# Machine Learning (CS 181): 8. Neural Networks 1

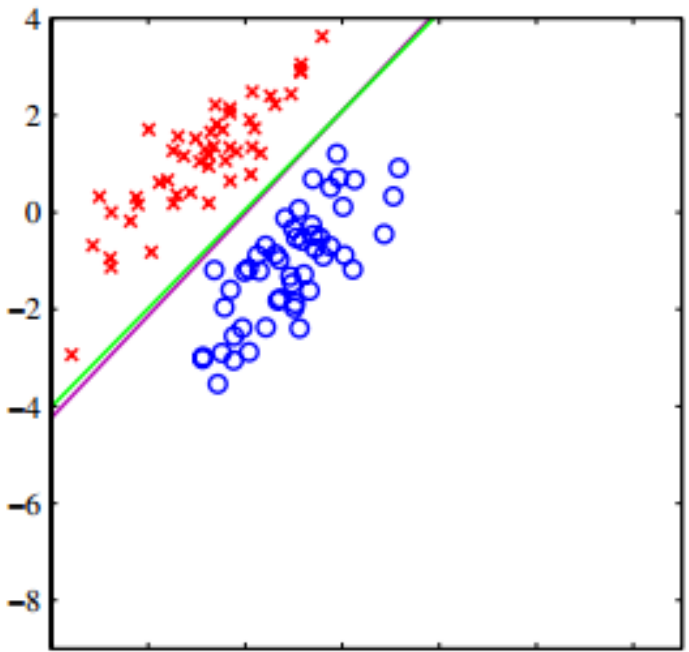
David Parkes and Sasha Rush

# Contents

# Overview: Linear Classification

- Perceptron - SGD, Perceptron algorithm
- Naive Bayes - Closed-form, counts, generative probabilistic
- Logistic Regression - SGD (today), discriminative probabilistic

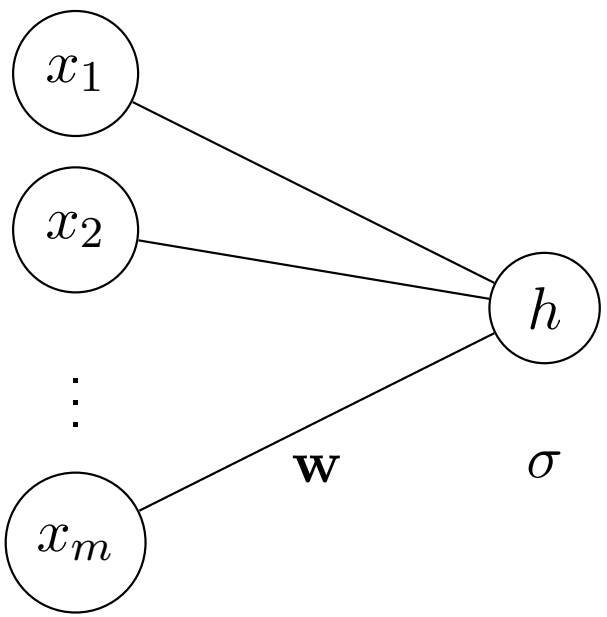
$$h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^\top \mathbf{x} + w_0$$



# Linear Model with Logistic

$$h(\mathbf{x}; \mathbf{w}) = \mathbf{x}^\top \mathbf{w} + w_0$$

$$p(y = 1|\mathbf{x}) = \sigma(h(\mathbf{x}; \mathbf{w}))$$



# Contents

# Linear Discriminative Model

We will require that the difference between classes in log space is linear:

$$h(\mathbf{x}; \mathbf{w}) = \ln p(y = 1|\mathbf{x}; \mathbf{w}) - \ln p(y = 0|\mathbf{x}; \mathbf{w})$$

Equivalently, $\ln(p(y = 1|\mathbf{x}; \mathbf{w})/(1 - p(y = 1|\mathbf{x}; \mathbf{w})) = h(\mathbf{x}; \mathbf{w})$, and:

$$\frac{p(y = 1|\mathbf{x}; \mathbf{w})}{1 - p(y = 1|\mathbf{x}; \mathbf{w})} = \exp(h(\mathbf{x}; \mathbf{w}))$$

Solving for $p(y = 1|\mathbf{x}; \mathbf{w})$, we have

$$p(y = 1|\mathbf{x}; \mathbf{w}) = \frac{\exp(h(\mathbf{x}; \mathbf{w}))}{1 + \exp(h(\mathbf{x}; \mathbf{w}))}, \tag{1}$$

$$p(y = 0|\mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(h(\mathbf{x}; \mathbf{w}))}$$

Finally, call (1) the logistic sigmoid activation:

$$\sigma(z) = (1 + \exp -z)^{-1}$$

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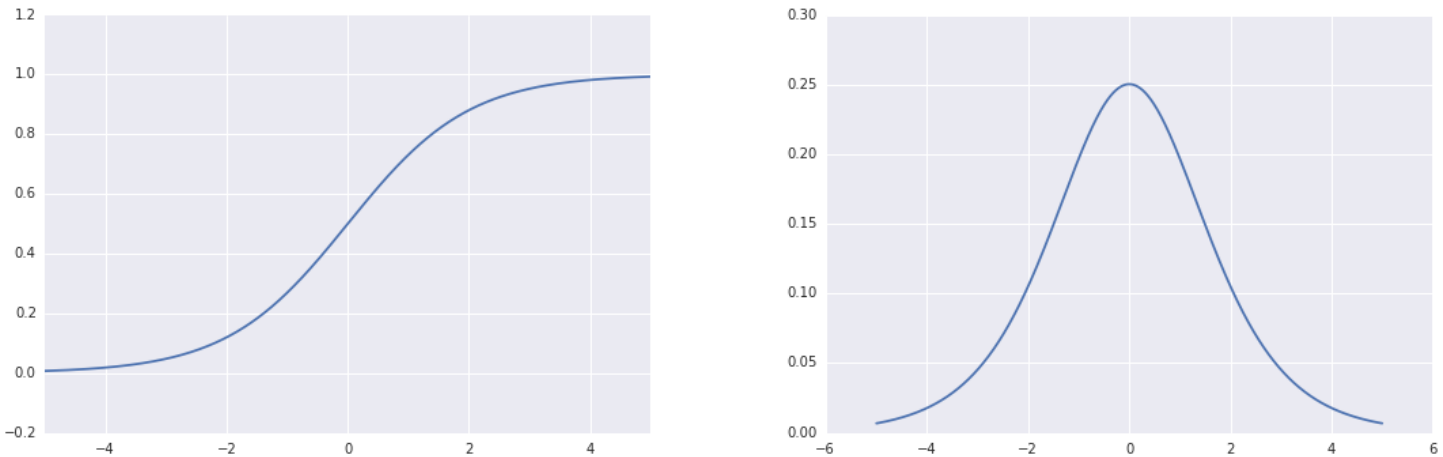
# (Logistic) Sigmoid Activation

$$\sigma(h) = (1 + \exp(-h))^{-1}$$

$$\sigma'(h) = \sigma(h)^2 \exp(-h)$$




Sigmoid Function and Derivative

- "Squashes" $\mathbb{R}$ to a probabilities.

# Logistic Regression

Linear model converted to probability estimated by sigmoid

$$p(y = 1|\mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^\top \mathbf{x} + w_0) = (1 + \exp(-h))^{-1}$$

$$p(y = 0|\mathbf{x}; \mathbf{w}) = 1 - \sigma(\mathbf{w}^\top \mathbf{x} + w_0) = (1 + \exp h)^{-1}$$

- Linear "Regression" transformed to probability estimate.
- Name is confusing, mostly used for *classification*.

# Fitting Model

Reminder:

$$p(y = 1|\mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^\top \mathbf{x} + w_0) = (1 + \exp(-h))^{-1}$$

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As this is now a probabilistic model, can fit with MLE.

$$\begin{aligned}
\mathcal{L}(\mathbf{w}) &= -\sum_{i=1}^{n} \ln p(y_i|\mathbf{x}_i; \mathbf{w}) = -\sum_{i=1}^{n} \ln \sigma(h_i)^{y_i} (1 - \sigma(h_i))^{1-y_i} \\
&= \sum_{i=1}^{n} y_i \ln(1 + \exp(-h_i)) + (1 - y_i) \ln(1 + \exp h_i)
\end{aligned}$$

# Likelihood and Estimation (1)

Reminder:

$$\begin{aligned} h(\mathbf{x}_i; \mathbf{w}) = h_i &= \mathbf{w}^\top \mathbf{x}_i + w_0 \\ \mathcal{L}(\mathbf{w}) &= \sum_{i=1}^{n} y_i \ln(1 + \exp(-h_i)) + (1 - y_i) \ln(1 + \exp h_i) \end{aligned}$$

Take gradients wrt $h_i$:

$$\frac{\partial}{\partial h_i} \ln(1 + \exp h_i) = \frac{\exp h_i}{1 + \exp h_i} = p(y_i = 1 | \mathbf{x}_i; \mathbf{w})$$

$$\frac{\partial}{\partial h_i} \ln(1 + \exp(-h_i)) = -\frac{\exp -h_i}{1 + \exp(-h_i)} = -p(y_i = 0 | \mathbf{x}_i; \mathbf{w})$$

Chain rule (with $h_i$ scalar function of $\mathbf{w}$):

$$\frac{\partial \mathcal{L}(\mathbf{w})}{\partial \mathbf{w}} = \frac{\partial h_i}{\partial \mathbf{w}} \frac{\partial \mathcal{L}(\mathbf{w})}{\partial h_i}$$

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# Likelihood and Estimation (2)

$$h_i = \mathbf{w}^\top \mathbf{x}_i + w_0$$

Take gradients wrt $\mathbf{w}$:

$$\frac{\partial}{\partial \mathbf{w}} \ln(1 + \exp h_i) = \frac{\partial h_i}{\partial \mathbf{w}} \times p(y_i = 1|\mathbf{x}; \mathbf{w}) = \mathbf{x}_i p(y_i = 1|\mathbf{x}; \mathbf{w})$$

$$\frac{\partial}{\partial \mathbf{w}} \ln(1 + \exp(-h_i)) = \frac{\partial h_i}{\partial \mathbf{w}} \times -p(y_i = 0|\mathbf{x}; \mathbf{w}) = -\mathbf{x}_i p(y_i = 0|\mathbf{x}; \mathbf{w})$$

$$\frac{\partial}{\partial \mathbf{w}} \mathcal{L}(\mathbf{w}) = \sum_{i=1}^{n} -y_i \mathbf{x}_i p(y_i = 0|\mathbf{x}_i) + (1 - y_i)\mathbf{x}_i p(y_i = 1|\mathbf{x}_i)$$

- If $y_i = 1$, gradient is $-\mathbf{x}_i p(y_i = 0|\mathbf{x}_i)$
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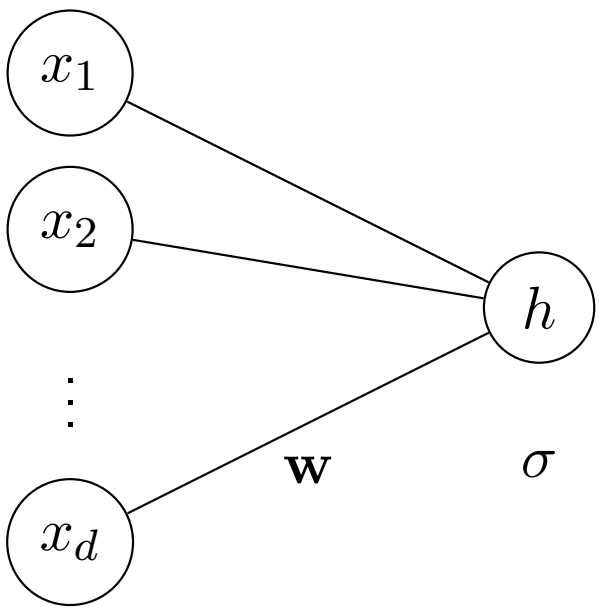
# High-Level Gradient Computation

Compute the loss function:

$$\mathbf{w} \rightarrow h(\mathbf{x}; \mathbf{w}) \rightarrow \mathcal{L}$$

Compute the gradient of loss wrt the weight, use chain rule:

$$\frac{\partial h}{\partial \mathbf{w}} \leftarrow \frac{\partial \mathcal{L}}{\partial h} \leftarrow \mathcal{L}$$



# Reminder: Stochastic Gradient Descent

Instead of computing gradient of entire loss, compute stochastic gradients.

1. Sample data point $i$, corresponding to $(\mathbf{x}_i, y_i)$
2. Compute loss and gradient for just that data point $\mathcal{L}^{(i)}(\mathbf{w})$
3. Update $\mathbf{w}$ based on this *stochastic gradient*

Similar to standard gradient descent, often more efficient in practice.

# SGD on Logistic Regression

(Exercise: derive)

1. Iterate over the data:
   - Compute $p(y_i = 1|\mathbf{x}_i)$.
   - If $(y_i = 1)$, add $\eta \times \mathbf{x}_i p(y_i = 0|\mathbf{x}_i)$ to $\mathbf{w}$
   - If $(y_i = 0)$, add $\eta \times -\mathbf{x}_i p(y_i = 1|\mathbf{x}_i)$ to $\mathbf{w}$
2. Repeat until convergence.

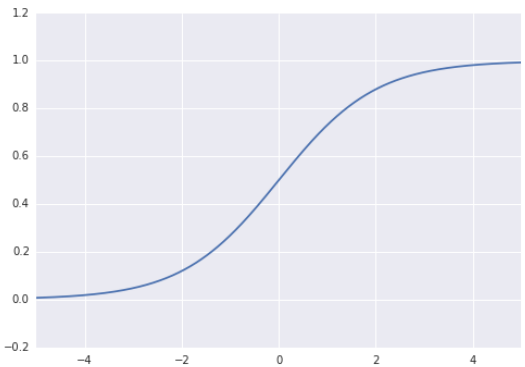
**Guaranteed** to maximize conditional likelihood of data.

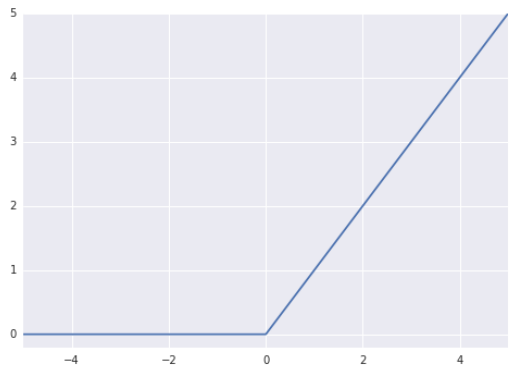
# Recall: Perceptron Algorithm

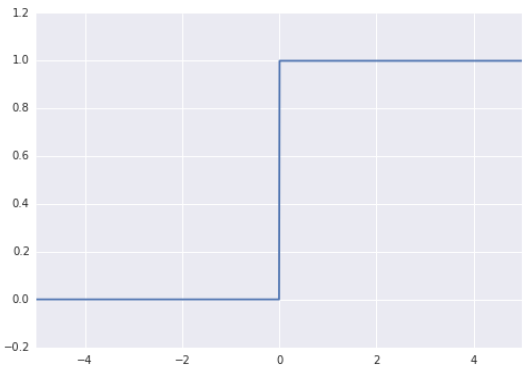
1. Iterate over the data:
   - If correct ($y_i = \hat{y}_i$), do nothing.
   - If incorrect, add/subtract $\eta \times \mathbf{x}_i$ to weights
2. If errors, repeat process.
3. Otherwise separator is found.

# Activation Functions

- Activation functions provide useful non-linear transformations of linear functions.
- Good activations also provide useful derivatives. (0/1 does not.)



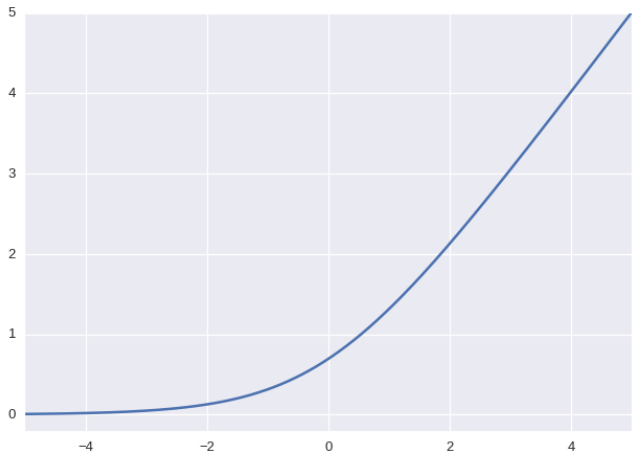



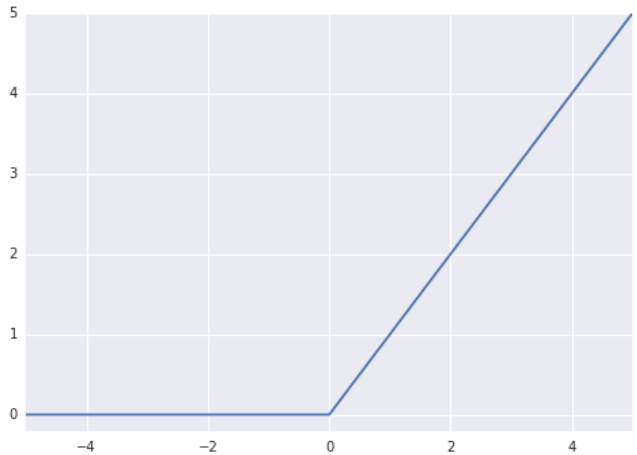




Sigmoid versus ReLU versus 0/1. x-axis input e.g $h(\mathbf{x}; \mathbf{w})$, y-axis output.

# Algorithms come from Loss Function

Direct comparison of negative ln $\sigma$ and ReLU in $\mathcal{Y} = \{0, 1\}$ notation




Logistic regression loss $\mathcal{L}_\sigma$ versus Perceptron loss $\mathcal{L}_{perc}$. $x$-axis is misclassification error, $y$-axis is increased loss.

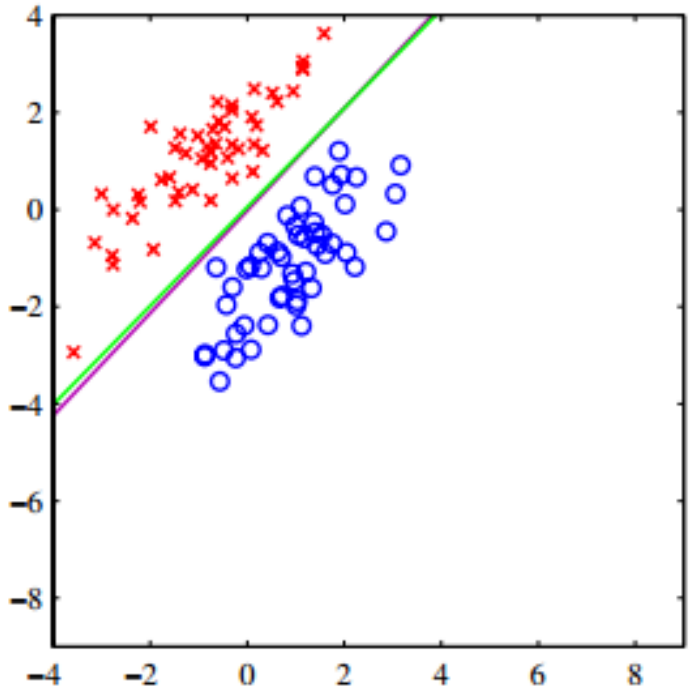
$$\mathcal{L}_\sigma(\mathbf{w}) = \sum_{i=1}^{n} -\ln \sigma(h_i)^{y_i} (1 - \sigma(h_i))^{1-y_i}$$

$$\mathcal{L}_{perc}(\mathbf{w}) = \sum_{i=1}^{n} f_{relu}(-h_i)^{y_i} f_{relu}(h_i)^{1-y_i}$$

# Contents

# Linear Models

- Linear models aren't very good for most problems.




Binary Classification

# Basis Functions

- What should we do?
- Our answer so far: use basis functions.

$$h(\mathbf{x}; \mathbf{w}, w_0) = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}) + w_0.$$

- Basis function provides another representation that makes it linear-separable (in $\mathbb{R}^d$)

# Downside of Basis Functions

Choosing basis functions is hard. Either need:

- Specific domain knowledge of the problem
  - Frequency domain in speech, visual detection for images, etc.
- Very large transformation with aggressive regularization.
  - Radial basis functions, high-degree polynomials

# Adaptive Basis Functions

Alternative approach: learn the basis functions from data.

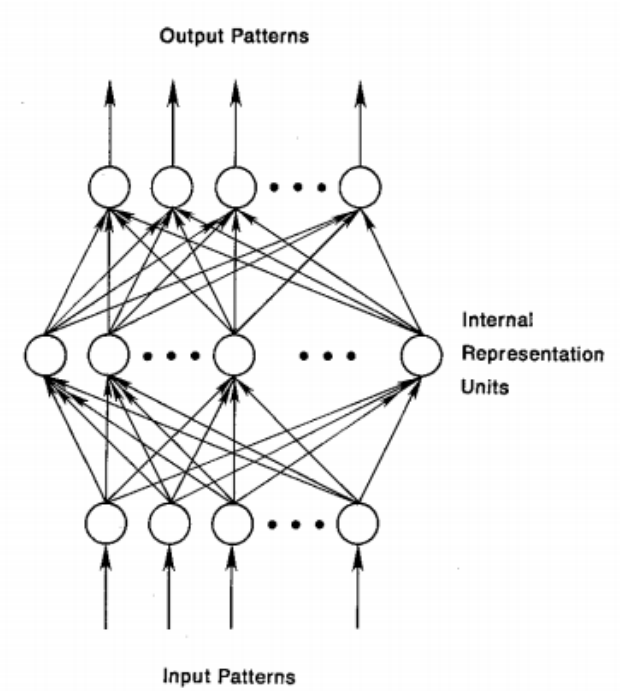
$$\boldsymbol{\phi}(\mathbf{x}; \mathbf{w}^1) : \mathbb{R}^m \mapsto \mathbb{R}^d$$

- Combines basis selection and learning.
- Several different approaches, we will focus on neural networks.
- Downside: Complicates the optimization problem.

# Contents

# Neural Networks: History 2

- AI Winter (post-perceptron)
- Paul Werbos (1974,1982)
- Popularized by work of Rumelhart et al (1986)




**Learning Internal Representations by Error Propagation**

D. E. RUMELHART, G. E. HINTON, and R. J. WILLIAMS

# Neural Networks: Formally

Define basis function as logistic regression:

For all $j \in \{1, \ldots, d\}$, define basis function as,

$$\phi_j(\mathbf{x}; \mathbf{w}_j^1, w_{j0}^1) = \sigma(\mathbf{w}_j^{1\top} \mathbf{x} + w_{j0}^1)$$

Where $\mathbf{w}_j^1 \in \mathbb{R}^{m \times 1}$

Interpretation:

- Predicting feature basis value.
- Different *linear* weight vector $\mathbf{w}_j$ for each basis dimension

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Interpretation:

- Predicting feature basis value.
- Different *linear* weight vector $\mathbf{w}_j$ for each basis dimension

# Neural Networks: Matrix-view

Define entire adaptive basis layer as $d$ problems,

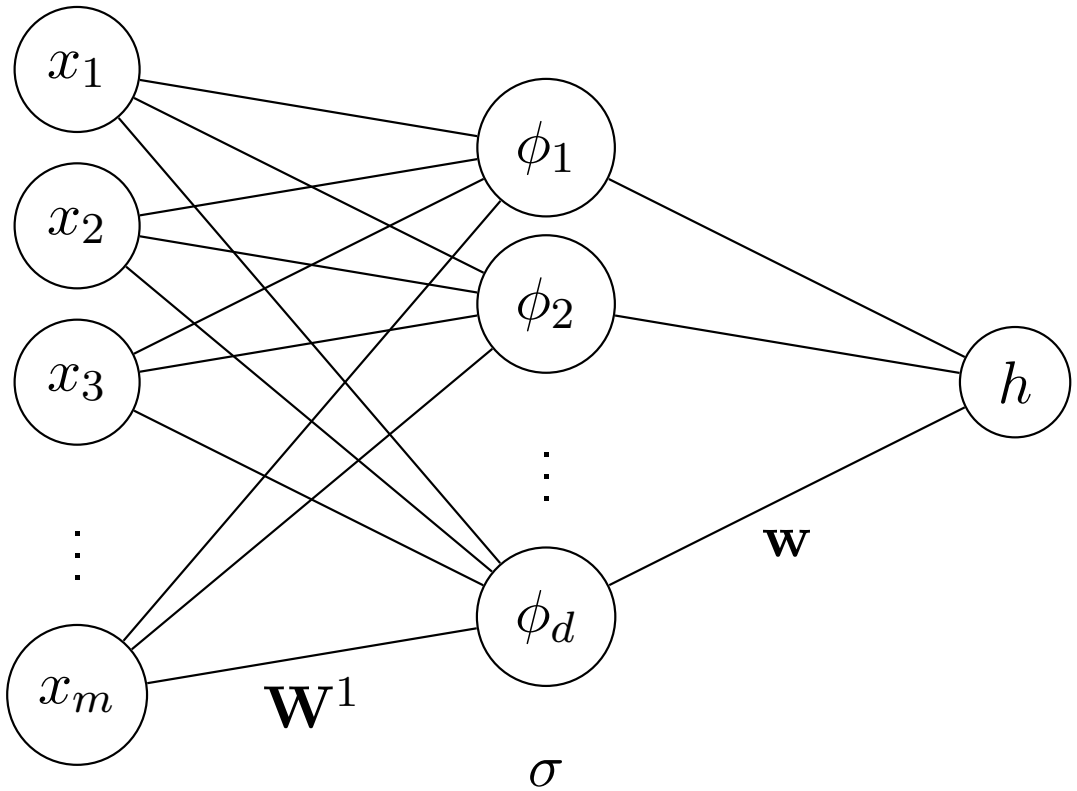
$$\boldsymbol{\phi}(\mathbf{x}; \mathbf{W}^1, \mathbf{w}_0^1) = \boldsymbol{\sigma}(\mathbf{W}^1\mathbf{x} + \mathbf{w}_0^1)$$

Where $\boldsymbol{\sigma}$ is pointwise sigmoid and $\mathbf{W}^1 \in \mathbb{R}^{d \times m}$

Full classification problem:

$$\begin{aligned} h(\mathbf{x}; \mathbf{w}, w_0, \mathbf{W}^1, \mathbf{w}_0^1) &= \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}; \mathbf{W}^1, \mathbf{w}_0^1) + w_0 \\ &= \mathbf{w}^\top \boldsymbol{\sigma}(\mathbf{W}^1\mathbf{x} + \mathbf{w}_0^1) + w_0 \end{aligned}$$

# Neural Network Diagram

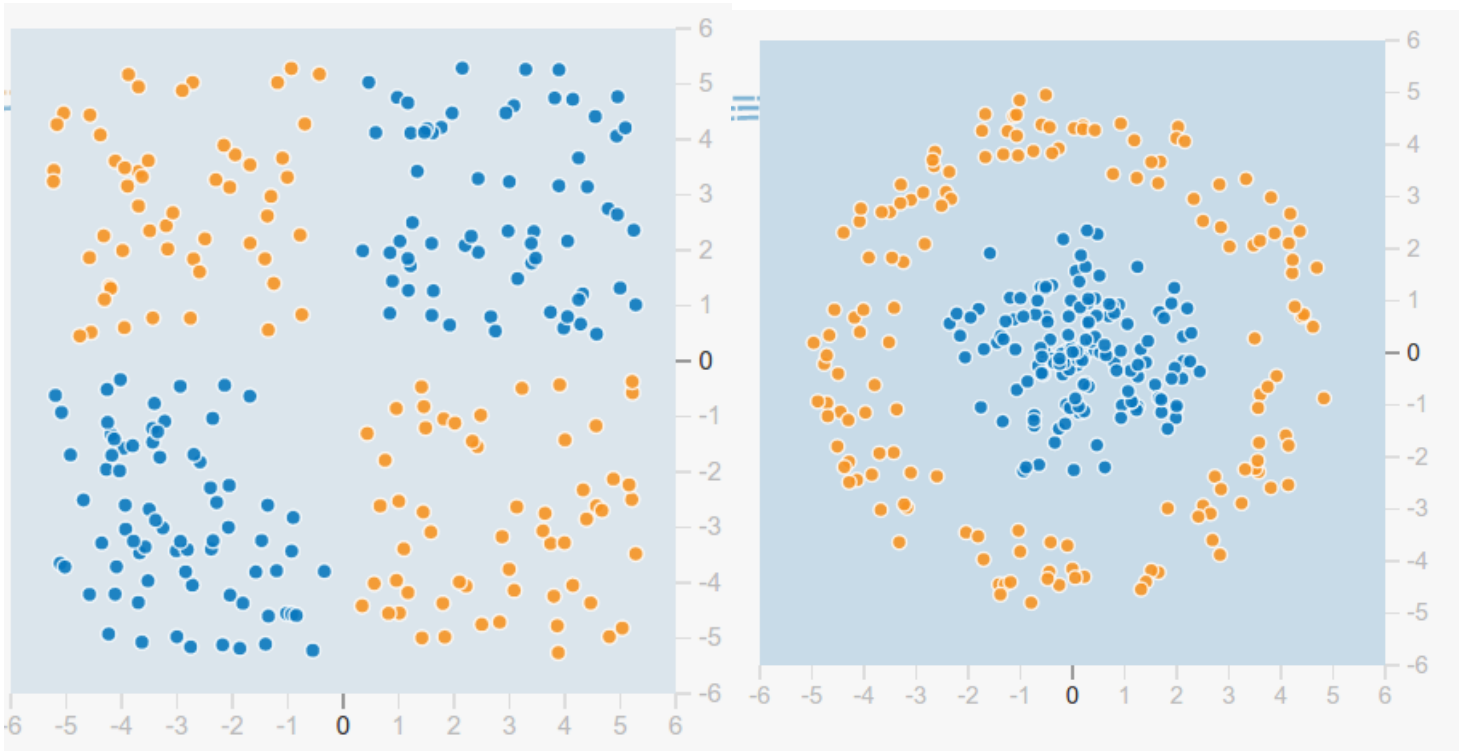



$$\boldsymbol{\phi}(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{W}^1\mathbf{x} + \mathbf{w}_0^1)$$

$$h(\mathbf{x}) = \mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}) + w_0$$

# Non-Linear Problems

- Clearly no linear separator.




Two class classification: (1) xor classification, (2) ring

# Exercise: XOR with Neural Network

- $\mathbf{x} = [0; 1]$ $\mathbf{x} = [1; 0]$ in class $y = 1$.
- $\mathbf{x} = [0; 0]$ $\mathbf{x} = [1; 1]$ in class $y = 0$.

$$\begin{aligned} \phi_1(x_1, x_2) &= \sigma(-x_1 - x_2 + 0.5) \\ \phi_2(x_1, x_2) &= \sigma(x_1 + x_2 - 1.5) \\ h(\mathbf{x}) &= -\phi_1 - \phi_2 + 0.5 \end{aligned}$$

- $\phi_1 > 0$, only $[0; 0]$
- $\phi_2 > 0$, only $[1; 1]$
- $h$, only $\phi_1 = 0$ and $\phi_2 = 0$

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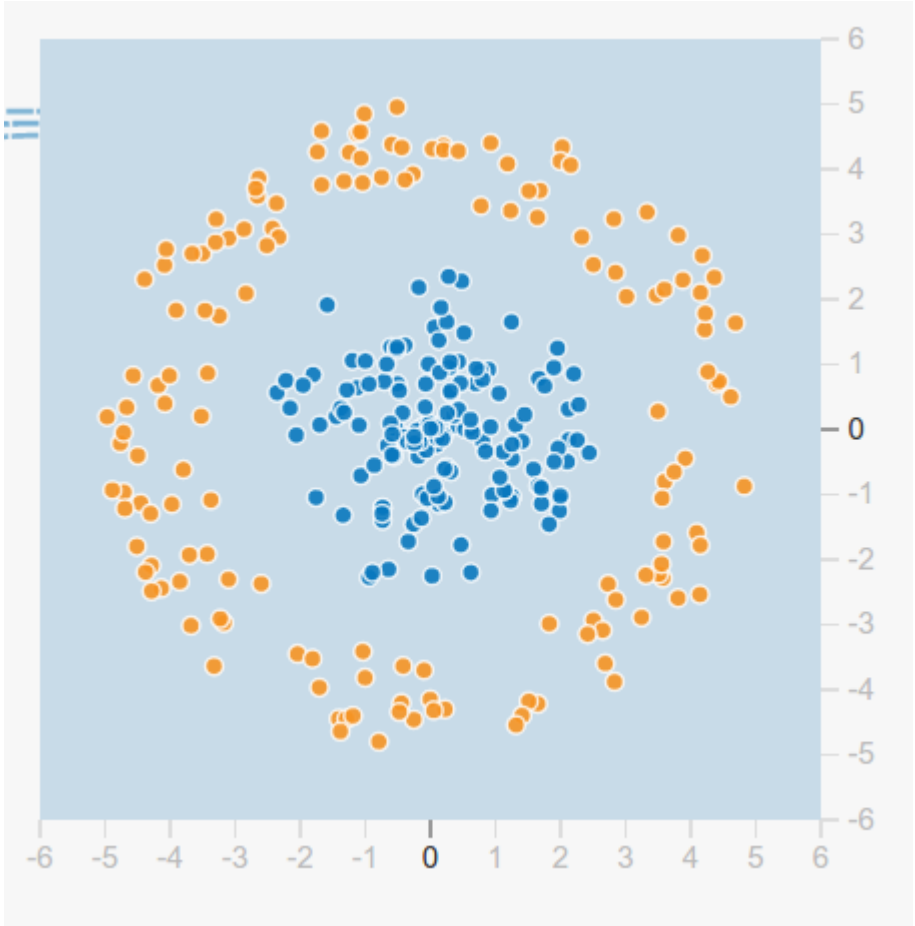
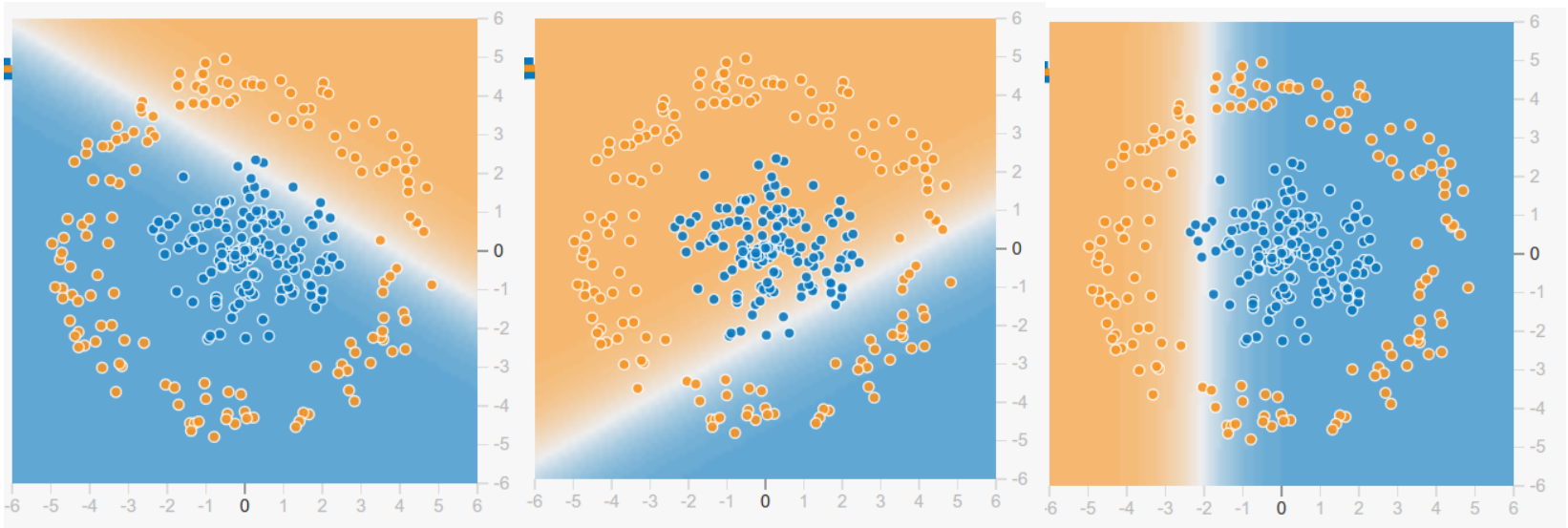
# Ring



# Visual Description

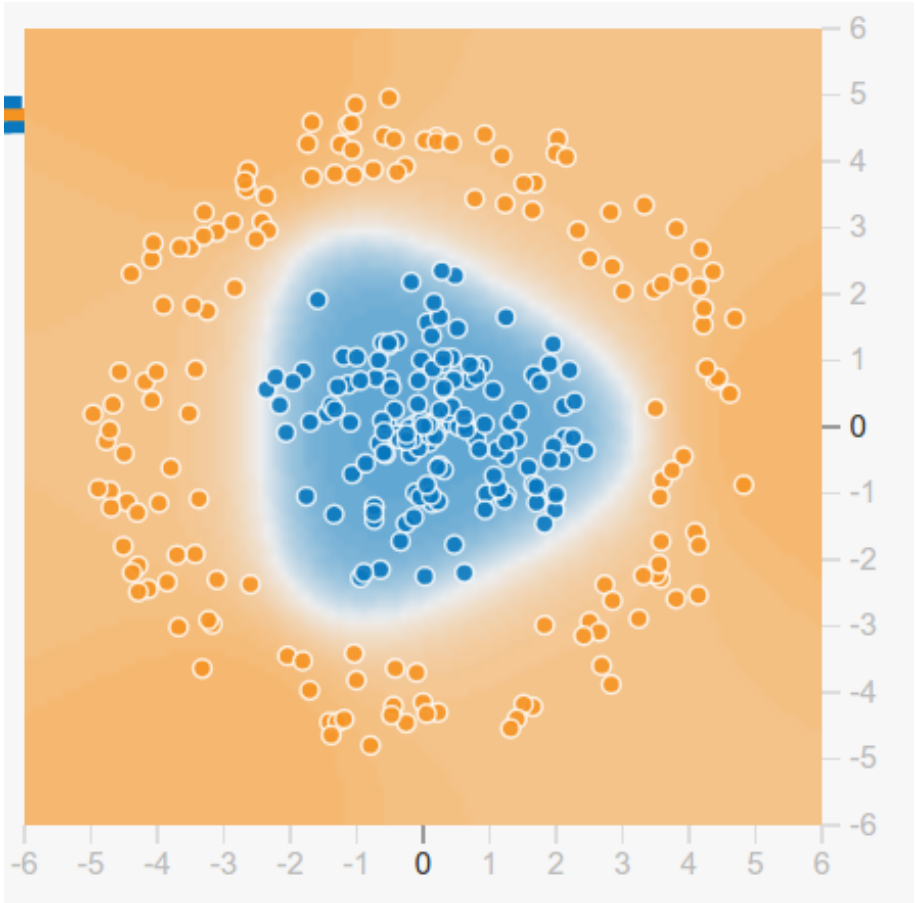
- $\phi$ is constructed by learned linear models.
- Logistic regression to select $\phi$ values.



Separators for learned features $\phi_1$, $\phi_2$, $\phi_3$.

# Final Non-Linear Output

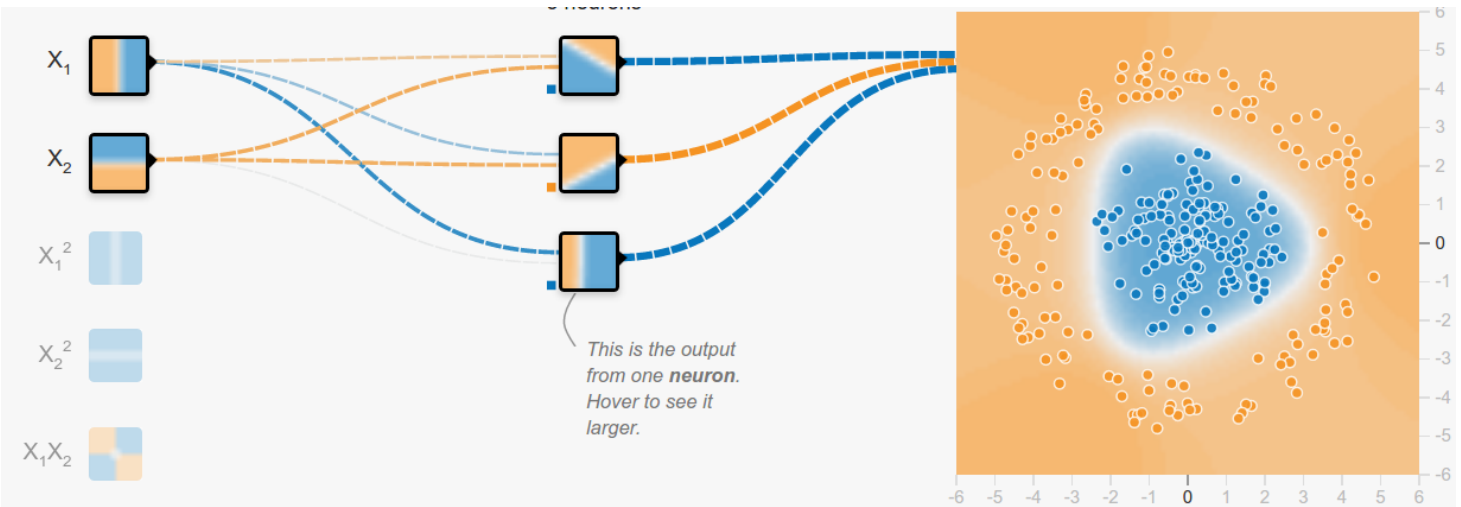
- Combining multiple layers give non-linear decision boundary.




Final classification $h$ using $\phi$ basis.

# Neural Network

- Multi-layer linear decisions for classification.




A 2-layer neural network

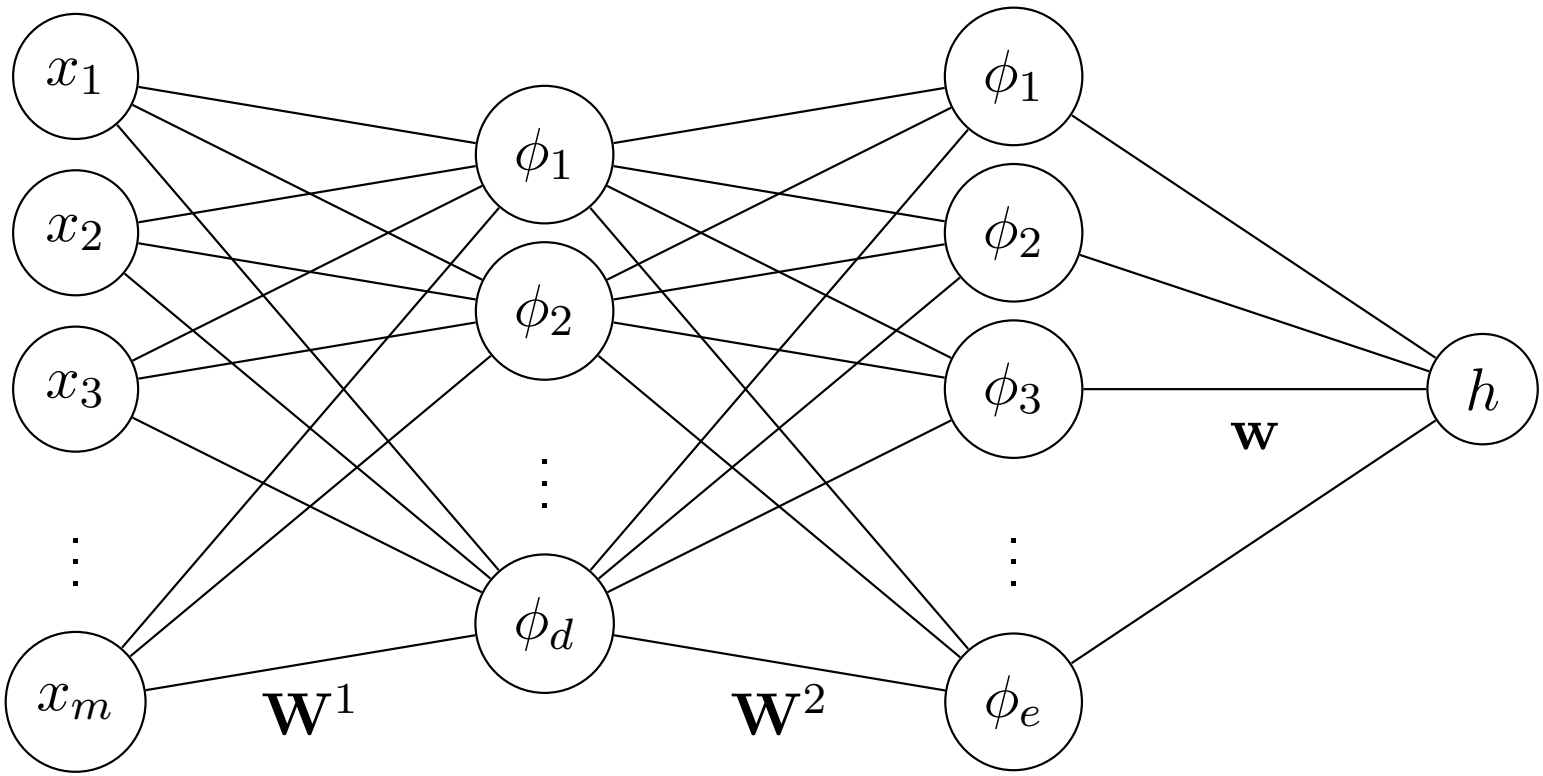
# Multilayer "Deep" Neural Networks

Can stack arbitrary layers of basis functions.

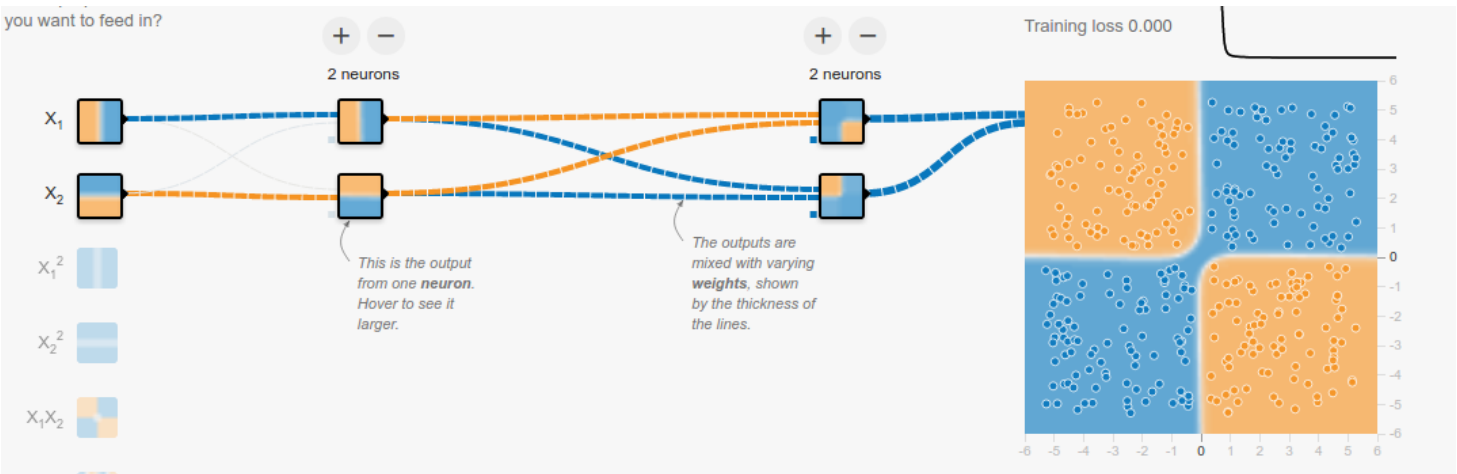
$$\boldsymbol{\phi}^l(\mathbf{x}; \mathbf{W}^l, \mathbf{w}_0^l) = \boldsymbol{\sigma}(\mathbf{W}^l \boldsymbol{\phi}^{(l-1)} + \mathbf{w}_0^l)$$

- Each layer learns adaptive basis based on previous layers.

# Multilayer NN



# 3-Layer Xor Network



# Demos