Support Vector Machines

Machine Learning

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Outline and References

- Outline
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  - Training [PRML 7.1.1]
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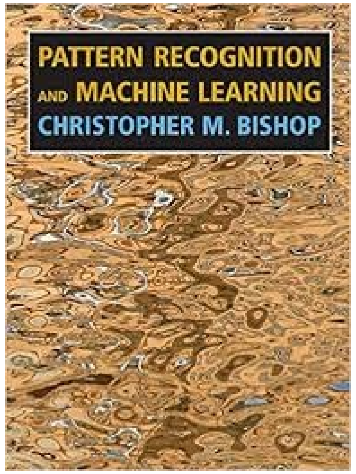
  - SVM for regression [PRML 7.1.4]

- References
  - Pattern Recognition and Machine Learning, Bishop [PRML]



Sparse Kernel Machines

- A significant limitation to kernel methods is that we need to compute the kernel function for each sample in the training set, that is often computationally unfeasible
- To deal with this issue, **sparse kernel methods** find **sparse** solutions, that rely only on a **subset** of the training samples
- The most well known among these methods are:
  - Support Vector Machines
  - Relevance Vector Machines

Sparse Kernel Machines

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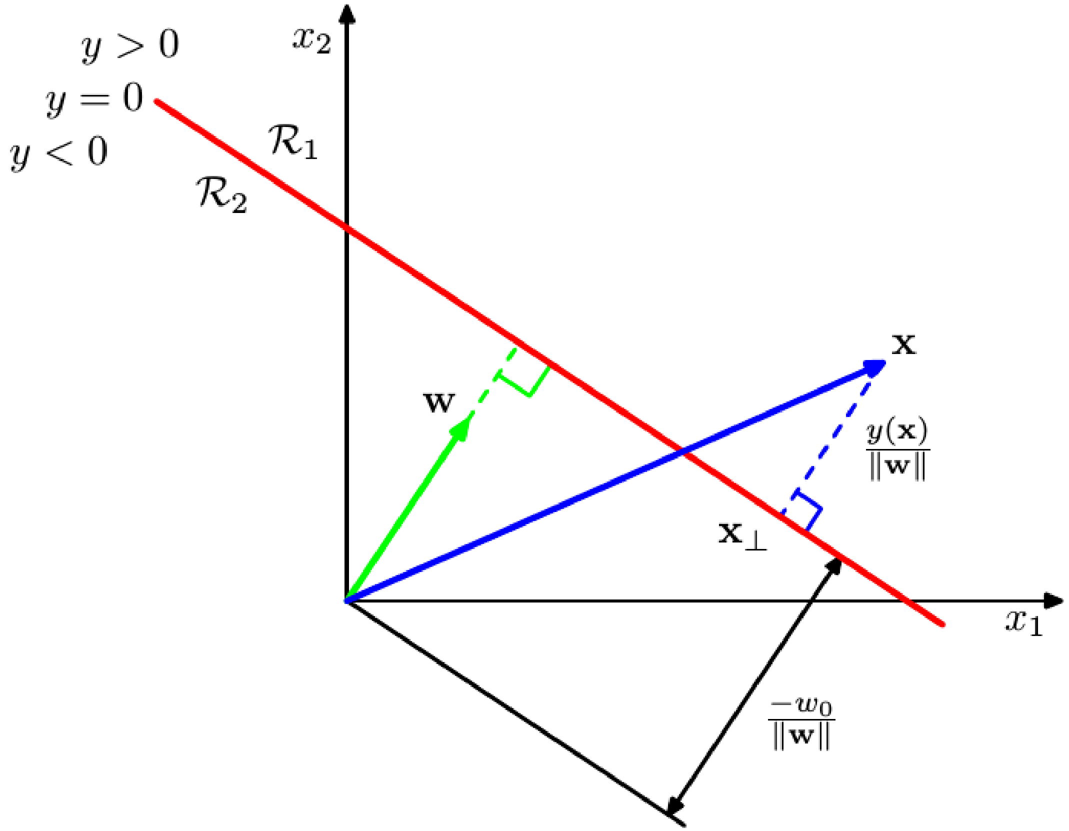
Separable Problems

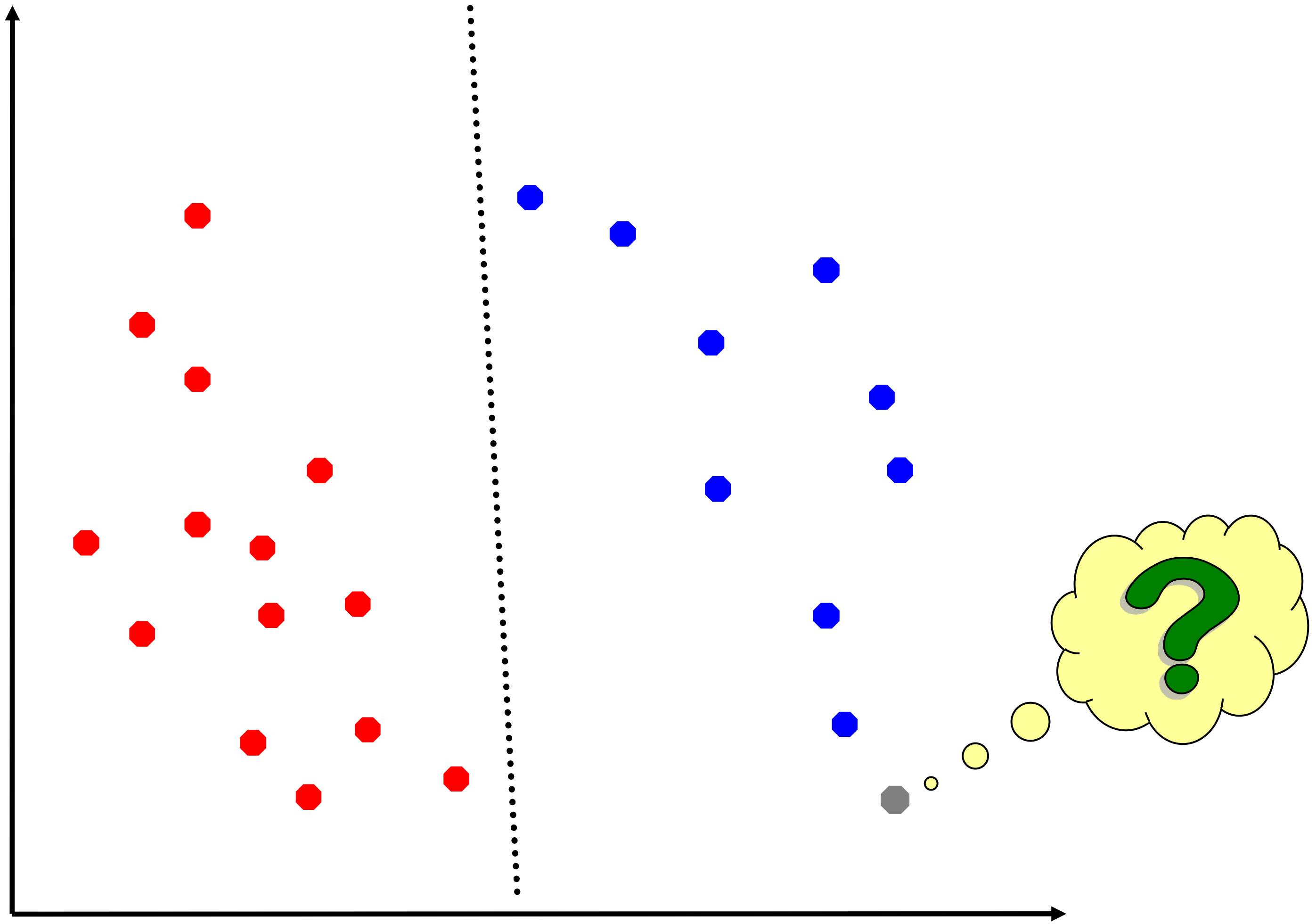
Do you remember the perceptron?

$$f(\mathbf{x}, \mathbf{w}) = \begin{cases} +1, & \text{if } \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + b \geq 0 \\ -1, & \text{otherwise} \end{cases}$$

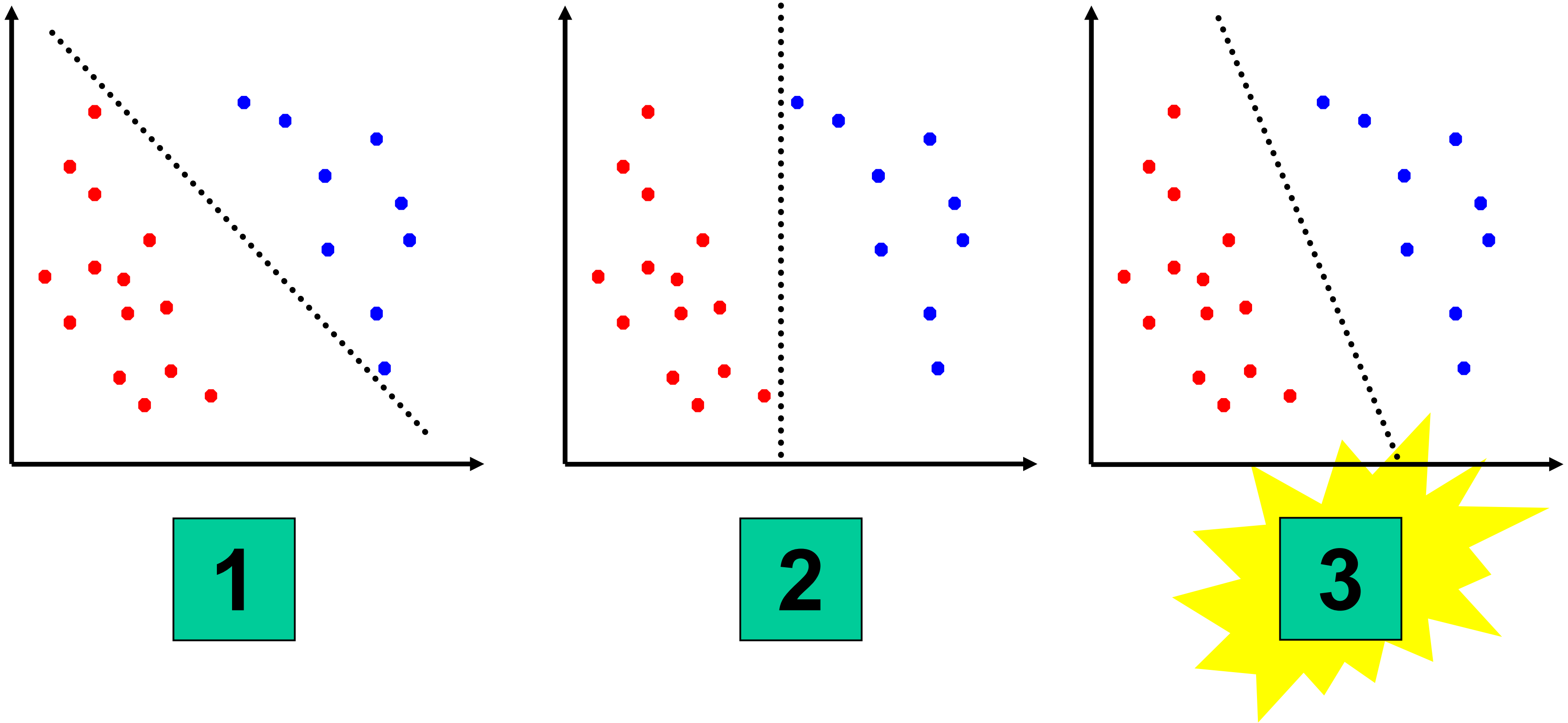


- Properties
  - DS is $y(\cdot) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + b = 0$
  - DS is orthogonal to $\mathbf{w}$
  - distance of DS from origin is $-\frac{w_0}{\|\mathbf{w}\|_2}$
  - distance of $\mathbf{x}$ from DS is $\frac{y(\mathbf{x})}{\|\mathbf{w}\|_2}$

The perceptron in action



Are all the solution equivalent?



Maximum Margin Classifier

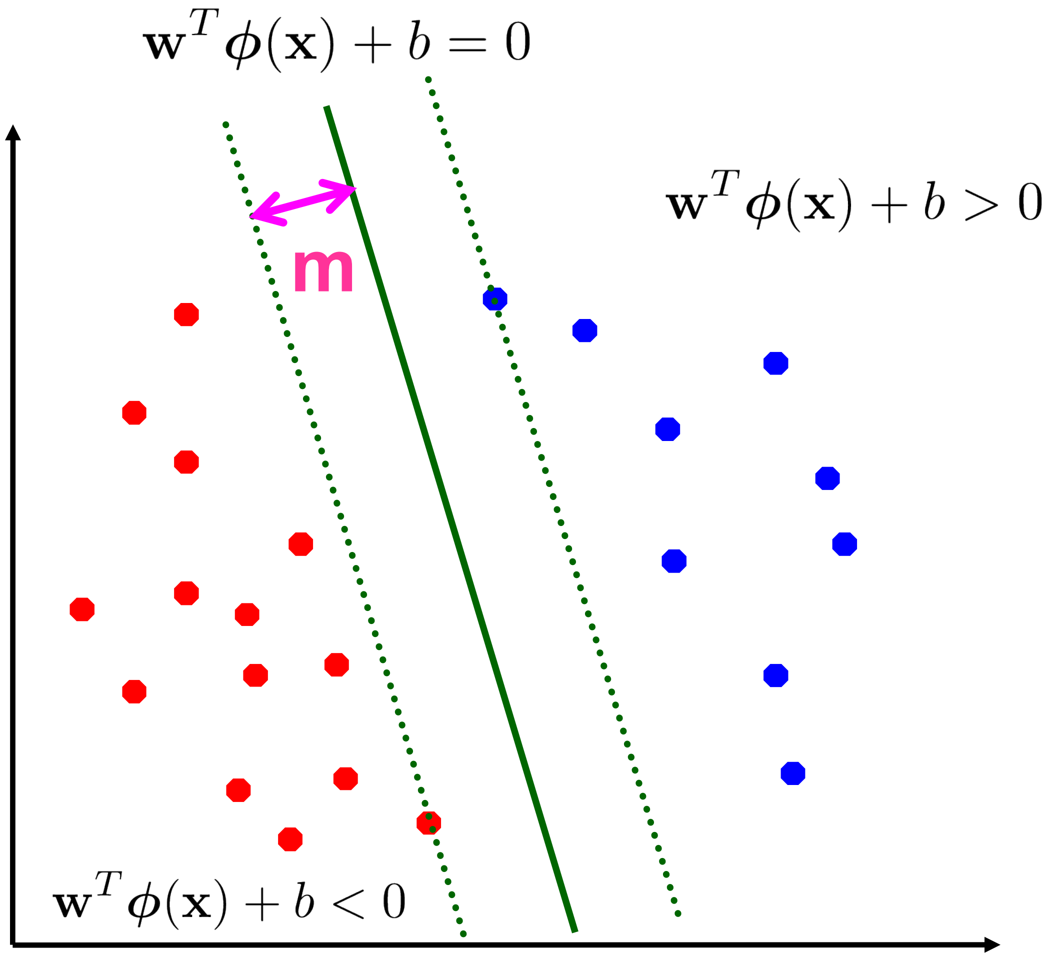
- The margin will be:

$$margin = \min_n \frac{t_n(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) + b)}{||\mathbf{w}||}$$

- Thus, the optimal **hyperplane** will be:

$$\arg\max_{\mathbf{w},b} \left\{ \min_n \left[\frac{t_n(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) + b)}{||\mathbf{w}||} \right] \right\}$$

- Unfortunately, solving this optimization problem would be very complex...



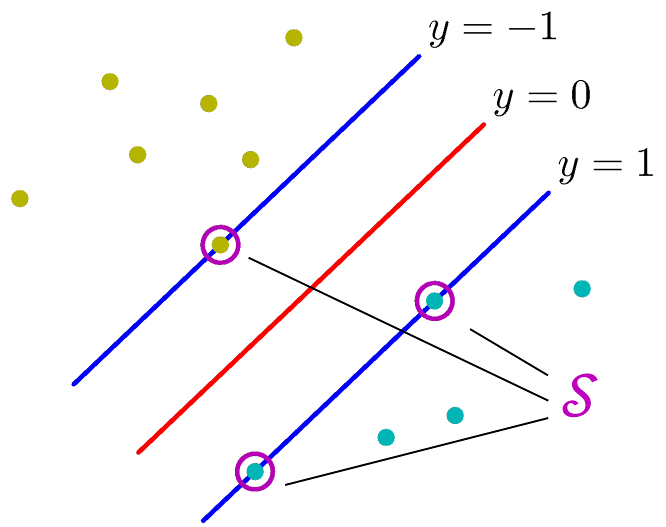
Equivalent constrained optimization problem

- **Canonical** hyperplane
  - There are infinite equivalent solutions:

$$\kappa \mathbf{w}^T \phi(\mathbf{x}) + \kappa b \quad \forall \kappa > 0$$

  - We will consider only solutions such that:

$$t_n(\mathbf{w}^T \phi(\mathbf{x}_n) + b) = 1 \quad \forall \mathbf{x}_n \in \mathcal{S}$$



- Equivalent **quadratic programming** problem

$$\begin{aligned} &\textbf{Minimize} \quad \frac{1}{2}\|\mathbf{w}\|_2^2 \\ &\textbf{Subject to} \quad t_n(\mathbf{w}^T \phi(\mathbf{x}_n) + b) \geq 1, \ \text{for all } n \end{aligned}$$

Derivation of dual problem

See [PRML - Appendix E]

- We can derive the dual problem using **Lagrance multipliers**:

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \left(t_i \left(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b\right) - 1\right)$$

- We need to maximize $\mathcal{L}$ with respect to α and minimize it with respect to $\mathbf{w}$ and b
- We can compute the gradient w.r.t. $\mathbf{w}$ and b and derive dual representation

$$\frac{\partial}{\partial \mathbf{w}}\mathcal{L} = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i t_i \boldsymbol{\phi}(\mathbf{x}_i)$$

$$\frac{\partial}{\partial b}\mathcal{L} = 0 \quad \Rightarrow \quad \sum_{i=1}^{n} \alpha_i t_i = 0$$

Dual Problem

- We can now rewrite the optimization problem as:

$$\textbf{Maximize} \quad \tilde{\mathcal{L}}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

$$\textbf{Subject to} \quad \alpha_n \geq 0 \text{ and } \sum_{n=1}^{N} \alpha_n t_n = 0, \qquad \text{for } n = 1, \ldots, N$$

  - where the explicit feature mapping does not appear explicitly anymore

Discriminant Function and Support Vectors

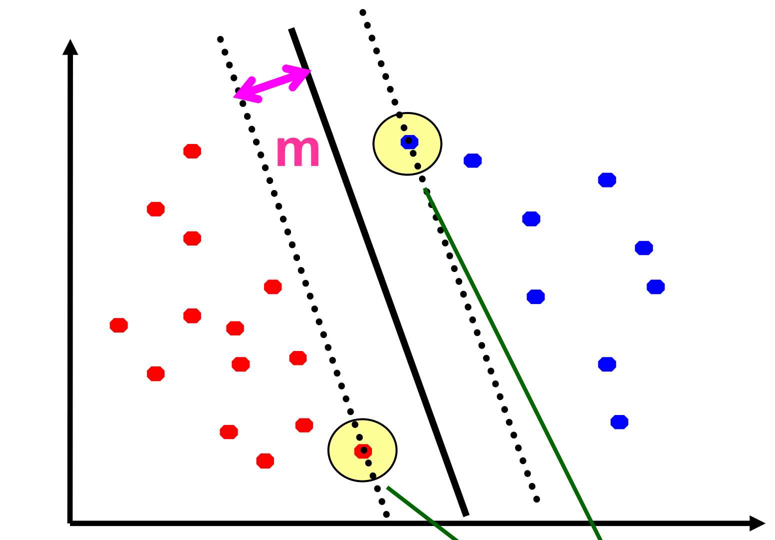
- The resulting discriminant function is:

$$y(\mathbf{x}) = \sum_{n=1}^{N} \alpha_n t_n k(\mathbf{x}, \mathbf{x}_n) + b$$

  - Only samples on the margin does contribute (i.e., $\alpha_i > 0$),
  - These samples are the Support Vectors
  - The bias is computed as:

$$b = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_n \in \mathcal{S}} \left(t_n - \sum_{\mathbf{x}_m \in \mathcal{S}} \alpha_m t_m k(\mathbf{x}_n, \mathbf{x}_m) \right)$$

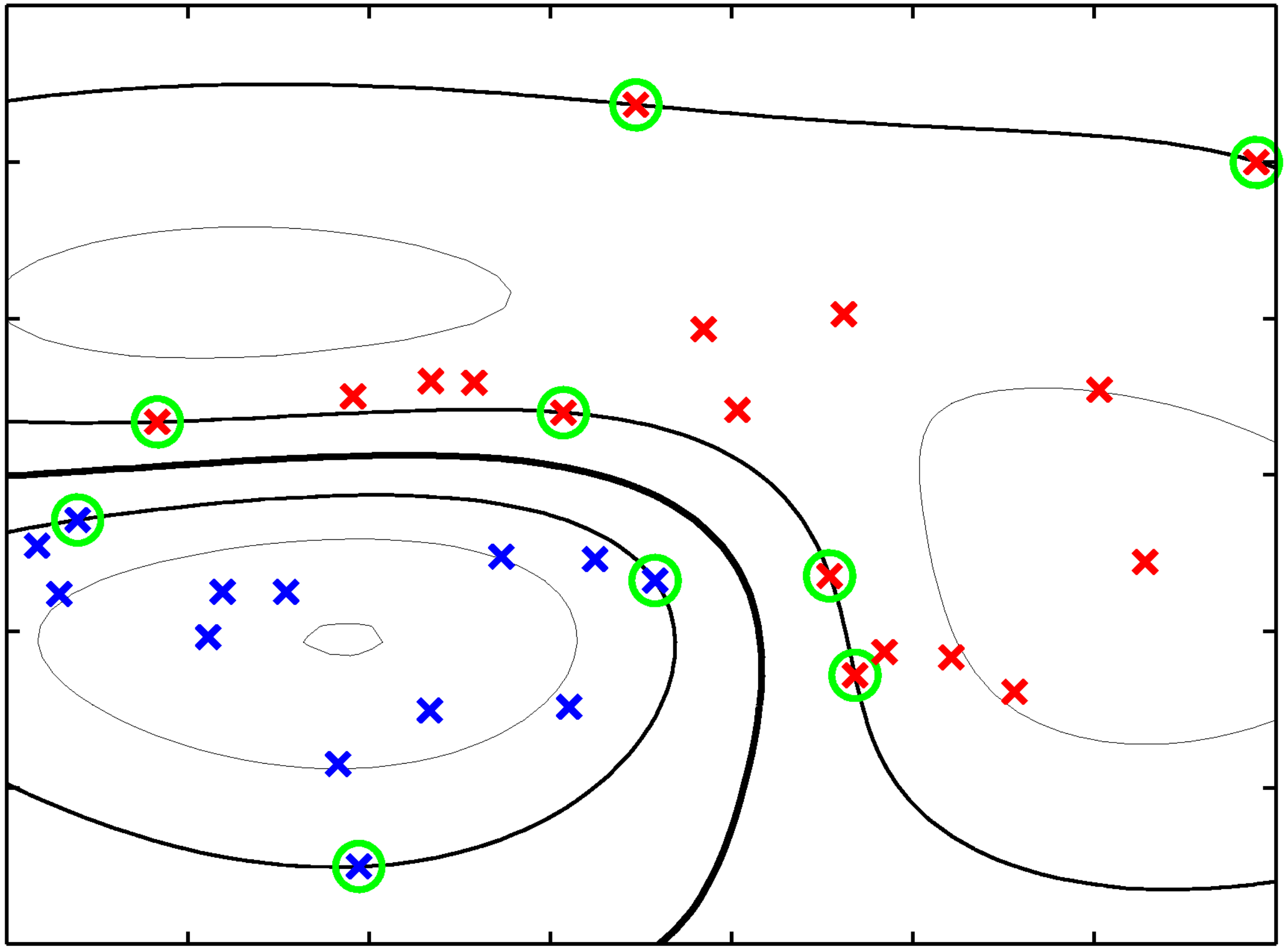
Support Vectors ($\mathcal{S}$)



$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \underbrace{\left(t_i \left(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b \right) - 1 \right)}_{0}$$

Example

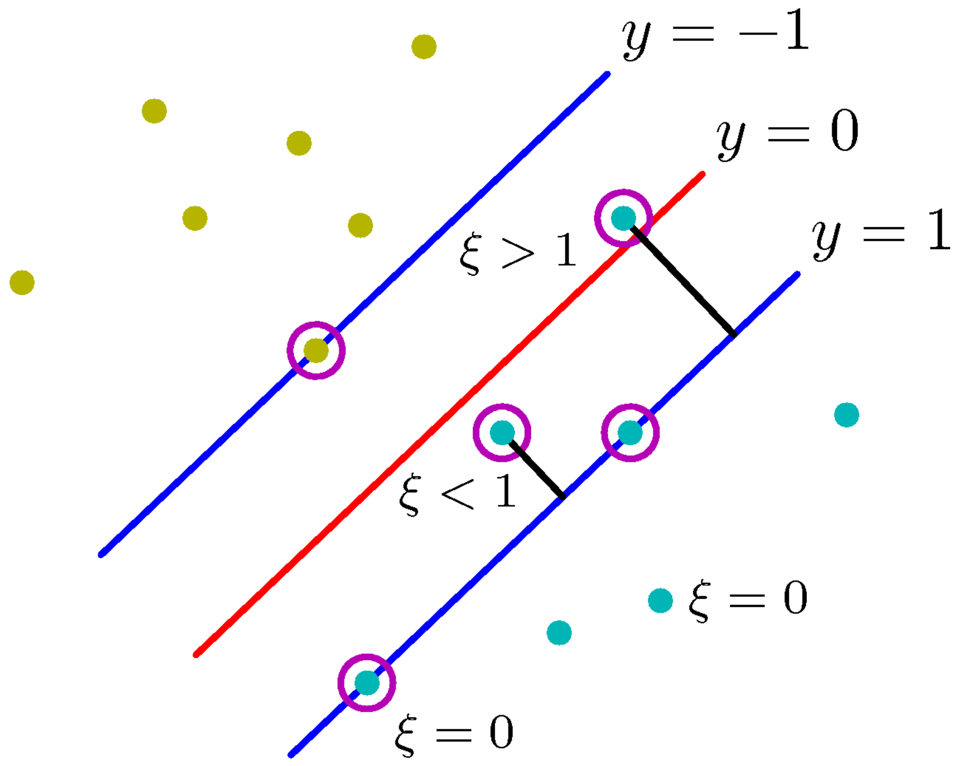
- An example of SVM discriminant function using Gaussian kernel function



Non-separable Problems

Non-Separable Problem

- So far, we assumed that samples are linearly separable in the feature space
- However, this is not always the case (e.g., noisy data)
- How to deal with such problems? We allow "error" (ξ_i) in classification:



Soft-Margin optimization problem

$$\begin{aligned} &\textbf{Minimize} \quad && \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N}\xi_n \\ &\textbf{Subject to} \quad && t_n(\mathbf{w}^T\phi(\mathbf{x}_n)+b) \geq 1-\xi_n, \qquad && \text{for all } n \\ & && \xi_n \geq 0, && \text{for all } n \end{aligned}$$

- ξ_n are called **slack variables** and represents **penalties** to **margin violation**
- *C* is a tradeoff parameter between error and margin
  - it allows to adjust the **bias-variance tradeoff**
  - **tuning** is required to find optimal value for C

Dual Representation (Box Constraints Problem)

$$\textbf{Maximize} \quad \tilde{\mathcal{L}}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

$$\textbf{Subject to} \quad 0 \leq \alpha_n \leq C, \qquad \text{for } n = 1, \ldots, N$$

$$\sum_{n=1}^{N} \alpha_n t_n = 0,$$

- As usual, **support vectors** are the samples for which $\alpha_n > 0$
  - If $\alpha_n < C \Rightarrow \xi_n = 0$, i.e., the sample is on the margin
  - If $\alpha_n = C$ the sample can be inside the margin and be either correctly classified ($\xi_n \leq 1$) or misclassified ($\xi_n > 1$)

Alternative formulation: ν-SVM

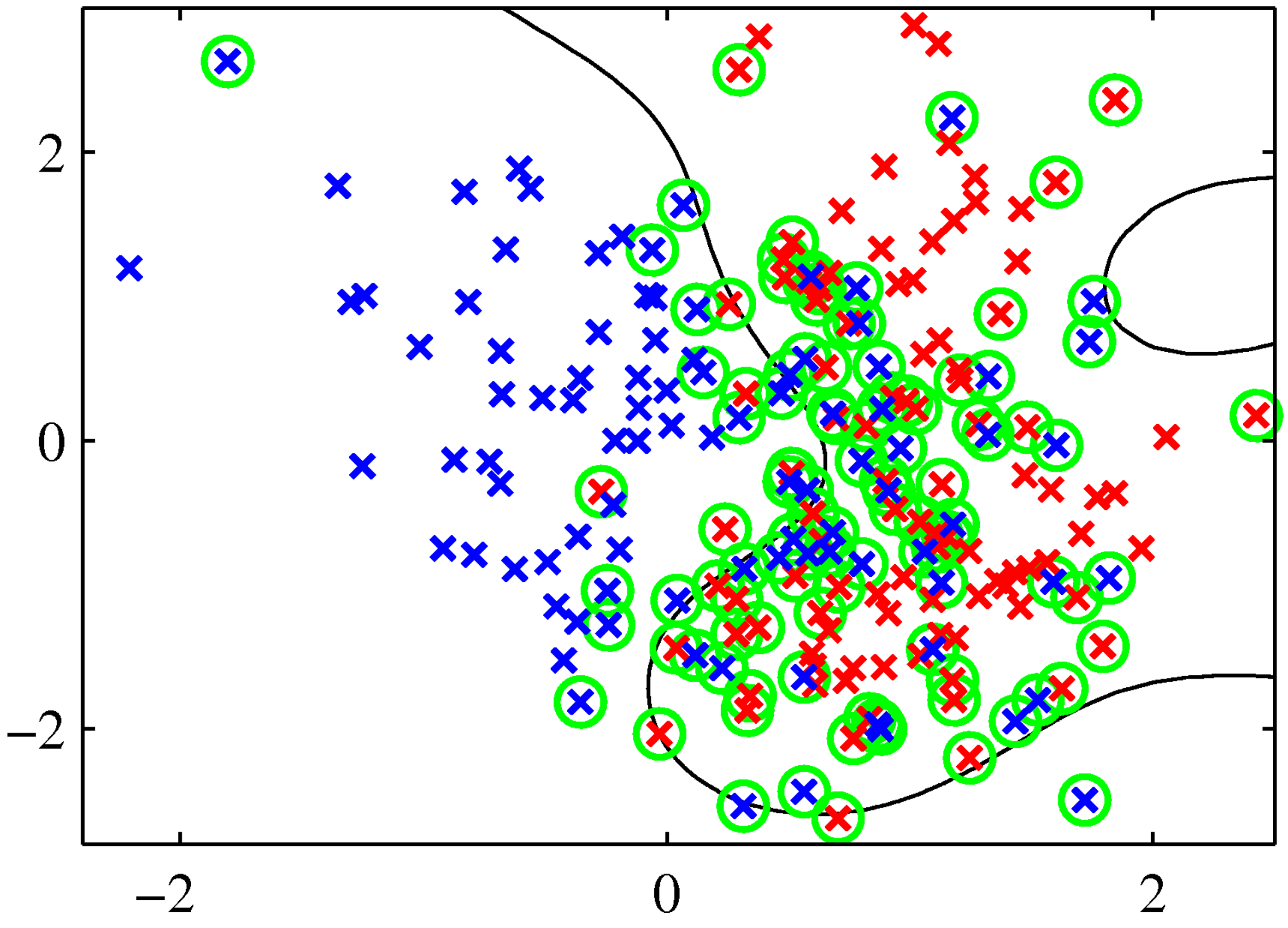
$$
\begin{aligned}
\textbf{Maximize} \quad & \tilde{\mathcal{L}}(\boldsymbol{\alpha}) = -\frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_n \alpha_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m) \\
\textbf{Subject to} \quad & 0 \leq \alpha_n \leq 1/N, \\
& \sum_{n=1}^{N} \alpha_n t_n = 0, \\
& \sum_{n=1}^{N} \alpha_n \geq \nu \qquad \text{for } n = 1, \ldots, N
\end{aligned}
$$

- Where $0 \leq \upsilon < 1$ is a user parameter that allow to control both the margin errors and the number of support vectors:

fraction of Margin Errors ≤ ν ≤ fraction of SVs

Example

- An example of ν-SVM discriminant function using Gaussian kernel function

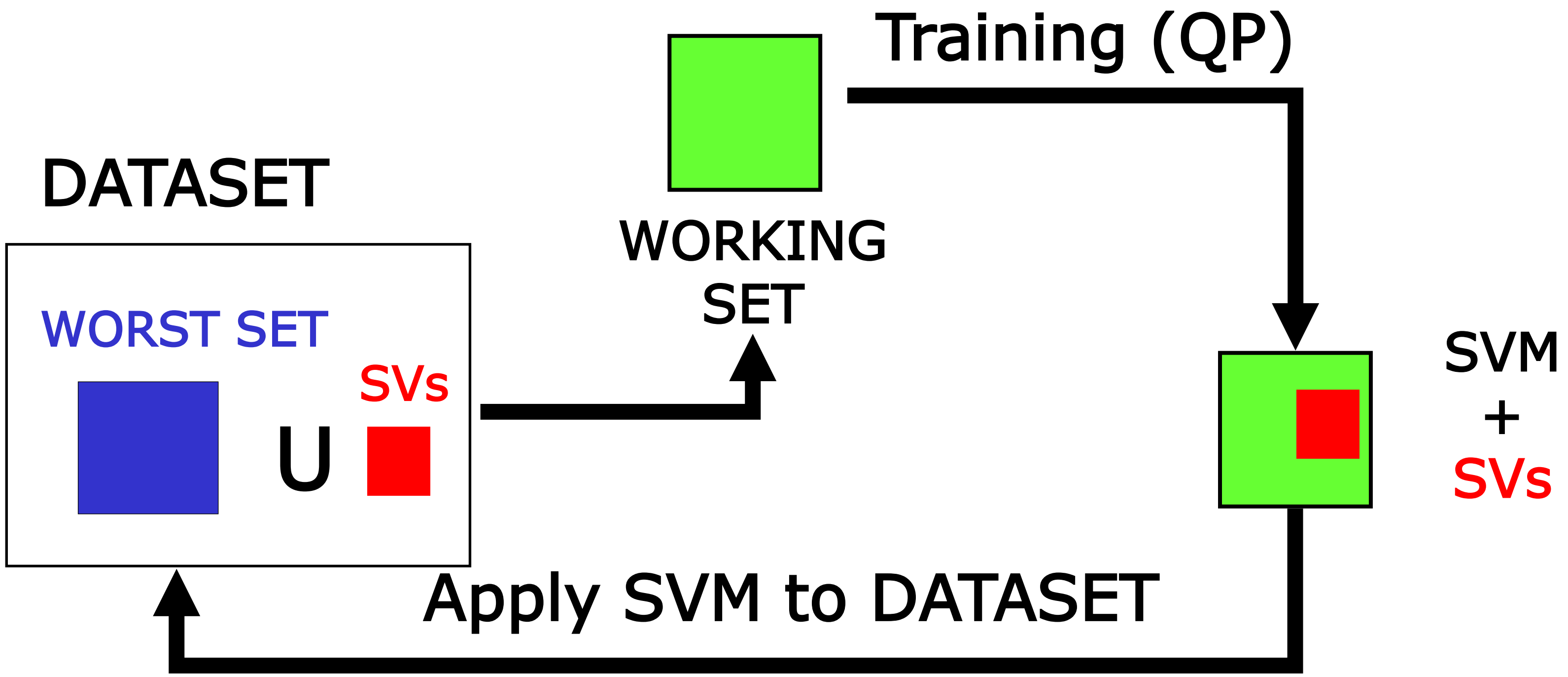


Training SVM in Practice

SVM Training

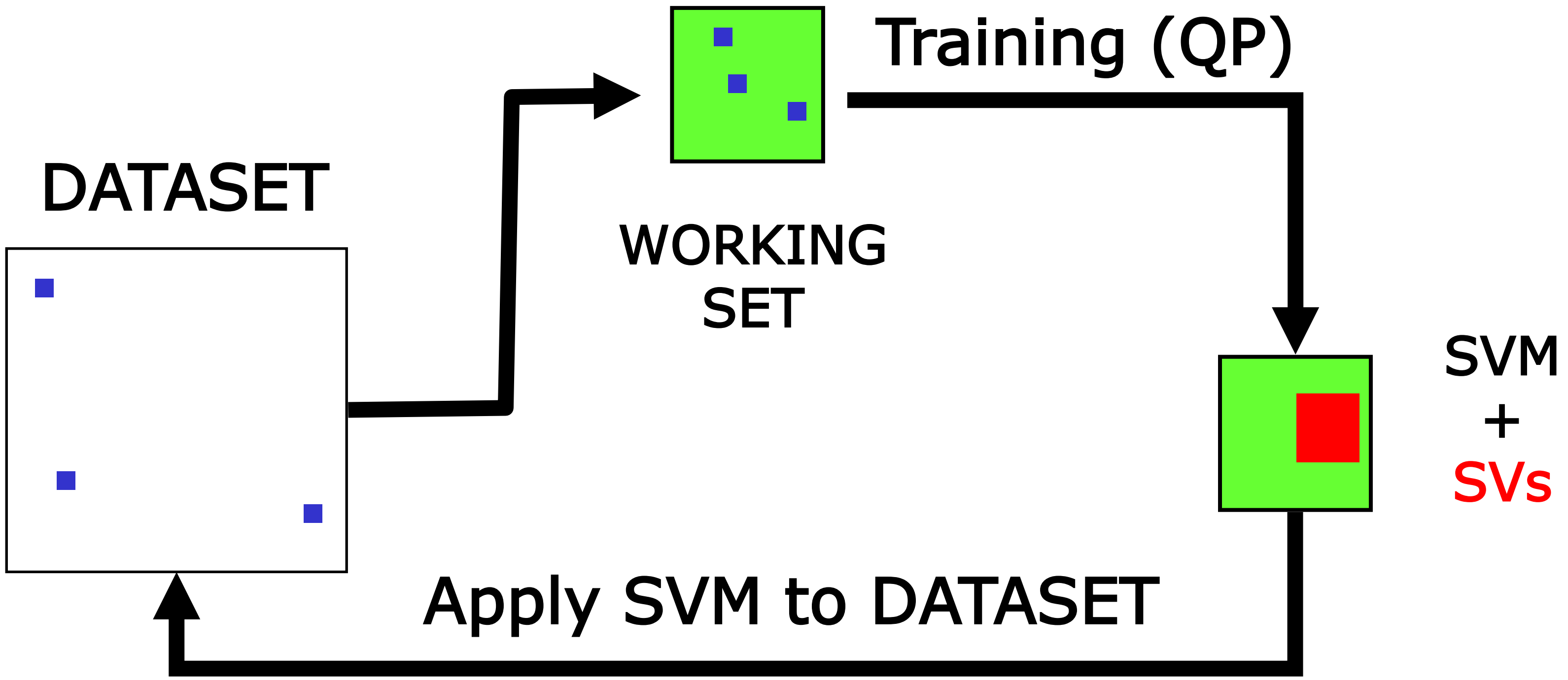
- Just solve the optimization problem to find α_i and b
- … but it is very expensive: $O(n^3)$ where n is the size of training set
- Faster approaches:
  - Chunking
  - Osuna’s methods
  - Sequential Minimal Optimization
- Online learning:
  - Chunking-based methods
  - Incremental methods

Chunking



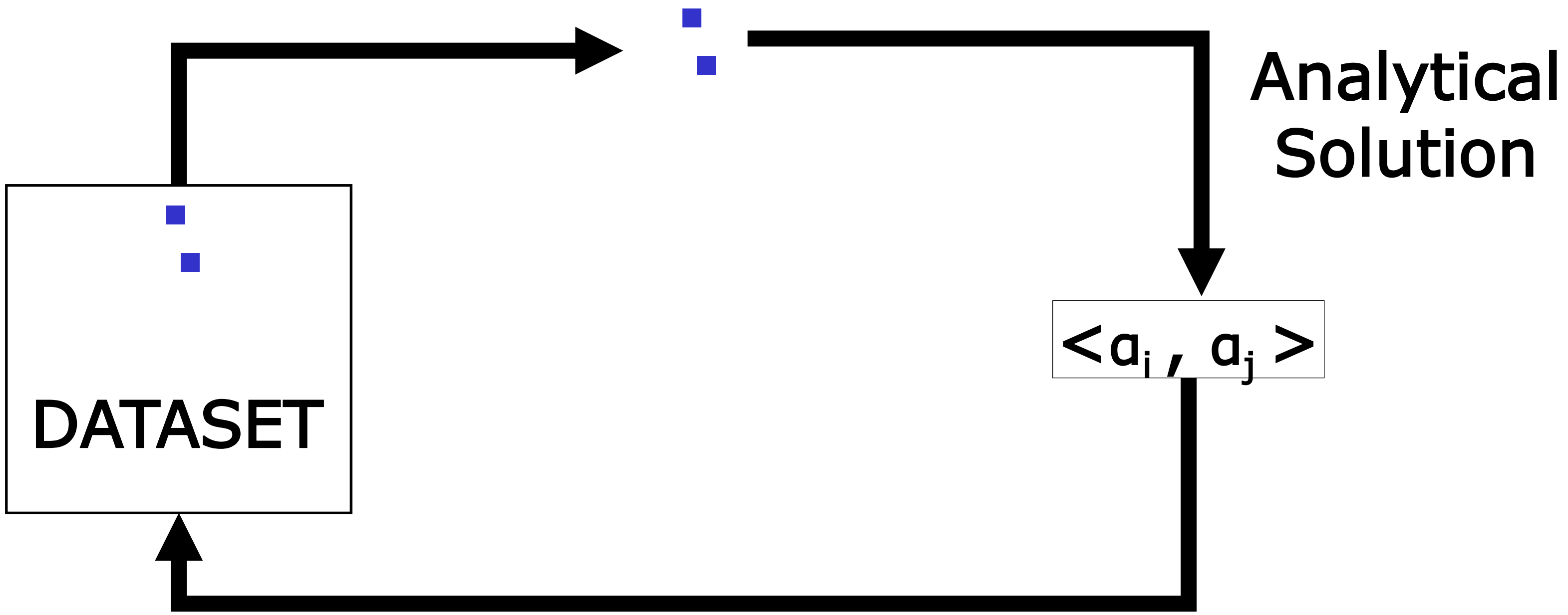
- Solves iteratively a sub-problem (working set)
- Build the working set with current SVs and the M samples with the bigger error (worst set)
- Size of the working set may increase!
- Converges to optimal solution!

Osuna's Method



- Solves iteratively a sub-problem (working set)
- Replace some samples in the working set with missclassified samples in data set
- Size of the working set is fixed!
- Converges to optimal solution!

Sequential Minimal Optimization

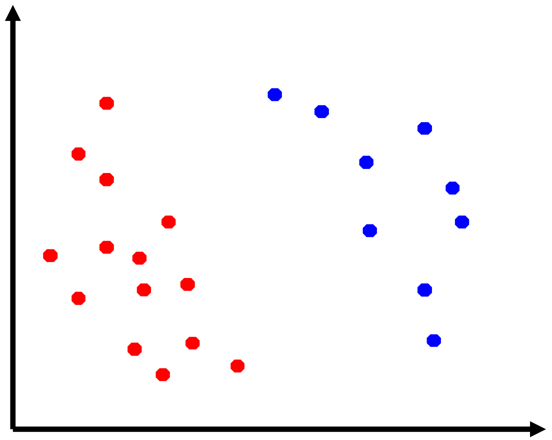


- Works iteratively only on two samples
- Size of the working set is minimal and multipliers are found analytically
- Converges to optimal solution!

Multi-class SVM

Multi-class SVM

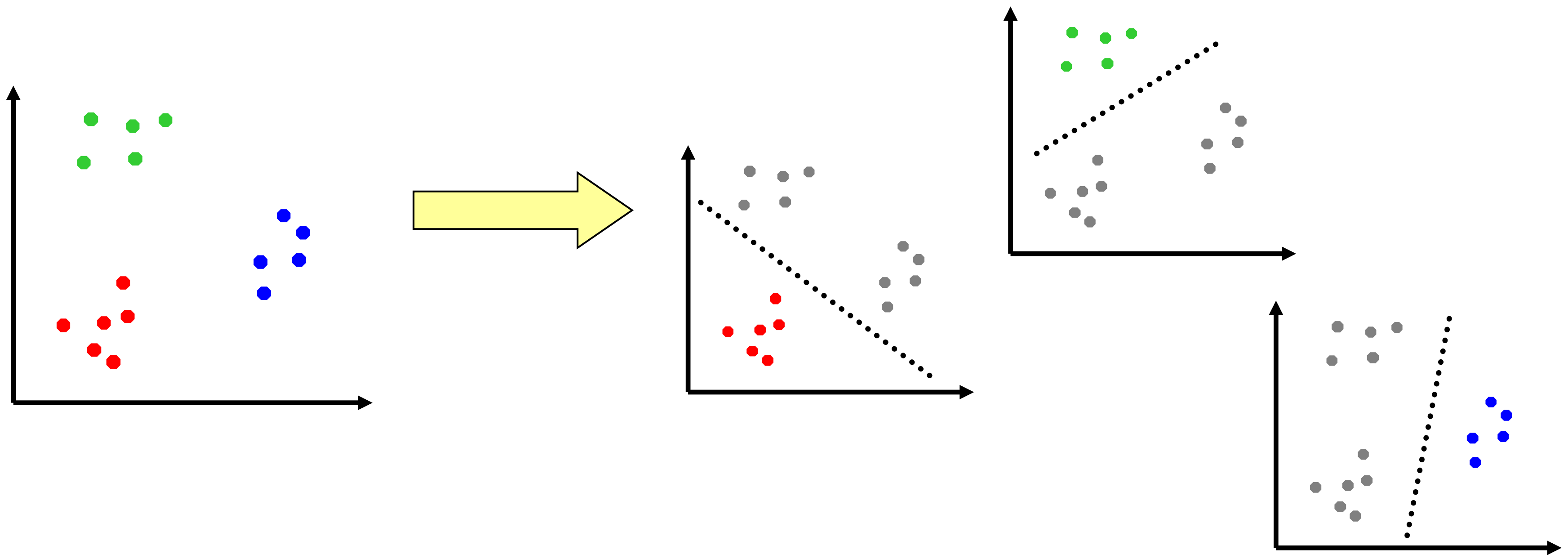
- So far we considered two-classes problems:



- How does SVM deal with multi-class problems?

One-against-all

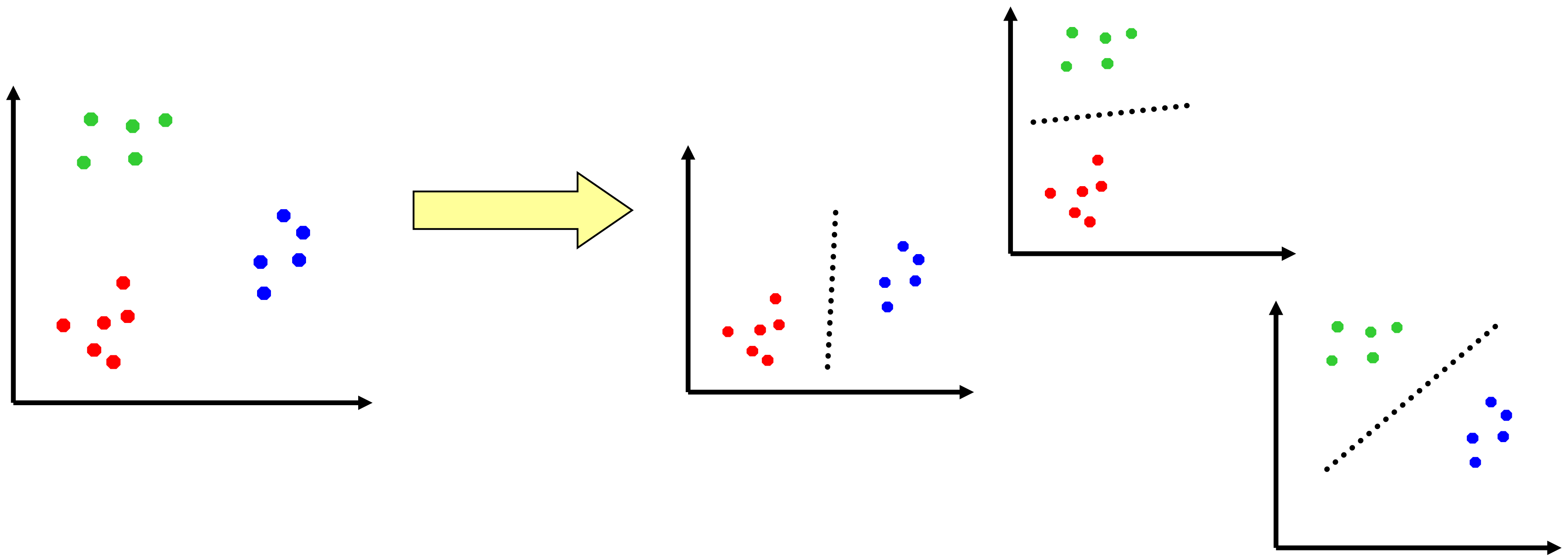
- A k-class problem is decomposed in k binary (2-class) problems



- Training is performed on the entire dataset and involves k SVM classifiers
- Test is performed choosing the class selected with the highest margin among the k SVM classifiers

One-against-one

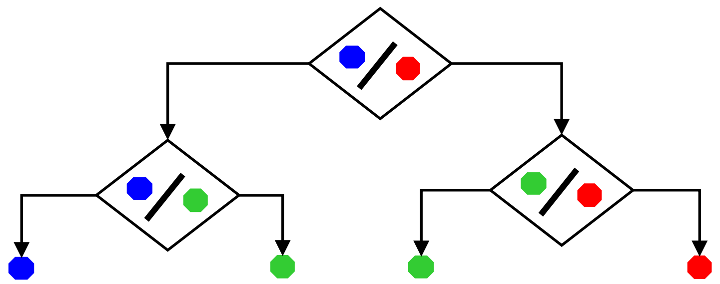
- A k-class problem is decomposed in k(k-1)/2 binary (2-class) problems



- The k(k-1)/2 SVM classifiers are trained on subsets of the dataset
- Test is performed by applying all the k(k-1)/2 classifiers to the new sample and the most voted label is chosen

DAGSVM

- In DAGSVM, the k-class problem is decomposed in k(k-1)/2 binary (2-class) problems as in one-against-one
- Training is performed as in one-against-one
- But test is performed using a Direct Acyclic Graph to reduce the number of SVM classifiers to apply:



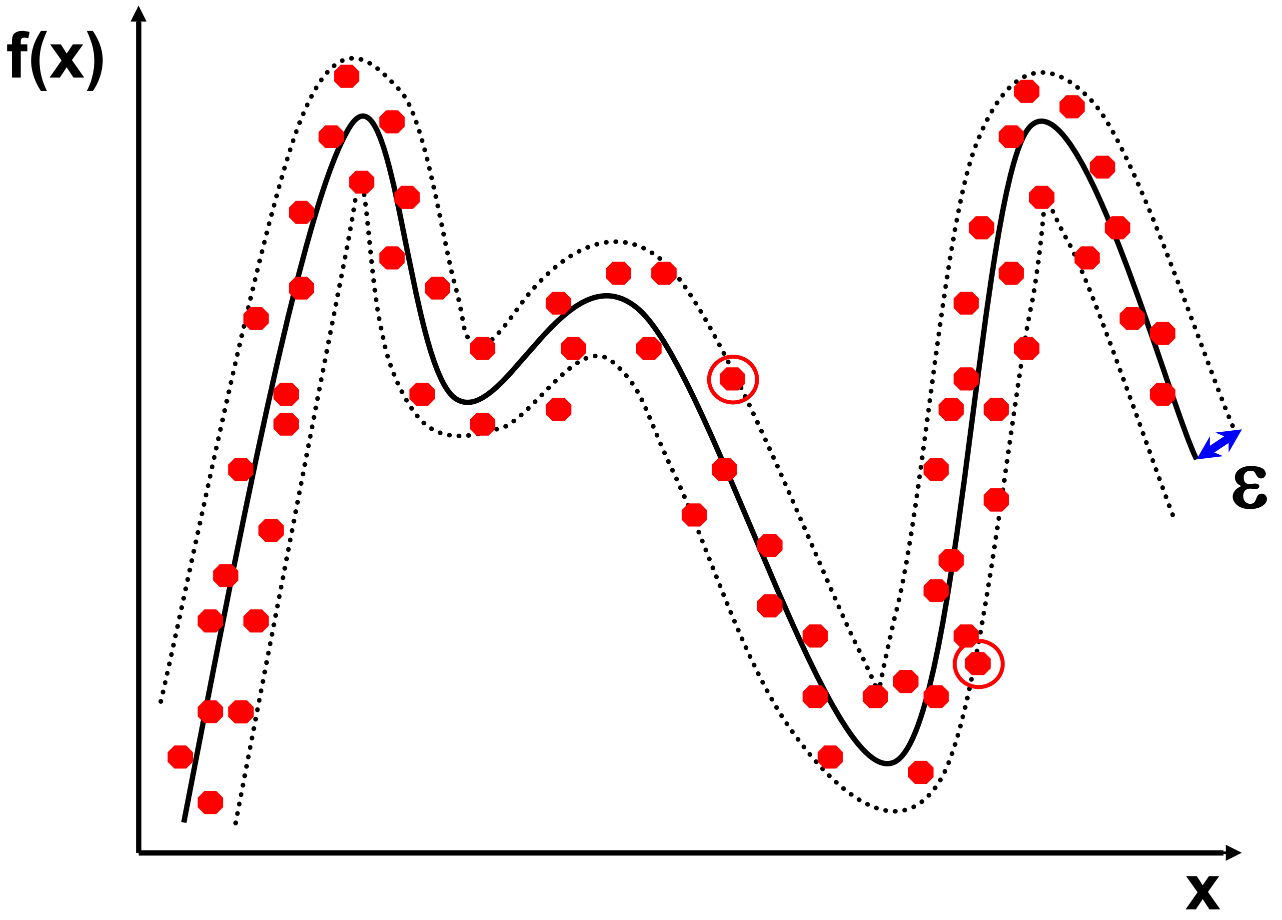
- The test process involves only k-1 binary SVM classifiers instead of k(k-1)/2 as in one-against-one approach

Multi-class SVM: summary

- One-against-all
  - **cheap** in terms of **memory** requirements
  - **expensive training** but **cheap test**
- One-against-one
  - **expensive** in terms of **memory** requirements
  - **expensive test** but **slightly cheap training**
- DAGSVM
  - **expensive** in terms of **memory** requirements
  - **slightly cheap training** and **cheap test**
- **One-against-one** is the **best performing** approach, due to the most effective decomposition
- **DAGSVM** is a **faster approximation** of one-against-one

SVM for Regression

Regression



Regression