Kernel Methods and Nonlinear Classification

Piyush Rai

CS5350/6350: Machine Learning

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Kernel Methods: Motivation

- Often we want to capture nonlinear patterns in the data
  - Nonlinear Regression: Input-output relationship may not be linear
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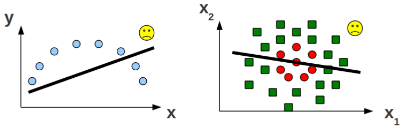

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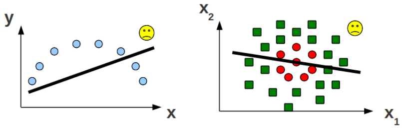

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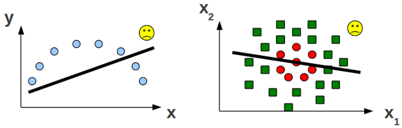

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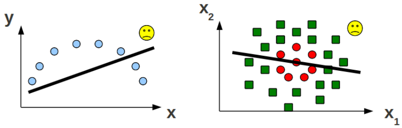

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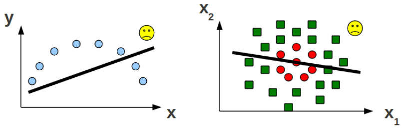

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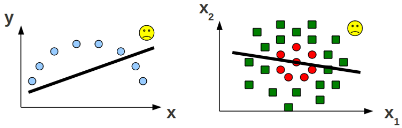

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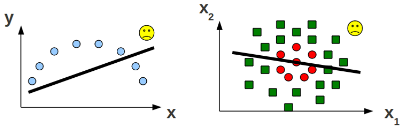

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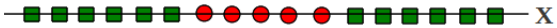
  - Kernels give such mappings for (almost) free
    - In most cases, the mappings need not be even computed
    - .. using the Kernel Trick!

Classifying non-linearly separable data

- Consider this binary classification problem



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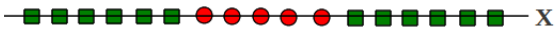

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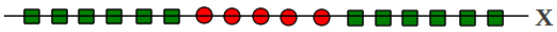

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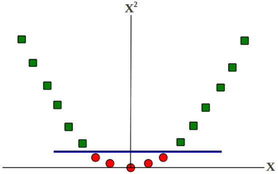

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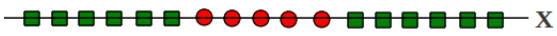

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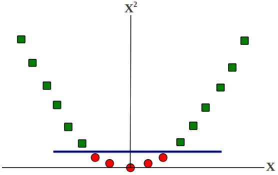
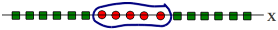


- Linear in the new representation $\equiv$ nonlinear in the old representation



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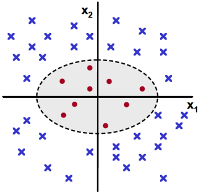

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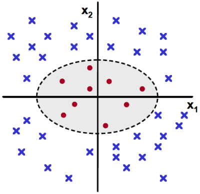

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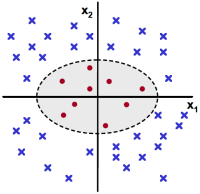

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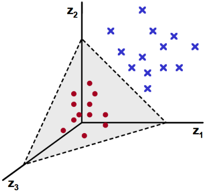

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- All kernel functions have these properties

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\begin{aligned}
\phi &: \mathcal{X} \to \mathcal{F} \\
k &: \mathcal{X} \times \mathcal{X} \to \mathbb{R}, \quad k(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^\top \phi(\mathbf{z})
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$$\begin{aligned} \phi &: \mathcal{X} \rightarrow \mathcal{F} \\ k &: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}, \quad k(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^\top \phi(\mathbf{z}) \end{aligned}$$

- $\mathcal{F}$ needs to be a *vector space* with a *dot product* defined on it
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    - No. It must satisfy **Mercer's Condition**

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  - Kernels can also be constructed by composing these rules

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Note: Kernel hyperparameters (e.g., d, γ) chosen via cross-validation

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  - Many of the unsupervised learning algorithms too can be kernelized (e.g., K-means clustering, Principal Component Analysis, etc.)

Kernelized SVM Training

- Recall the SVM dual Lagrangian:

$$\text{Maximize} \quad L_D(\mathbf{w}, b, \xi, \alpha, \beta) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\mathbf{x}_m^T \mathbf{x}_n)$$

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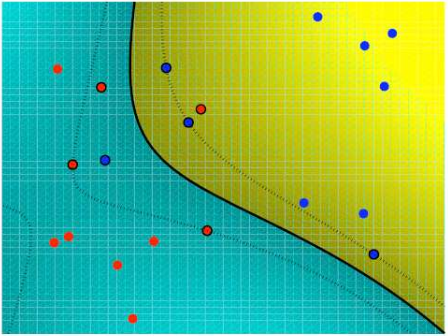
SVM with an RBF Kernel



- The learned decision boundary in the original space is nonlinear

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Next class..

- Intro to probabilistic methods for supervised learning
  - Linear Regression (probabilistic version)
  - Logistic Regression