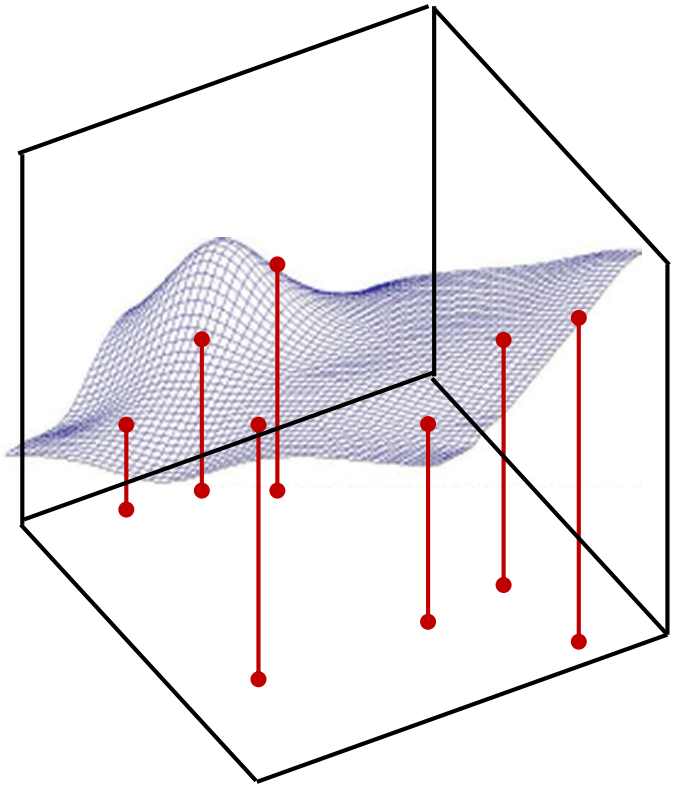
Neural Networks

Representations

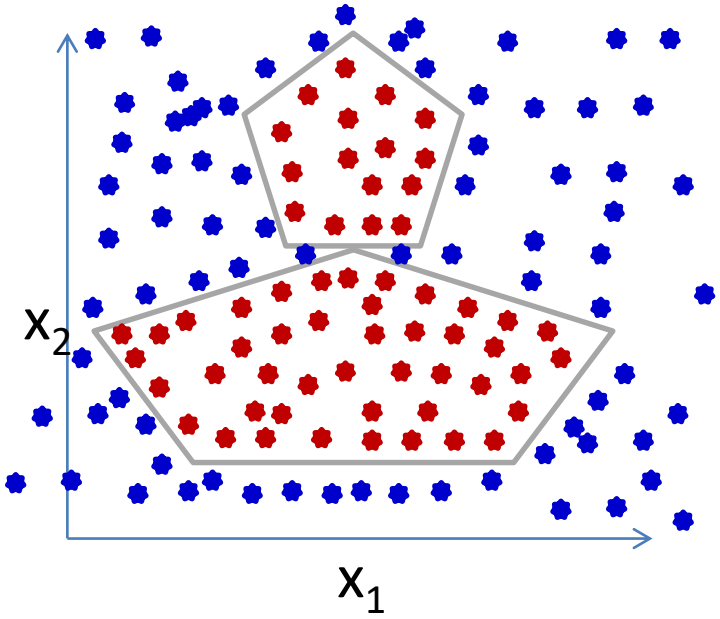
Fall 2017

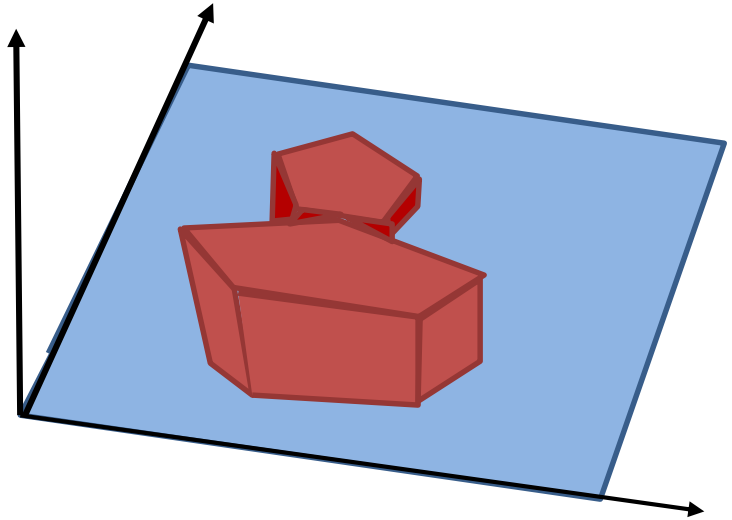
Learning in the net



- Problem: Given a collection of input-output pairs, learn the function

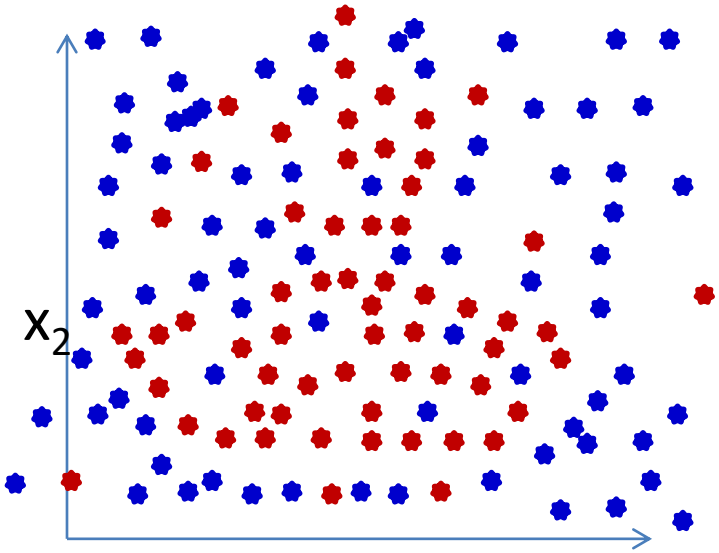
Learning for classification

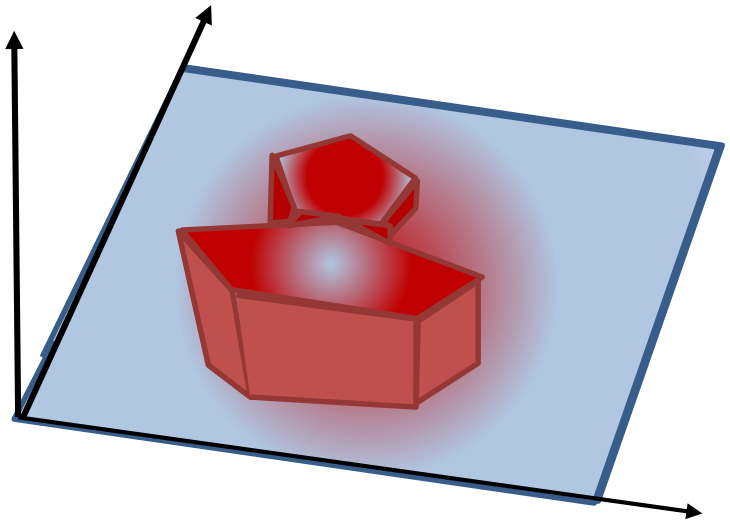




- When the net must learn to classify..

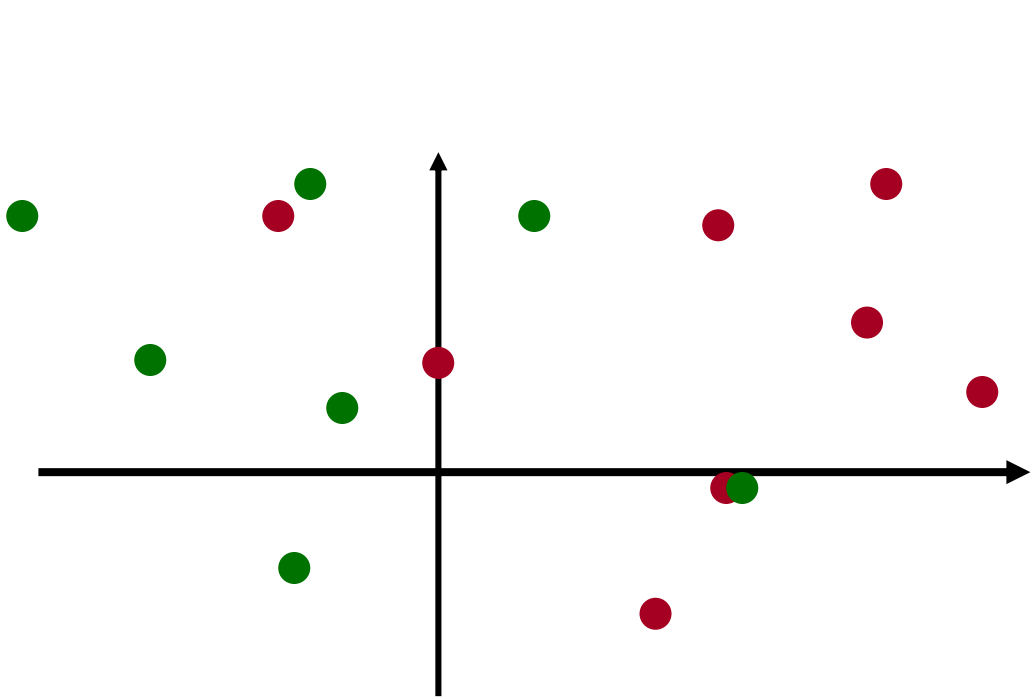
Learning for classification

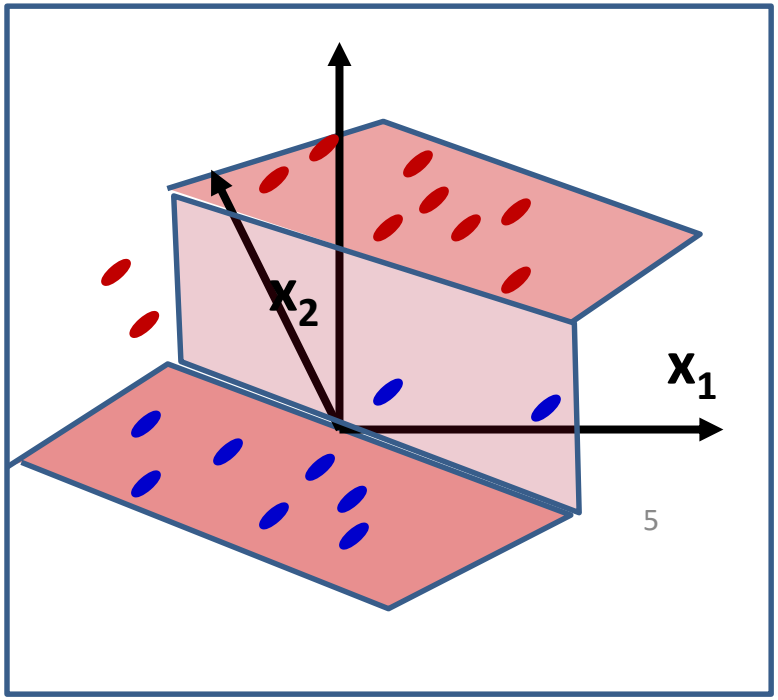




- In reality
  - In general not really cleanly separated
    - So what is the function we learn?

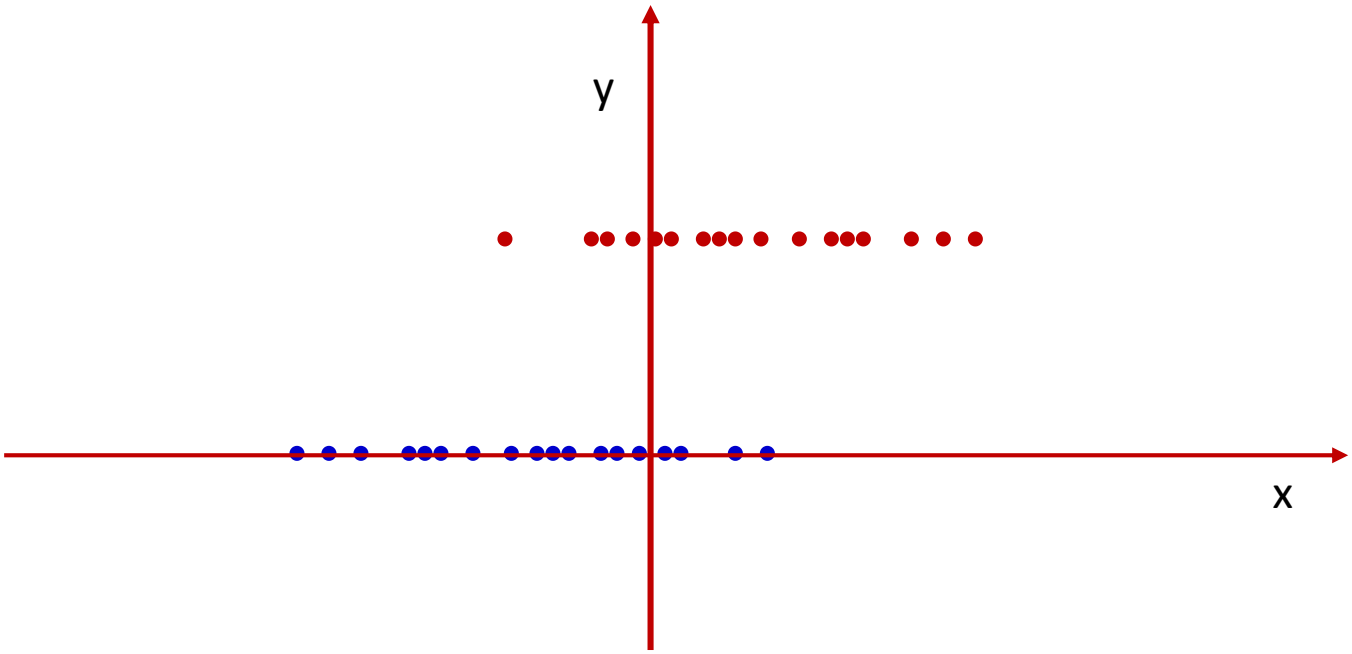
In reality: Trivial linear example





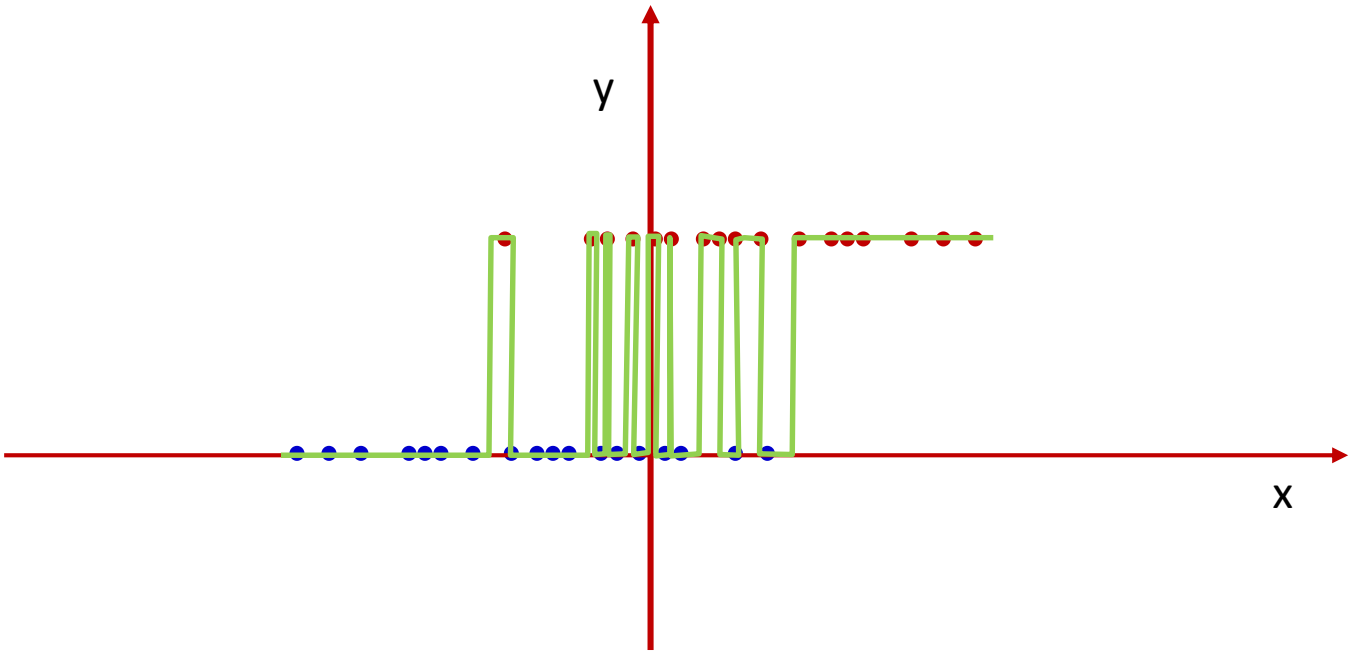
- Two-dimensional example
  - Blue dots (on the floor) on the "red" side
  - Red dots (suspended at Y=1) on the "blue" side
  - No line will cleanly separate the two colors

Non-linearly separable data: 1-D example



- One-dimensional example for visualization
  - All (red) dots at Y=1 represent instances of class Y=1
  - All (blue) dots at Y=0 are from class Y=0
  - The data are not linearly separable
    - In this 1-D example, a linear separator is a threshold
    - No threshold will cleanly separate red and blue dots

Undesired Function



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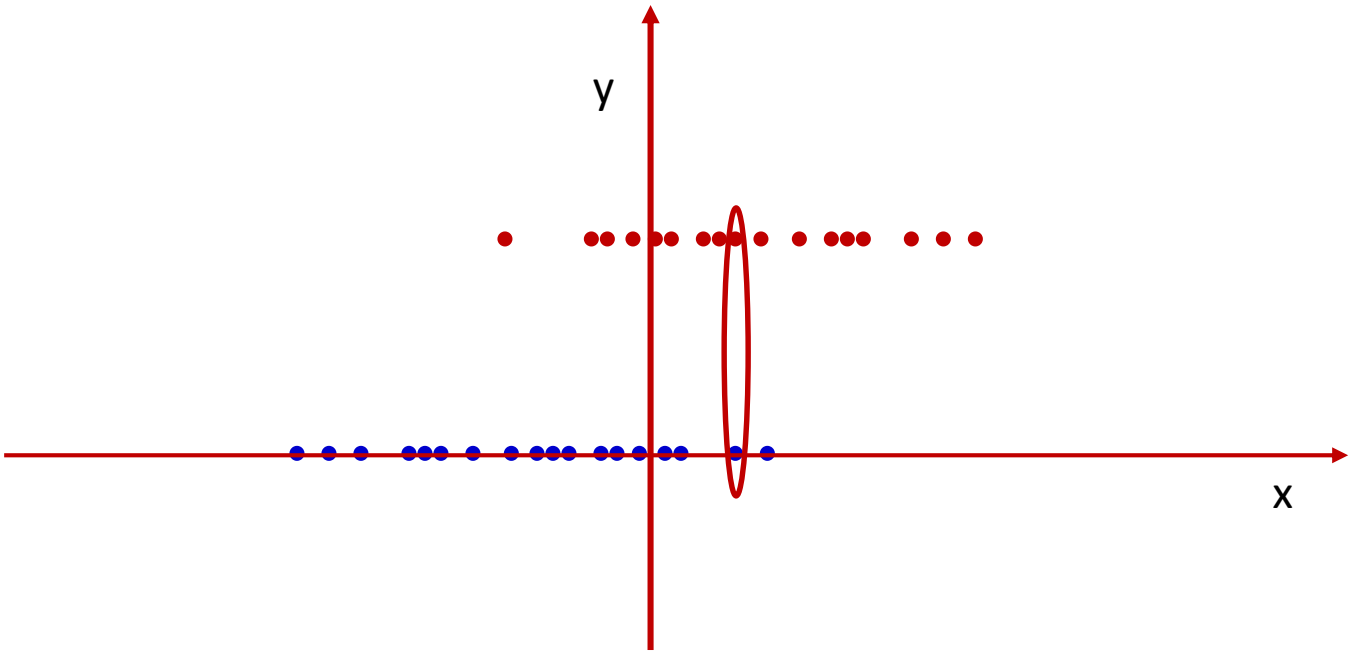

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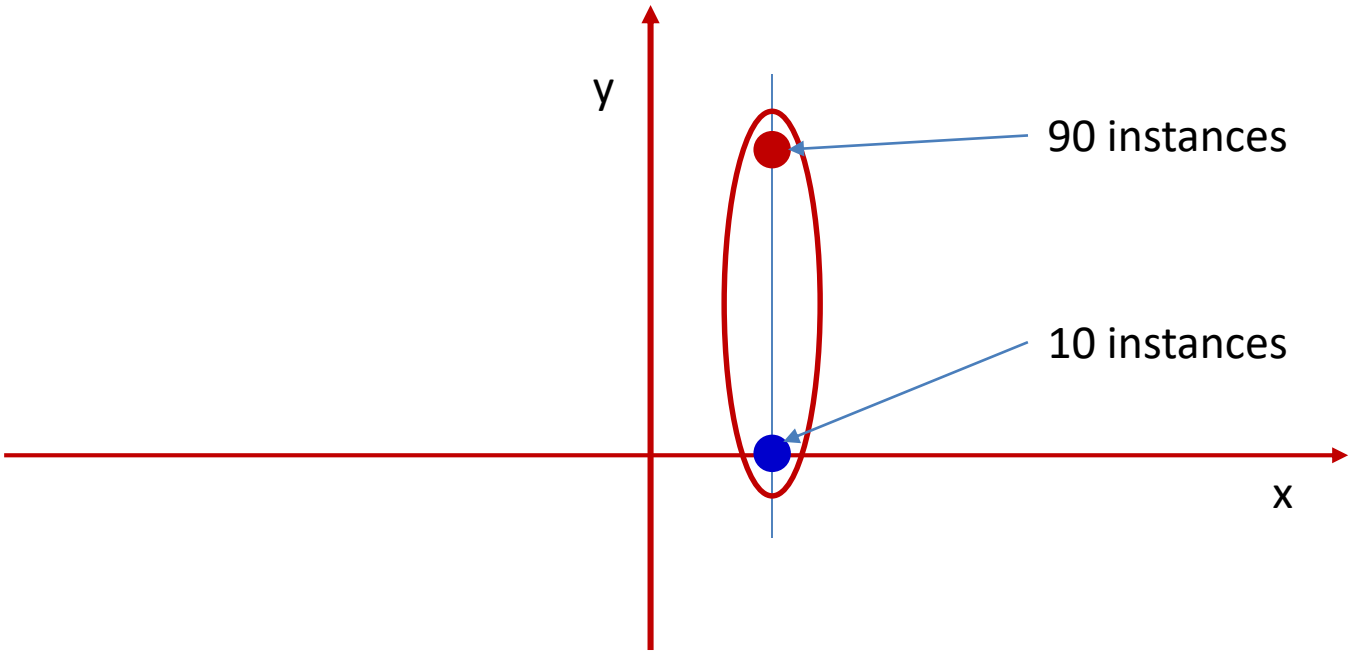

- What must the value of the function be at this X?
  - 1 because red dominates?
  - 0.9 : The average?

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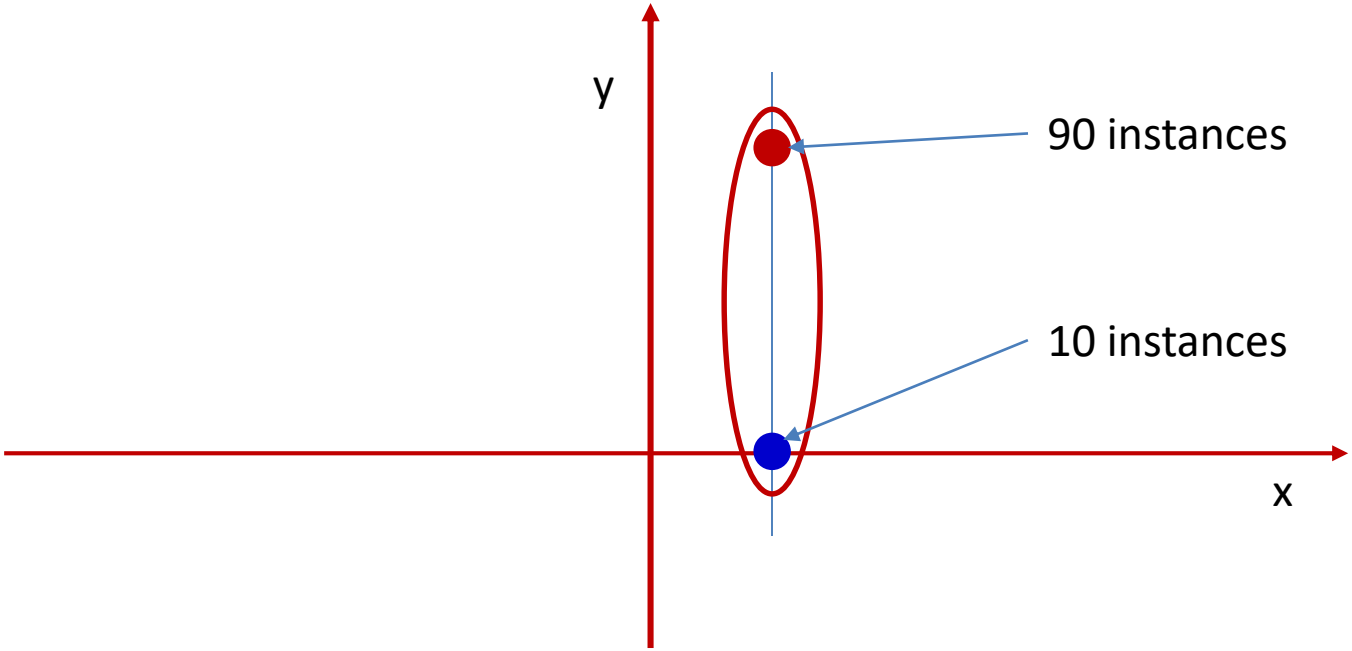

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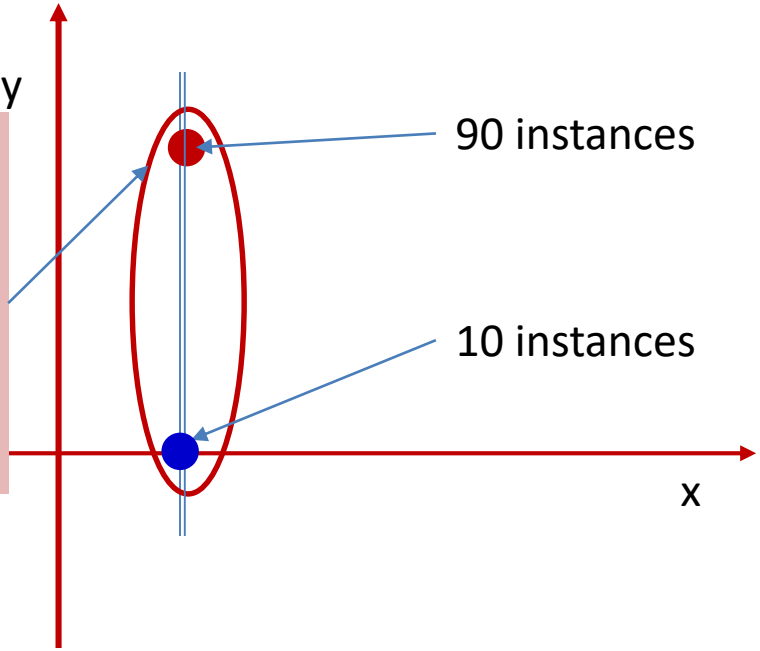
Estimate: $\approx P(1|X)$

Potentially much more useful than a simple 1/0 decision
Also, potentially more realistic

What if?

Should an infinitesimal nudge of the red dot change the function estimate entirely?

If not, how do we estimate $P(1|X)$?
(since the positions of the red and blue X Values are different)



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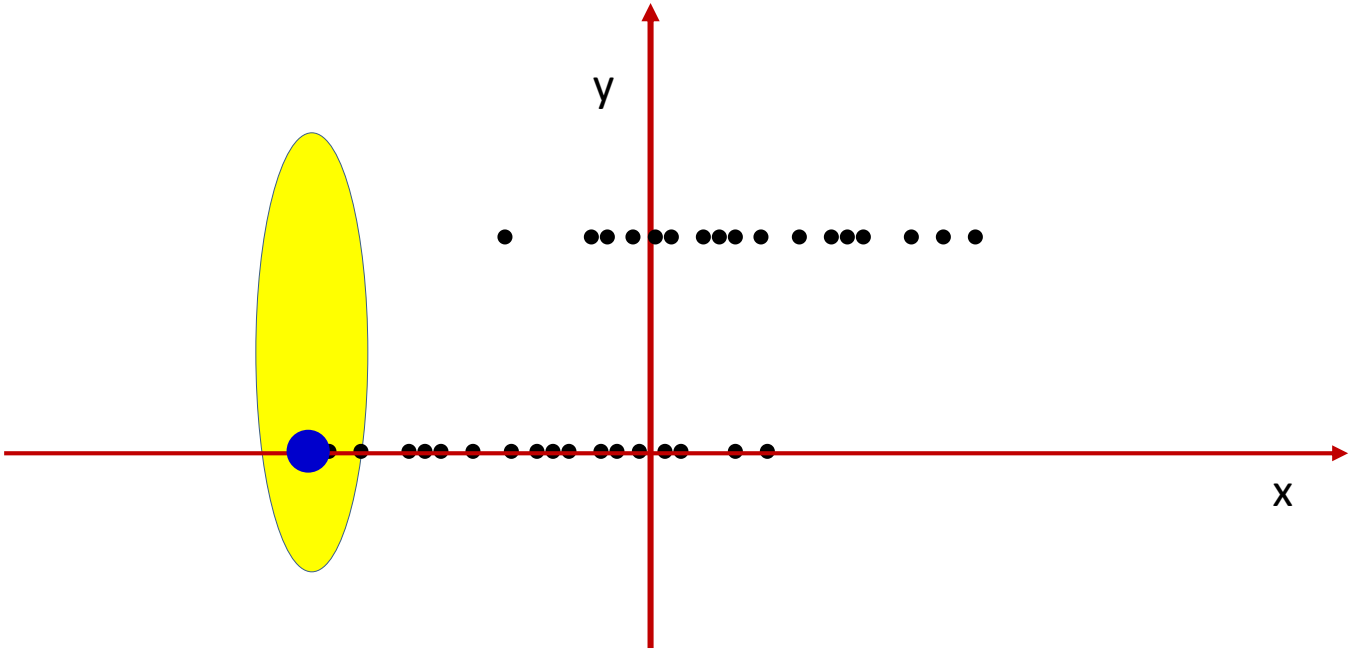
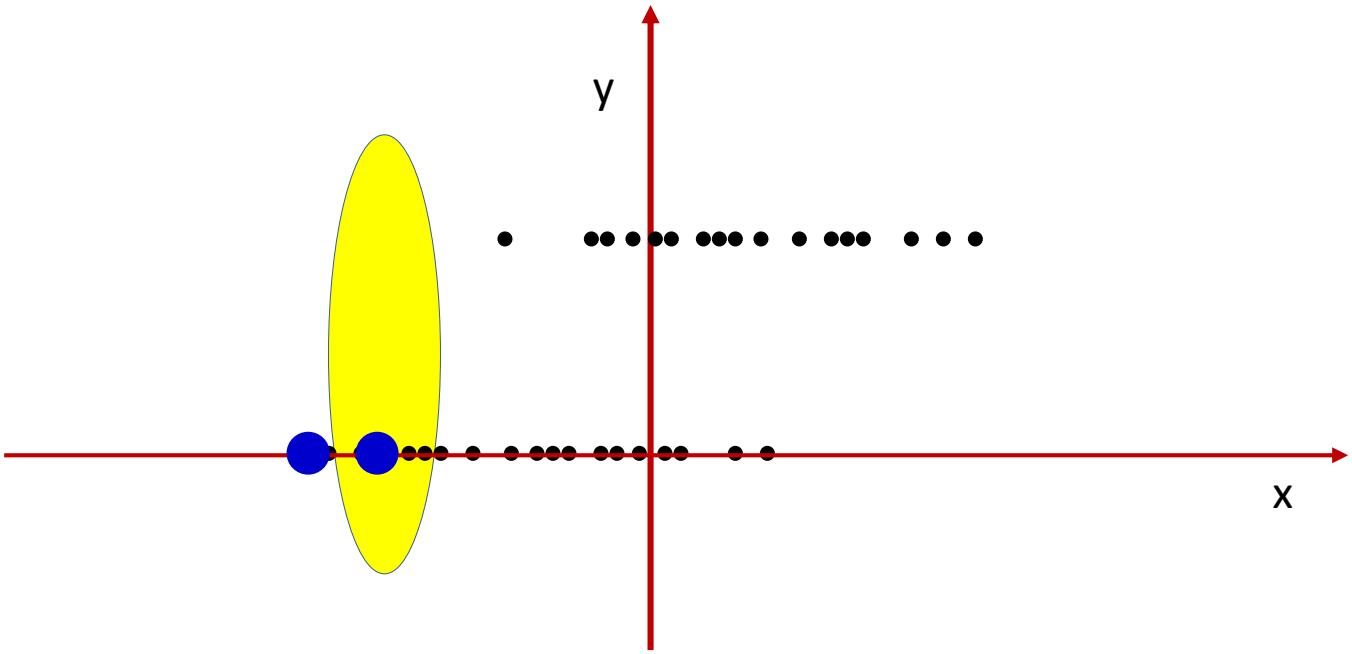
The *probability* of y=1



- Consider this differently: at each point look at a small window around that point
- Plot the average value within the window
  - This is an approximation of the *probability* of Y=1 at that point

The *probability* of y=1



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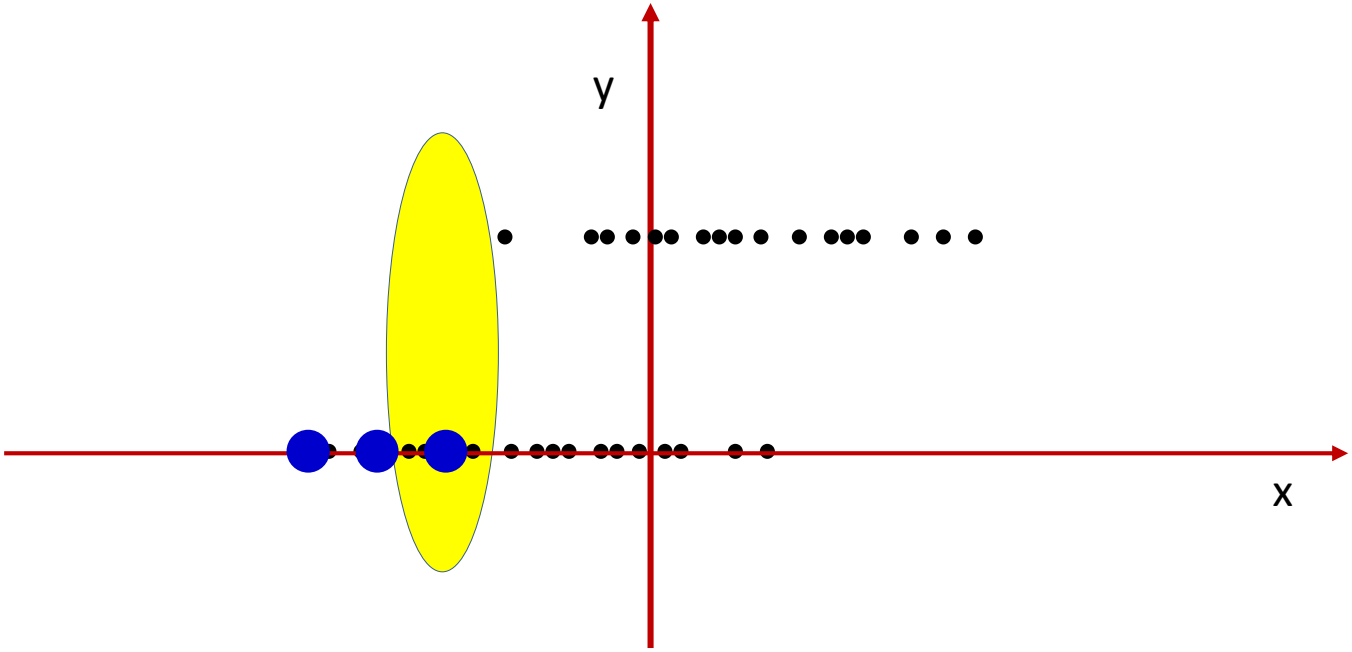

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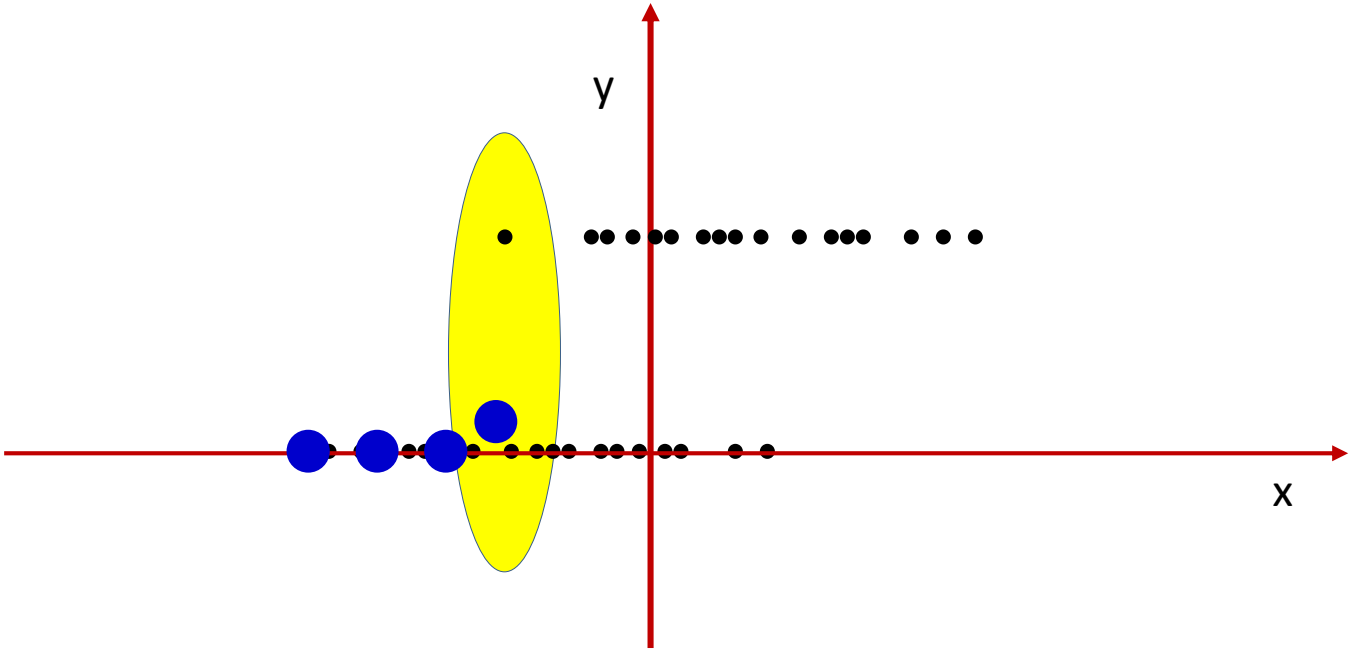

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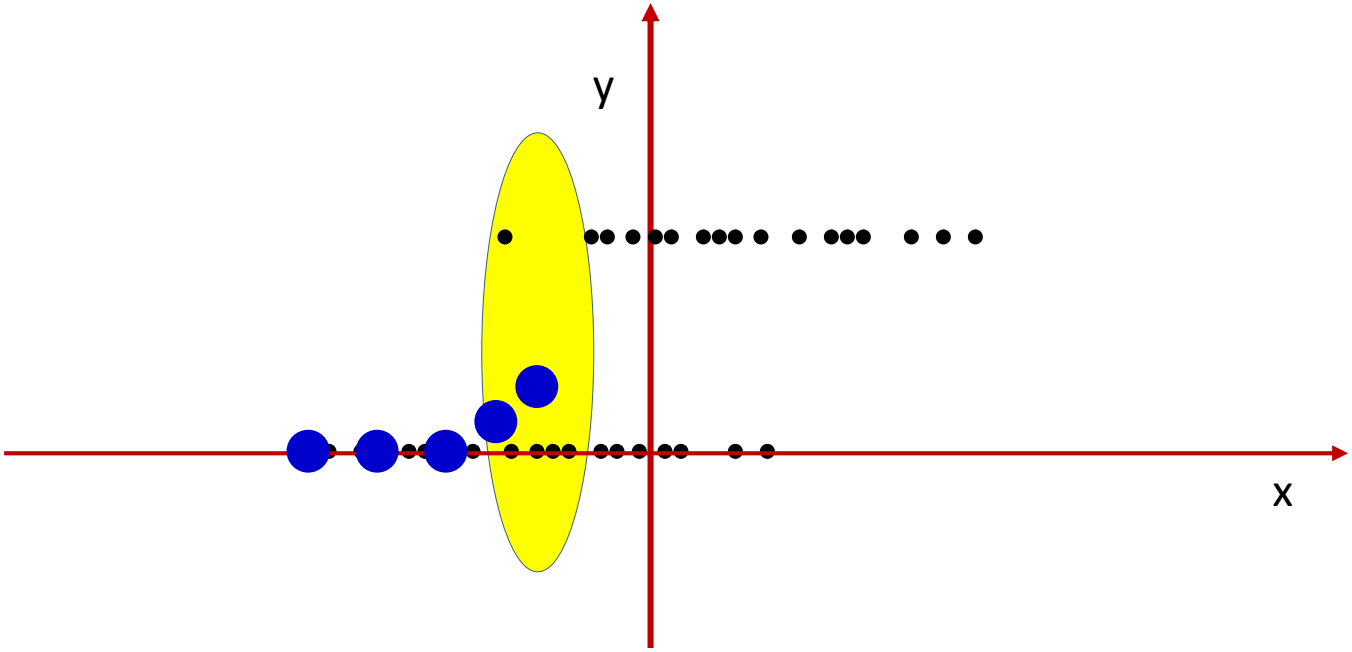

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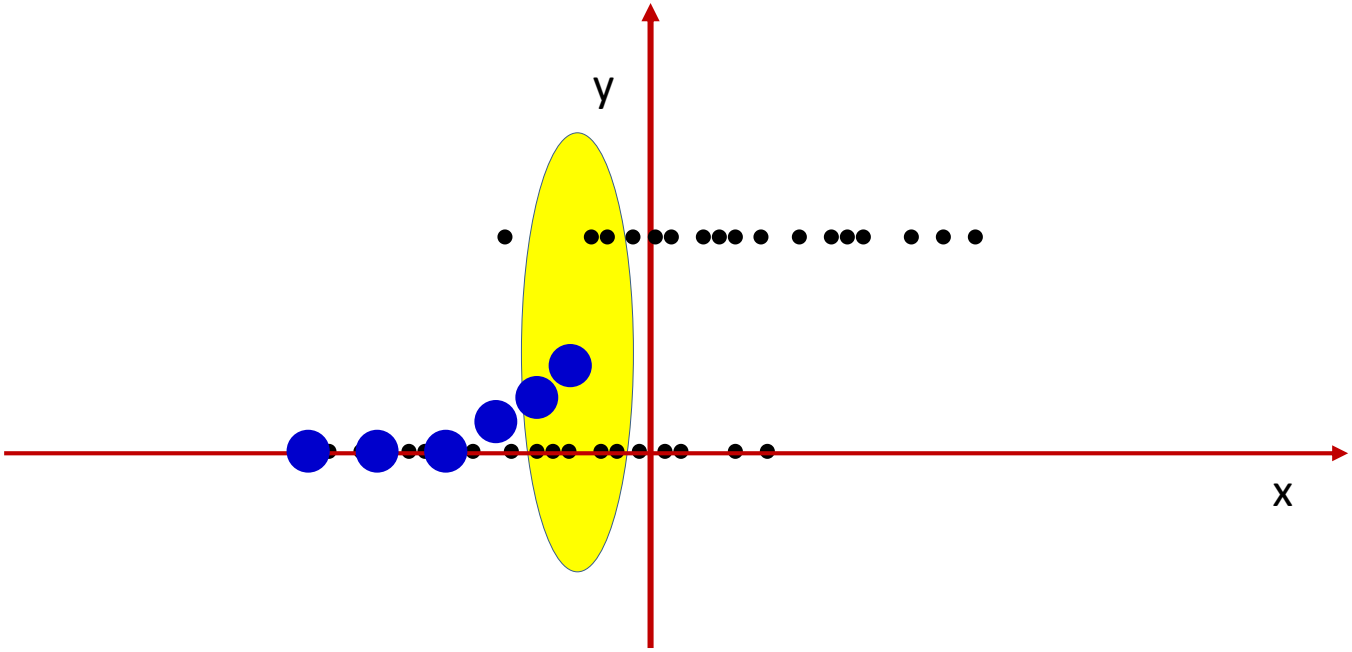

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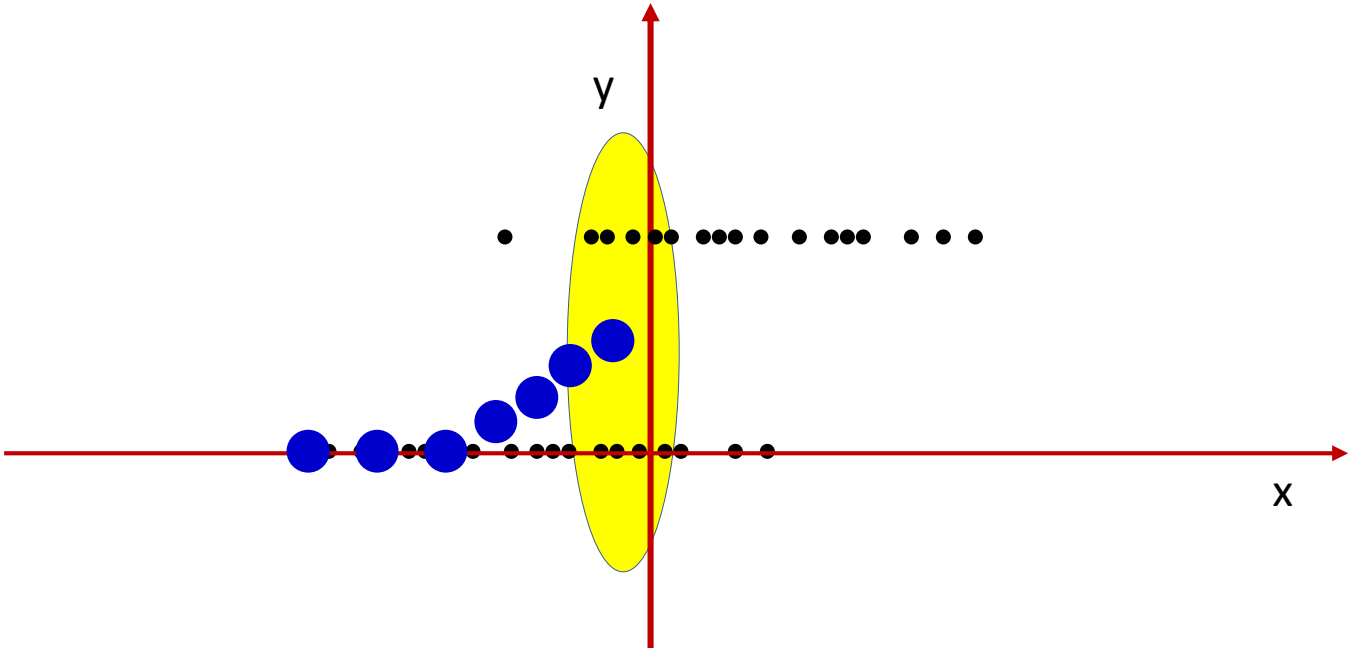

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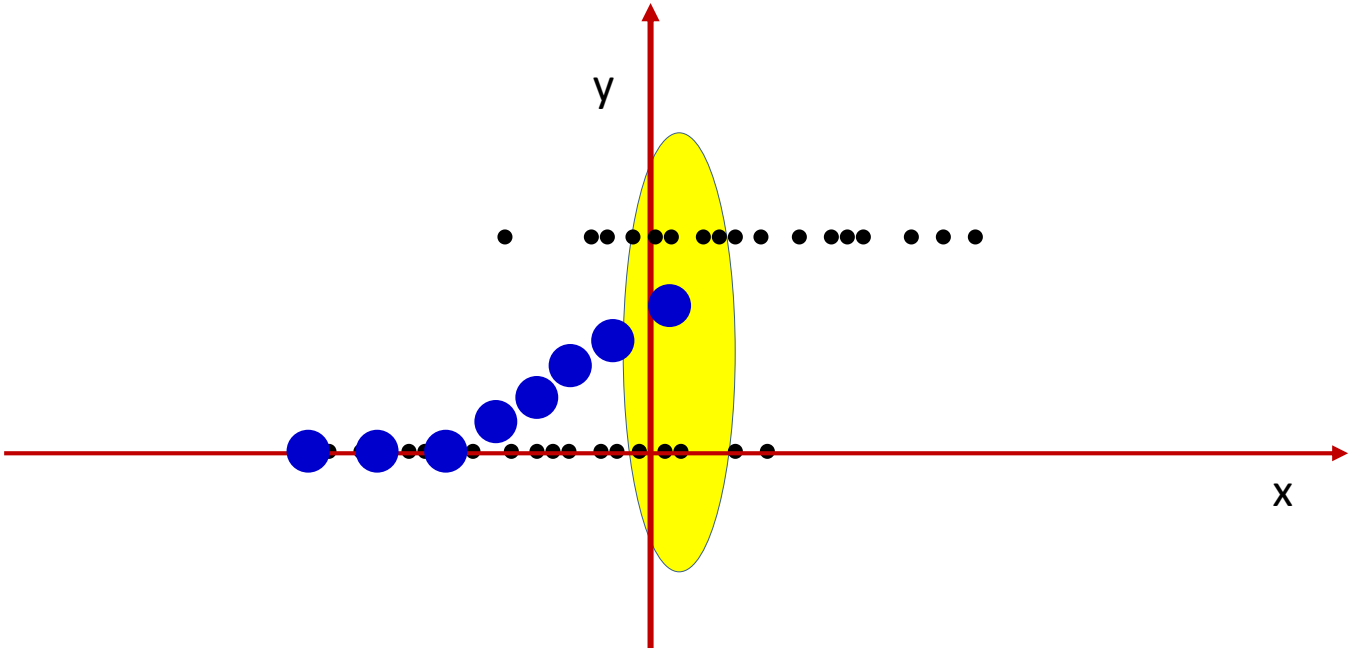

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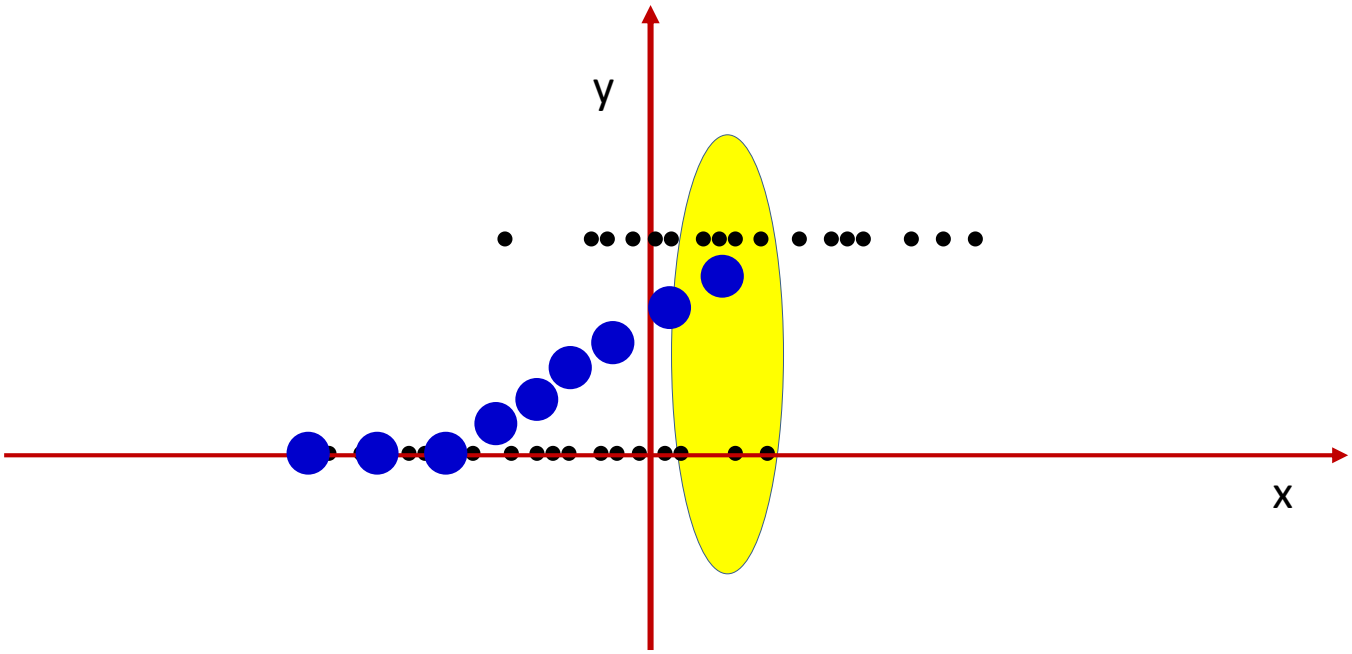

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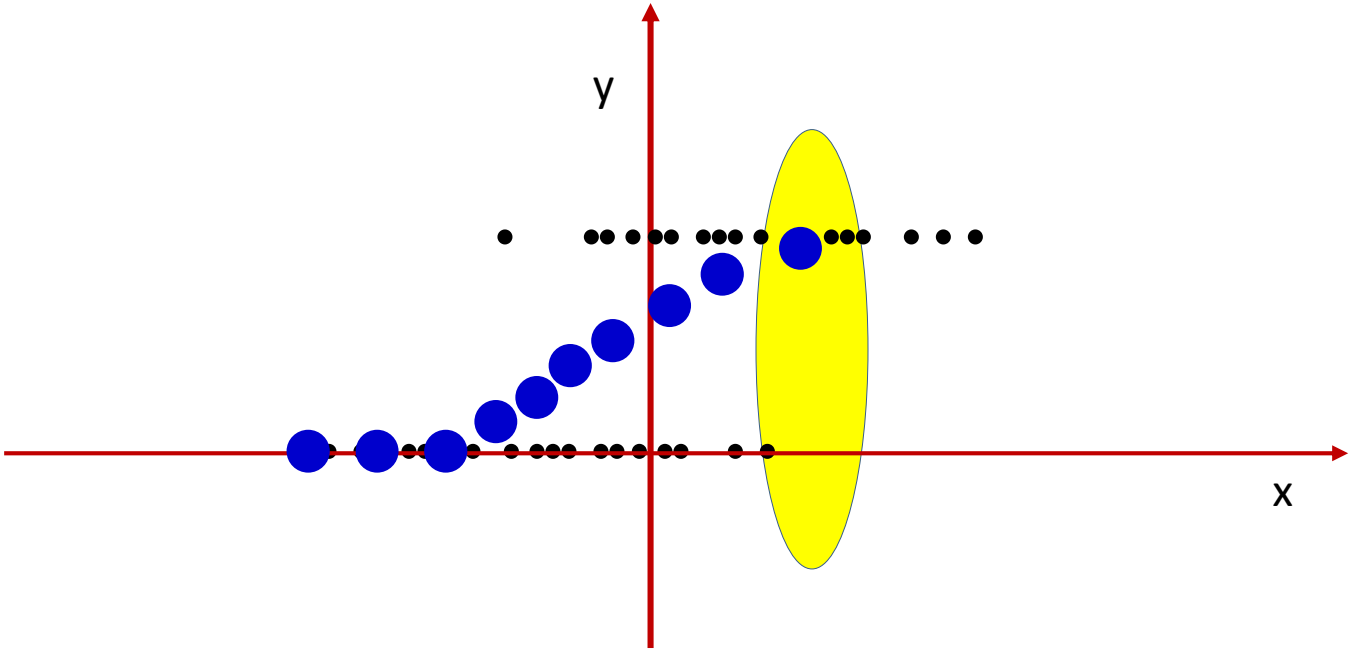

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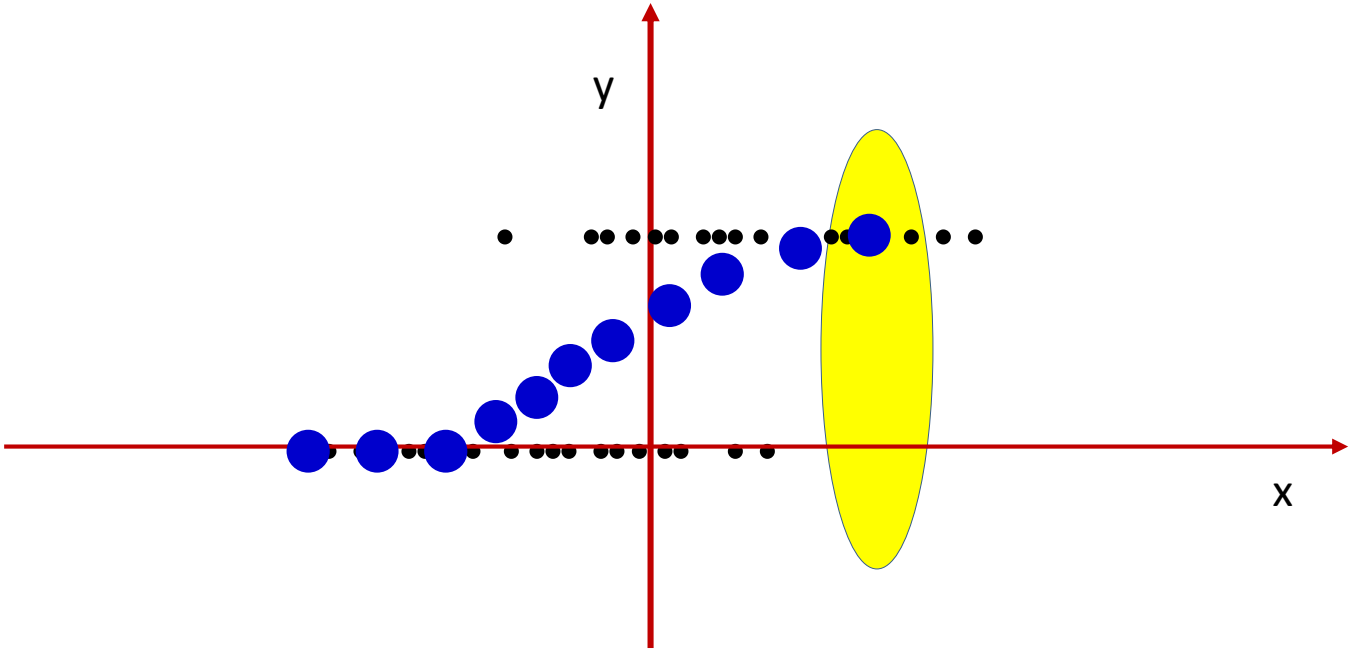

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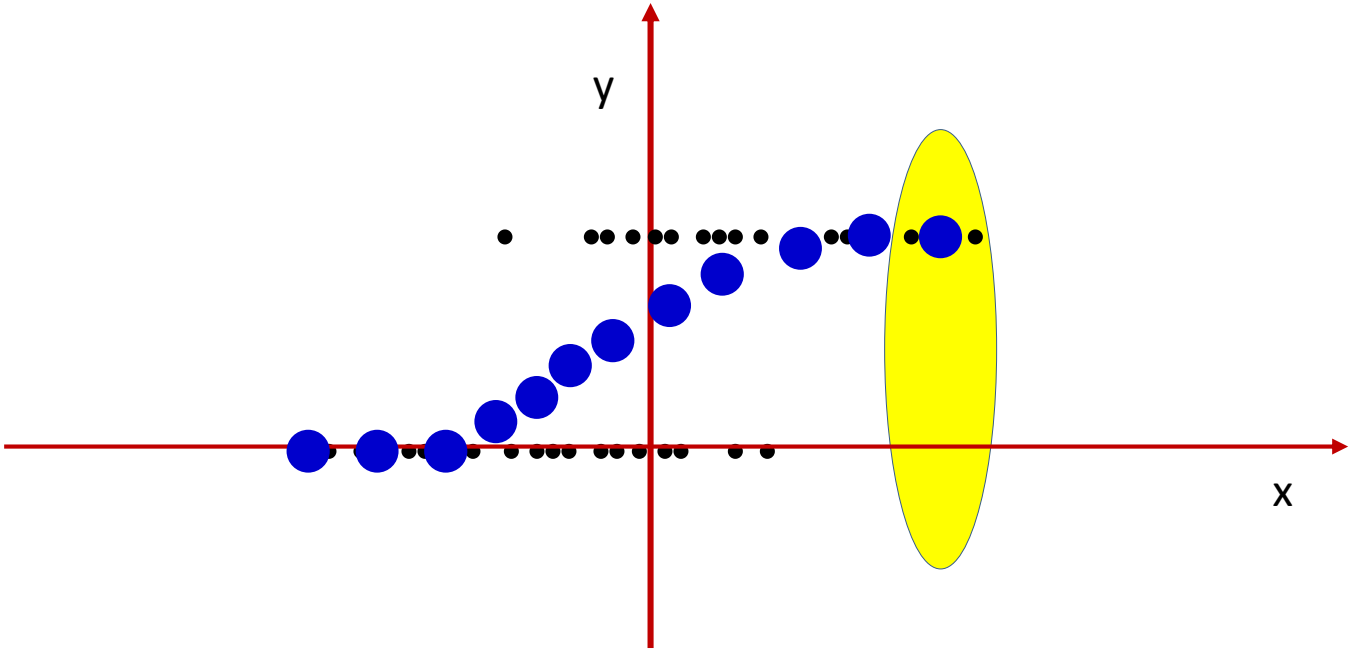

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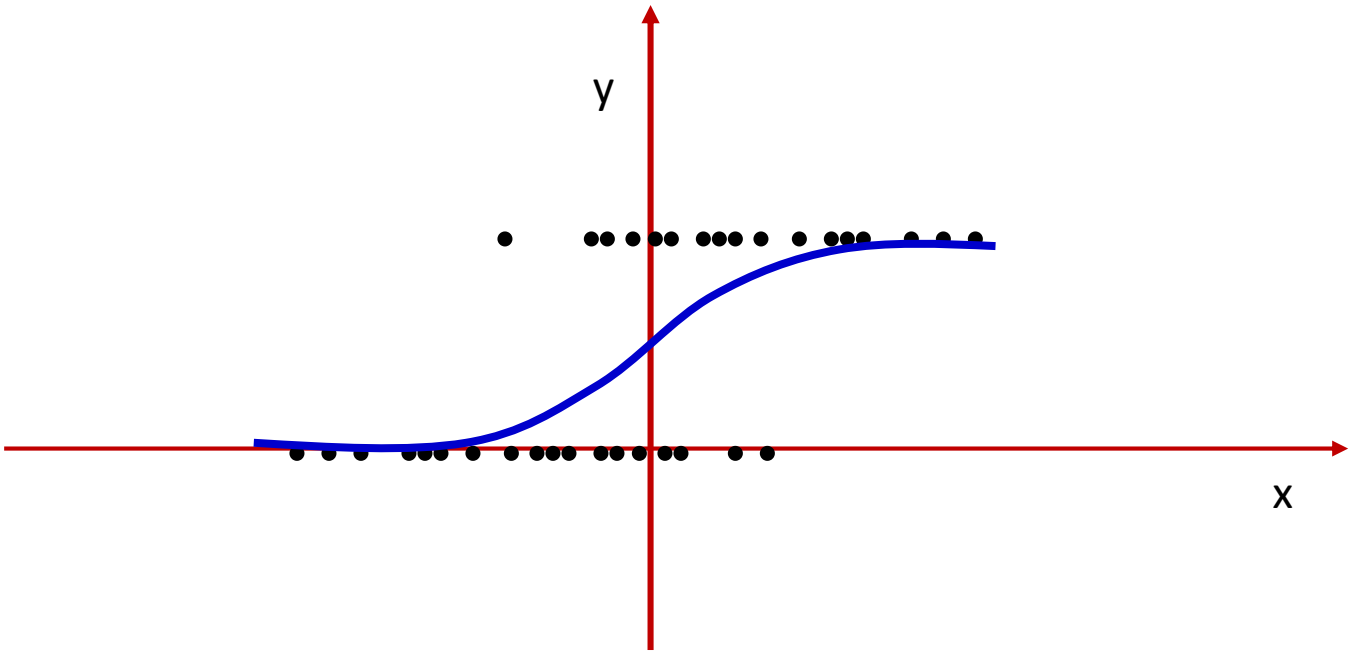

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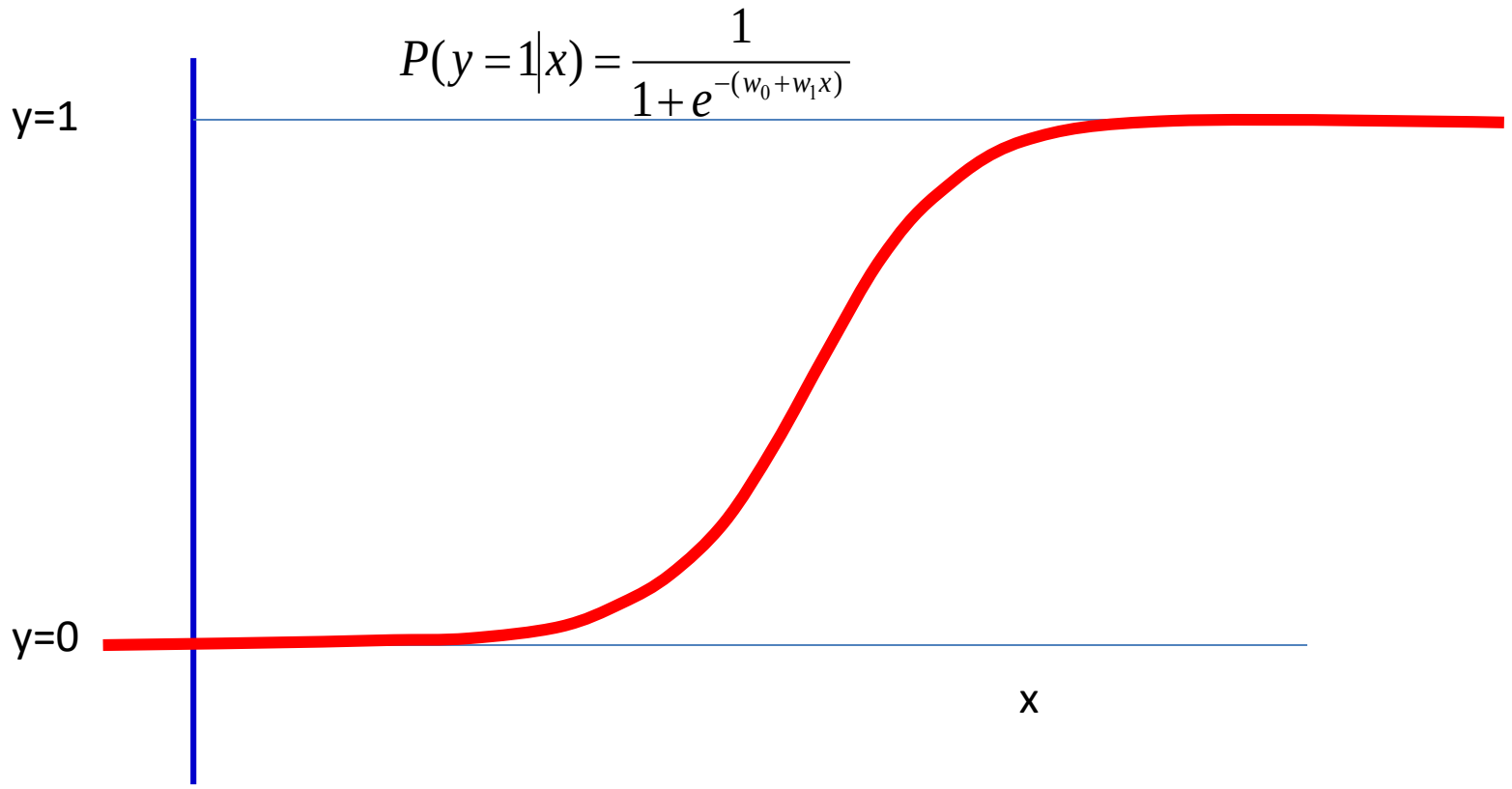
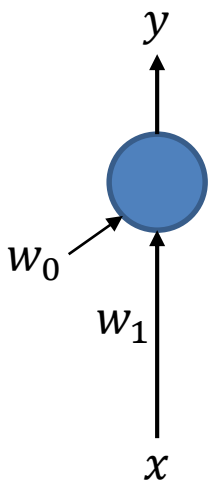
The logistic regression model



- Class 1 becomes increasingly probable going left to right
  - Very typical in many problems

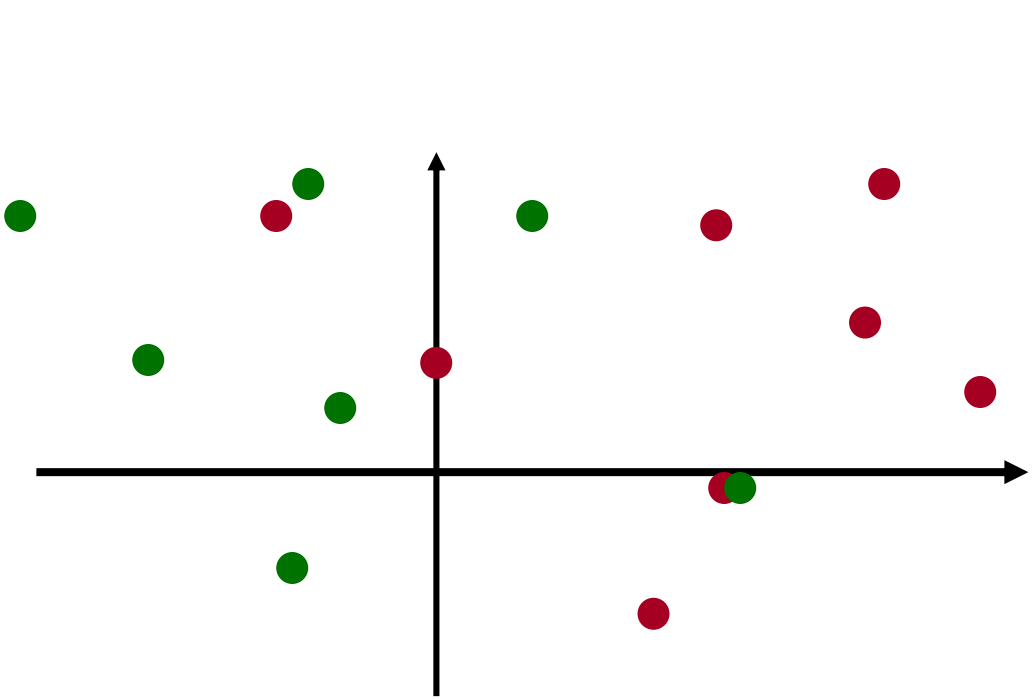
The logistic perceptron

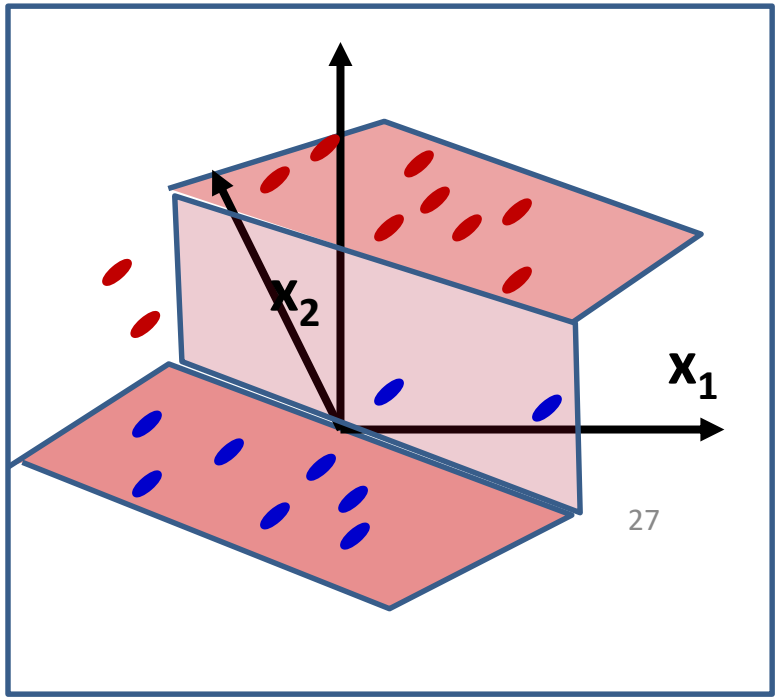


$$P(y|x) = \frac{1}{1+e^{-(w_0+w_1 x)}}$$

- A sigmoid perceptron with a single input models the *a posteriori* probability of the class given the input

Non-linearly separable data





- Two-dimensional example
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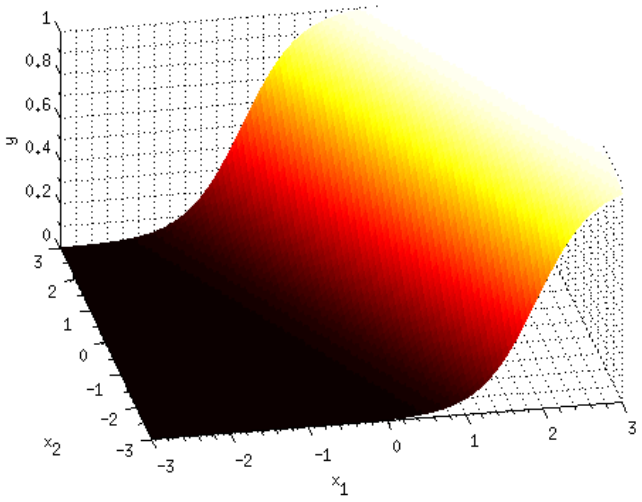
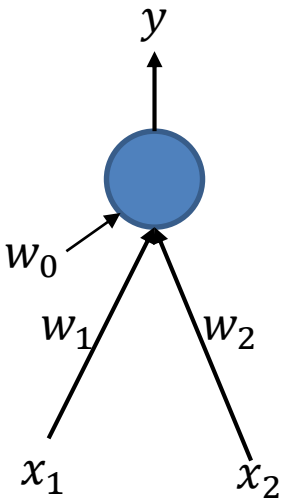
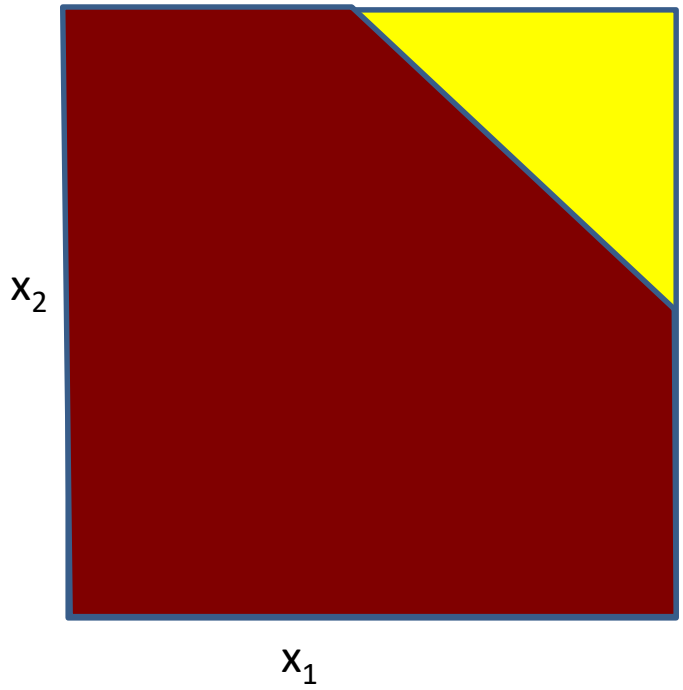
Logistic regression





Decision: y > 0.5?

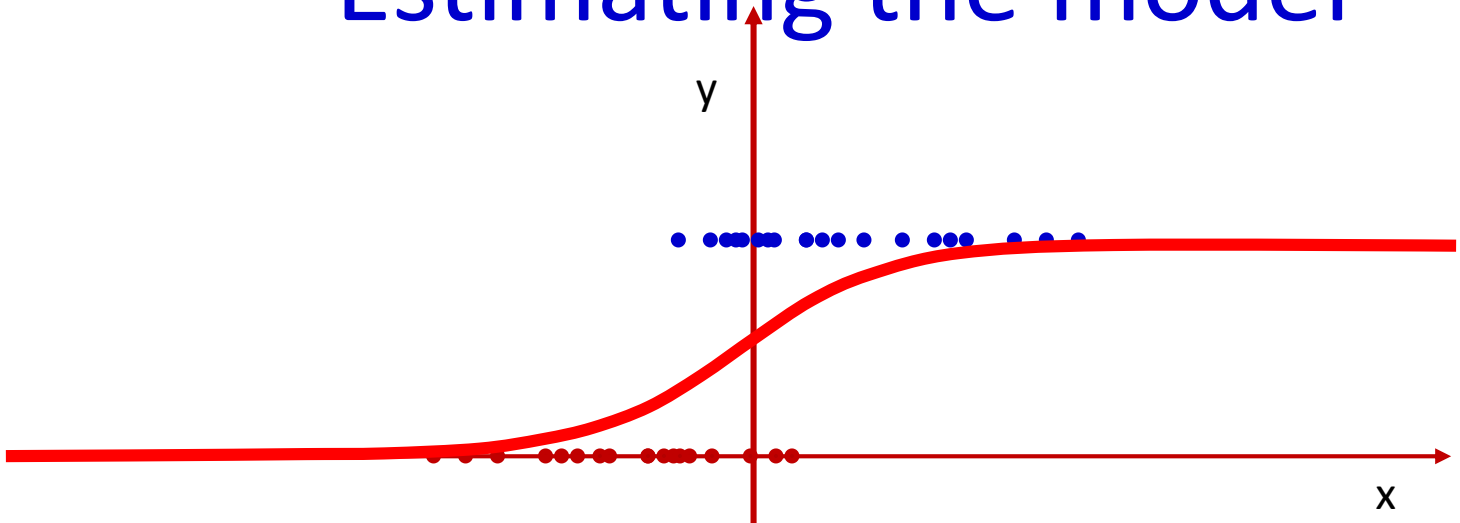


When X is a 2-D variable

$$P(Y=1|X)=\frac{1}{1+\exp\left(-\left(\sum_i w_i x_i + w_0\right)\right)}$$

- This the perceptron with a sigmoid activation
  - It actually computes the *probability* that the input belongs to class 1

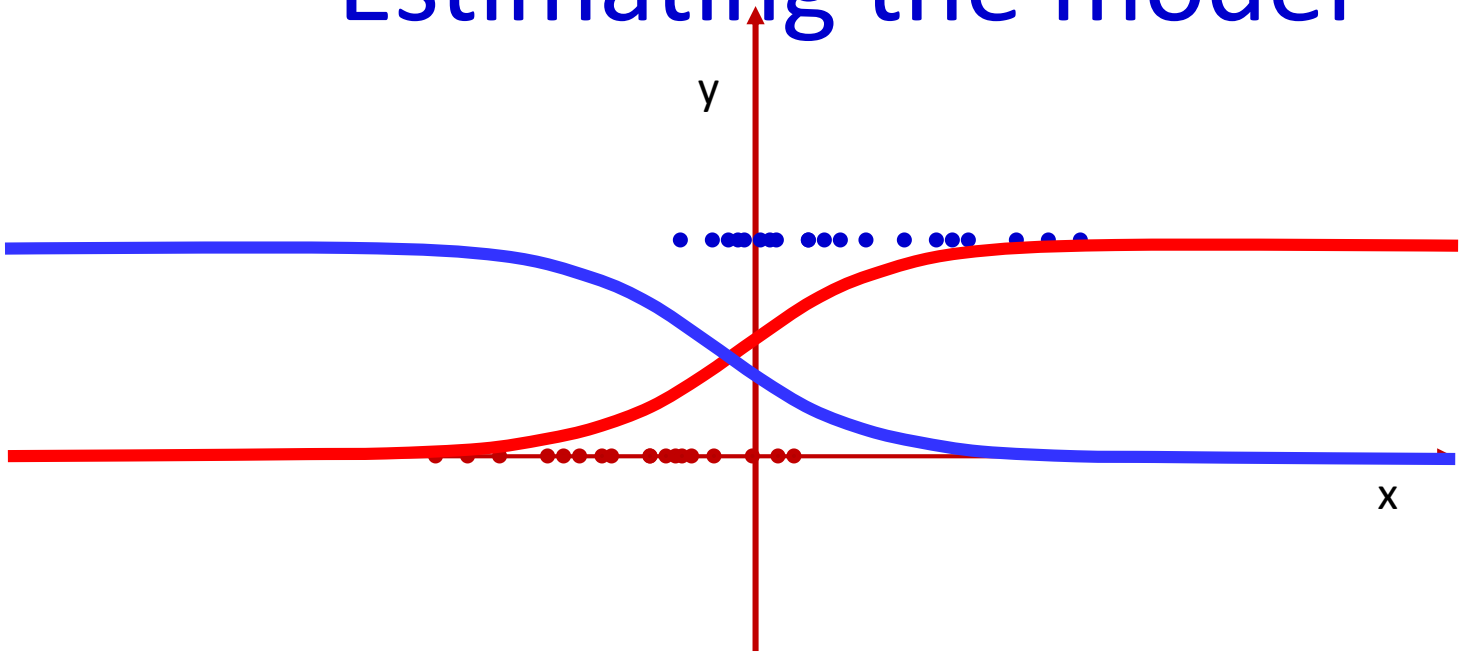
Estimating the model



$$P(y|x) = f(x) = \frac{1}{1+e^{-(w_0+w_1x)}}$$

- Given the training data (many (x, y) pairs represented by the dots), estimate w_0 and w_1 for the curve

Estimating the model



- Easier to represent using a y = +1/-1 notation

$$P(y=1|x)=\frac{1}{1+e^{-(w_0+w_1x)}}$$

$$P(y=-1|x)=\frac{1}{1+e^{(w_0+w_1x)}}$$

$$P(y|x)=\frac{1}{1+e^{-y(w_0+w_1x)}}$$

Estimating the model

- Given: Training data

$$(X_1, y_1), (X_2, y_2), \ldots, (X_N, y_N)$$

- Xs are vectors, ys are binary (0/1) class values
- Total probability of data

$$P\big((X_1, y_1), (X_2, y_2), \ldots, (X_N, y_N)\big) = \prod_i P(X_i, y_i)$$

$$= \prod_i P(y_i | X_i)\, P(X_i) = \prod_i \frac{1}{1 + e^{-y_i(w_0 + w^T X_i)}} P(X_i)$$

Estimating the model

- Likelihood

$$P(Training\ data) = \prod_i \frac{1}{1 + e^{-y_i(w_0 + w^T X_i)}} P(X_i)$$

- Log likelihood

$$\log P(Training\ data) =$$

$$\sum_i \log P(X_i) - \sum_i \log\left(1 + e^{-y_i(w_0 + w^T X_i)}\right)$$

Maximum Likelihood Estimate

$$\widehat{w}_0, \widehat{w}_1 = \underset{w_0, w_1}{\operatorname{argmax}} \log P(Training\ data)$$

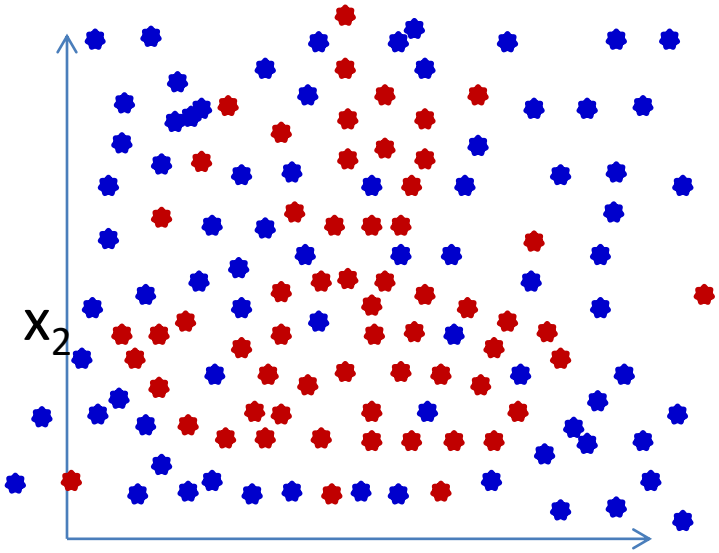
- Equals (note argmin rather than argmax)

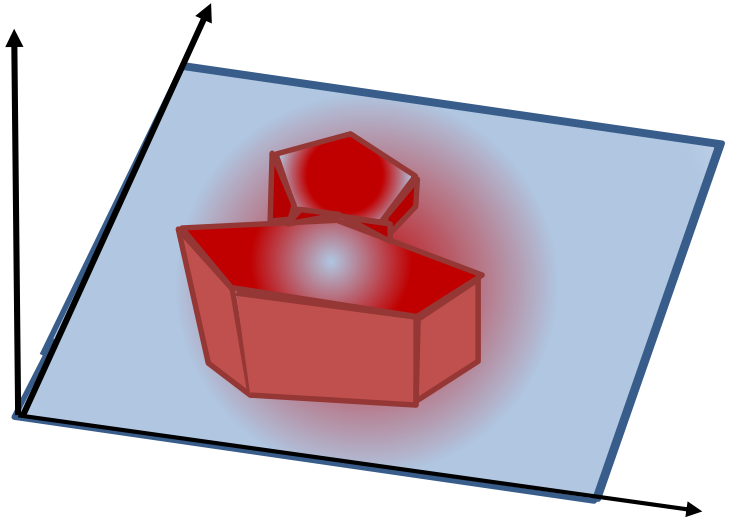
$$\widehat{w}_0, \widehat{w}_1 = \underset{w_0, w}{\operatorname{argmin}} \sum_i \log\left(1 + e^{-y_i(w_0 + w^T X_i)}\right)$$

- Identical to minimizing the KL divergence between the desired output y and actual output $\frac{1}{1+e^{-(w_0+w^T X_i)}}$

- Cannot be solved directly, needs gradient descent

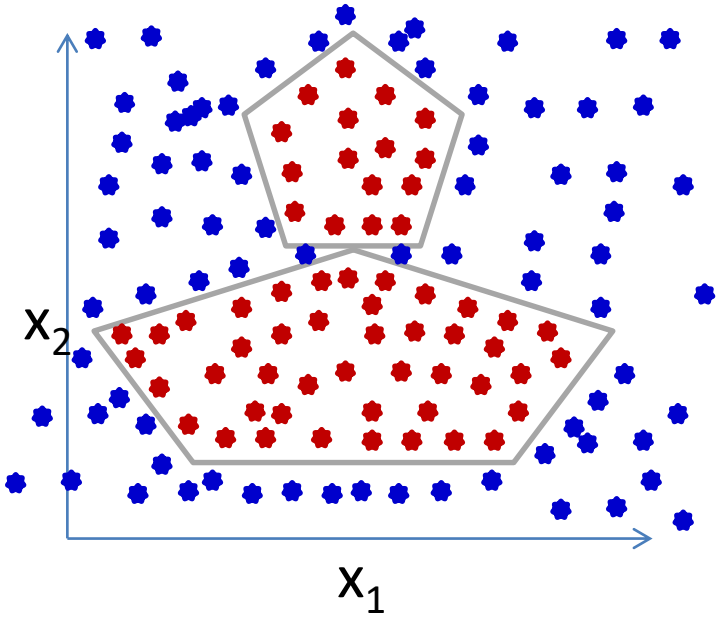
So what about this one?

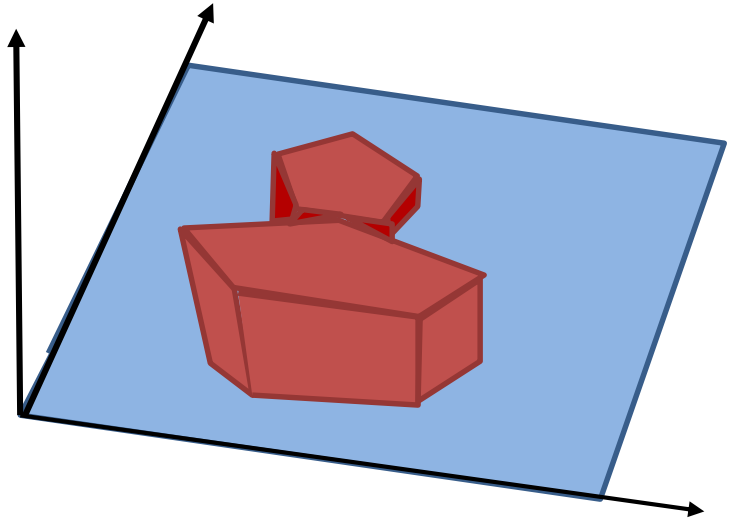




- Non-linear classifiers..

First consider the separable case..





- When the net must learn to classify..

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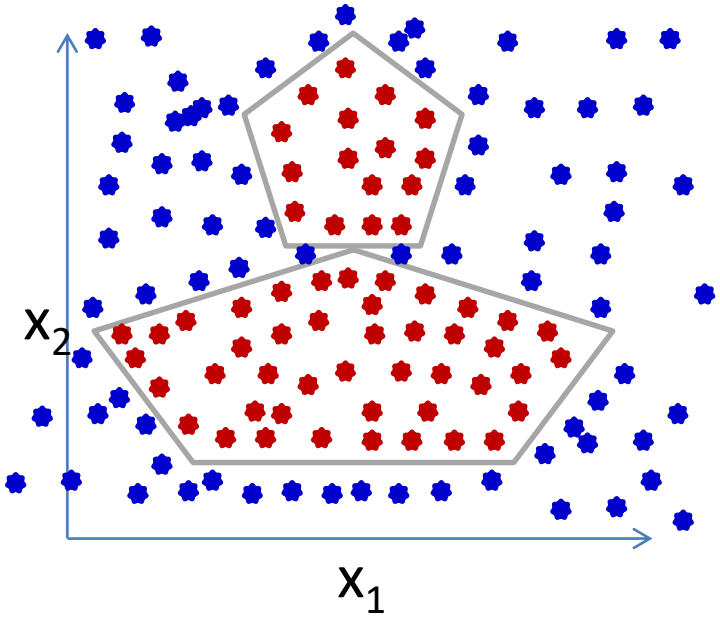
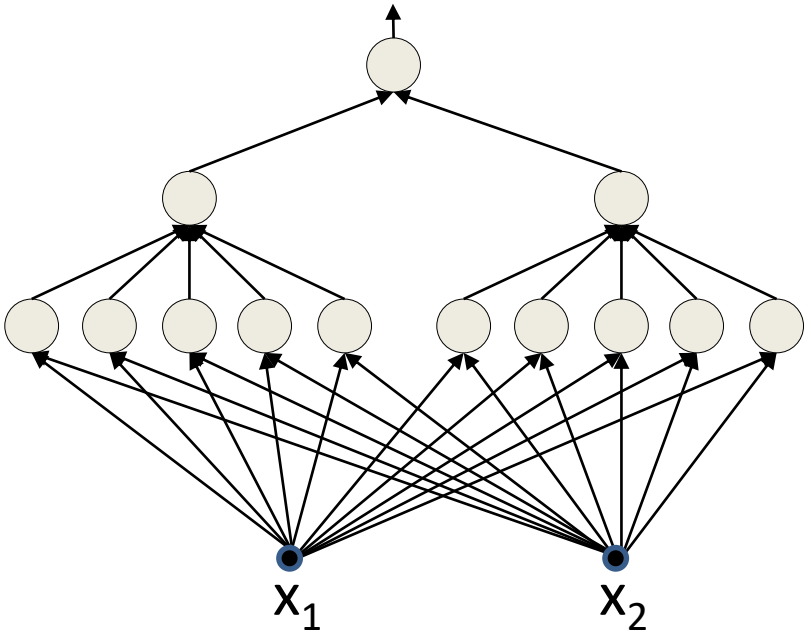
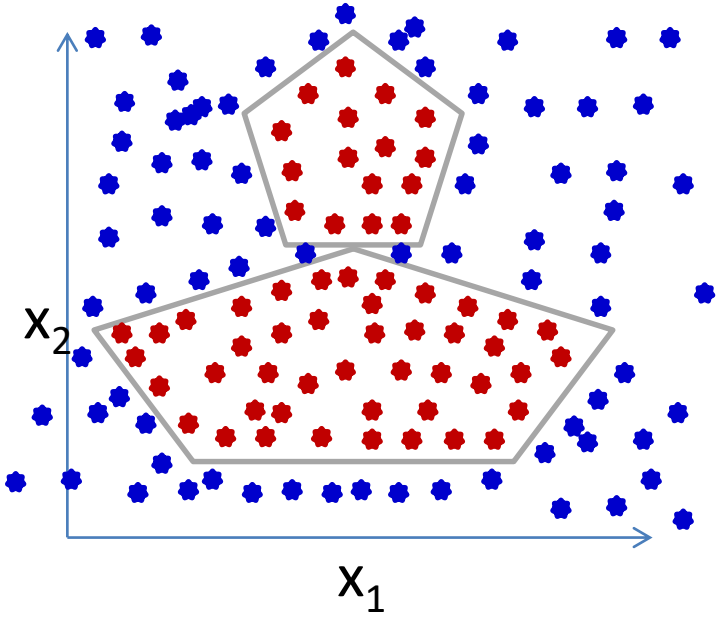
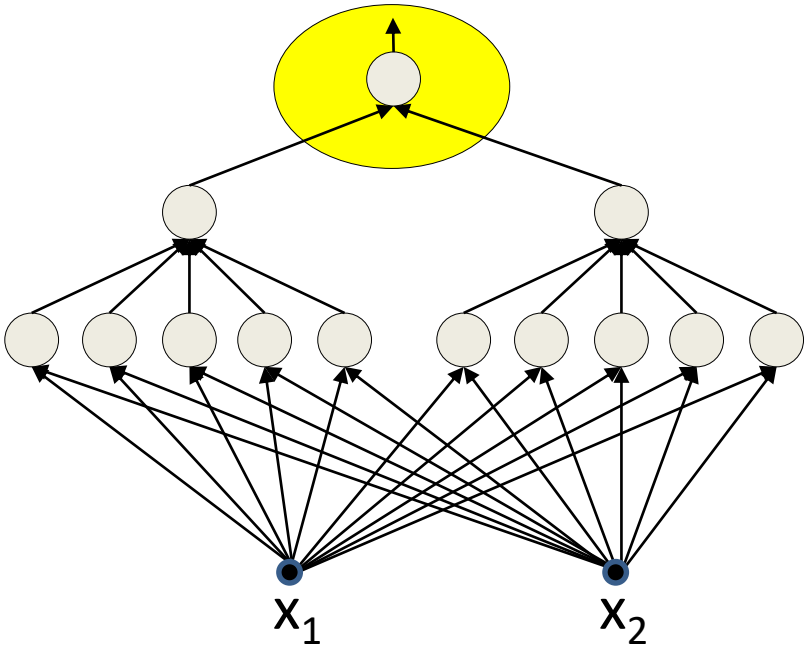




- For a “sufficient” net

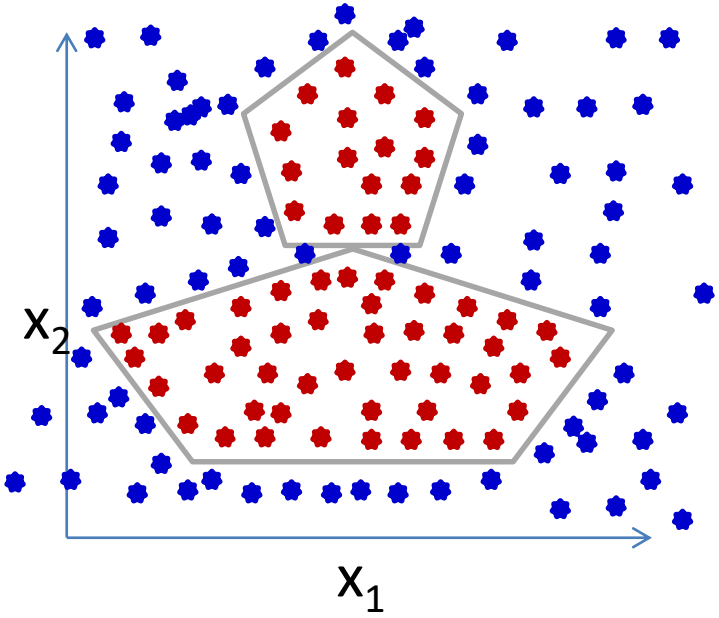
First consider the separable case..

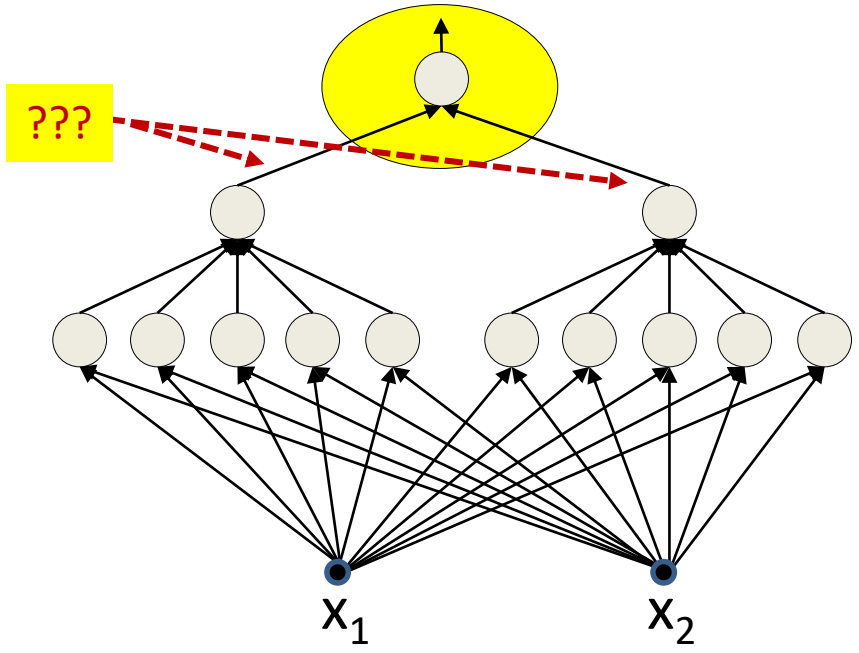




- For a “sufficient” net
- This final perceptron is a linear classifier

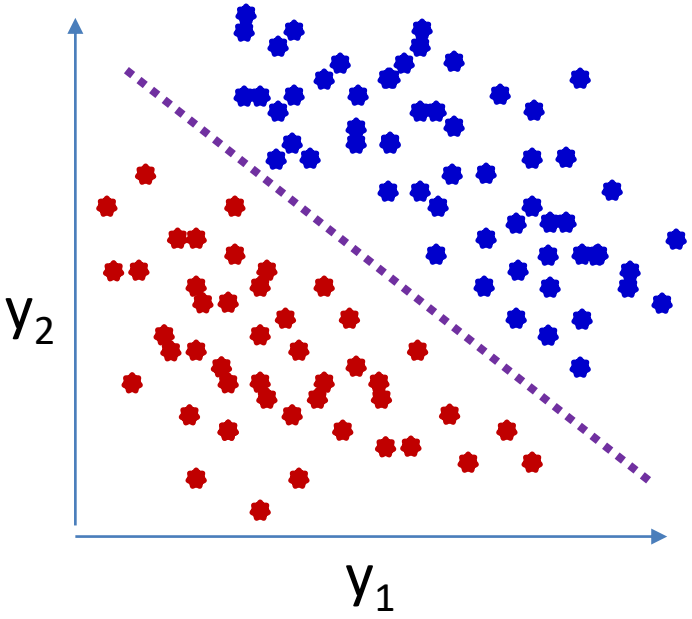
First consider the separable case..

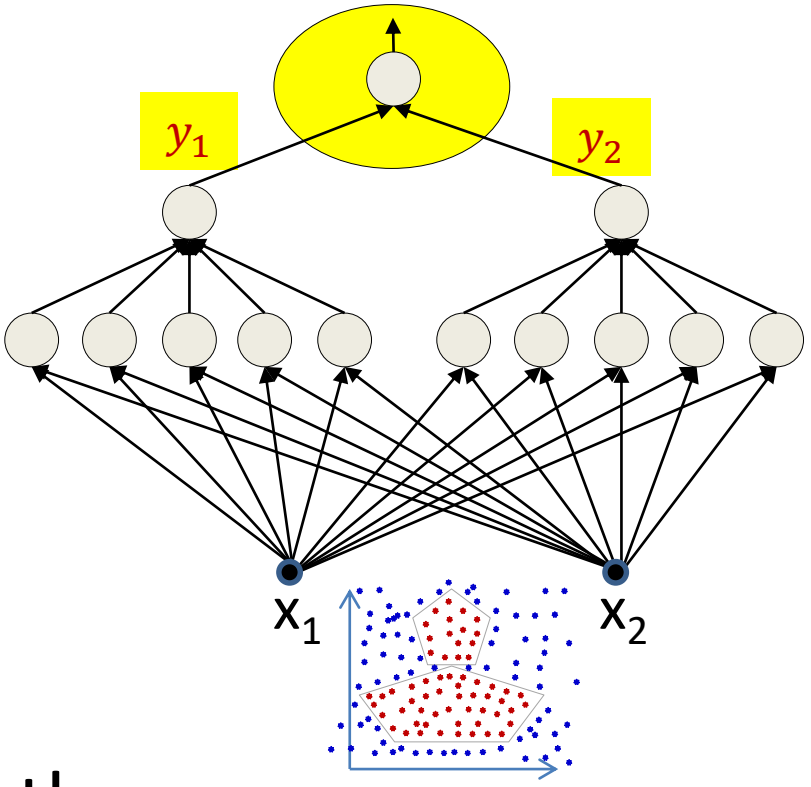




- For a “sufficient” net
- This final perceptron is a linear classifier over the output of the penultimate layer

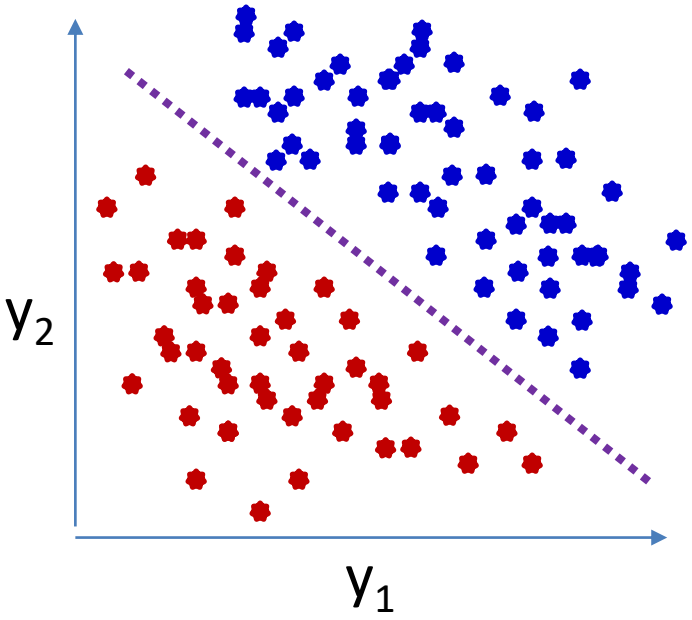
First consider the separable case..

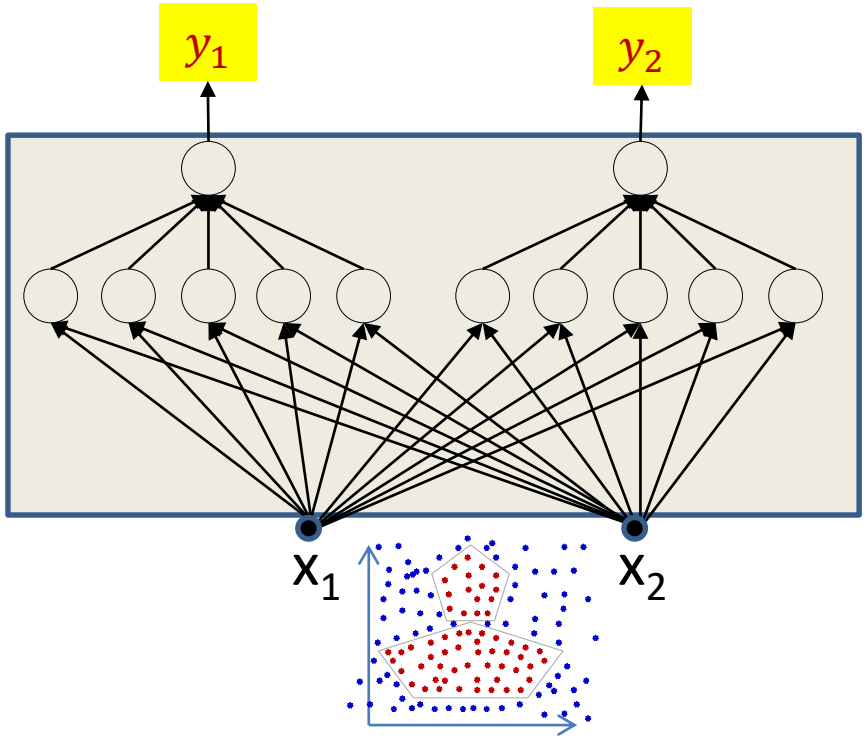




- For perfect classification the output of the penultimate layer must be linearly separable

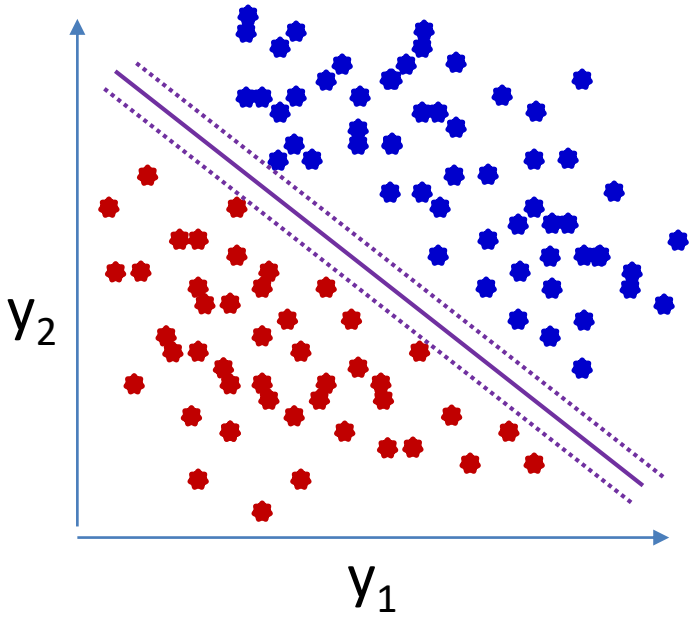
First consider the separable case..

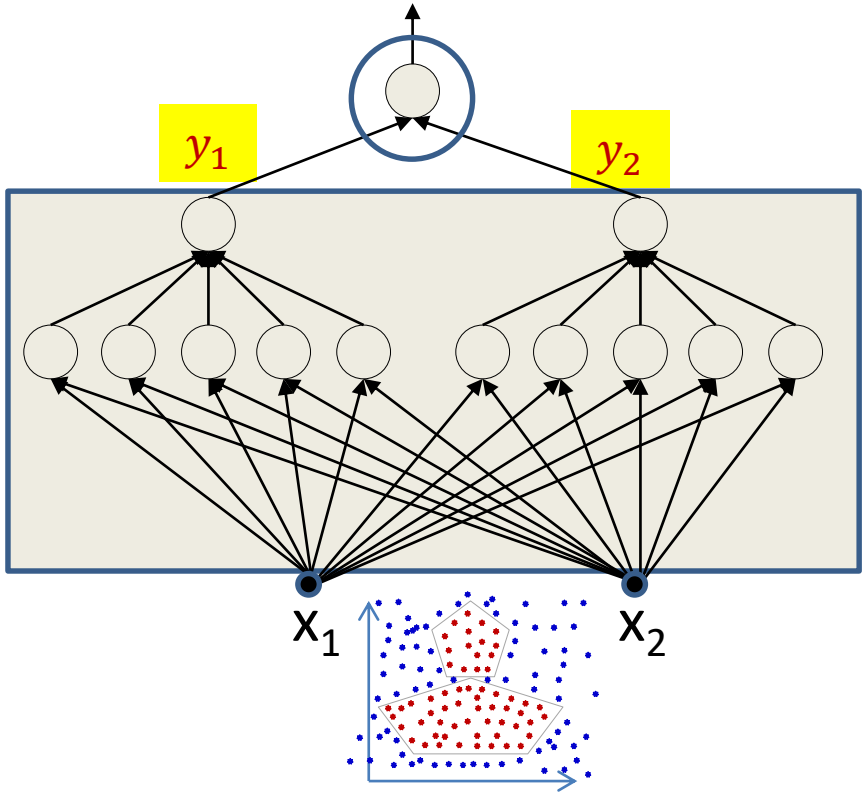




- The rest of the network may be viewed as a transformation that transforms data from non-linear classes to linearly separable features

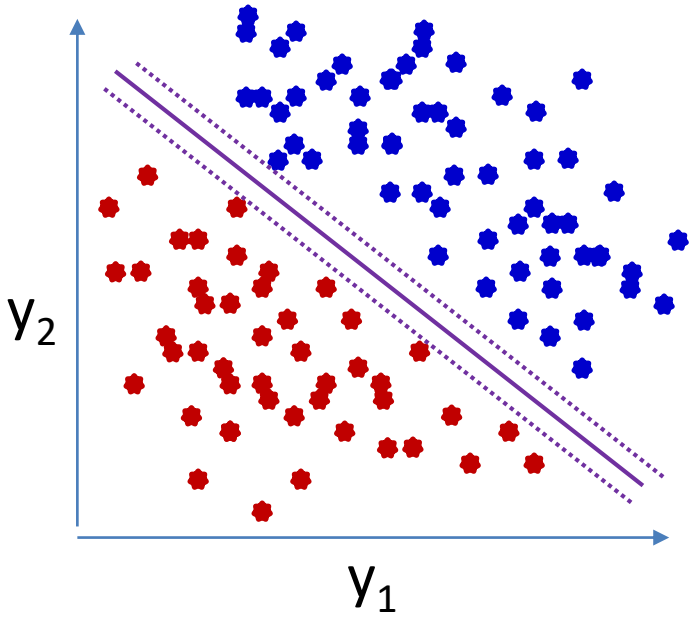
First consider the separable case..

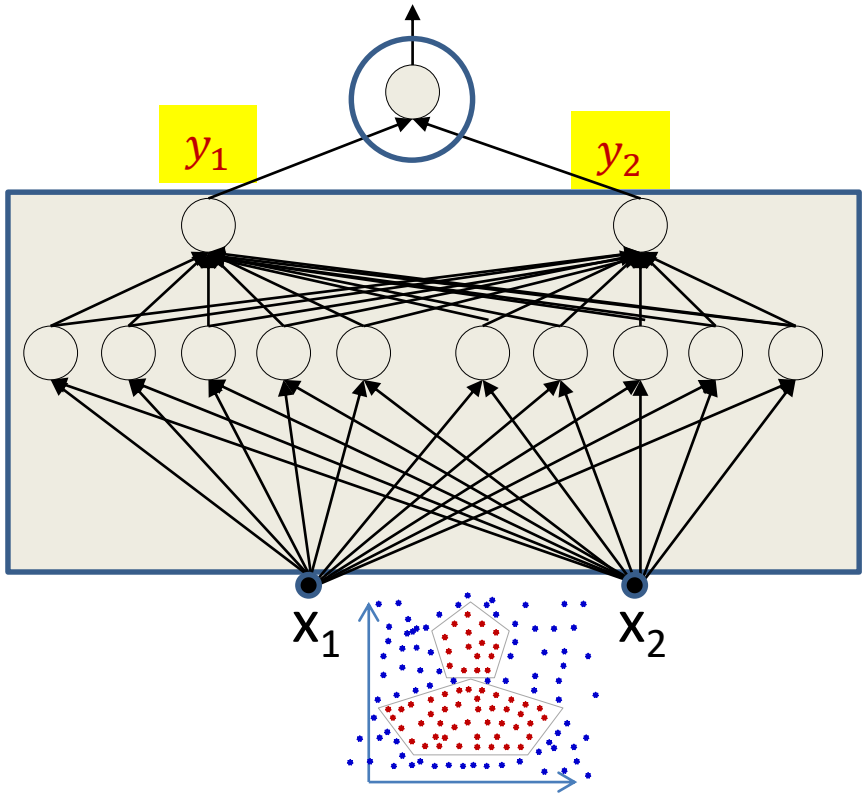




- The rest of the network may be viewed as a transformation that transforms data from non-linear classes to linearly separable features
  - We can now attach *any* linear classifier above it for perfect classification
  - Need not be a perceptron
  - In fact, for ***binary*** classifiers an SVM on top of the features may be more generalizable!

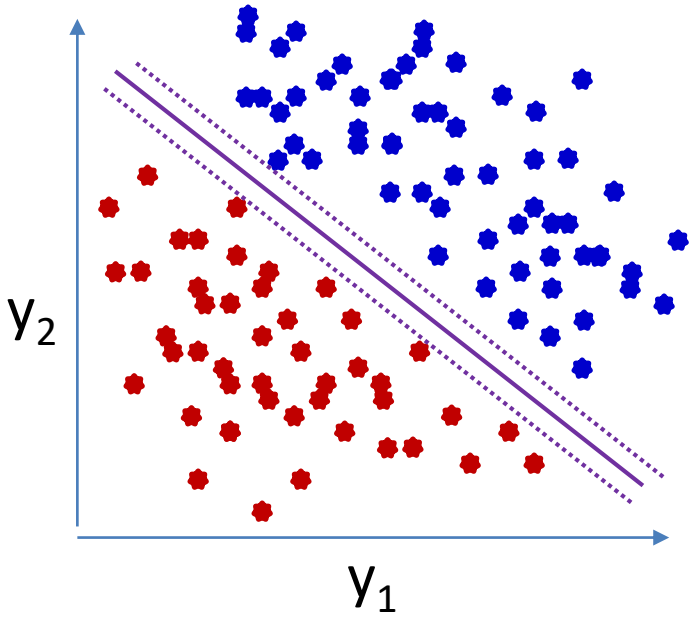
First consider the separable case..

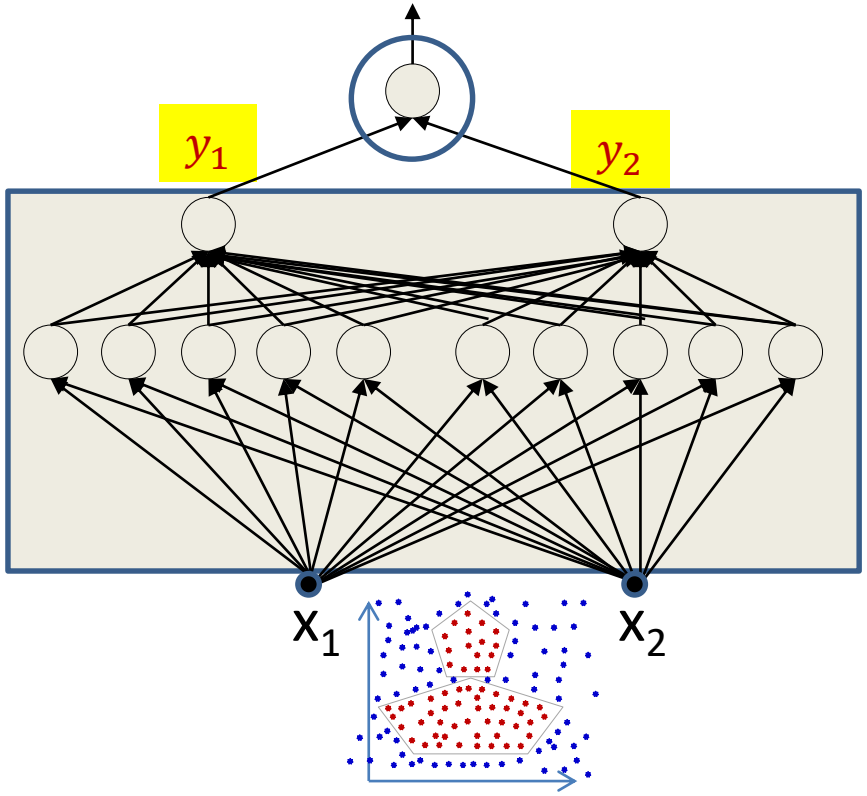




- This is true of *any* sufficient structure
  - Not just the optimal one
  - For *insufficient* structures, the network may *attempt* to transform the inputs to linearly separable features
    - But not be perfect
      - Still, for binary problems, using an SVM with slack may be more effective than a final perceptron!

First consider the separable case..



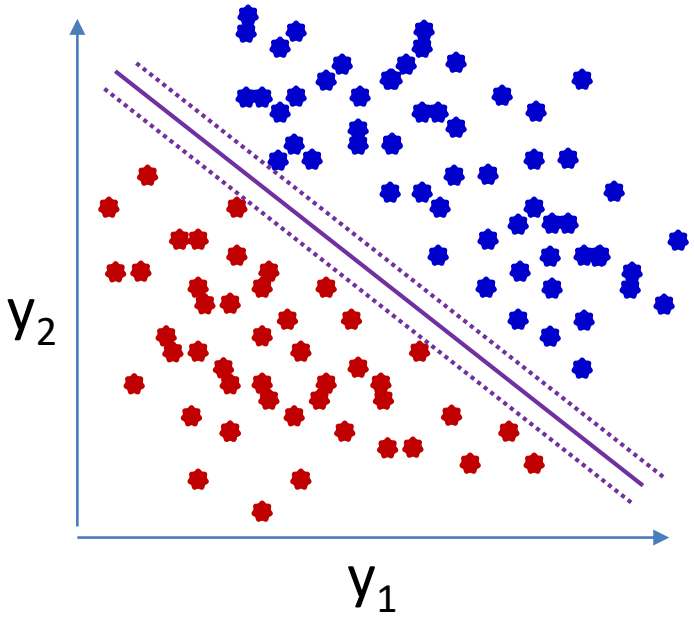


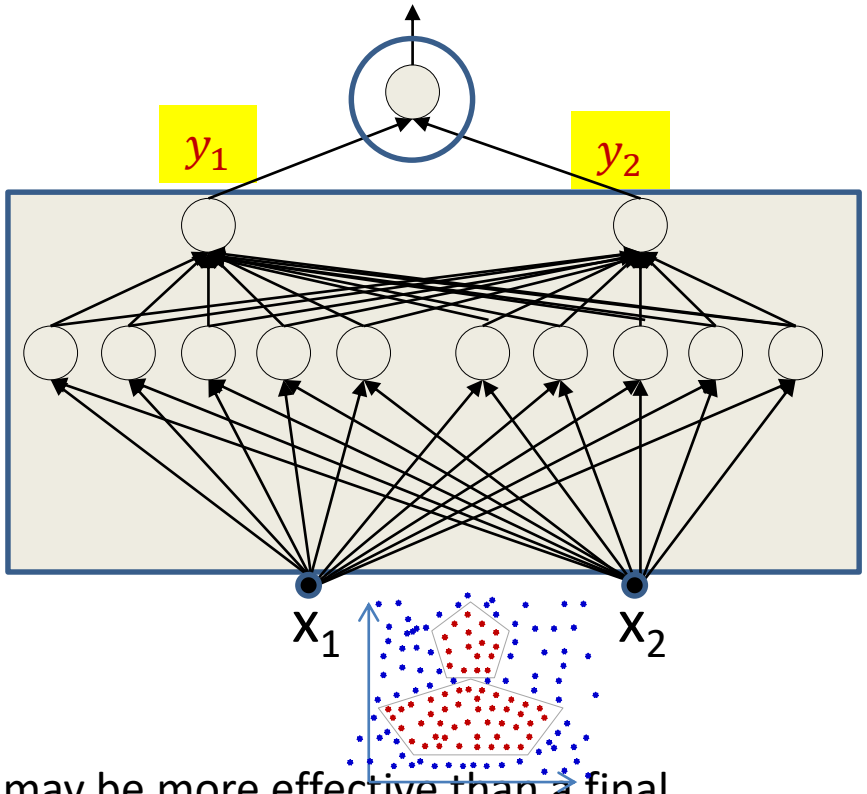
- This is true of *any* sufficient structure
  - Not just the optimal one
- For *insufficient* structures, the network may *attempt* to transform the inputs to linearly separable features
  - Will fail to separate
  - Still, for binary problems, using an SVM with slack may be more effective than a final perceptron!

Story so far

- A classification MLP actually comprises two components
  - A "feature extraction network" that converts the inputs into linearly separable features
    - Or *nearly* linearly separable features
  - A final linear classifier that operates on the linearly separable features

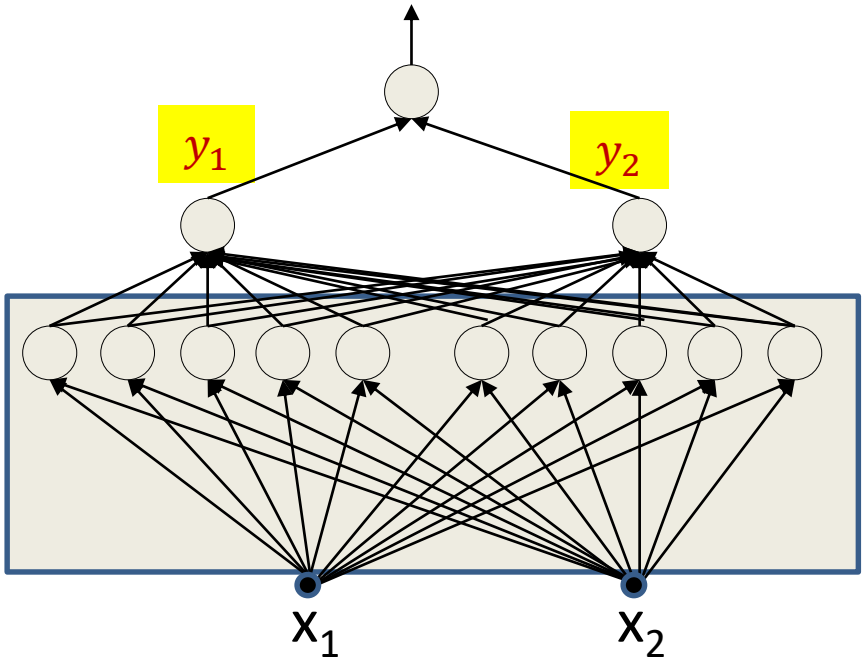
An SVM at the output?





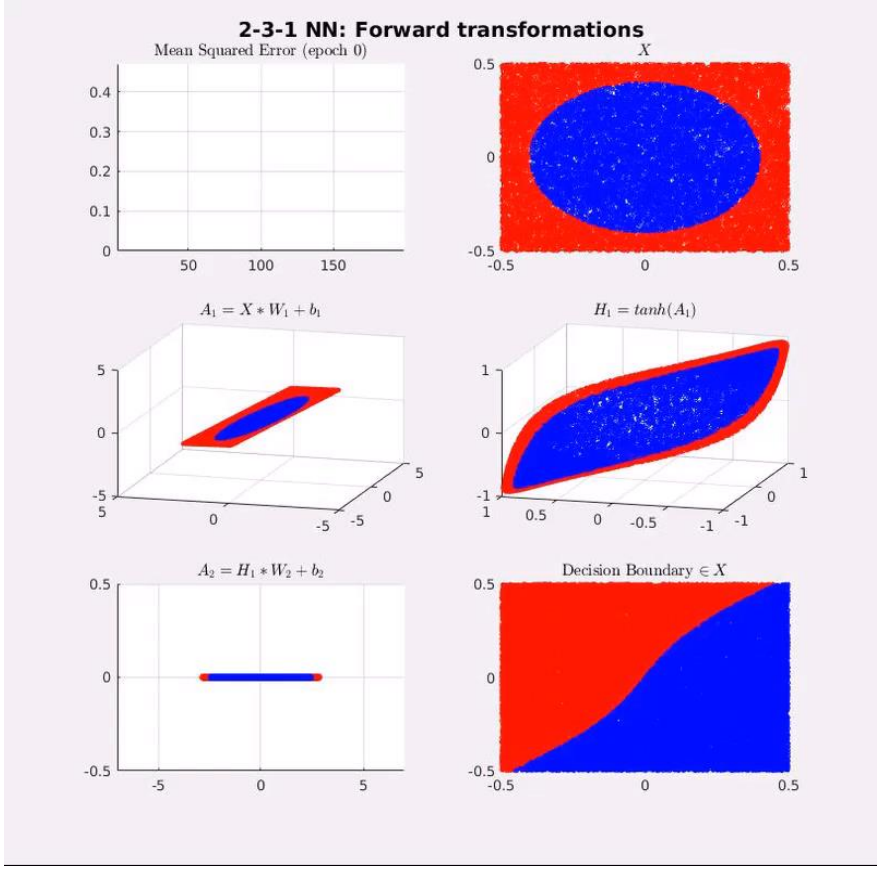
- For binary problems, using an SVM with slack may be more effective than a final perceptron!
- How does that work??
  - *Option 1: First* train the MLP with a perceptron at the output, then detach the feature extraction, compute features, and train an SVM
  - *Option 2:* Directly employ a max-margin rule at the output, and optimize the entire network
    - Left as an exercise for the curious

How about the lower layers?



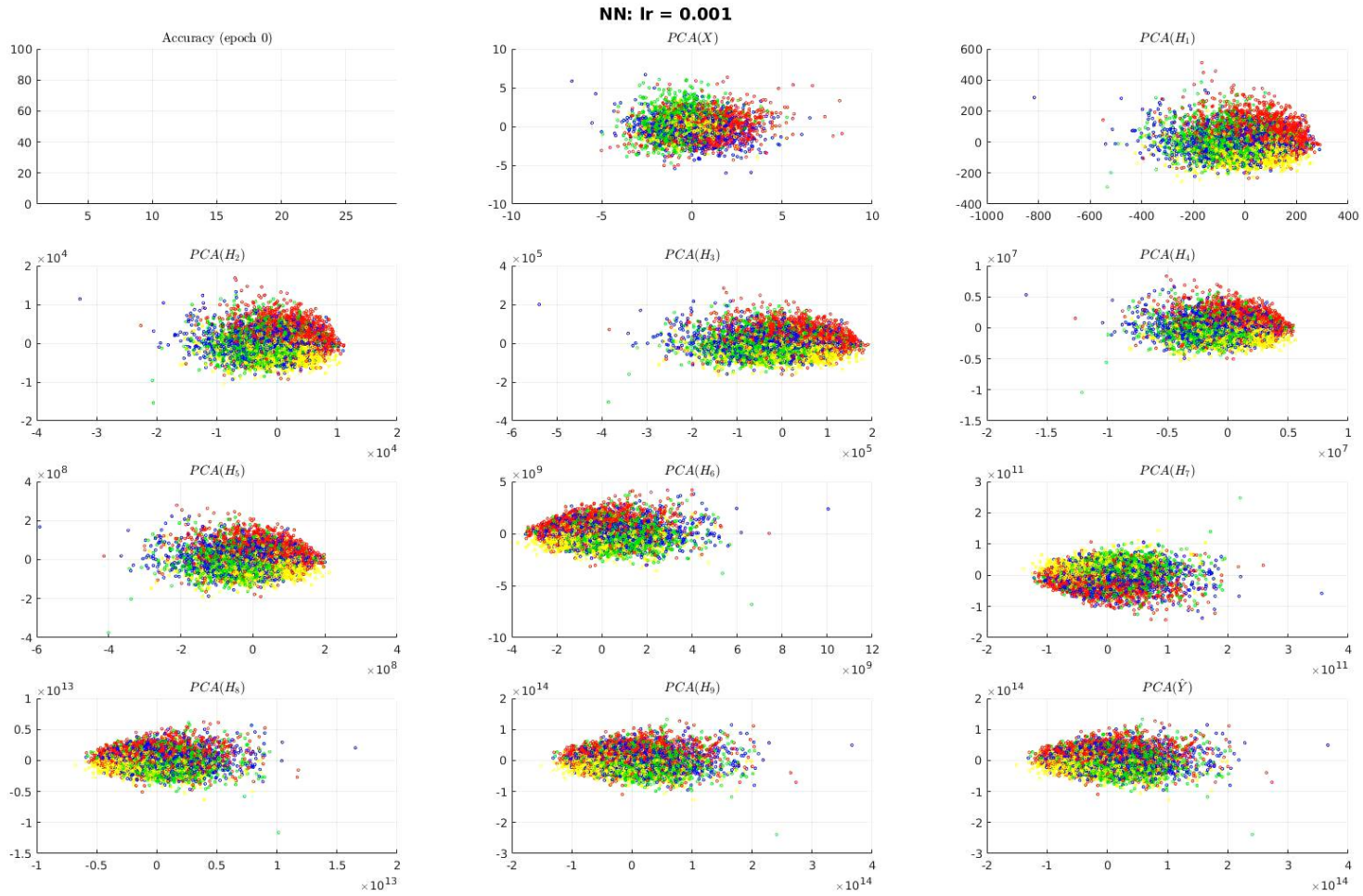
- How do the lower layers respond?
  - They too compute features
  - But how do they look
- Manifold hypothesis: For separable classes, the classes are linearly separable on a non-linear manifold
- Layers sequentially “straighten” the data manifold
  - Until the final layer, which fully linearizes it

The behavior of the layers



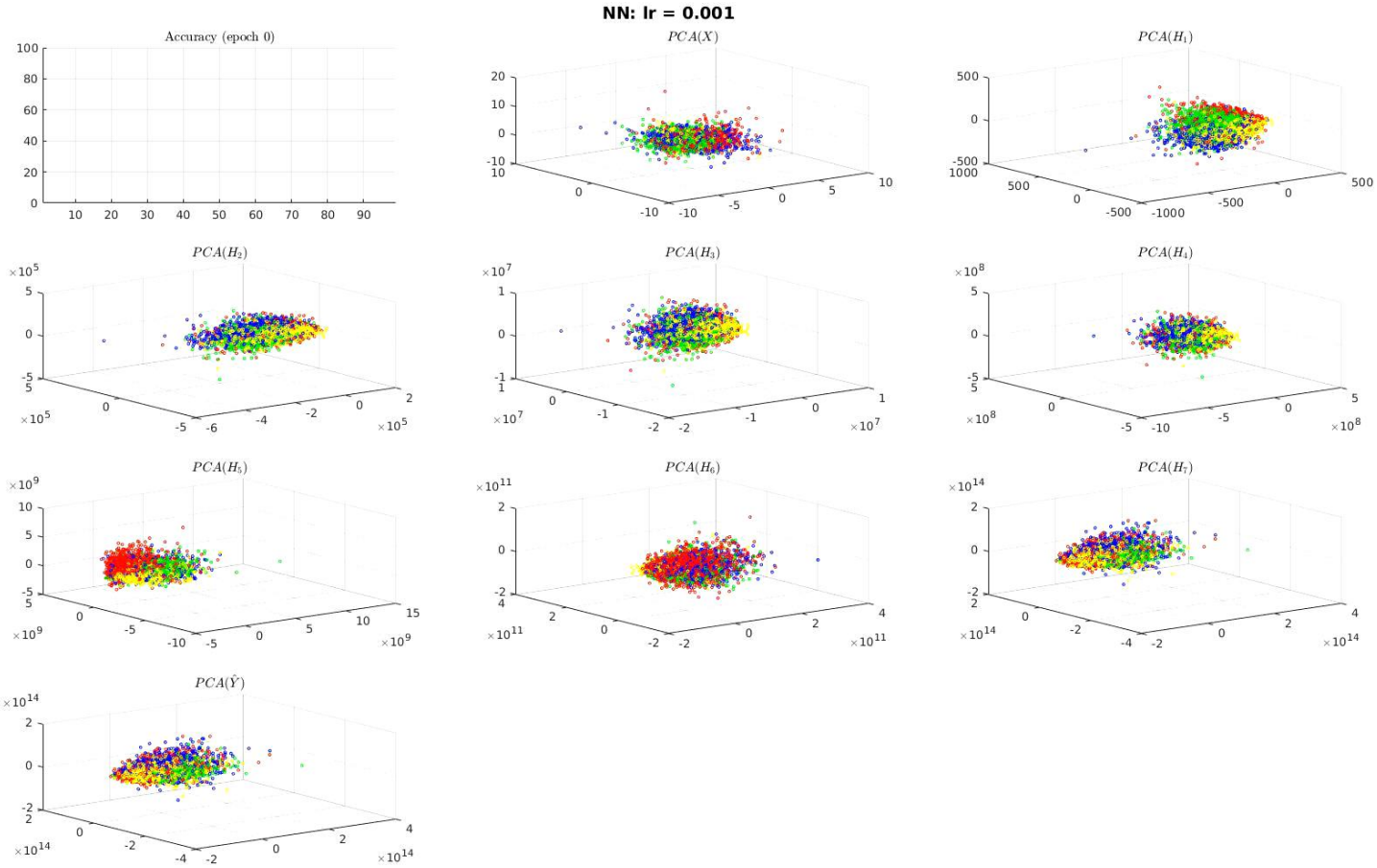
- Synthetic example: Feature space

The behavior of the layers



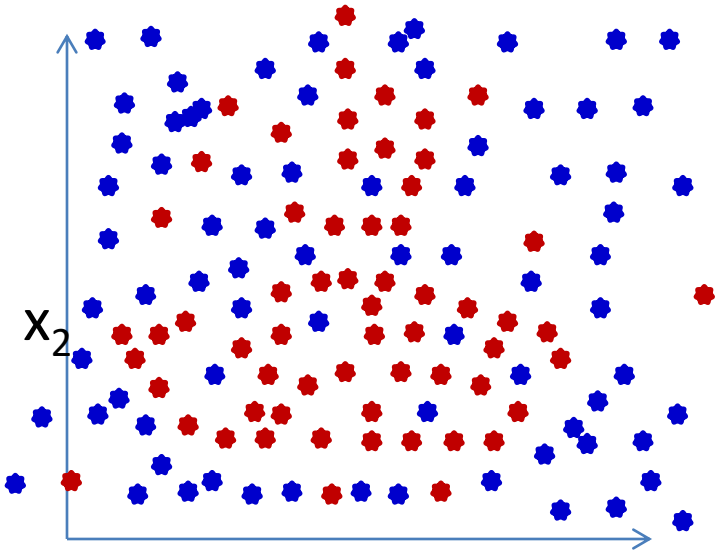
- CIFAR

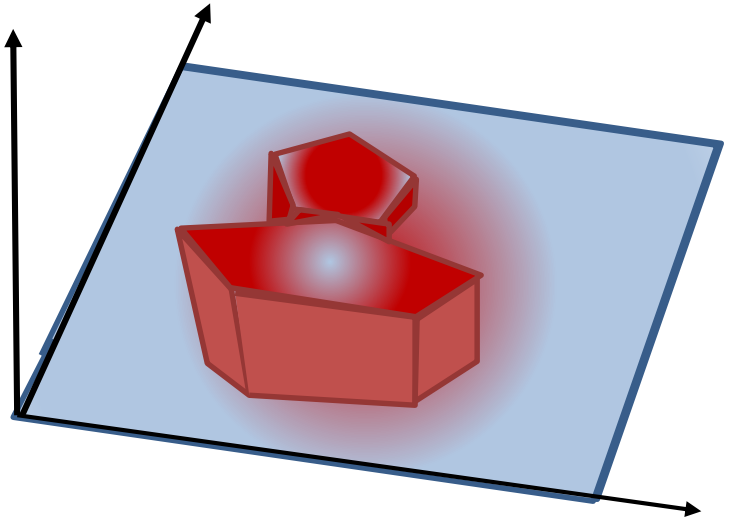
The behavior of the layers



- CIFAR

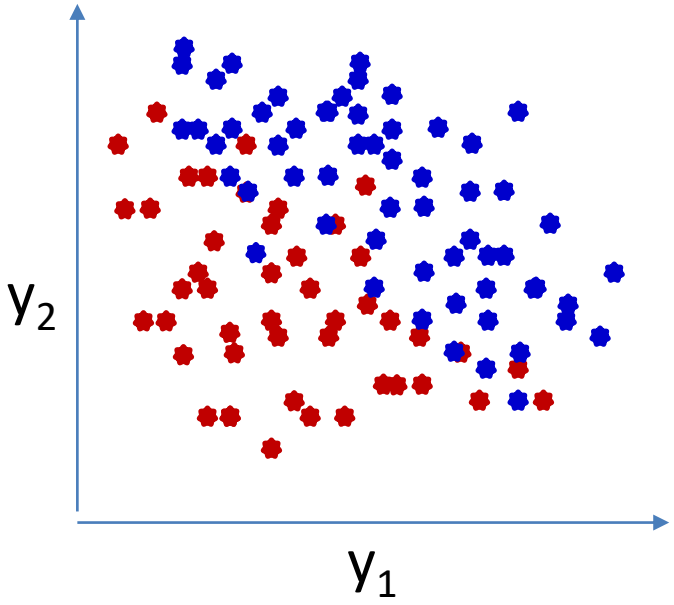
When the data are not separable and boundaries are not linear..

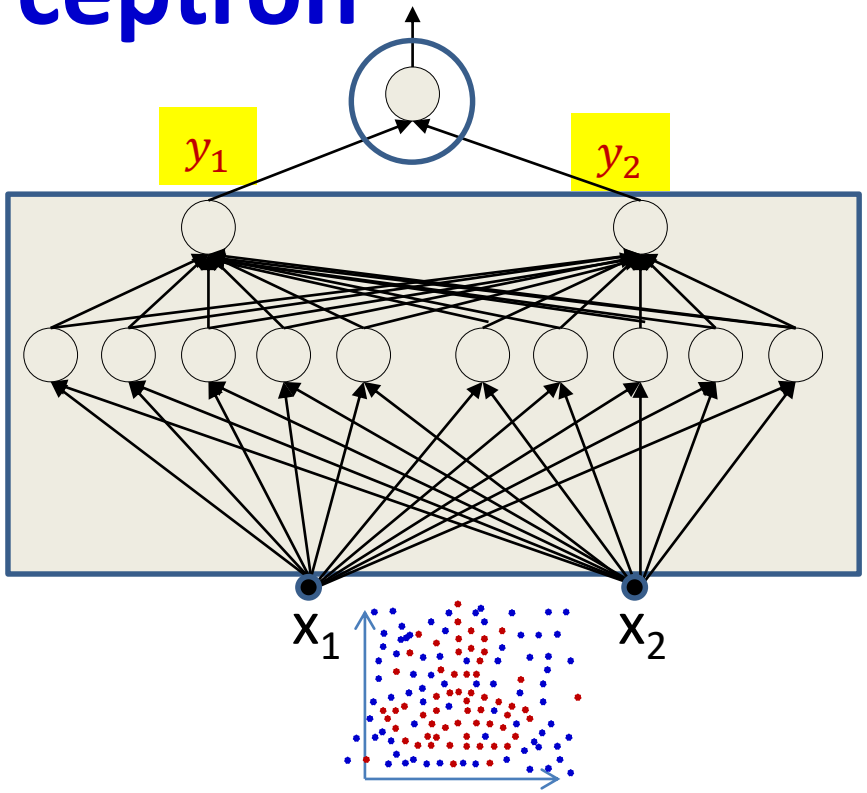




- More typical setting for classification problems

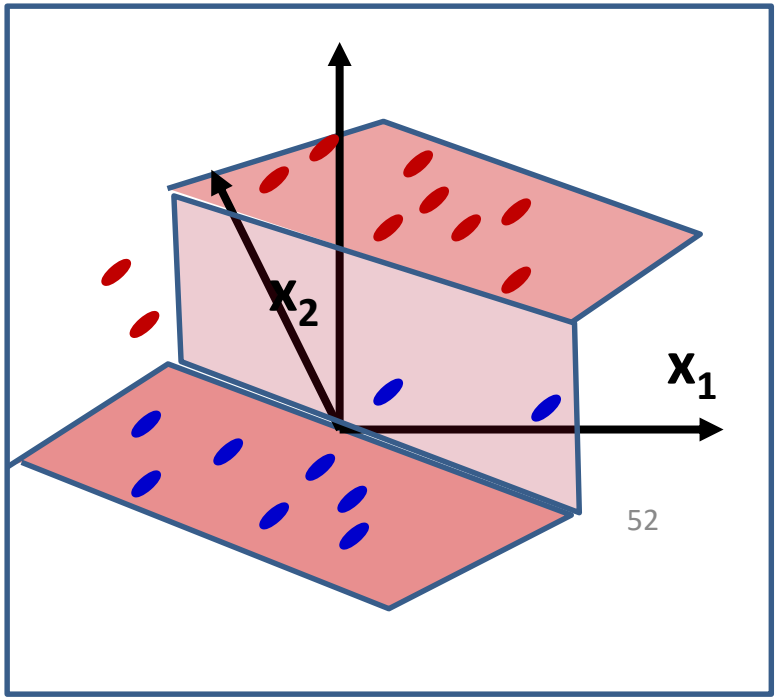
Inseparable classes with an output logistic perceptron

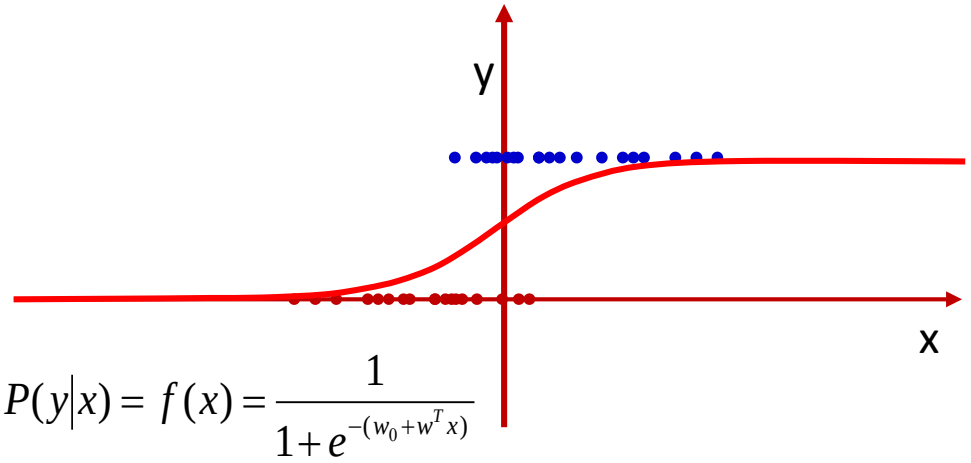




- The “feature extraction” layer transforms the data such that the posterior probability may now be modelled by a logistic

Inseparable classes with an output logistic perceptron

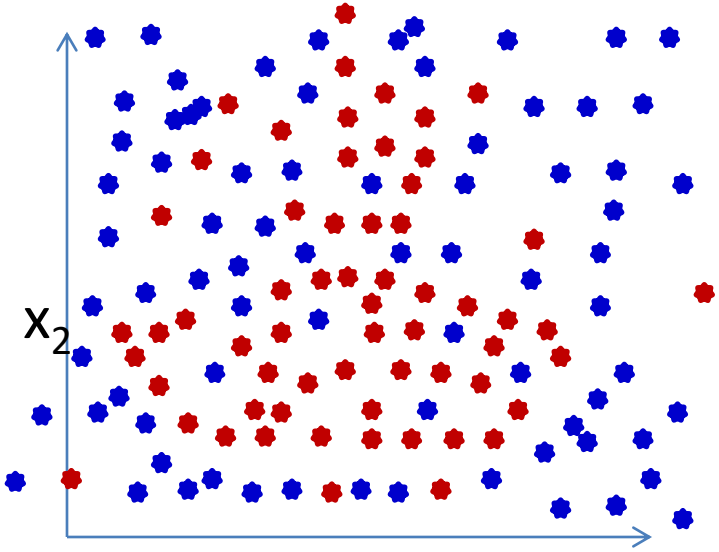


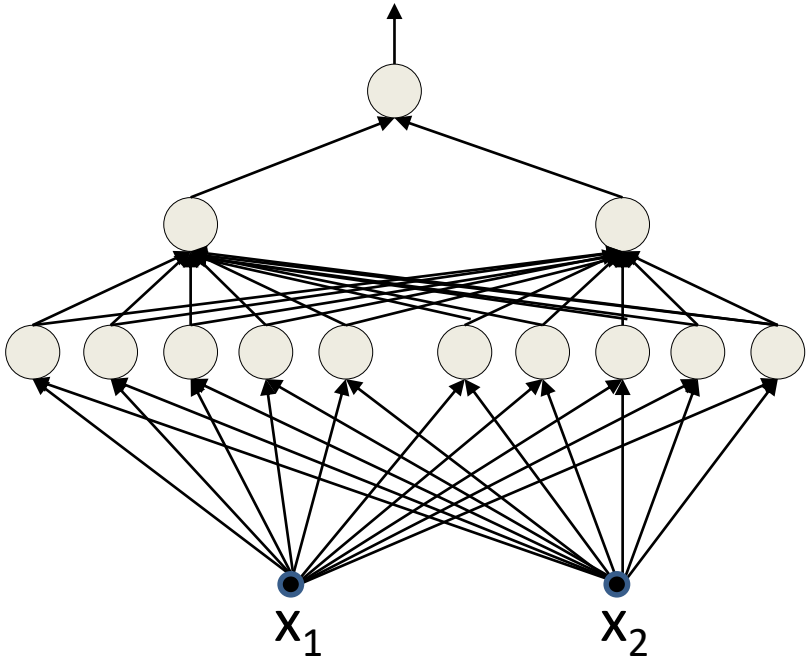


$$P(y|x) = f(x) = \frac{1}{1+e^{-(w_0+w^T x)}}$$

- The "feature extraction" layer transforms the data such that the posterior probability may now be modelled by a logistic
  - The output logistic computes the posterior probability of the class given the input

When the data are not separable and boundaries are not linear..

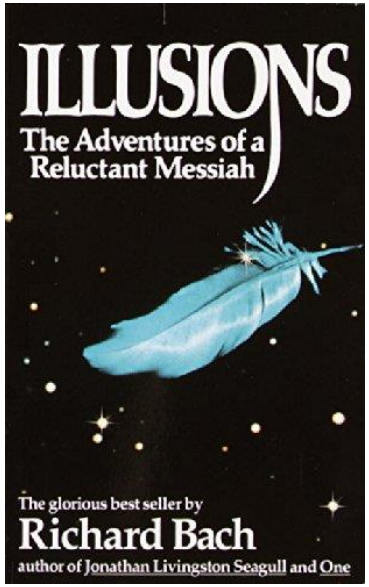




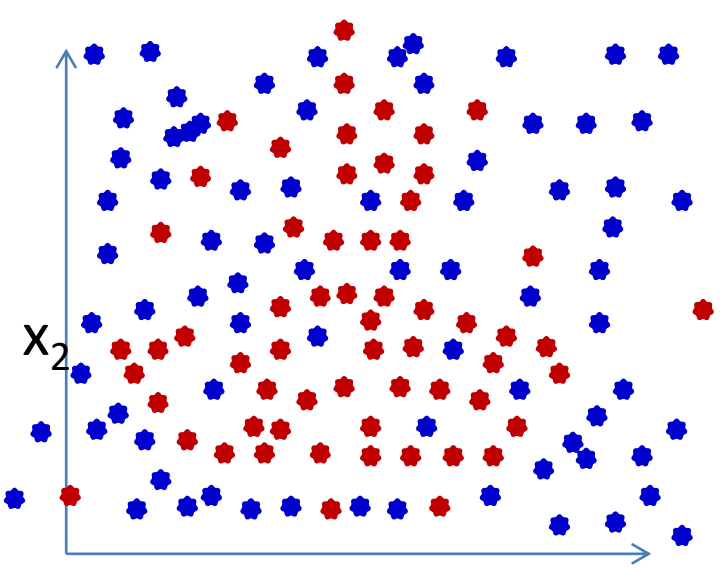
- The output of the network is $P(y|x)$
  - For multi-class networks, it will be the *vector* of a posteriori class probabilities

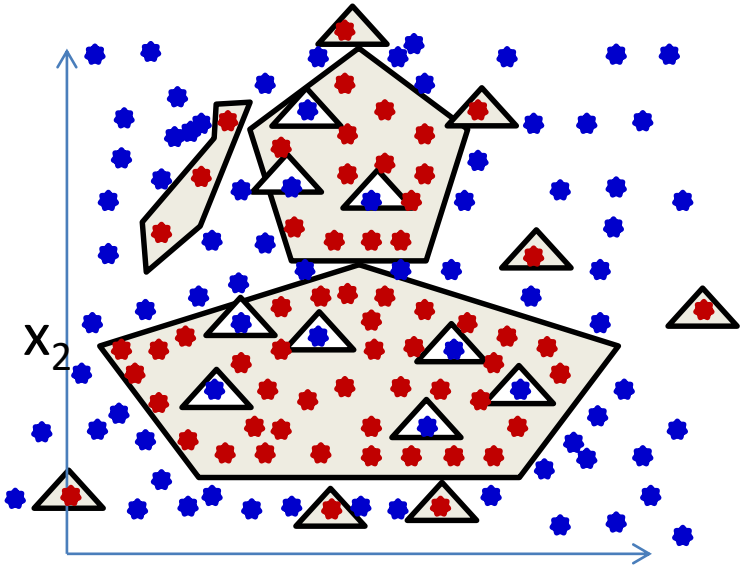
Everything in this book may be wrong!

- Richard Bach (Illusions)



There's no such thing as inseparable classes

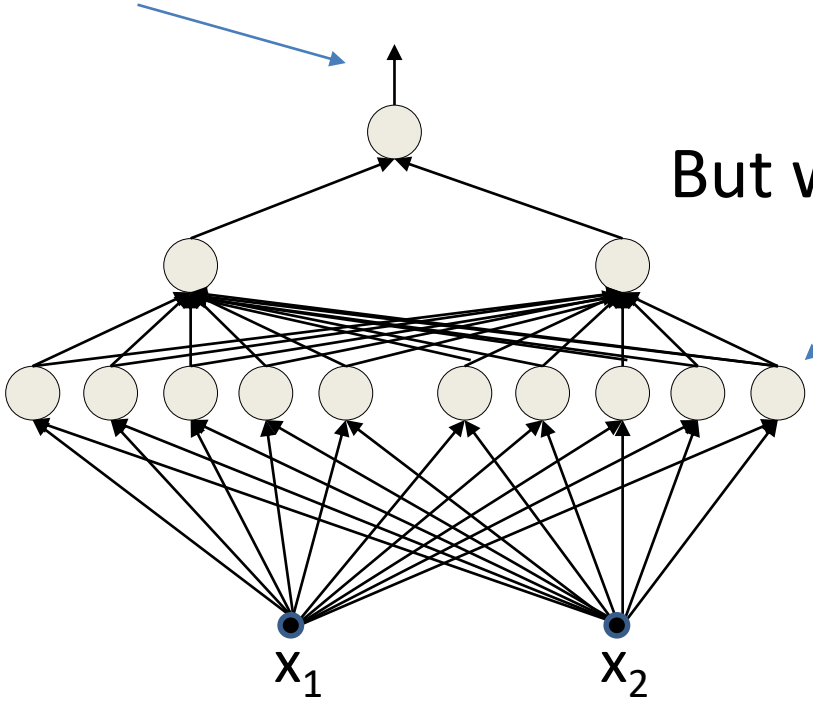




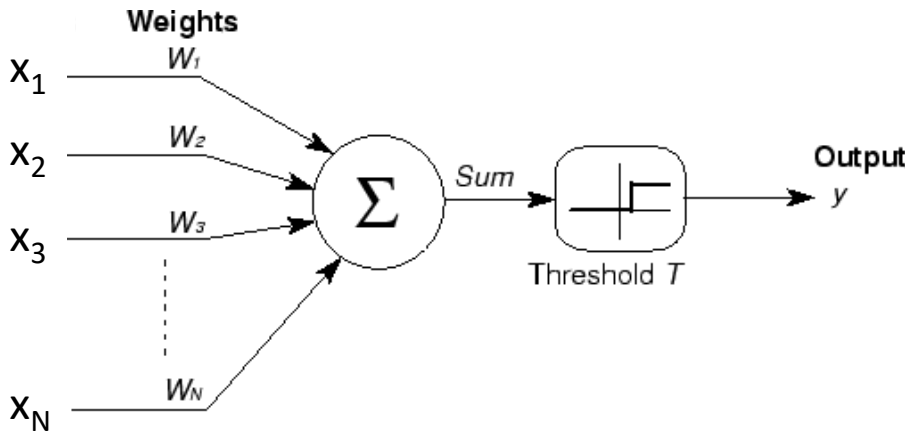
- A sufficiently detailed architecture can separate *any* arrangement of points
  - "Correctness" of the suggested intuitions subject to various parameters, such as regularization, detail of network, training paradigm, convergence etc..

Changing gears..

We've seen what the network learns here



Recall: The basic perceptron

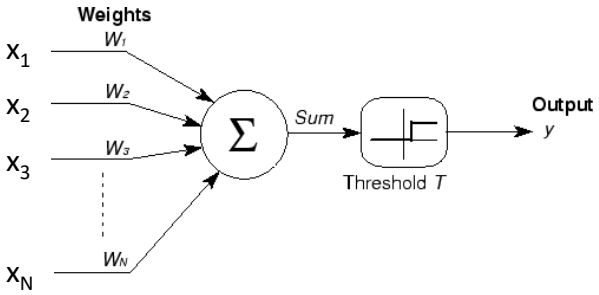


$$y = \begin{cases} 1 \; if \; \sum_i w_i x_i \geq T \\ 0 \; else \end{cases}$$

$$y = \begin{cases} 1 \; if \; \mathbf{x}^T \mathbf{w} \geq T \\ 0 \; else \end{cases}$$

- What do the *weights* tell us?
  - The neuron fires if the inner product between the weights and the inputs exceeds a threshold

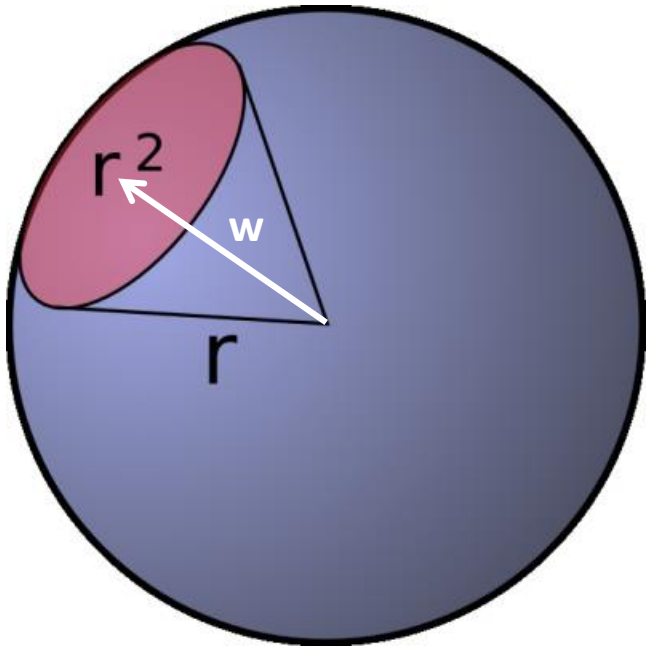
Recall: The weight as a "template"



$$X^T W > T$$

$$\cos\theta > \frac{T}{|X|}$$

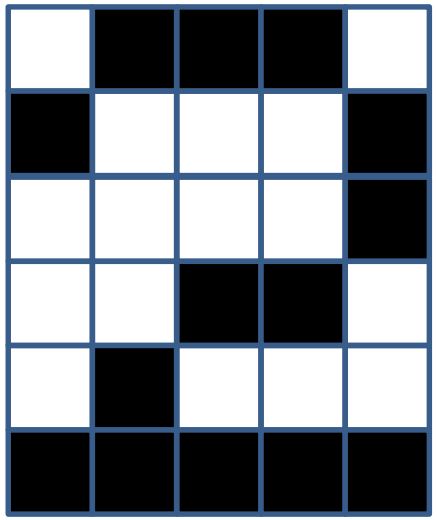
$$\theta < cos^{-1}\left(\frac{T}{|X|}\right)$$



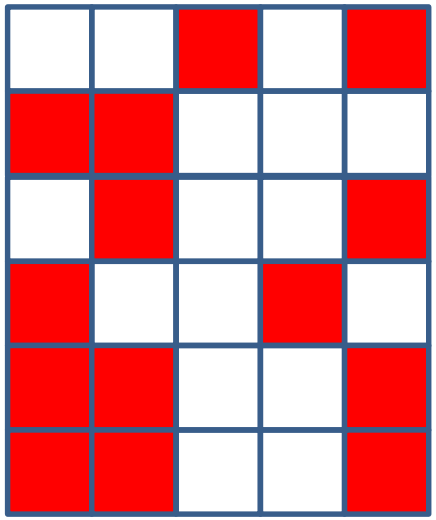
- The perceptron fires if the input is within a specified angle of the weight
  - Represents a convex region on the surface of the sphere!
  - The network is a Boolean function over these regions.
    - The overall decision region can be arbitrarily nonconvex
- Neuron fires if the input vector is close enough to the weight vector.
  - If the input pattern matches the weight pattern closely enough

Recall: The weight as a template

W

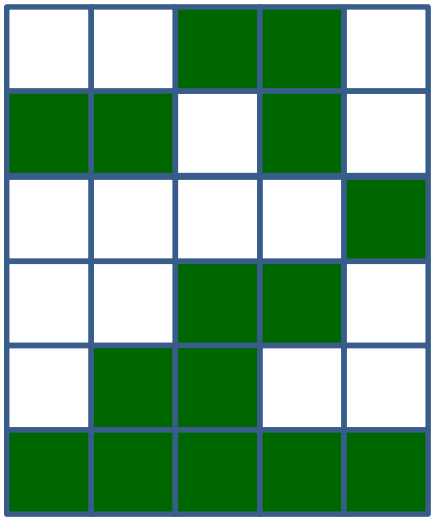


X



Correlation = 0.57

X

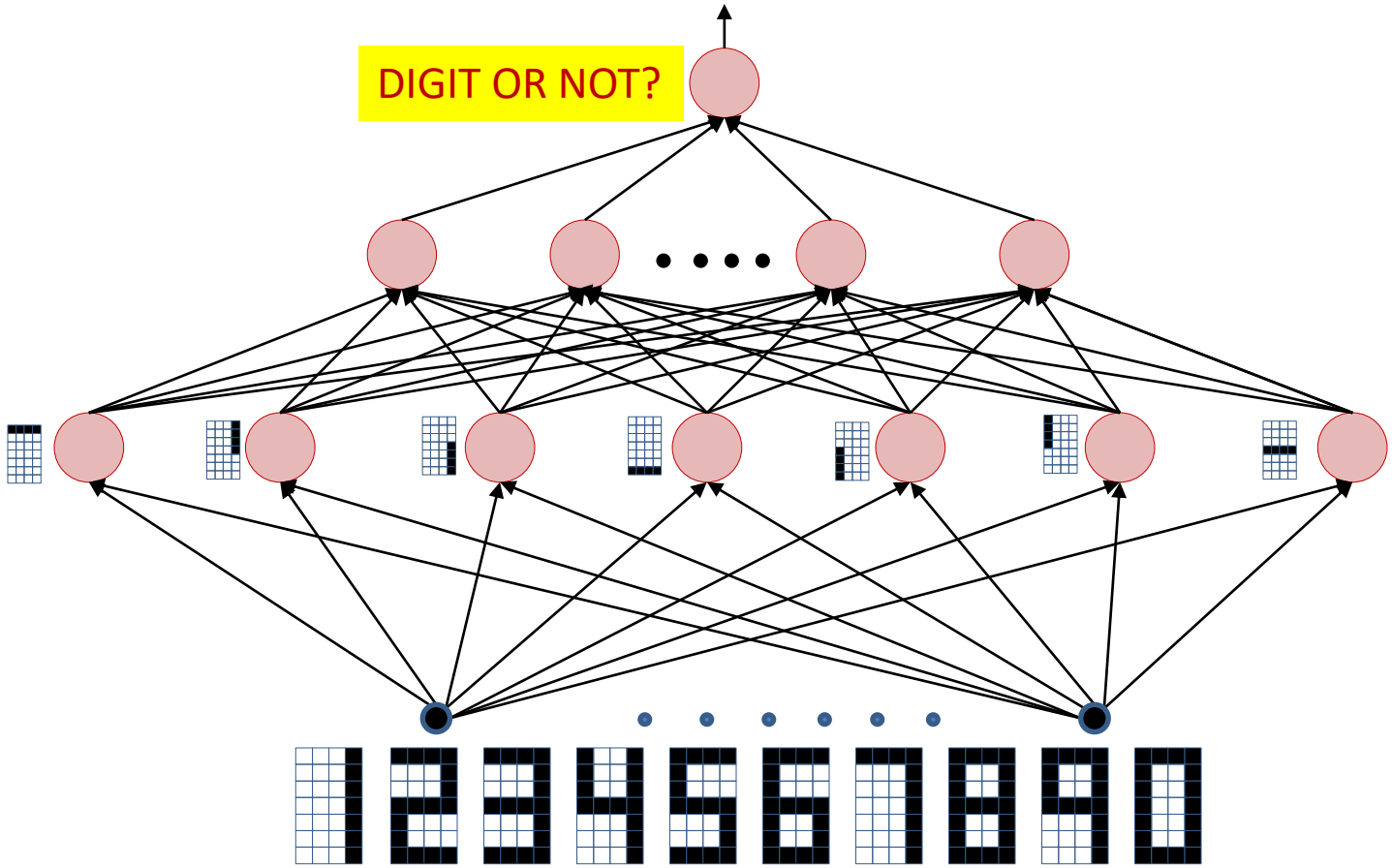


Correlation = 0.82

$$y = \begin{cases} 1 \; if \sum_i w_i x_i \geq T \\ 0 \; else \end{cases}$$

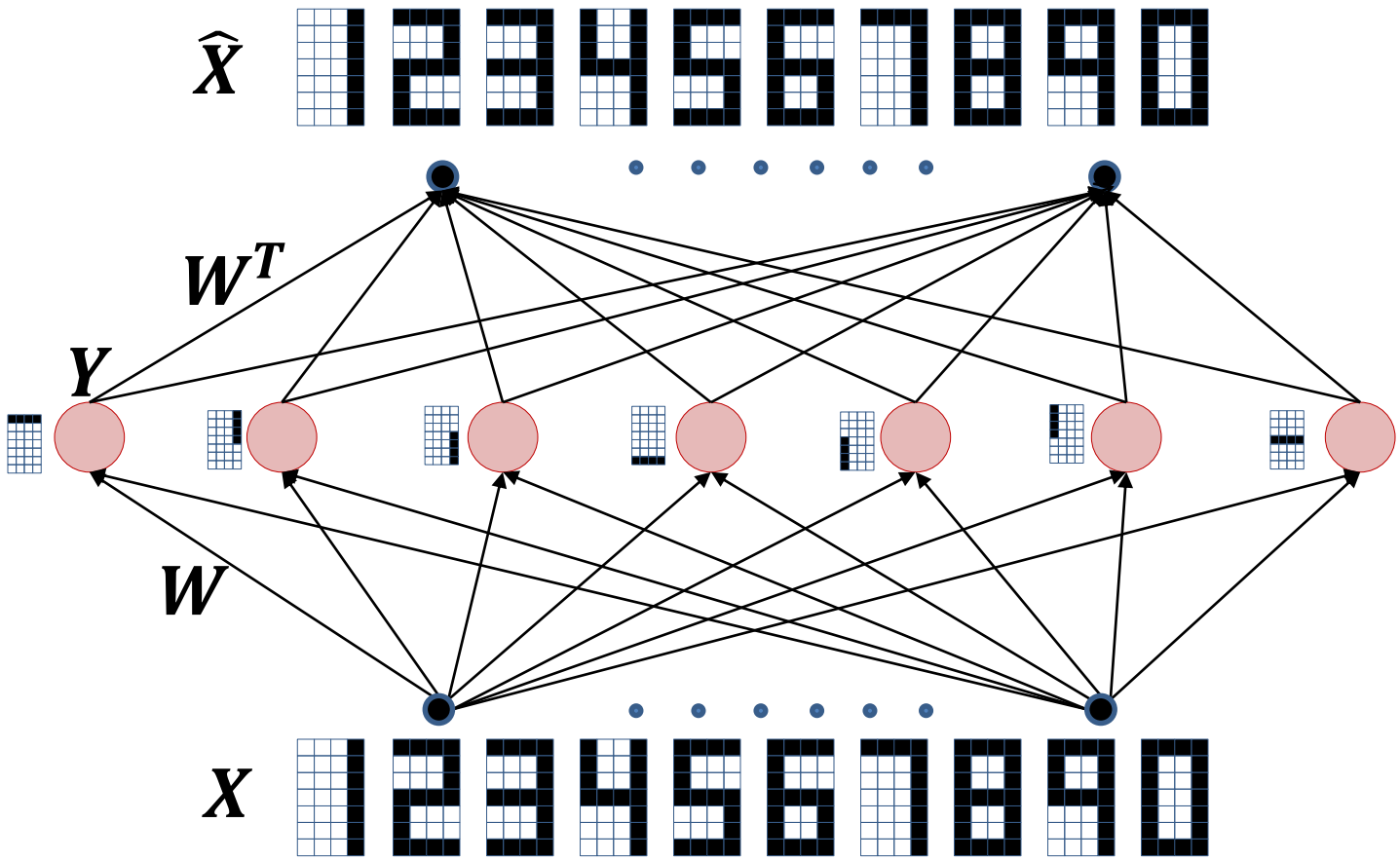
- If the *correlation* between the weight pattern and the inputs exceeds a threshold, fire
- The perceptron is a *correlation filter!*

Recall: MLP features



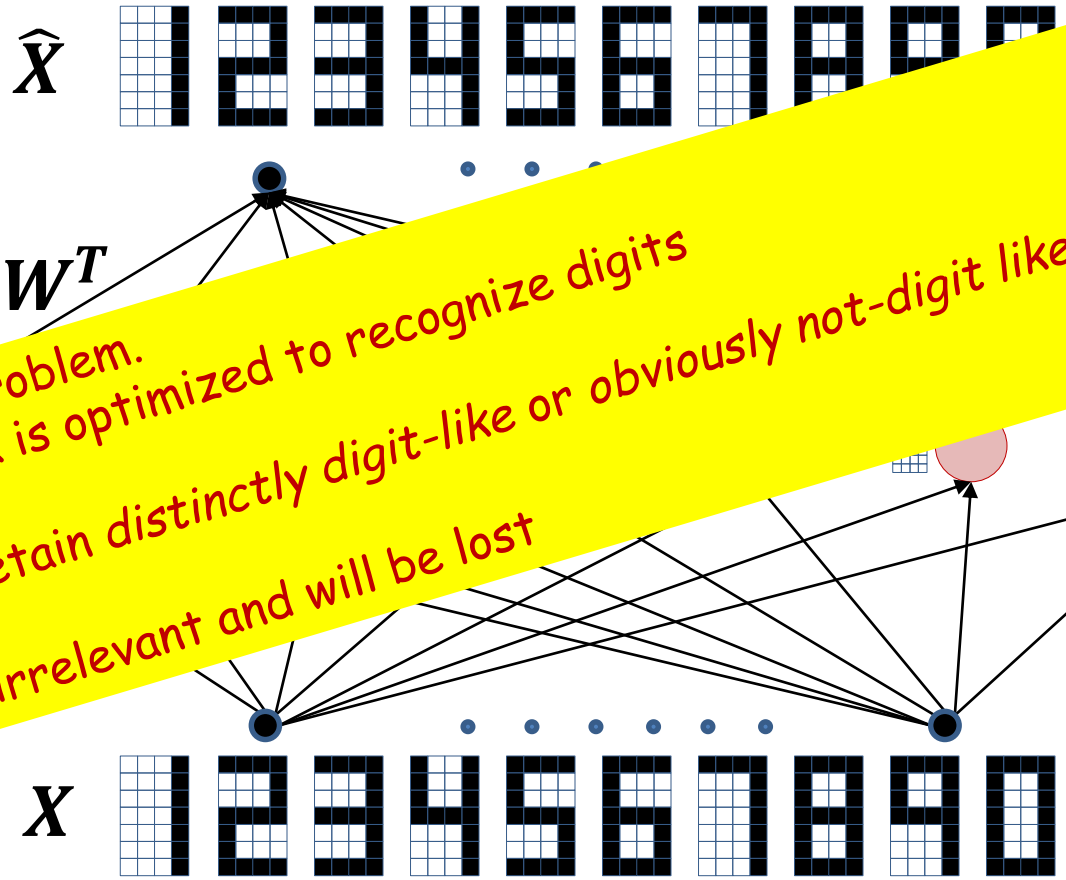
- The lowest layers of a network detect significant features in the signal
- **The signal could be (partially) reconstructed using these features**
  - **Will retain all the significant components of the signal**

Making it explicit



- **The signal could be (partially) reconstructed using these features**
  - **Will retain all the significant components of the signal**
- Simply *recompose* the detected features
  - Will this work?

Making it explicit



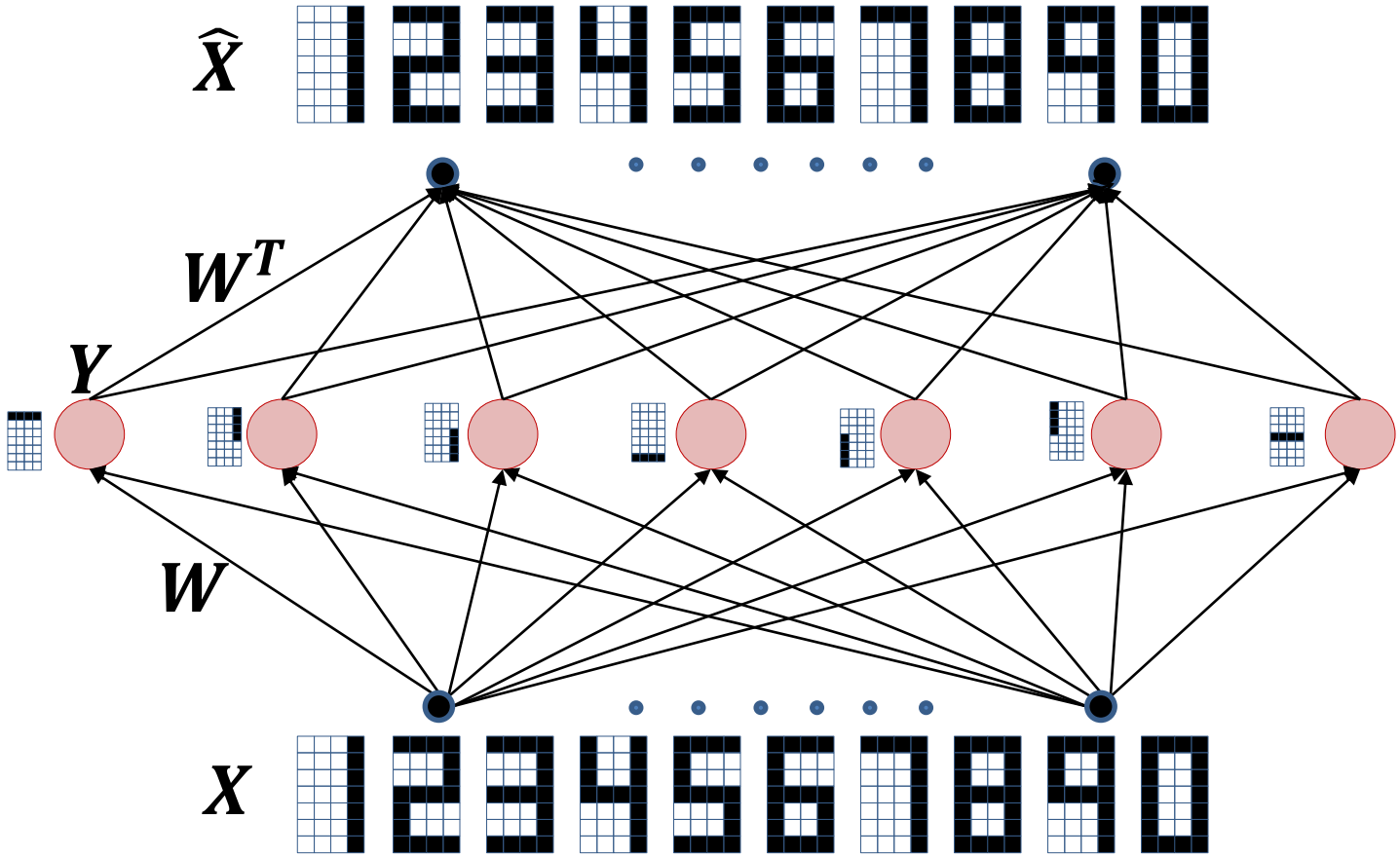
Not in this problem.
The network is optimized to recognize digits

Will only retain distinctly digit-like or obviously not-digit like features

Rest are irrelevant and will be lost

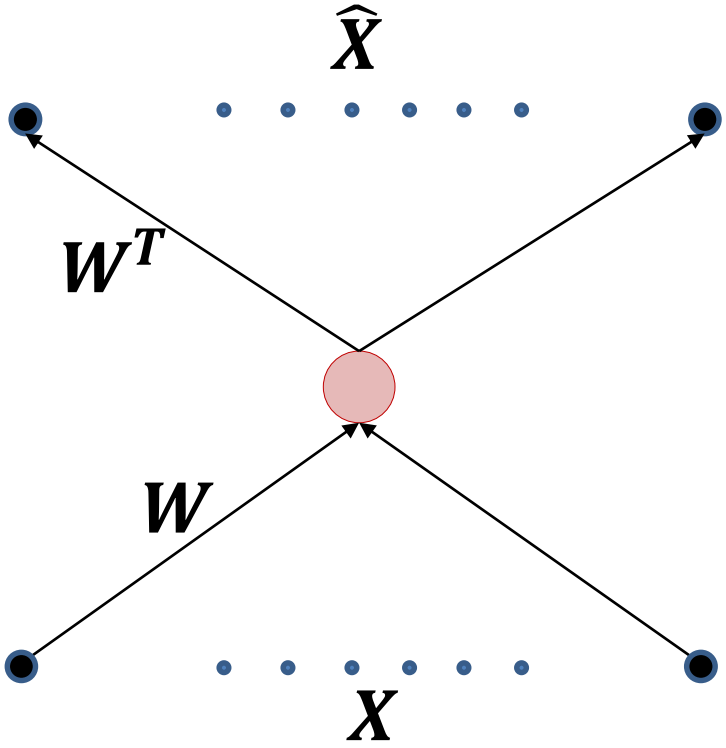
- **The signal could be (partially) reconstructed using these features**
  - **Will retain all the significant components of the signal**
- Simply *recompose* the detected features
  - Will this work?

Making it explicit: an autoencoder



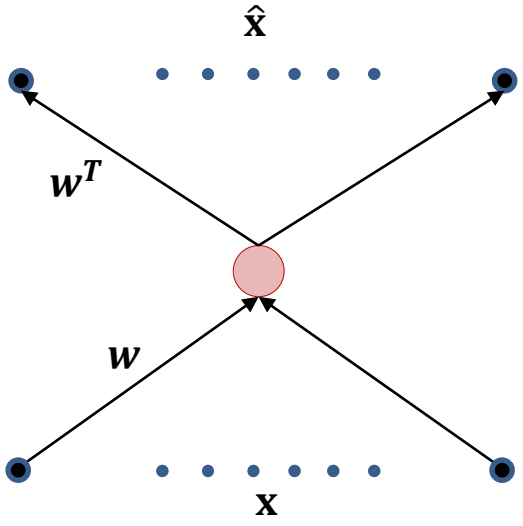
- A neural network can be trained to predict the input itself
- This is an *autoencoder*
- An *encoder* learns to detect all the most significant patterns in the signals
- A *decoder* recomposes the signal from the patterns

The Simplest Autencoder



- A single hidden unit
- Hidden unit has *linear* activation
- What will this learn?

The Simplest Autencoder



Training: Learning W by minimizing L2 divergence

$$\hat{\mathrm{x}} = w^T w \mathrm{x}$$

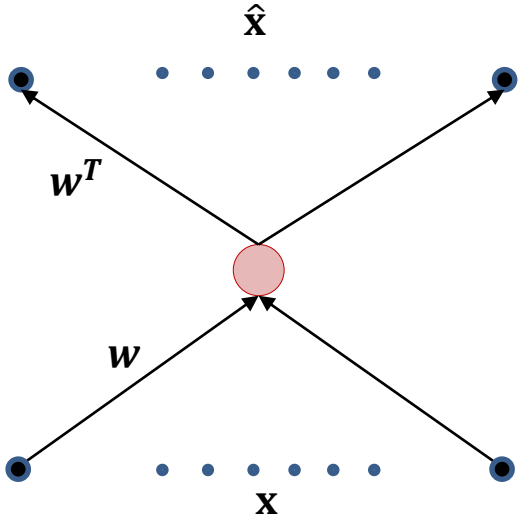
$$div(\hat{\mathrm{x}}, \mathrm{x}) = \|\mathrm{x} - \hat{\mathrm{x}}\|^2 = \|\mathrm{x} - \mathrm{w}^T w \mathrm{x}\|^2$$

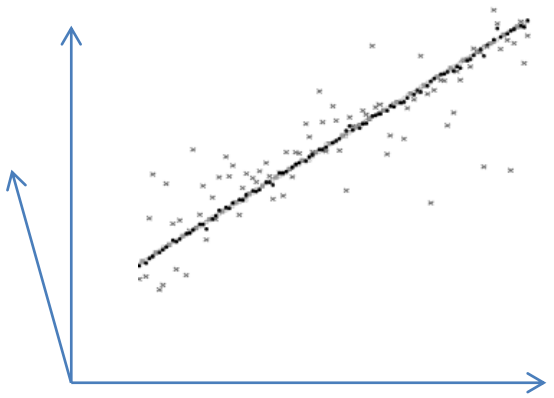
$$\widehat{W} = \underset{W}{\operatorname{argmin}}\, E[div(\hat{\mathrm{x}}, \mathrm{x})]$$

$$\widehat{W} = \underset{W}{\operatorname{argmin}}\, E[\|\mathrm{x} - \mathrm{w}^T w \mathrm{x}\|^2]$$

- This is just PCA!

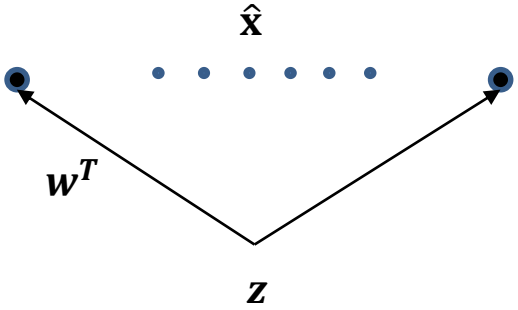
The Simplest Autencoder

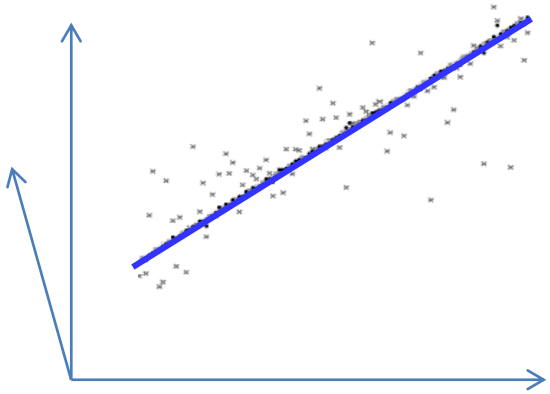




- The autoencoder finds the direction of maximum energy
  - Variance if the input is a zero-mean RV
- All input vectors are mapped onto a point on the principal axis

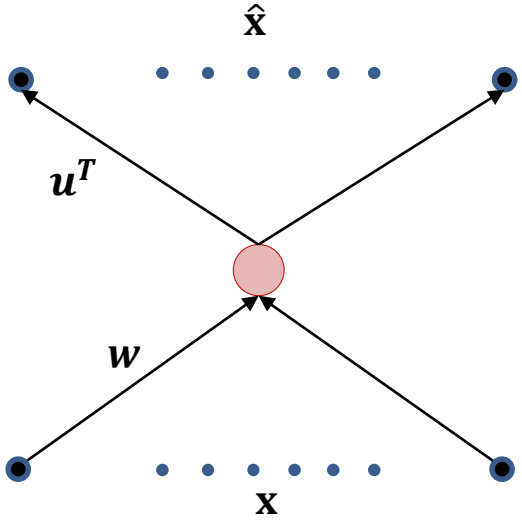
The Simplest Autencoder

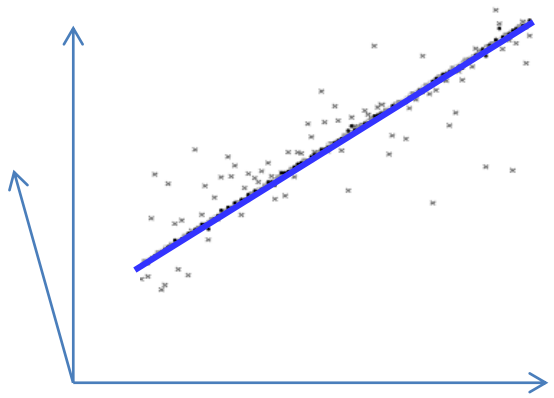




- Simply varying the hidden representation will result in an output that lies along the major axis

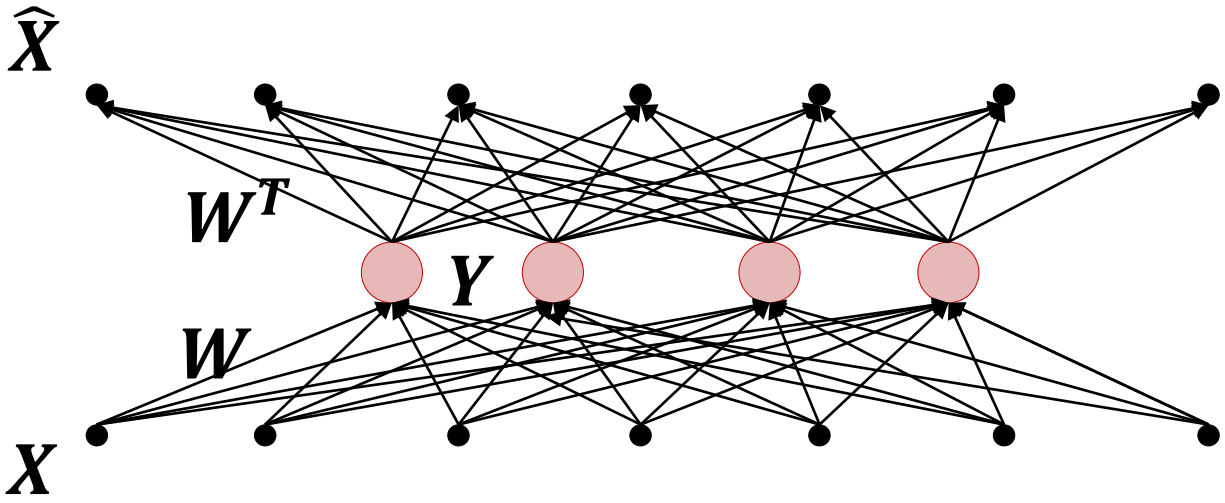
The Simplest Autencoder

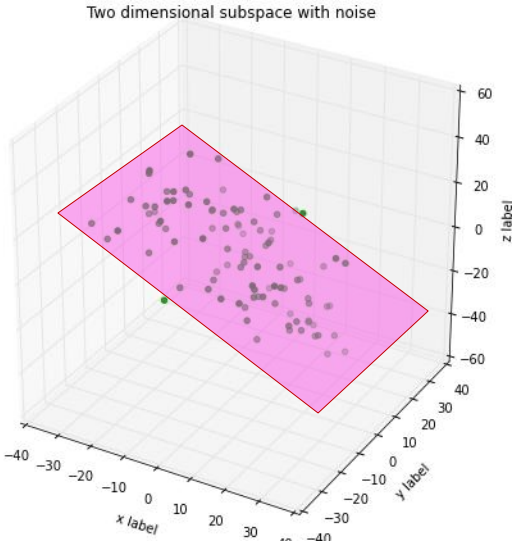




- Simply varying the hidden representation will result in an output that lies along the major axis
- This will happen even if the learned output weight is separate from the input weight
  - The minimum-error direction *is* the principal eigen vector

For more detailed AEs without a non-linearity

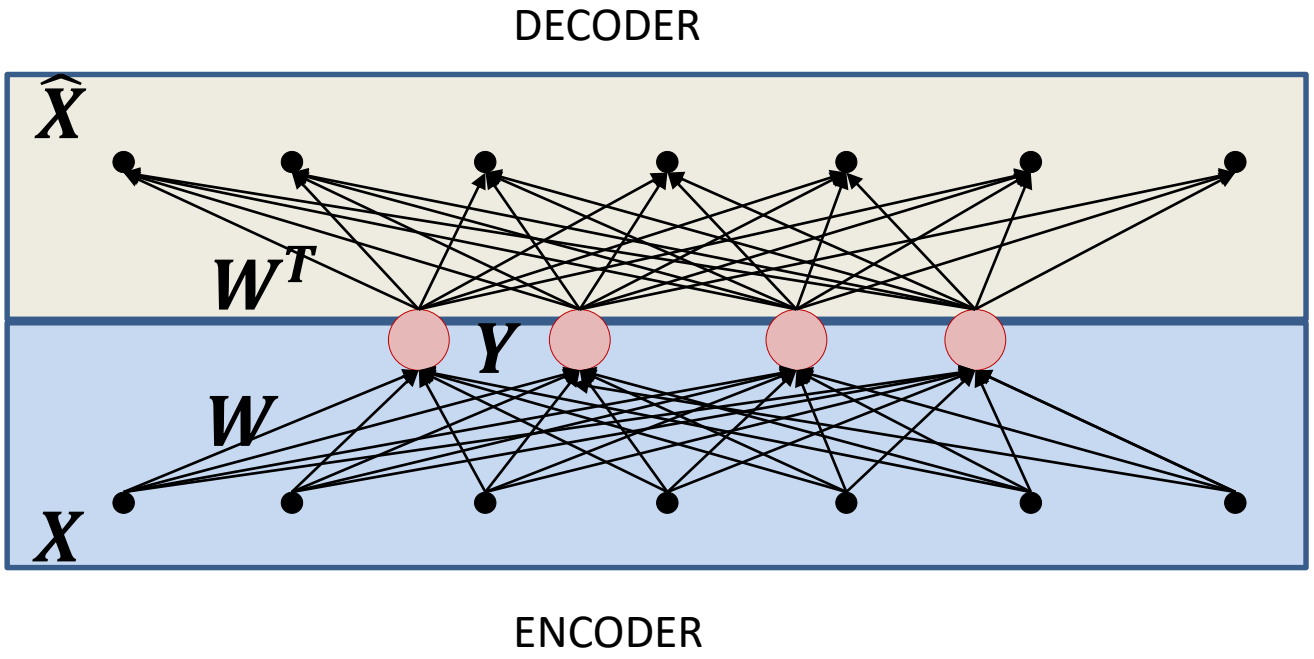




$\mathbf{Y} = \mathbf{W}\mathbf{X}$ $\hat{\mathbf{X}} = \mathbf{W}^T\mathbf{Y}$ $E = \|\mathbf{X} - \mathbf{W}^T\mathbf{W}\mathbf{X}\|^2$ Find W to minimize Avg[E]

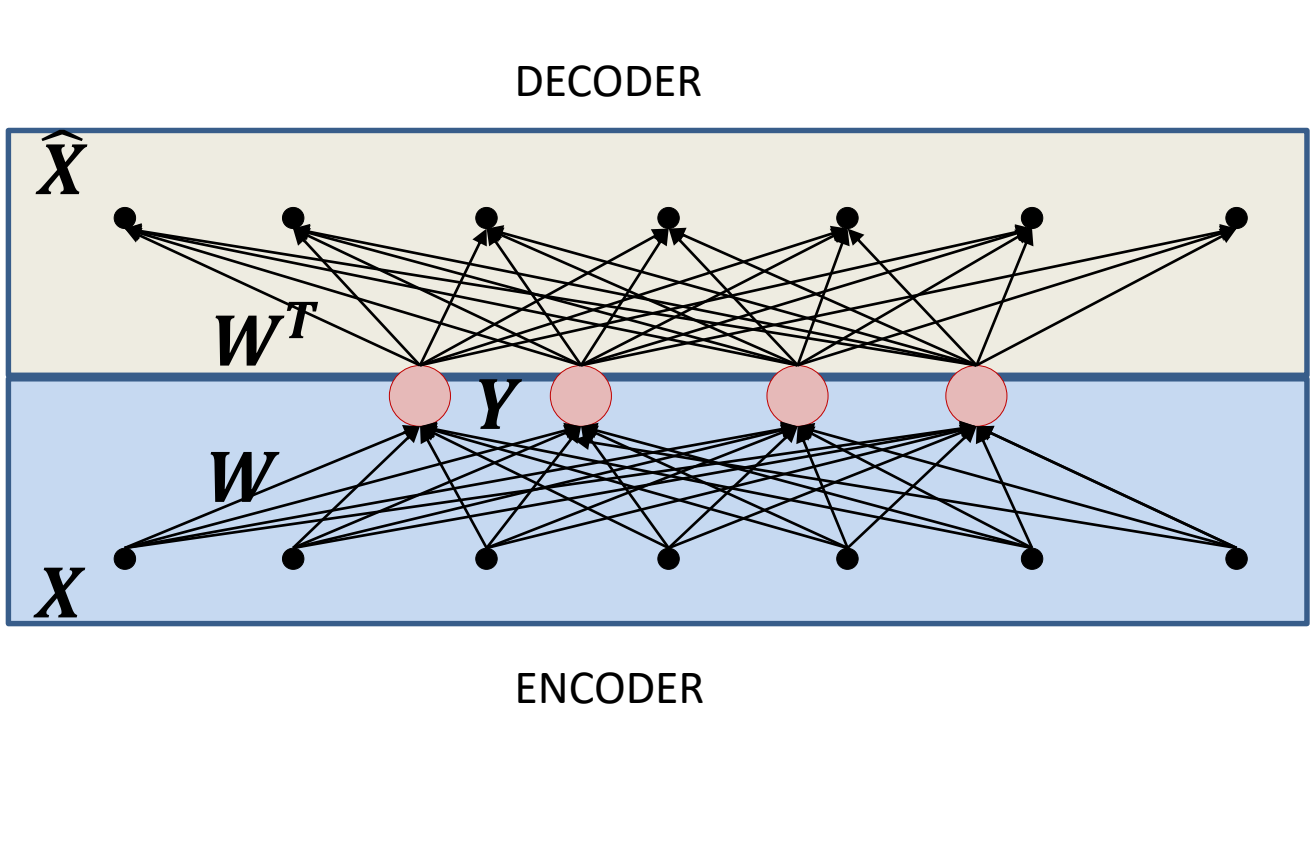
- This is still just PCA
  - The output of the hidden layer will be in the principal subspace
    - Even if the recomposition weights are different from the "analysis" weights

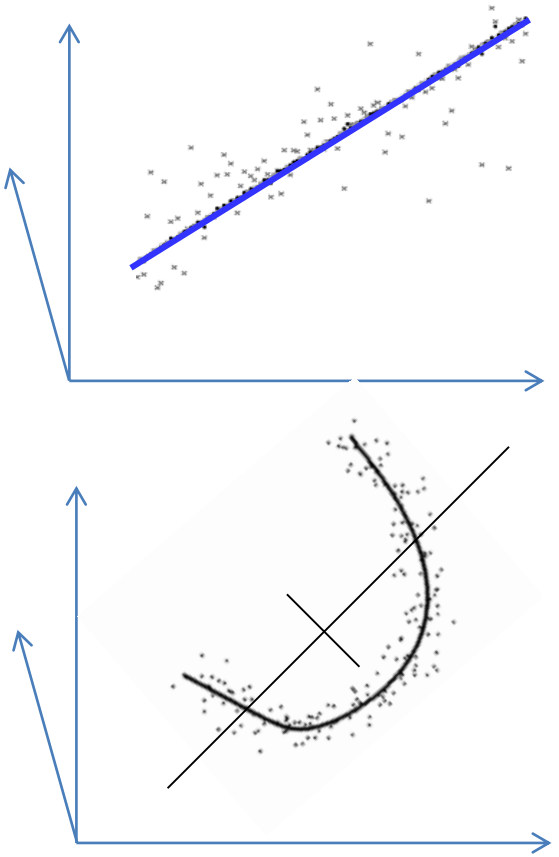
Terminology



- Terminology:
  - **Encoder:** The "Analysis" net which computes the hidden representation
  - **Decoder:** The "Synthesis" which recomposes the data from the hidden representation

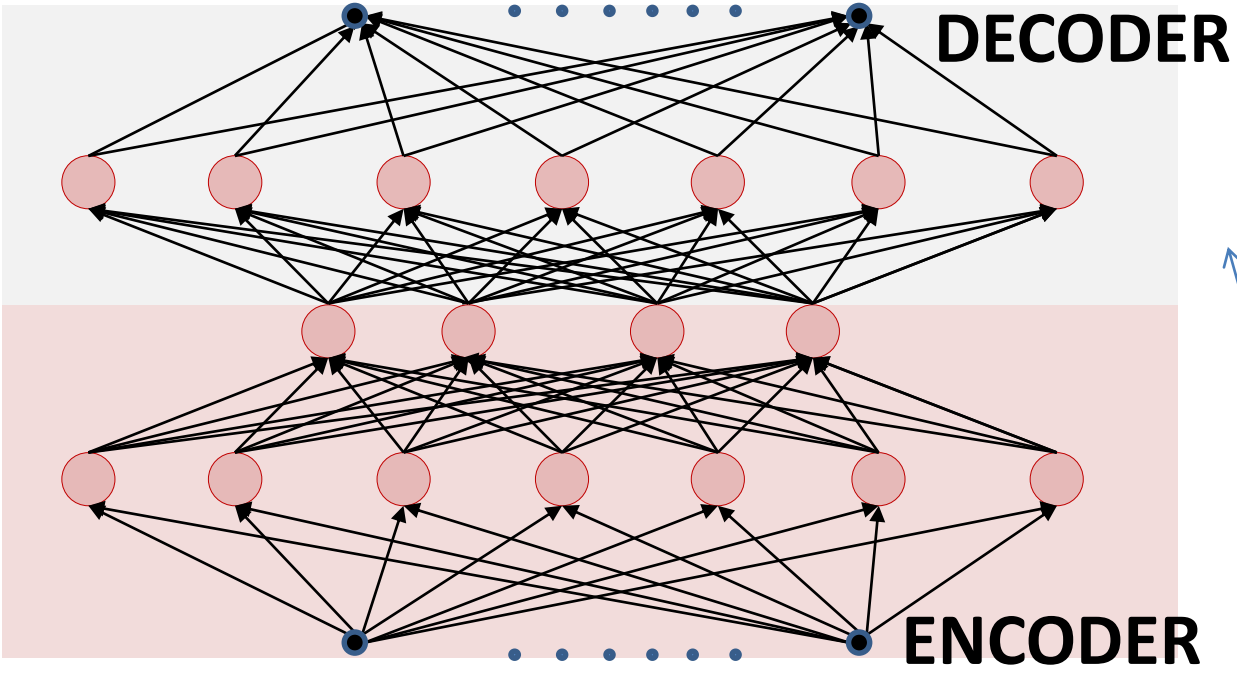
Introducing *nonlinearity*

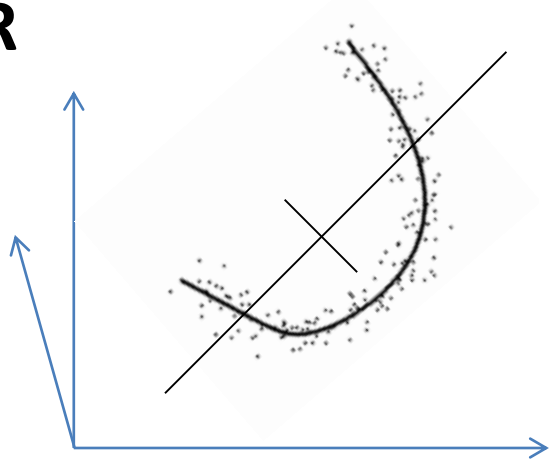




- When the hidden layer has a *linear* activation the decoder represents the best *linear* manifold to fit the data
  - Varying the hidden value will move along this linear manifold
- **When the hidden layer has non-linear activation, the net performs *nonlinear PCA***
  - The decoder represents the best non-linear manifold to fit the data
  - Varying the hidden value will move along this non-linear manifold

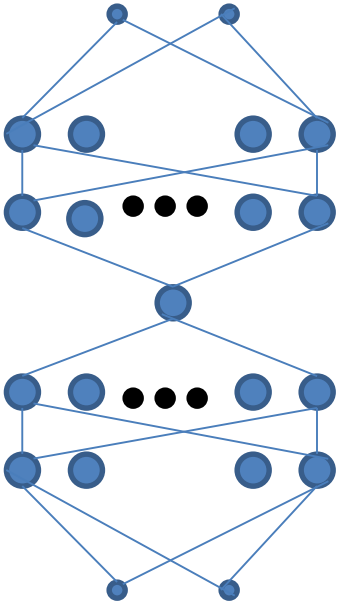
The AE

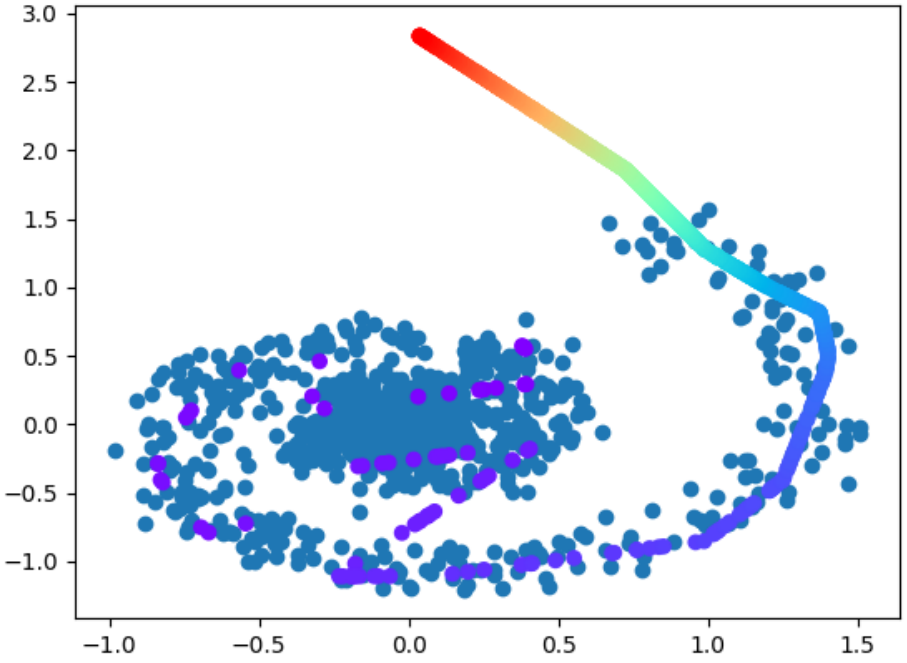




- With non-linearity
  - "Non linear" PCA
  - Deeper networks can capture more complicated manifolds
    - "Deep" autoencoders

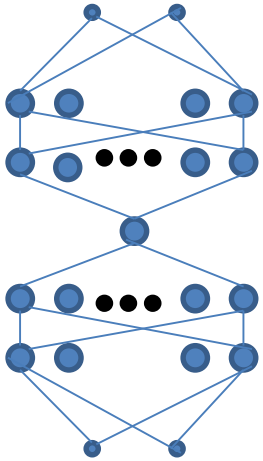
Some examples

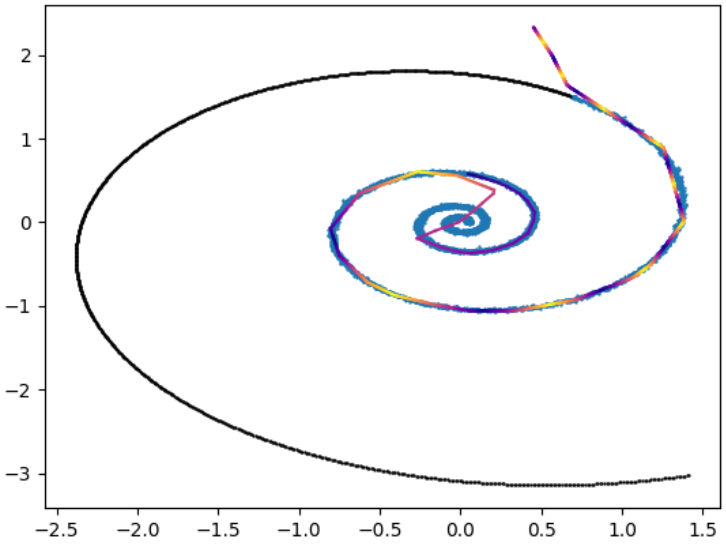


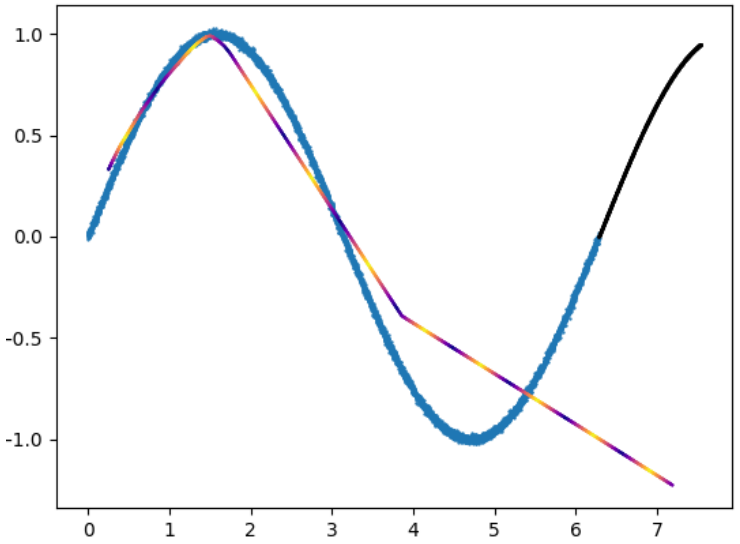


- 2-D input
- Encoder and decoder have 2 hidden layers of 100 neurons, but hidden representation is unidimensional
- Extending the hidden “z” value beyond the values seen in training extends the helix linearly

Some examples

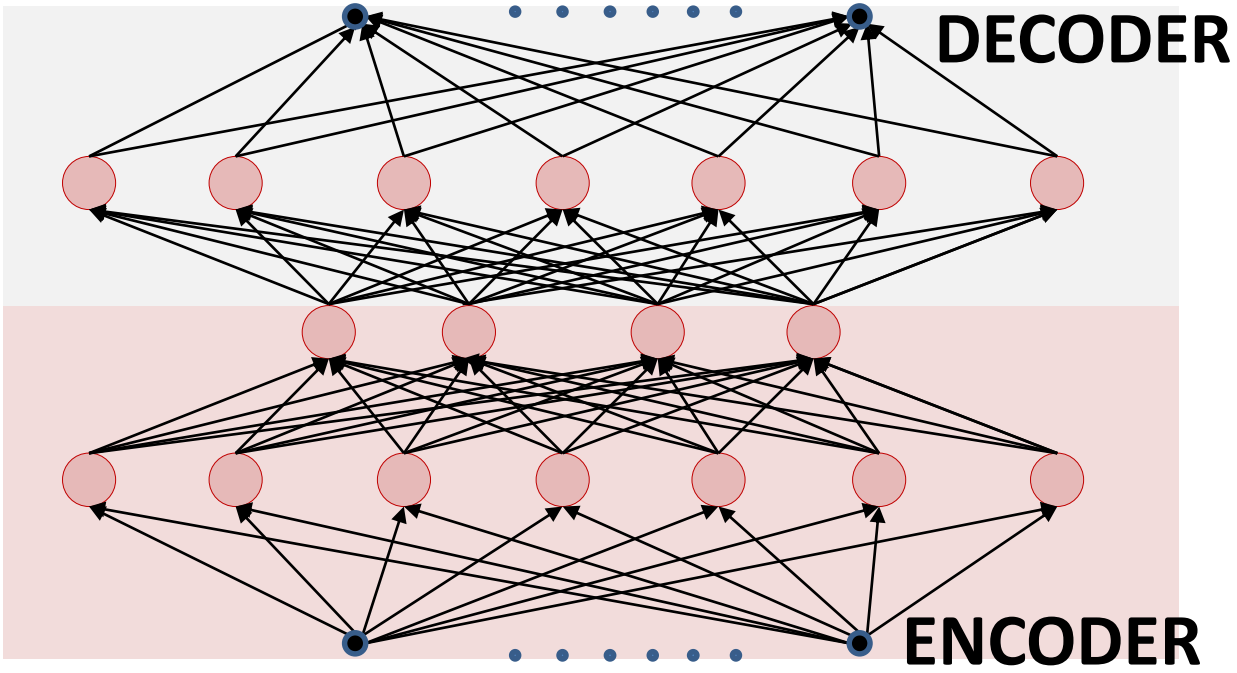






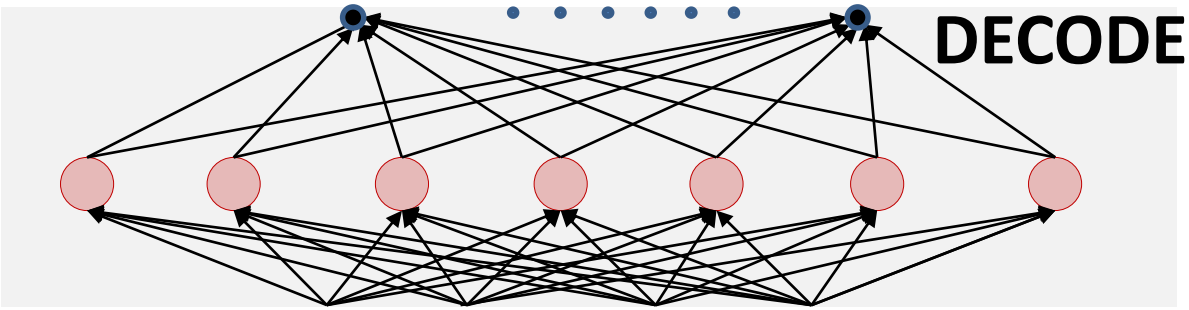
- The model is discriminative..
  - Varying the hidden layer value only generates data along the learned manifold
    - May be poorly learned
  - *Any input* will result in an output along the learned manifold

The AE



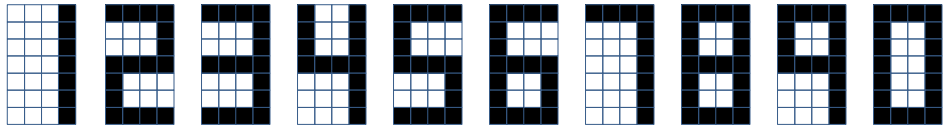
- When the hidden representation is of lower dimensionality than the input, often called a "**bottleneck**" network
  - Nonlinear PCA
  - Learns the manifold for the data
    - If properly trained

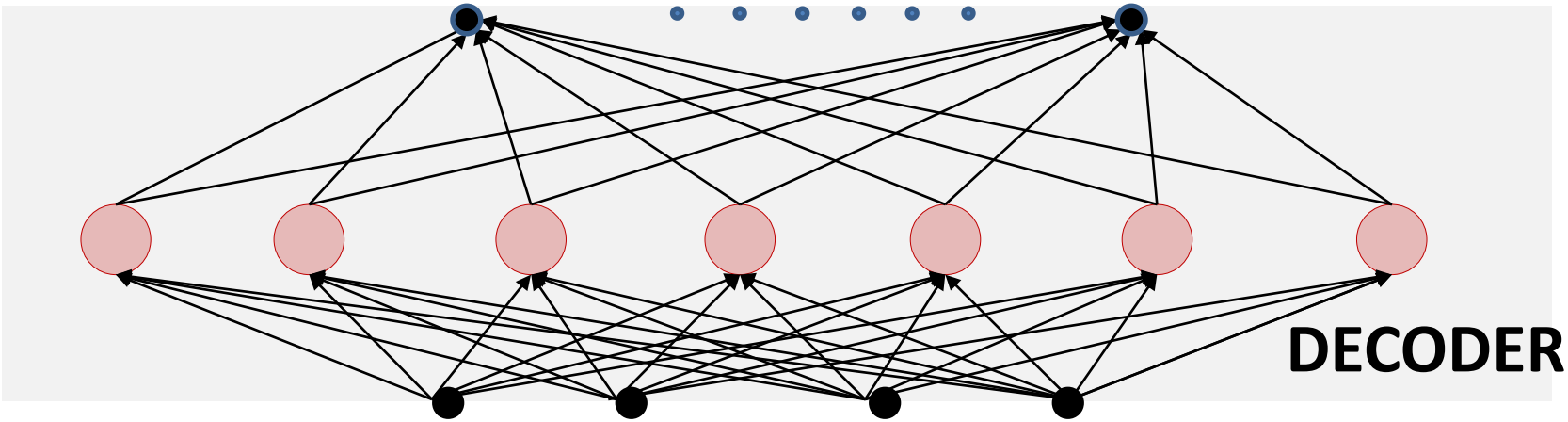
The AE



- The decoder can only generate data on the manifold that the training data lie on
- This also makes it an excellent "generator" of the distribution of the training data
  - Any values applied to the (hidden) input to the decoder will produce data similar to the training data

The Decoder:

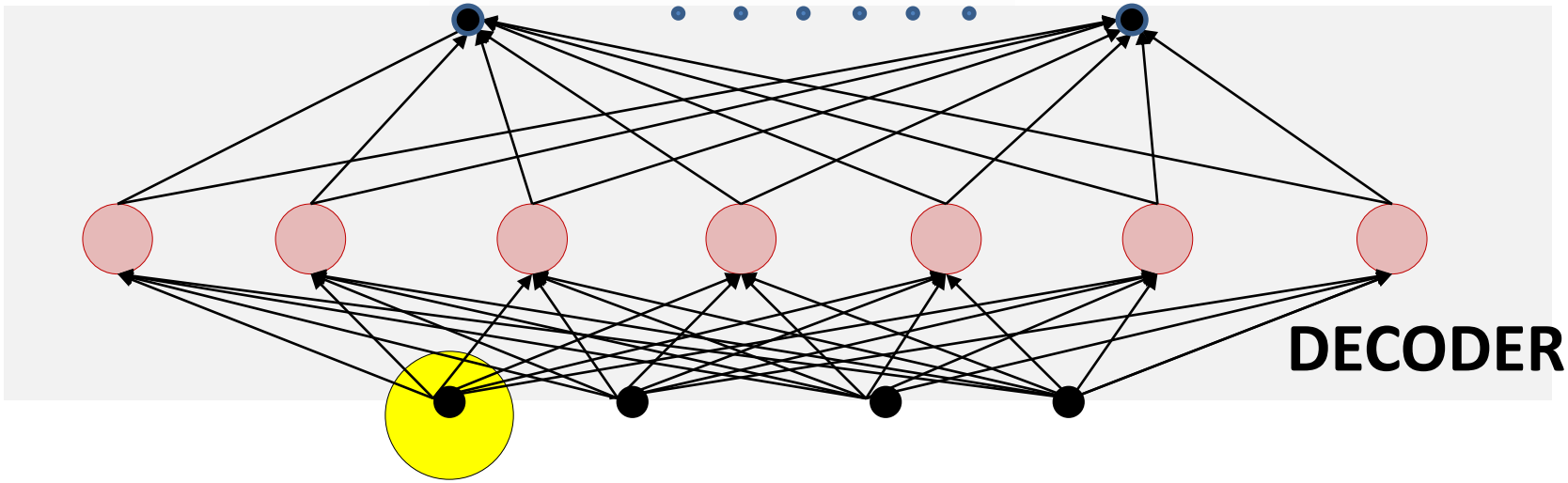




- The decoder represents a source-specific generative *dictionary*
- Exciting it will produce typical data from the source!

The Decoder:

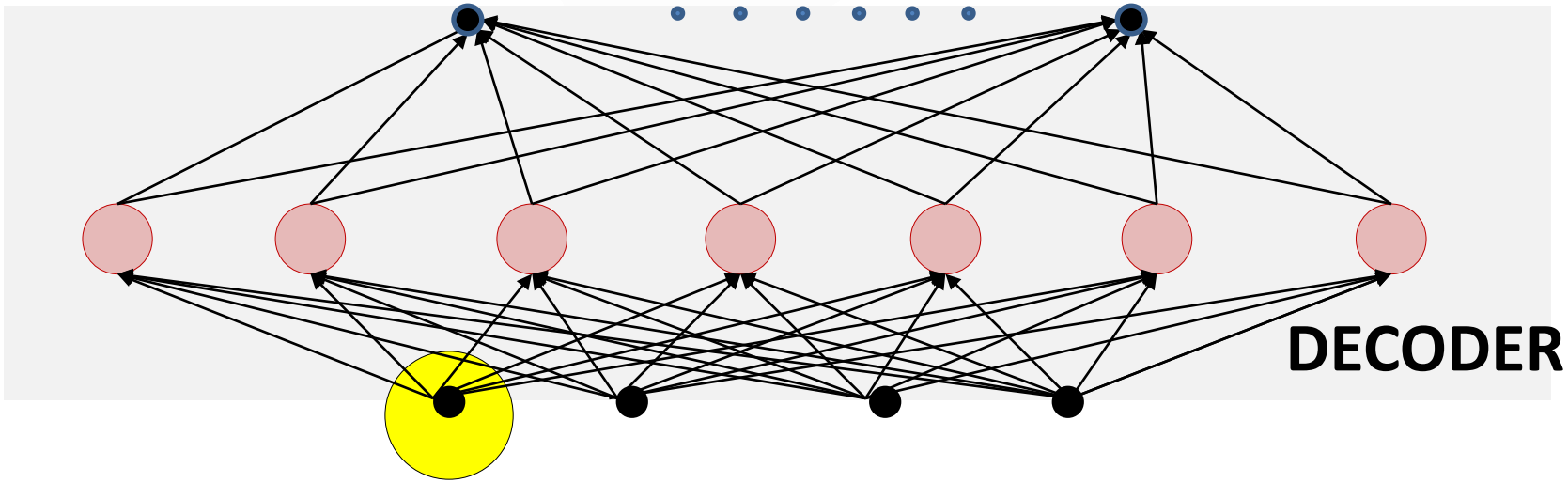
Sax dictionary



- The decoder represents a source-specific generative *dictionary*
- Exciting it will produce typical data from the source!

The Decoder:

Clarinet dictionary



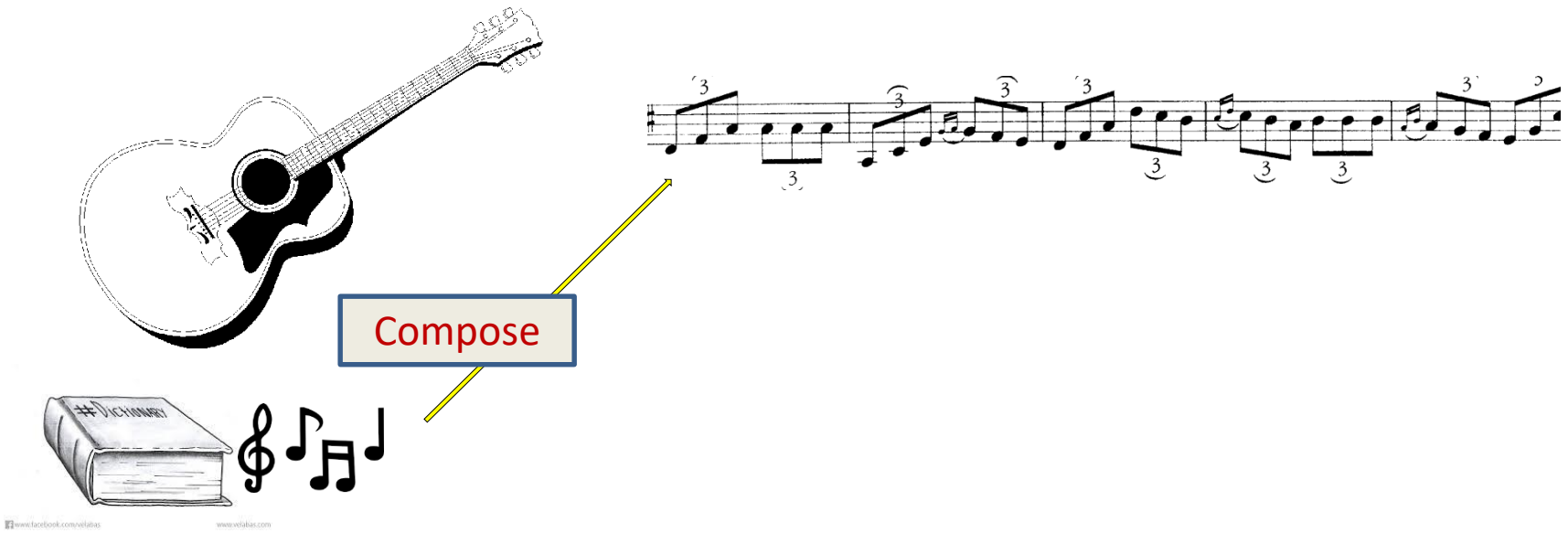
- The decoder represents a source-specific generative *dictionary*
- Exciting it will produce typical data from the source!

A cute application..

- Signal separation…

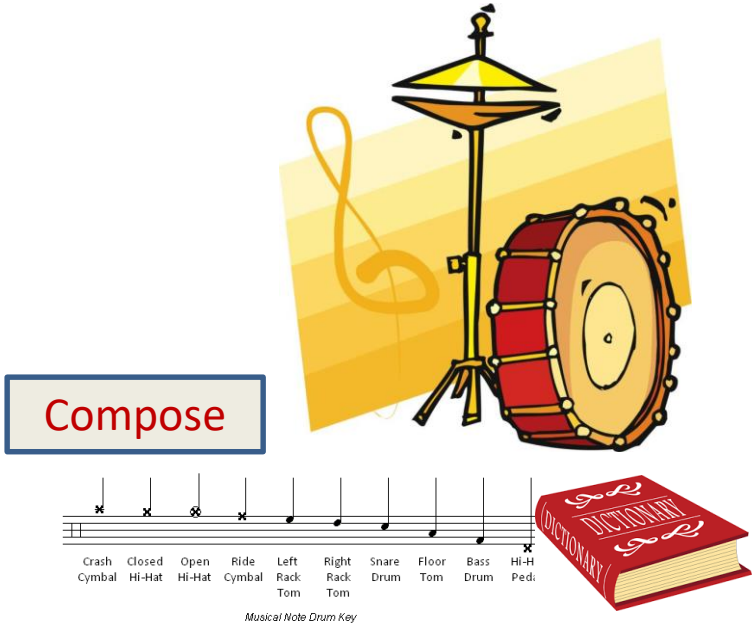
- Given a mixed sound from multiple sources, separate out the sources

Dictionary-based techniques



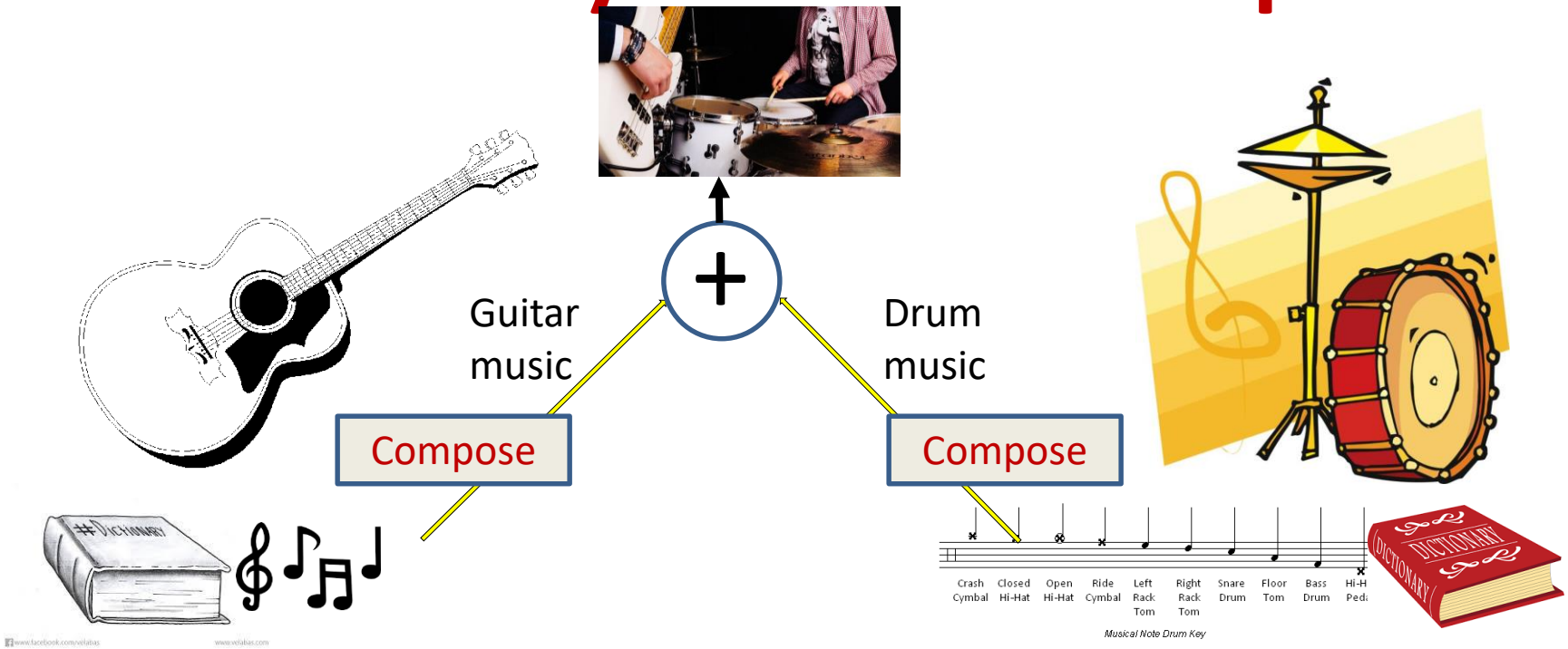
- Basic idea: Learn a dictionary of “building blocks” for each sound source
- All signals by the source are composed from entries from the dictionary for the source

Dictionary-based techniques



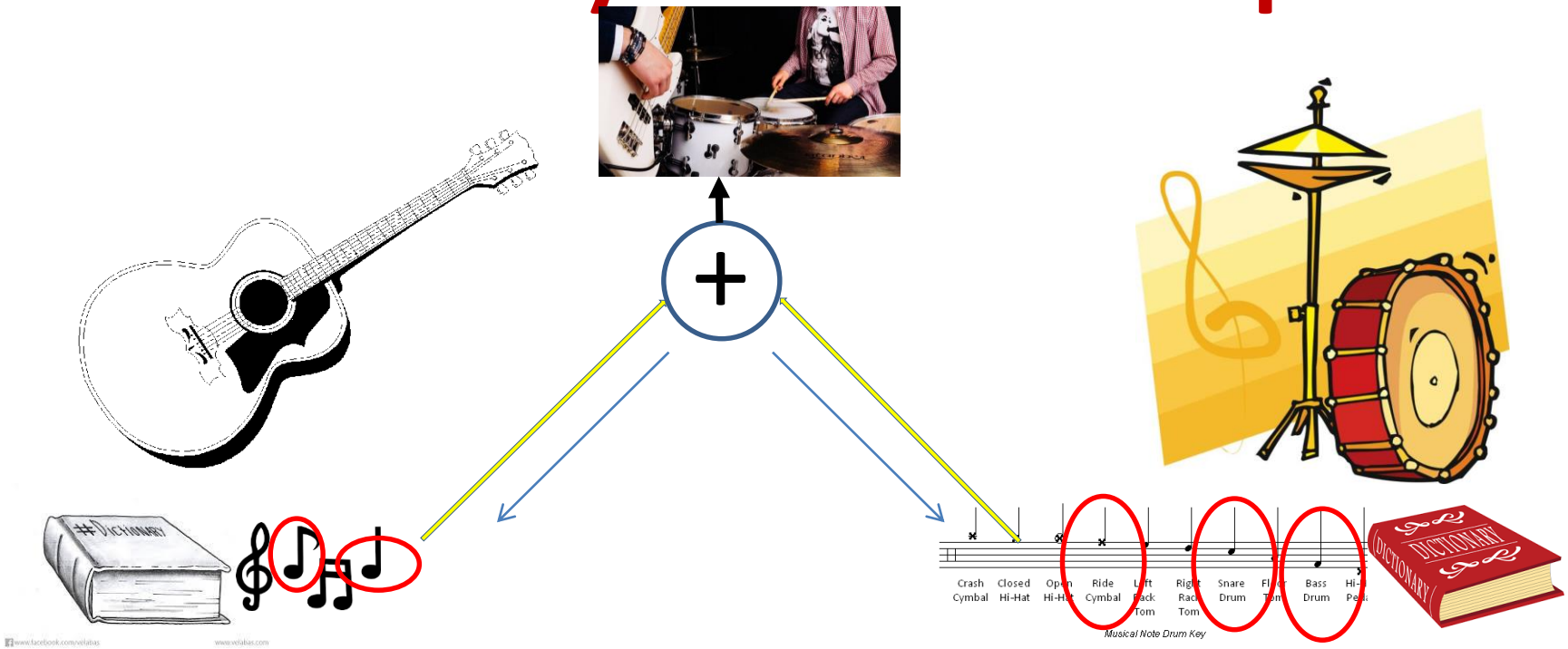
- Learn a similar dictionary for all sources expected in the signal

Dictionary-based techniques



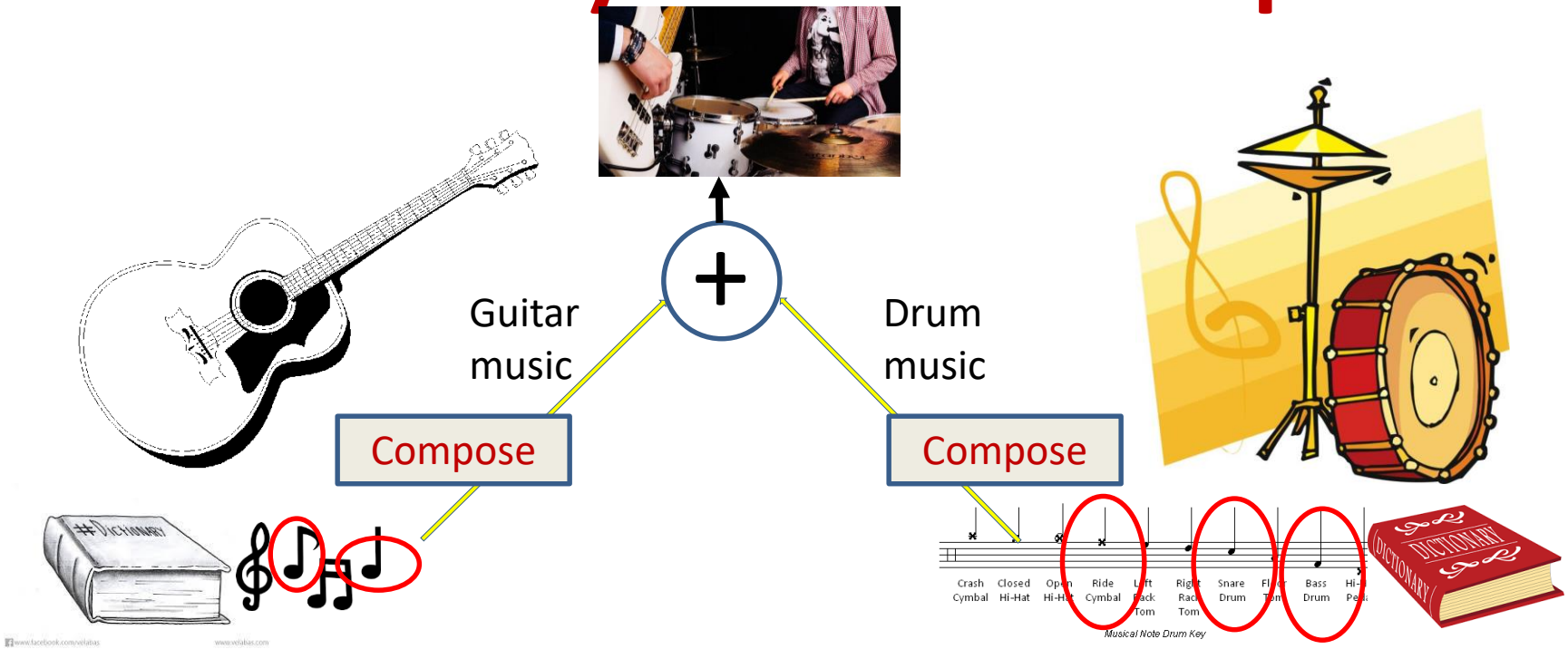
- A mixed signal is the linear combination of signals from the individual sources
  - Which are in turn composed of entries from its dictionary

Dictionary-based techniques



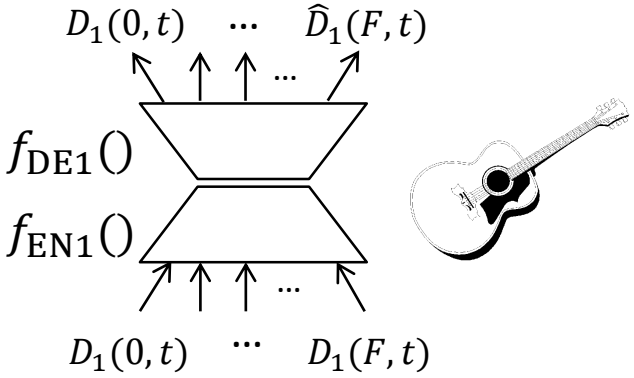
- Separation: Identify the combination of entries from both dictionaries that compose the mixed signal

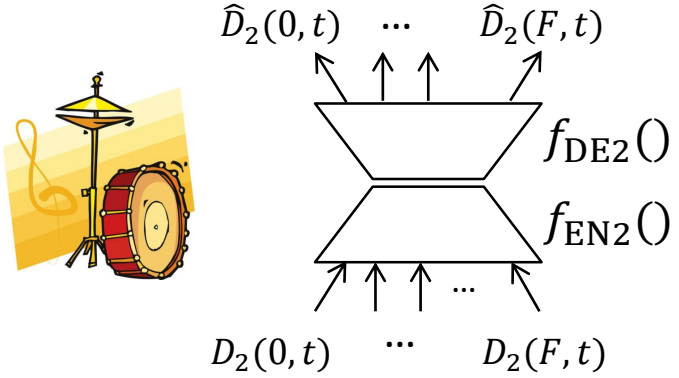
Dictionary-based techniques



- Separation: Identify the combination of entries from both dictionaries that compose the mixed signal
  - The composition from the identified dictionary entries gives you the separated signals

Learning Dictionaries

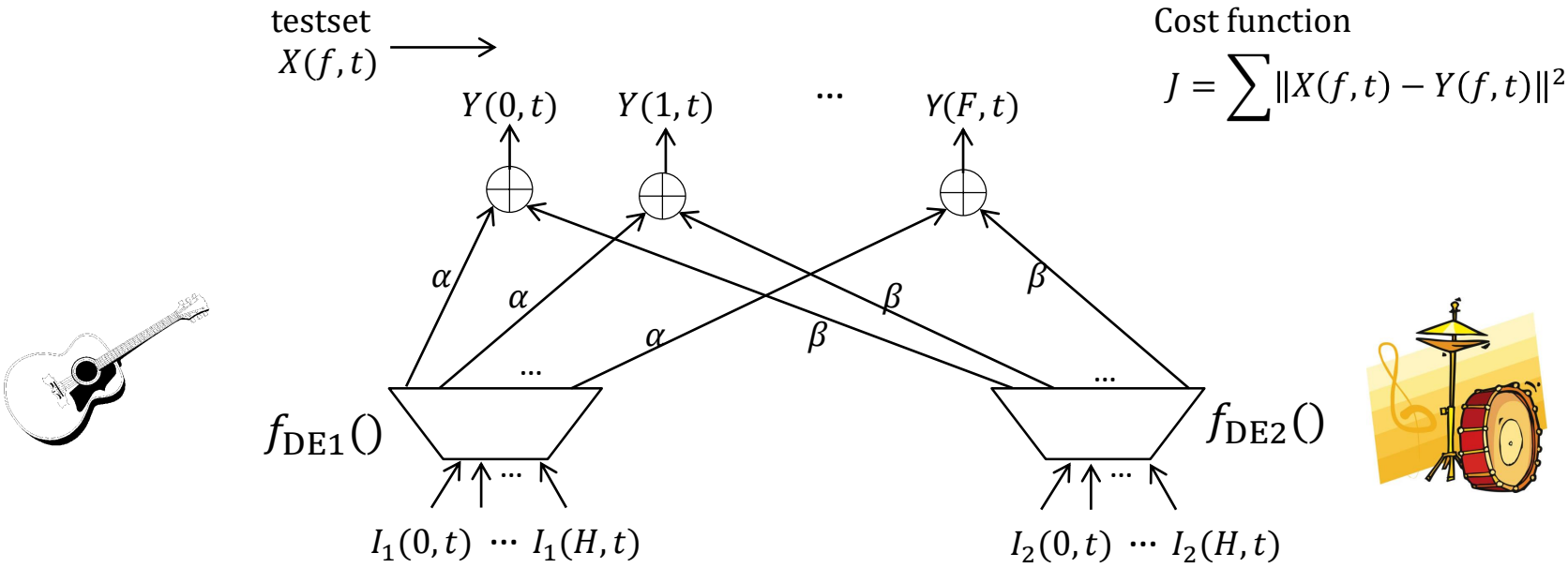




- Autoencoder dictionaries for each source
  - Operating on (magnitude) spectrograms

- For a well-trained network, the “decoder” dictionary is highly specialized to creating sounds for that source

Model for mixed signal



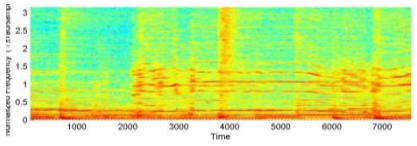
Estimate $I_1()$ and $I_2()$ to minimize cost function $J()$

- The sum of the outputs of both neural dictionaries
  - For some unknown input

Separation

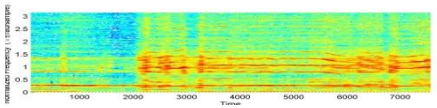
Test Process

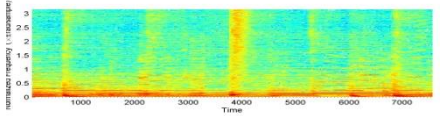
testset $X(f,t)$



Cost function

$$J = \sum \|X(f,t) - Y(f,t)\|^2$$



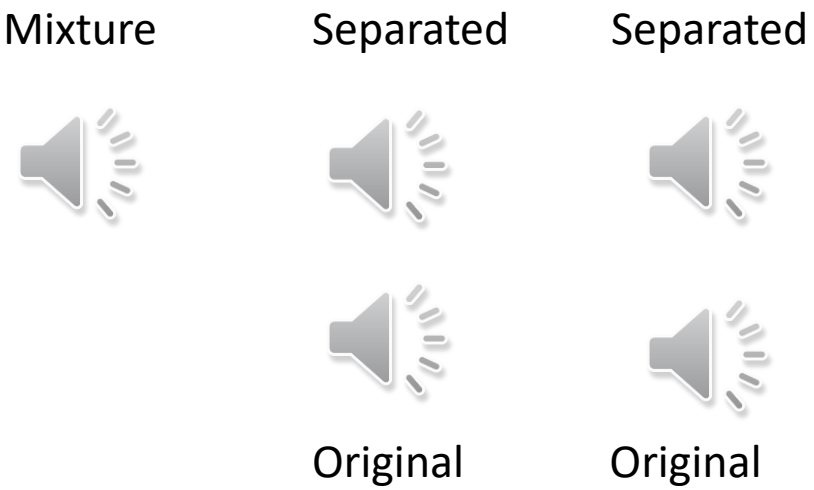


H : Hidden layer size

Estimate $I_1()$ and $I_2()$ to minimize cost function $J()$

- Given mixed signal and source dictionaries, find excitation that best recreates mixed signal
  - Simple backpropagation
- Intermediate results are separated signals

Example Results



5-layer dictionary, 600 units wide

- Separating music

Story for the day

- Classification networks learn to predict the *a posteriori* probabilities of classes
  - The network until the final layer is a feature extractor that converts the input data to be (almost) linearly separable
  - The final layer is a classifier/predictor that operates on linearly separable data

- Neural networks can be used to perform linear or non-linear PCA
  - "Autoencoders"
  - Can also be used to compose constructive dictionaries for data
    - Which, in turn can be used to model data distributions