Linear Discriminant Analysis vs. Kernel Fisher Discriminant Analysis

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- LDA is based on quite simple assumptions
- Extension by Kernels allows solving more complex problems efficiently

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- But what means "best"??

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- **Problem:** Typically the hypothesis space $\mathcal{H}$ is extremely large.
- **Possible solution:** Restrict $\mathcal{H}$ to a special class of parameterized hypotheses and try to learn the parameters (e.g. polynomial base functions).

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- Best hypothesis class is strongly depending on problem
- $\rightarrow$ class seperability!

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- Nice to have, but quite rare
- In all other cases we will need nonlinear discriminant functions

Examples (1)

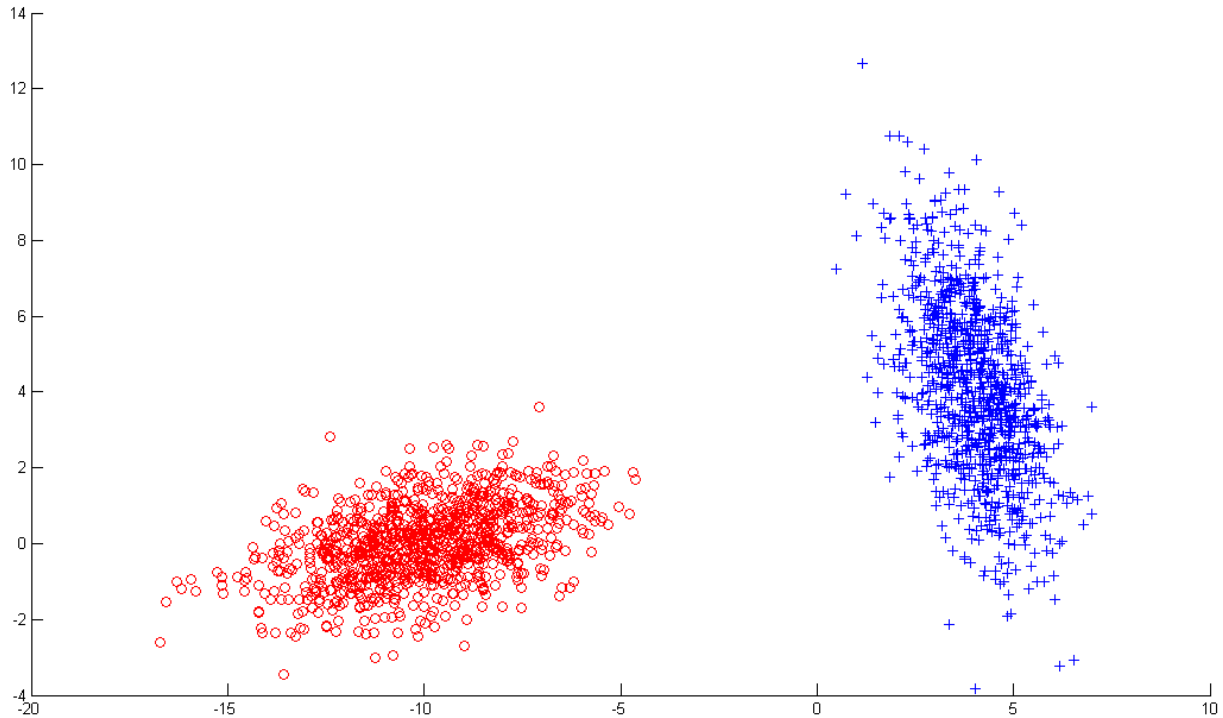

Figure: Two classes which are linearely seperable

Examples (2)

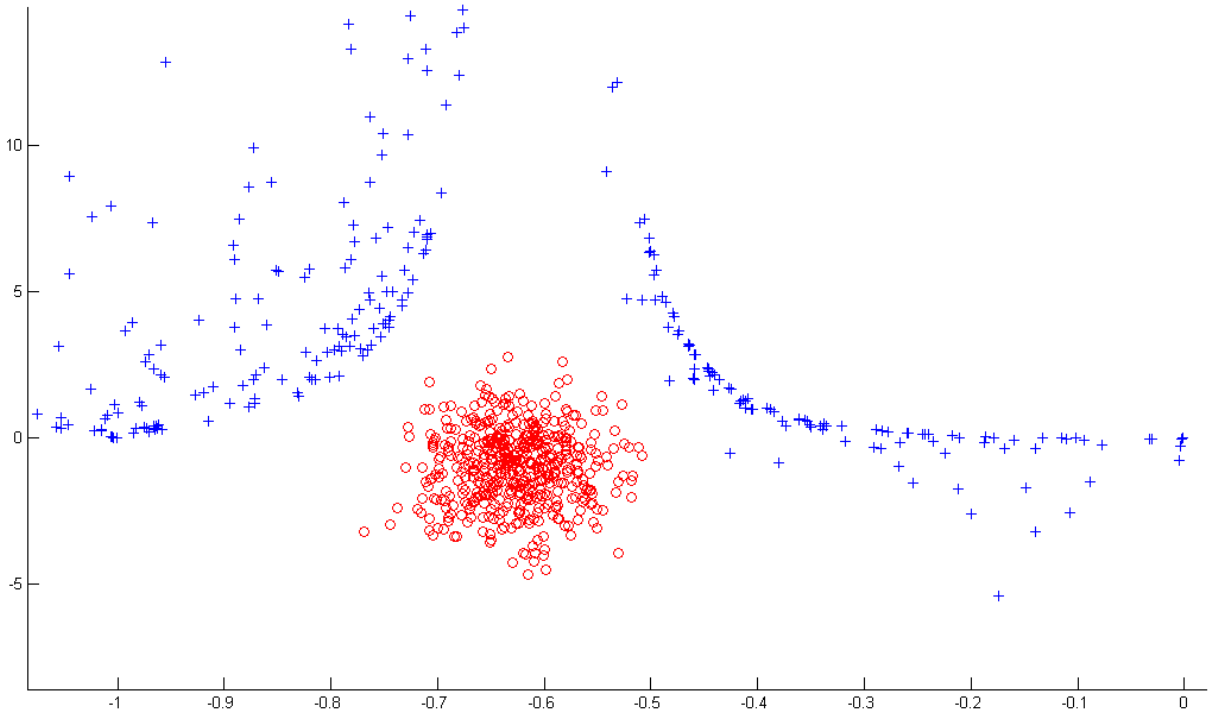

Figure: Two classes which are not linearely seperable

What it is...

- Common method in statistics / machine learning

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Definition (binary case)

Given an N-dimensional feature space $\mathcal{X}$, examples $\mathbf{x}_1^i \in \mathcal{X}$ belonging to class 1 and examples $\mathbf{x}_2^j \in \mathcal{X}$ belonging to class 2, find a linear $(N-1)$-dimensional subspace $\hat{\mathcal{X}} \subseteq \mathcal{X}$ which best seperates classes 1 and 2.

The subspace $\hat{\mathcal{X}}$ is represented by its normal vector $\mathbf{w}^T$ ($\mathbf{w}^T\mathbf{x} = const.$).

Illustration

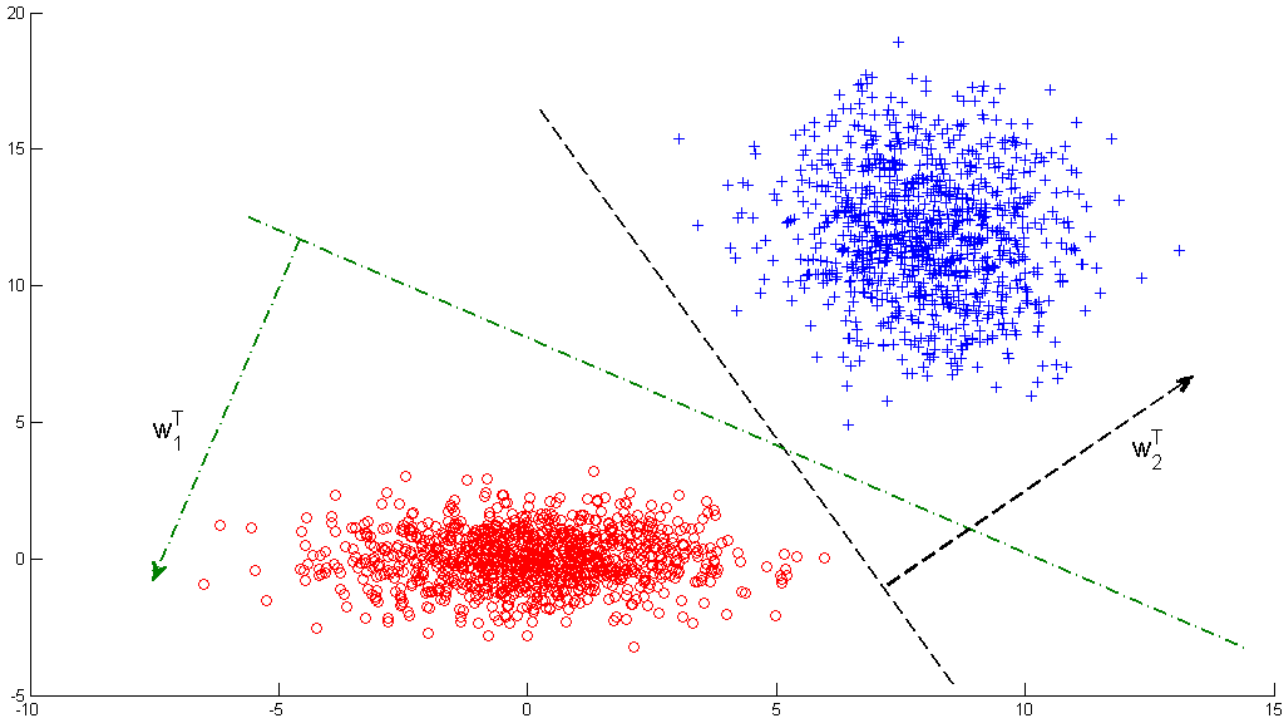

Figure: Many possibilities for seperation

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- But typically LDA is associated with Fisher's Discriminant Analysis
- In this presentation we will consider FDA

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- Definition of an optimality criterion which allows us to determine $\mathbf{w}^T$

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Fisher's Optimality Criterion

Choose a direction $\mathbf{w}^T$ that maximizes the *Within Class Variance* while minimizing the *Between Class Variance*.

Illustration of the FDA principle

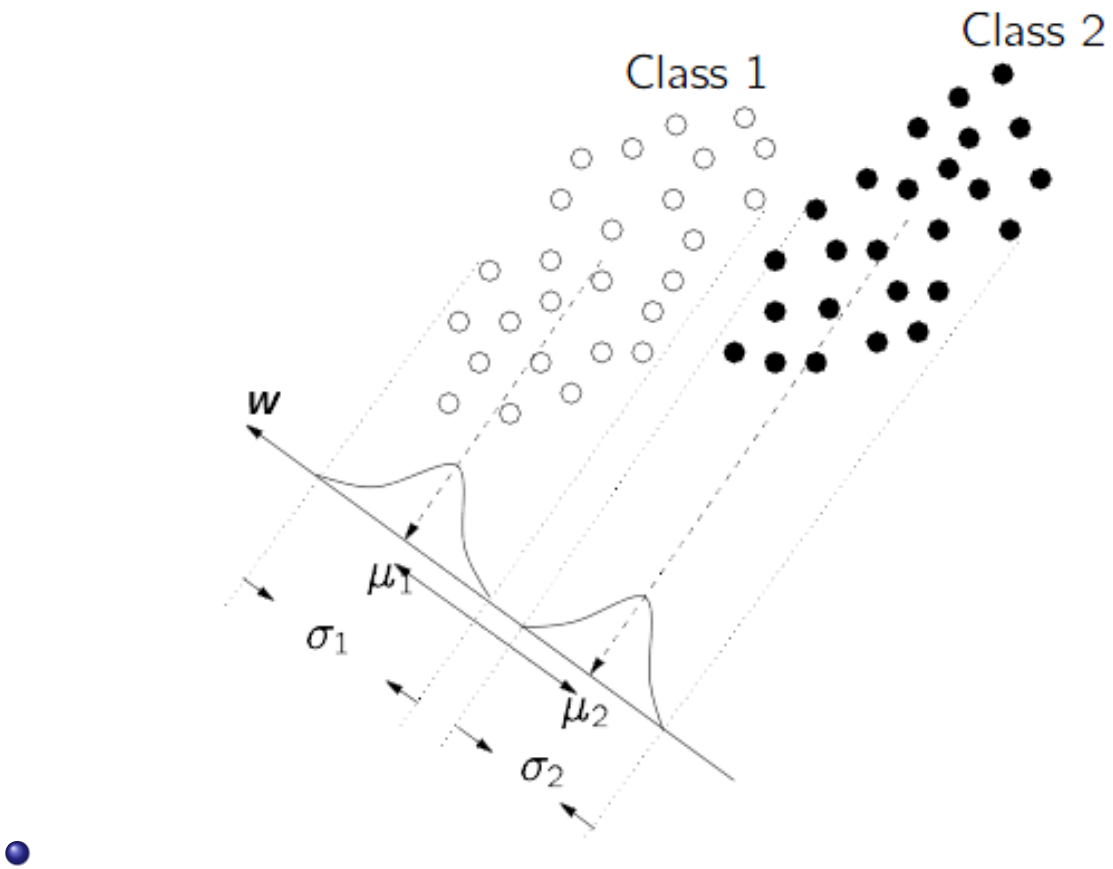

Figure: Source: [Mika, 2002]

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  - Mean of Class 1: $\mathbf{m}_1 = E\{\mathbf{x}_1\}$
  - Mean of Class 2: $\mathbf{m}_2 = E\{\mathbf{x}_2\}$
  - Projected Mean of Class 1: $\mu_1 = \mathbf{w}^T\mathbf{m}_1$
  - Projected Mean of Class 2: $\mu_2 = \mathbf{w}^T\mathbf{m}_2$
  - Variance of projected Class 1: $\sigma_1^2 = E\left\{(\mathbf{w}^T\mathbf{x}_1 - \mu_1)^2\right\}$
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- We consider the ratio of between class variance and within class variance

$$J(\mathbf{w}) = \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2} \tag{2}$$

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$$J(\mathbf{w}) = \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2} \tag{2}$$

- gives us the following optimization problem:

$$\mathbf{w} = \underset{\mathbf{w}\in\mathcal{X}}{arg\ max}\ J(\mathbf{w}) \tag{3}$$

Determining **w**

- It can be shown (blackboard) that

$$J(\mathbf{w}) = \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2} = \frac{\mathbf{w}^T \mathbf{S}_b \mathbf{w}}{\mathbf{w}^T \mathbf{S}_w \mathbf{w}} \tag{4}$$

with

$$\mathbf{S}_b = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T \tag{5}$$

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- which can be maximized in closed form with respect to **w**

Determining **w** (2)

Solution

Fisher's optimal direction can be determined as

$$\mathbf{w} = \mathbf{S}_w^{-1}(\mathbf{m}_1 - \mathbf{m}_2) \tag{7}$$

The discriminant function is then given by

$$\mathbf{w}^T\mathbf{x} = w_0 = \frac{\mathbf{w}^T(\mathbf{m}_1 + \mathbf{m}_2)}{2} \tag{8}$$

Classifying new Data Points

- Check if the data point $\mathbf{x}_{new}$ lies "above" or "below" the resulting hyperplane

$$H_{LDA} : \mathcal{X} \rightarrow \mathcal{Y} = \begin{cases} Class1 & \mathbf{w}^T \mathbf{x}_{new} < w_0 \\ Class2 & \mathbf{w}^T \mathbf{x}_{new} \geq w_0 \end{cases} \tag{9}$$

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- Can also be interpreted as projecting the data point onto $\mathbf{w}$ and checking the decision threshhold w_0 in the reduced subspace (see MATLAB demo!)

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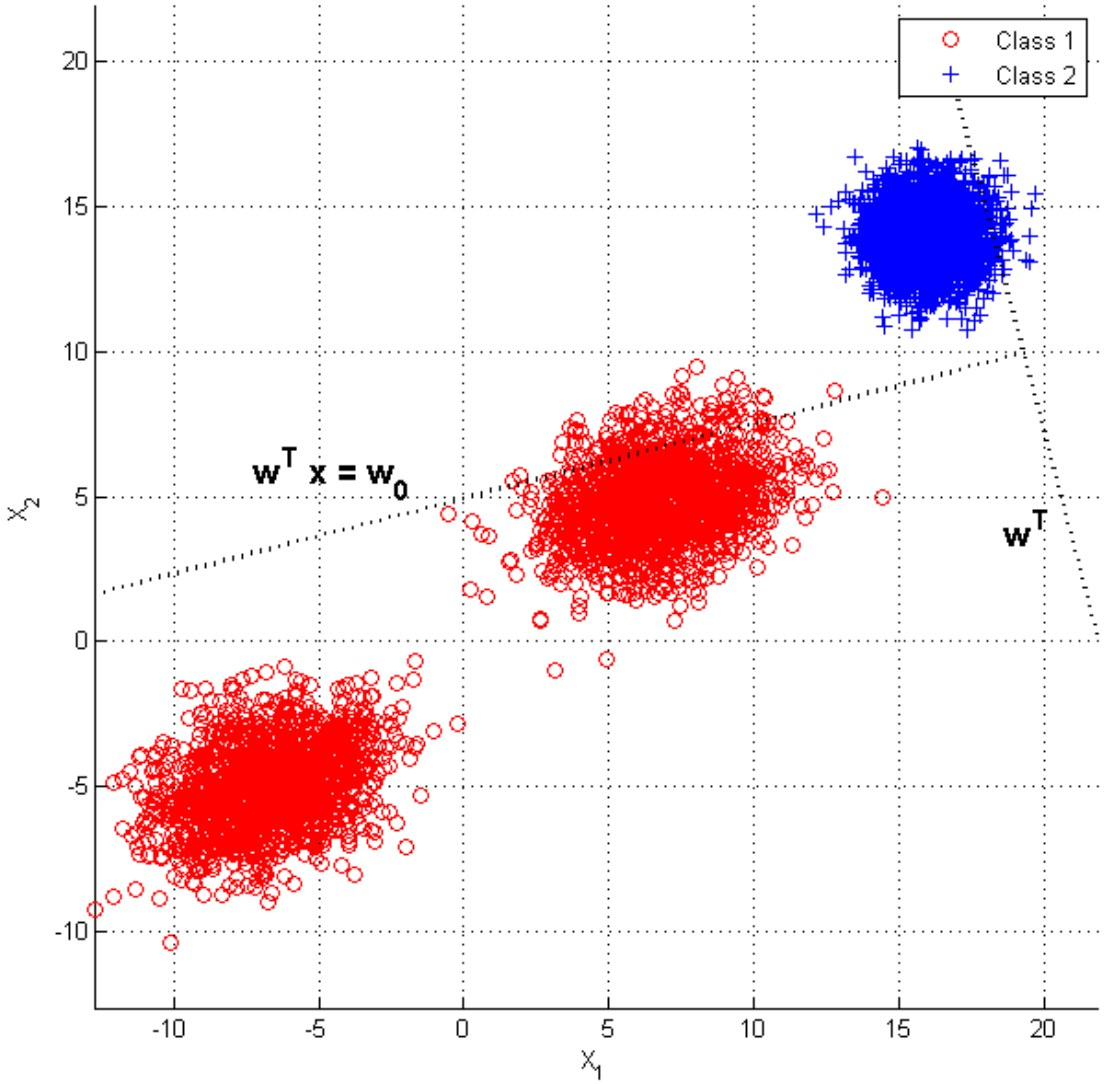
- Can be really bad, even if data is linearly separable
- Often if underlying densities are *complex* (e.g. multi-modal)

Example where LDA fails



Demo

MATLAB Demo...

Shortcomings of Fisher Discriminant

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- ...limited in complexity of problems which can be solved

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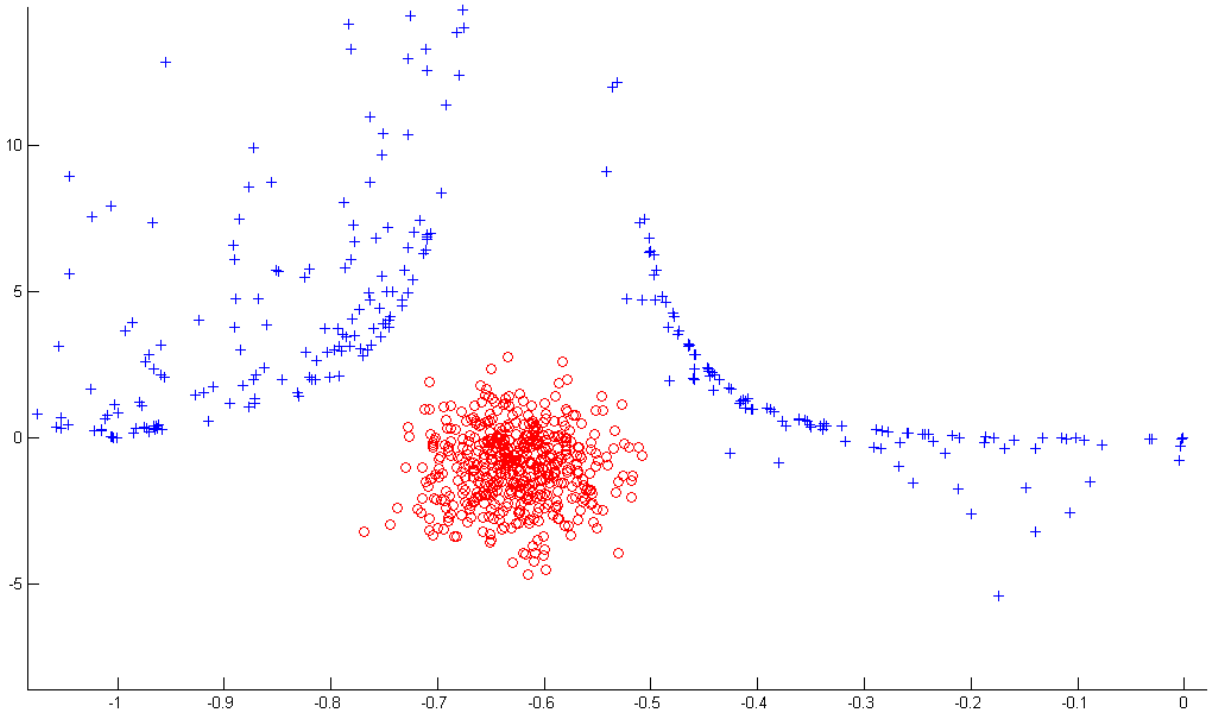

Figure: Two classes which are not linearly separable

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- Computational benefits
- Kernels are not restricted to vectorial data - e.g. Strings ([Blaz, 2004], [Lodhi et al., 2002]) or Graphs ([Zhou et al., 2009])

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- As linear discriminants are not enough for real world data...
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- Map the data non-linearly to a feature space $\mathcal{F}$...
- ...compute Fisher Discriminant there, yielding a non-linear discriminant in input space

Recap

- For the Fisher Discriminant we had to optimize:

$$J(\mathbf{w}) = \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2} = \frac{\mathbf{w}^T \mathbf{S}_b \mathbf{w}}{\mathbf{w}^T \mathbf{S}_w \mathbf{w}} \tag{12}$$

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and

$$\mathbf{m}_i = E\{\mathbf{x}_i\} \tag{15}$$

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Formulation of the non-linear mapping Φ

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- BUT NOW: $\mathbf{w} \in \mathcal{F}$

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- Need a formulation of $\frac{\mathbf{w}^T \mathbf{S}_b^\Phi \mathbf{w}}{\mathbf{w}^T \mathbf{S}_w^\Phi \mathbf{w}}$ with only dot-products $\langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle \rightarrow k(\mathbf{x}, \mathbf{y})$

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- Then we can use different kernels (RBF, Polynomial, ...) to do the computation efficiently, without explicitly map to the feature space $\mathcal{F}$
- As numerator and denominator are both scalars, reformulation can be done independently

Reformulation of numerator

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  $\mathbf{N} = E\left\{(\mathbf{K}_{x_1} - \mathbf{K}_{\bar{x}_1})(\mathbf{K}_{x_1} - \mathbf{K}_{\bar{x}_1})^T\right\} + E\left\{(\mathbf{K}_{x_2} - \mathbf{K}_{\bar{x}_2})(\mathbf{K}_{x_2} - \mathbf{K}_{\bar{x}_2})^T\right\}$

Kernel Fisher Discriminant Solution

- Solving the Kernel Fisher Discriminant by:

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Some useful facts

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Example to KFD from ([Knaf, 2007])

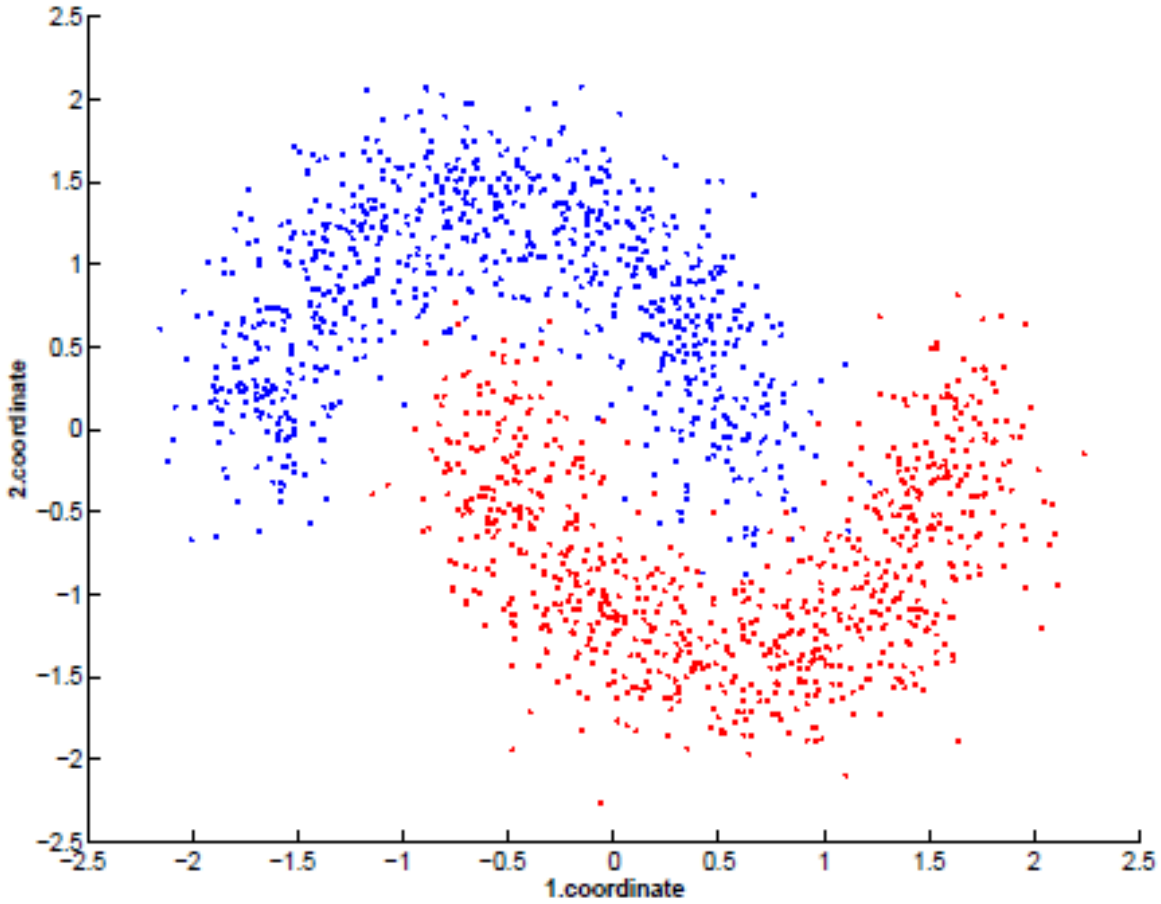

Figure: Input data $\mathcal{X} = \mathcal{X}_1 \cup \mathcal{X}_2$, Source: [Knaf, 2007]

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- Comparison to simple Fisher Discriminant

Discriminant function of the KFD with Gauss-Kernel

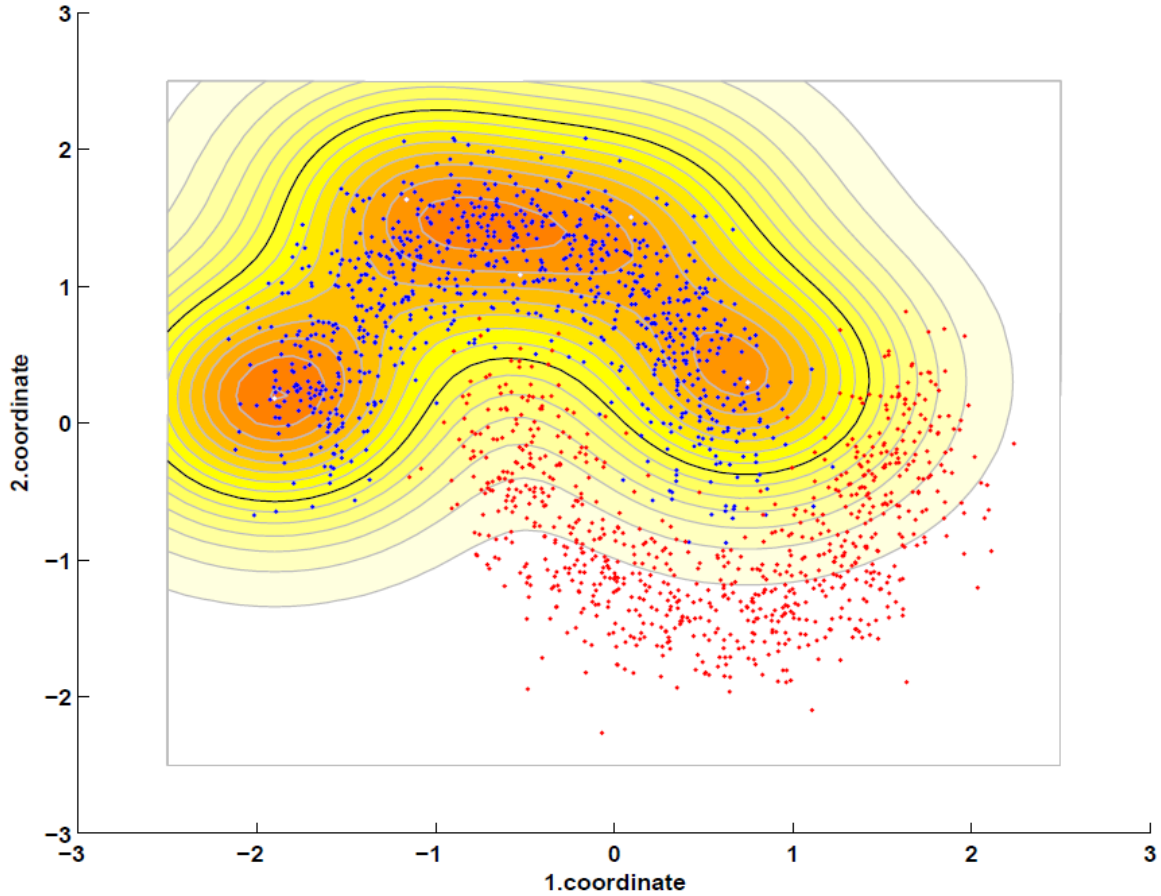


Figure: Source: [Knaf, 2007]

Discriminant function of the KFD with Polynomial-Kernel

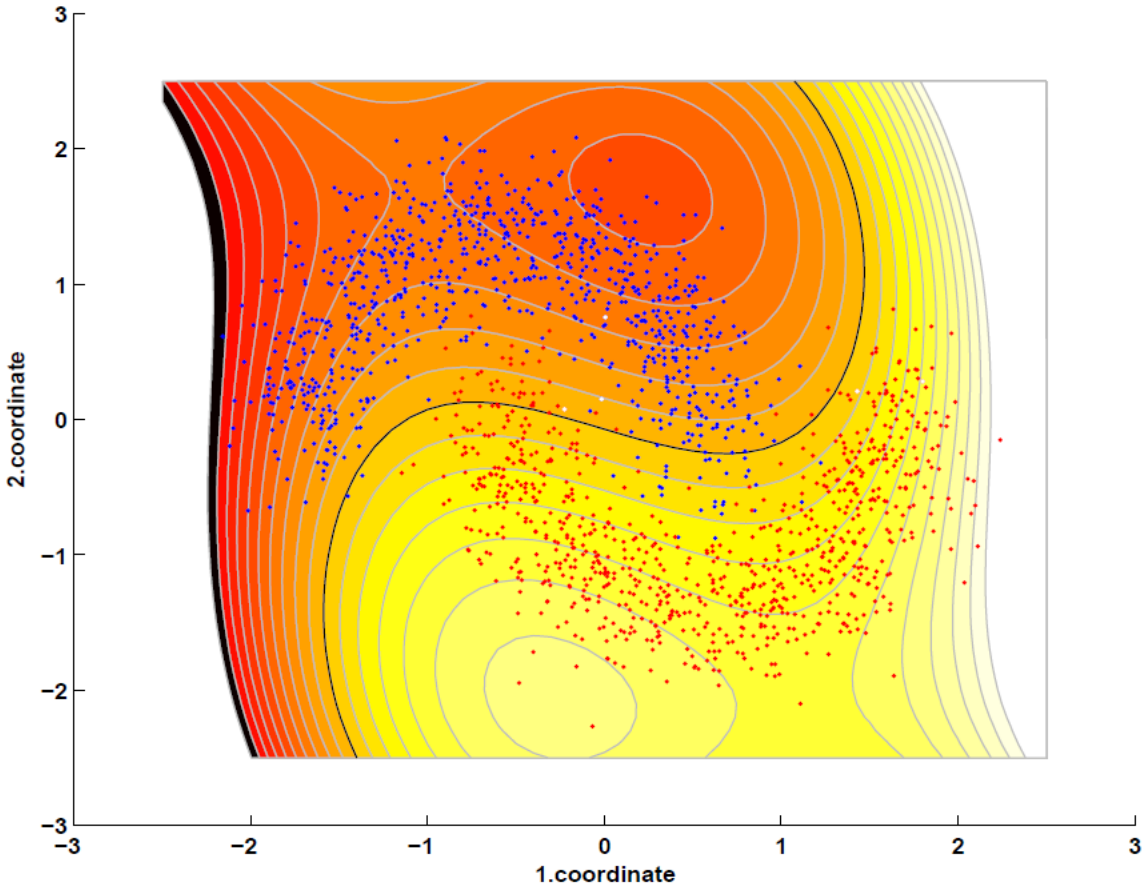


Figure: Source: [Knaf, 2007]

Distributions of the data points projected on the discriminant functions

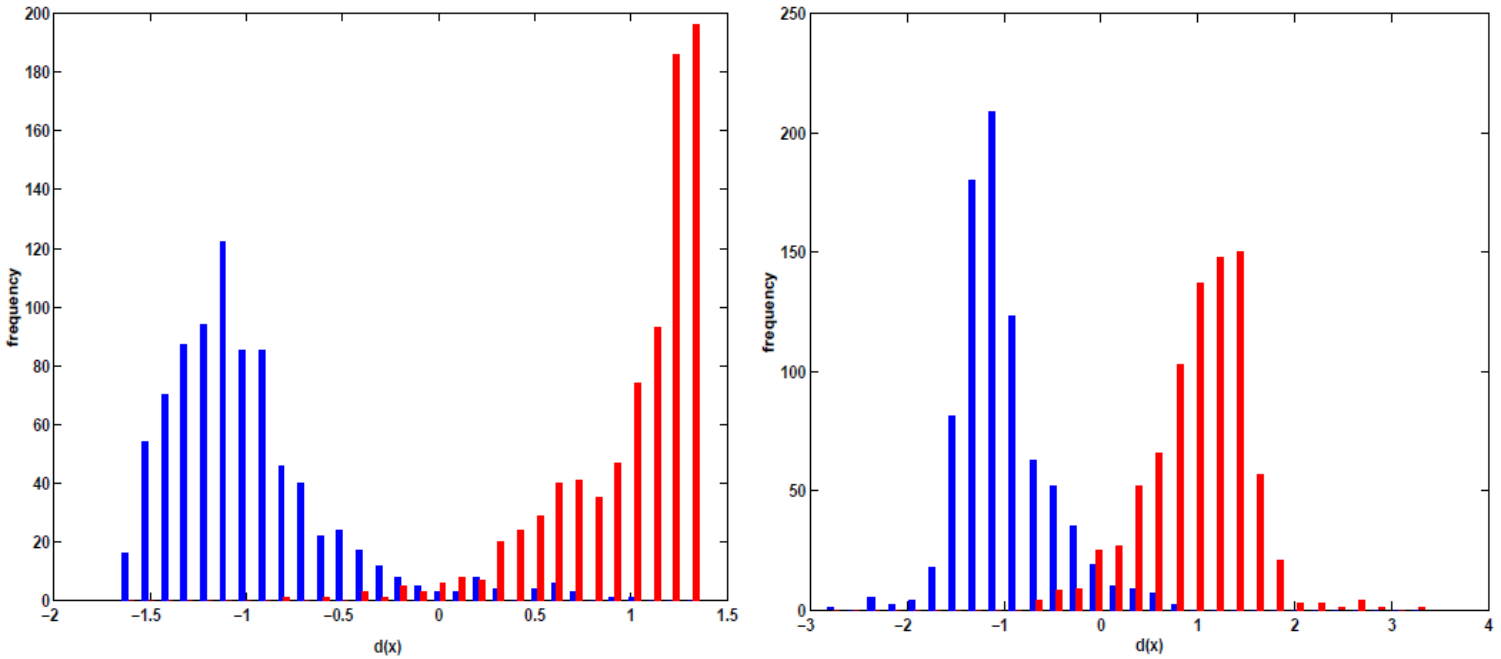
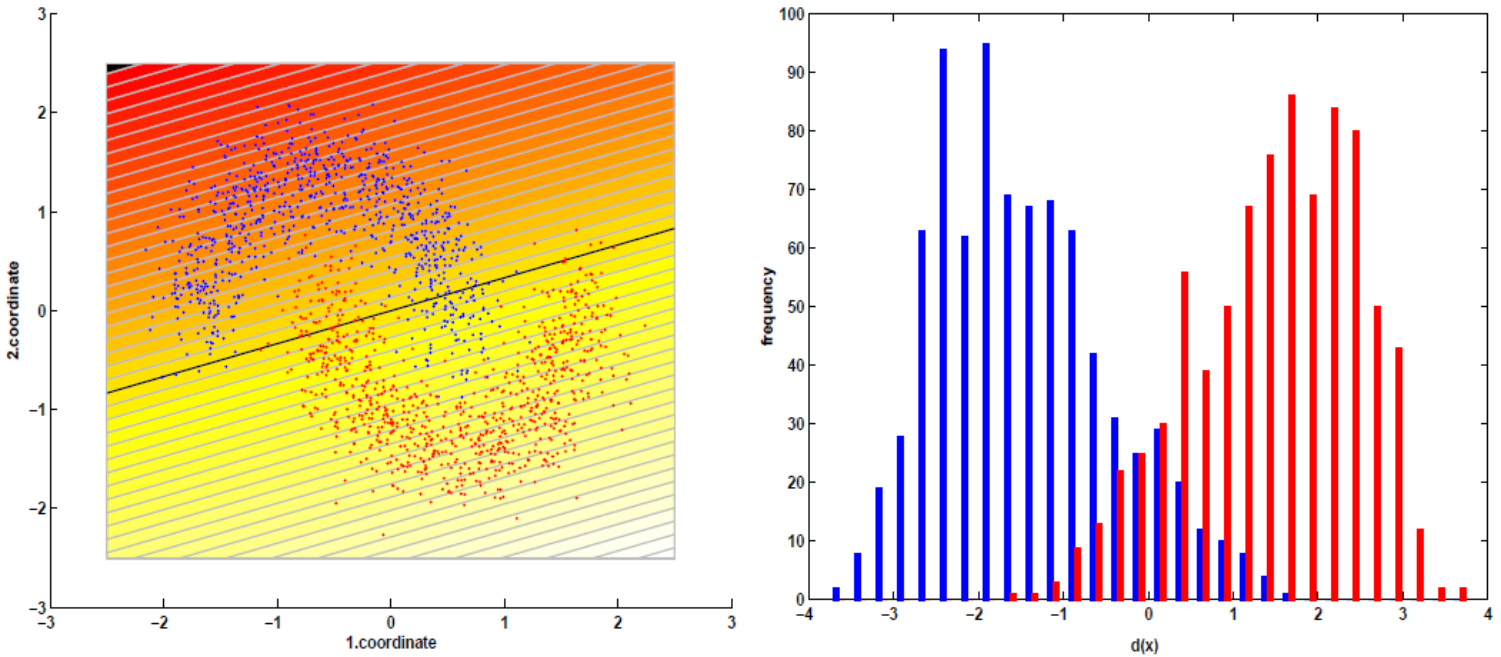


Figure: Source: [Knaf, 2007]

Solution of the simple Fisher discriminant function



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Demo

MATLAB Demo...

Summary

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