Week 8

Machine Learning and Big Data - DATA622

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Support Vector Machines

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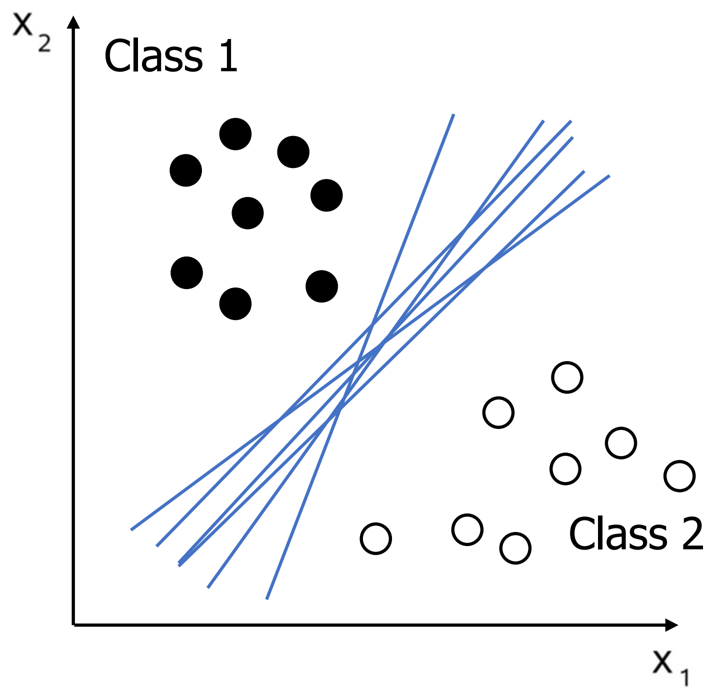
Support Vector Machines

How do you find the right decision boundary?



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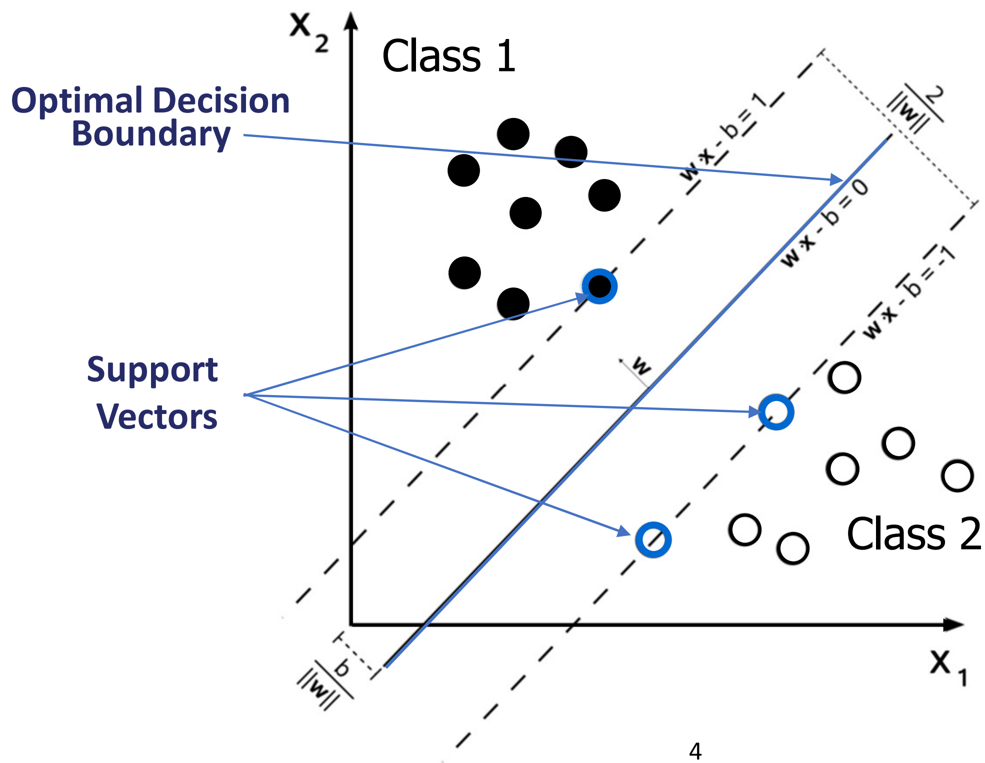
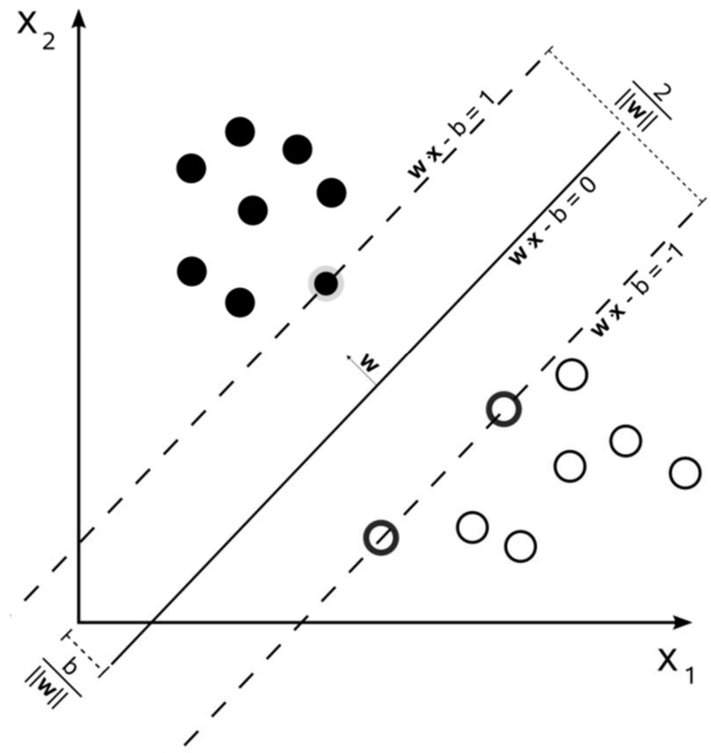
Support Vector Machines

SVM approach: Maximize the margin, to define the decision boundary



Support Vector Machines



$$\max \frac{2}{\|w\|}$$

subject to

$$y_n \begin{cases} +1 & w^T x + b \geq 1 \\ -1 & w^T x + b \leq -1 \end{cases}$$

which we can write as $y_n(w^T x + b) \geq 1$

$$max\frac{2}{||w||} = max\frac{1}{||w||} = min||w|| = min\frac{1}{2}||w||^2$$

$$b = \frac{1}{S}\sum_{i=1}^{S}(y_i - w \cdot x)$$

$$w = \sum_{i=1}^{m} \alpha_i y_i x_i$$

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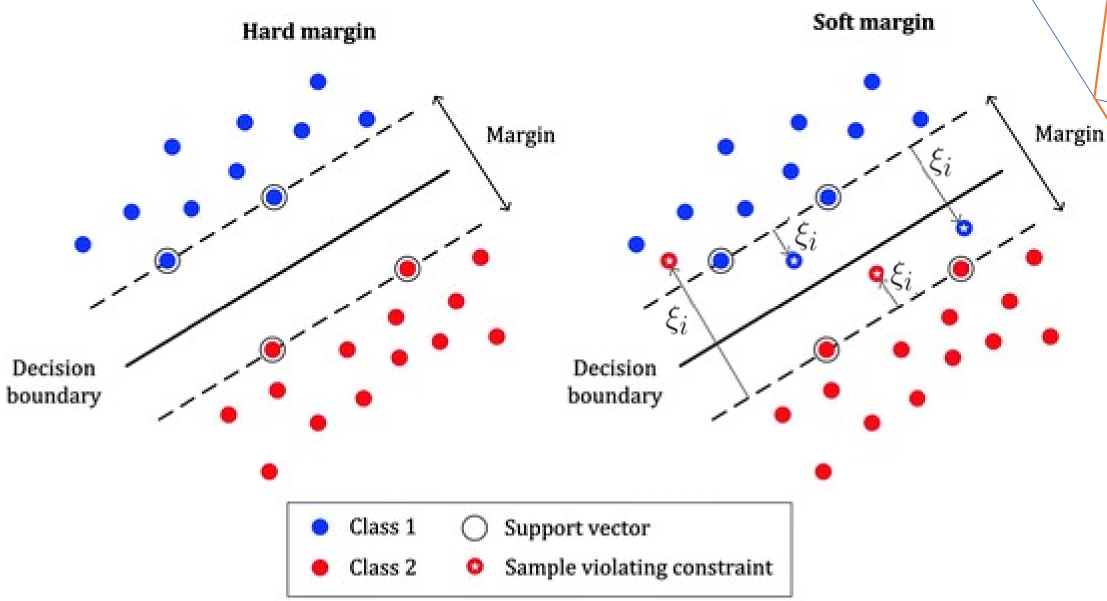
Soft-margin SVM

So far we have considered the case with no errors (hard margin).
How do we handle the case where there is is overlap?

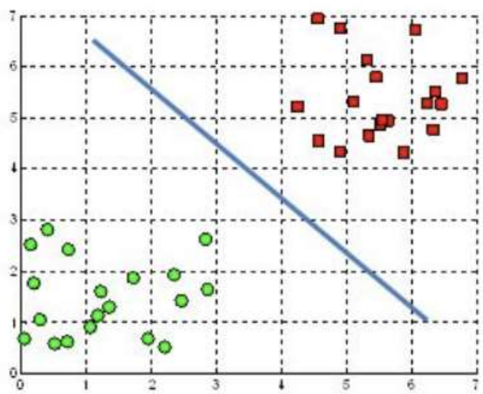


$$\underbrace{\min \frac{1}{2}\|w\|^2}_{\text{regularizer}} + \underbrace{C_i \sum_{i=1}^{n} \xi_i}_{\text{error term}}$$

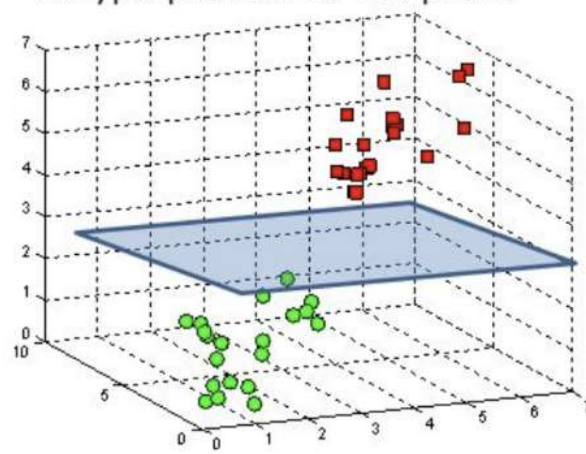
Hyperplanes

A decision boundary is defined by a hyperplane

A hyperplane in $\mathbb{R}^2$ is a line



A hyperplane in $\mathbb{R}^3$ is a plane

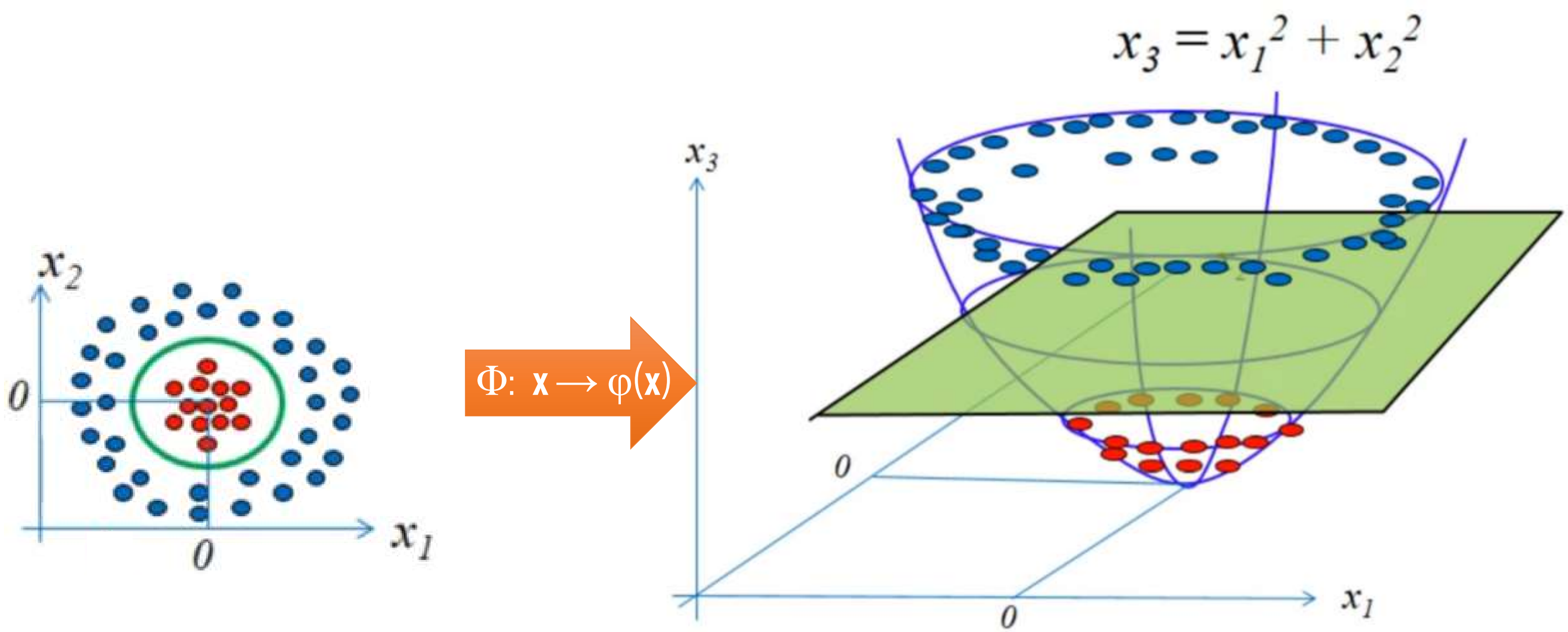


Kernels

What do we do about non-linear decision boundaries?

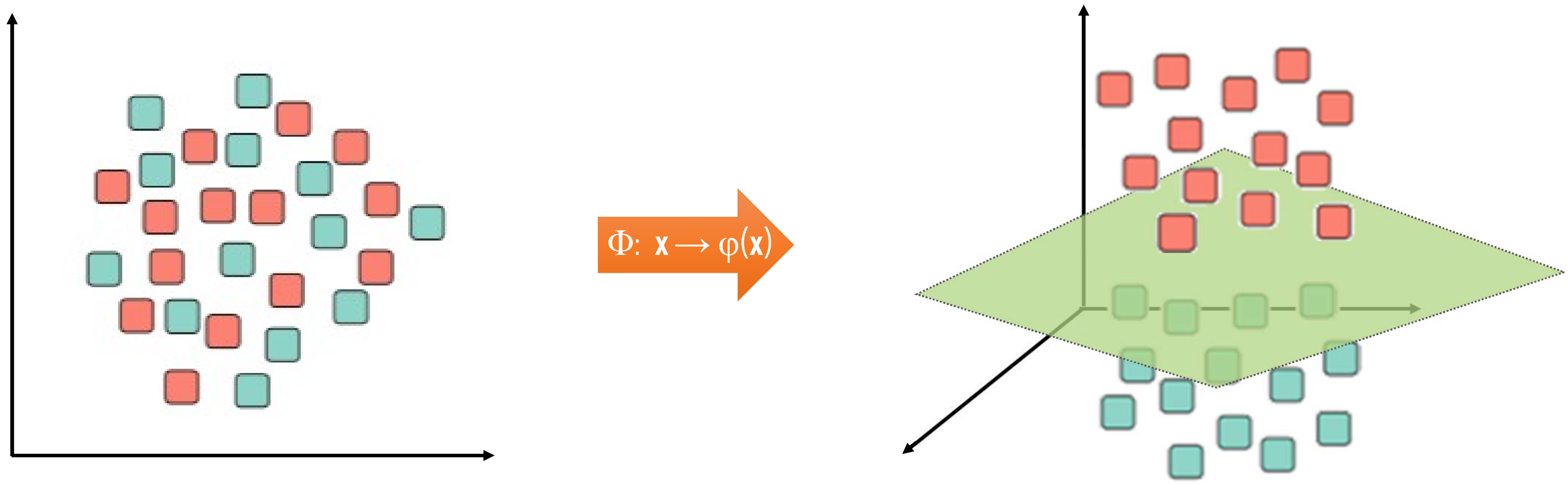
Non-linear decision boundaries

- Map the original input space to a higher-dimensional feature space where the training set is separable.



The "kernel trick"

- Kernels allow us to keep using a linear classifier – because we have embedded the data in a higher-dimensional feature space



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The “kernel trick’

- The linear classifier relies on dot product between vectors:
  $$K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i \cdot \mathbf{x}_j$$
- If every data point is mapped into high-dimensional space via some transformation
  $$\Phi: \mathbf{x}_i \rightarrow \varphi(\mathbf{x}_i)$$
  the dot product becomes:
  $$K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i) \cdot \varphi(\mathbf{x}_j)$$
- A *kernel function* is similarity function that corresponds to an inner product in some expanded feature space
- *The kernel trick*: instead of explicitly computing the lifting transformation $\varphi(\mathbf{x})$, define a kernel function K such that:
  $$K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i) \cdot \varphi(\mathbf{x}_j)$$
- Goal: Avoid having to directly construct $\varphi()$ at any point in the algorithm

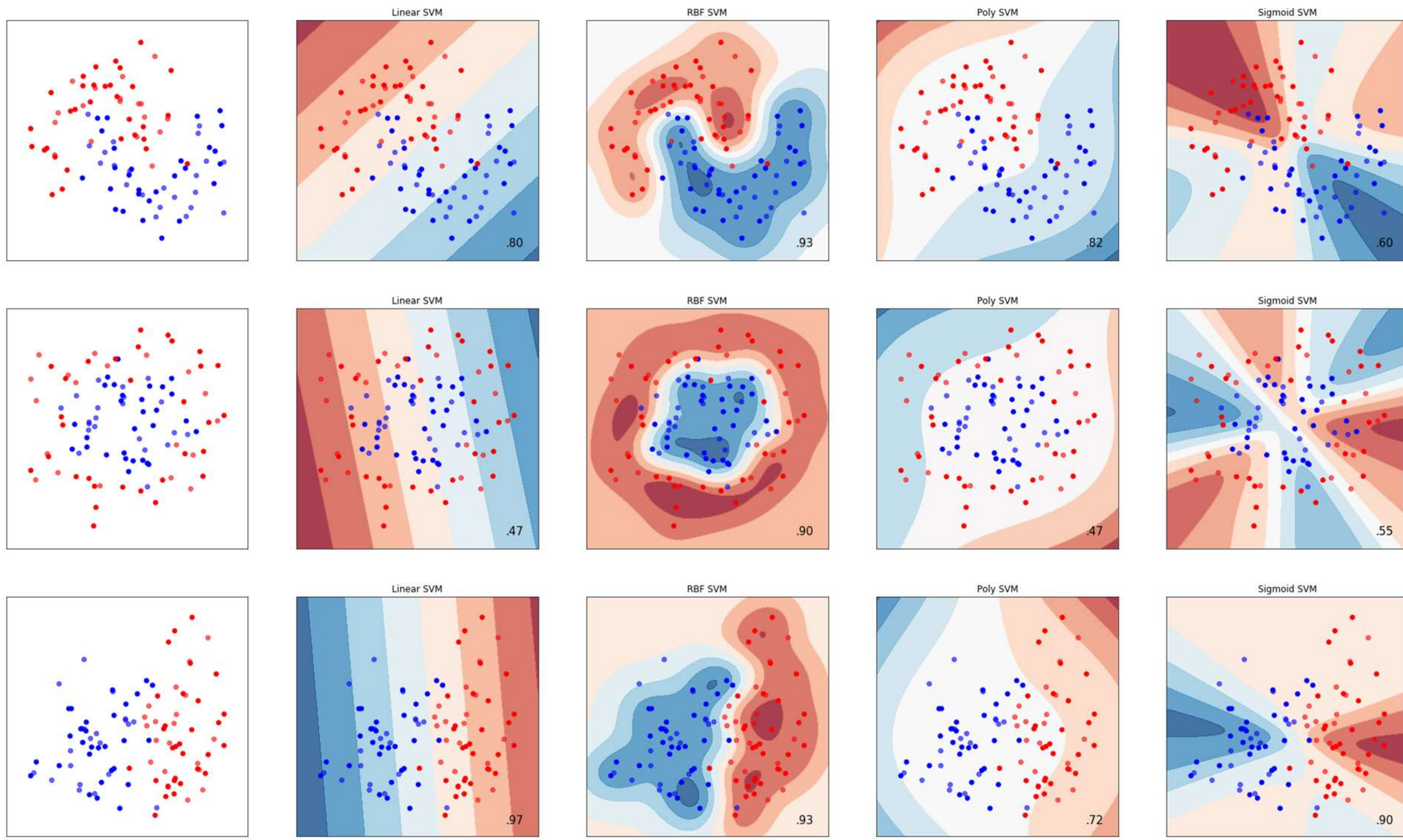
The “kernel trick’

- Kernel trick is allows extremely complex ϕ( ) while keeping K(a,b) simple
- Goal: Avoid having to directly construct ϕ( ) at any point in the algorithm

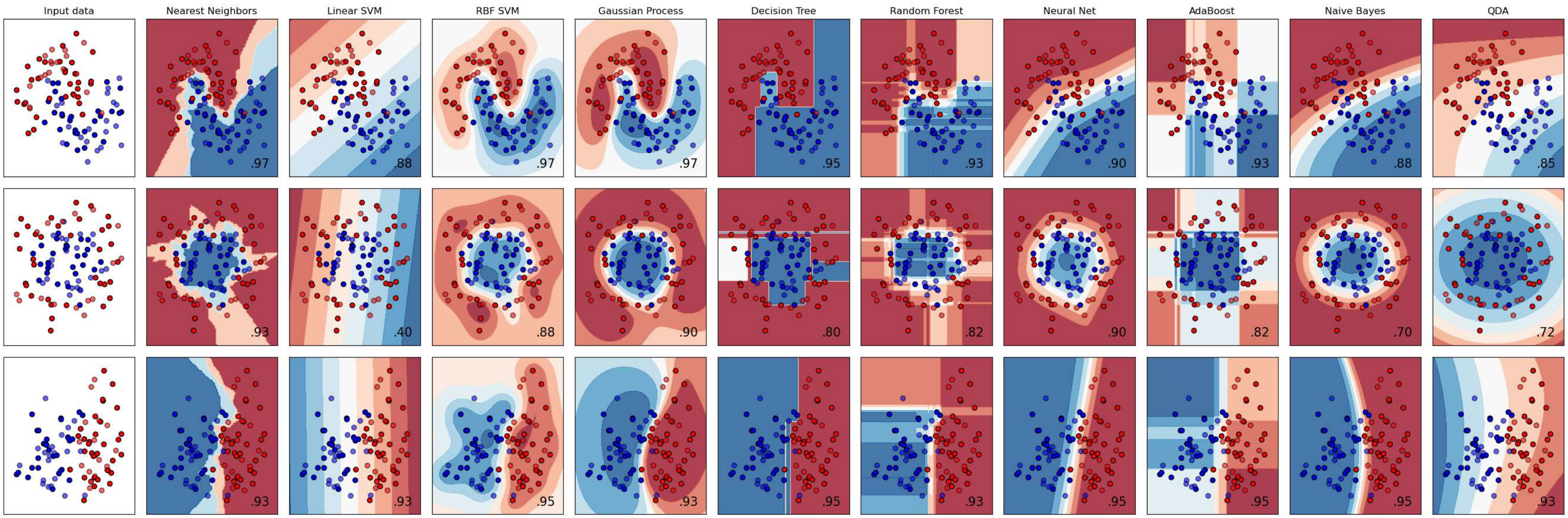
Common kernels

1. Polynomial kernel: $k(\mathbf{x_i}, \mathbf{x_j}) = (\mathbf{x_i} \cdot \mathbf{x_j} + 1)^d$
2. Gaussian kernel: $k(x, y) = \exp\left(-\frac{||x-y||^2}{2\sigma^2}\right)$
3. Gaussian radial basis function (RBF): $k(\mathbf{x_i}, \mathbf{x_j}) = \exp(-\gamma ||\mathbf{x_i} - \mathbf{x_j}||^2)$
4. Laplace RBF kernel: $k(x, y) = \exp\left(-\frac{||x-y||}{\sigma}\right)$
5. Sigmoid kernel: $k(x, y) = \frac{J_{v+1}(\sigma ||x-y||)}{||x-y||^{-n(v+1)}}$
6. ANOVA radial basis kernel: $k(x, y) = \sum_{k=1}^{n} \exp(-\sigma(x^k - y^k)^2)^d$
7. Linear splines kernel in one-dimension: $k(x, y) = 1 + xy + xy\ min(x, y) - \frac{x+y}{2}\ min(x, y)^2 + \frac{1}{3}\min(x, y)^3$

Comparison of kernels



Comparison of kernels



Source: https://scikit-learn.org/stable/auto_examples/classification/plot_classifier_comparison.html

Multi-class Classification

Turning a binary classifier into a multi-class classifier

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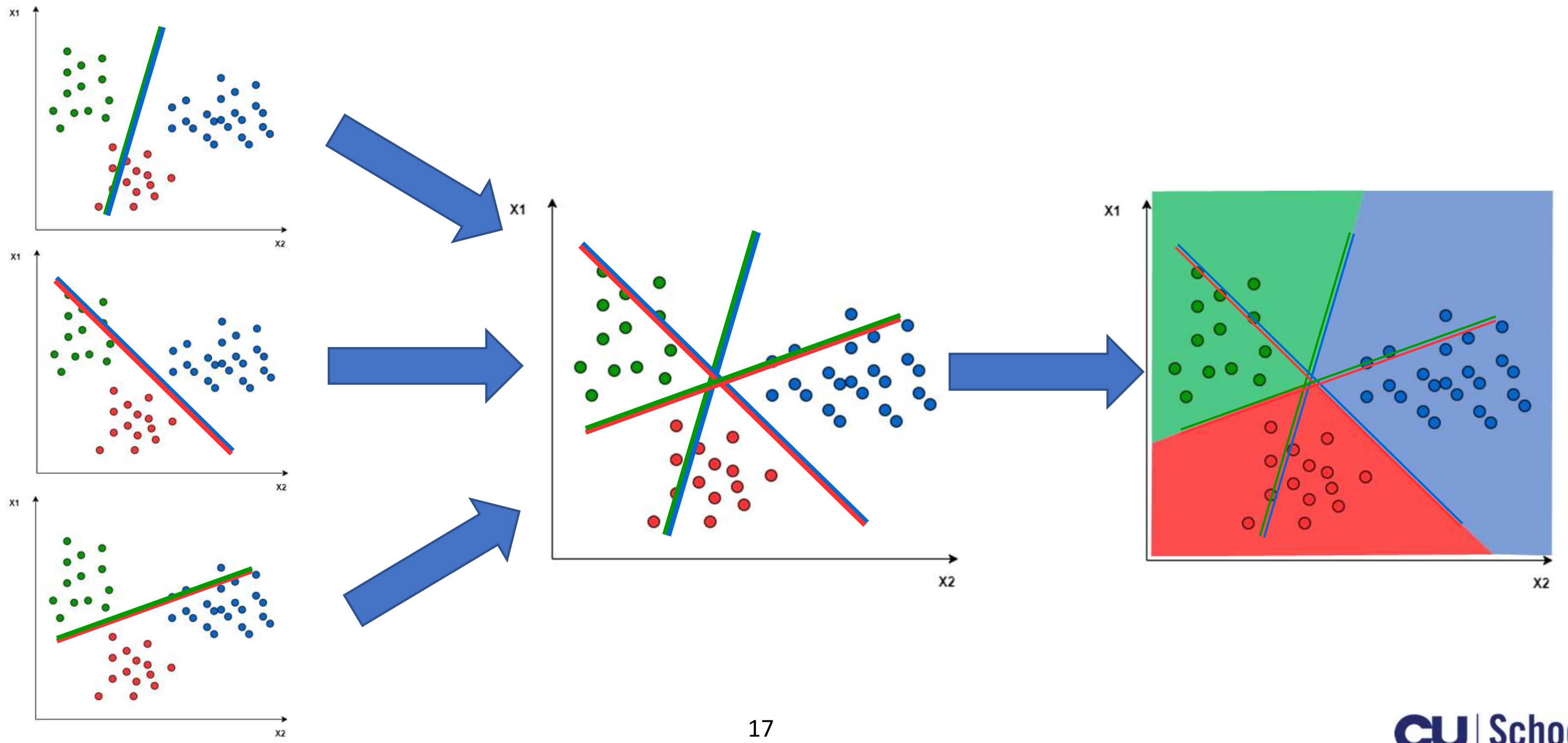
Multi-class SVM: One-vs-one

A hyperplane is generated between every two classes, neglecting the points of the third class.



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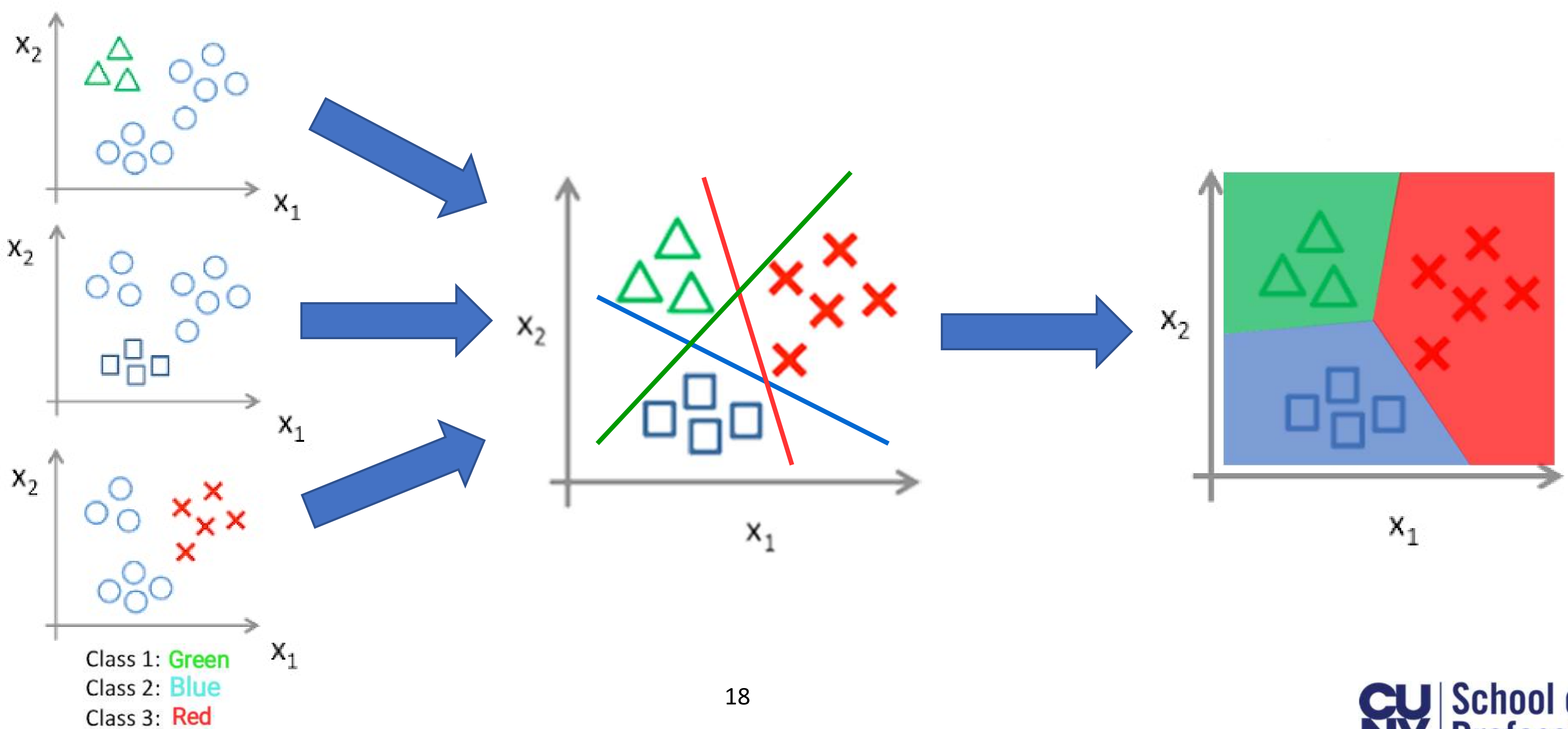
Multi-class SVM: One-vs-rest

A hyperplane is generated each class and all other classes at once.



Properties of SVMs

Benefits and weaknesses of SVMs

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Benefits of SVMs

- Works well on smaller cleaner datasets
- It can be more efficient because it uses a subset of training points
- Different kernel functions can be specified for the decision function
- Sparseness of solution when dealing with large data sets
  - Only support vectors are used to specify the separating hyperplane
- Ability to handle large feature spaces
  - Complexity does not depend on the dimensionality of the feature space
- Overfitting can be controlled by soft margin approach
- Guaranteed to converge to a single global solution (convex optimization)

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Weakness of SVMs

- Sensitive to noise
  - A relatively small number of mislabeled examples can dramatically decrease the performance
- Essentially a binary classifier
- Isn’t suited to larger datasets as the training time with SVMs can be high
- Less effective on noisier datasets with overlapping classes
- If the number of features is a lot bigger than the number of data points, avoiding over-fitting when choosing kernel functions and regularization term is crucial.

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