Support Vector Machines

Machine Learning

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Outline and References

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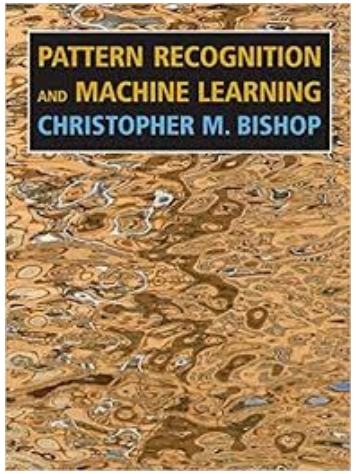
  - SVM for regression [PRML 7.1.4]

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



Sparse Kernel Machines

allows us not to have to compute the feature vectors, even if high dimensional.

- 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 → we have to compute the Gram matrix: $K = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \dots \\ k(x_2, x_1) & & \\ \vdots & & k(x_N, x_N) \end{bmatrix}$ $[N \times N]$ } computational expensive.
- To deal with this issue, **sparse kernel methods** find **sparse** solutions, that rely only on a **subset** of the training samples

  only a few samples in the dataset will correspond to a ≠0 weight:

  Prediction: { $y(x) = w^T \phi(x)$

  a lot of elements will be zero.
- The most well known among these methods are:
  - Support Vector Machines
  - Relevance Vector Machines

We work on this

Separable Problems

Do you remember the perceptron?

Recap on perceptron :

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

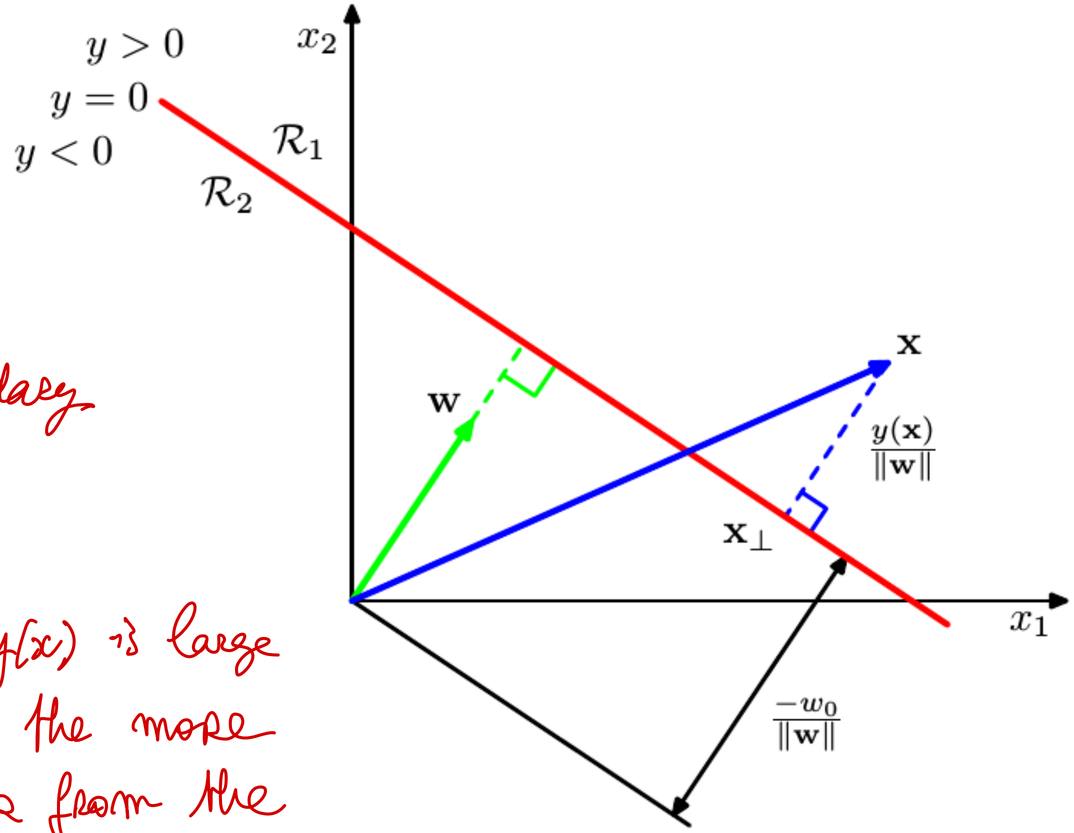
- Properties
  - DS is $y(\cdot) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + b = 0$
  - DS is orthogonal to $\mathbf{w}$

  } Decision boundary

  - 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 more $y(x)$ is large (in $|.|$), the more x is far from the boundary.

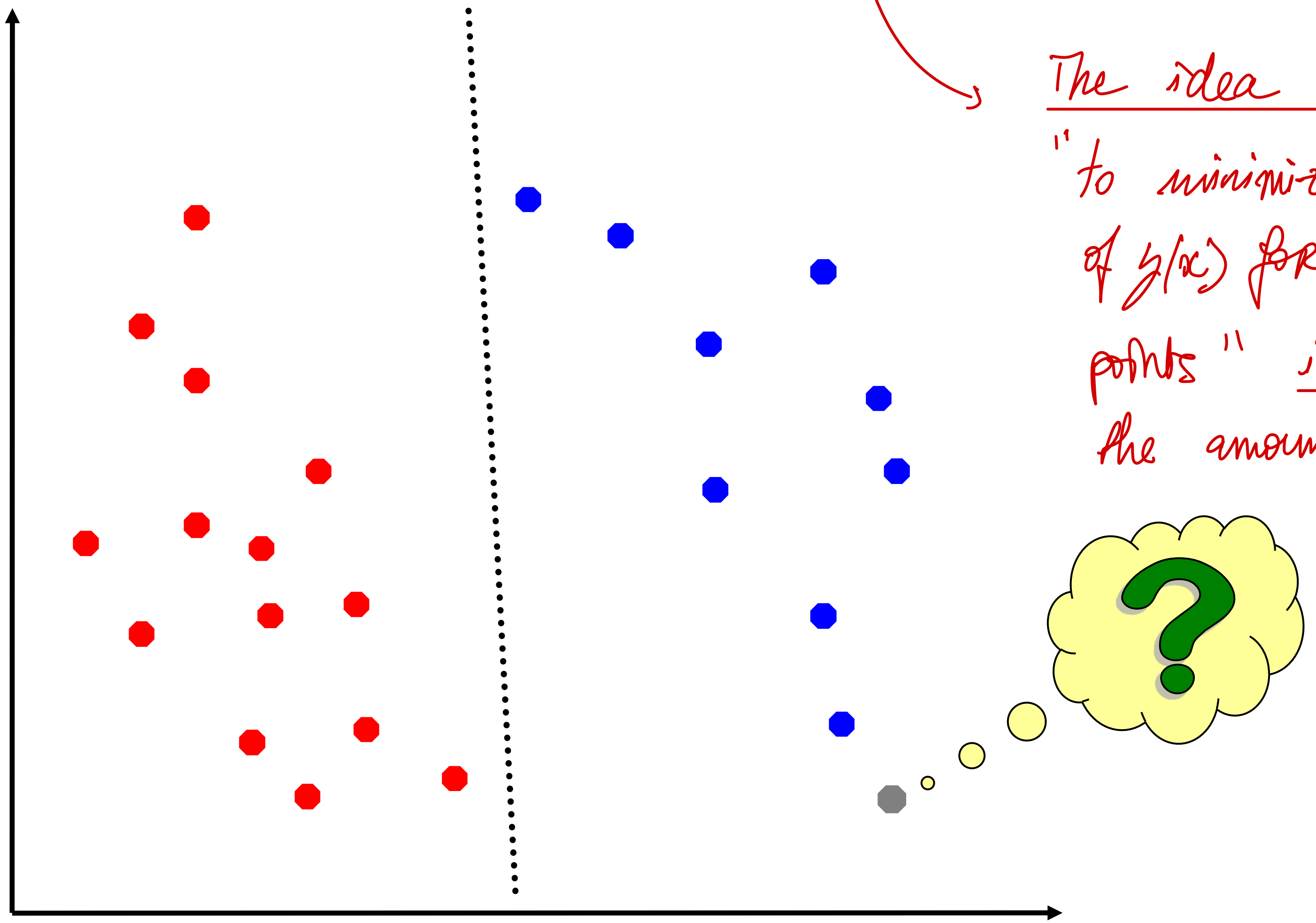
distance but with a sign.

"How far a point is far from decision boundary?"



The perceptron in action

Perceptron was only working when the pb was linearly separable ...!

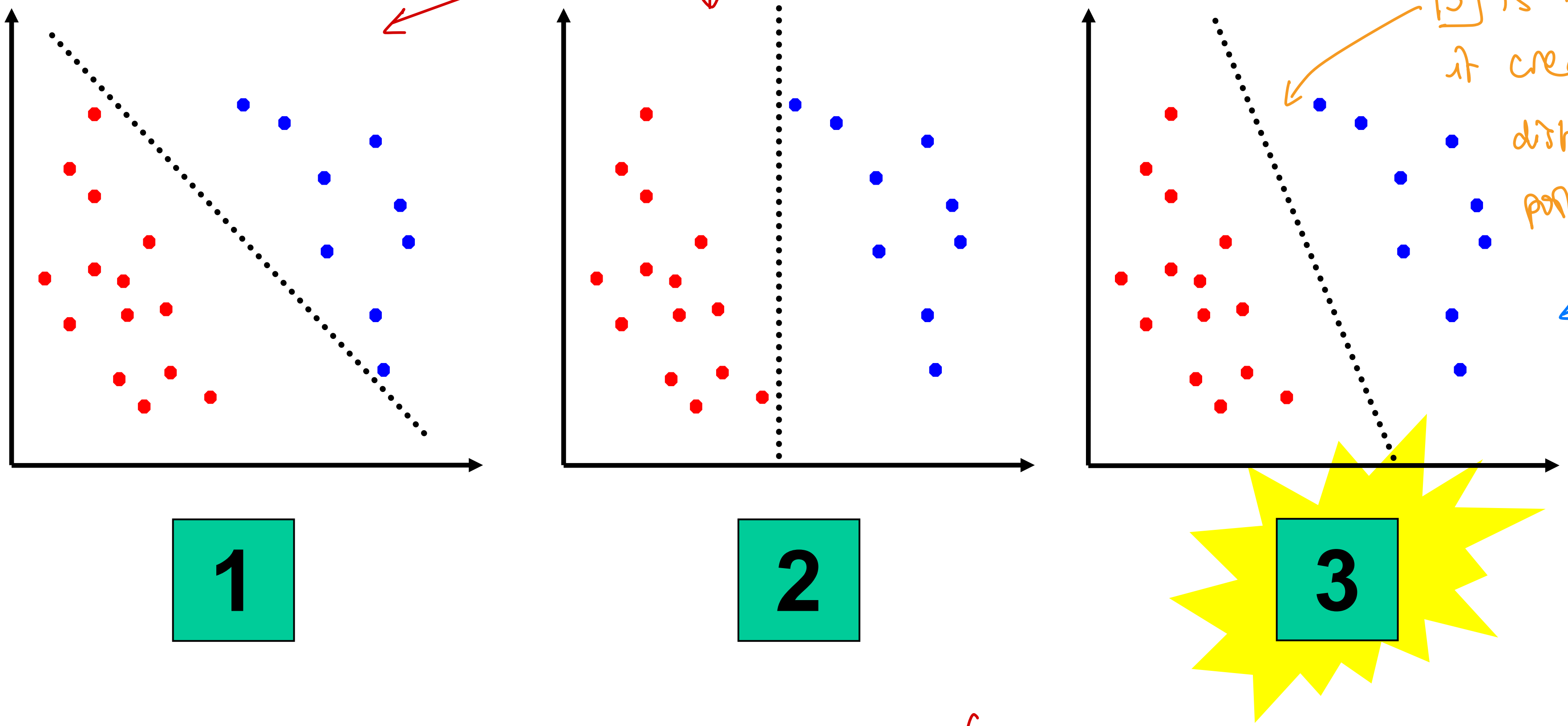


The idea of perceptron:

"to minimize the value of $y(x)$ for the misclassified points" i.e "to minimize the amount of mistake we are doing".

Are all the solution equivalent?

⚠ Any solution here has the same probability to be discovered by the perceptron...



$\boxed{3}$ is the best because it creates a "large" distance between points & boundary.

The SVM will introduce a "sort of bias" to prefer a solution vs the others.

... the one you'll get just depends on
- initialisation;
- order of data.

Maximum Margin Classifier

see @ slide 5: "distance x-to-decision bdary":
$= \frac{y(x)}{\|W\|_2}$.
Here we take the MIN.

- The margin will be:

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

To make it positive → "true distance".

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

we want to max. the margin wrt w, b.

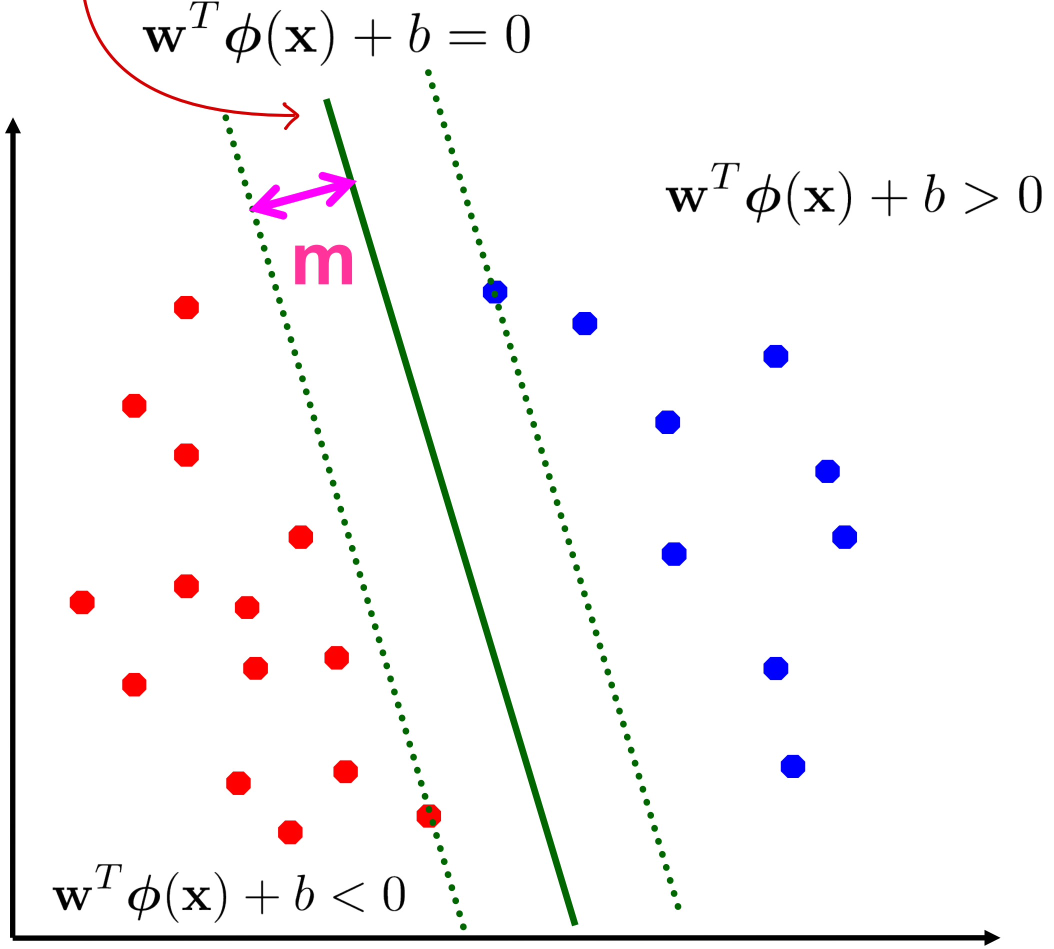
$$\arg\max_{\mathbf{w},b} \left\{ \min_n \left[\frac{t_n(\mathbf{w}^T \phi(\mathbf{x}_n) + b)}{||\mathbf{w}||} \right] \right\}$$

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

↓

So we need to simplify the problem.

The boundary is necessarily in the middle between blue dots & red dots (otherwise you move it a bit to reach equality).



Equivalent constrained optimization problem

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

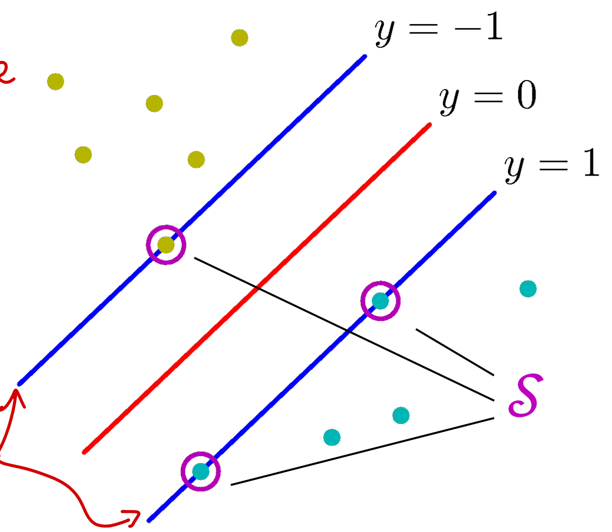
$$\kappa \mathbf{w}^T \phi(\mathbf{x}) + \kappa b \quad \forall \kappa > 0$$

The equation of the boundary doesn't change if $\begin{cases} w \leftarrow \kappa w \\ b \leftarrow \kappa b \end{cases}$, $\kappa > 0$.

  - We will consider only solutions such that:

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

The value of the y fct on the margin $= \pm 1$.



using that: only one solution (one w, one b).

- Equivalent **quadratic programming** problem

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

(squared version: easier opti).

↳ $= 1$ for S, > 1 for the others.

→ Indeed, if we re-write the "optimal hyperplane" (cf previous slide): $\underset{w,b}{\arg\max} \left(\frac{1}{\|w\|} \right)$.

Derivation of dual problem

See [PRML - Appendix E]

optimization technique

- We can derive the dual problem using **Lagrance multipliers**: $(\forall \alpha_i,\ \alpha_i \geq 0)$

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

- 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

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

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

inject those in the above equation to get the dual problem.

Dual Problem

- We can now rewrite the optimization problem as:

comes from the $\langle . | . \rangle$ between feature vectors.

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

- where the explicit feature mapping does not appear explicitly anymore

Optimization problem only wrt α.

we are able to solve the pb with only the knowledge of the kernel function & not the feature space.

Discriminant Function and Support Vectors

- The resulting discriminant function is:

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

mainly zeros here.

solution of the optimization pb.

STILL SPARSE !!

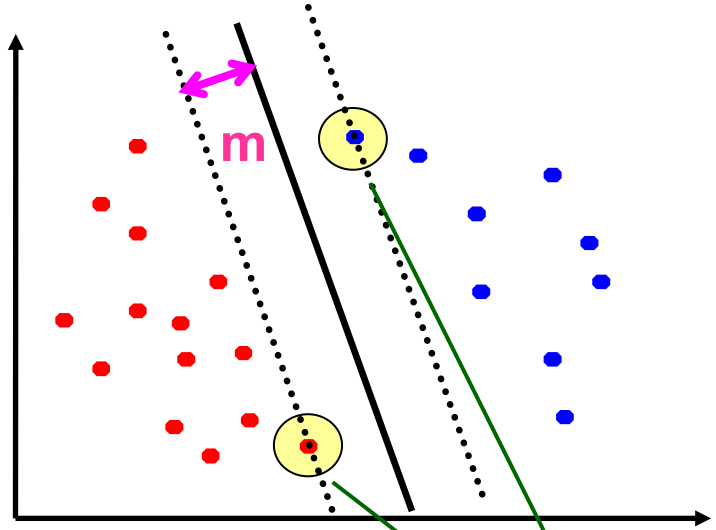
comes from the Lagrange Multiplier... (more details in the Bishop book).

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

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

bias is computed via averaging on S.

Support Vectors ($\mathcal{S}$)

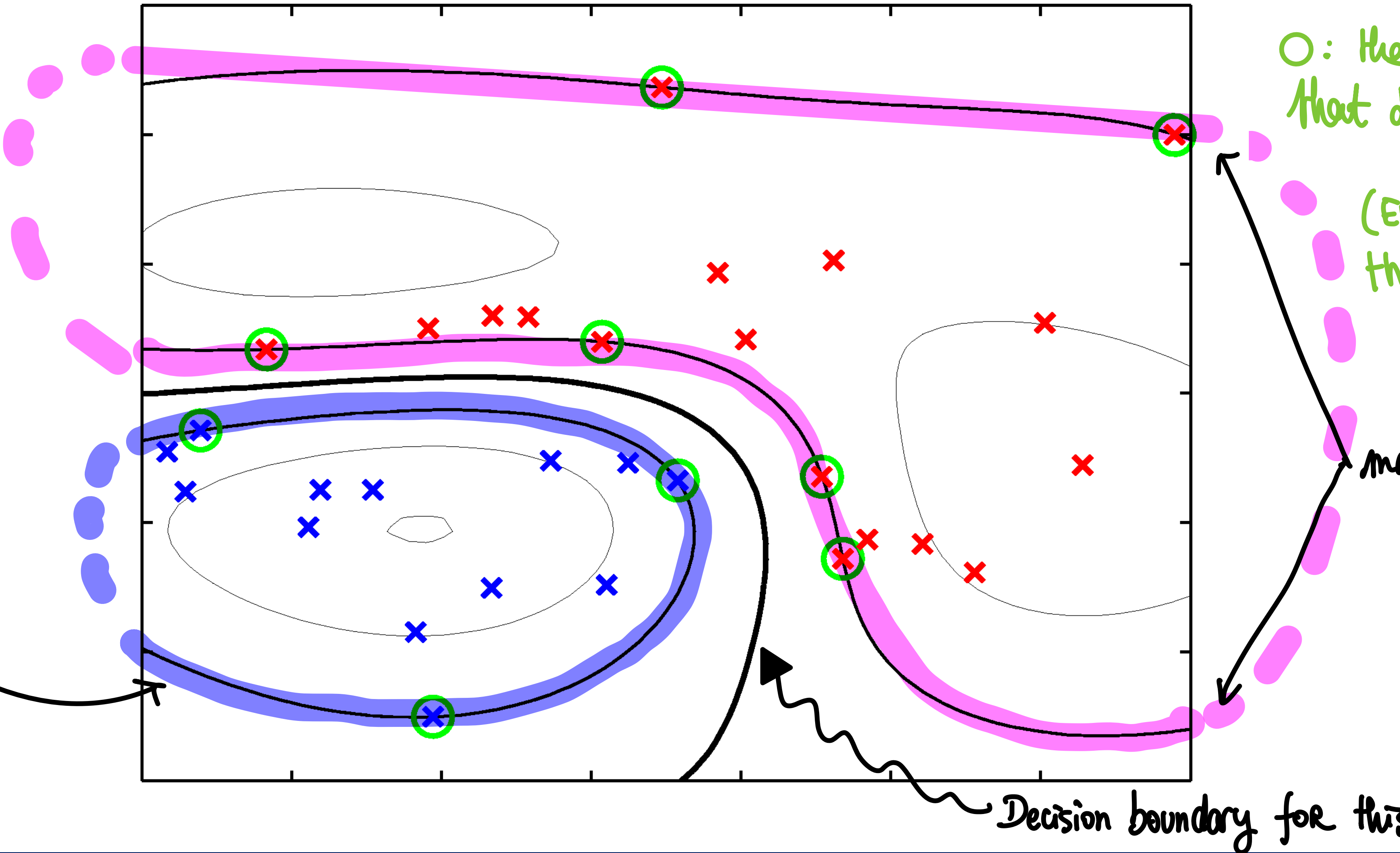


$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \underbrace{\left(t_i \left(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b\right) - 1\right)}_{0}$$

Example

- An example of SVM discriminant function using Gaussian kernel function

As we can see, this SVM technique can have a very complex solution (which is great!).



O: the only points that define this solution! (Even if we had thousands of pts).

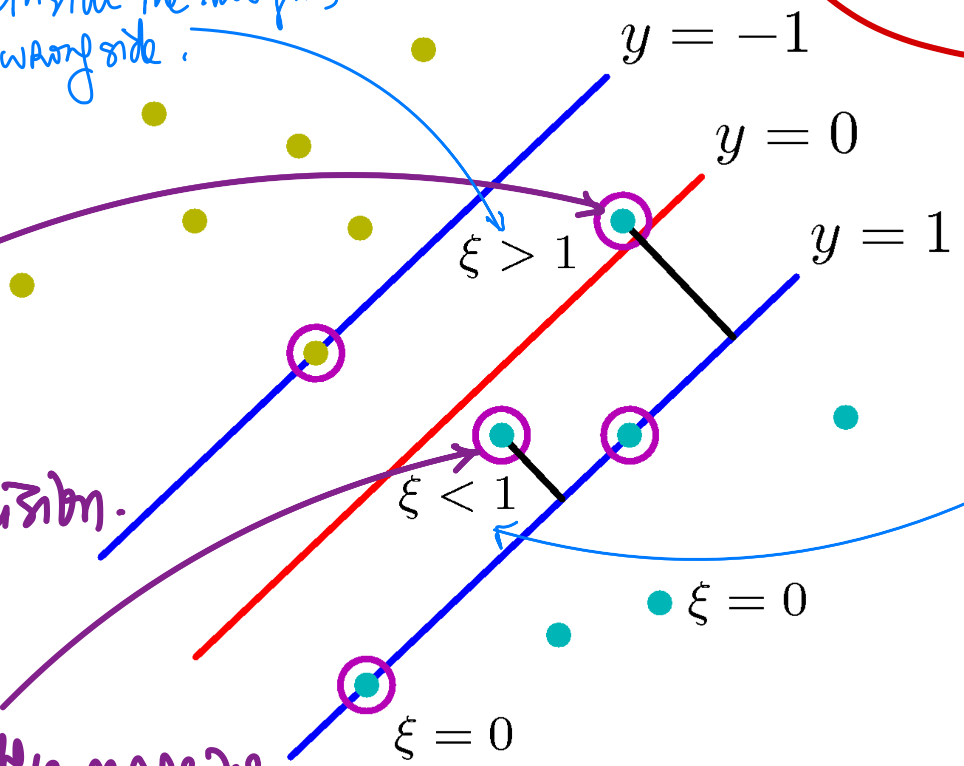
Non-separable Problems

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 SVM".

since it is inside the margins AND on the wrong side.



Even worse: points on the wrong side of the boundary decision.

since it is inside the margins BUT on the right side.

Some points inside the margins.

Soft-Margin optimization problem

To penalize when there are some "mistakes".

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

- 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

$C \uparrow \rightarrow Var \uparrow, Bias \downarrow$

↳ the larger C, the lower regularization.

Dual Representation (Box Constraints Problem)

of the "Soft Margin" version of the problem.

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

- As usual, **support vectors** are the samples for which $\alpha_n > 0$
  - If $\alpha_n < C \implies \xi_n = 0$, 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

[no use of C here]

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

$$\textbf{Subject to} \quad 0 \leq \alpha_n \leq 1/N,$$

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

$$\sum_{n=1}^{N} \alpha_n \geq \nu \qquad \text{for } n = 1, \ldots, N$$

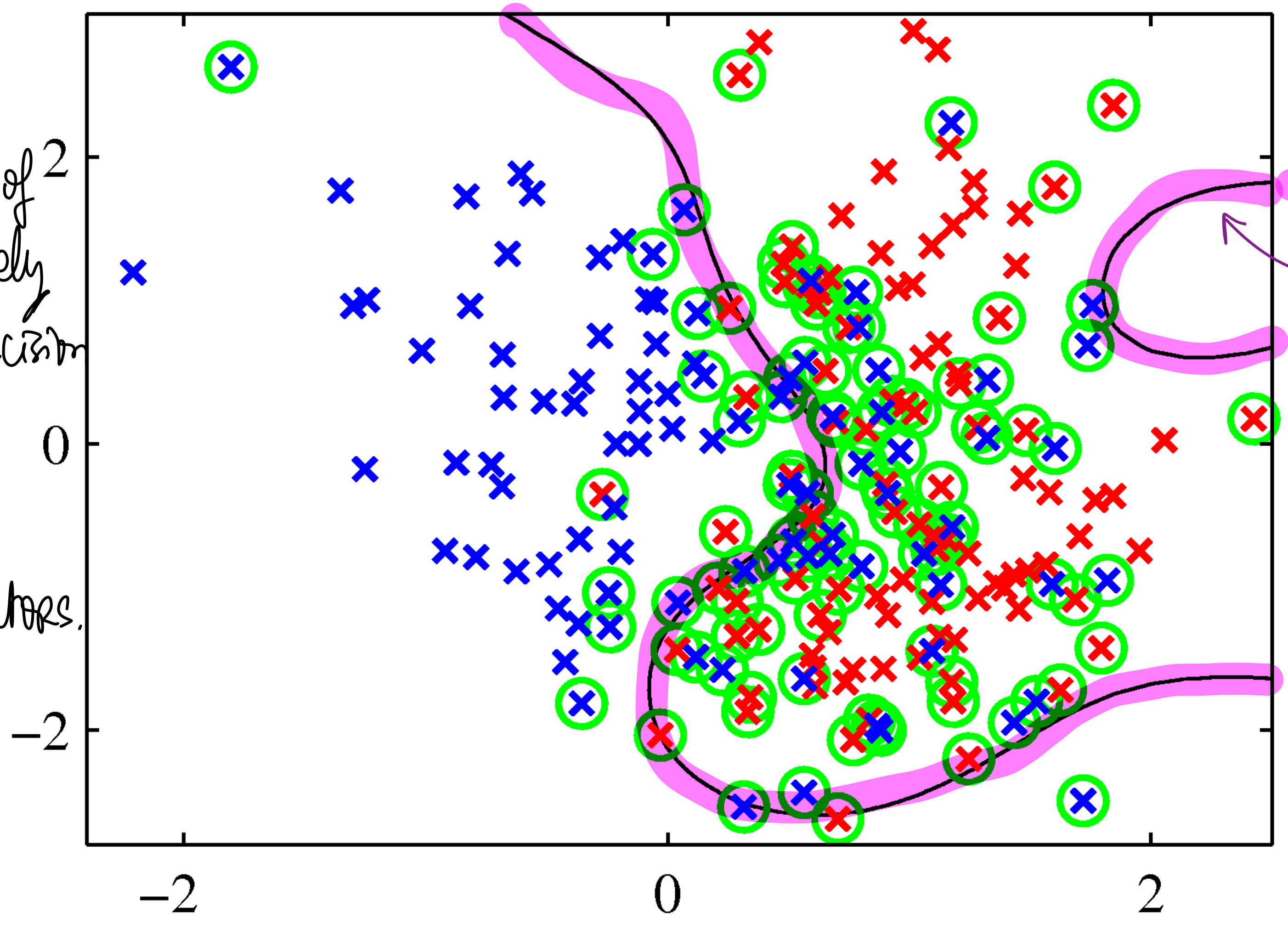
- Where $0 \leq \upsilon < 1$ is a user parameter that allow to control both the margin errors and the number of support vectors:

fraction of Margin Errors ≤ ν ≤ fraction of SVs

Example ⇝ Very complex real example !!

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

Of course, introduction of soft margins will likely result in smoother decision boundary but will likely increase the number of support vectors.



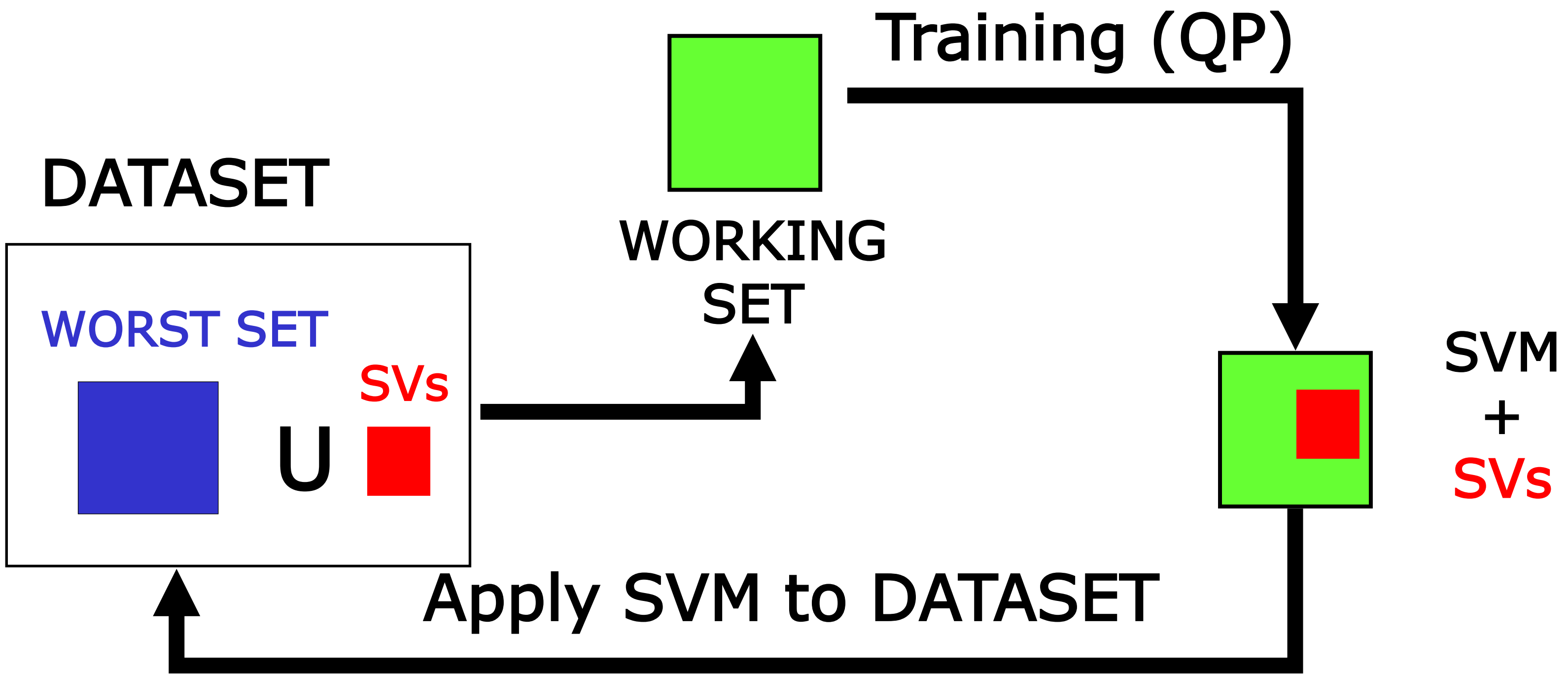
only the decision boundary is shown here.

Training SVM in Practice

SVM Training

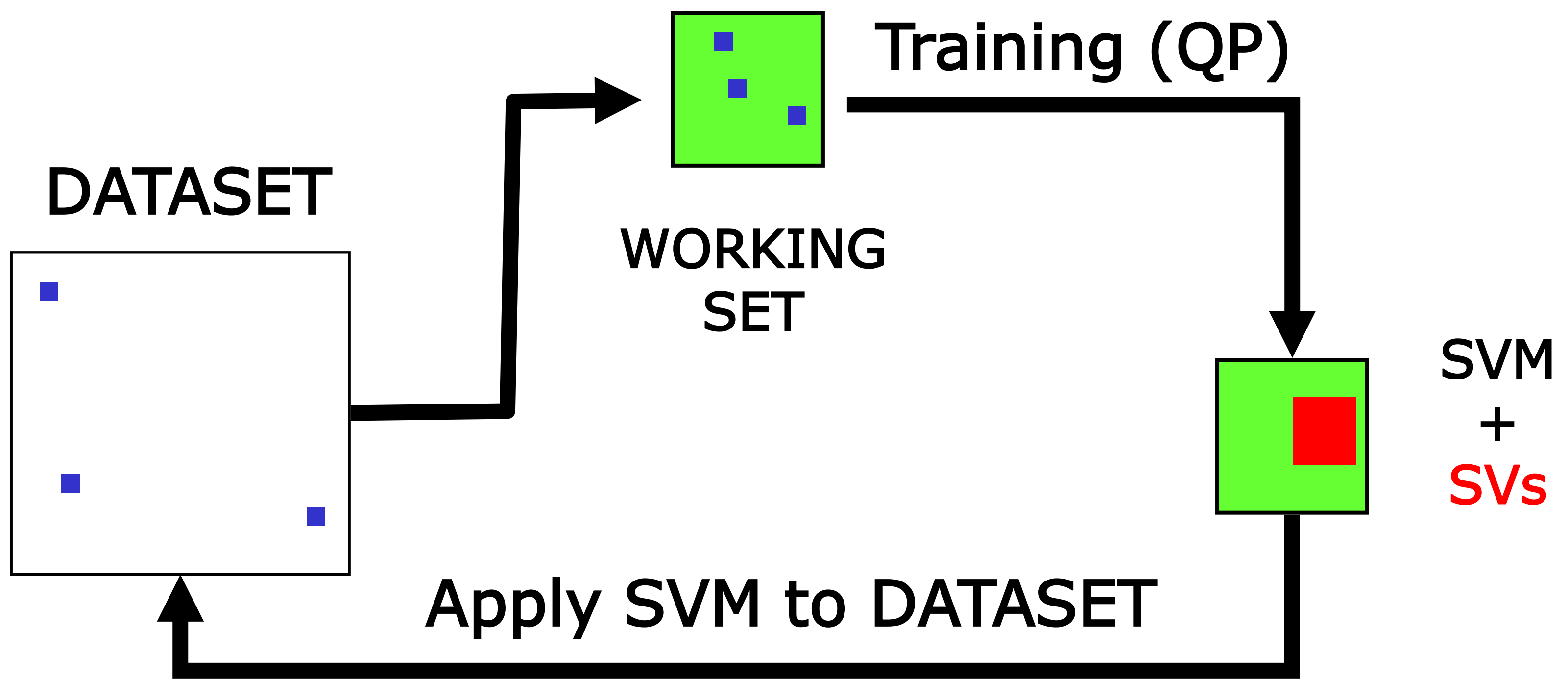
- Just solve the optimization problem to find α_i and b
- … but it is very expensive: $O(n^3)$ where n is the size of training set
- Faster approaches:
  - Chunking
  - Osuna’s methods
  - Sequential Minimal Optimization
- Online learning:
  - Chunking-based methods
  - Incremental methods

Chunking



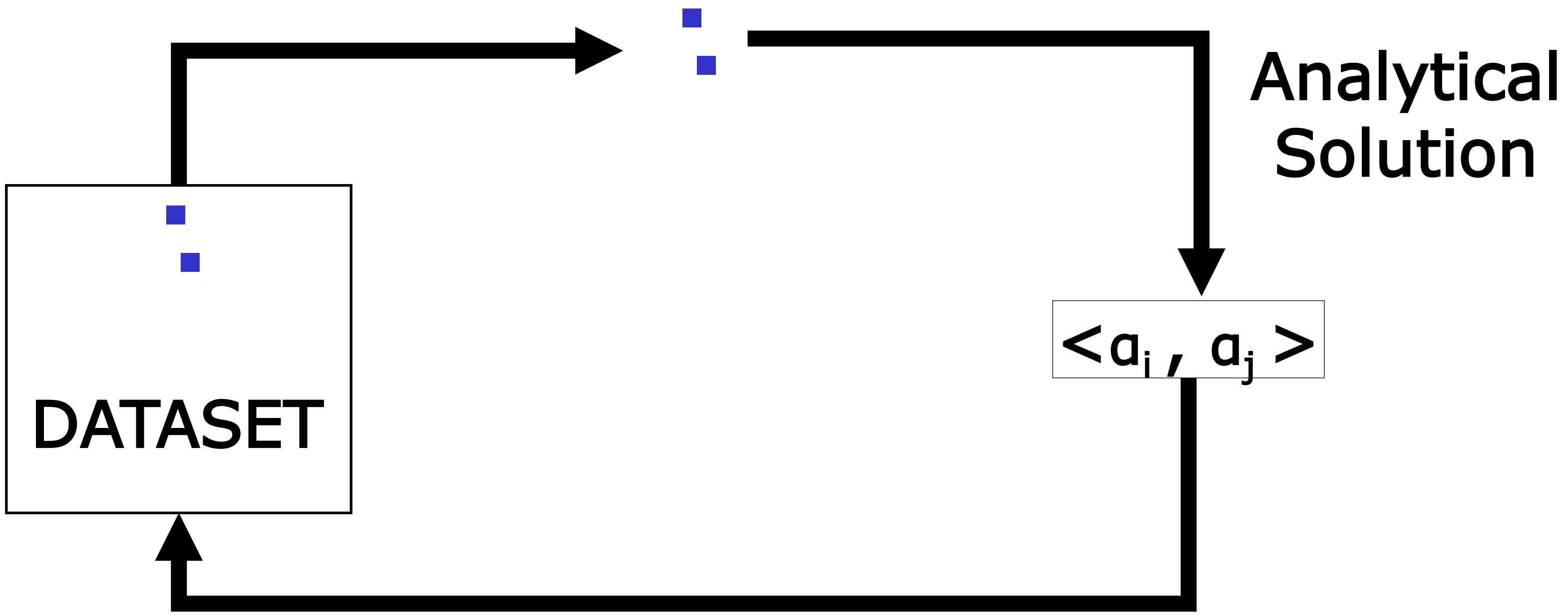
- Solves iteratively a sub-problem (working set)
- Build the working set with current SVs and the M samples with the bigger error (worst set)
- Size of the working set may increase!
- Converges to optimal solution!

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

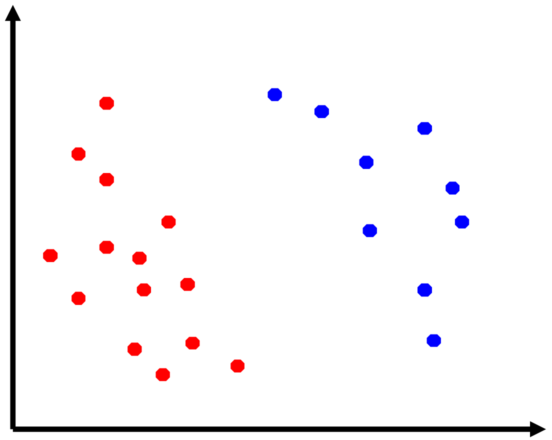


- Works iteratively only on two samples
- Size of the working set is minimal and multipliers are found analytically
- Converges to optimal solution!

Multi-class SVM

Multi-class SVM

- So far we considered two-classes problems:

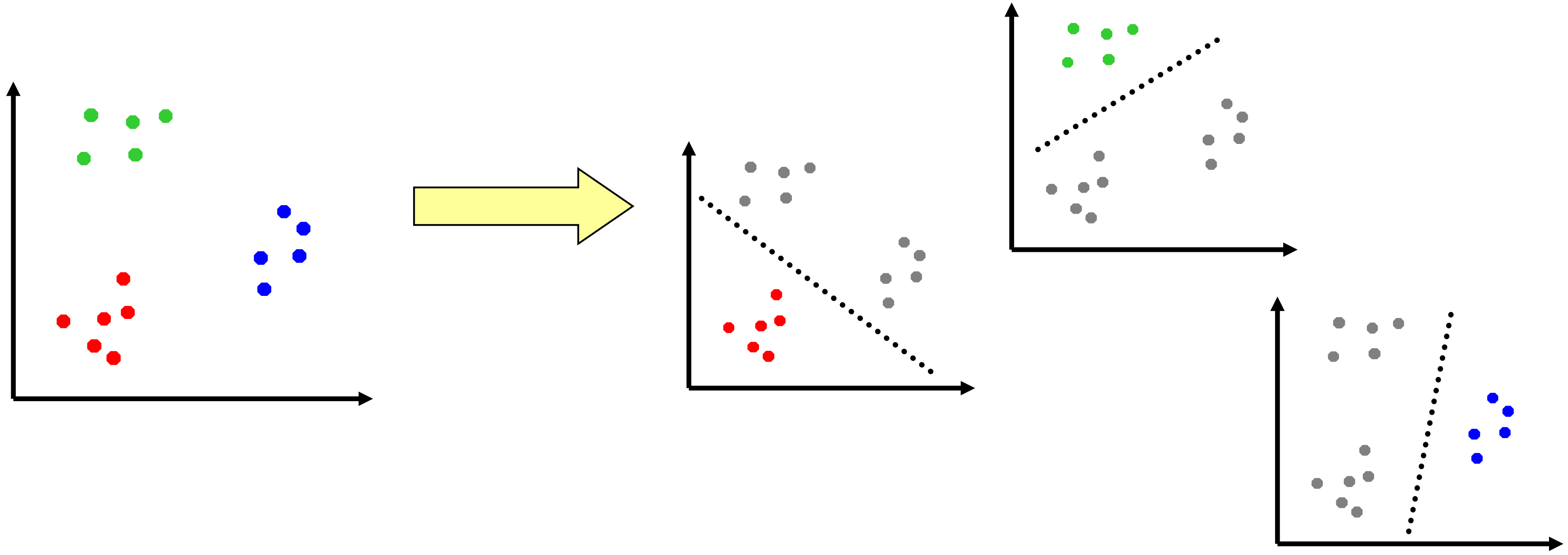


- How does SVM deal with multi-class problems?

Not easy to extend !!

One-against-all

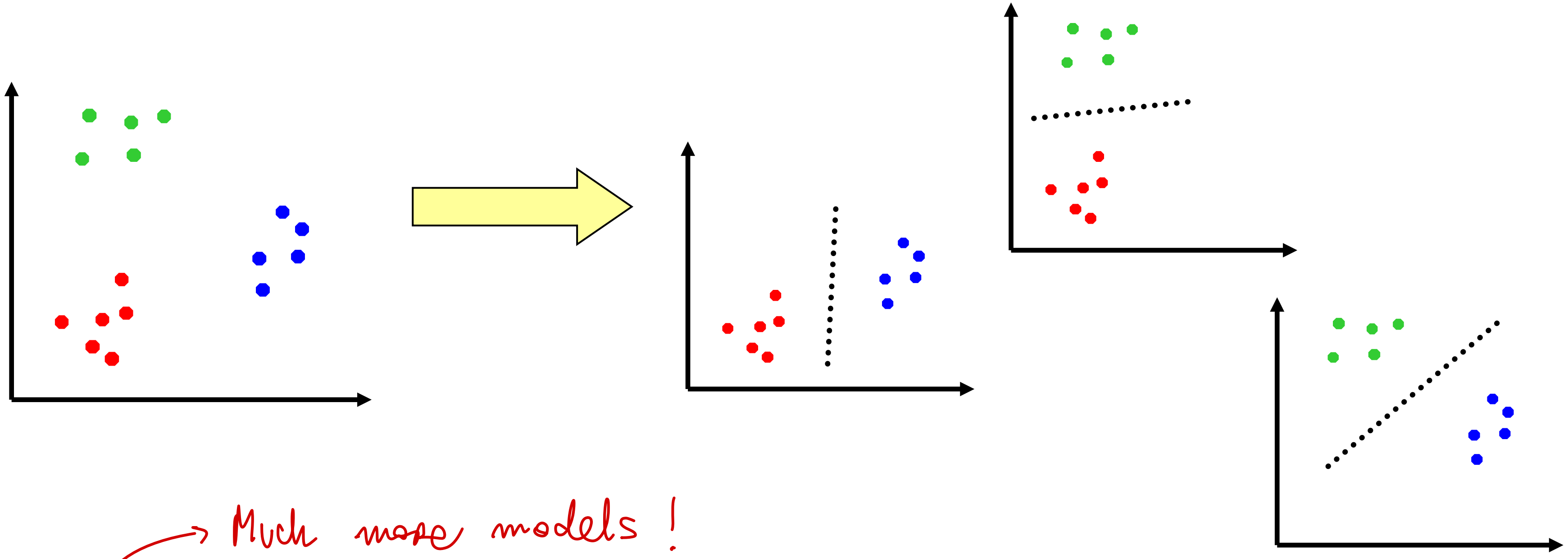
- A k-class problem is decomposed in k binary (2-class) problems



- 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



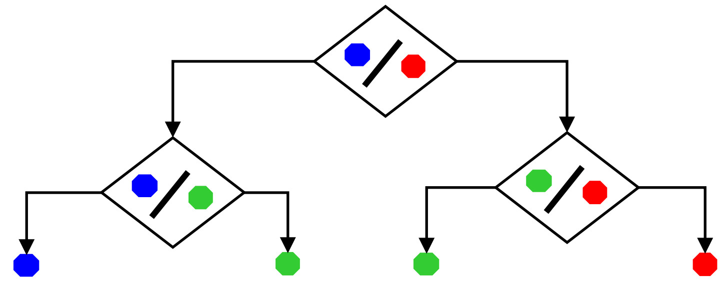
Much more models!

- 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

→ Training : as in "one-against-one"
→ Testing is different !!

- 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

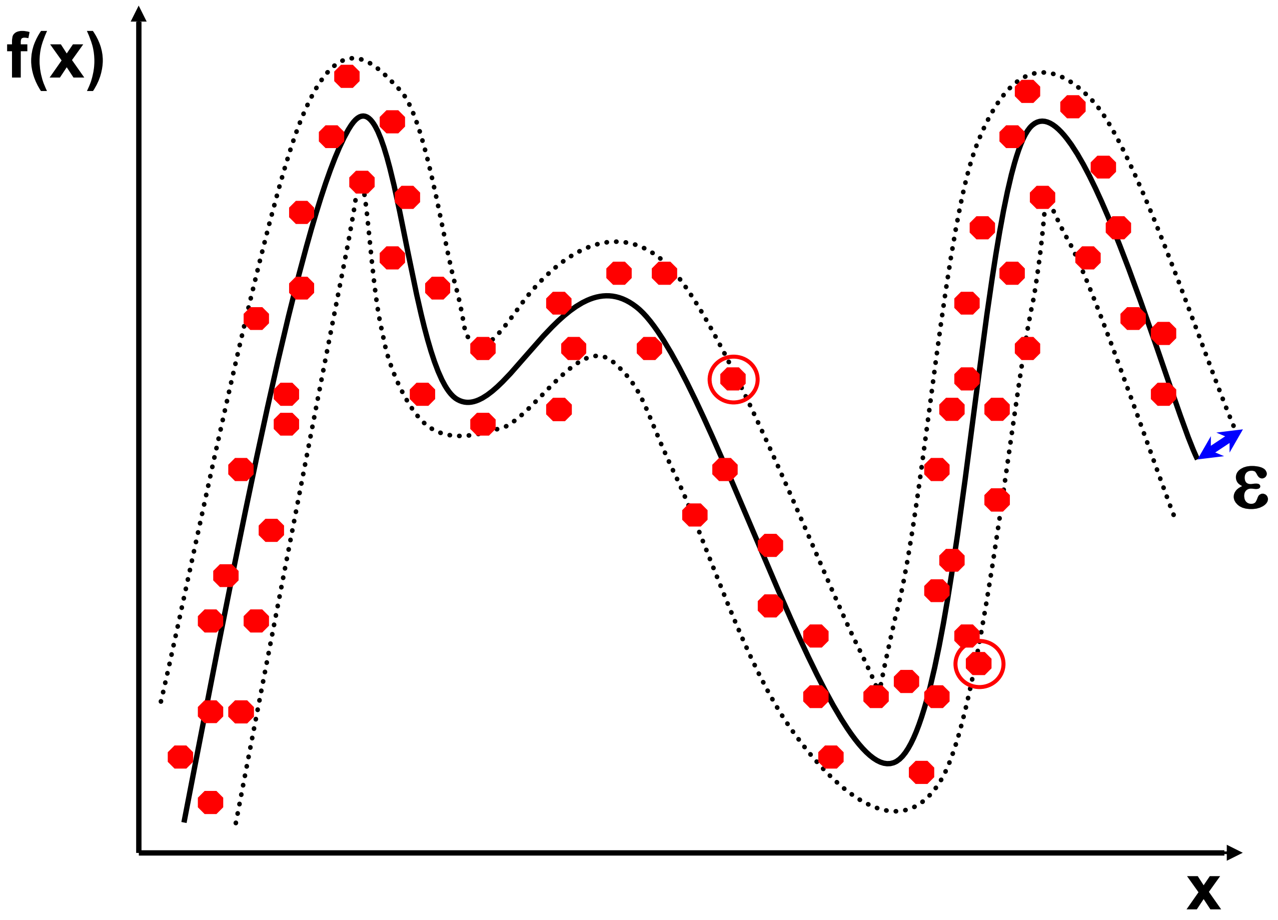
SVM for Regression

Regression

⇝ margin ~~as separation~~

↓

instead : margin as "amount of mistake you allow".



Regression