Machine Learning
ITCS 4156

The Perceptron Algorithm

The Kernel Trick

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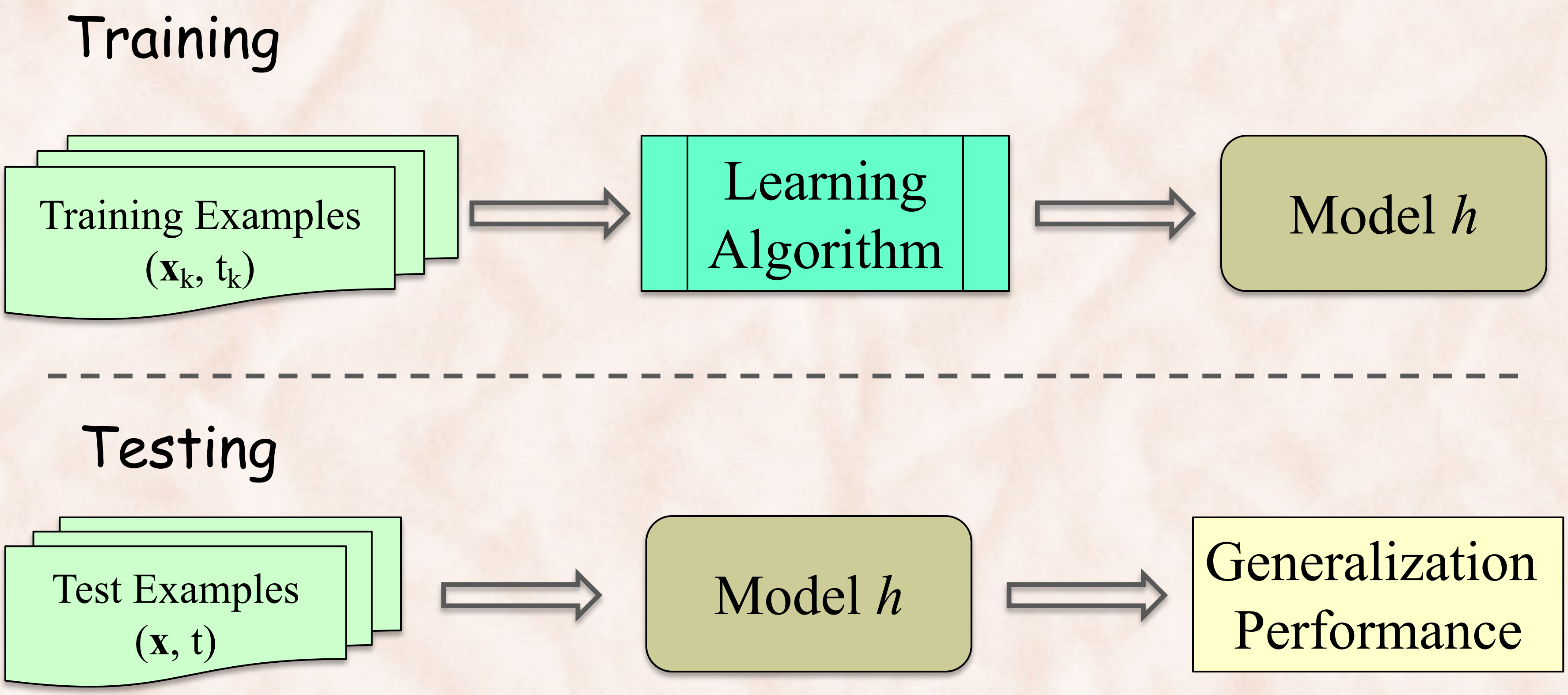
Supervised Learning



Supervised Learning

- **Task** = learn an (unkown) function $t : X \rightarrow T$ that maps input instances $\mathbf{x} \in X$ to output targets $t(\mathbf{x}) \in T$:
  - **Classification**:
    - The output $t(\mathbf{x}) \in T$ is one of a finite set of discrete categories.
  - **Regression**:
    - The output $t(\mathbf{x}) \in T$ is continuous, or has a continuous component.

- Target function $t(\mathbf{x})$ is known (only) through (noisy) set of training examples:

$$(\mathbf{x}_1,t_1), (\mathbf{x}_2,t_2), \ldots (\mathbf{x}_n,t_n)$$

Three Parametric Approaches to Classification

1) Discriminant Functions: construct $f: X \rightarrow T$ that directly assigns a vector $\mathbf{x}$ to a specific class C_k.
   - Inference and decision combined into a single learning problem.
   - *Linear Discriminant*: the decision surface is a hyperplane in X:
     - Perceptron
     - Support Vector Machines
     - Fisher 's Linear Discriminant

Three Parametric Approaches to Classification

2) Probabilistic Discriminative Models: directly model the posterior class probabilities $p(C_k \mid \mathbf{x})$.
   - Inference and decision are separate.
   - Less data needed to estimate $p(C_k \mid \mathbf{x})$ than $p(\mathbf{x} \mid C_k)$.
   - Can accommodate many overlapping features.
     - Logistic Regression
     - Conditional Random Fields

Three Parametric Approaches to Classification

3) Probabilistic Generative Models:

- Model class-conditional $p(\mathbf{x} \mid C_k)$ as well as the priors $p(C_k)$, then use Bayes's theorem to find $p(C_k \mid \mathbf{x})$.
  - or model $p(\mathbf{x}, C_k)$ directly, then marginalize to obtain the posterior probabilities $p(C_k \mid \mathbf{x})$.
- Inference and decision are separate.
- Can use $p(\mathbf{x})$ for *outlier* or *novelty detection*.
- Need to model dependencies between features.
  - Naïve Bayes.
  - Hidden Markov Models.

Generative and Discriminative Classifiers

Suppose we're distinguishing cat from dog images

ImageNet

ImageNet

Generative Classifier:

- Build a model of what's in a cat image
  - Knows about whiskers, ears, eyes
  - Assigns a probability to any image:
    - how cat-y is this image?

Also build a model for dog images

Given a new image:

Run both models and see which one fits better.

Discriminative Classifier

Just try to distinguish dogs from cats

Oh look, dogs have collars!

Let's ignore everything else.

Finding the correct class c from a document d in Generative vs Discriminative Classifiers

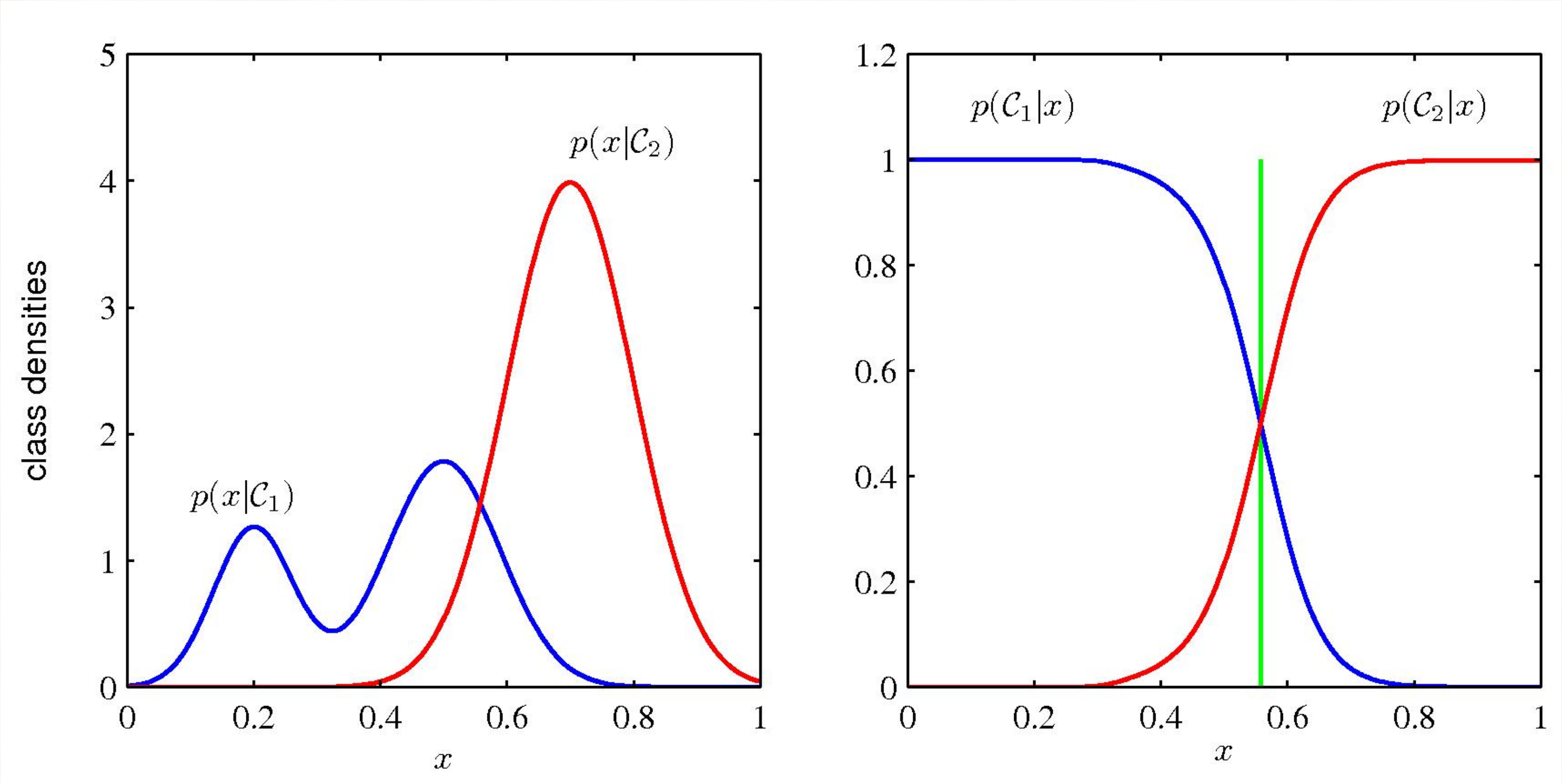
- Naive Bayes

$$\hat{c} = \underset{c \in C}{\operatorname{argmax}} \; \overbrace{P(d|c)}^{\text{likelihood}} \; \overbrace{P(c)}^{\text{prior}}$$

- Logistic Regression

$$\hat{c} = \underset{c \in C}{\operatorname{argmax}} \; \overset{\text{posterior}}{P(c|d)}$$

Generative vs. Discriminative



Left-hand mode has no effect on posterior class probabilities.

Three Parametric Approaches to Classification

1) Discriminant Functions: construct h: X $\rightarrow$ T that directly assigns a vector $\mathbf{x}$ to a specific class C_k.
   - Inference and decision combined into a single learning problem.
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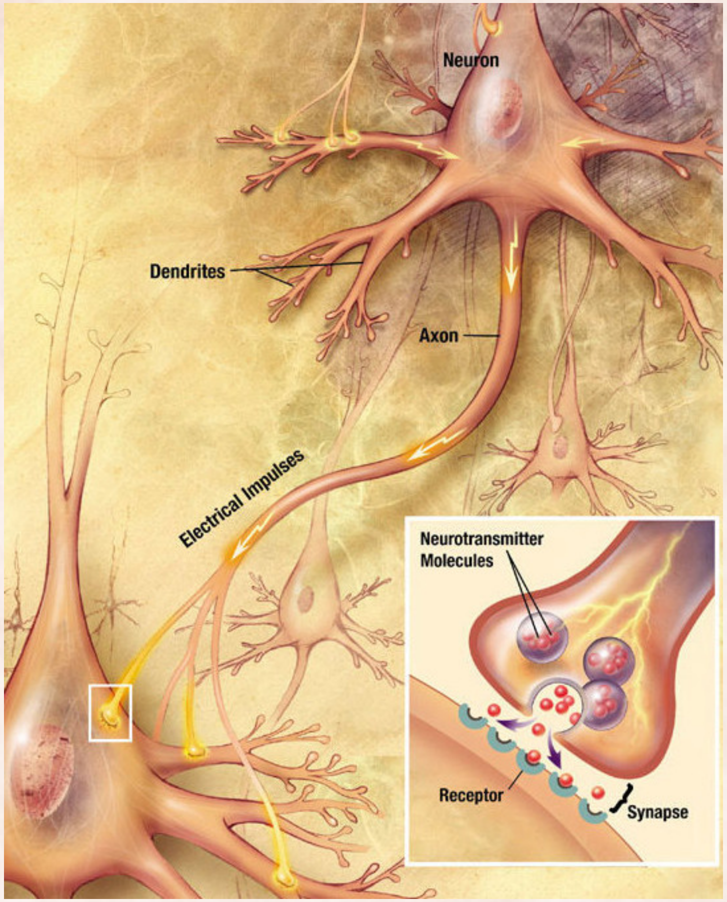
Discriminant Function Approach to Classification

- **Task** = build a function $h(\mathbf{x})$ such that:
  - h matches t well on the training data:
    => h is able to fit data that it has seen.
  - h also matches t well on test data:
    => h is able to **generalize to unseen data**.

- **Task** = choose h from a "nice" *class of functions* that depend on a vector of parameters $\mathbf{w}$:
  - $h(\mathbf{x}) \equiv h_{\mathbf{w}}(\mathbf{x}) \equiv h(\mathbf{w},\mathbf{x})$
  - **what classes of functions are "nice"?**

Neurons



Soma is the central part of the neuron:
- *where the input signals are combined.*

Dendrites are cellular extensions:
- *where majority of the input occurs.*

Axon is a fine, long projection:
- *carries nerve signals to other neurons.*

Synapses are molecular structures between axon terminals and other neurons:
- *where the communication takes place.*

Neuron Models

https://www.research.ibm.com/software/IBMResearch/multimedia/IJCNN2013.neuron-model.pdf

Year	Model Name	Reference
1907	Integrate and fire	[13]
1943	McCulloch and Pitts	[11]
1952	Hodgkin-Huxley	[12]
1958	Perceptron	[14]
1961	Fitzhugh-Nagumo	[15]
1965	Leaky integrate-and-fire	[16]
1981	Morris-Lecar	[17]
1986	Quadratic integrate-and-fire	[18]
1989	Hindmarsh-Rose	[19]
1998	Time-varying integrate-and-fire model	[20]
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2003	Exponential integrate-and-fire	[25]
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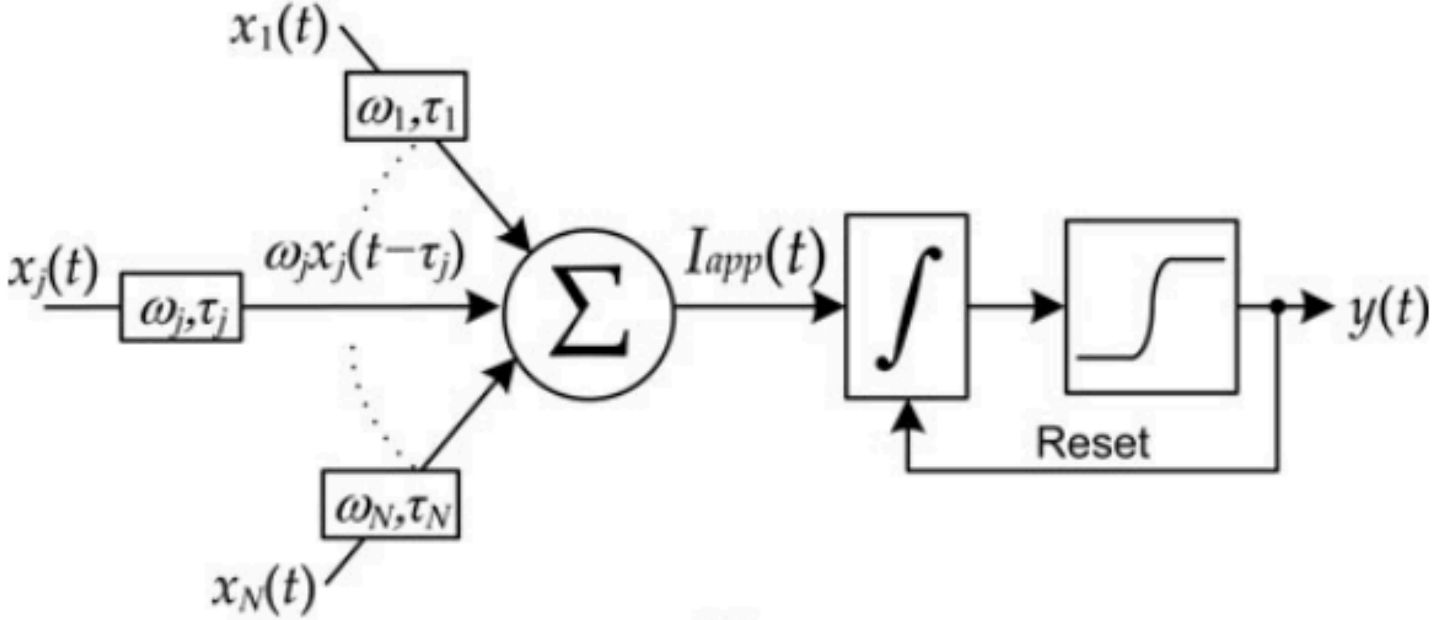
2005	Adaptive exponential integrate-and-fire	[27]
2009	Mihalas-Neibur	[28]

Spiking/LIF Neuron Function

http://ee.princeton.edu/research/prucnal/sites/default/files/06497478.pdf



(b)

Fig. 2. (a) Illustration and (b) functional description of a leaky integrate-and-fire neuron. Weighted and delayed input signals are summed into the input current $I_{\text{app}}(t)$, which travel to the soma and perturb the internal state variable, the voltage V. Since V is hysteric, the soma performs integration and then applies a threshold to make a spike or no-spike decision. After a spike is released, the voltage V is reset to a value V_{reset}. The resulting spike is sent to other neurons in the network.

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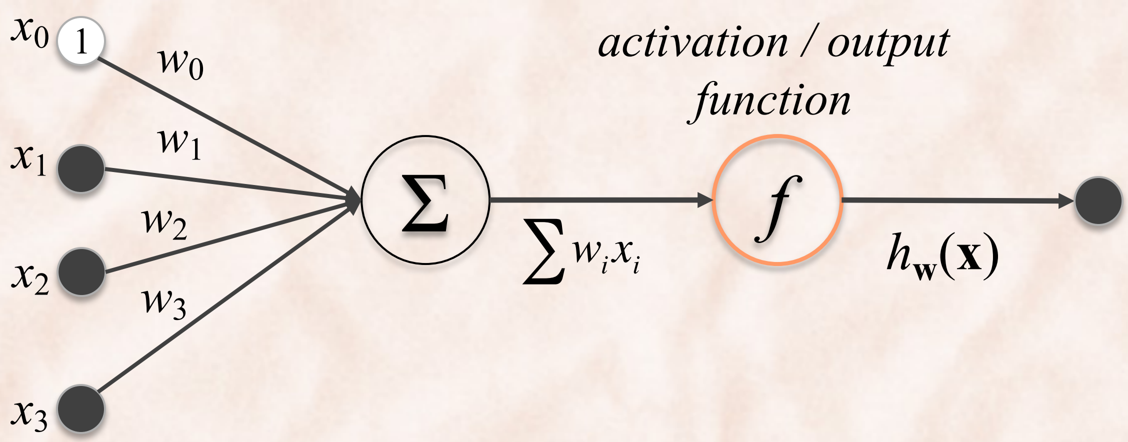
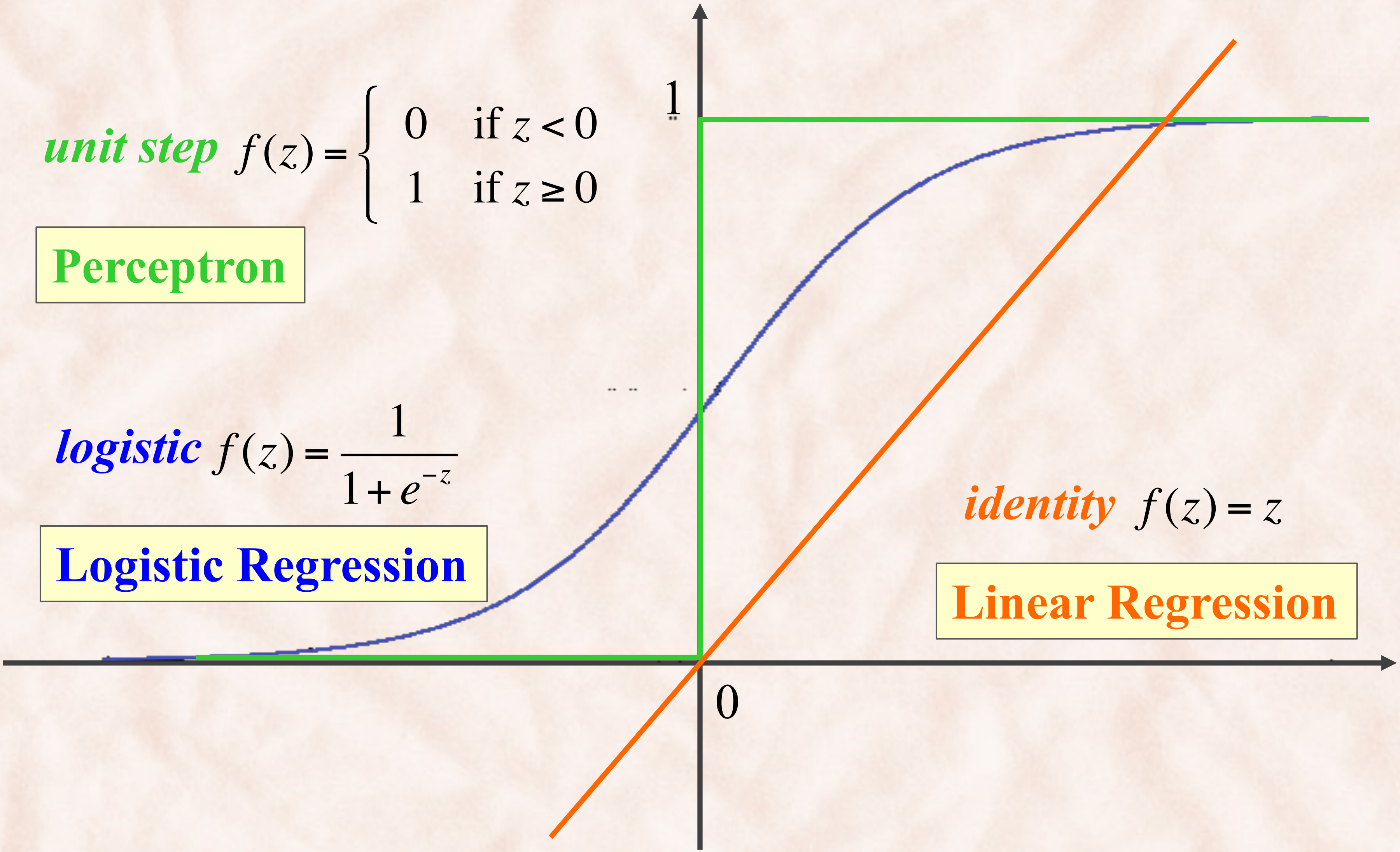
McCulloch-Pitts Neuron Function

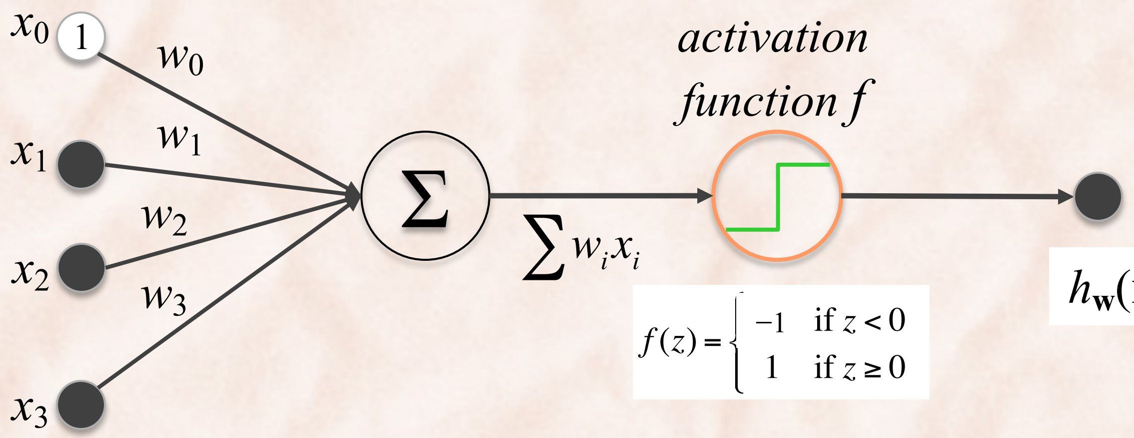


- Algebraic interpretation:
  - The output of the neuron is a **linear combination** of inputs from other neurons, **rescaled by** the synaptic **weights**.
    - weights w_i correspond to the synaptic weights (activating or inhibiting).
    - summation corresponds to combination of signals in the soma.
  - It is often transformed through a monotonic **activation function**.

Activation/Output Functions



Perceptron



$$f(z) = \begin{cases} -1 & \text{if } z < 0 \\ 1 & \text{if } z \geq 0 \end{cases}$$

$$h_{\mathbf{w}}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w}^T\mathbf{x} > 0 \\ -1 & \text{otherwise} \end{cases}$$

- Assume classes $T = \{c_1, c_2\} = \{1, -1\}$.
- Training set is $(\mathbf{x}_1, t_1), (\mathbf{x}_2, t_2), \ldots (\mathbf{x}_n, t_n)$.

  $\mathbf{x} = [1, x_1, x_2, ..., x_k]^T$

  $h(\mathbf{x}) = sgn(\mathbf{w}^T\mathbf{x}) = sgn(w_0 + w_1\, x_1 + \ldots + w_k\, x_k)$

a linear discriminant function

Linear Discriminant Functions

- Use a linear function of the input vector:

$$h(\mathbf{x}) = \mathbf{w}^T \varphi(\mathbf{x}) + w_0$$

weight vector

bias = − threshold

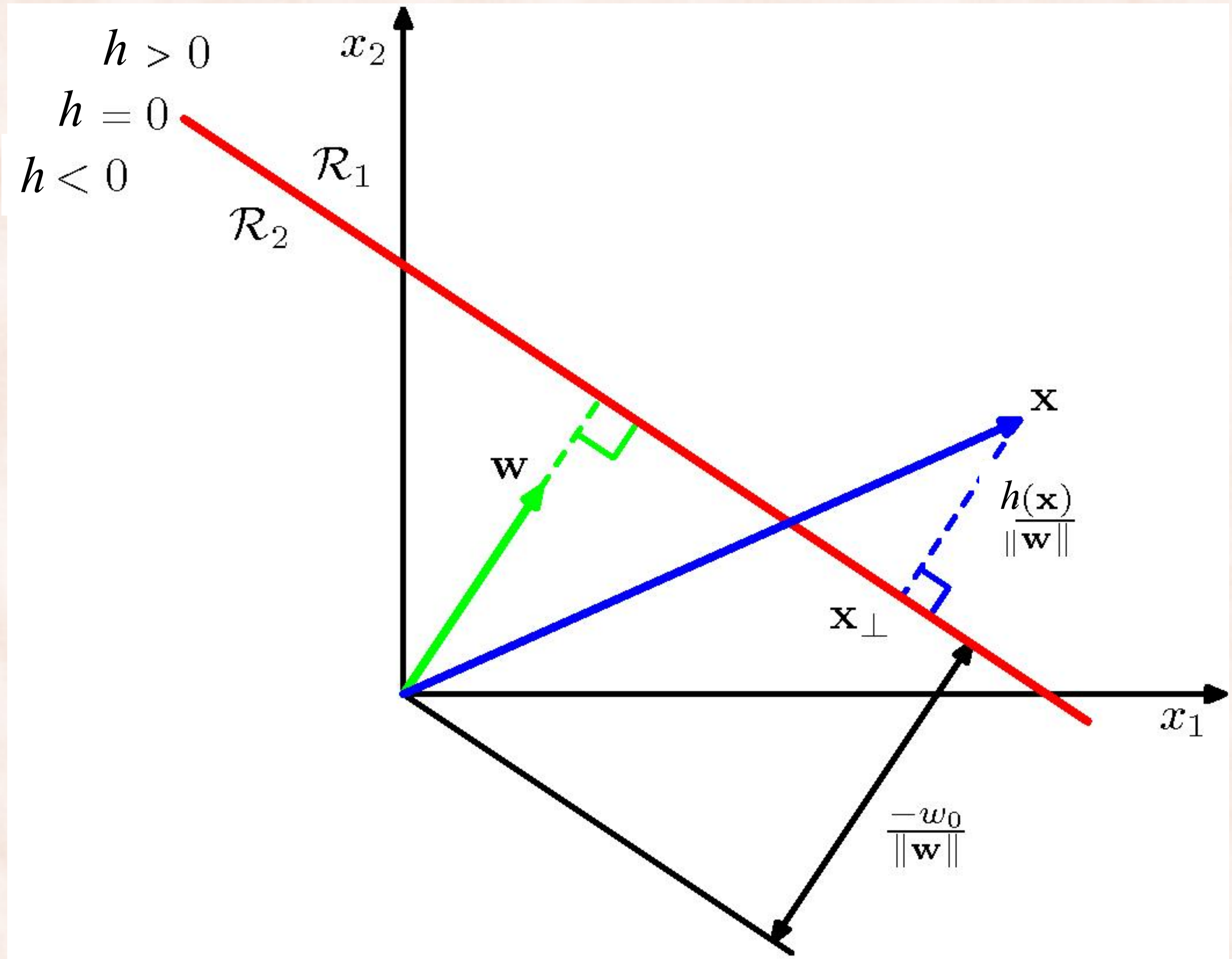
- Decision:

$\mathbf{x} \in C_1$ if $h(\mathbf{x}) \geq 0$, otherwise $\mathbf{x} \in C_2$.

$\Rightarrow$ decision boundary is hyperplane $h(\mathbf{x}) = 0$.

- Properties:
  - $\mathbf{w}$ is orthogonal to vectors lying within the decision surface.
  - w_0 controls the location of the decision hyperplane.

Geometric Interpretation



Linear Discriminant Functions: Two Classes (K = 2)

- What algorithms can be used to learn $y(\mathbf{x}) = \mathbf{w}^T\varphi(\mathbf{x}) + w_0$?

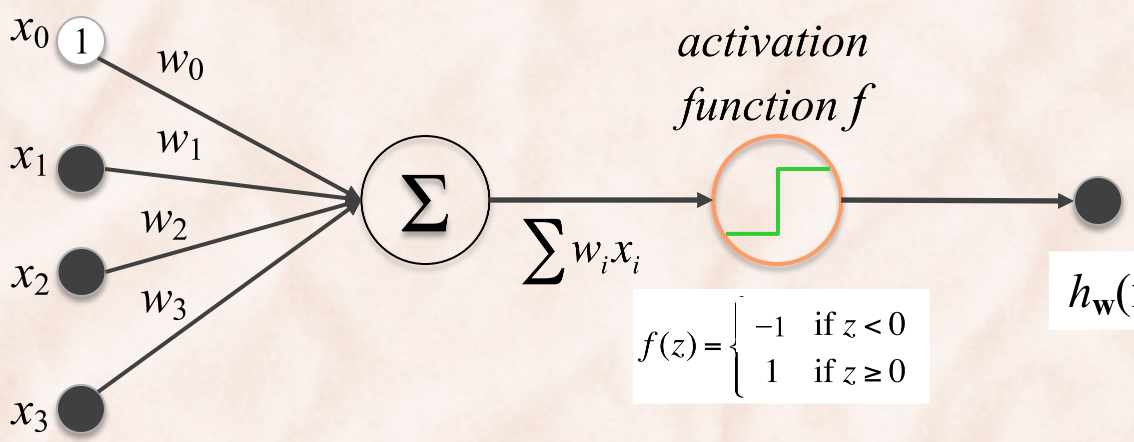
  Assume a training dataset of $N = N_1 + N_2$ examples in C_1 and C_2.

  – Perceptron:
    - Voted/Averaged Perceptron
    - Kernel Perceptron

  – Support Vector Machines:
    - Linear
    - Kernel

  – Fisher's Linear Discriminant

Perceptron



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- Assume classes $T = \{c_1, c_2\} = \{1, -1\}$.
- Training set is $(\mathbf{x}_1, t_1), (\mathbf{x}_2, t_2), \ldots (\mathbf{x}_n, t_n)$.

  $\mathbf{x} = [1, x_1, x_2, \ldots, x_k]^T$

  $h(\mathbf{x}) = sgn(\mathbf{w}^T\mathbf{x}) = sgn(w_0 + w_1 x_1 + \ldots + w_k x_k)$

a linear discriminant function

Perceptron Learning

- Learning = finding the "right" parameters $\mathbf{w}^T = [w_0, w_1, \ldots, w_k]$
  - Find $\mathbf{w}$ that minimizes an *error function* $E(\mathbf{w})$ which measures the misfit between $h(\mathbf{x}_n, \mathbf{w})$ and t_n.
  - Expect that $h(\mathbf{x},\mathbf{w})$ performing well on training examples $x_n \Rightarrow h(x,\mathbf{w})$ will perform well on arbitrary test examples $\mathbf{x} \in X$.

- **Least Squares** error function?

$$E(\mathbf{w}) = \frac{1}{2}\boxed{\sum_{n=1}^{N}\{h(\mathbf{x}_n,\mathbf{w}) - t_n\}^2}$$

2 x # of mistakes

Least Squares vs. Perceptron Criterion

- **Least Squares** => cost is # of misclassified patterns:
  - Piecewise constant function of $\mathbf{w}$ with discontinuities.
  - Cannot find closed form solution for $\mathbf{w}$ that minimizes cost.
  - Cannot use gradient methods (gradient zero almost everywhere).

- **Perceptron Criterion**:
  - Set labels to be +1 and − 1. Want $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n > 0$ for $t_n = 1$, and $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n < 0$ for $t_n = -1$.

    $\Rightarrow$ would like to have $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n t_n > 0$ for all patterns.

    $\Rightarrow$ want to minimize $-\mathbf{w}^{\mathrm{T}}\mathbf{x}_n t_n$ for all missclassified patterns M.

$$\boxed{\Rightarrow \text{minimize } E_p(\mathbf{w}) = -\sum_{n\in M} \mathbf{w}^T \mathbf{x}_n t_n}$$

Stochastic Gradient Descent

- **Perceptron Criterion**:

$$\boxed{\text{minimize } E_p(\mathbf{w}) = -\sum_{n \in M} \mathbf{w}^T \mathbf{x}_n t_n}$$

- Update parameters **w** sequentially **after each mistake**:

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_P(\mathbf{w}^{(\tau)}, \mathbf{x}_n)$$
$$= \mathbf{w}^{(\tau)} + \eta \mathbf{x}_n t_n$$

- The magnitude of **w** is inconsequential => set $\eta = 1$.

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \mathbf{x}_n t_n$$

The Perceptron Algorithm: Two Classes

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $n = 1 \ldots N$
3. $\boxed{h_n = sgn(\mathbf{w}^T \mathbf{x}_n)}$
4. $\boxed{\textbf{if } h_n \neq t_n \textbf{ then}}$
5. $\mathbf{w} = \mathbf{w} + t_n \mathbf{x}_n$

$$sgn(z) = \begin{cases} +1 & \text{if } z > 0, \\ 0 & \text{if } z = 0, \\ -1 & \text{if } z < 0 \end{cases}$$

Repeat:
a) until convergence.
b) for a number of epochs E.

Theorem [Rosenblatt, 1962]:

If the training dataset is linearly separable, the perceptron learning algorithm is guaranteed to find a solution in a finite number of steps.

- see Theorem 1 (Block, Novikoff) in [Freund & Schapire, 1999].

The Perceptron Algorithm: Two Classes

$$sgn(z) = \begin{cases} +1 & \text{if } z > 0, \\ 0 & \text{if } z = 0, \\ -1 & \text{if } z < 0 \end{cases}$$

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $n = 1 \ldots \mathrm{N}$
3. $h_n = \mathbf{w}^{\mathrm{T}}\mathbf{x}_n$
4. **if** $h_{\mathrm{n}} t_n \leq 0$ **then**
5. $\mathbf{w} = \mathbf{w} + t_n \mathbf{x}_n$

Repeat:
a) until convergence.
b) for a number of epochs E.

Theorem [Rosenblatt, 1962]:

If the training dataset is linearly separable, the perceptron learning algorithm is guaranteed to find a solution in a finite number of steps.

- see Theorem 1 (Block, Novikoff) in [Freund & Schapire, 1999].

The Perceptron Algorithm: Two Classes

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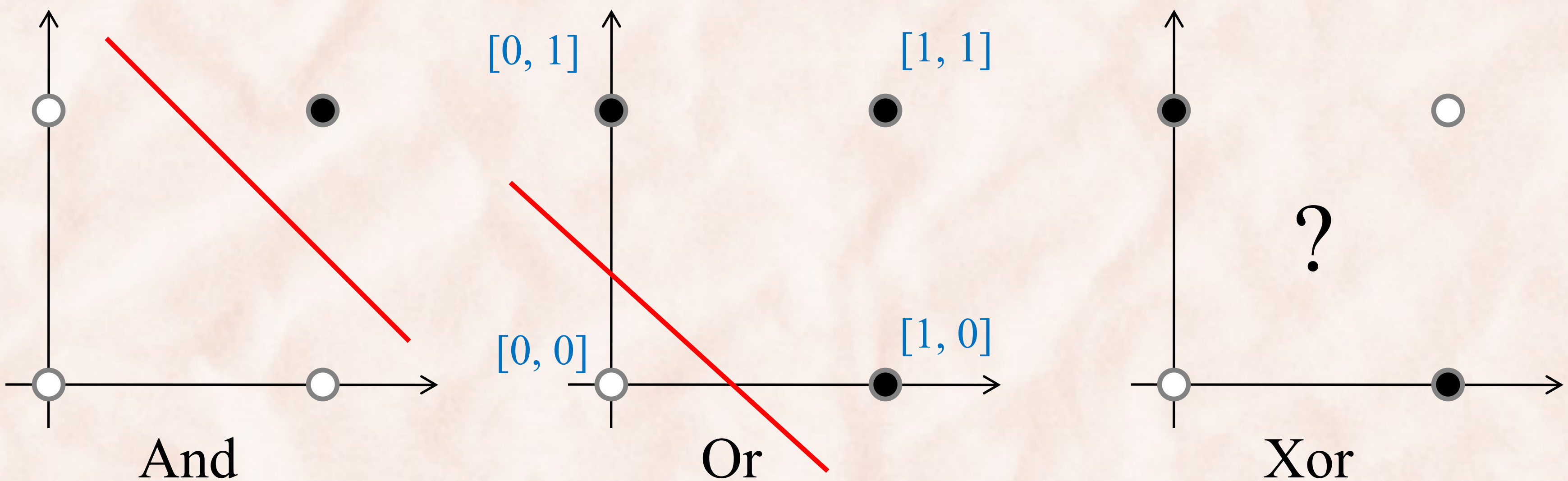
2. **for** $n = 1 \ldots N$
3. $\quad h_n = \mathbf{w}^T \mathbf{x}_n$
4. $\quad$ **if** $h_n \geq 0$ and $t_n = -1$
5. $\quad\quad \mathbf{w} = \mathbf{w} - \mathbf{x}_n$
6. $\quad$ **if** $h_n \leq 0$ and $t_n = +1$
7. $\quad\quad \mathbf{w} = \mathbf{w} + \mathbf{x}_n$

Repeat:
a) until convergence.
b) for a number of epochs E.

What is the impact of the perceptron update on the score $\mathbf{w}^T \mathbf{x}_n$ of the misclassified example $\mathbf{x}_n$?

Linear vs. Non-linear Decision Boundaries



$$\left.\begin{aligned}\varphi(\mathbf{x}) &= [1, x_1, x_2]^T \\ \mathbf{w} &= [w_0, w_1, w_2]^T\end{aligned}\right\} \Rightarrow \mathbf{w}^T\varphi(\mathbf{x}) = [w_1, w_2]^T[x_1, x_2] + w_0$$

How to Find Non-linear Decision Boundaries

1) Perceptron with manually engineered features:
   – Quadratic features.

2) Kernel methods (e.g. SVMs) with non-linear kernels:
   – Quadratic kernels, Gaussian kernels.

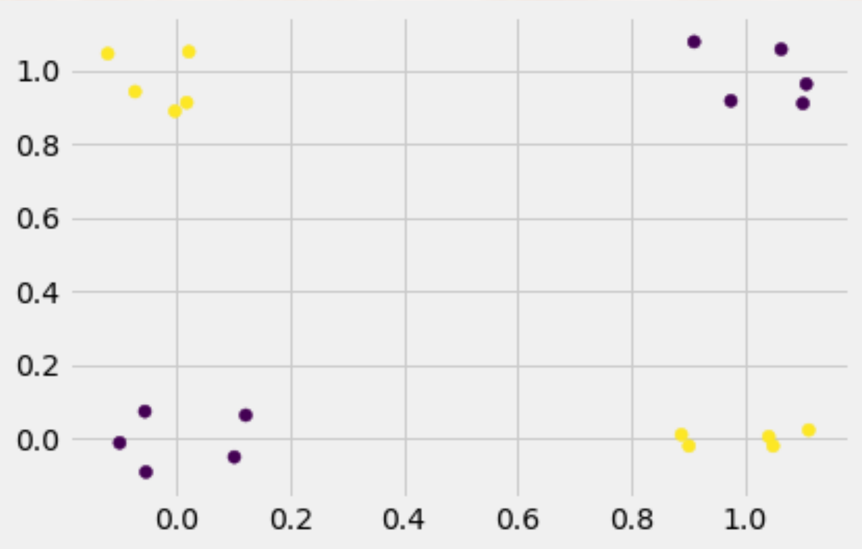
Deep Learning class

3) Unsupervised feature learning (e.g. auto-encoders):
   – Plug learned features in any linear classifier.

4) Neural Networks with one or more hidden layers:
   – Automatically learned features.

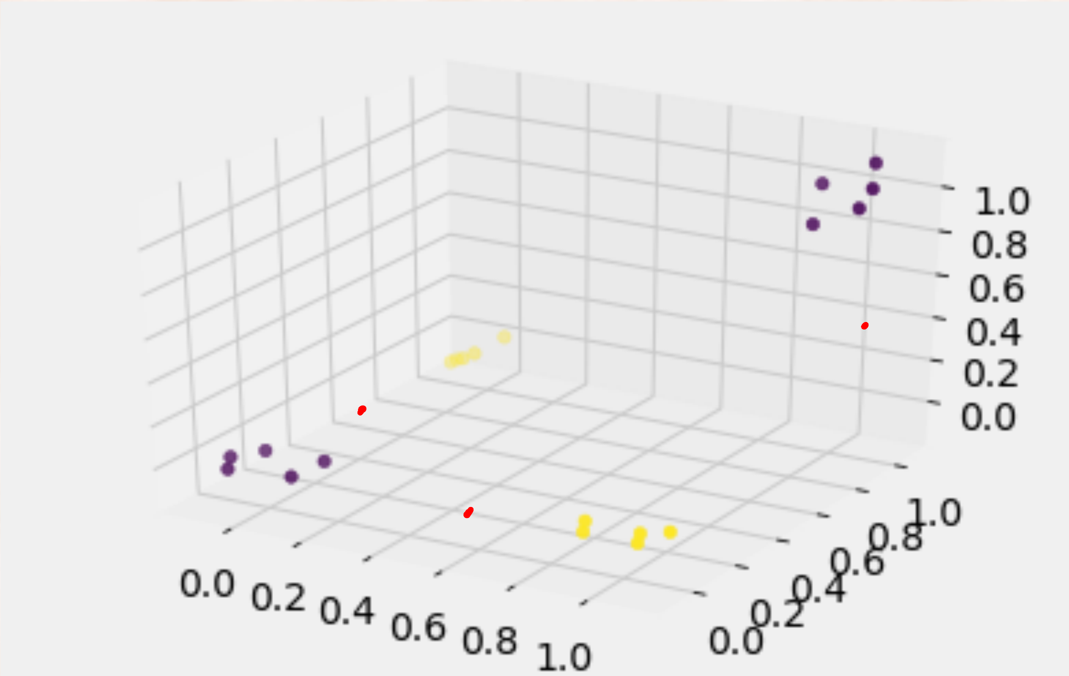
Non-Linear Classification: XOR Dataset

$$\mathbf{x} = [x_1, x_2]$$



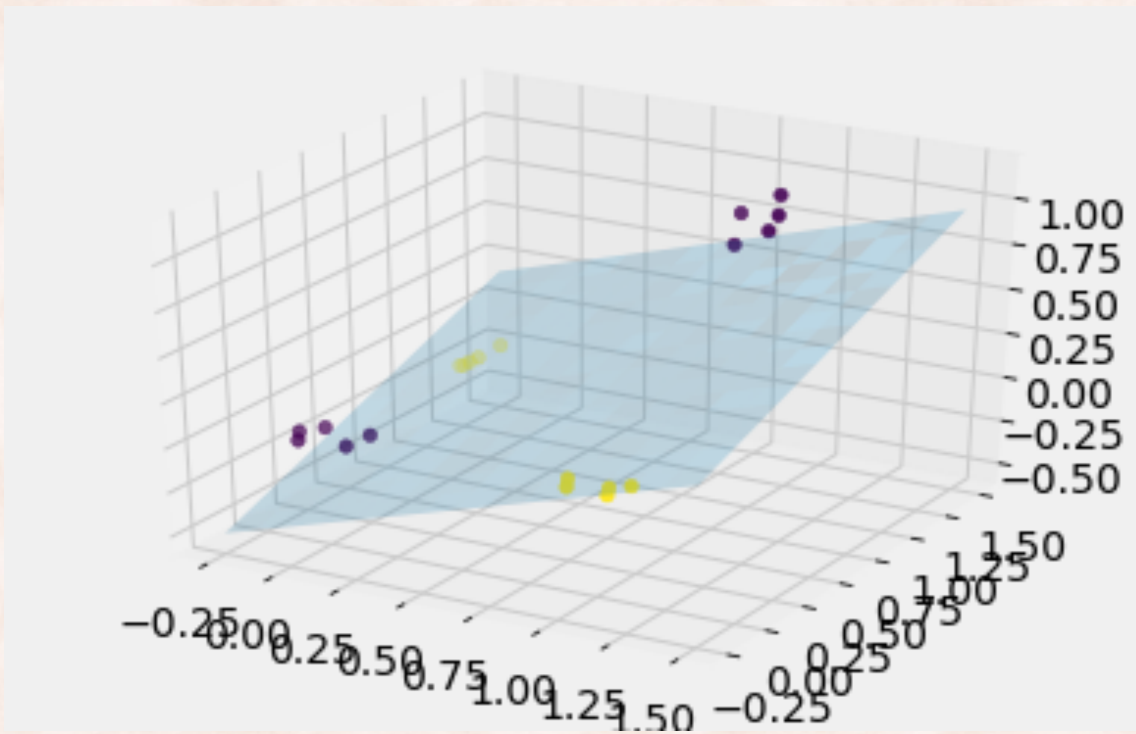
1) Manually Engineered Features: Add $x_1 x_2$

$$\mathbf{x} = [x_1, x_2, x_1 x_2]$$



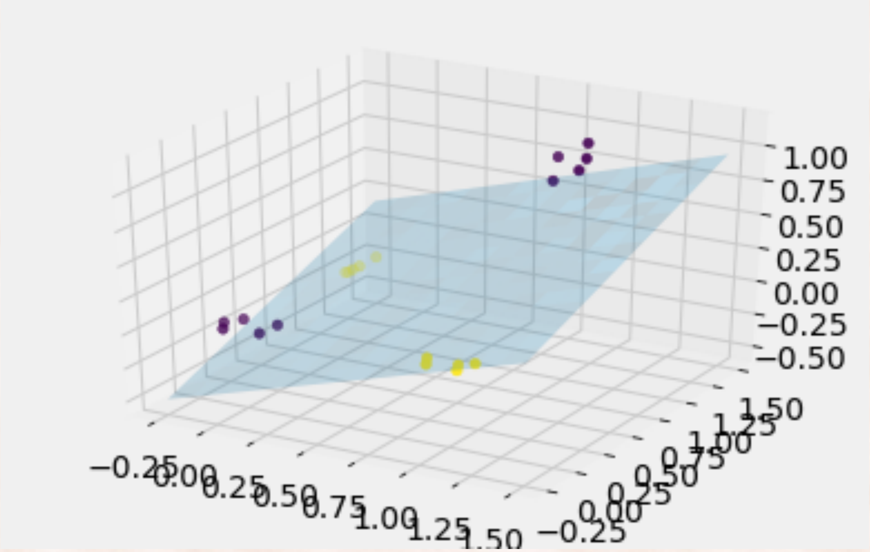
Logistic Regression with Manually Engineered Features

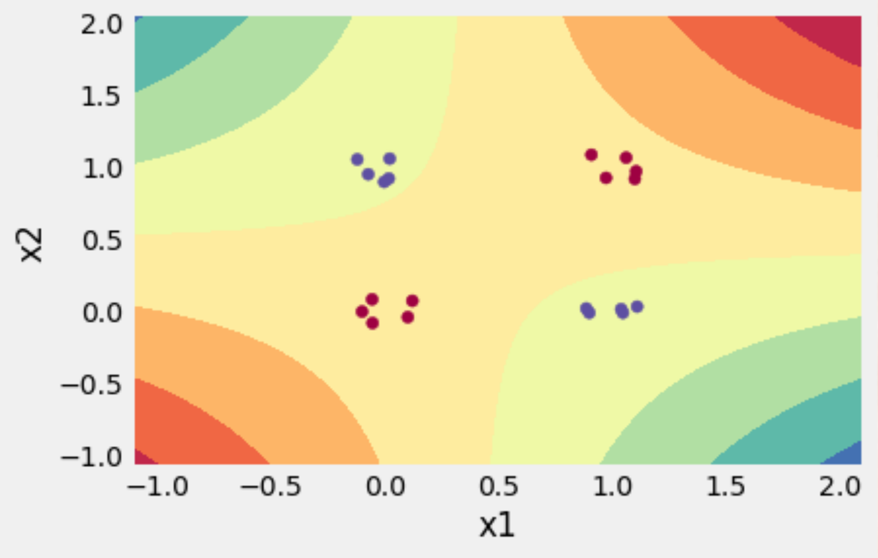
$$\mathbf{x} = [x_1, x_2, x_1 x_2]$$



Perceptron with Manually Engineered Features

Project $\mathbf{x} = [x_1, x_2, x_1x_2]$ and decision hyperplane back to $\mathbf{x} = [x_1, x_2]$





Averaged Perceptron: Two Classes

initialize parameters $\mathbf{w} = 0$, $\tau = 1$, $\overline{\mathbf{w}} = 0$

for $n = 1 \ldots \mathrm{N}$

  $h_n = sgn(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n)$

  if $h_n \neq t_n$ **then**

    $\mathbf{w} = \mathbf{w} + t_n\mathbf{x}_n$

  $\overline{\mathbf{w}} = \overline{\mathbf{w}} + \mathbf{w}$

  $\tau = \tau + 1$

return $\overline{\mathbf{w}} / \tau$

$$sgn(z) = \begin{cases} +1 & \text{if } z > 0, \\ 0 & \text{if } z = 0, \\ -1 & \text{if } z < 0 \end{cases}$$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing: $\mathrm{h}(\mathbf{x}) = sgn(\overline{\mathbf{w}}^T\mathbf{x})$

2) Kernel Methods with Non-Linear Kernels

- Perceptrons, SVMs can be '*kernelized*':
  1. Re-write the algorithm such that during training and testing feature vectors $\mathbf{x}$, $\mathbf{y}$ appear only in dot-products $\mathbf{x}^T\mathbf{y}$.
  2. Replace dot-products $\mathbf{x}^T\mathbf{y}$ with *non-linear kernels* $K(\mathbf{x}, \mathbf{y})$:
     - K is a kernel if and only if $\exists\varphi$ such that $K(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x})^T \varphi(\mathbf{y})$
       - φ can be in a much higher dimensional space.
         - » e.g. combinations of up to k original features
       - $\varphi(\mathbf{x})^T \varphi(\mathbf{y})$ can be computed efficiently without enumerating $\varphi(\mathbf{x})$ or $\varphi(\mathbf{y})$.

The Perceptron Algorithm: Two Classes

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $n = 1 \ldots \mathrm{N}$
3. $\quad h_n = sgn(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n)$
4. $\quad$ **if** $h_n \neq t_n$ **then**
5. $\qquad \mathbf{w} = \mathbf{w} + t_n\mathbf{x}_{\mathrm{n}}$

Repeat:

a) until convergence.

b) for a number of epochs E.

Loop invariant: **w** is a weighted sum of training vectors:

$$\mathbf{w} = \sum_{n=1..N} \alpha_n t_n \mathbf{x}_n \Rightarrow \mathbf{w}^T\mathbf{x} = \sum_{n=1..N} \alpha_n t_n \mathbf{x}_n^T \mathbf{x}$$

Kernel Perceptron: Two Classes

1. **define** $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_{j=1..N} \alpha_j t_j \mathbf{x}_j^T \mathbf{x} = \sum_{j=1..N} \alpha_j t_j K(\mathbf{x}_j, \mathbf{x})$
2. **initialize** dual parameters $\alpha_n = 0$
3. **for** $n = 1 \ldots N$
4. $\quad h_n = sgn\, f(\mathbf{x}_n)$
5. $\quad$ **if** $h_n \neq t_n$ **then**
6. $\quad\quad \alpha_n = \alpha_n + 1$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing: $h(\mathbf{x}) = sgn\, f(\mathbf{x})$

Kernel Perceptron: Two Classes

1. **define** $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_{j=1..N} \alpha_j t_j \mathbf{x}_j^T \mathbf{x} = \sum_{j=1..N} \alpha_j t_j K(\mathbf{x}_j, \mathbf{x})$
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6. $\quad\quad \alpha_n = \alpha_n + 1$

Repeat:
a) until convergence.
b) for a number of epochs E.

Let $S = \{j | \alpha_j \neq 0\}$ be the set of *support vectors*. Then $f(\mathbf{x}) = \sum_{j \in S} \alpha_j t_j K(\mathbf{x}_j, \mathbf{x})$

During testing: $h(\mathbf{x}) = sgn\, f(\mathbf{x})$

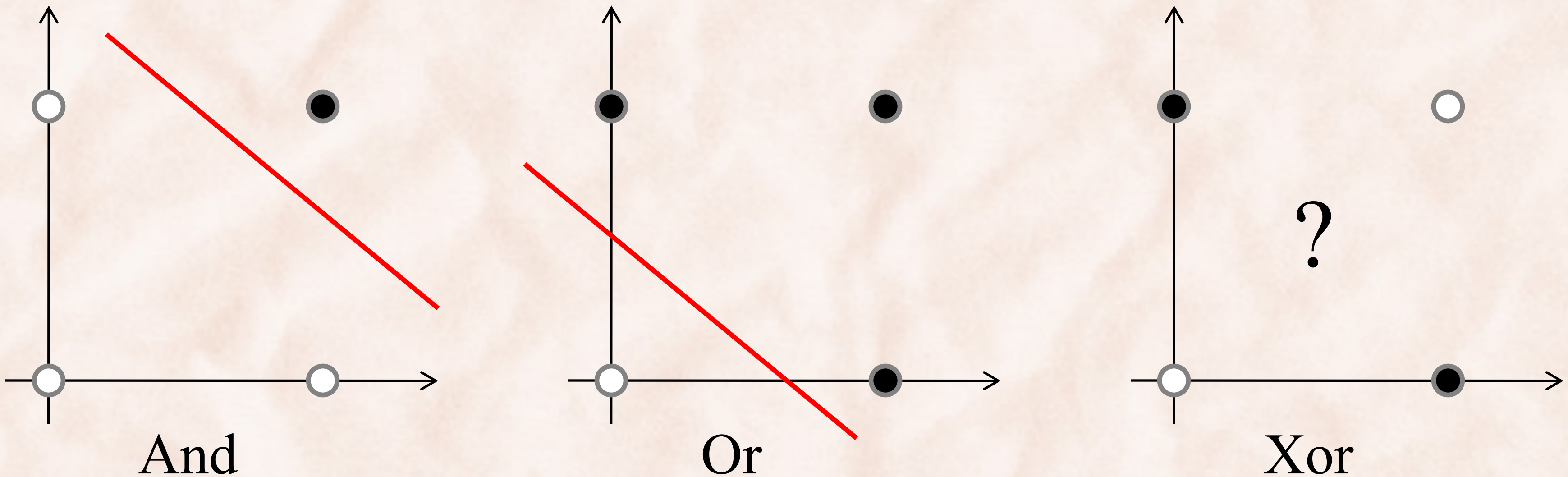
Kernel Perceptron: Equivalent Formulation

1. **define** $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_j \alpha_j \mathbf{x}_j^T \mathbf{x} = \sum_j \alpha_j K(\mathbf{x}_j, \mathbf{x})$
2. **initialize** dual parameters $\alpha_n = 0$
3. **for** $n = 1 \ldots \mathrm{N}$
4. $\quad h_n = sgn\, f(\mathbf{x}_n)$
5. $\quad$ **if** $h_n \neq t_n$ **then**
6. $\qquad \alpha_n = \alpha_n + t_n$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing: $h(\mathbf{x}) = sgn\, f(\mathbf{x})$

The Perceptron vs. Boolean Functions



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Perceptron with Quadratic Kernel

- Discriminant function:

$$f(\mathbf{x}) = \sum_i \alpha_i t_i \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}) = \sum_i \alpha_i t_i K(\mathbf{x}_i, \mathbf{x})$$

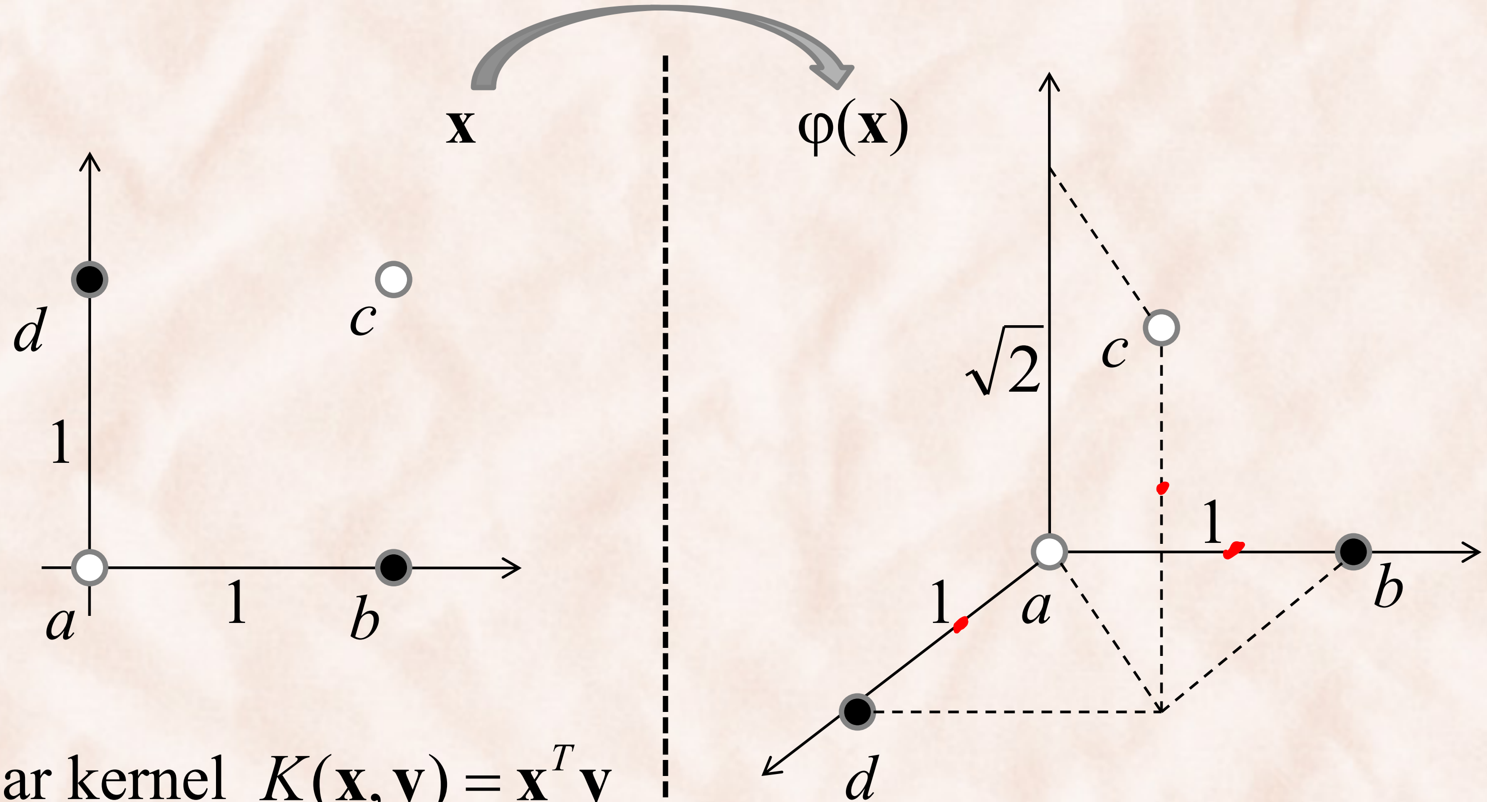
- Quadratic kernel:

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T \mathbf{y})^2 = (x_1 y_1 + x_2 y_2)^2$$

$\Rightarrow$ corresponding feature space $\varphi(\mathbf{x}) = ?$

conjunctions of two atomic features

Perceptron with Quadratic Kernel



Linear kernel $K(\mathbf{x},\mathbf{y}) = \mathbf{x}^T\mathbf{y}$

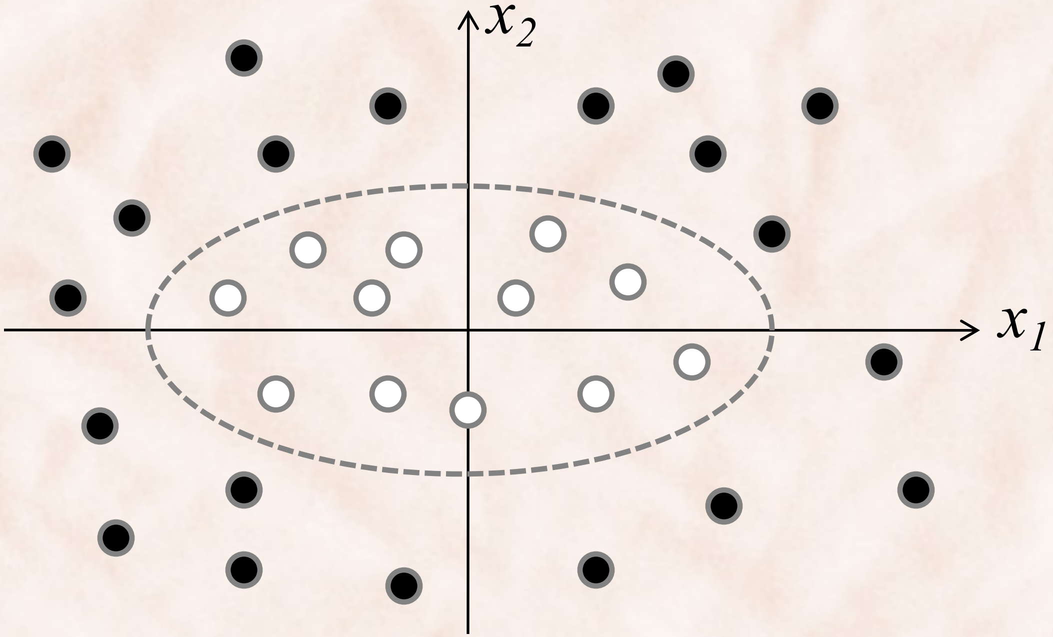
Quadratic kernel $K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y})^2$

Quadratic Kernels

- Circles, hyperbolas, and ellipses as separating surfaces:

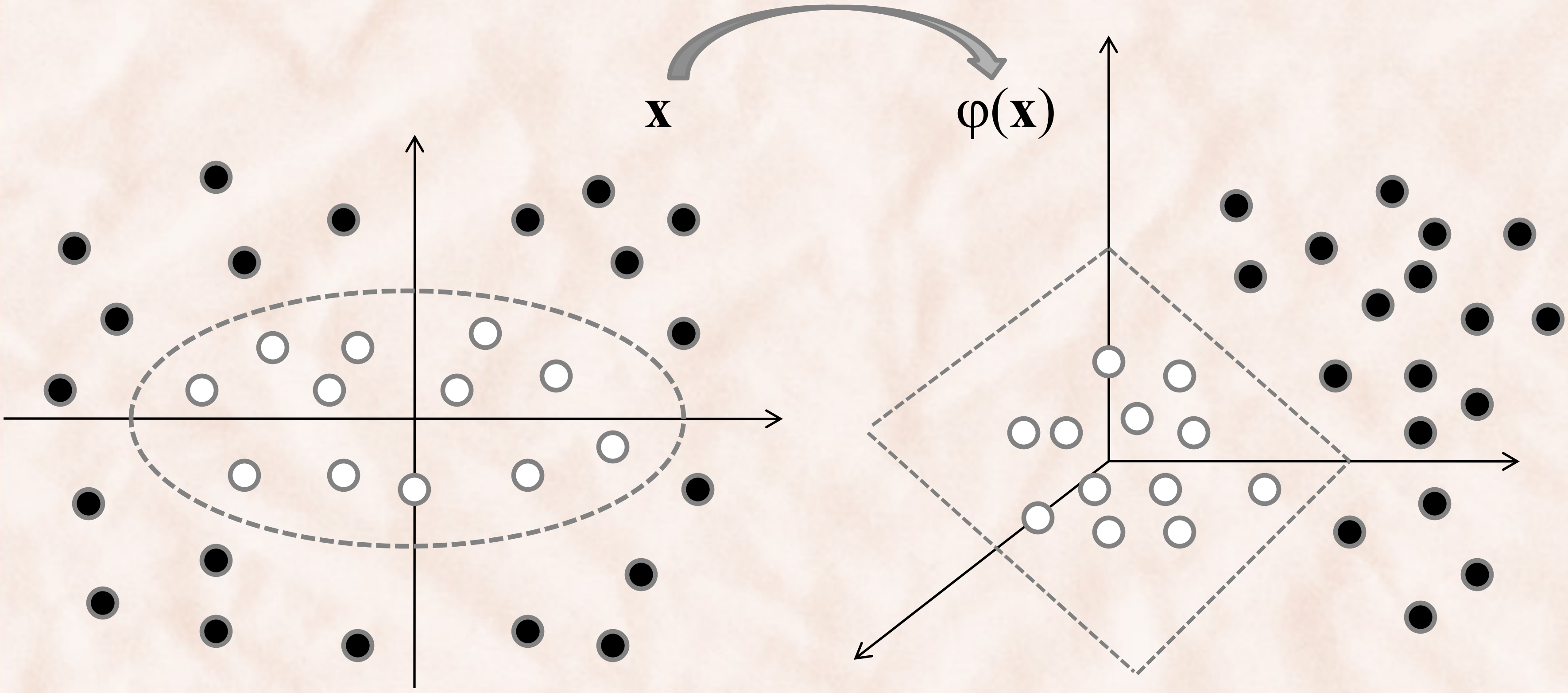
$$K(\mathbf{x},\mathbf{y}) = (1+\mathbf{x}^T\mathbf{y})^2 = \varphi(x)^T\varphi(y)$$

$$\varphi(x) = [1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2]^T$$



Quadratic Kernels

$$K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y})^2 = \varphi(\mathbf{x})^T\varphi(\mathbf{y})$$



Explicit Features vs. Kernels

- Explicitly enumerating features can be prohibitive:
  - 1,000 basic features for $\mathbf{x}^T\mathbf{y}$ => 500,500 quadratic features for $(\mathbf{x}^T\mathbf{y})^2$
  - Much worse for higher order features.

- Solution:
  - Do not compute the feature vectors, compute kernels instead (i.e. compute dot products between implicit feature vectors).
    - $(\mathbf{x}^T\mathbf{y})^2$ takes 1001 multiplications.
    - $\varphi(\mathbf{x})^T \varphi(\mathbf{y})$ in feature space takes 500,500 multiplications.

Kernel Functions

- Definition:

  A function $k : X \times X \rightarrow R$ is a kernel function if there exists a feature mapping $\varphi : X \rightarrow R^n$ such that:

  $$k(\mathbf{x},\mathbf{y}) = \varphi(\mathbf{x})^T \varphi(\mathbf{y})$$

- Theorem:

  $k : X \times X \rightarrow R$ is a valid kernel $\Leftrightarrow$ the Gram matrix K whose elements are given by $k(\mathbf{x}_n,\mathbf{x}_m)$ is *positive semidefinite* for all possible choices of the set $\{\mathbf{x}_n\}$.

Kernel Examples

- Linear kernel: $K(\mathbf{x},\mathbf{y}) = \mathbf{x}^T\mathbf{y}$
- Quadratic kernel: $K(\mathbf{x},\mathbf{y}) = (c + \mathbf{x}^T\mathbf{y})^2$
  - contains constant, linear terms and terms of order two (c > 0).
- Polynomial kernel: $K(\mathbf{x},\mathbf{y}) = (c + \mathbf{x}^T\mathbf{y})^M$
  - contains all terms up to degree M (c > 0).
- Gaussian kernel: $K(\mathbf{x},\mathbf{y}) = \exp(-\|\mathbf{x}-\mathbf{y}\|^2 / 2\sigma^2)$
  - corresponding feature space has infinite dimensionality.

Techniques for Constructing Kernels

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

$$k(\mathbf{x}, \mathbf{x}') = ck_1(\mathbf{x}, \mathbf{x}') \tag{6.13}$$

$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}') \tag{6.14}$$

$$k(\mathbf{x}, \mathbf{x}') = q\left(k_1(\mathbf{x}, \mathbf{x}')\right) \tag{6.15}$$

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) \tag{6.16}$$

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') \tag{6.17}$$

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') \tag{6.18}$$

$$k(\mathbf{x}, \mathbf{x}') = k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) \tag{6.19}$$

$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}' \tag{6.20}$$

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}_a') + k_b(\mathbf{x}_b, \mathbf{x}_b') \tag{6.21}$$

$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}_a')k_b(\mathbf{x}_b, \mathbf{x}_b') \tag{6.22}$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

Kernels over Discrete Structures

- Subsequence Kernels [Lodhi et al., JMLR 2002]:
  - Σ is a finite alphabet (set of symbols).
  - $\mathbf{x},\mathbf{y} \in \Sigma^*$ are two sequences of symbols with lengths $|\mathbf{x}|$ and $|\mathbf{y}|$
  - $k(\mathbf{x},\mathbf{y})$ is defined as the number of common substrings of length n.
  - $k(\mathbf{x},\mathbf{y})$ can be computed in $O(n|\mathbf{x}||\mathbf{y}|)$ time complexity.

- Tree Kernels [Collins and Duffy, NIPS 2001]:
  - T_1 and T_2 are two trees with N_1 and N_2 nodes respectively.
  - $k(T_1, T_2)$ is defined as the number of common subtrees.
  - $k(T_1, T_2)$ can be computed in $O(N_1 N_2)$ time complexity.
  - in practice, time is linear in the size of the trees.

Supplementary Reading

- PRML Chapter 6:
  - Section 6.1 on dual representations for linear regression models.
  - Section 6.2 on techniques for constructing new kernels.

Linear Discriminant Functions: Multiple Classes (K > 2)

1) Train K or K–1 *one-versus-the-rest* classifiers.
2) Train K(K–1)/2 *one-versus-one* classifiers.

3) Train K linear functions:

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \varphi(\mathbf{x}) + w_{k0}$$

- Decision:

  $\mathbf{x} \in C_k$ if $y_k(\mathbf{x}) > y_j(\mathbf{x})$, for all $j \neq k$.

  $\Rightarrow$ decision boundary between classes C_k and C_j is hyperplane defined by $y_k(\mathbf{x}) = y_j(\mathbf{x})$ i.e. $(\mathbf{w}_k - \mathbf{w}_j)^T \varphi(\mathbf{x}) + (w_{k0} - w_{j0}) = 0$

  $\Rightarrow$ same geometrical properties as in binary case.

Linear Discriminant Functions: Multiple Classes (K > 2)

4) More general ranking approach:

$$y(\mathbf{x}) = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}, t) \quad \text{where} \quad T = \{c_1, c_2 \ldots, c_K\}$$

- It subsumes the approach with K separate linear functions.

- Useful when T is very large (e.g. exponential in the size of input **x**), assuming inference can be done efficiently.

The Perceptron Algorithm: K classes

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $i = 1 \ldots n$
3. $\quad y_\mathrm{i} = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}_i, t)$
4. $\quad$ **if** $y_\mathrm{i} \neq t_i$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + \varphi(\mathbf{x}_\mathrm{i}, t_i) - \varphi(\mathbf{x}_\mathrm{i}, y_\mathrm{i})$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing:

$$t^* = \arg\max_{t \in T} \mathbf{w}^T \phi(\mathbf{x}, t)$$

Averaged Perceptron: K classes

1. **initialize** parameters $\mathbf{w} = 0$, $\tau = 1$, $\overline{\mathbf{w}} = 0$
2. **for** $i = 1 \ldots n$
3. $\quad y_i = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}_i, t)$
4. $\quad$ **if** $y_i \neq t_i$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + \varphi(\mathbf{x}_i, t_i) - \varphi(\mathbf{x}_i, y_i)$
6. $\quad \overline{\mathbf{w}} = \overline{\mathbf{w}} + \mathbf{w}$
7. $\quad \tau = \tau + 1$
8. **return** $\overline{\mathbf{w}} / \tau$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing: $t^* = \arg\max_{t \in T} \overline{\mathbf{w}}^T \varphi(\mathbf{x}, t)$

The Perceptron Algorithm: K classes

1. **initialize** parameters $\mathbf{w} = 0$
2. **for** $i = 1 \ldots n$
3. $\quad c_j = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}_i, t)$
4. $\quad$ **if** $c_j \neq t_i$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + \varphi(\mathbf{x}_i, t_i) - \varphi(\mathbf{x}_i, c_j)$

Repeat:
a) until convergence.
b) for a number of epochs E.

Loop invariant: **w** is a weighted sum of training vectors:

$$\mathbf{w} = \sum_{i,j} \alpha_{ij} (\phi(\mathbf{x}_i, t_i) - \phi(\mathbf{x}_i, c_j))$$

$$\Rightarrow \quad \mathbf{w}^T \phi(\mathbf{x}, t) = \sum_{i,j} \alpha_{ij} (\phi(\mathbf{x}_i, t_i)^T \phi(\mathbf{x}, t) - \phi(\mathbf{x}_i, c_j)^T \phi(\mathbf{x}, t))$$

Kernel Perceptron: K classes

1. **define** $f(\mathbf{x},t) = \sum_{i,j} \alpha_{ij} (\phi(\mathbf{x}_i, t_i)^T \phi(\mathbf{x},t) - \phi(\mathbf{x}_i, c_j)^T \phi(\mathbf{x},t))$
2. **initialize** dual parameters $\alpha_{ij} = 0$
3. **for** $i = 1 \dots n$
4. $\quad c_j = \arg\max_{t \in T} f(\mathbf{x}_i, t)$
5. $\quad$ **if** $y_i \neq t_i$ **then**
6. $\quad\quad \alpha_{ij} = \alpha_{ij} + 1$

Repeat:
a) until convergence.
b) for a number of epochs E.

During testing:

$$t^* = \arg\max_{t \in T} f(\mathbf{x}, t)$$

Kernel Perceptron: K classes

- Discriminant function:

$$f(\mathbf{x},t) = \sum_{i,j} \alpha_{i,j} (\phi(\mathbf{x}_i,\, t_i)^T \phi(\mathbf{x},t) - \phi(\mathbf{x}_i,c_j)^T \phi(\mathbf{x},t))$$

$$= \sum_{i,j} \alpha_{ij} (K(\mathbf{x}_i,\, t_i,\mathbf{x},t) - K(\mathbf{x}_i,c_j,\mathbf{x},t))$$

where:

$$K(\mathbf{x}_i,t_i,\mathbf{x},t) = \varphi^T(\mathbf{x}_i,t_i)\varphi(\mathbf{x},t)$$

$$K(\mathbf{x}_i,y_i,\mathbf{x},t) = \phi^T(\mathbf{x}_i,y_i)\phi(\mathbf{x},t)$$