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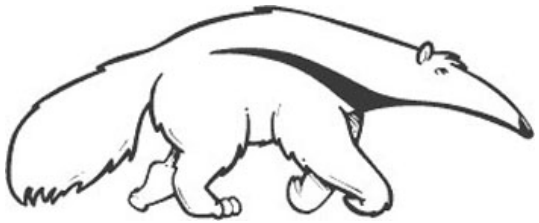
CS178: Machine Learning and Data Mining

Neural Networks

Prof. Alexander Ihler



Machine Learning

Multi-Layer Perceptrons

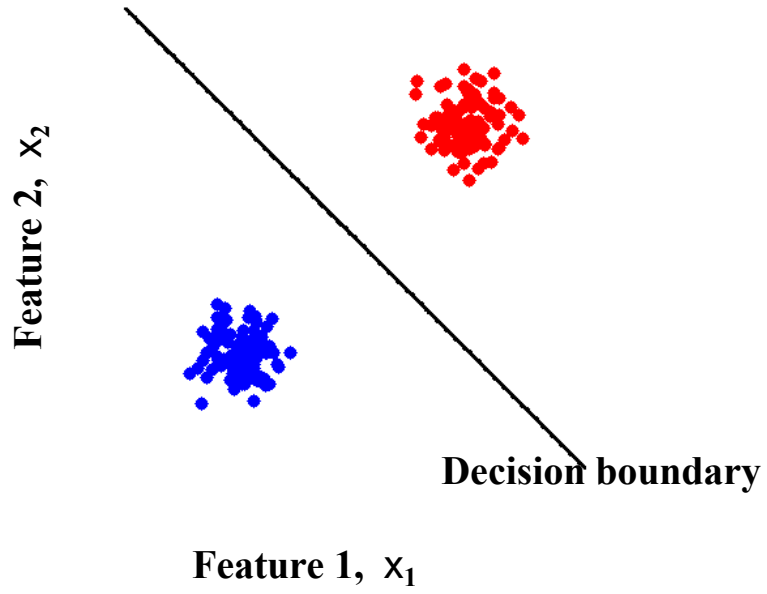
Backpropagation Learning

Convolutional Neural Networks

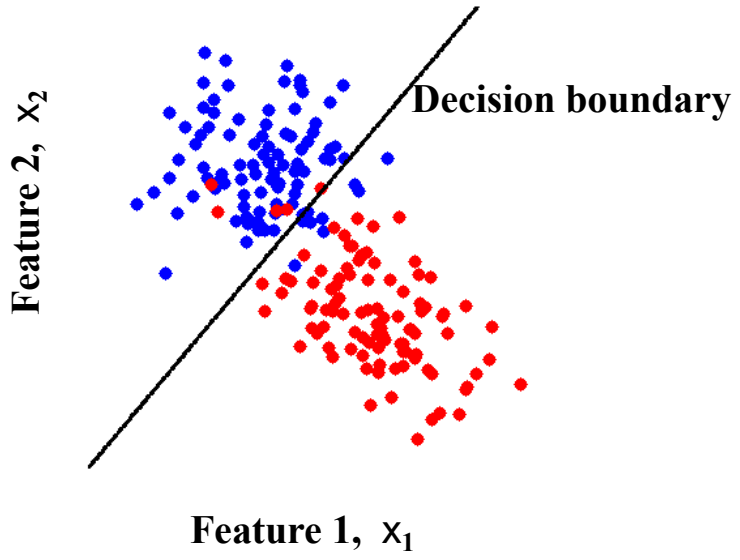
Linear classifiers (perceptrons)

- 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

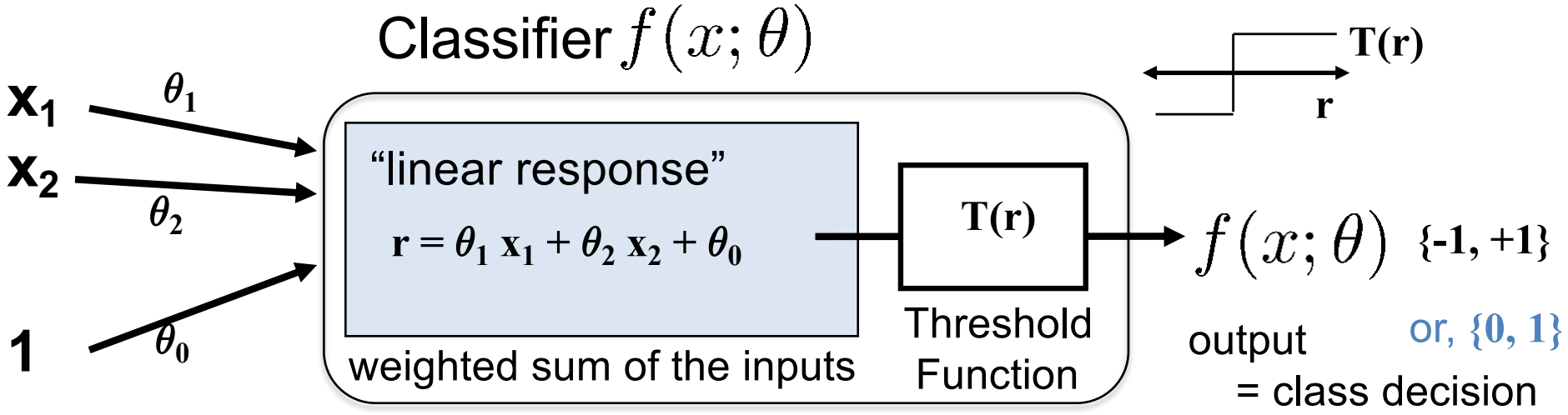
Linearly separable data



Linearly non-separable data



Perceptron Classifier (2 features)

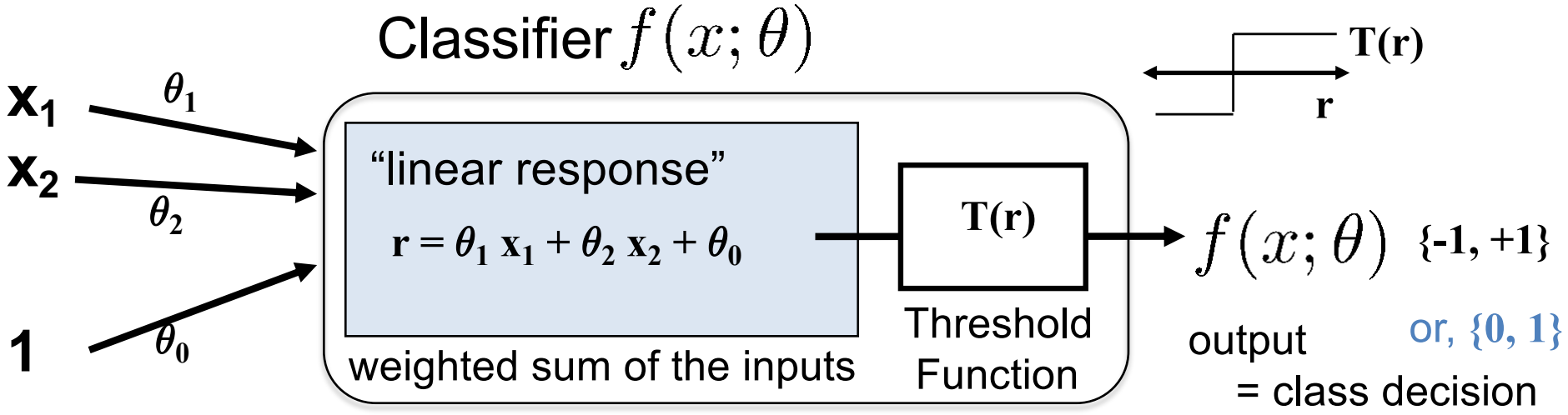



```
r = X.dot( theta.T )          # compute linear response
Yhat = 2*(r > 0)-1            # "sign": predict +1 / -1
```

Decision Boundary at r(x) = 0

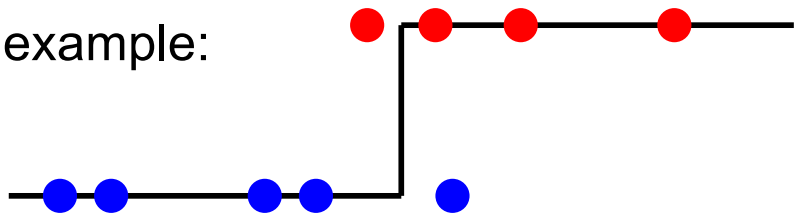
Solve: $X_2 = -w_1/w_2\ X_1 - w_0/w_2$ (Line)

Perceptron Classifier (2 features)




```
r = X.dot( theta.T )          # compute linear response
Yhat = 2*(r > 0)-1            # "sign": predict +1 / -1
```

1D example:

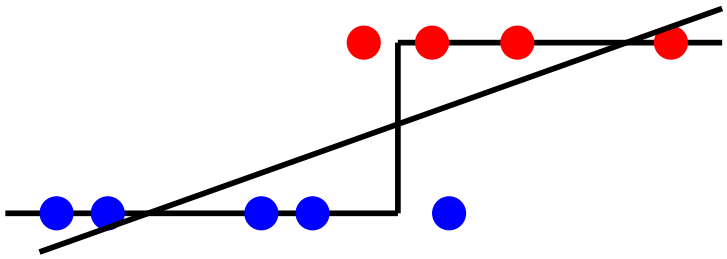


T(r) = -1 if r < 0
T(r) = +1 if r > 0

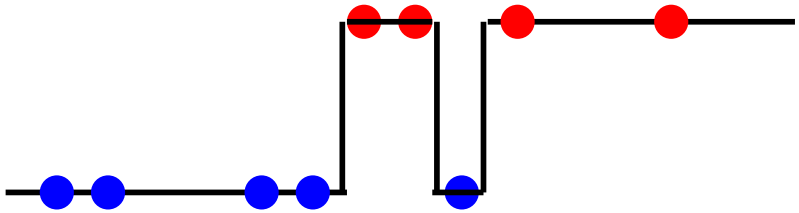
Decision boundary = "x such that T(w_1 x + w_0) transitions"

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?

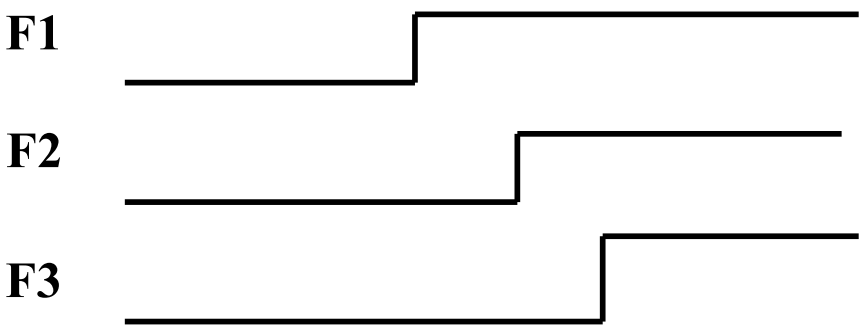


Features and perceptrons

- 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?

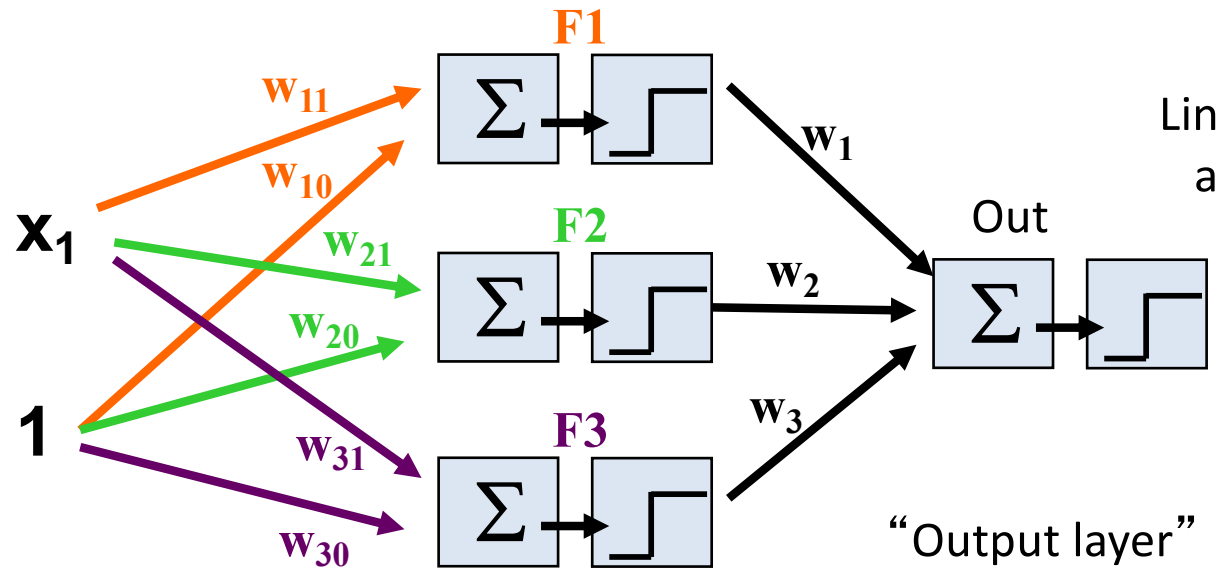


Linear function of features
a F1 + b F2 + c F3 + d

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



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

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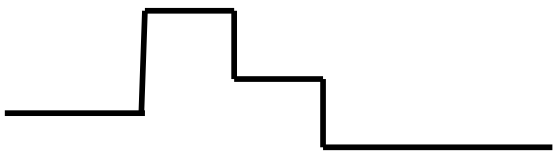


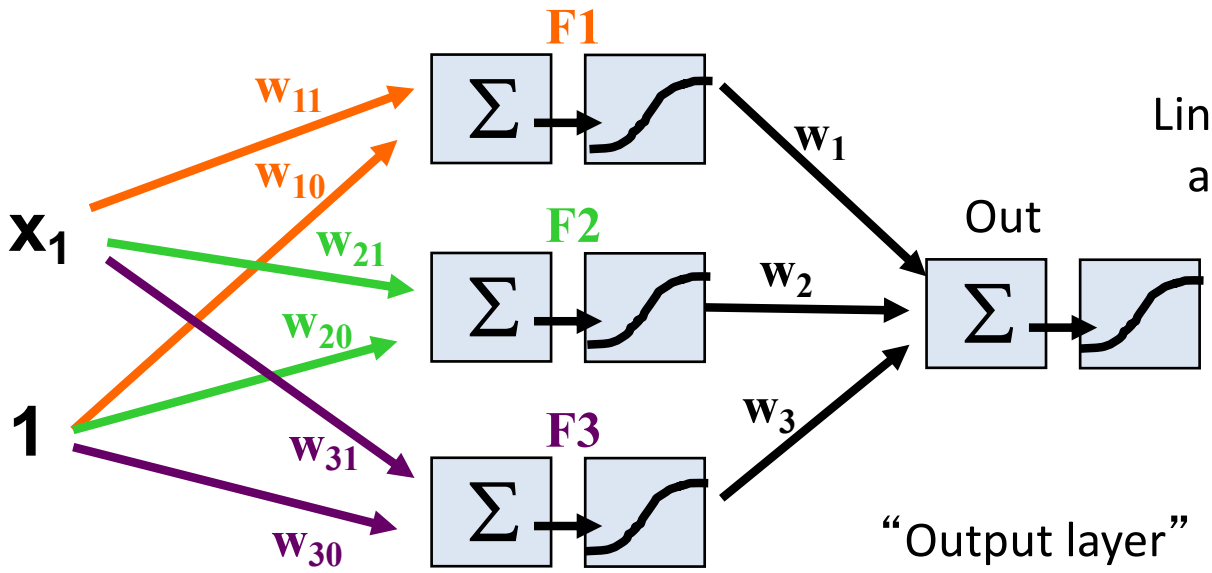
$$W^1 = \begin{matrix} w_{10} & w_{11} \\ w_{20} & w_{21} \\ w_{30} & w_{31} \end{matrix}$$

$$W^2 = w_1 \; w_2 \; w_3$$

Multi-layer perceptron model

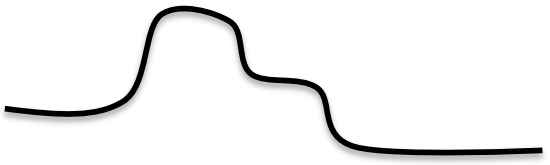
- Step functions are just perceptrons!
  - "Features" are outputs of a perceptron
  - Combination of features output of another

Regression version:
Remove activation function from output



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

Ex: F1 – F2 + F3

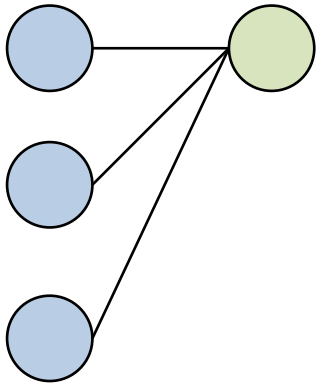


$$W^1 = \begin{matrix} w_{10} & w_{11} \\ w_{20} & w_{21} \\ w_{30} & w_{31} \end{matrix}$$

$$W^2 = w_1 \; w_2 \; w_3$$

Features of MLPs

- Simple building blocks
  - Each element is just a perceptron function
- Can build upwards

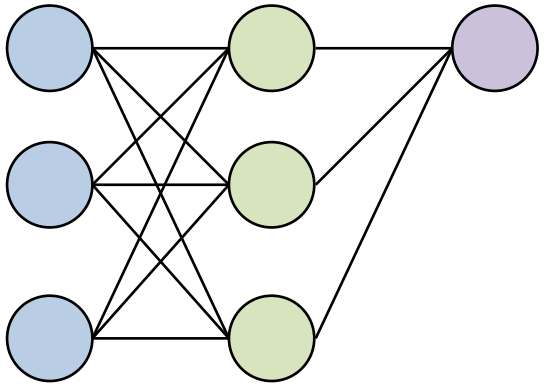


Input Features

Perceptron:
Step function /
Linear partition

Features of MLPs

- Simple building blocks
  - Each element is just a perceptron function
- Can build upwards

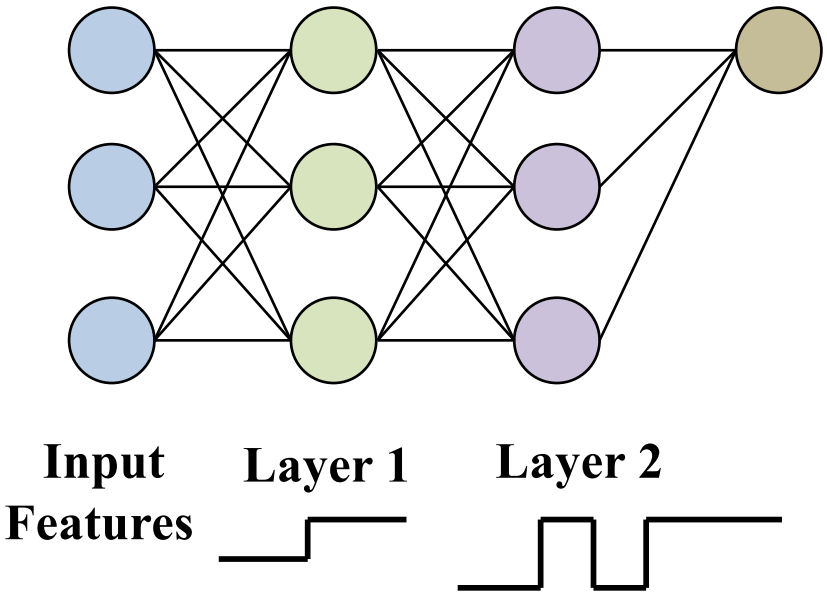


Input Features **Layer 1**

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

Features of MLPs

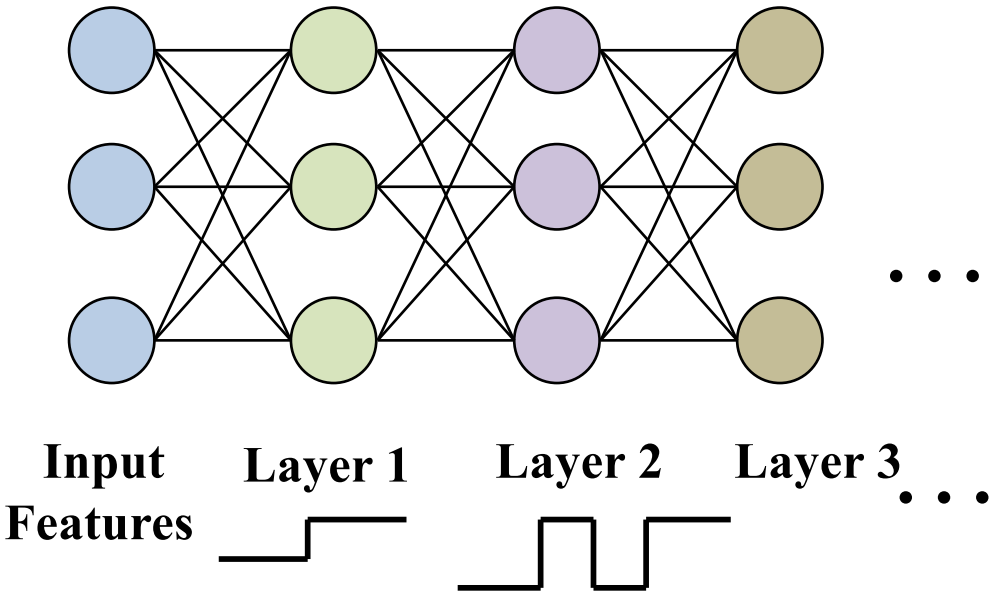
- Simple building blocks
  - Each element is just a perceptron function
- Can build upwards



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

Features of MLPs

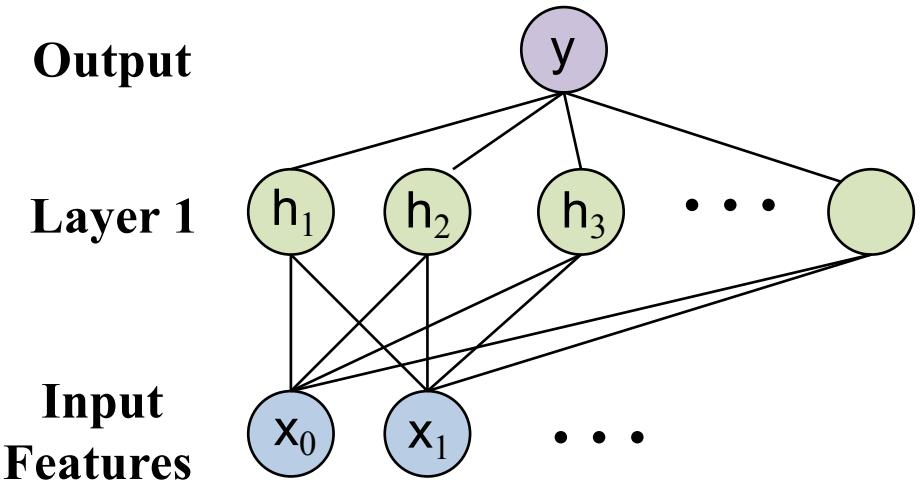
- Simple building blocks
  - Each element is just a perceptron function
- Can build upwards

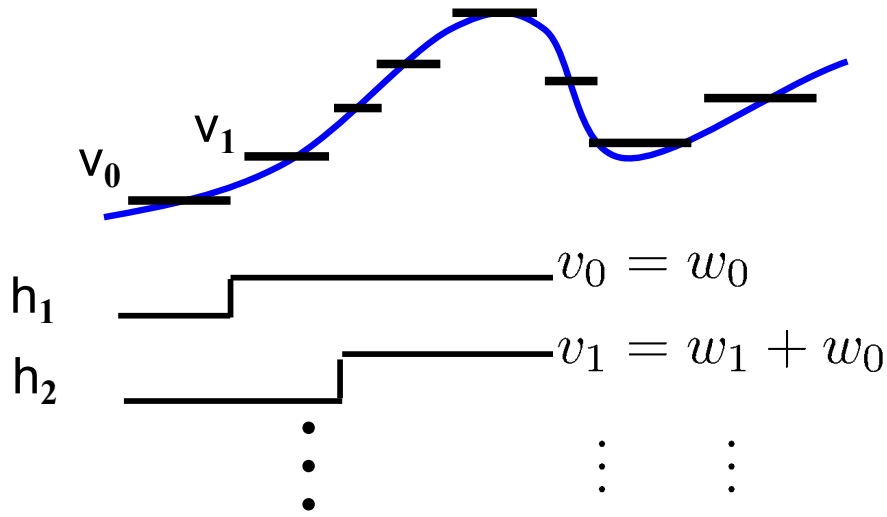


Current research:
"Deep" architectures
(many layers)

Features of MLPs

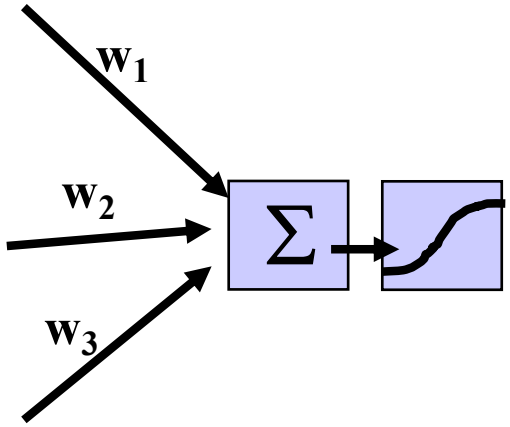
- Simple building blocks
  - Each element is just a perceptron function
- Can build upwards
- Flexible function approximation
  - Approximate arbitrary functions with enough hidden nodes



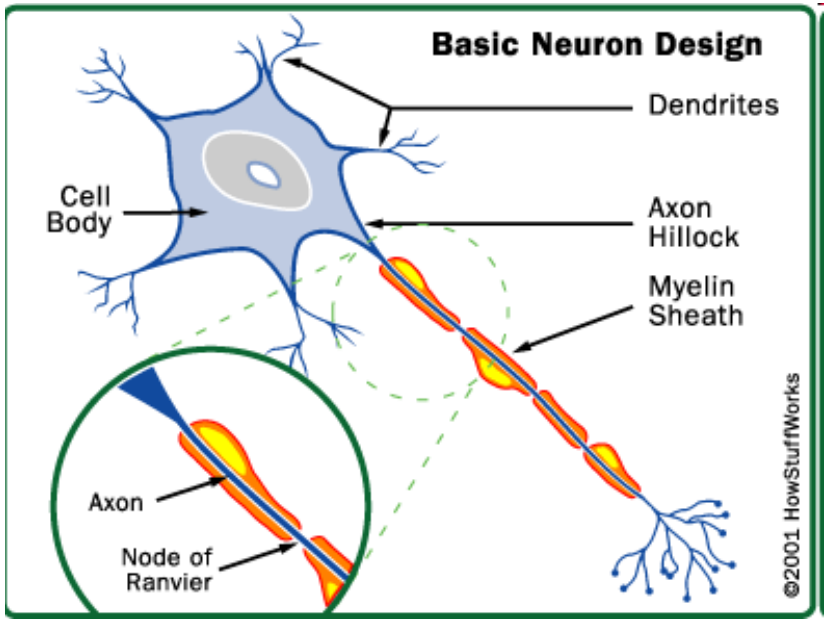


Neural networks

- Another term for MLPs
- Biological motivation

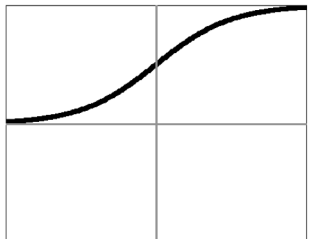
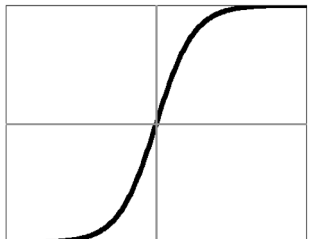
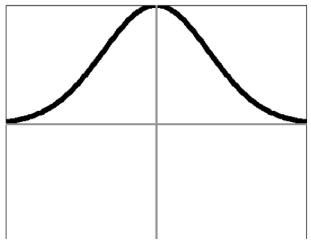
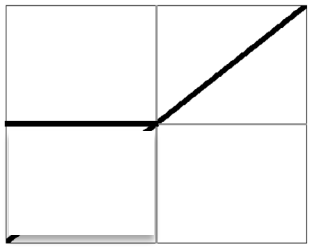


- Neurons
  - "Simple" cells
  - Dendrites sense charge
  - Cell weighs inputs
  - "Fires" axon



"How stuff works: the brain"

Activation functions

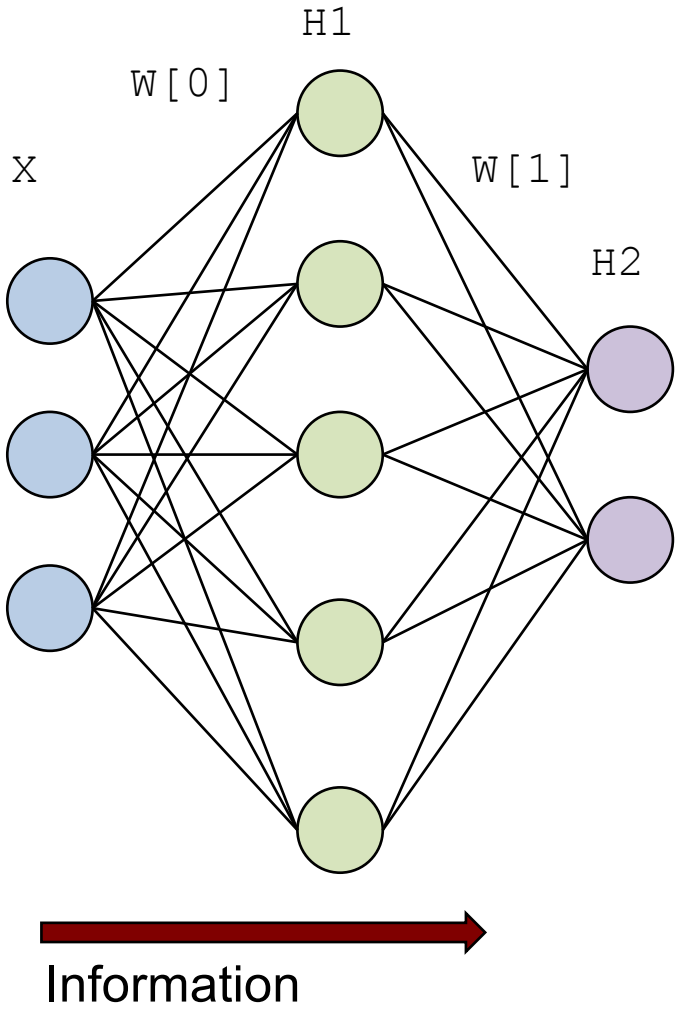
Logistic	$\sigma(z) = \frac{1}{1+\exp(-z)}$		$\frac{\partial \sigma}{\partial z}(z) = \sigma(z)(1-\sigma(z))$
Hyperbolic Tangent	$\sigma(z) = \frac{1-\exp(-2z)}{1+\exp(-2z)}$		$\frac{\partial \sigma}{\partial z}(z) = 1-(\sigma(z))^2$
Gaussian	$\sigma(z) = \exp(-z^2/2)$		$\frac{\partial \sigma}{\partial z}(z) = -z\sigma(z)$
ReLU (rectified linear)	$\sigma(z) = \max(0, z)$		$\frac{\partial \sigma}{\partial z}(z) = \mathbb{1}[z > 0]$
Linear	$\sigma(z) = z$		and many others…

Feed-forward networks

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

```
R = X.dot(W[0])+B[0] # linear response
H1= Sig( R )         # activation f'n

S = H1.dot(W[1])+B[1] # linear response
H2 = Sig( S )         # activation f'n
```

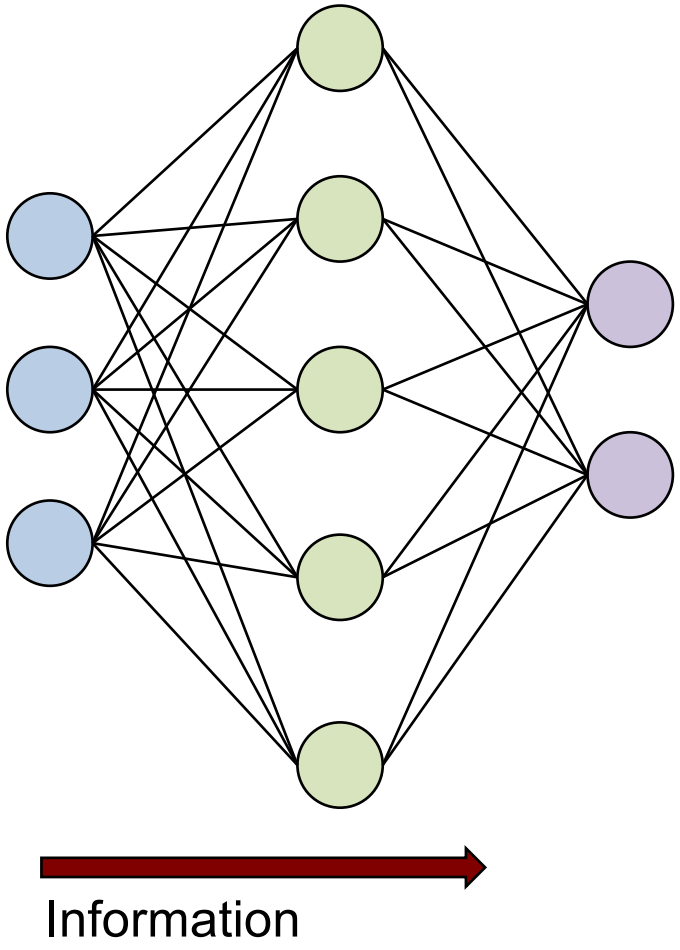


Feed-forward networks

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

Multi-Layer Perceptrons

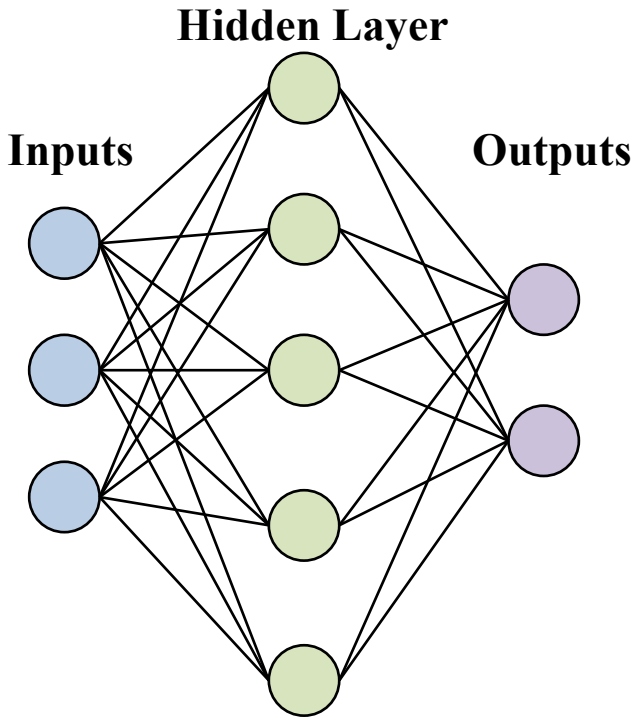
Backpropagation Learning

Convolutional Neural Networks

Training MLPs

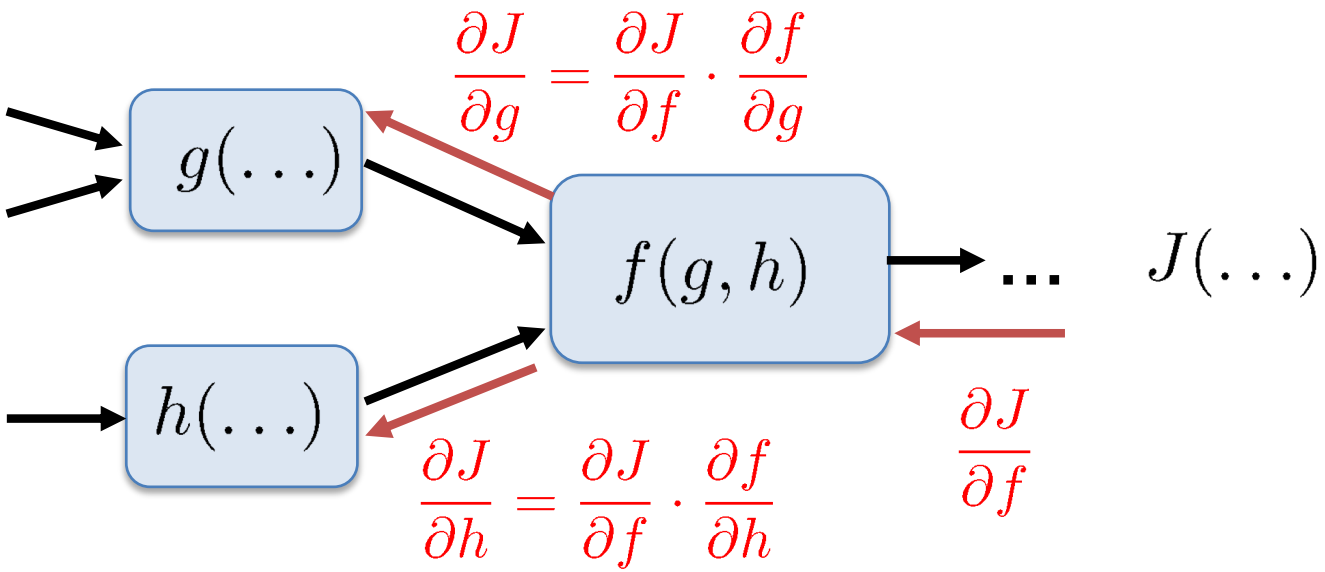
- Observe features “x” with target “y”
- Push “x” through NN = output is “ŷ”
- Error: $(y- \hat{y})^2$ (Can use different loss functions if desired…)
- How should we update the weights to improve?

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



Gradient calculations

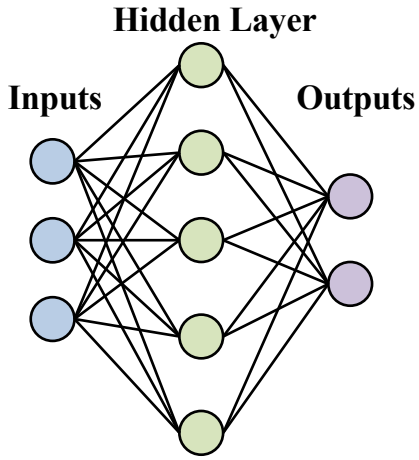
- Think of NNs as "schematics" made of smaller functions
  - Building blocks: summations & nonlinearities
  - For derivatives, just apply the chain rule, etc!



Ex: $f(g,h) = g^2 h$

$$\frac{\partial J}{\partial g} = \frac{\partial J}{\partial f} \cdot 2\, g(\cdot)\, h(\cdot) \qquad \frac{\partial J}{\partial h} = \frac{\partial J}{\partial f} \cdot g^2(\cdot)$$

save & reuse info (g,h) from forward computation!



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

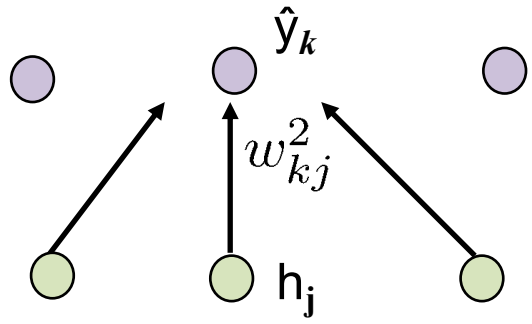
$$J_i(W) = \sum_k \; (y_k^{(i)} - \hat{y}_k^{(i)})^2$$

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

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

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

$$\beta_k^2$$

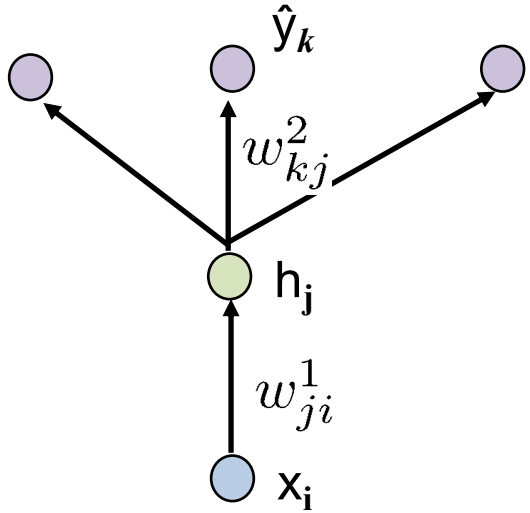
(Identical to logistic mse regression with inputs "h_j")

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

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

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

$$\beta_k^2$$



Backpropagation

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

$$\frac{\partial J}{\partial w^2_{kj}} = \boxed{-2(y_k - \hat{y}_k)\ \sigma'(s_k)}\ h_j$$

$$\frac{\partial J}{\partial w^1_{ji}} = \sum_k \boxed{-2(y_k - \hat{y}_k)\ \sigma'(s_k)}\ w^2_{kj}\ \sigma'(t_j)\ x_i$$

β^2_k

Forward pass

Loss function

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

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)
# W1  : (N2xN1)
H   = Sig(X.dot(W[0]))
# H   : (1xN2)
# W2  : (N3xN21)
Yh  = Sig(H.dot(W[1]))
# Yh  : (1xN3)
```

```
B2 = (Y-Yhat) * dSig(S)    #(1xN3)

G2 = B2.T.dot( H )         #(N3x1)*(1xN2)=(N3xN2)

B1 = B2.dot(W[1])*dSig(T)  #(1xN3)*(N3xN2)=(1xN2)

G1 = B1.T.dot( X )         #(N2xN1)
```

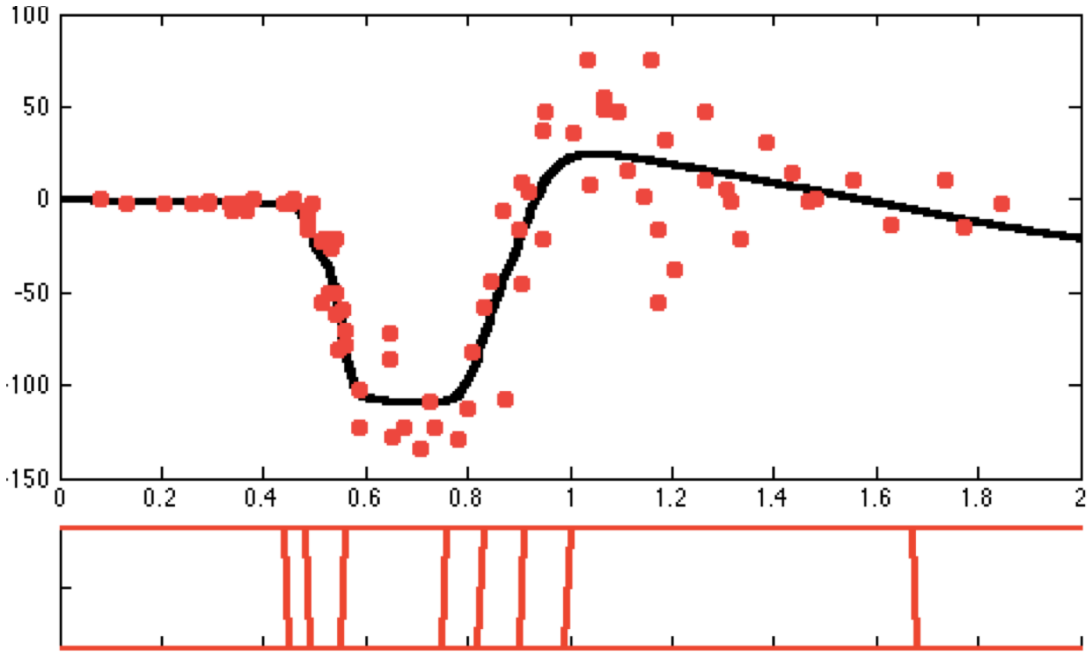
Example: Regression, MCycle data

- 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:

+

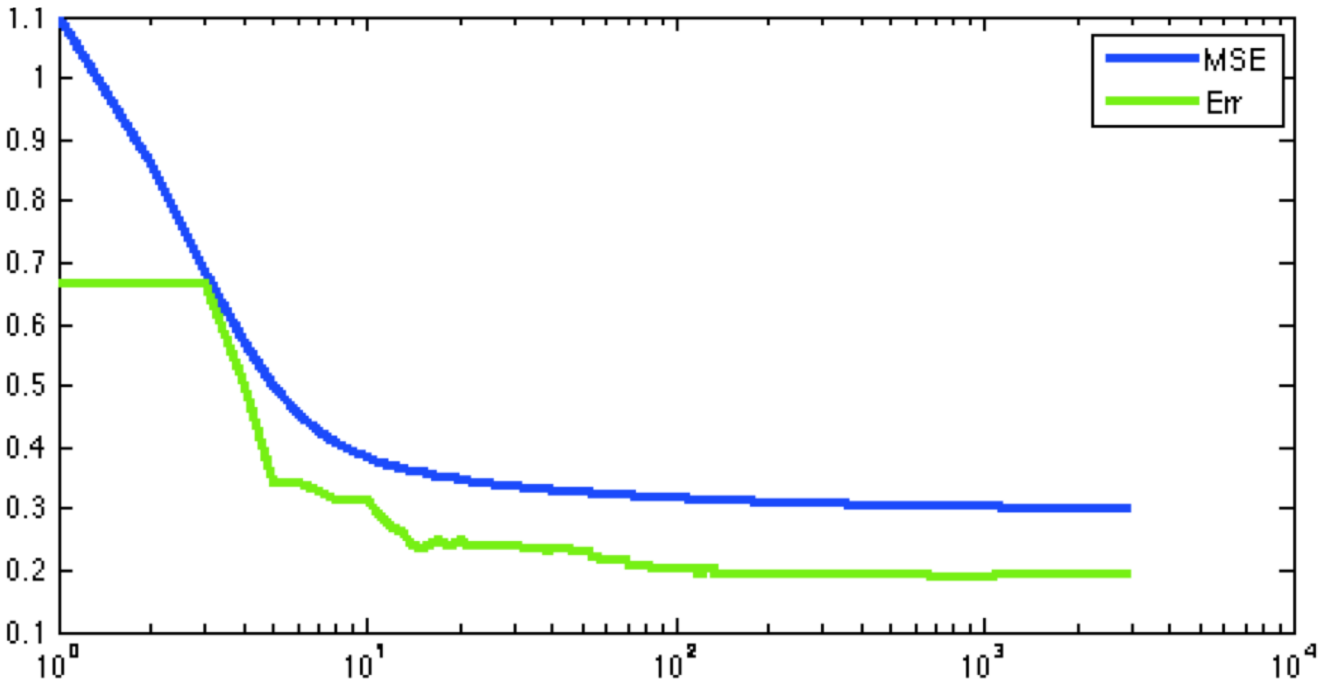
learned prediction f'n:

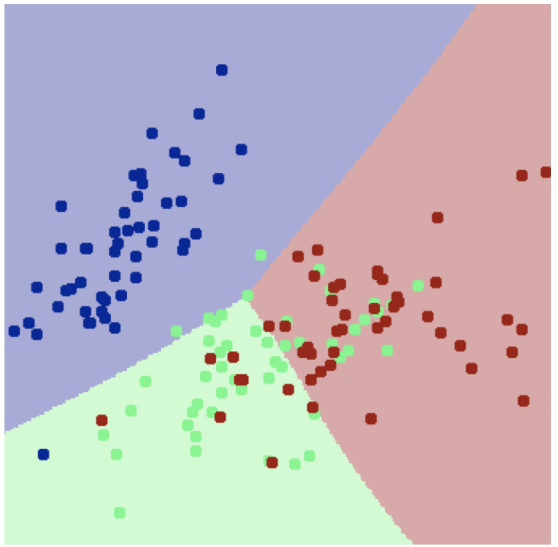


Responses of hidden nodes
(= features of linear regression):
select out useful regions of "x"

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

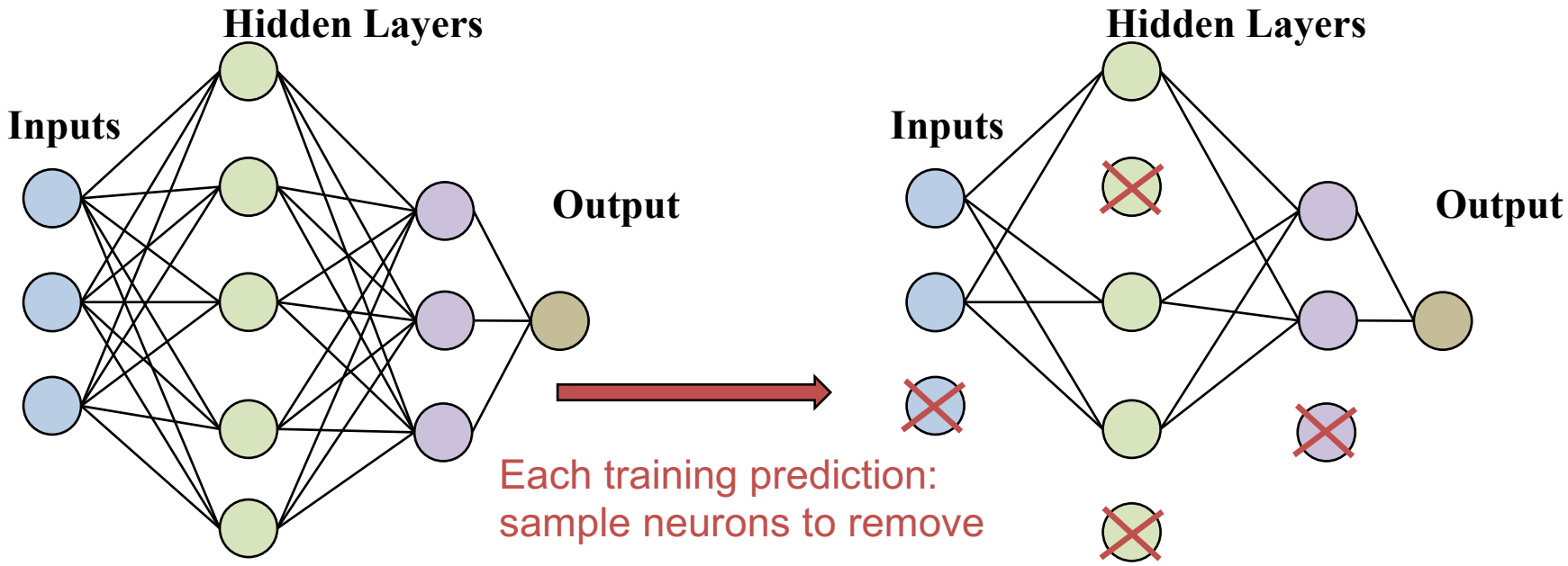




Dropout

[Srivastava et al 2014]

- Another recent technique
  - Randomly "block" some neurons at each step
  - Trains model to have redundancy (predictions must be robust to blocking)



Each training prediction:
sample neurons to remove

```
# ... during training ...
R = X.dot(W[0])+B[0];       # linear response
H1= Sig( R );               # activation f'n
H1 *= np.random.rand(*H1.shape)<p; #drop out!
```

Demo Time!

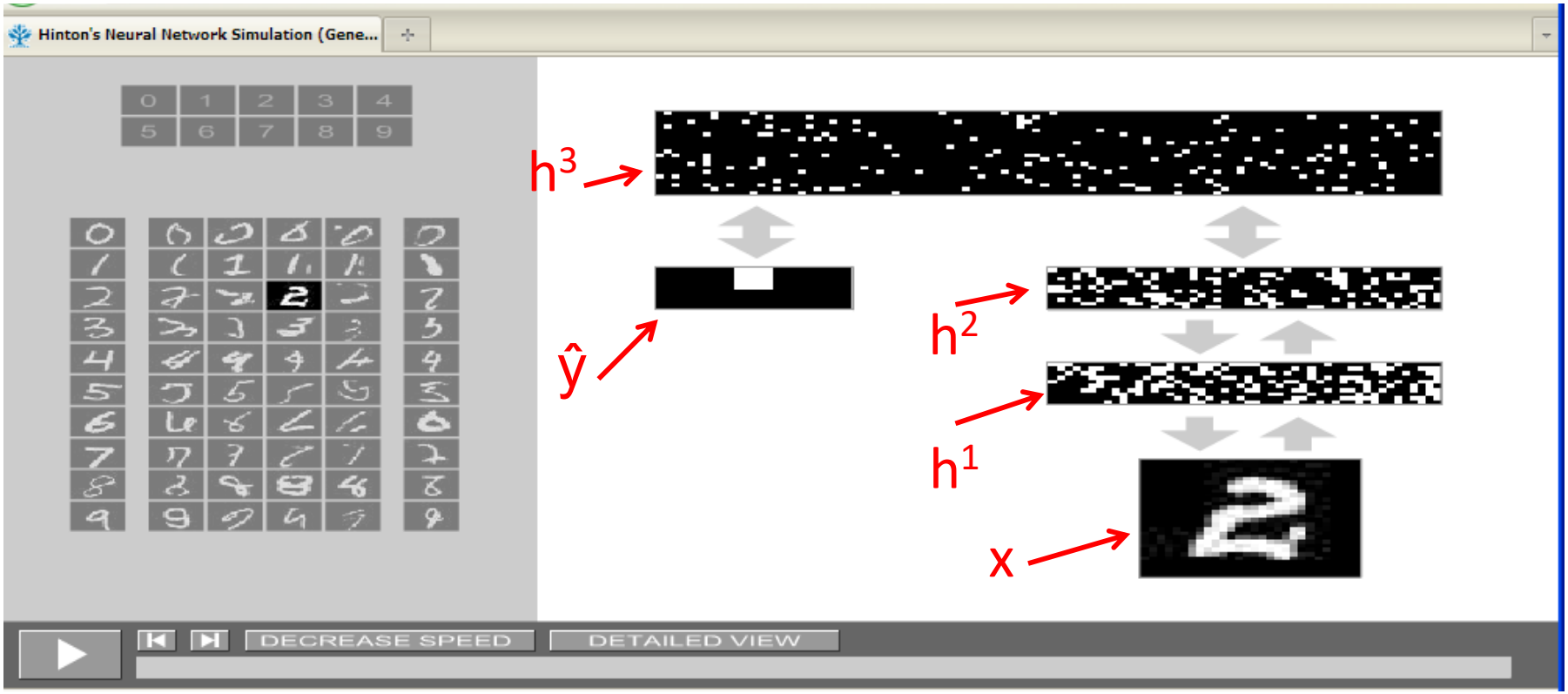
http://playground.tensorflow.org/

MLPs in practice

[Hinton et al. 2007]

- Example: Deep belief nets
  - Handwriting recognition
  - Online demo
  - 784 pixels ⇔ 500 mid ⇔ 500 high ⇔ 2000 top ⇔ 10 labels

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



MLPs in practice

[Hinton et al. 2007]

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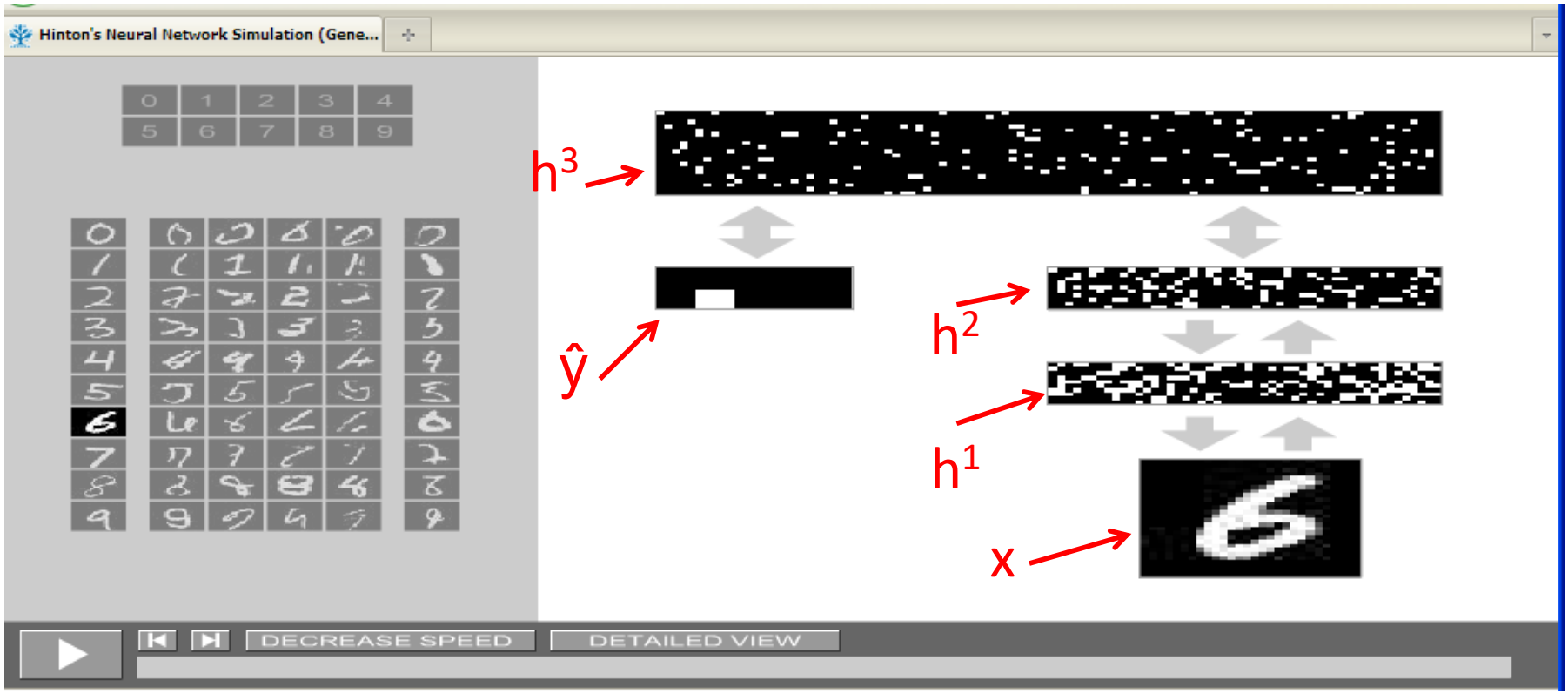


Machine Learning

Multi-Layer Perceptrons

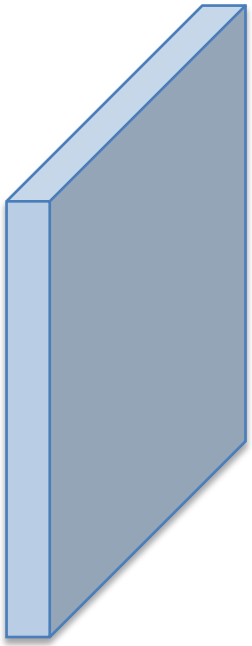
Backpropagation Learning

Convolutional Neural Networks

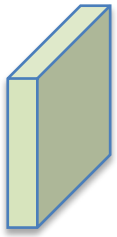
Convolutional networks

- Organize & share the NN's weights (vs "dense")
- Group weights into "filters"

Input: 28x28 image



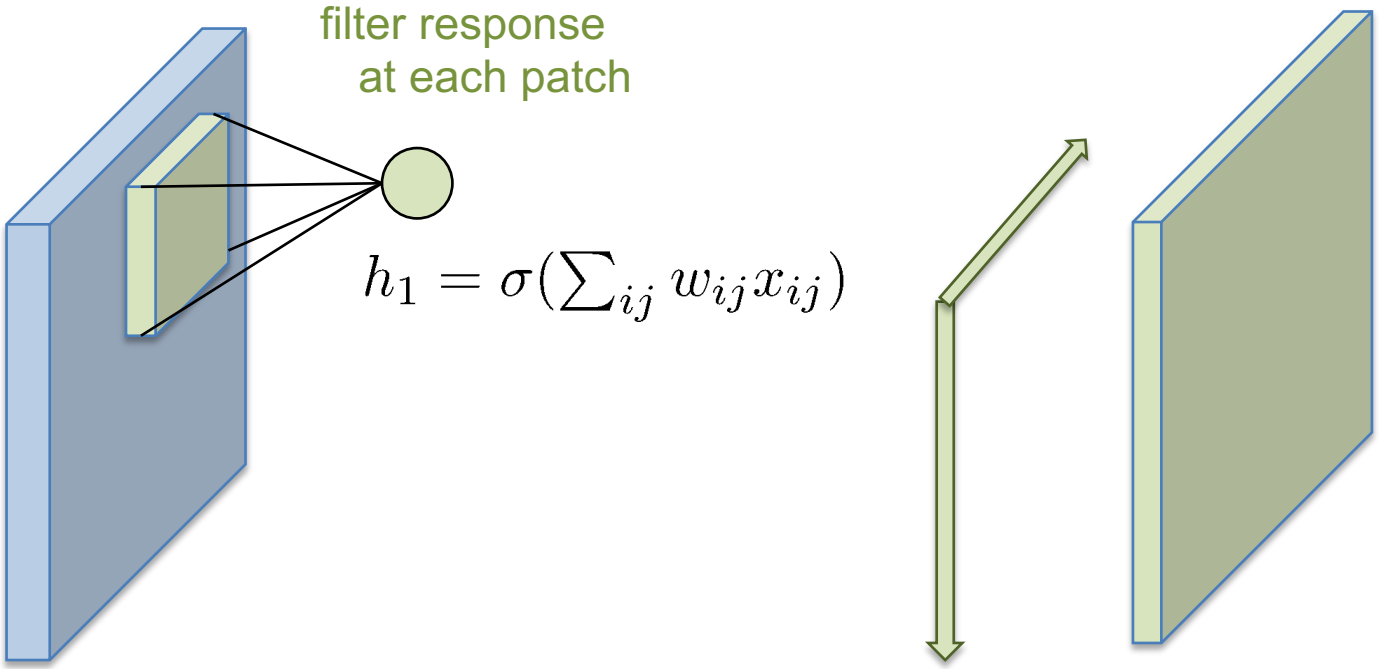
Weights: 5x5



Convolutional networks

- Organize & share the NN's weights (vs "dense")
- Group weights into "filters" & convolve across input image

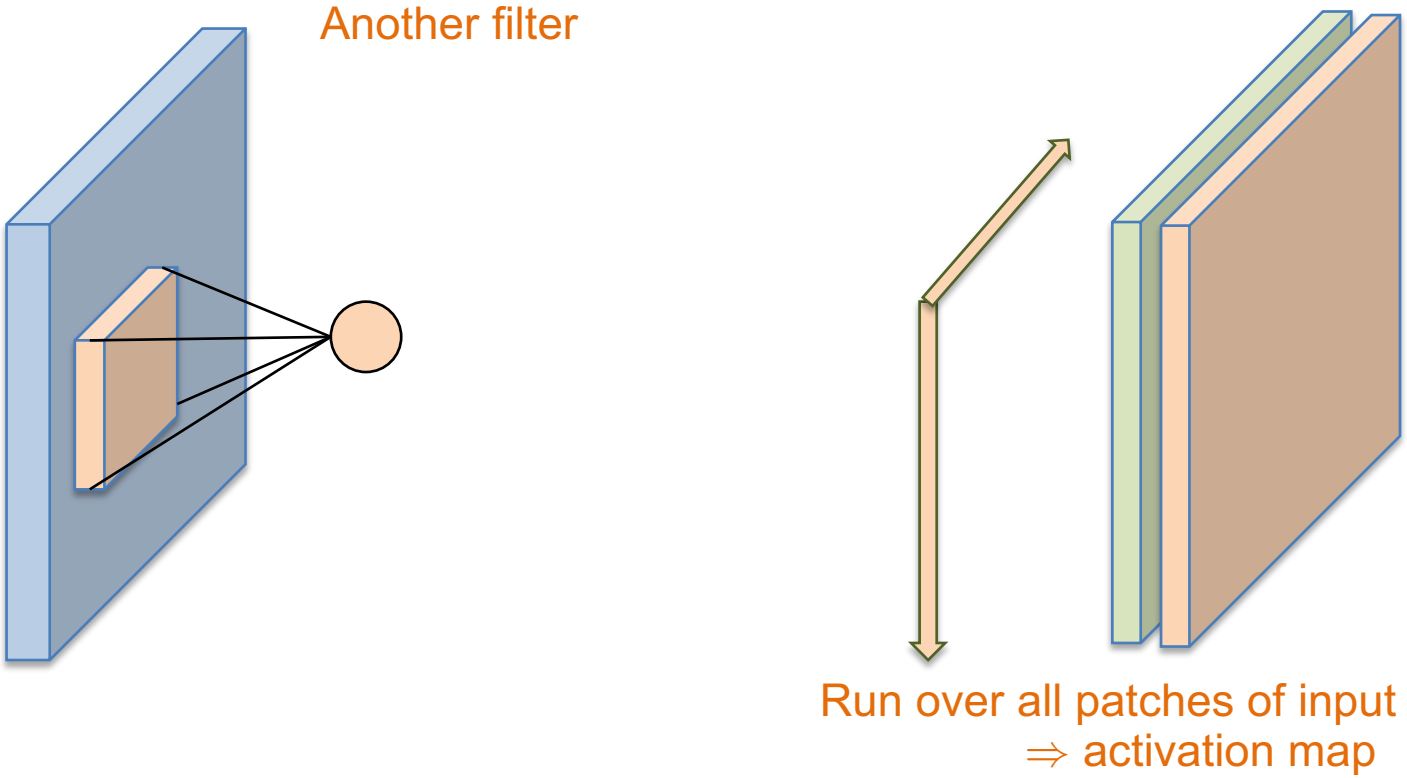
Input: 28x28 image Weights: 5x5 24x24 image



Convolutional networks

- Organize & share the NN's weights (vs "dense")
- Group weights into "filters" & convolve across input image

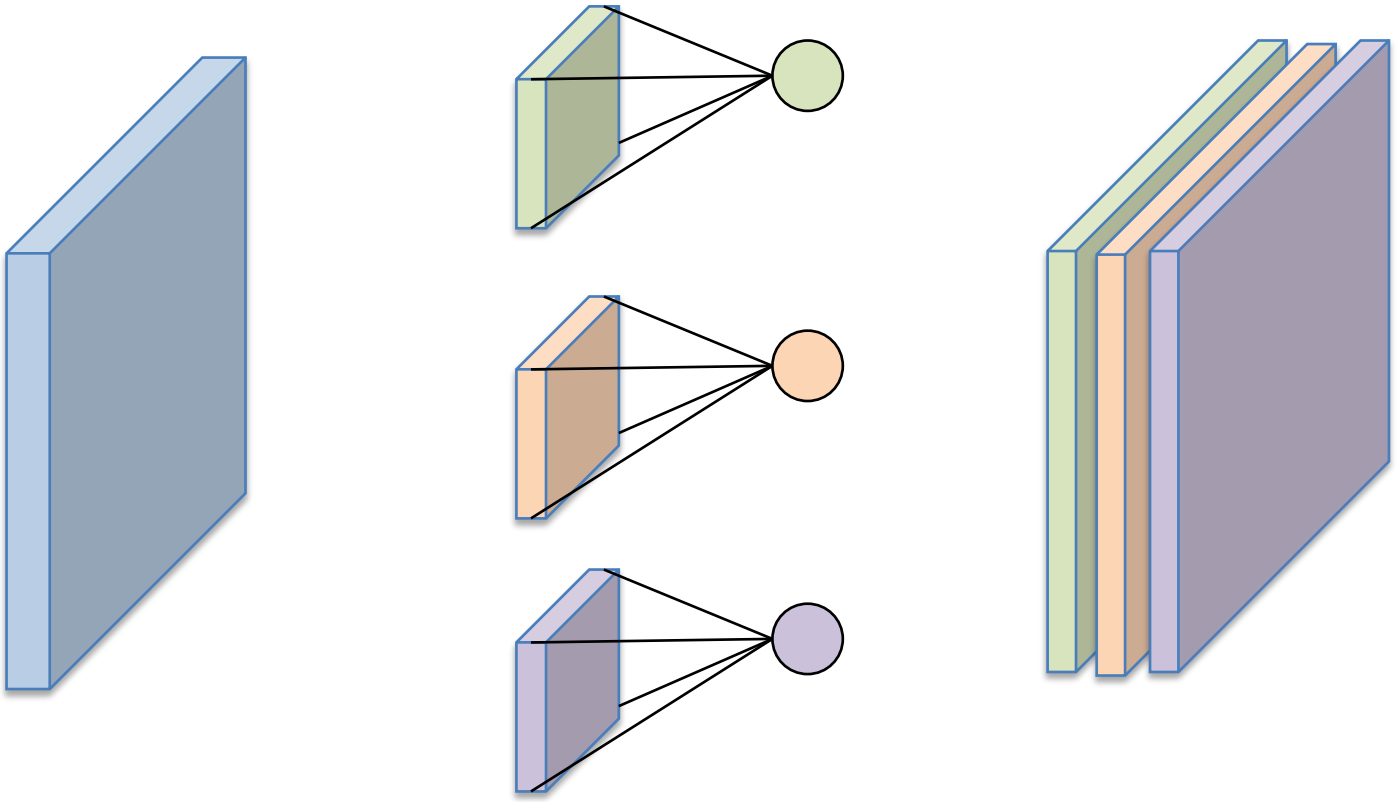
Input: 28x28 image Weights: 5x5



Convolutional networks

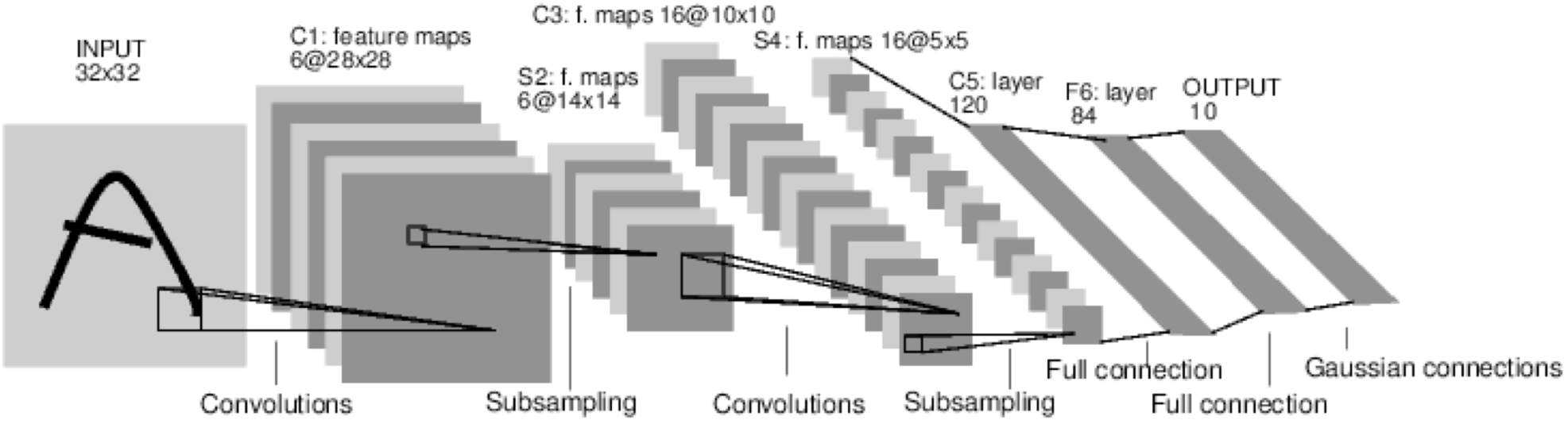
- Organize & share the NN's weights (vs "dense")
- Group weights into "filters" & convolve across input image
- Many hidden nodes, but few parameters!

Input: 28x28 image Weights: 5x5 Hidden layer 1



Convolutional networks

- Again, can view components as building blocks
- Design overall, deep structure from parts
  - Convolutional layers
  - “Max-pooling” (sub-sampling) layers
  - Densely connected layers

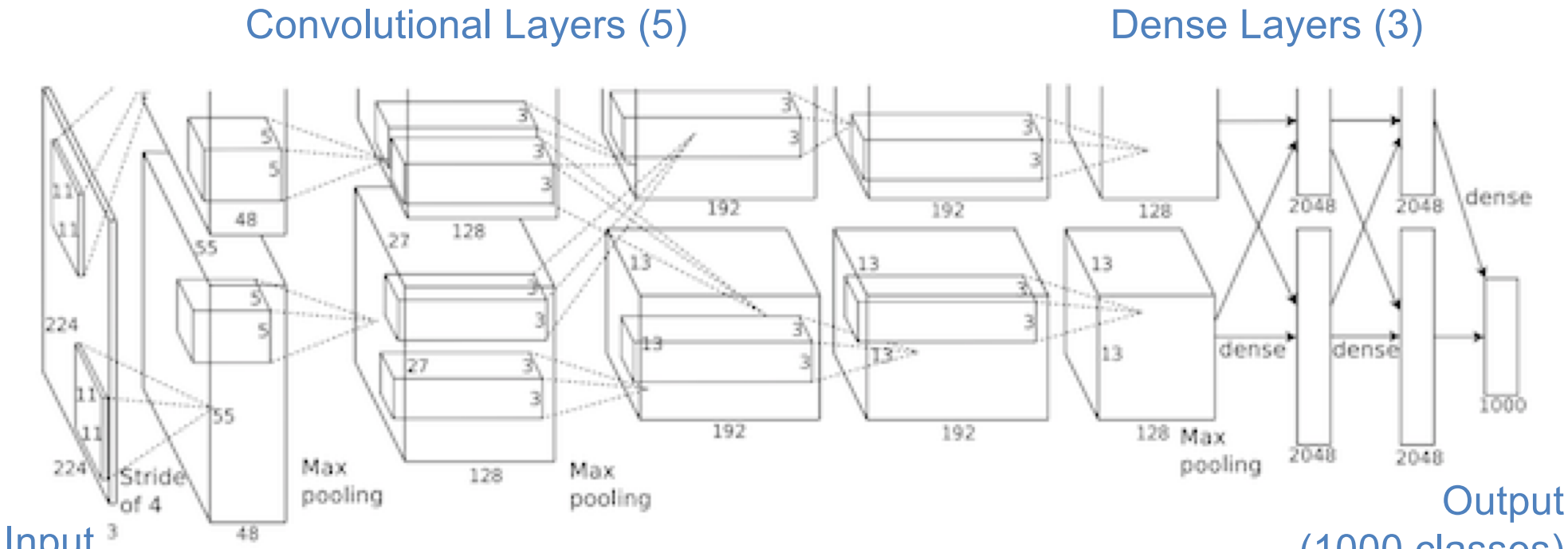


LeNet-5 [LeCun 1980]

Ex: AlexNet

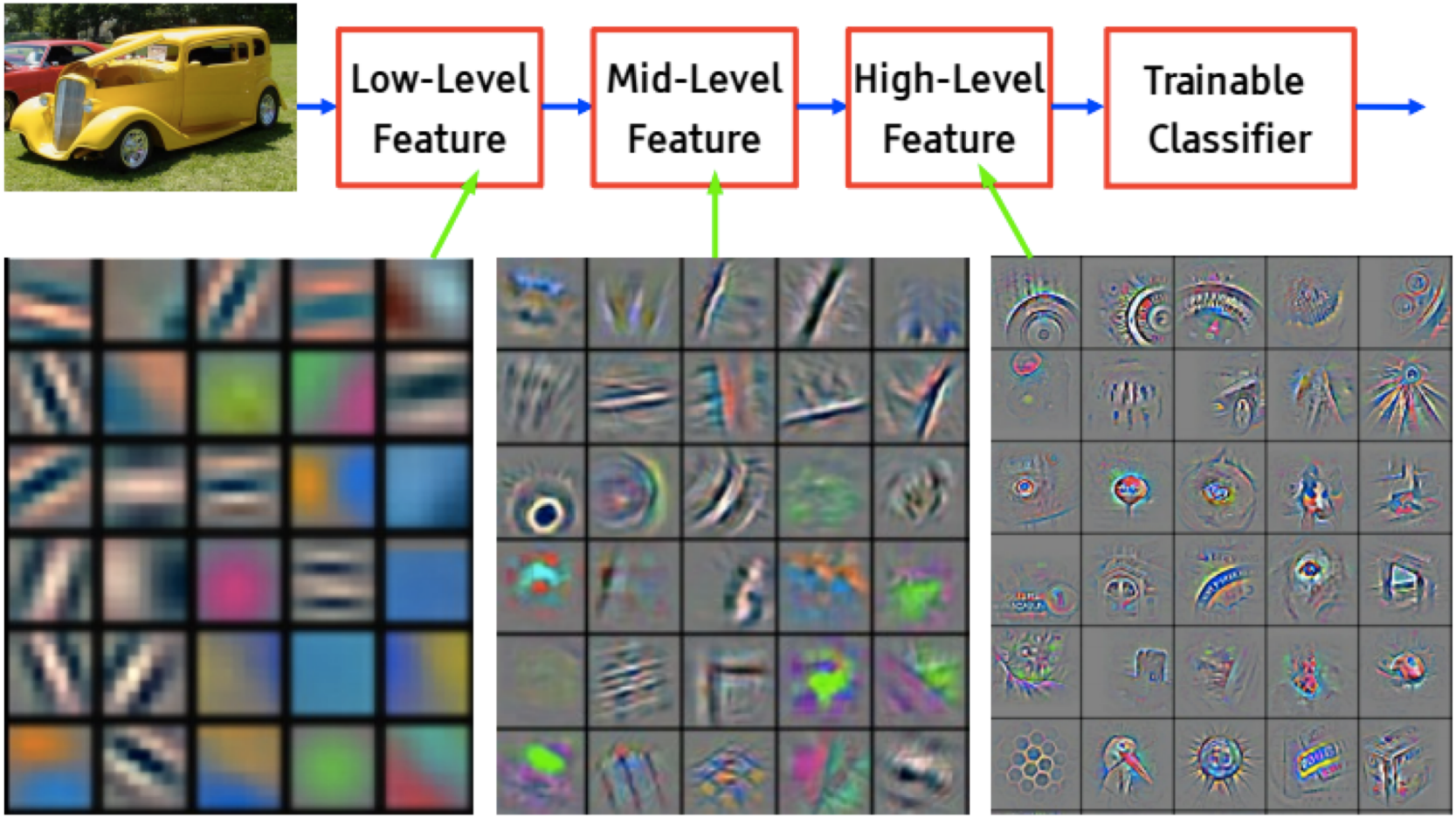
[Krizhevsky et al. 2012]

- Deep NN model for ImageNet classification
  - 650k units; 60m parameters
  - 1m data; 1 week training (GPUs)



Hidden layers as “features”

- Visualizing a convolutional network’s filters [Zeiler & Fergus 2013]



Slide image from Yann LeCun:
https://drive.google.com/open?id=0BxKBnD5y2M8NclFWSXNxa0JlZTg

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. Building block view.
- Advanced: deep nets, conv nets, dropout, …