CS434a/541a: Pattern Recognition
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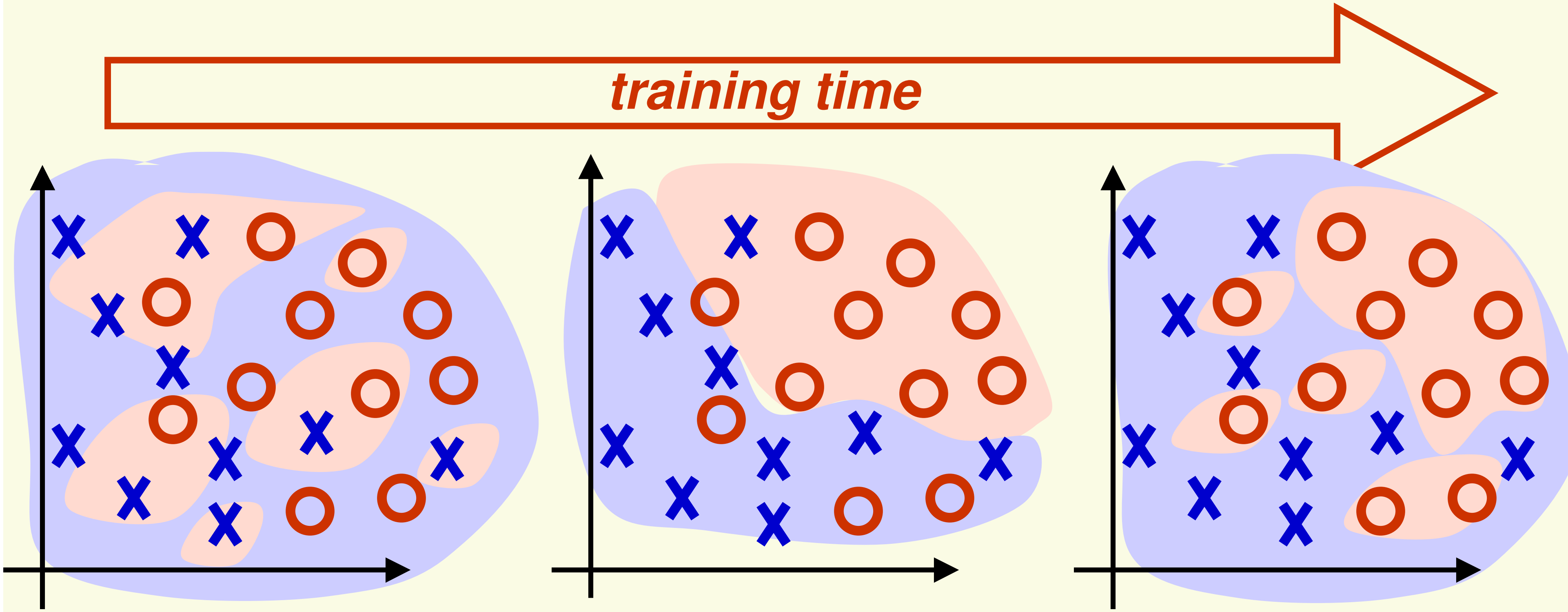
Lecture 14

Today

- Continue Multilayer Neural Networks (MNN)
  - Training/testing/validation curves
  - Practical Tips for Implementation
  - Concluding Remarks on MNN

MNN Training



Large training error: *in the beginning random decision regions*

Small training error: *decision regions improve with time*

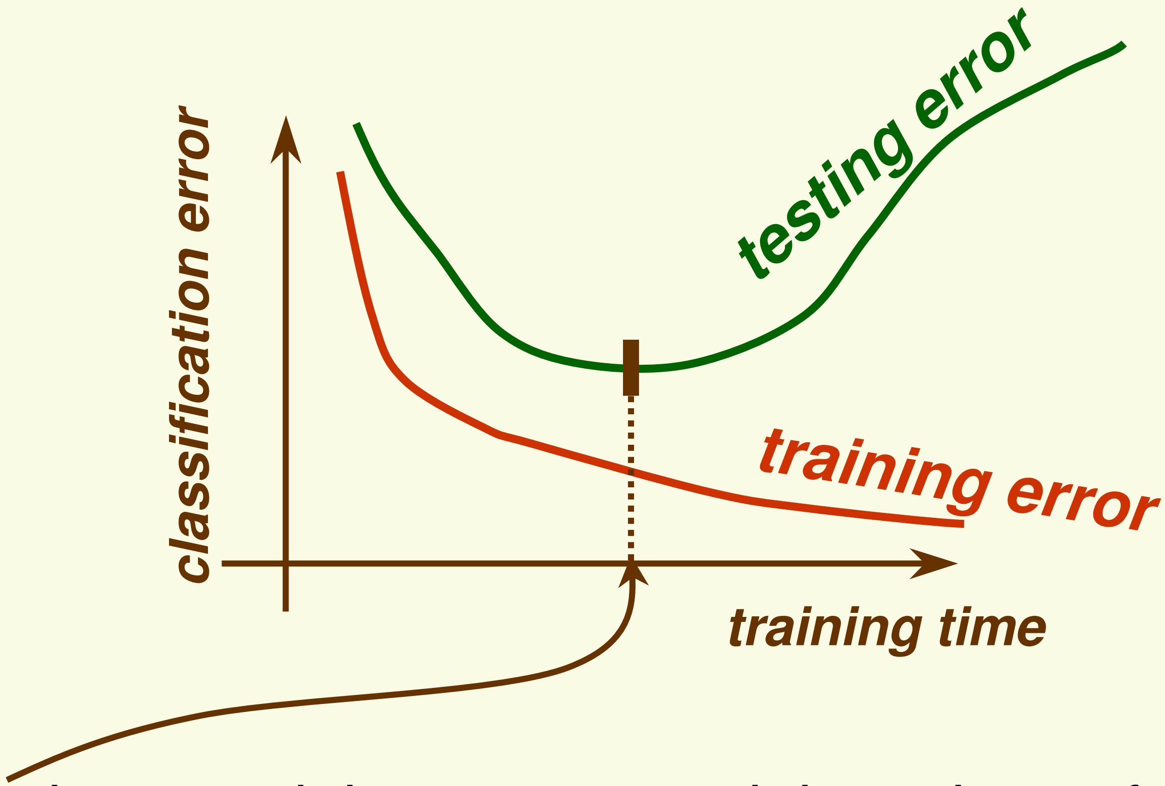
Zero training error: *decision regions separate training data perfectly, but we overfited the network*

MNN Learning Curves

- ***Training data***: data on which learning (gradient descent for MNN) is performed
- ***Test data***: used to assess network generalization capabilities
- Training error typically goes down, since with enough hidden units, can find discriminant function which classifies training patterns exactly

- Test error first goes down, but then goes up since at some point we start to ***overfit*** the network to the training data

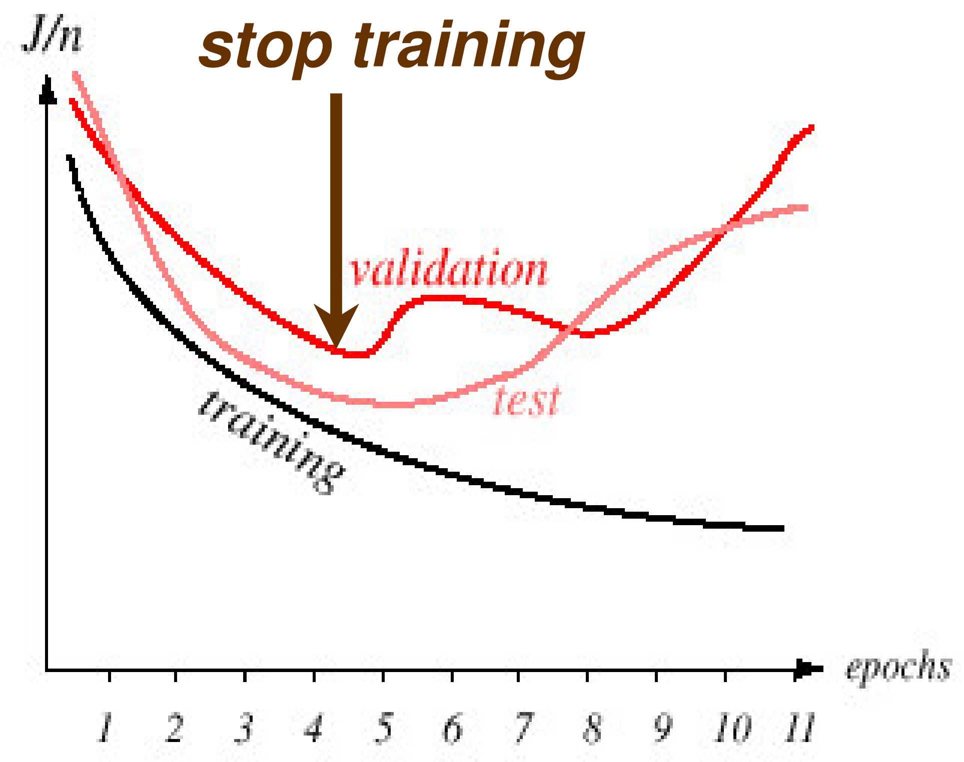
Learning Curves



- this is a good time to stop training, since after this time we start to overfit
- However, stopping criterion is part of training phase, ***we cannot use test data for anything that has to do with the learning phase***

Learning Curves

- Create a third separate data set called ***validation data***:
- validation data is used to determine "parameters", in this case when learning should stop



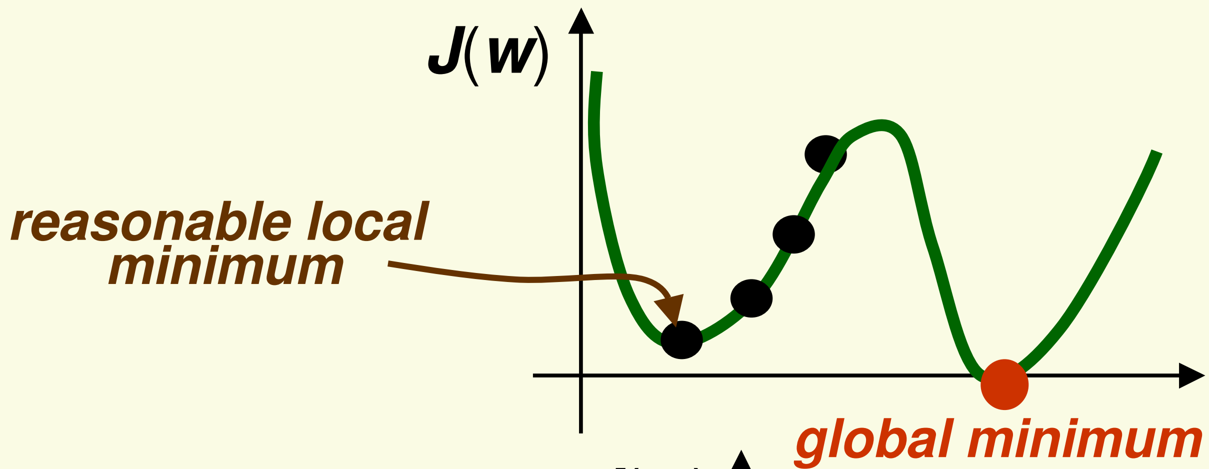
- Stop training after the first local minimum on validation data
  - We are assuming performance on test data will be similar to performance on validation data

Data Sets

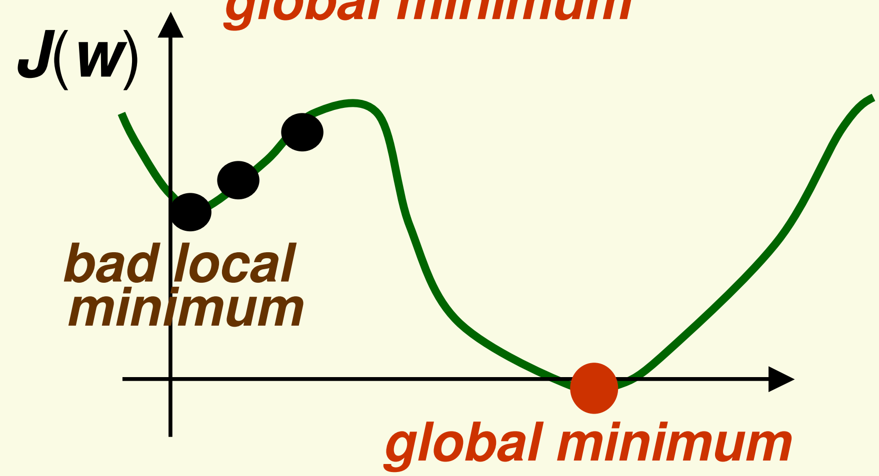
- ***Training data***
  - data on which learning is performed
- ***Validation data***
  - validation data is used to determine any free parameters of the classifier
    - ***k*** in the knn neighbor classifier
    - ***h*** for parzen windows
    - number of hidden layers in the MNN
    - etc
- ***Test data***
  - used to assess network generalization capabilities

Practical Tips for BP: Momentum

- Gradient descent finds only a local minima
  - not a problem if $\boldsymbol{J}(\boldsymbol{w})$ is small at a local minima. Indeed, we do not wish to find $\boldsymbol{w}$ s.t. $\boldsymbol{J}(\boldsymbol{w}) = 0$ due to overfitting



  - problem if $\boldsymbol{J}(\boldsymbol{w})$ is large at a local minimum $\boldsymbol{w}$



Practical Tips for BP: Momentum

- Momentum: popular method to avoid local minima and also speeds up descent in plateau regions
  - weight update at time $\boldsymbol{t}$ is $\Delta \boldsymbol{w}^{(t)} = \boldsymbol{w}^{(t)} - \boldsymbol{w}^{(t-1)}$
  - add temporal average direction in which weights have been moving recently

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + (1-\alpha)\underbrace{\left[\eta \frac{\partial \boldsymbol{J}}{\partial \boldsymbol{w}}\right]}_{\text{steepest descent direction}} + \alpha \underbrace{\Delta \boldsymbol{w}^{(t-1)}}_{\text{previous direction}}$$

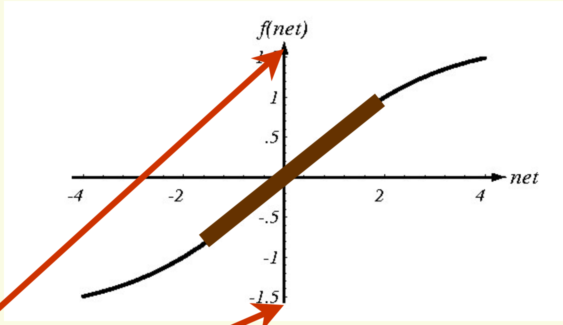
  - at $\alpha = 0$, equivalent to gradient descent
  - at $\alpha = 1$, gradient descent is ignored, weight update continues in the direction in which it was moving previously (momentum)
  - usually, α is around 0.9

Practical Tips for BP: Activation Function

- Gradient descent will work with any continuous ***f*** however some choices are better than others
- Desirable properties of ***f*** :
  - Continuous and differentiable Nonlinearity to express nonlinear decision boundaries
  - Saturation, that is ***f*** has minimum and maximum values (-***a*** and ***b***). Keeps and weights ***w***, ***v*** bounded, thus training time down
  - Monotonicity so that activation function itself does not introduce additional local minima
  - Linearity for a small values of net, so that network can produce linear model, if data supports it
  - antisymmetric, that is ***f***(-1) = -***f***(1), leads to faster learning

Practical Tips for BP: Activation Function

- Sigmoid activation function ***f*** satisfies all of the above properties



$$\boldsymbol{f}(\boldsymbol{net}) = \alpha \frac{e^{\beta \cdot net} - e^{-\beta \cdot net}}{e^{\beta \cdot net} + e^{-\beta \cdot net}}$$

- Convenient to set $\alpha = 1.716$, $\beta = 2/3$
- Asymptotic values ∓ 1.716
- Linear range is roughly for $-1 < \boldsymbol{net} < 1$

Practical Tips for BP: Target Values

- For sigmoid function, to represent class ***c***, use

$$\boldsymbol{t}^{(\boldsymbol{c})} = \begin{bmatrix} -1 \\ \vdots \\ 1 \\ \vdots \\ -1 \end{bmatrix} \leftarrow \boldsymbol{c}\text{th row}$$

- Always use values less than asymptotic values for target
  - For small error, need ***t*** to be close to $\boldsymbol{z} = \boldsymbol{f}(\boldsymbol{net})$
  - For any finite value of ***net***, ***f***(***net***) never reaches the asymptotic value
  - The error will always be too large, training will never stop, and weights ***w***, ***v*** will go to infinity

Practical Tips for BP: Normalization

- Each feature of input data should be normalized
- Suppose we measure fish length in meters and weight in grams
  - Typical sample [length = 0.5, weight = 3000]
  - Feature length will be basically ignored by the network
  - If length is in fact important, learning will be VERY slow

Practical Tips for BP: Normalization

- Normalize each feature ***i*** to be of mean ***0*** and variance ***1***
  - First for each feature ***i***, compute ***var*** [$x^{(i)}$] and ***mean*** [$x^{(i)}$]
  - Then

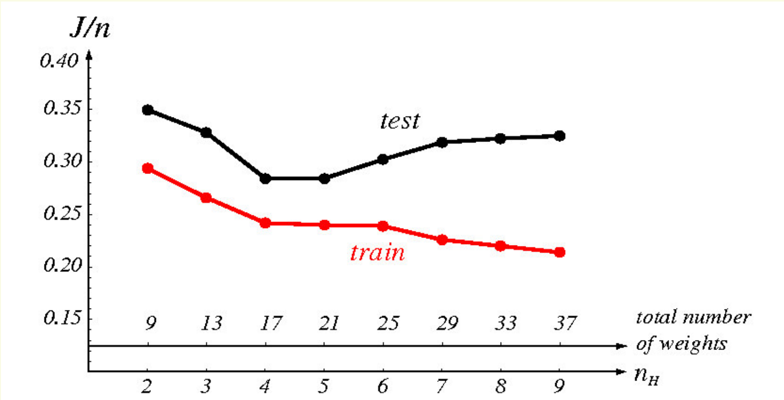
$$x_k^{(i)} \leftarrow \frac{x_k^{(i)} - mean\left(x^{(i)}\right)}{\sqrt{var\left(x^{(i)}\right)}}$$

  - Cannot do this for online version of the algorithm since data is not available all at once

- If there are a lot of highly correlated or redundant features, can reduce dimensionality with PCA
- Test samples should be subjected to the same transformations as the training samples

Practical Tips for BP: # of Hidden Units

- # of input units = number of features, # output units = # classes. How to choose N_H, the # of hidden units?
- N_H determines the expressive power of the network
  - Too small N_H may not be sufficient to learn complex decision boundaries
  - Too large N_H may overfit the training data resulting in poor generalization



Practical Tips for BP: # of Hidden Units

- Choosing N_H is not a solved problem
- Rule of thumb
  - if total number of training samples is n, choose N_H so that the total number of weights is $n/10$
  - total number of weights = (# of w) + (# of v)
- Can choose N_H which gives the best performance on the validation data

Practical Tips for BP: Initializing Weights

- Do not set either $\boldsymbol{w}$ or $\boldsymbol{v}$ to 0
- Rule of thumb for our sigmoid function
  - Choose random weights from the range

$$-\frac{1}{\sqrt{d}} < w_{ji} < \frac{1}{\sqrt{d}}$$

$$-\frac{1}{\sqrt{N_H}} < v_{kj} < \frac{1}{\sqrt{N_H}}$$

Practical Tips for BP: Learning Rate

- As any gradient descent algorithm, backpropagation depends on the learning rate η
- Rule of thumb $\eta = 0.1$
- However we can adjust η at the training time
- The objective function ***J*** should decrease during gradient descent
  - If it oscillates, η is too large, decrease it
  - If it goes down but very slowly, η is too small,increase it

Practical Tips for BP: Weight Decay

- To simplify the network and avoid overfitting, it is recommended to keep the weights small
- Implement weight decay after each weight update:

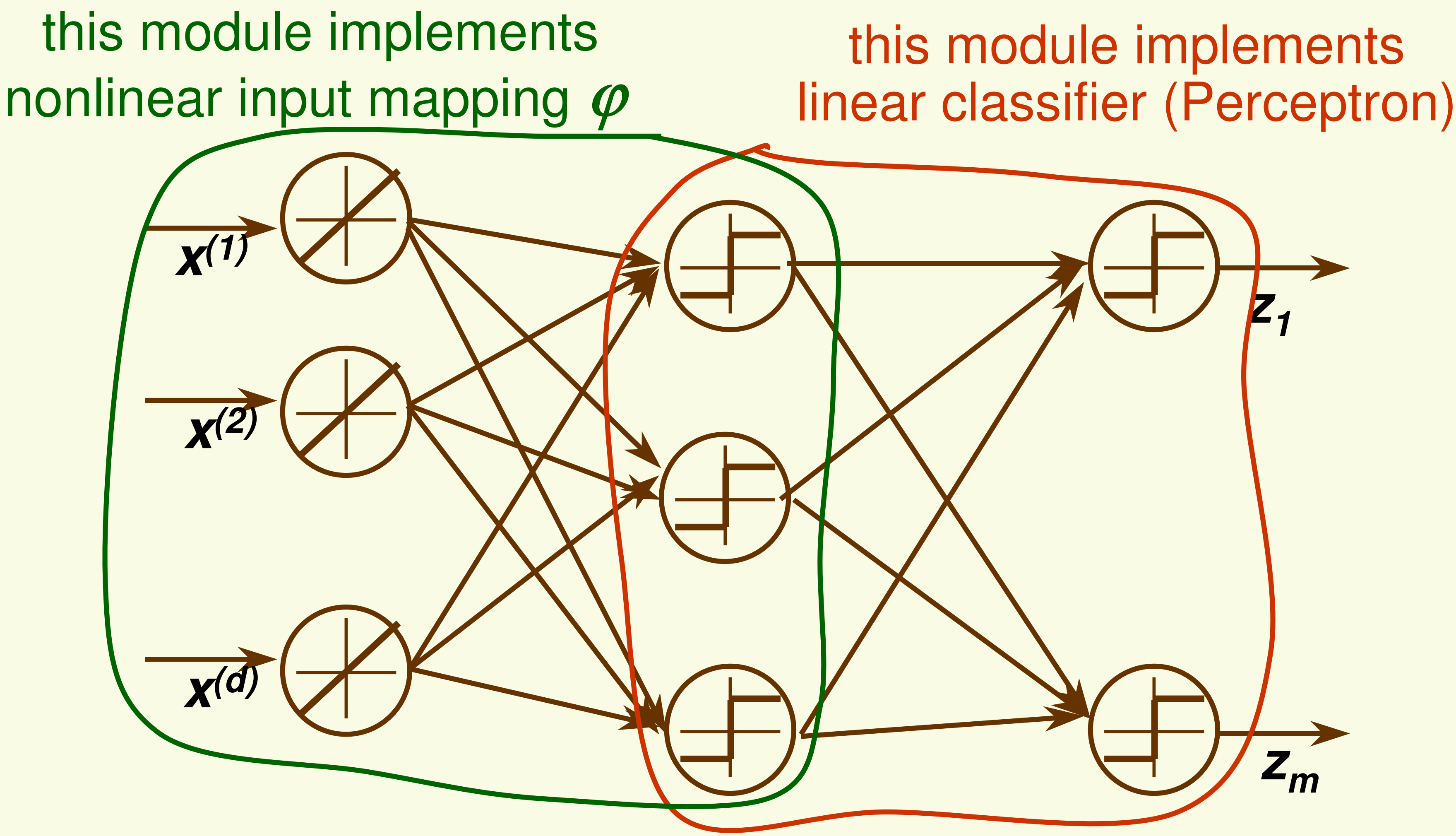
$$w^{new} = w^{old}(1-\varepsilon), \quad 0 < \varepsilon < 1$$

- Additional benefit is that “unused” weights grow small and may be eliminated altogether
  - A weight is “unused” if it is left almost unchanged by the backpropagation algorithm

Practical Tips for BP: # Hidden Layers

- Network with 1 hidden layer has the same expressive power as with several hidden layers
- For some applications, having more than 1 hidden layer may result in faster learning and less hidden units overall
- However networks with more than 1 hidden layer are more prone to the local minima problem

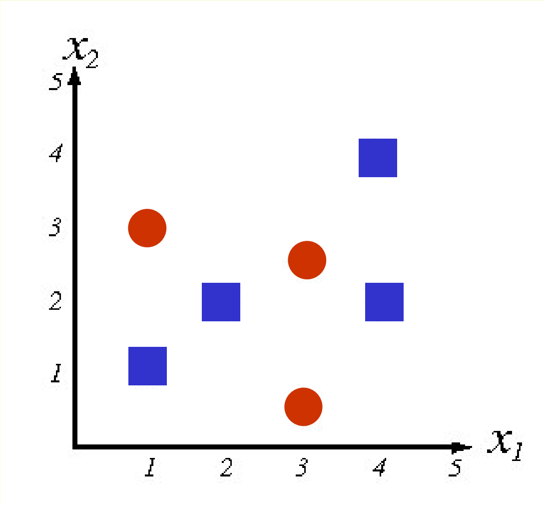
MNN as Nonlinear Mapping



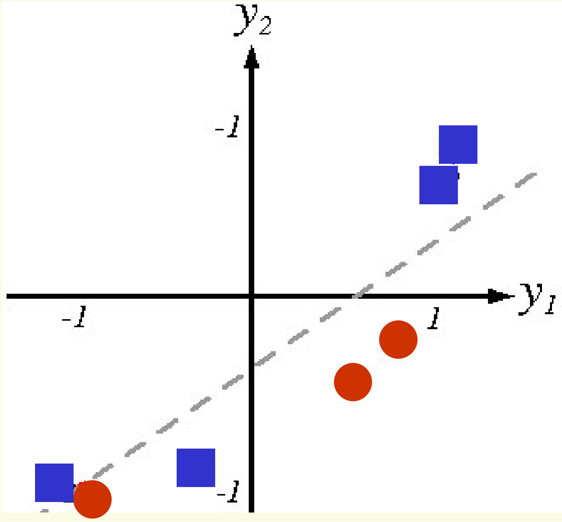
MNN as Nonlinear Mapping

- Thus MNN can be thought as learning 2 things at the same time
  - the nonlinear mapping of the inputs
  - linear classifier of the nonlinearly mapped inputs

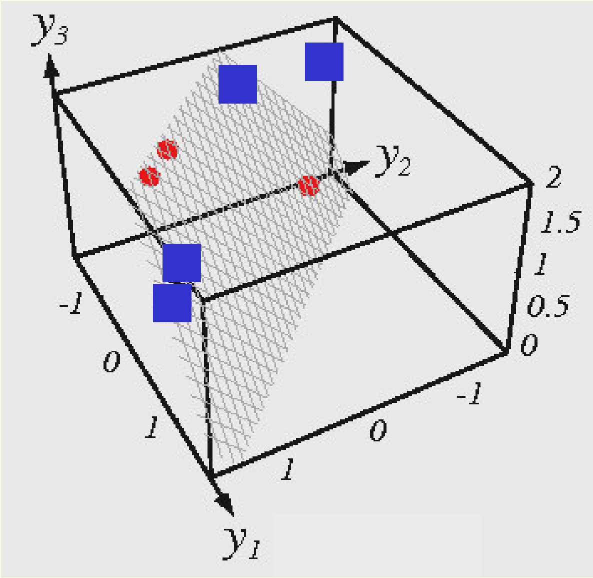
MNN as Nonlinear Mapping



original feature space ***x****; patterns are not linearly separable*



MNN finds nonlinear mapping ***y****=φ(****x****) to 2 dimensions (2 hidden units); patterns are almost linearly separable*



MNN finds nonlinear mapping ***y****=φ(****x****) to 3 dimensions (3 hidden units) that; patterns are linearly separable*

Concluding Remarks

- Advantages
  - MNN can learn complex mappings from inputs to outputs, based only on the training samples
  - Easy to use
  - Easy to incorporate a lot of heuristics
- Disadvantages
  - It is a “black box”, that is difficult to analyze and predict its behavior
  - May take a long time to train
  - May get trapped in a bad local minima
  - A lot of “tricks” to implement for the best performance