ITCS 5356: Intro to Machine Learning

The Average Perceptron

The Kernel Trick

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Linear Discriminant Functions: Two classes (K = 2)

- Use a linear function of the input vector:

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

weight vector

bias = – threshold

- Decision:

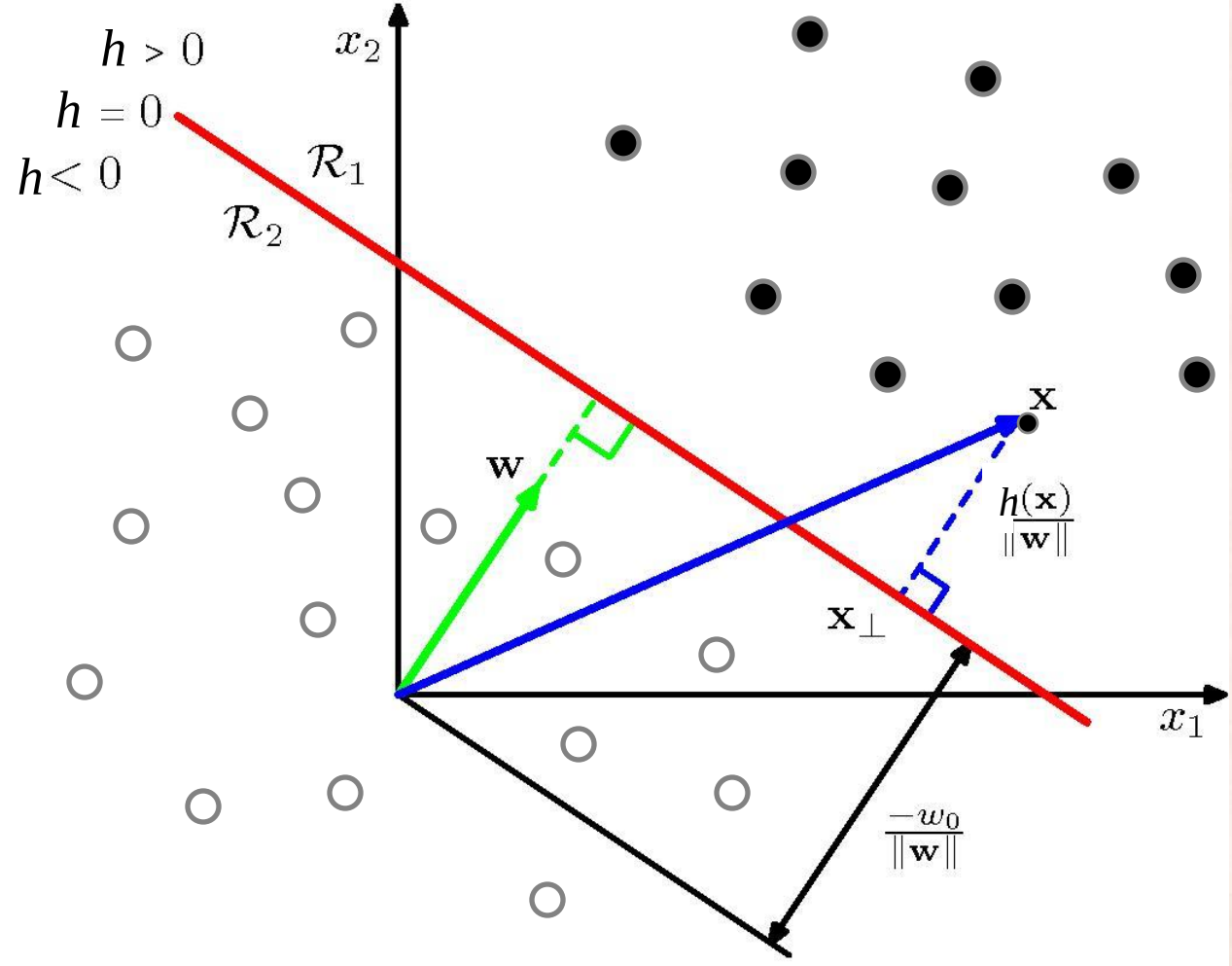
  $\mathbf{x} \in C_1$ if $h(\mathbf{x}) \geq 0$, otherwise $\mathbf{x} \in C_2$.

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

- Properties:
  - **w** is orthogonal to vectors lying within the decision surface.
  - w_0 controls the location of the decision hyperplane.

Geometric Interpretation

$$h(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 = w_1x_1 + w_2x_2 + w_0$$



Linear Models for Classification

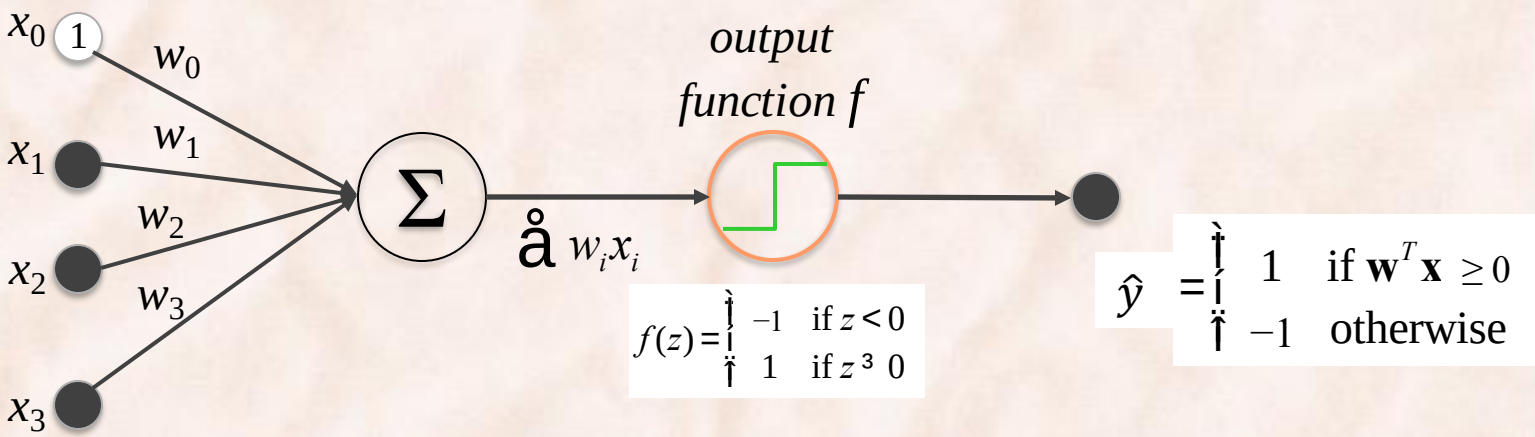
- We want to use a linear function of the feature vector:

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

- How to find **w** automatically? Use ML!
  - **Perceptron**.
  - **Logistic Regression**.

- What if the data is not linearly separable? Make it!
  - Engineer new features (LR) or use kernels (Perceptron).
  - Learn new features (**Neural Networks**).

Linear Discriminant Classification



- Assume classes T = $\{c_1, c_2\} = \{1, -1\}$.
- Training set is $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots (\mathbf{x}_n, y_n)$.

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

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

a linear discriminant function

Linear Discriminant Classification: Objective Function

- 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 $\hat{t}(\mathbf{x}_n)$ and t_n.

- **Least Squares** error function?

$$J(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}(\hat{y}_n - y_n)^2$$

$$\hat{y} = \begin{cases} 1 & \text{if } \mathbf{w}^T\mathbf{x} \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

4 times # of mistakes

Least Squares vs. Perceptron Criterion

- **Least Squares** => cost is # of misclassified patterns:
  - Piecewise constant function of **w** with discontinuities.
  - Cannot find closed form solution for **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 $y_n = 1$, and $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n < 0$ for $y_n = -1$.
    - $\Rightarrow$ would like to have $\mathbf{w}^{\mathrm{T}}\mathbf{x}_n y_n > 0$ for all patterns.
    - $\Rightarrow$ want to minimize $-\mathbf{w}^{\mathrm{T}}\mathbf{x}_n y_n$ for all missclassified patterns M.

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

Stochastic Gradient Descent

- **Perceptron Criterion**:

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

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

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

$$= \mathbf{w}^{(\tau)} + \eta \mathbf{x}_n y_n$$

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

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

Prove it.

The Perceptron Algorithm: Two Classes

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

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 $\mathbf{x}_n$?

The Perceptron Algorithm: Two Classes

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

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

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

$$\mathbf{w} = \sum_n \alpha_n y_n \mathbf{x}_n \quad \Rightarrow \quad \mathbf{w}^T \mathbf{x} = \sum_n \alpha_n y_n \mathbf{x}_n^T \mathbf{x}$$

The Perceptron Algorithm: Two Classes

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

$sgn(h) = +1$ if $h > 0$,
0 if $h = 0$,
-1 if $h < 0$

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

initialize parameters $\mathbf{w} = 0$

for epoch $e = 1 \ldots E$

  mistakes = 0

  for example $n = 1 \ldots N$

    $\hat{y}_n = sgn(\mathbf{w}^T\mathbf{x}_n)$

    if $\hat{y}_n \neq y_n$ **then**

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

      mistakes = mistakes + 1

  if mistakes = 0

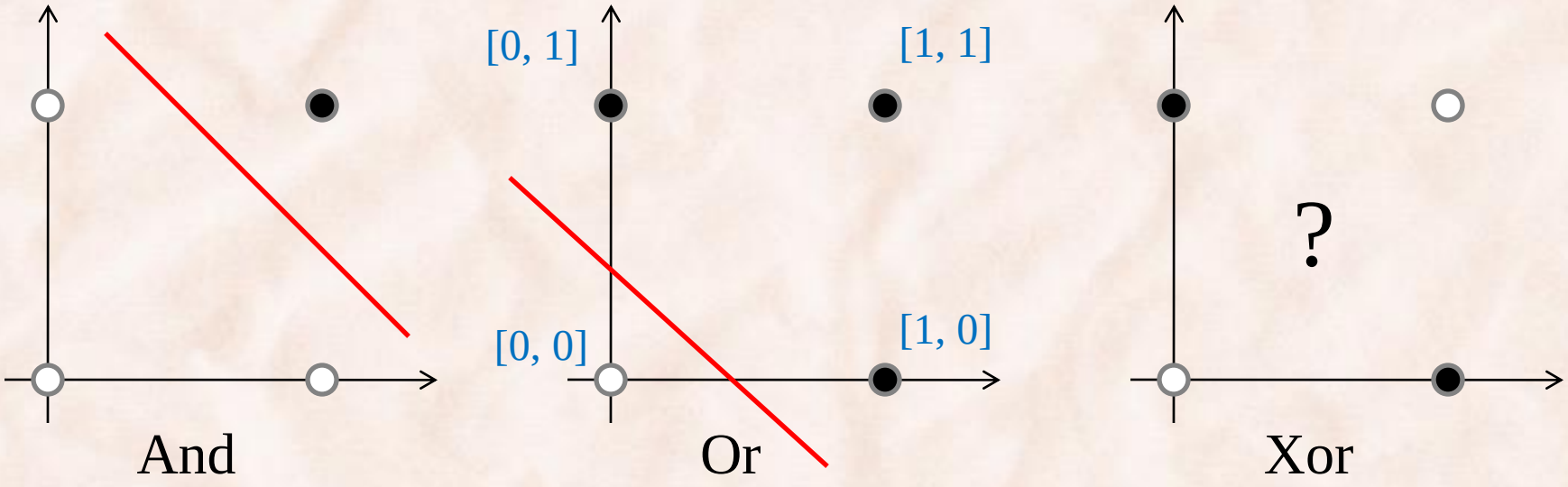
    break

Converged!

$sgn(h) = +1$ if $h > 0$,
0 if $h = 0$,
-1 if $h < 0$

1 epoch = one pass over all training examples.

Linear vs. Non-linear Decision Boundaries



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

How to Find Non-linear Decision Boundaries

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

2) **Kernel methods with non-linear kernels**:
   - Quadratic kernels, Gaussian kernels.

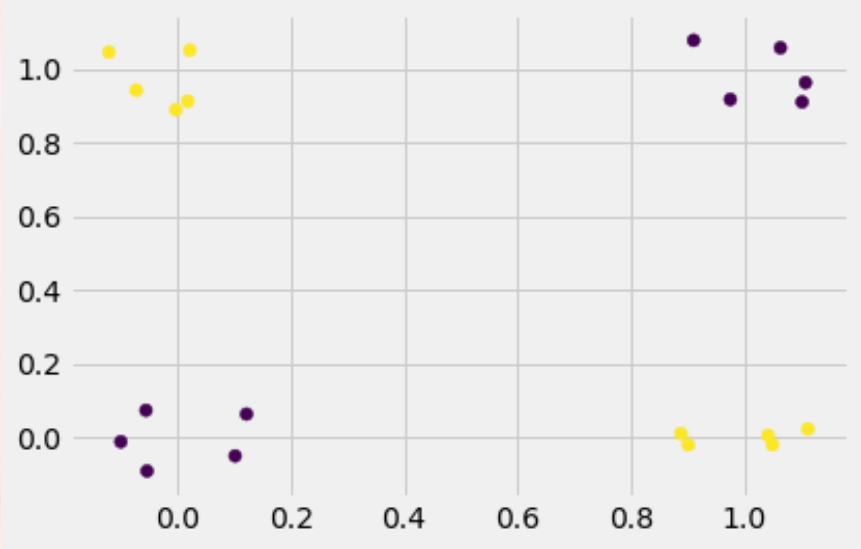
Deep Learning

3) Self-supervised 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.

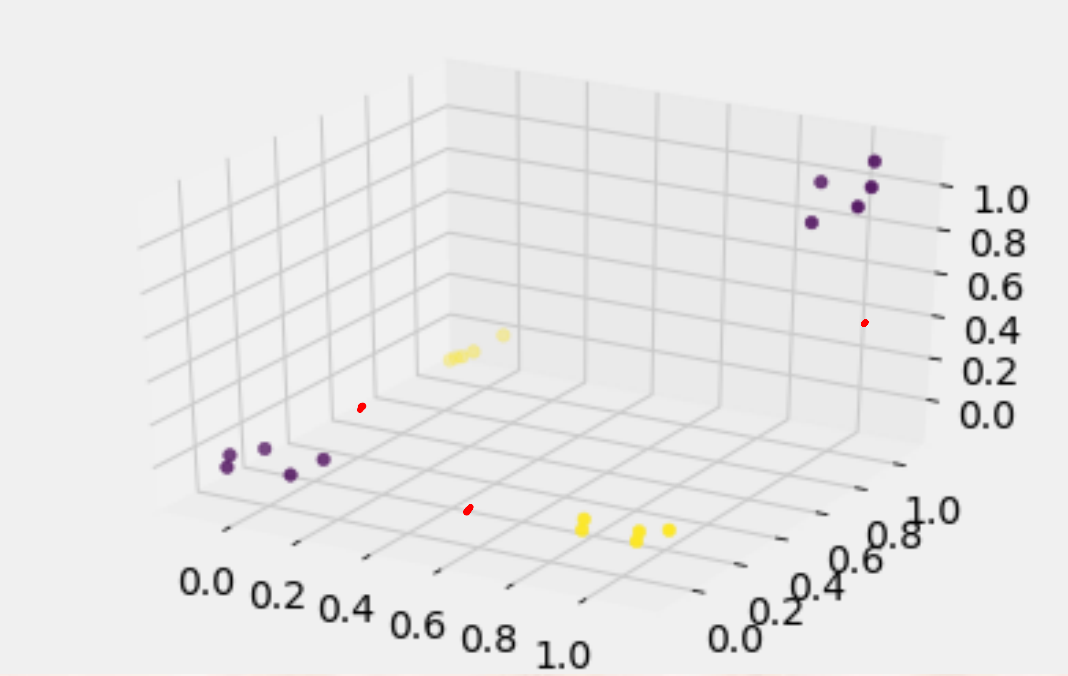
Non-Linear Classification: XOR Dataset

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



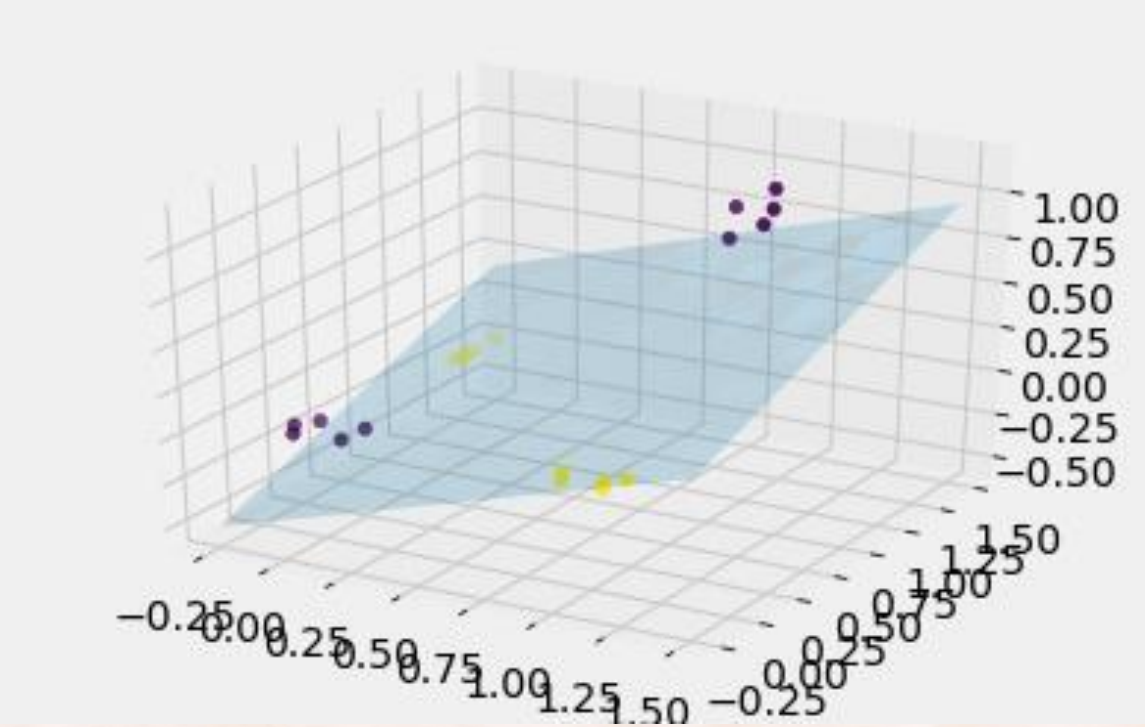
1) Manually Engineered Features: Add x_1x_2

$$\mathbf{x} = [x_1, x_2, x_1x_2]$$



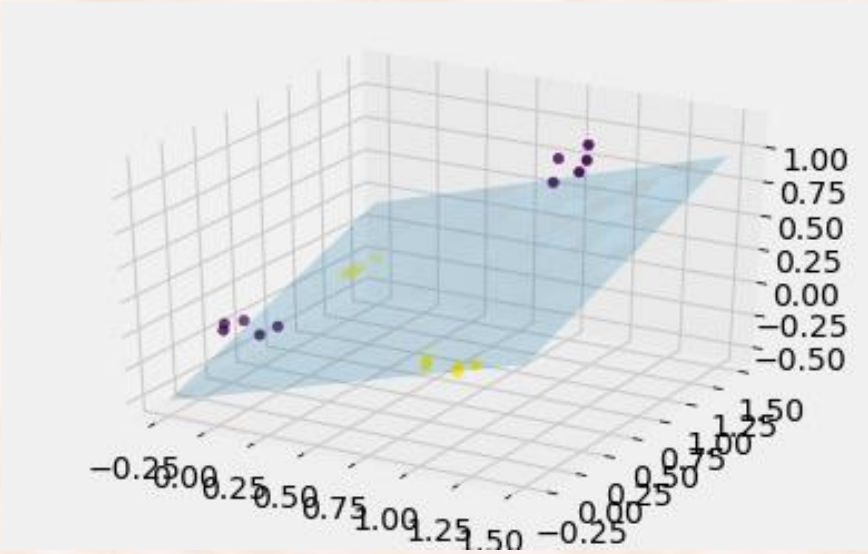
Logistic Regression with Manually Engineered Features

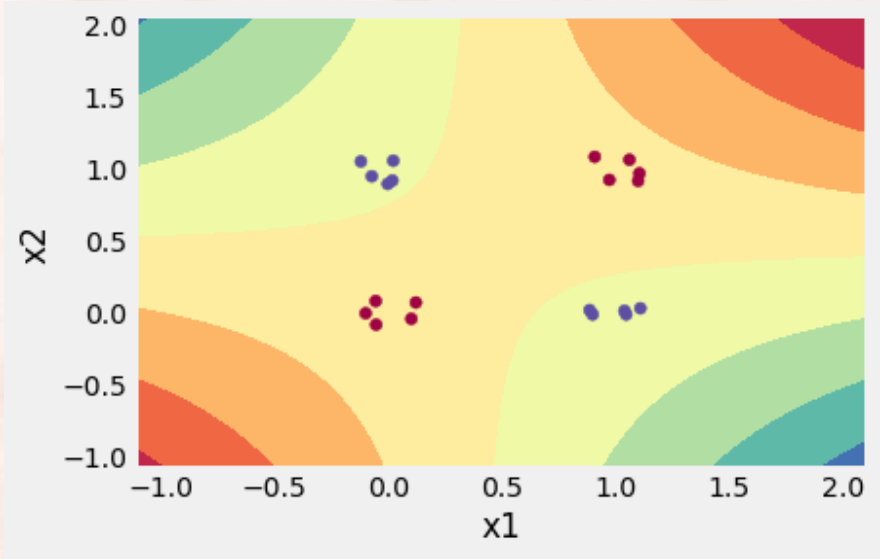
$$\mathbf{x} = [x_1, x_2, x_1 x_2]$$



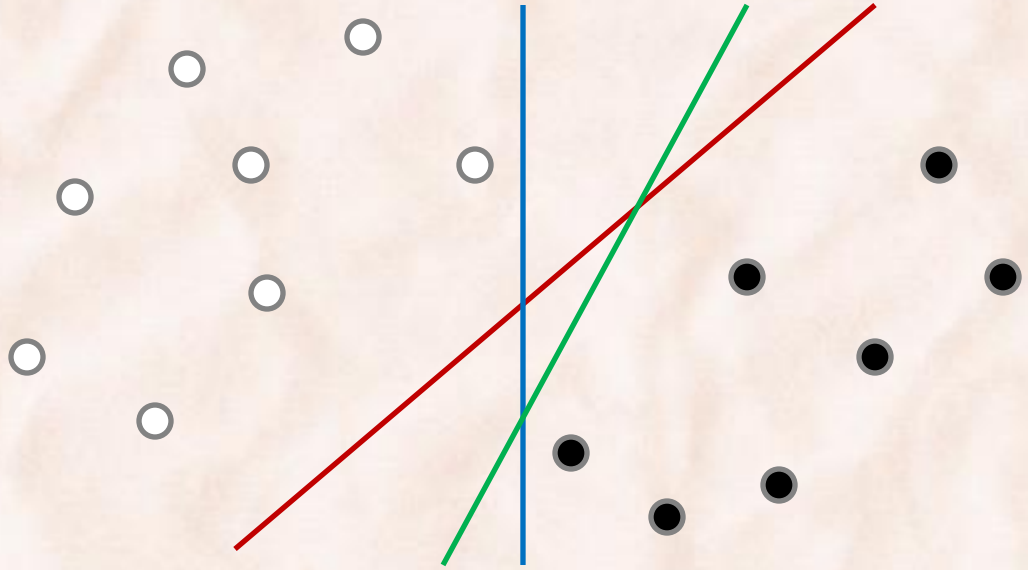
Perceptron with Manually Engineered Features

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





Classifiers & Margin



- Which classifier has the smallest generalization error?
  - The one that maximizes the margin [Computational Learning Theory]
    - **margin** = the distance between the decision boundary and the closest sample.

Averaged Perceptron: Two Classes

1. **initialize** parameters $\mathbf{w} = 0$, $\tau = 1$, $\bar{\mathbf{w}} = 0$
2. **for** $n = 1 \ldots N$
3. $\quad \hat{y}_n = sgn(\mathbf{w}^T \mathbf{x}_n)$
4. $\quad$ **if** $\hat{y}_n \neq y_n$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + y_n \mathbf{x}_n$
6. $\quad \bar{\mathbf{w}} = \bar{\mathbf{w}} + \mathbf{w}$
7. $\quad \tau = \tau + 1$
8. **return** $\bar{\mathbf{w}}/\tau$

$sgn(z) = +1$ if $z > 0$,
0 if $z = 0$,
-1 if $z < 0$

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

During testing: $\hat{y} = sgn(\bar{\mathbf{w}}^T \mathbf{x})$

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 **x**, **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 Representer Theorem

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

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

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

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

Kernel Perceptron: Two Classes

define $\mathbf{w} = \sum_{n=1..N} \alpha_n y_n \mathbf{x}_n$

1. **initialize** dual parameters $\alpha_n = 0$
2. **for** $n = 1 \ldots N$
3. $\quad \hat{y}_n = sgn\,(\mathbf{w}^T \mathbf{x}_n)$
4. $\quad$ **if** $\hat{y}_n \neq y_n$ **then**
5. $\quad\quad \alpha_n = \alpha_n + 1$

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

Inference: $\hat{y} = sgn\,(\mathbf{w}^T \mathbf{x})$

where $\mathbf{w}^T \mathbf{x} = \sum_{j=1..N} \alpha_j y_j \mathbf{x}_j^T \mathbf{x} = \sum_{j=1..N} \alpha_j y_j K(\mathbf{x}_j, \mathbf{x})$

Kernel Perceptron: Two Classes

define $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_{j=1..N} \alpha_j y_j \mathbf{x}_j^T\mathbf{x} = \sum_{j=1..N} \alpha_j y_j K(\mathbf{x}_j, \mathbf{x})$

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

1. **initialize** dual parameters $\alpha_n = 0$
2. **for** $n = 1 \ldots N$
3. $\quad \hat{y}_n = sgn\ f(\mathbf{x}_n)$
4. $\quad$ **if** $\hat{y}_n \neq y_n$ **then**
5. $\quad\quad \alpha_n = \alpha_n + 1$

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 $h(\mathbf{x}) = \sum_{j \in S} \alpha_j y_j K(\mathbf{x}_j, \mathbf{x})$

During testing: $\hat{y} = sgn\ h(\mathbf{x})$

$$\mathbf{w} = \sum_{j \in S} \alpha_j y_j \varphi(\mathbf{x}_j)$$

Kernel Perceptron: Complete Pseudocode

initialize dual parameters $\boldsymbol{\alpha} = 0$
for epoch $e = 1 \ldots E$
    mistakes = 0
    for example $n = 1 \ldots N$
        $\hat{y}_n = sgn\ h(\mathbf{x}_n)$
        if $\hat{y}_n \neq y_n$ **then**
            $\alpha_n = \alpha_n + 1$
            mistakes = mistakes + 1
    if mistakes = 0
        break
return $\boldsymbol{\alpha}$

$sgn(h) = +1$ if $h > 0$,
0 if $h = 0$,
-1 if $h < 0$

1 epoch = one pass over all training examples.

$$h(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_j \alpha_j y_j \mathbf{x}_j^T \mathbf{x} = \sum_j \alpha_j y_j K(\mathbf{x}_j, \mathbf{x})$$

Kernel Perceptron: Alternative Formulation

define $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x} = \sum_j \alpha_j \mathbf{x}_j^T\mathbf{x} = \sum_j \alpha_j K(\mathbf{x}_j, \mathbf{x})$

no y_j anymore

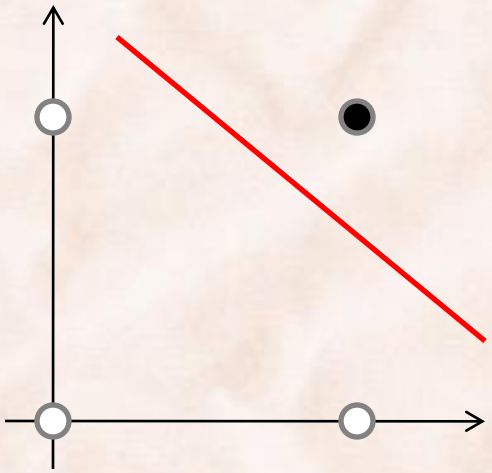
1. **initialize** dual parameters $\alpha_n = 0$
2. **for** $n = 1 \ldots N$
3. $\hat{y}_n = sgn\ h(\mathbf{x}_n)$
4. **if** $\hat{y}_n \neq y_n$ **then**
5. $\alpha_n = \alpha_n + y_n$

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

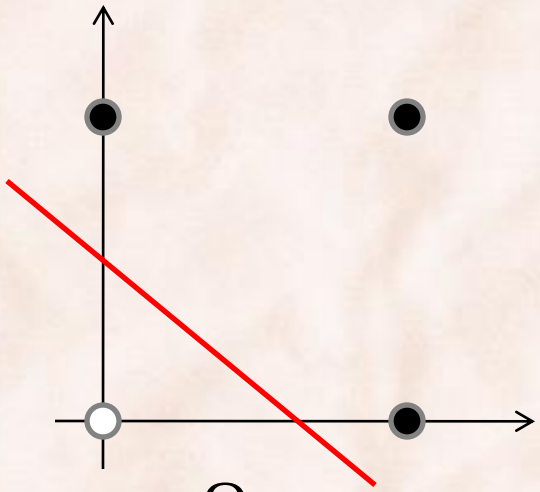
add y_n instead of 1

During testing: $\hat{y} = sgn\ h(\mathbf{x})$

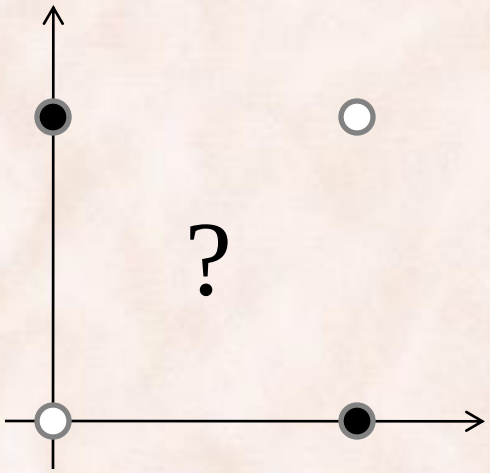
The Perceptron vs. Boolean Functions



And



Or



Xor

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

Perceptron with Quadratic Kernel

- Discriminant function:

$$h(\mathbf{x}) = \sum_{j=1..N} \alpha_j y_j \varphi(\mathbf{x}_j)^T \varphi(\mathbf{x}) = \sum_{j=1..N} \alpha_j y_j K(\mathbf{x}_j, \mathbf{x})$$

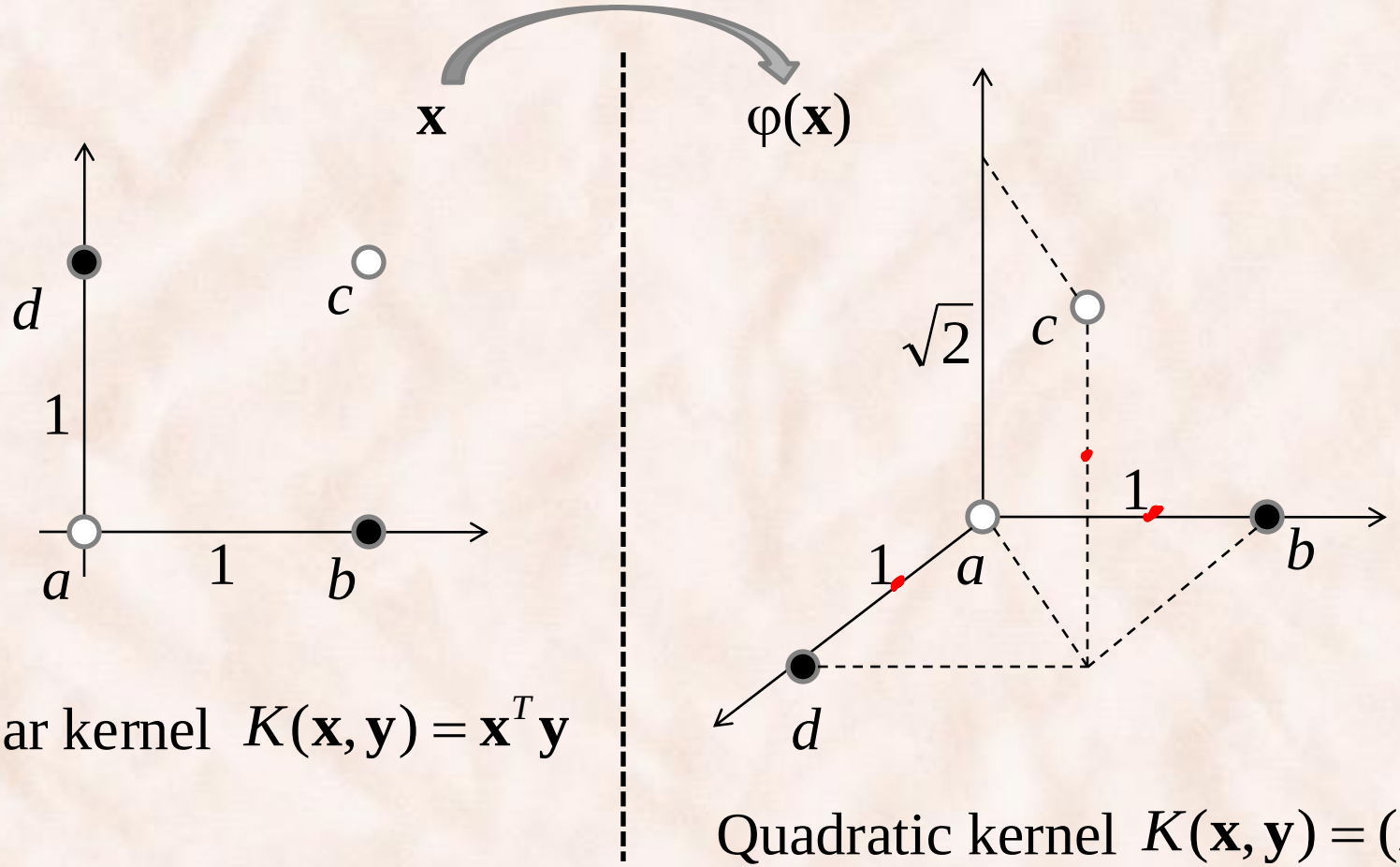
- Quadratic kernel:

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

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

conjunctions of two atomic features

Perceptron with Quadratic Kernel



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

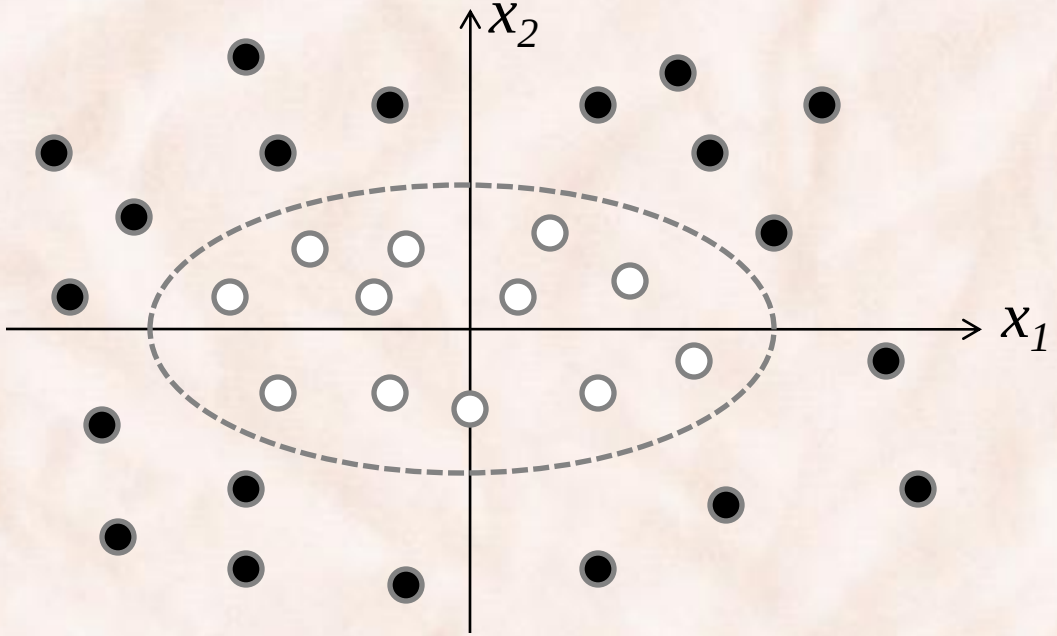
Quadratic kernel $K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y})^2$

Quadratic Kernels

- Circles, hyperbolas, and ellipses as separating surfaces:

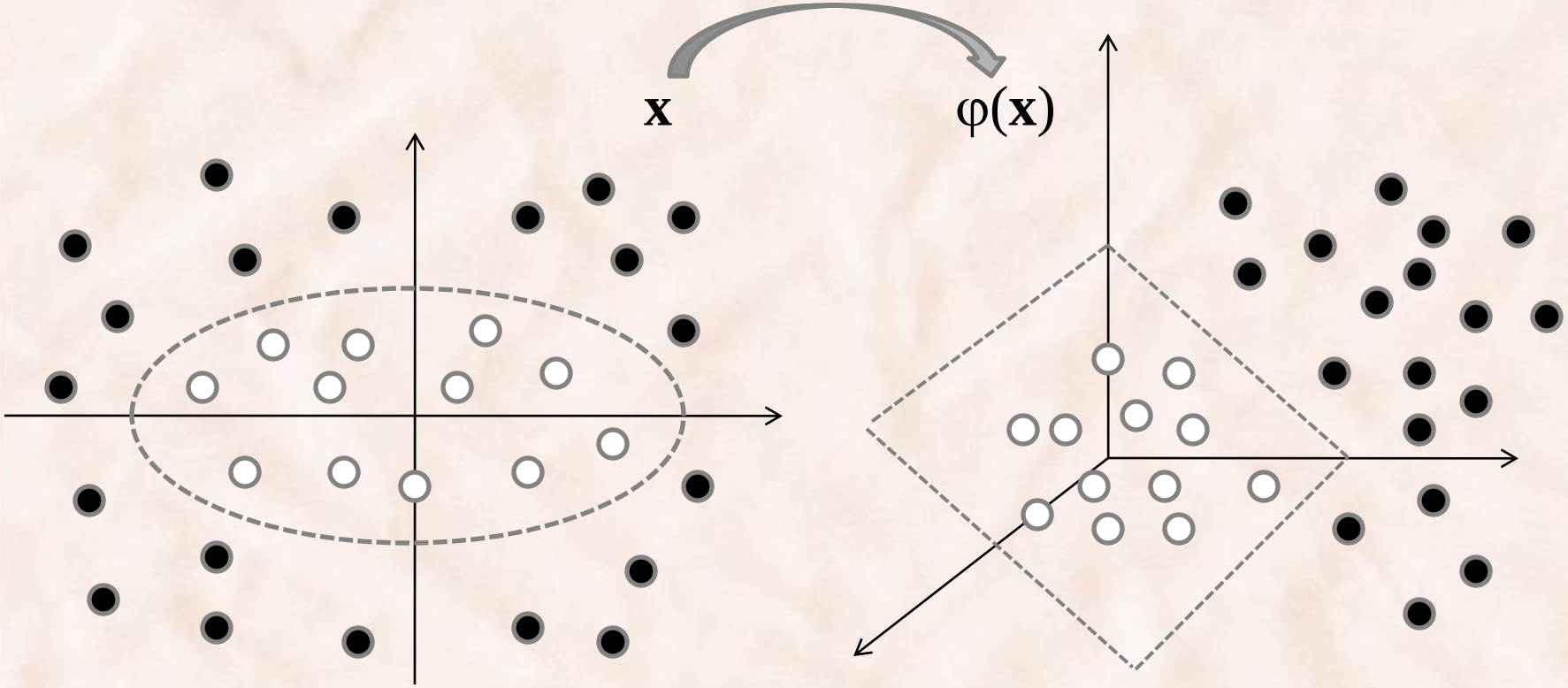
$$K(\mathbf{x},\mathbf{y}) = (1+\mathbf{x}^T\mathbf{y})^2 = \varphi(x)^T\varphi(y)$$

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



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.
  - Prove using Taylor expansion of exponential.

$$\varphi(x) = e^{-\gamma x^2}\left[1, \sqrt{2\gamma}x\,, \sqrt{2}\gamma x^2, \ldots\right]$$

also called r or γ

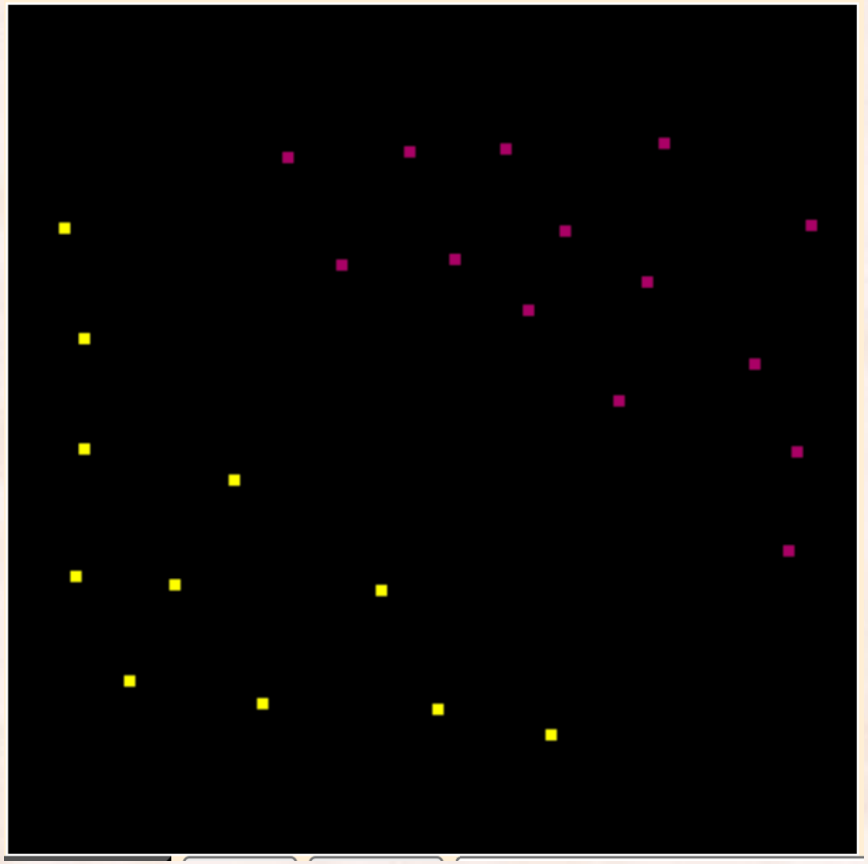
Techniques for Constructing Kernels

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

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= c k_1(\mathbf{x}, \mathbf{x}') && (6.13)\\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') && (6.14)\\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.15)\\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.16)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') && (6.17)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}') && (6.18)\\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) && (6.19)\\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}' && (6.20)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.21)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.22)
\end{aligned}
$$

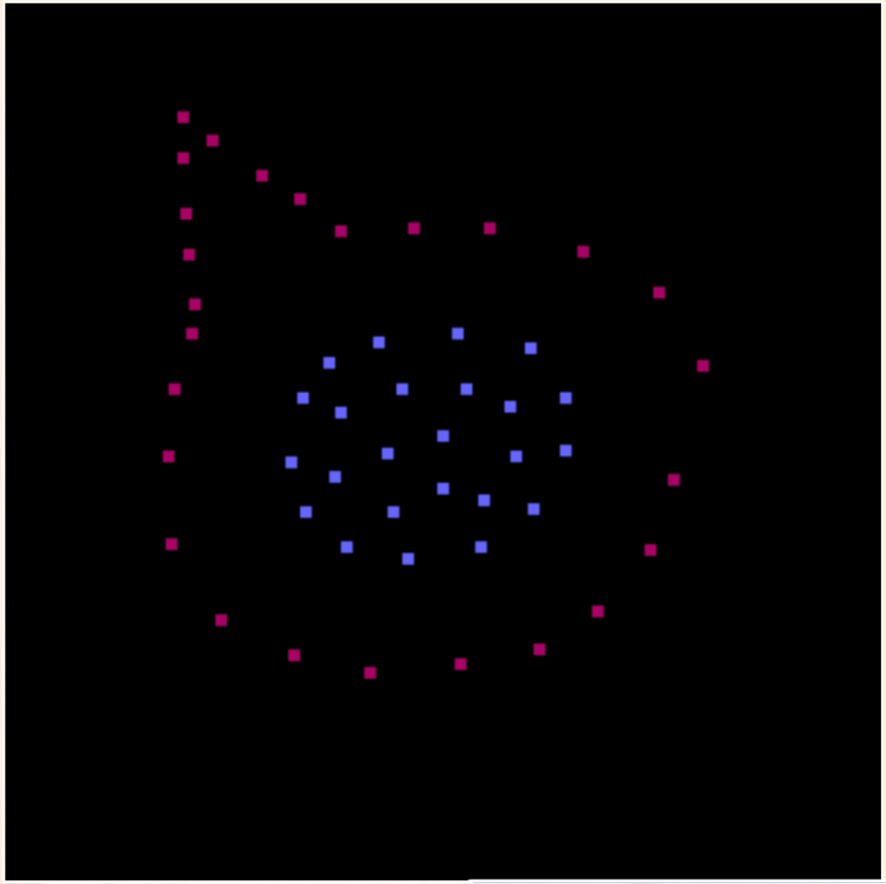
where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite 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.

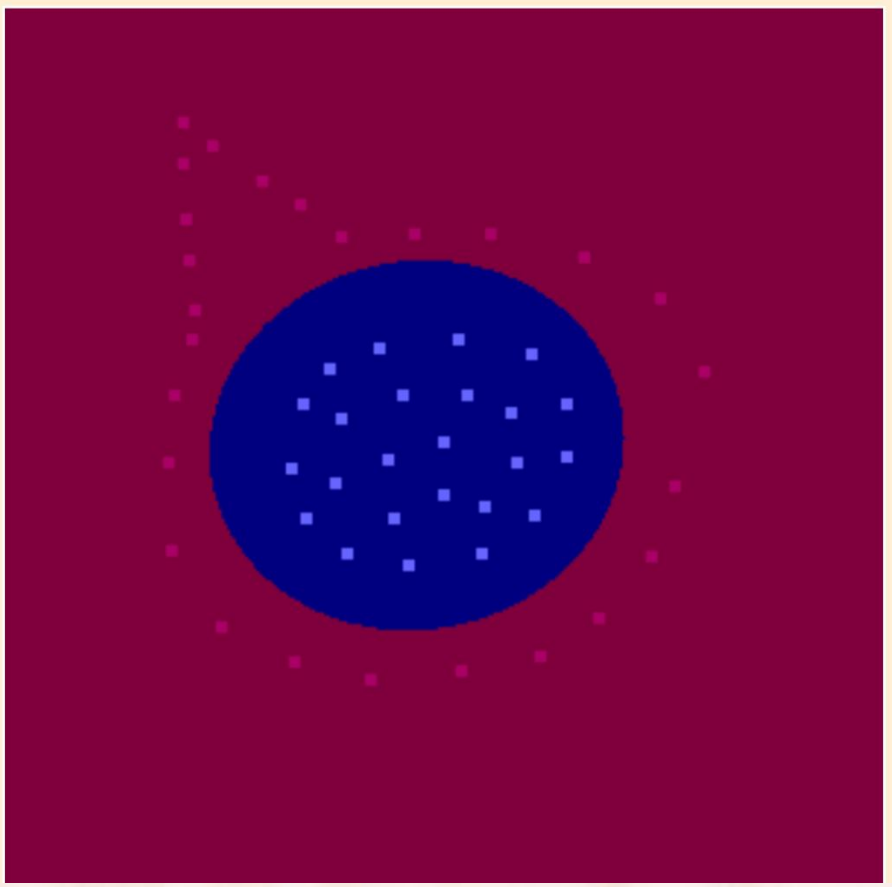
Linear Kernel $\mathbf{x}^T\mathbf{y}, C = 100$



https://www.csie.ntu.edu.tw/~cjlin/libsvm/

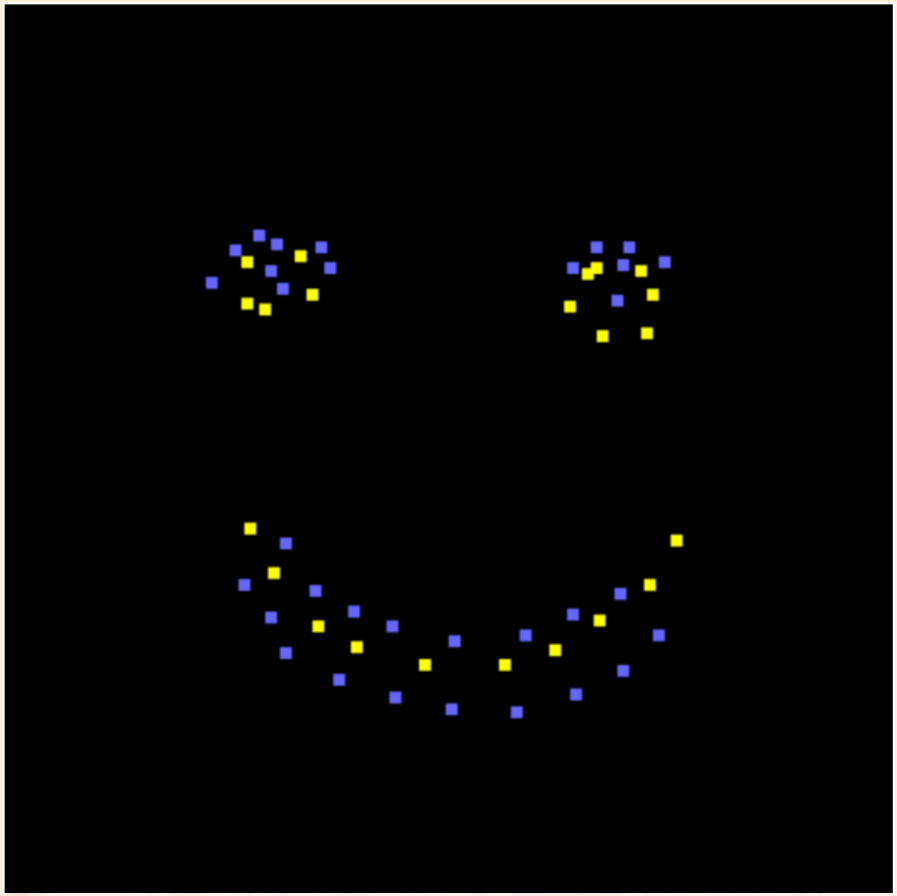
Quadratic kernel $(1 + \mathbf{x}^T\mathbf{y})^2, C = 500$

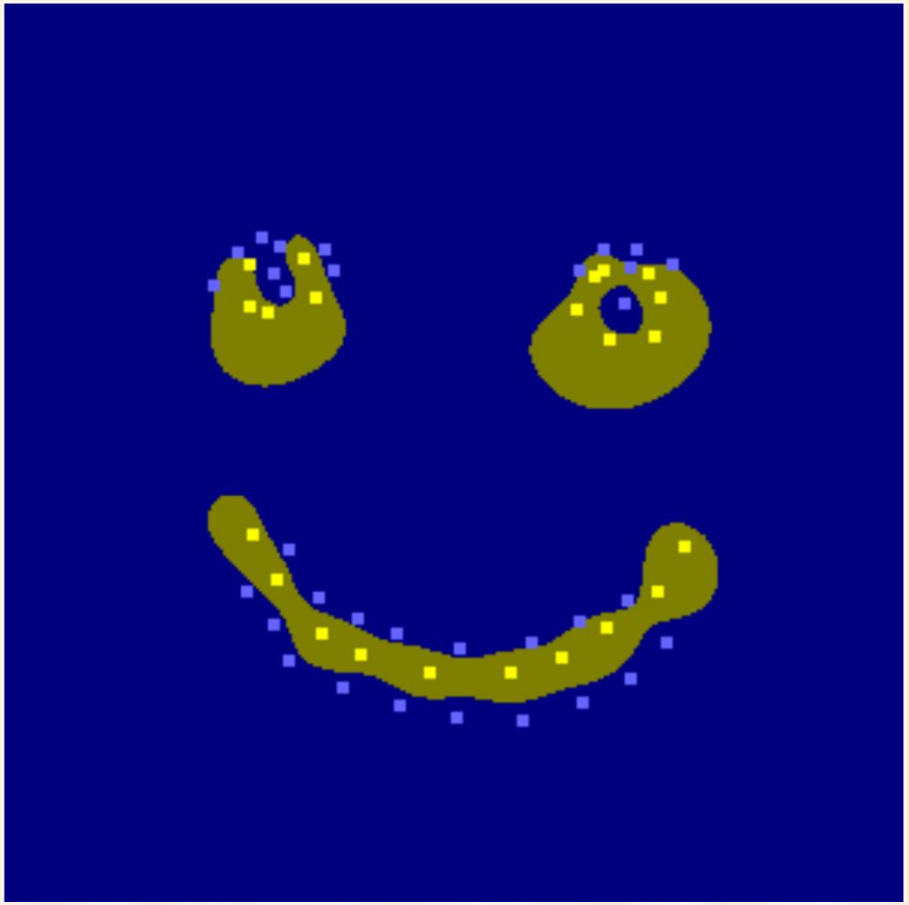




https://www.csie.ntu.edu.tw/~cjlin/libsvm/

Gaussian kernel with $\frac{1}{2\sigma^2} = 250, C = 100$





https://www.csie.ntu.edu.tw/~cjlin/libsvm/

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.

Readings

1. [Required] Peter Flach's ML textbook, chapter 7:
   - Section 7.1 on the Least-squares method.
   - Section 7.2 on the Perceptron.
   - Section 7.5 on Kernels and the Kernel Perceptron.

2. [Optional] Bishop, 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* binary classifiers.
2) Train K(K–1)/2 *one-versus-one* binary 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:

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

- 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. $\quad y_i = \arg\max_{t \in T} \mathbf{w}^T \varphi(\mathbf{x}_i, t)$
4. $\quad$ **if** $y_i \neq t_i$ **then**
5. $\quad\quad \mathbf{w} = \mathbf{w} + \varphi(\mathbf{x}_i, t_i) - \varphi(\mathbf{x}_i, y_i)$

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

During testing:

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

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:

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

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

Kernel Perceptron: K classes

1. **define** $f(\mathbf{x},t) = \sum_{i,j} a_{ij}(f(\mathbf{x}_i, t_i)^T f(\mathbf{x},t) - f(\mathbf{x}_i, c_j)^T f(\mathbf{x},t))$
2. **initialize** dual parameters $\alpha_{ij} = 0$
3. **for** $i = 1 \ldots n$
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:

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

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

where:

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

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