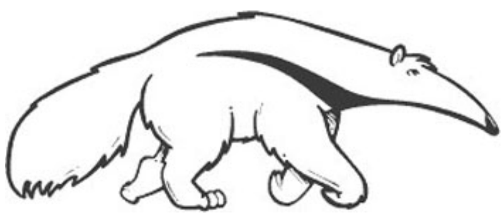

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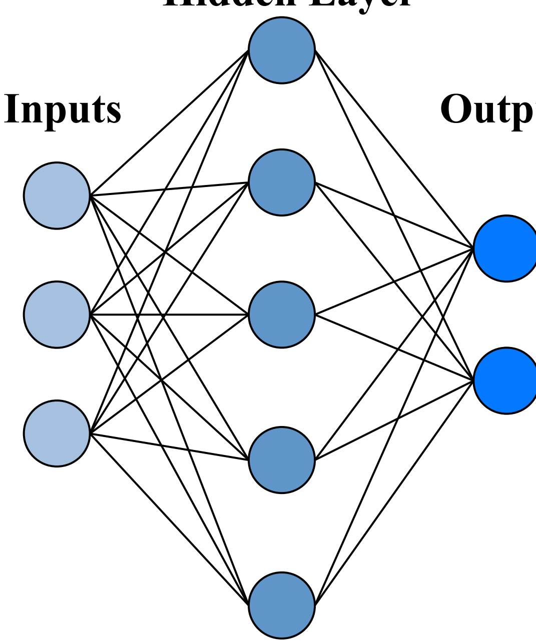
Training MLPs

- Observe features "x" with target "y"
- Push "x" through NN = output is "ŷ"
- Error: $(y - \hat{y})^2$ (Can use different loss functions if desired…)
- How should we update the weights to improve?

- Single layer
  - Logistic sigmoid function
  - Smooth, differentiable
- Optimize using:
  - Batch gradient descent
  - Stochastic gradient descent



Backpropagation

- Just gradient descent…
- Apply the chain rule to the MLP

$$\frac{\partial J}{\partial w_{kj}^2} = -2 \sum_{k'} (y_{k'} - \hat{y}_{k'})\ (\partial \hat{y}_{k'})$$

$$= -2(y_k - \hat{y}_k)\ \sigma'(s_k)\ h_j$$

(Identical to logistic mse regression with inputs "h_j")

Forward pass

Loss function

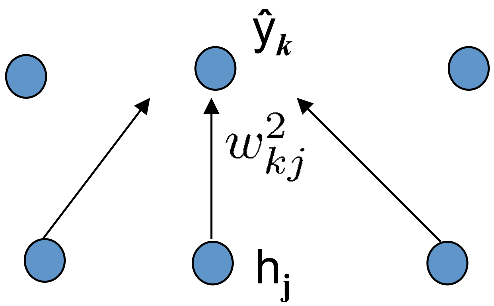
$$J_i(W) = \sum_k\ (y^{(i)} - \hat{y}_k^{(i)})^2$$

Output layer

$$\hat{y}_k = \sigma(s_k) = \sigma(\sum_j w_{kj}^2 h_j)$$

Hidden layer

$$h_j = \sigma(t_j) = \sigma(\sum_i w_{ji}^1 x_i)$$



Backpropagation

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$$\frac{\partial J}{\partial w^2_{kj}} = -2 \sum_{k'} (y_{k'} - \hat{y}_{k'}) \; (\partial \hat{y}_{k'})$$

$$= \underbrace{\boxed{-2(y_k - \hat{y}_k) \; \sigma'(s_k)}}_{\beta^2_k} \; h_j$$

(Identical to logistic mse regression with inputs "h_j")

Forward pass

Loss function

$$J_i(W) = \textstyle\sum_k \; (y^{(i)} - \hat{y}^{(i)}_k)^2$$

Output layer

$$\hat{y}_k = \sigma(s_k) = \sigma(\textstyle\sum_j w^2_{kj} h_j)$$

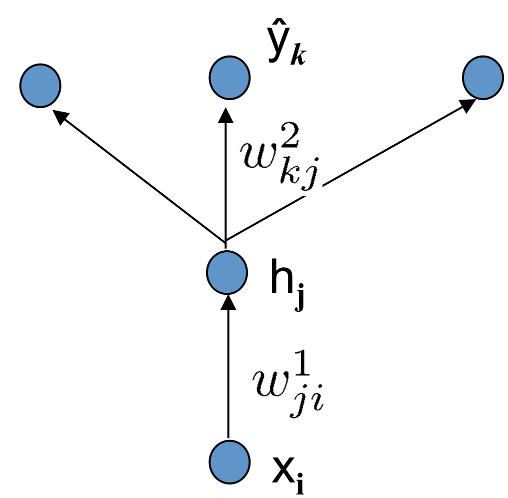
Hidden layer

$$h_j = \sigma(t_j) = \sigma(\textstyle\sum_i w^1_{ji} x_i)$$

$$\frac{\partial J}{\partial w^1_{ji}} = \sum_k -2(y_k - \hat{y}_k) \; (\partial \hat{y}_k)$$

$$= \sum_k -2(y_k - \hat{y}_k) \; \sigma'(s_k) \; w_{kj} \; \partial h_j$$

$$= \sum_k \underbrace{\boxed{-2(y_k - \hat{y}_k) \; \sigma'(s_k)}}_{\beta^2_k} \; w_{kj} \; \sigma'(t_j) \; x_i$$



Backpropagation

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Forward pass

Loss function

$$J_i(W) = \sum_k (y^{(i)} - \hat{y}^{(i)}_k)^2$$

Output layer

$$\hat{y}_k = \sigma(s_k) = \sigma(\sum_j w^2_{kj} h_j)$$

Hidden layer

$$h_j = \sigma(t_j) = \sigma(\sum_i w^1_{ji} x_i)$$

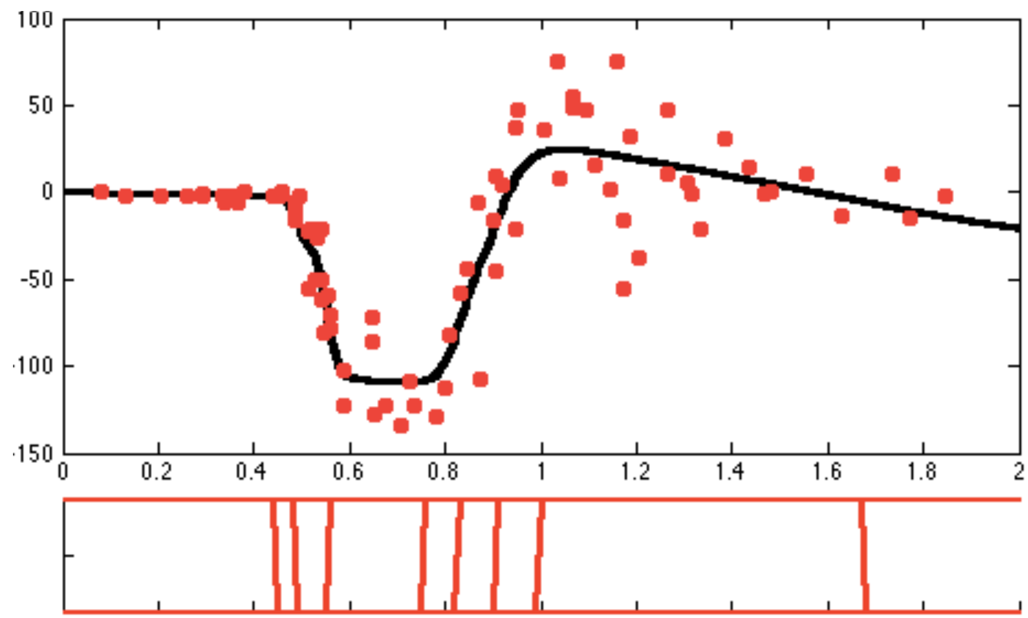
```
% X  : (1xN1)
H  = Sig( W1 * X1');
% W1 : (N2 x N1+1)
% H  : (1xN2)
Yh = Sig( W2 * H1');
% W2 : (N3 x N2+1)
% Yh : (1xN3)
```

```
B2 = (Y-Yhat) .* dSig(S);%(1xN3)

G2 = B' * H;             %(N3x1)*(1xN2)=(N3xN2)

B1 = (B*W2)' .* dSig(T); %(1xN3)*(N3*N2).*(1xN2)

G1 = B' * X;             %(N2 x N1+1)
```

Example: Regression, MCycle data

- Train NN model, 2 layer
  - 1 input features => 1 input units
  - 10 hidden units
  - 1 target => 1 output units
  - Logistic sigmoid activation for hidden layer, linear for output layer

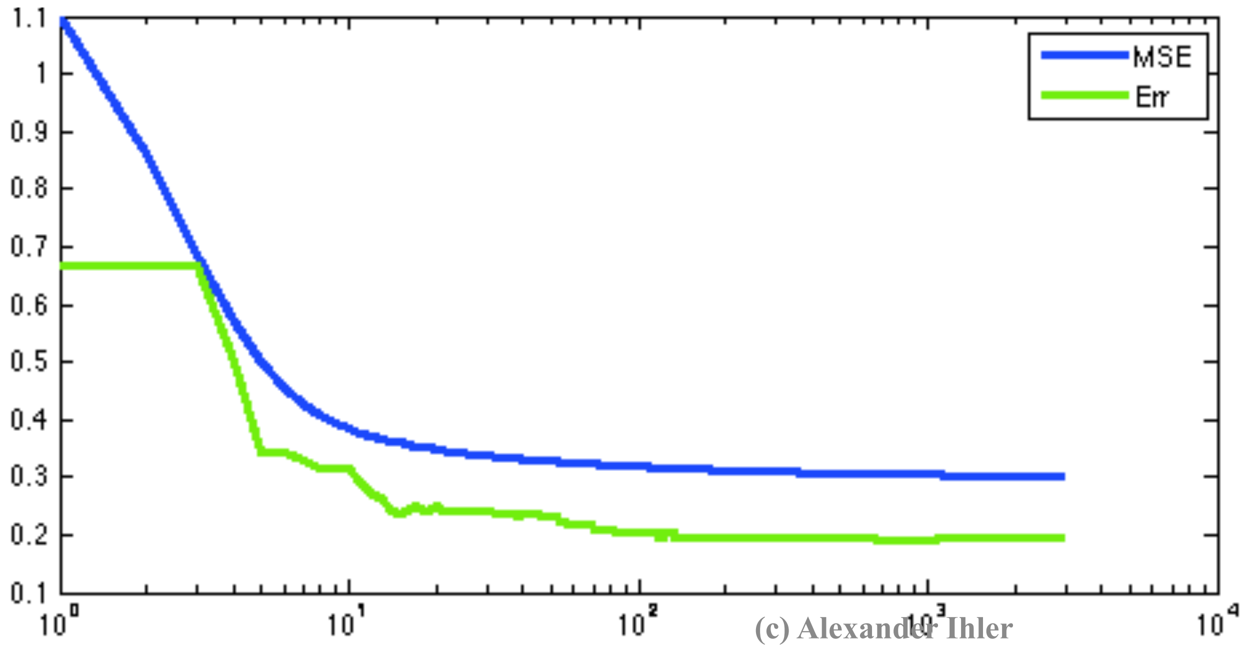
Data:
+
learned prediction f'n:

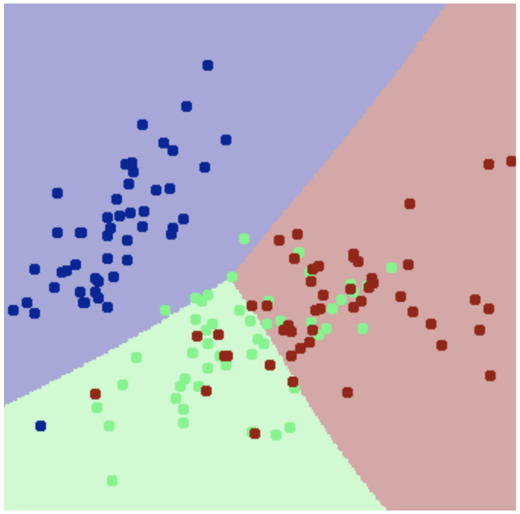


Responses of hidden nodes
(= features of linear regression):
select out useful regions of "x"

Example: Classification, Iris data

- Train NN model, 2 layer
  - 2 input features => 2 input units
  - 10 hidden units
  - 3 classes => 3 output units   (y = [0 0 1], etc.)
  - Logistic sigmoid activation functions
  - Optimize MSE of predictions using stochastic gradient

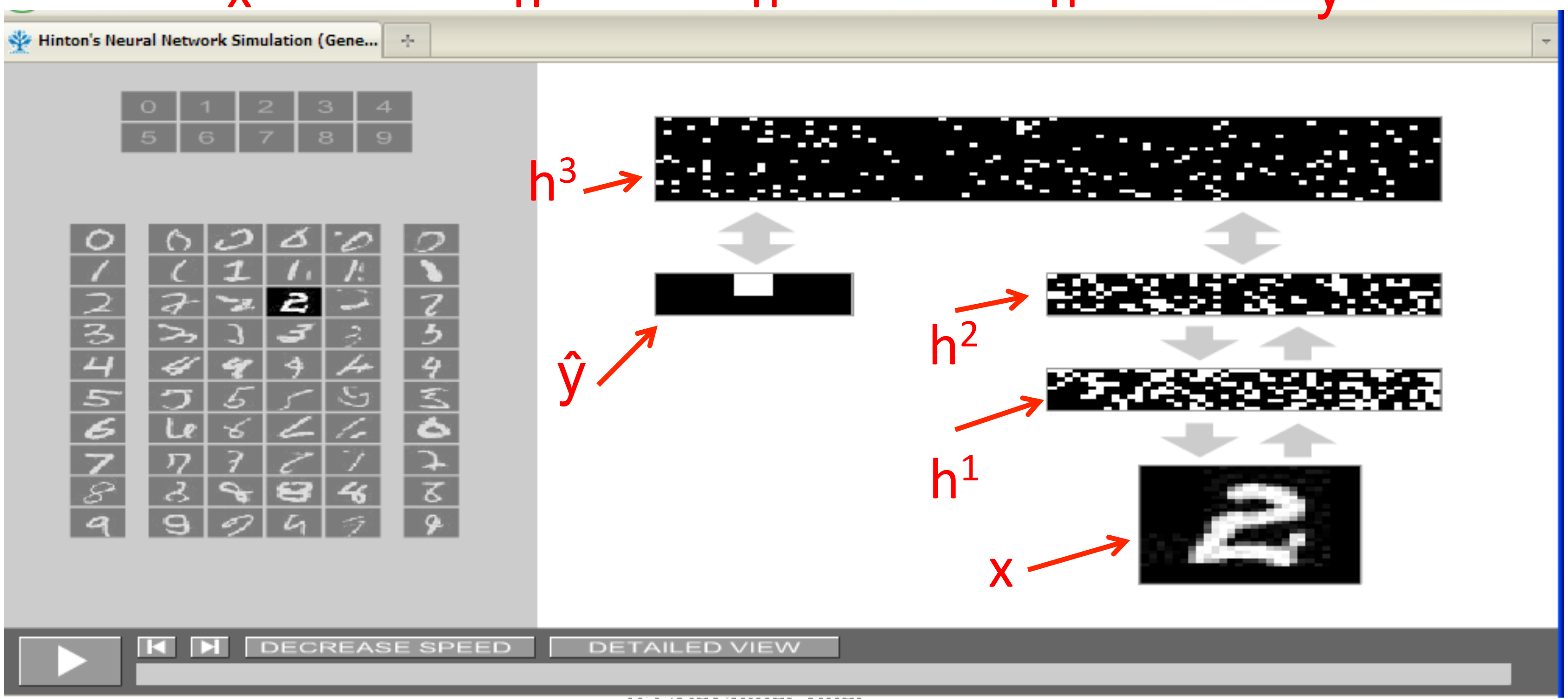




MLPs in practice

- Example: Deep belief nets (Hinton et al. 2007)
  - Handwriting recognition
  - Online demo
  - 784 pixels ⇔ 500 mid ⇔ 500 high ⇔ 2000 top ⇔ 10 labels

x h^1 h^2 h^3 $\hat{y}$



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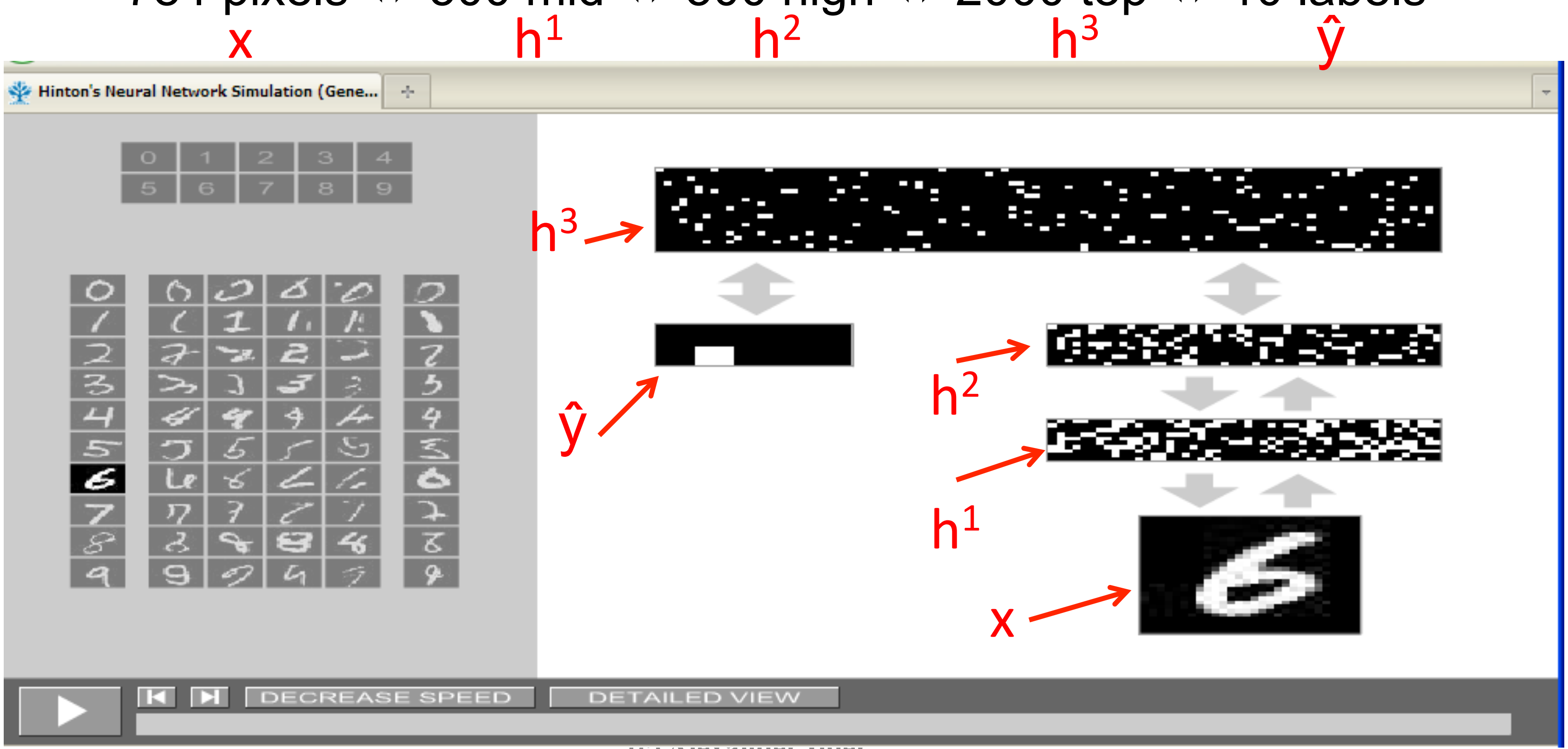

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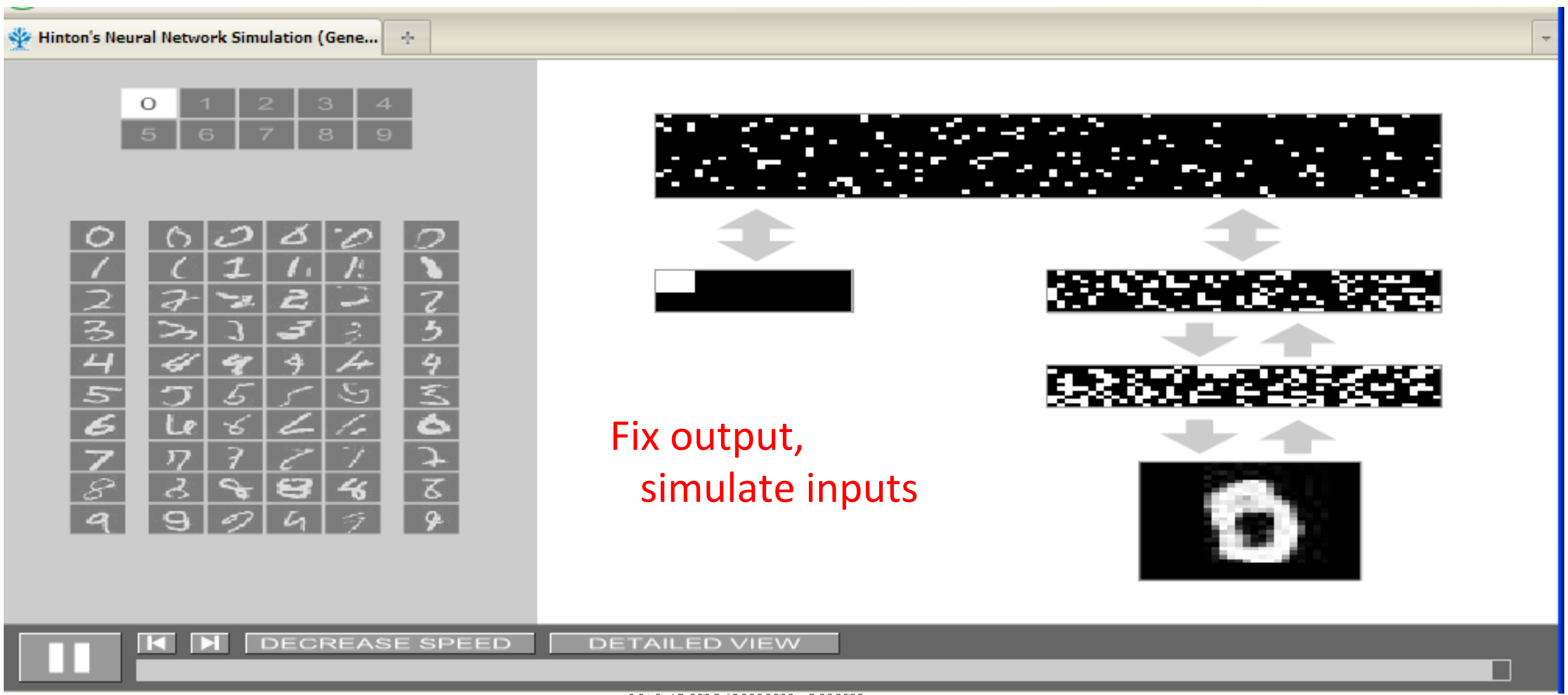

Neural networks & DBNs

- Want to try them out?
- Matlab "Deep Learning Toolbox"

  https://github.com/rasmusbergpalm/DeepLearnToolbox

  rasmusbergpalm / **DeepLearnToolbox**

  Matlab/Octave toolbox for deep learning. Includes Deep Belief Nets, Stacked Autoencoders, Convolutional Neural Nets, Convolutional Autoencoders and vanilla Neural Nets. Each method has examples to get you started.

- Also:
  - A built-in toolbox for Matlab: need a license…
  - Netlab: free but older, not updated in some time

Summary

- Neural networks, multi-layer perceptrons
- Cascade of simple perceptrons
  - Each just a linear classifier
  - Hidden units used to create new features
- Together, general function approximators
  - Enough hidden units (features) = any function
  - Can create nonlinear classifiers
  - Also used for function approximation, regression, …
- Training via backprop
  - Gradient descent; logistic; apply chain rule