SVM: Support Vector Machine

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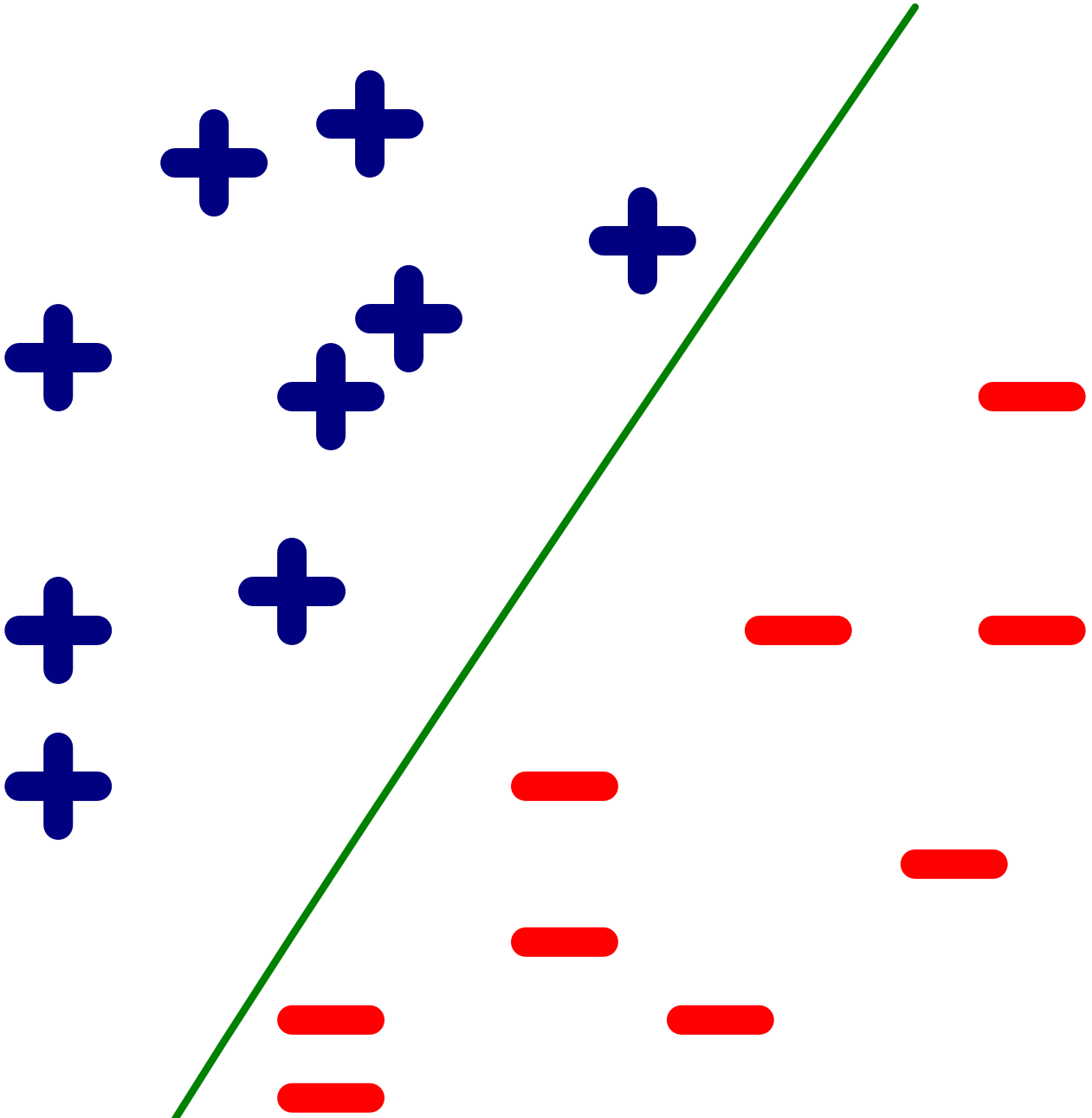
Outline

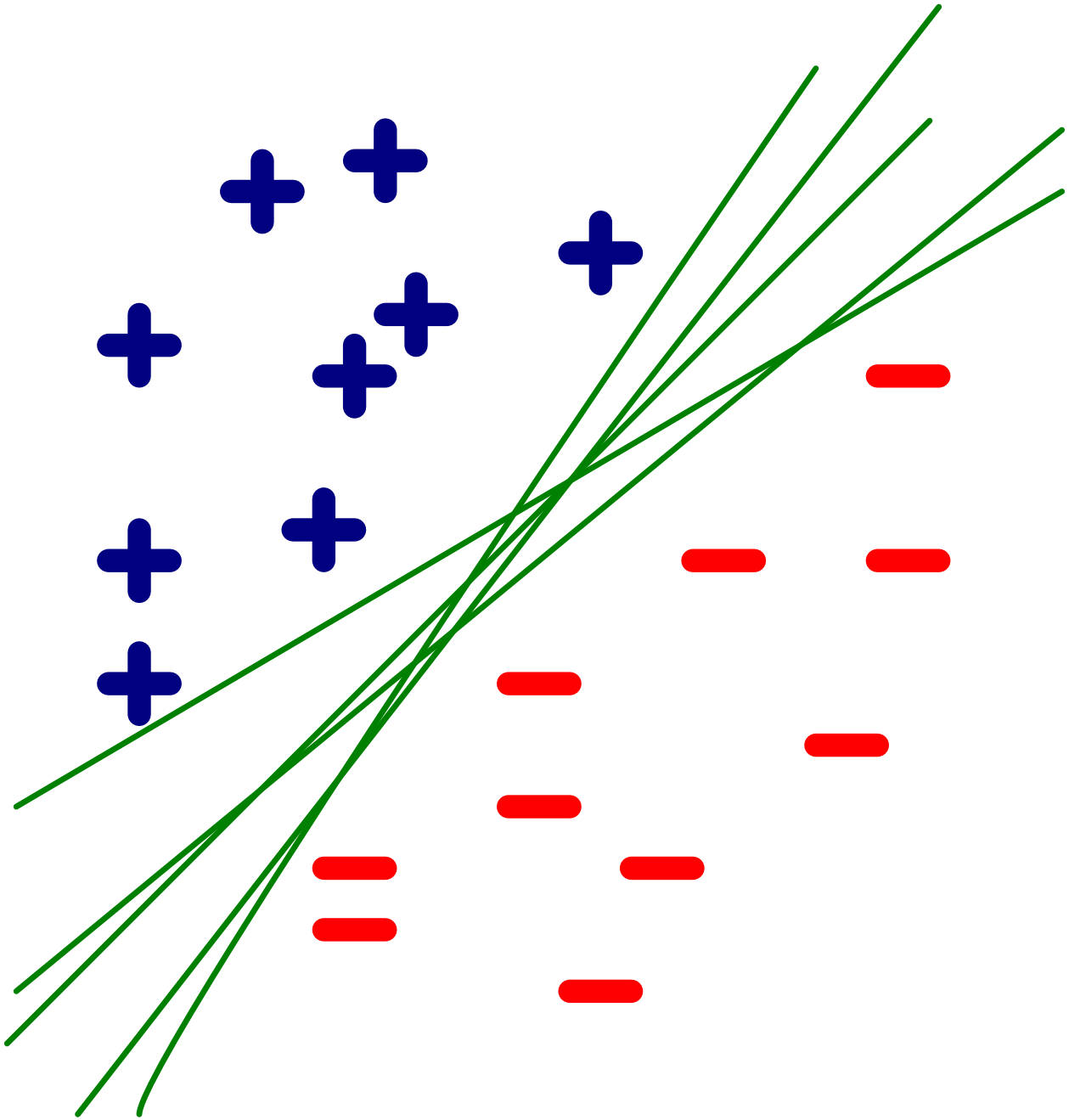
Introduction

- Context
  - supervised learning
  - classification (or regression)
    - binary
    - extension : multiclass
- Why SVM ? Is that deep ?
- SVMs are important because of
  - theoretical reasons :
    - Robust to very large number of variables and small set of samples
    - Can learn both simple and highly complex classification models
    - Employ sophisticated mathematical principles to avoid overfitting
  - superior empirical results

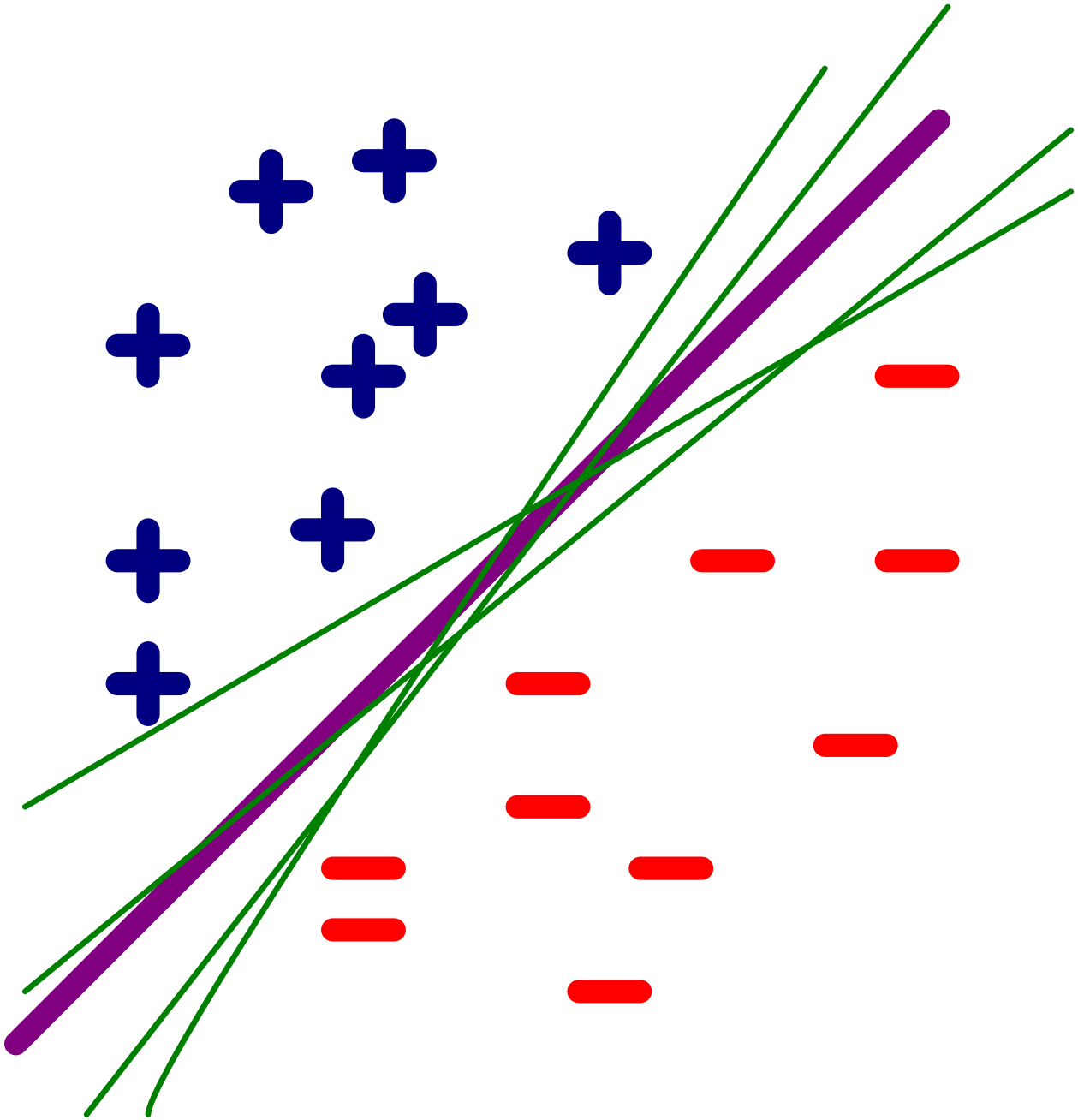
Principle : linear separation



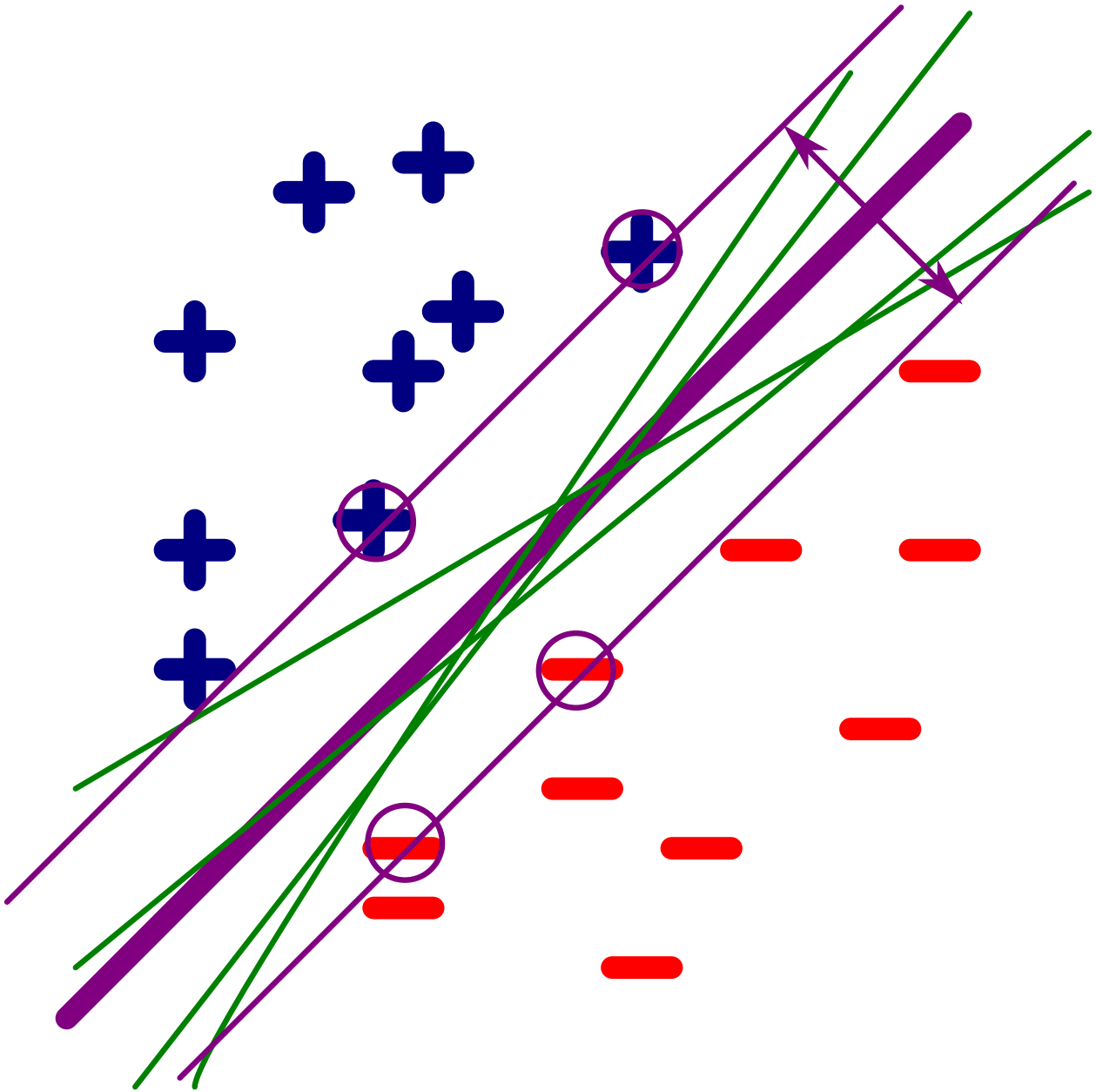
Principle : many solution



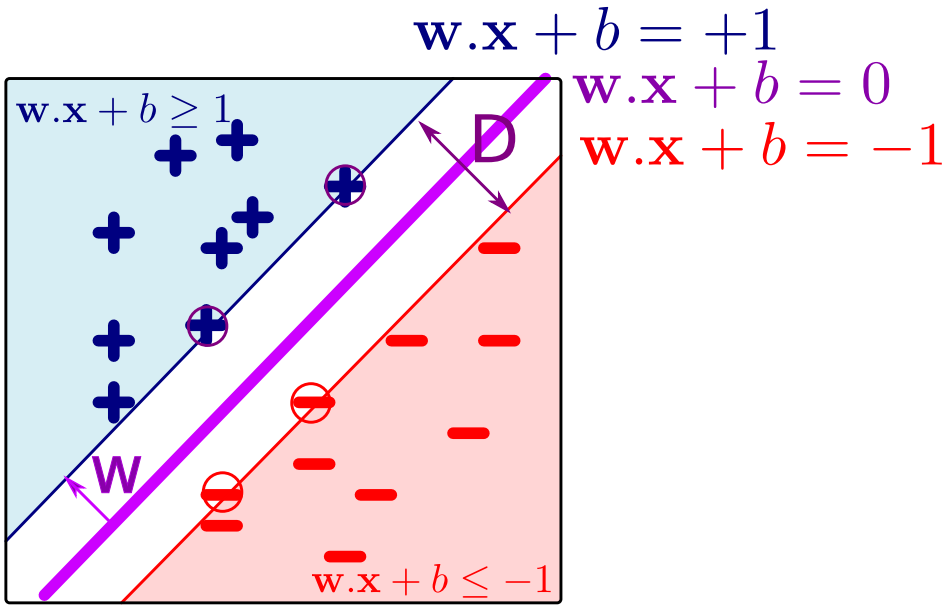
Principle : find the best one



Principle : maximising the margin



Problem formalisation



- Margin maximisation : $D = \frac{2}{\|\mathrm{w}\|}$
  - minimization of $\|\mathrm{w}\|$ or $\frac{1}{2}\|\mathrm{w}\|^2$
- Labeled data :
  - positive samples : $y = +1$
    - $\mathrm{w.x} + b \geq 1$
  - negative samples : $y = -1$
    - $\mathrm{w.x} + b \leq -1$
  - thus : $y\,(\mathrm{w.x} + b) \geq 1$

SVM problem :

minimisation of $\frac{1}{2}\|\mathrm{w}\|^2$ under the constraint $\forall i,\ y_i\,(\mathrm{w.x}_i + b) \geq 1$

Prediction : $sign(\mathrm{w.x} + b)$

dual problem

- Lagrangian : maximisation of $\frac{1}{2}\|\mathrm{w}\|^2 - \sum_i \alpha_i(y_i\,(\mathrm{w}.\mathrm{x}_i + b) - 1)$ with $\forall i\ \alpha_i \geq 0$
- annulation of derivatives with respect to w and b :
  - $\mathrm{w} = \sum_i \alpha_i y_i \mathrm{x_i}$
  - $\sum_i \alpha_i y_i = 0$
- the dual problem is :

dual problem

maximisation of $\sum_i \alpha_i - \frac{1}{2}\sum_i \sum_k \alpha_i \alpha_k y_i y_k \mathrm{x_i}\mathrm{x_k}$ under the contraints $\forall i\ \alpha_i \geq 0$ and $\sum_i \alpha_i y_i = 0$

SVM : a unique solution

If, to the dual problem, we add the Karush–Kuhn–Tucker condition :

$$\forall i \ \alpha_i (y_i \, (\mathrm{w}.\mathrm{x}_i + b) - 1) = 0$$

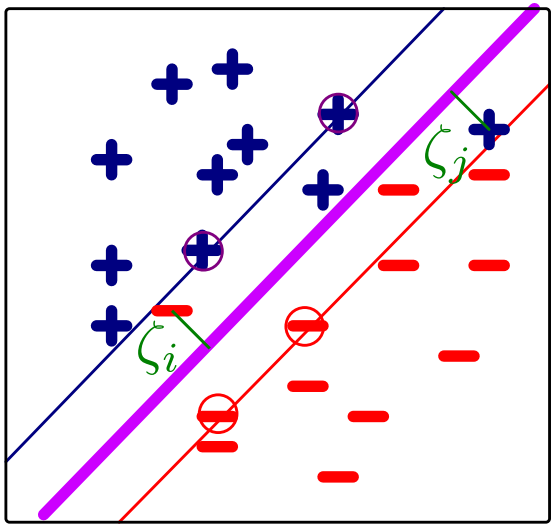
there exists an optimal solution

- if $\alpha_i > 0$: $y_i \, (\mathrm{w}.\mathrm{x}_i + b) - 1 = 0$: on the margin
- if $y_i \, (\mathrm{w}.\mathrm{x}_i + b) > 1$: $\alpha_i = 0$
- thus $\mathrm{w} = \sum_{i, \alpha_i > 0} \alpha_i y_i \mathrm{x}_i$
- for a new data x : $sign(\mathrm{w}.\mathrm{x} + b) = sign(\sum_{i, \alpha_i > 0} \alpha_i y_i \mathrm{x}_i.\mathrm{x} + b)$

First step in SVM using python : using scikitlearn

```
# pip3 install scikit-learn
from sklearn import svm
X = [[0, 0], [1, 1]]
y = [0,1]
classif = svm.SVC(kernel='linear')
classif.fit(X, y)
print('prediction class for [2,2]', classif.predict([[2., 2.]]
print('support vectors: ', classif.support_vectors_)
```

Accepting errors : soft margin



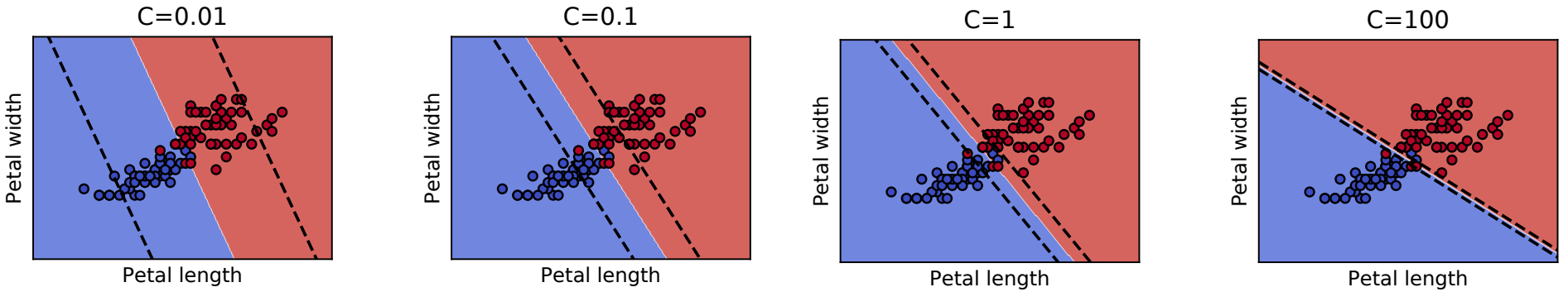
Soft margin

minimisation of $\frac{1}{2}\|\mathrm{w}\|^2 + C\sum_i \zeta_i$ under the constraint
$\forall i\ y_i\,(\mathrm{w}.\mathrm{x}_i + b) \geq 1 - \zeta_i$ and $\forall i\ \zeta_i \geq 0$

Dual formulation

maximisation of $\sum_i \alpha_i - \frac{1}{2}\sum_i \sum_k \alpha_i \alpha_k y_i y_k \mathrm{x_i x_k}$ under the contraints
$\forall i\ C \geq \alpha_i \geq 0$ and $\sum_i \alpha_i y_i = 0$

Soft margin : parameter C

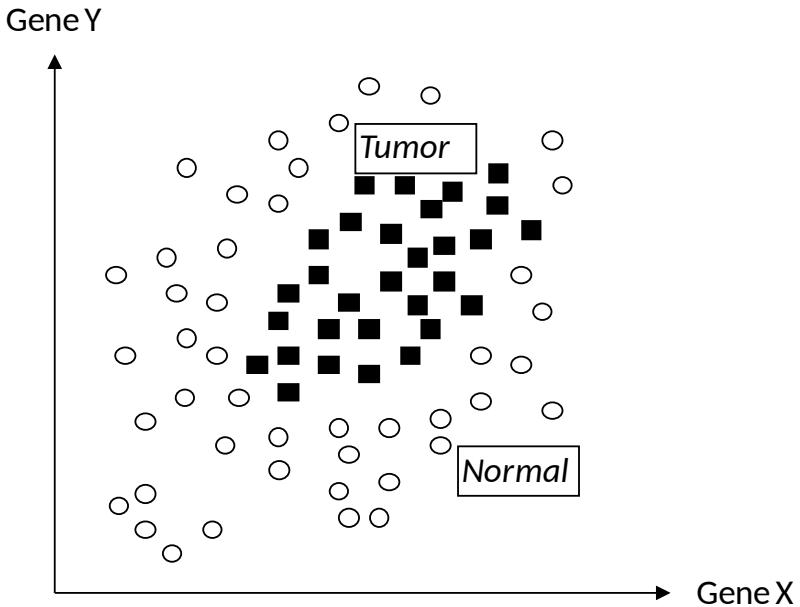


- A small C value will give a wider margin, at the cost of some misclassifications.
- A huge C value will give the hard margin classifier and tolerates zero constraint violation.
- Find the C value such that noisy data does not impact the solution too much.

Unbalanced data

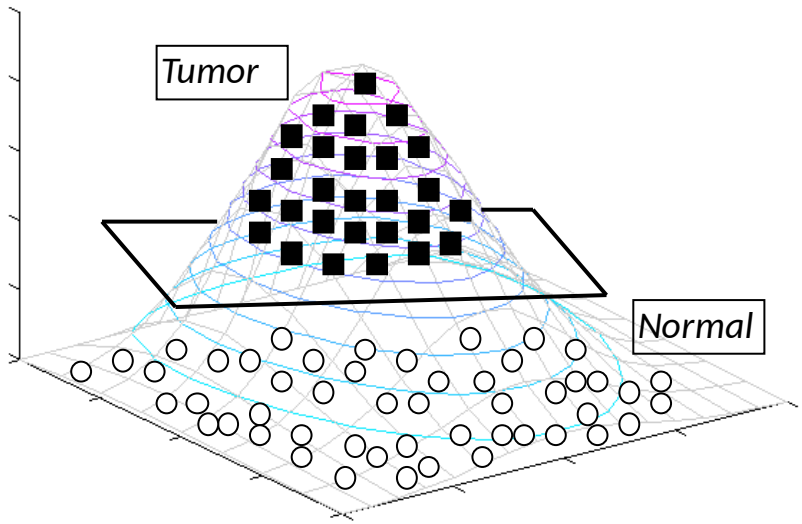
- the idea is to increase the cost of bad classification for the smallest class
- C is replaced by C^+ for positive data and C^- for negative data.
- implementation in `sklearn` (from the documentation)
  - SVC implements a keyword `class_weight` in the fit method. It's a dictionary of the form `class_label : value`, where `value` is a floating point number strictly positive that sets the parameter C of class `class_label` to `C * value`.
  - SVC implements also weights for individual samples in method fit through keyword `sample_weight`. Similar to `class_weight`, these set the parameter C for the i^{th} example to `C * sample_weight[i]`.

Non linearly separable data : the kernel trick



kernel

Φ



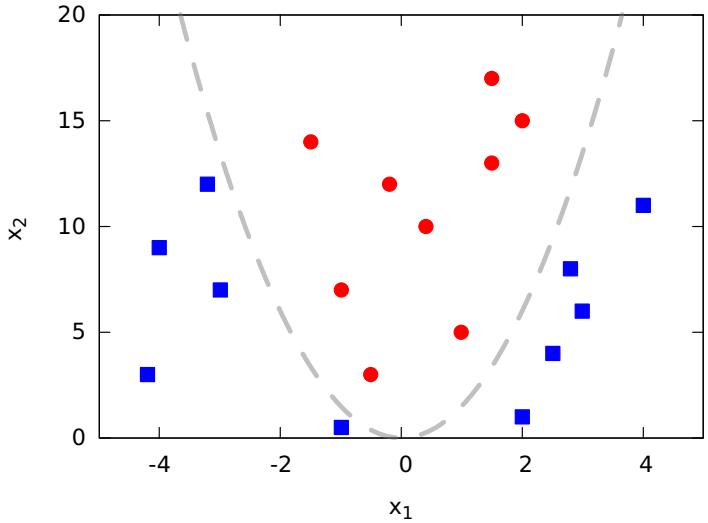
Data is not linearly separable in the input space

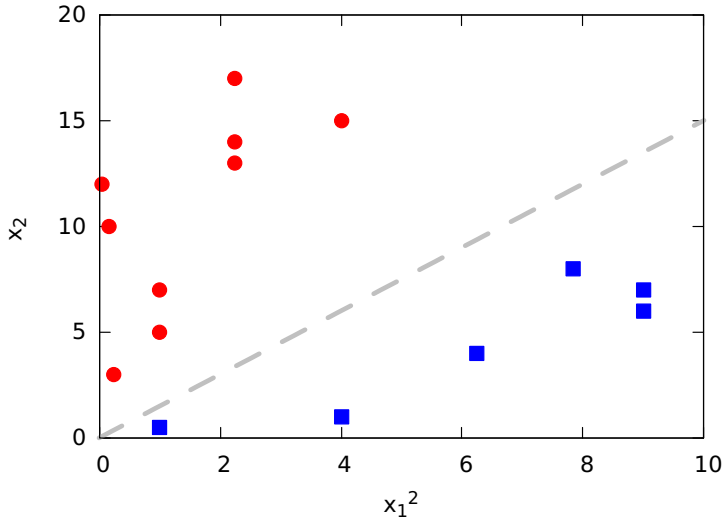
Data is linearly separable in the feature space obtained by a kernel

$$\Phi : \mathbf{R}^N \longrightarrow \mathbf{H}$$

kernel trick

- Here, we define Φ explicitely
  - input space $x = [x_1, x_2]$ (2 dimensions)
  - feature space $\Phi(x) = [x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, 1]$ (6 dimensions)





kernel trick

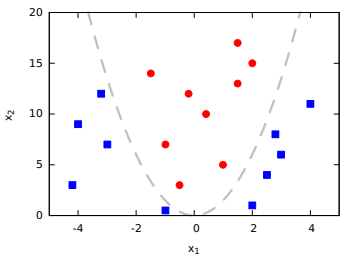
- SVM solution in the induced space (feature space) :

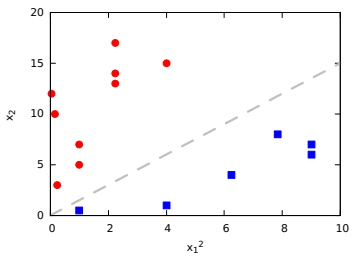
$$f(x) = \sum_{isupp.vect} \alpha_i (y_i \Phi(x_i).\Phi(x) + b)$$

- Instead of explicitely defining Φ, we rather define K :

$$K(x, x') = \Phi(x).\Phi(x')$$

- Allow avoiding computation in the input space
  - useful, mainly if $dim(\Phi) = \infty$
- Back to our example :





$$\Phi(x) = [x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, 1]$$
$$\Phi(x') = [x'^2_1, x'^2_2, \sqrt{2}x'_1, \sqrt{2}x'_2, \sqrt{2}x'_1x'_2, 1]$$
$$K(x, x') = (x.x' + 1)^2$$

Kernels

Dual formulation

maximisation of $\sum_i \alpha_i - \frac{1}{2} \sum_i \sum_k \alpha_i \alpha_k y_i y_k K(\mathrm{x_i}, \mathrm{x_k})$ under the contraints

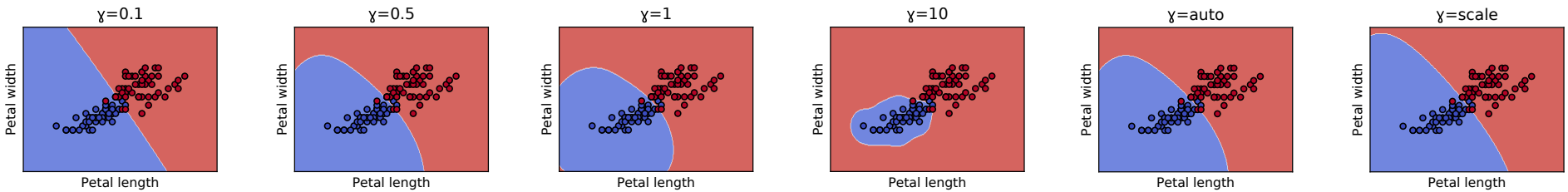
$\forall i \ C \geq \alpha_i \geq 0$ and $\sum_i \alpha_i y_i = 0$

Prediction

$$\mathrm{sign}\left(\sum_{j \ supp.vect} \alpha_j y_j K(\mathrm{x_j}, \mathrm{x}) + b \right)$$

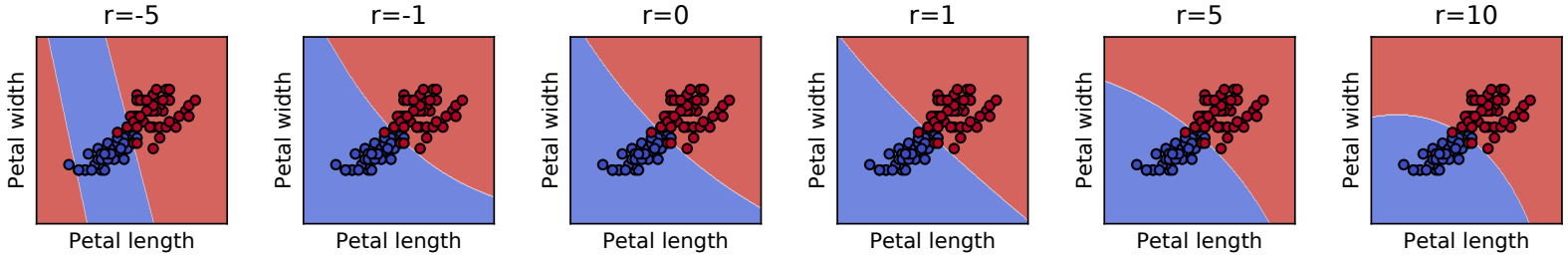
Predefined kernels (1)

- `'linear'`
- `'rbf'` (radial basis function) :
  - $\exp\left(-\gamma\|x - x'\|^2\right)$ (`gamma` for γ)
  - in `scikit-learn` :
    - `gamma = 'auto'` : $\frac{1}{n}$ where n is the dimension of samples
    - `gamma = 'scale'` : $\frac{1}{\sigma n}$ where σ is the standard variation of x
  - Examples using a RBF kernel with $C = 1$:

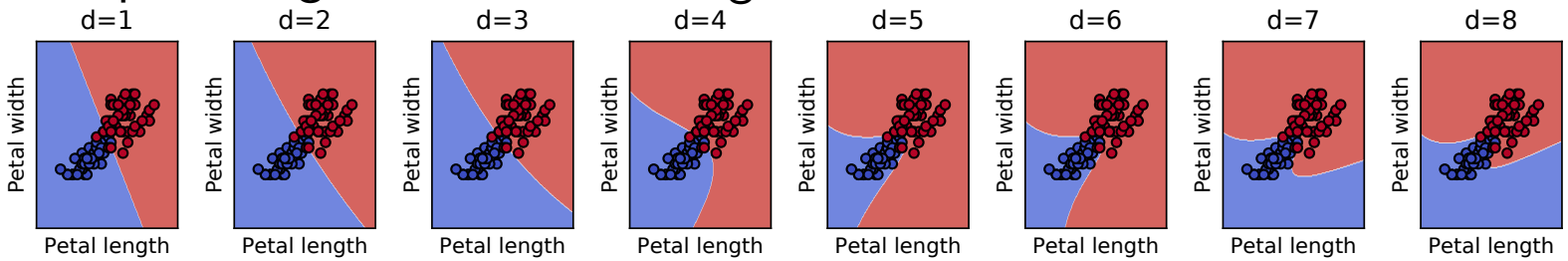


Predefined kernels (2)

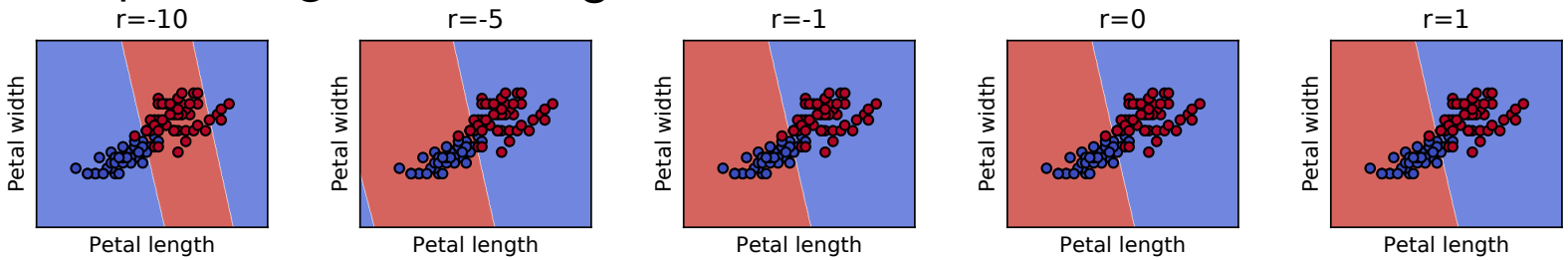
- 'polynomial' :
  - $(\gamma < x, x' > +r)^d$ (degree for d ; coef0 for r)
    - examples using degree 3, $C = 1$ and gamma = 'scale'



    - examples using $r = 0$, $C = 1$ and gamma = 'scale'



- 'sigmoid'
  - $tanh(\gamma < x, x' > +r)$
    - examples using $C = 1$ and gamma = 'scale'



Kernels in practice

- need to find the best kernel for your problem
- compare kernels with best parameters
  - C, γ, ...
- methods of parameters estimation
  - exhaustive search (`GridSearchCV`)

```
param_grid = [
{'C':[0.1, 0.2, 0.5, 1, 2, 5, 10], 'kernel':['linear']},
{'C':[0.5, 1, 5, 10],'degree':[2,3],'coef0':[-1,0,1],'kernel':['poly']}
]
```

  - randomized search (`RandomizedSearchCV`)
    - distributions for parameters

Custom kernels

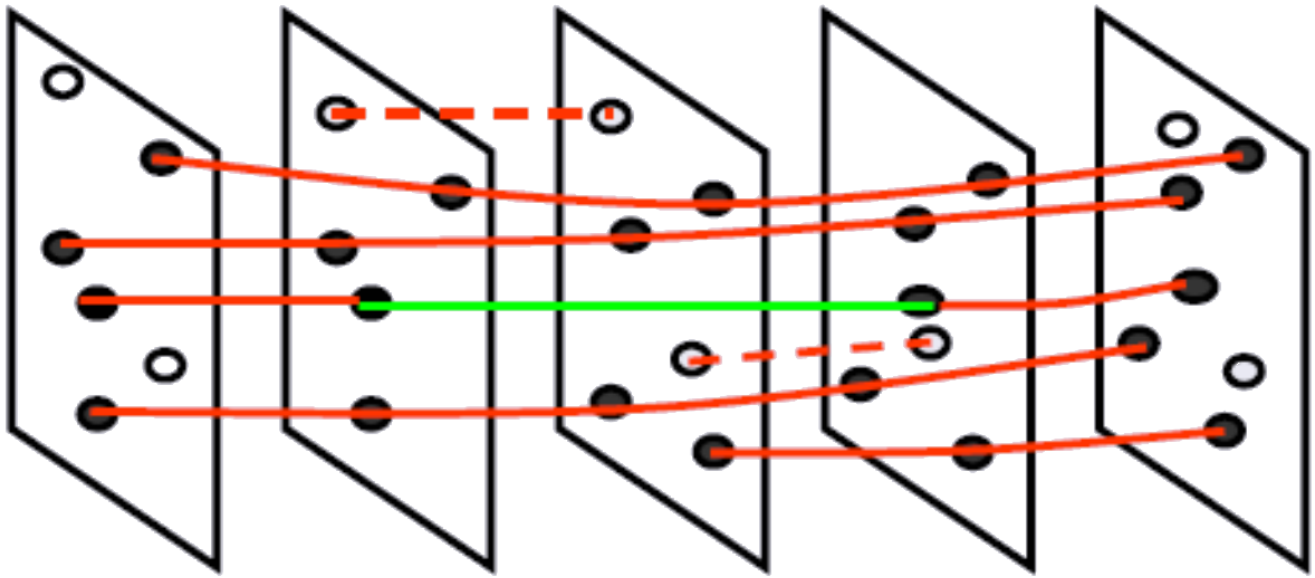
hand make kernel

```
def my_kernel(X, Y):
    return np.dot(X, Y)
classif = svm.SVC(kernel=my_kernel)
```

- for text or genes
- example for image : `https://www.tensorflow.org/tutorials/representation/kernel_methods` (Fourier kernel)
- for video

a video kernel (1)

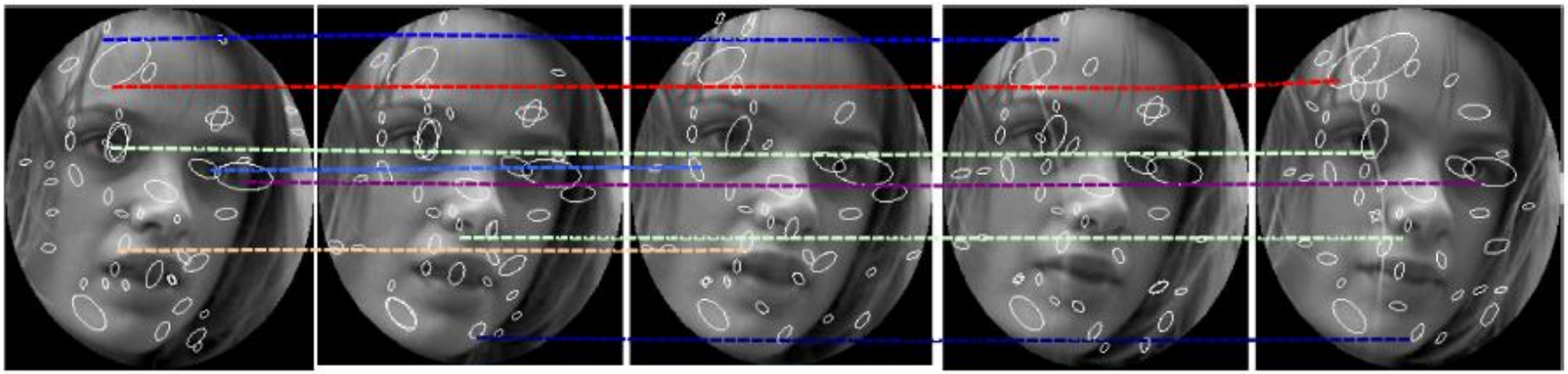
- intra-tube chain tracking
- consistent chain extraction



Solid lines: consistent chains, dash lines: noise, green lines: linking two short chain

- Tube T_i : a set of chains C_{ri} of SIFT descriptors
- $T_i = \{C_{1i}, \ldots, K_{ki}\}$ and $C_{ri} = \{SIFT_{1r_i}, \ldots SIFT_{pr_i}\}$

a video kernel (2)



The major kernel on tubes is then defined as:

$$K'_{pow}(T_i, T_j) = \left(\sum_r \sum_s \frac{|C_{ri}|}{\sqrt{|T_i|}} \frac{|C_{sj}|}{\sqrt{|T_j|}} k'(C_{ri}, C_{sj})^q \right)^{\frac{1}{q}} \quad (1)$$

with the following minor kernel on chains:

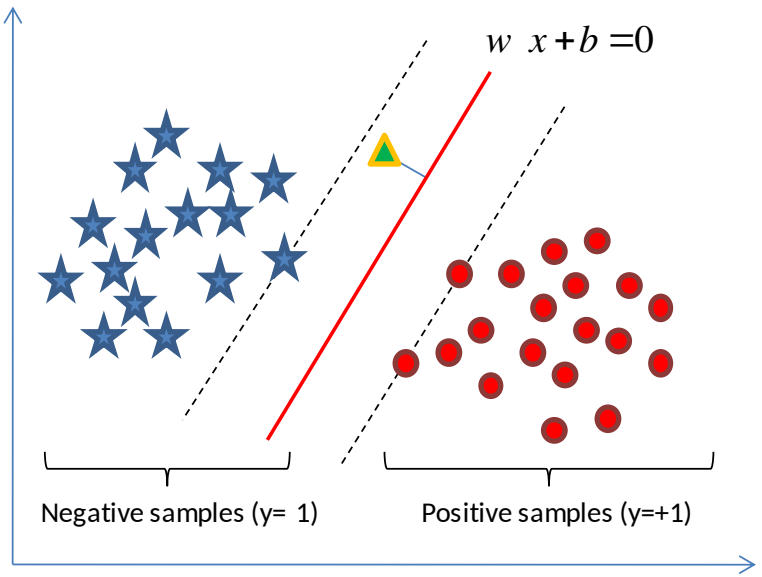
$$k'(C_{ri}, C_{sj}) = exp\left(-\frac{1}{2\sigma^2} \chi^2 \left(\overline{C}_{ri}, \overline{C}_{sj} \right) \right) e^{-\frac{\left(\overline{x}_{ri} - \overline{x}_{sj}\right)^2 + \left(\overline{y}_{ri} - \overline{y}_{sj}\right)^2}{2\sigma_2^2}}$$

Output of SVM

- not a probability
- need to be transformed (Platt)
- `sklearn` constructor option `probability` set to `True`

Output of SVM classifier

1. SVMs output a class label (positive or negative) for each sample $\text{sign}(w.x + b)$
2. One can also compute distance from the hyperplane that separates classes, e.g. $w.x + b$. These distances can be used to compute performance metrics.



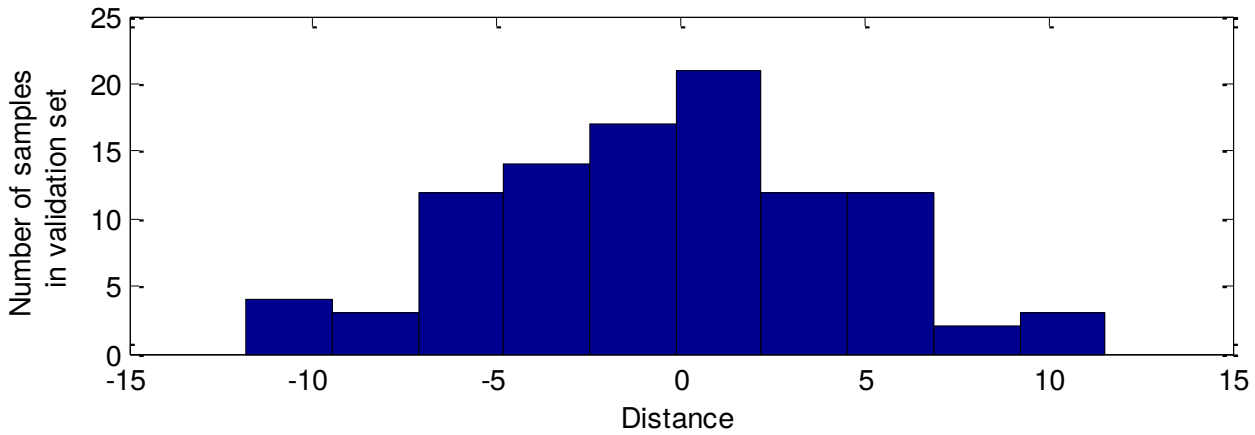
- Question : How can one use SVMs to estimate posterio class probabilities, i.e. $P(\text{positive class} \mid \text{sample } x)$?

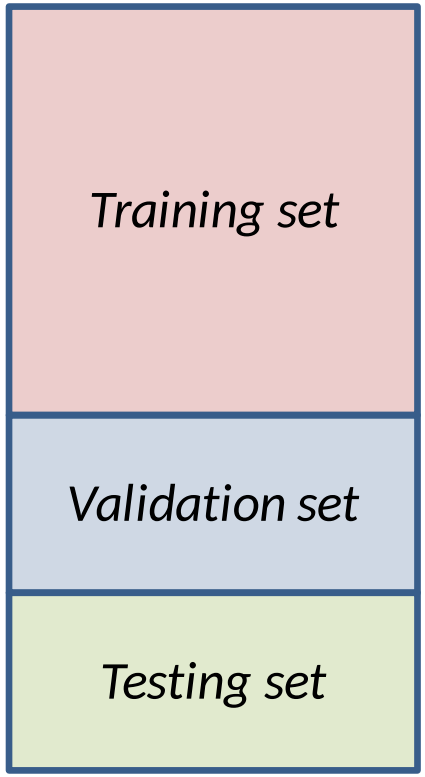
Simple binning method

1. Train SVM classifier in the *Training set*.
2. Apply it to the *Validation set* and compute distances from the hyperplane to each sample.

Sample #	1	2	3	4	5	...	98	99	100
Distance	2	1	8	3	4		2	0.3	0.8

3. Create a histogram with Q (e.g., say 10) bins using the above distances. Each bin has an upper and lower value in terms of distance.

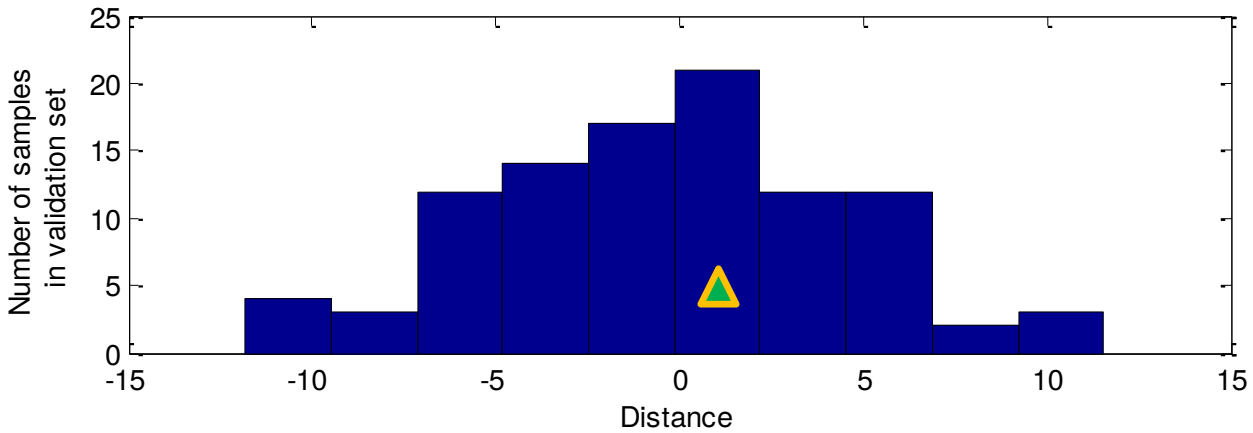


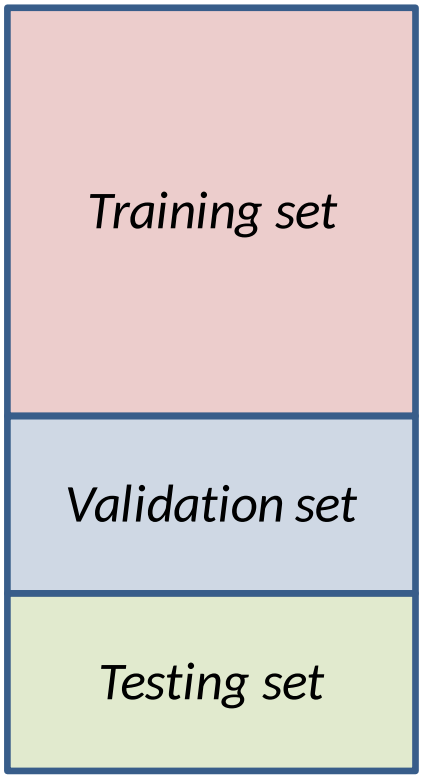


Simple binning method

4. Given a new sample from the *Testing set*, place it in the corresponding bin.

   E.g., sample #382 has distance to hyperplane = 1, so it is placed in the bin [0, 2.5]





5. Compute probability P(positive class | sample #382) as a fraction of true positives in this bin.

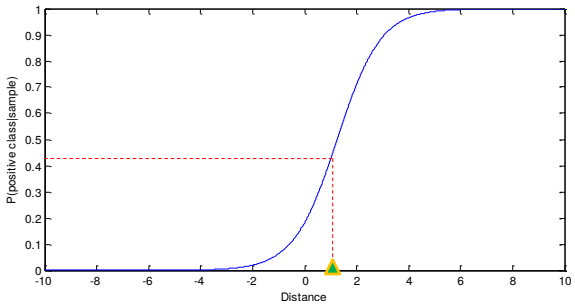
   E.g., this bin has 22 samples (from the *Validation set*), out of which 17 are positive ones , so we compute P(positive class | sample #382) = 17/22 = 0.77

Platts's method

- convert distances output by SVM to probabilities :
  - sigmoid filter :

$$P(\text{positive class}|\text{sample}) = \frac{1}{1+\exp(Ad+B)}$$

where d is the distance from hyperplane, A and B parameters



  - target probabilities : $t_i = \frac{y_i+1}{2}$
  - minimization :

$$\min -\sum_i t_i \log(p_i) + (1-p_i)\log(1-t_i) \text{ where } p_i = \frac{1}{1+\exp(Ad_i+B)}$$

Platt's method

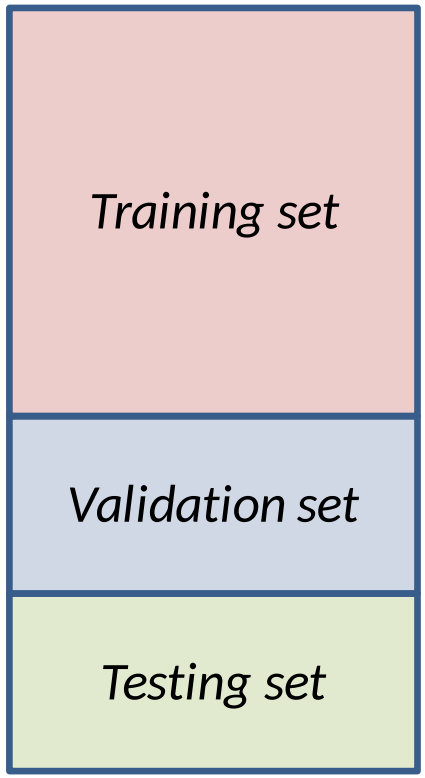
1. Train SVM classifier in the *Training set*.

2. Apply it to the *Validation set* and compute distances from the hyperplane to each sample.

Sample #	1	2	3	4	5	...	98	99	100
Distance	2	1	8	3	4		2	0.3	0.8

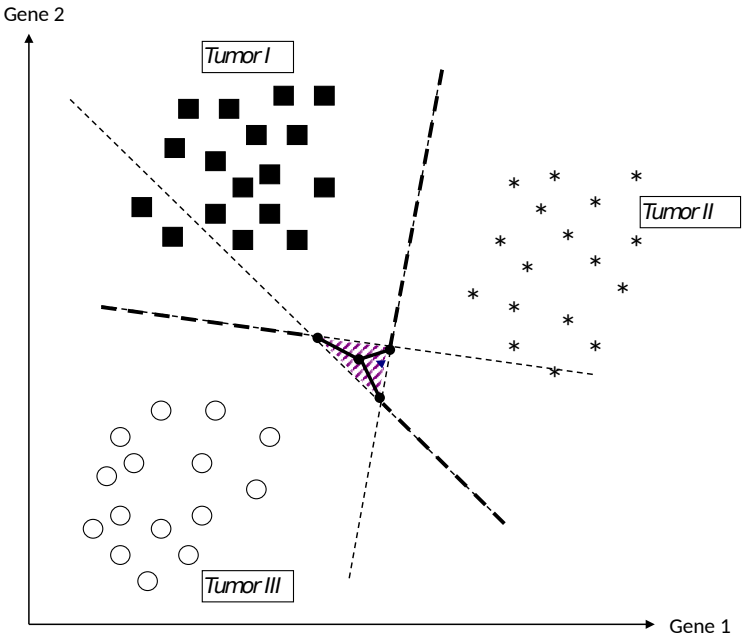
3. Determine parameters A and B of the sigmoid function by minimizing the negative log likelihood of the data from the *Validation set*.

4. Given a new sample from the *Testing set*, compute its posterior probability using sigmoid function.

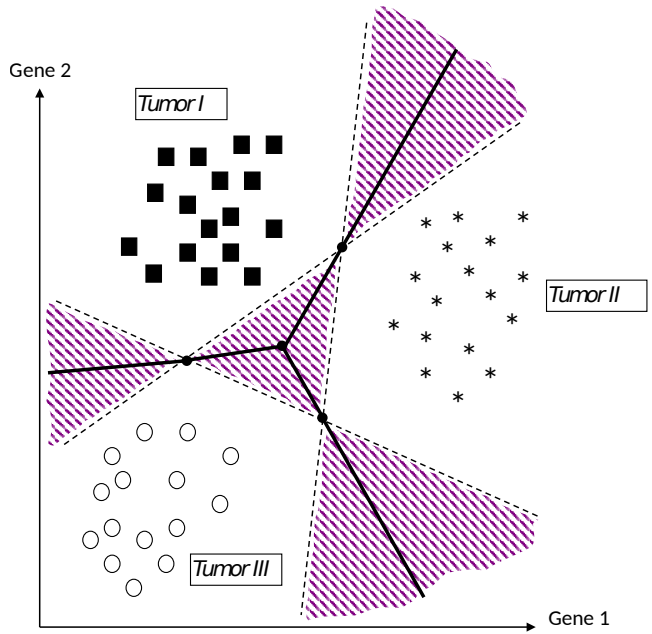


Multiclass SVM

- n classes
- two methods (`decision_function_shape(...)`)

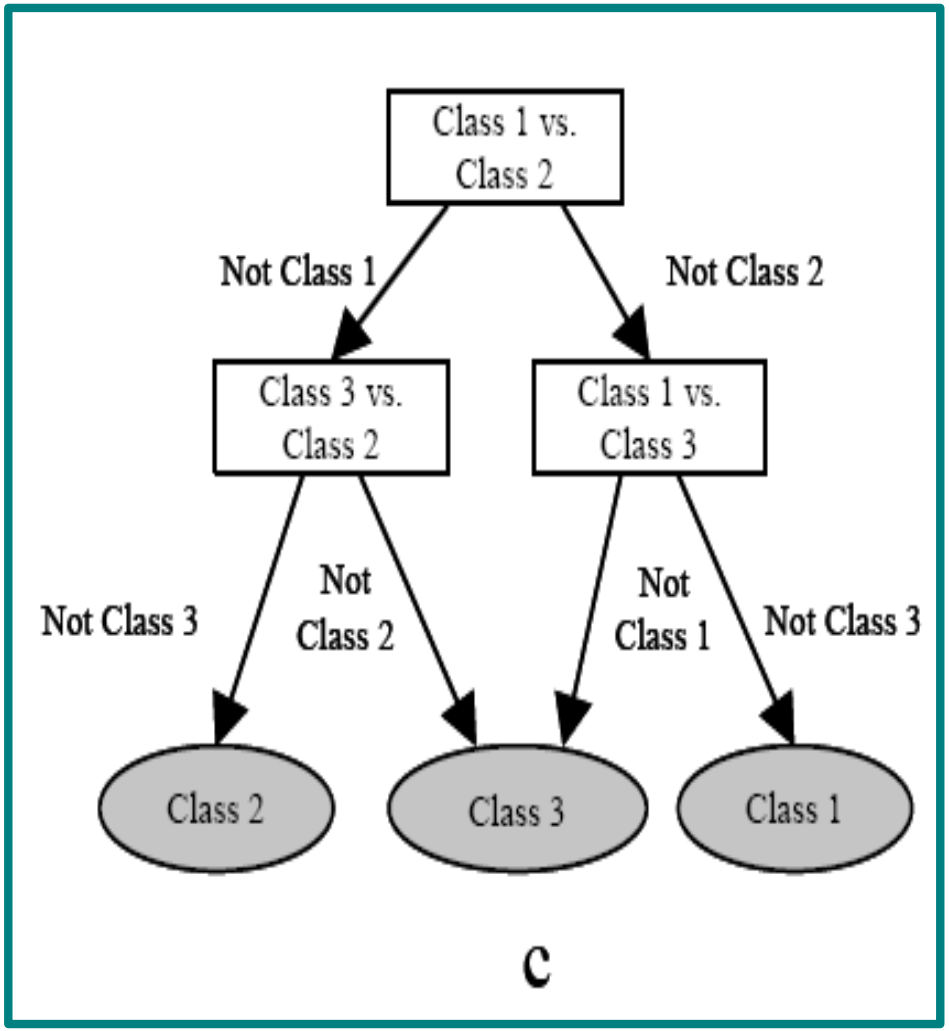


- one versus one (`'ovo'`)
  - build $n(n-1)/2$ SVM classifiers
  - maximum vote from classifiers



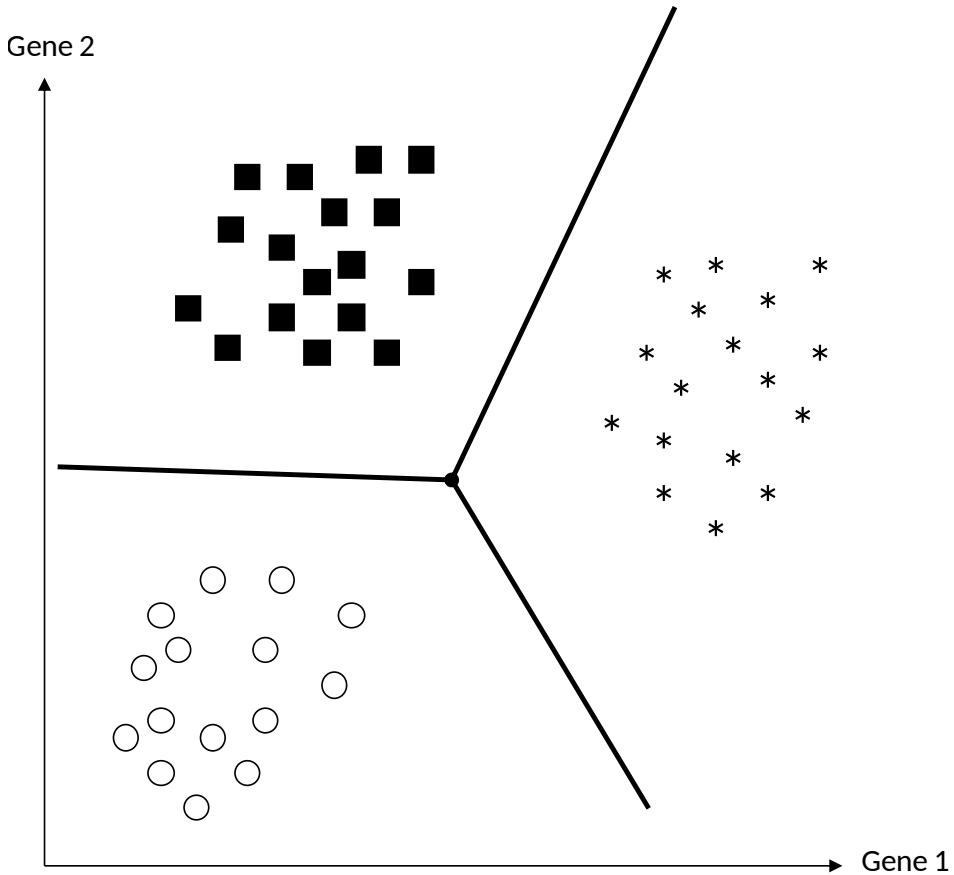
- one versus the rest (`'ovr'`)
  - build n SVM classifiers
  - unbalanced classes

DAGSVM multicategory



- Constructs a decision tree
- Each node is a binary SVM for a pair of classes
- k leaves : k classification decisions
- non-leaf (p, q) : two edges
  - left edge : not p decision
  - right edge : not q decision

SVM multicategory methods by Weston and Watkins and by Crammer and Singer

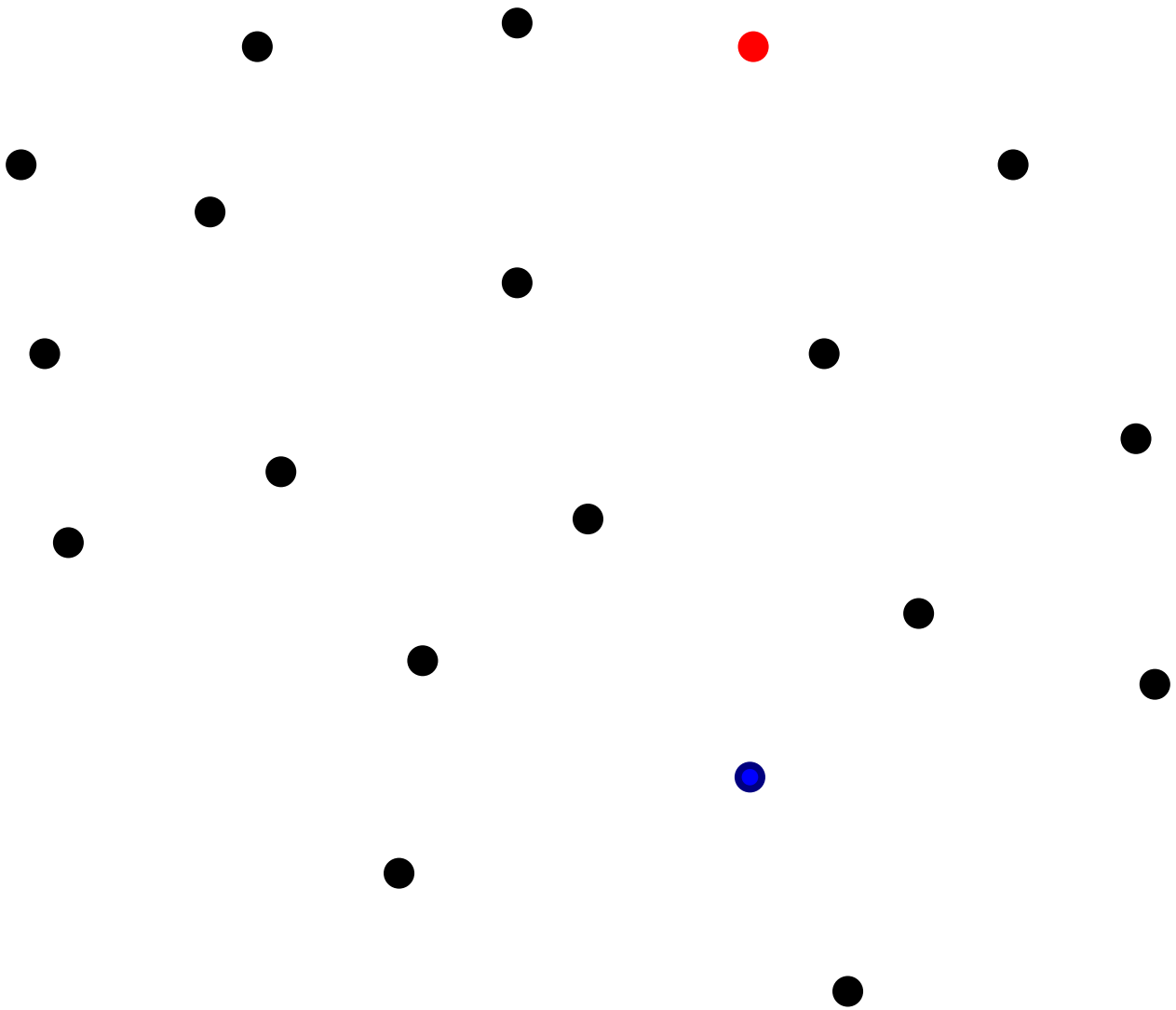


- Constructs a single classifier by maximizing the margin between all the classes simultaneously
- Both require the solution of a single QP problem of size (k-1)n, but the CS MC-SVM uses less slack variables in the constraints of the optimization problem, thereby making it computationally less expensive

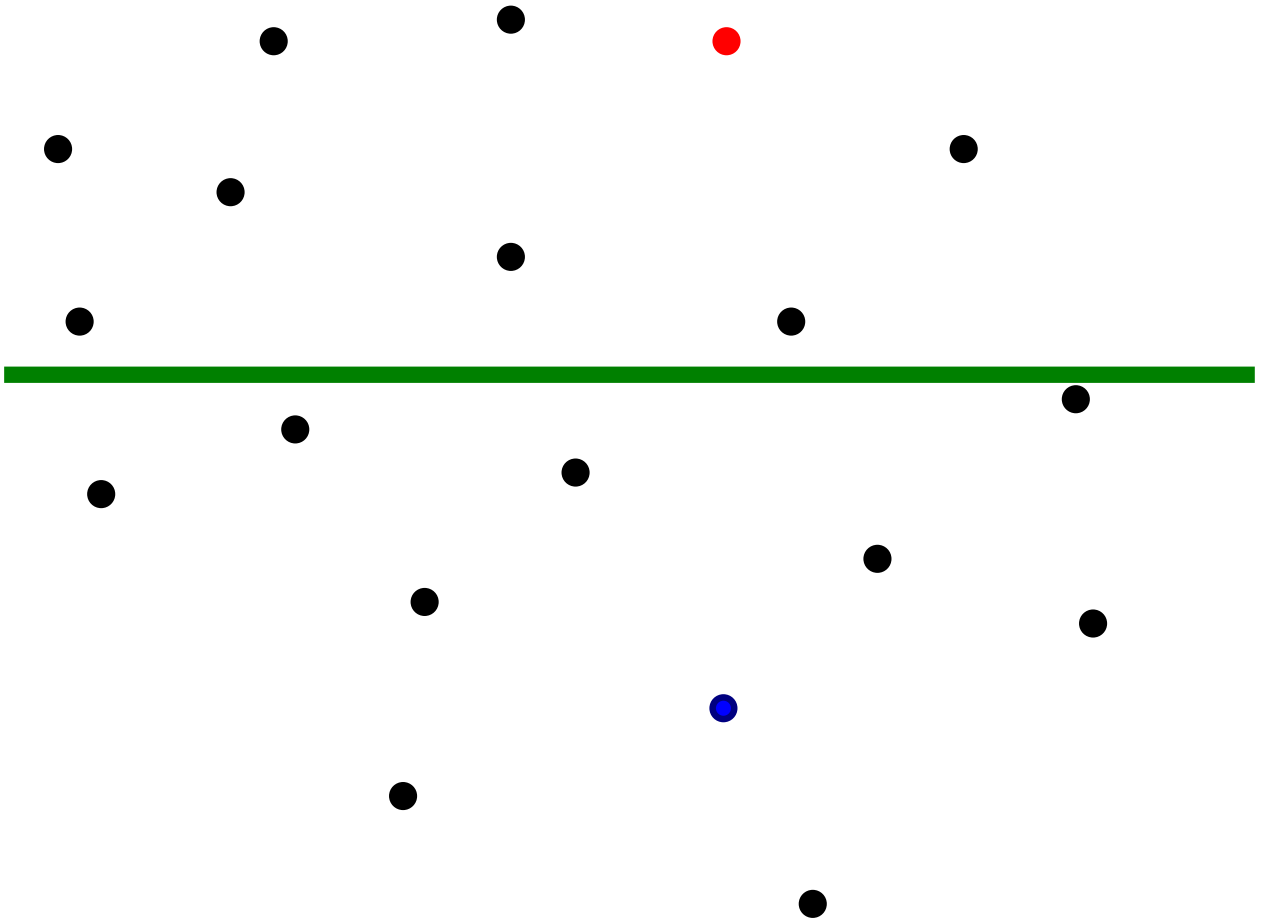
Active learning with SVM

- hyperplane estimation using small set of labelled data
- estimation of distance for non-labelled data
- selection of data close to the hyperplane (could use a constraint on diversity)
  - ask the user for label (or to correct labels)
- refine the estimation

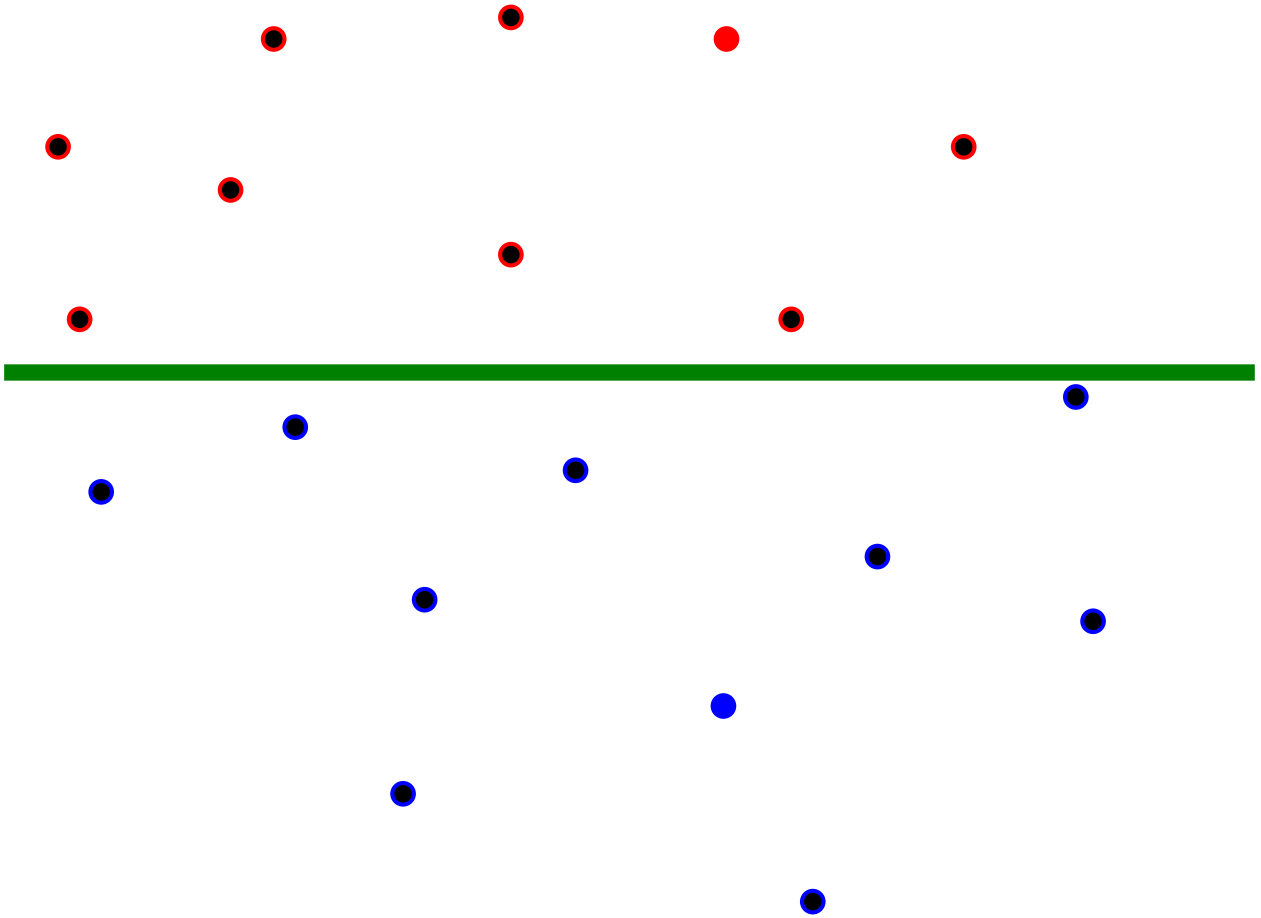
Active learning example : start with 2 annoted samples



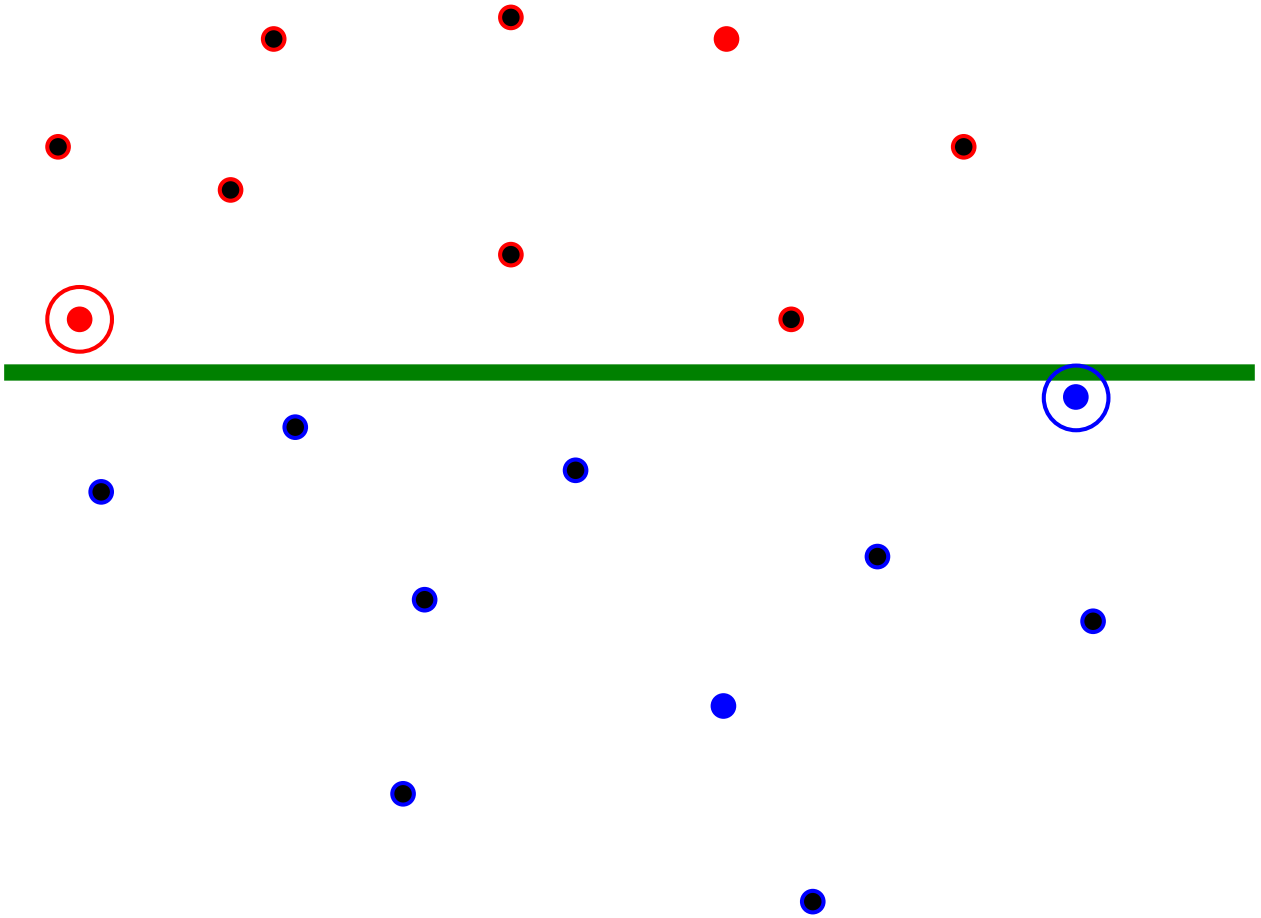
Active learning example : linear SVM classification



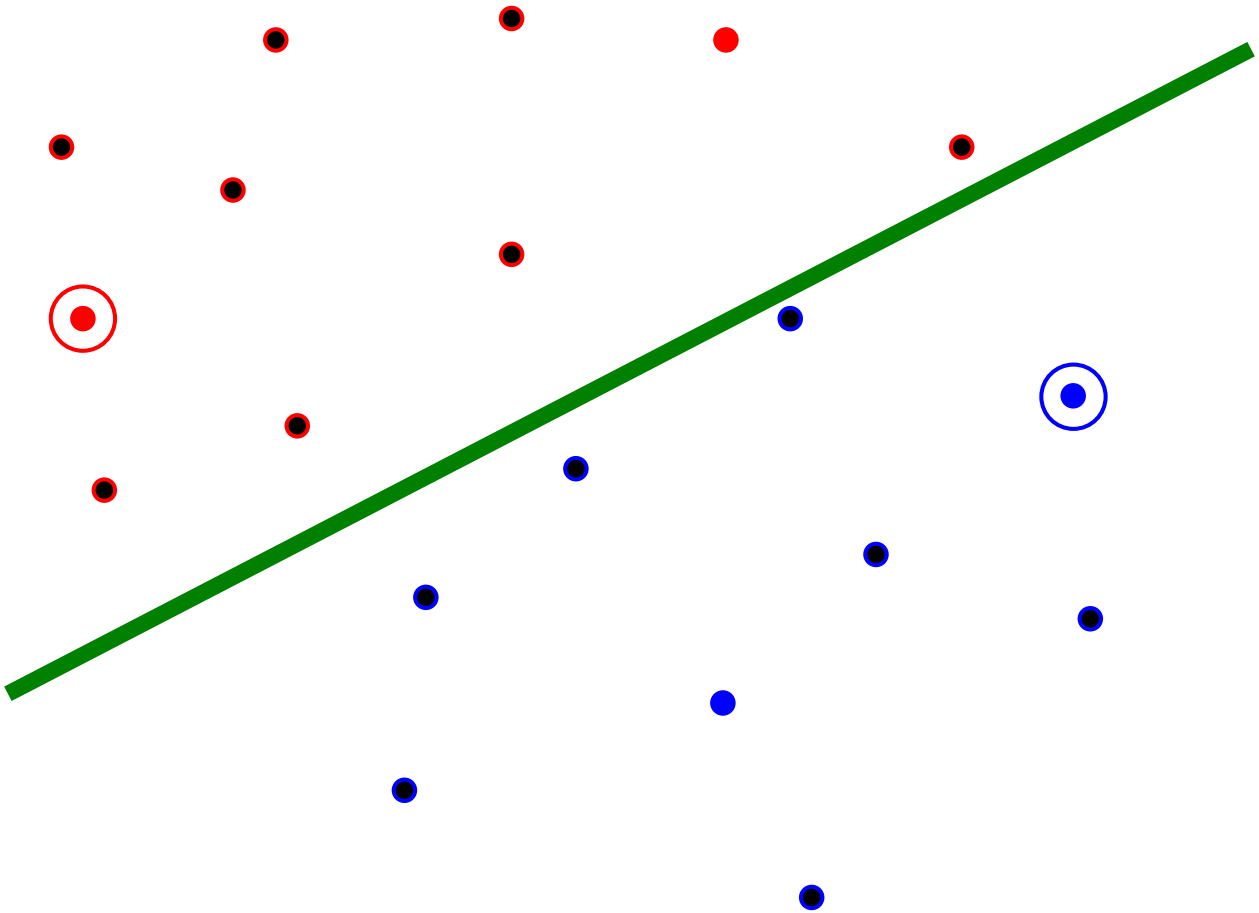
Active learning example : label all data



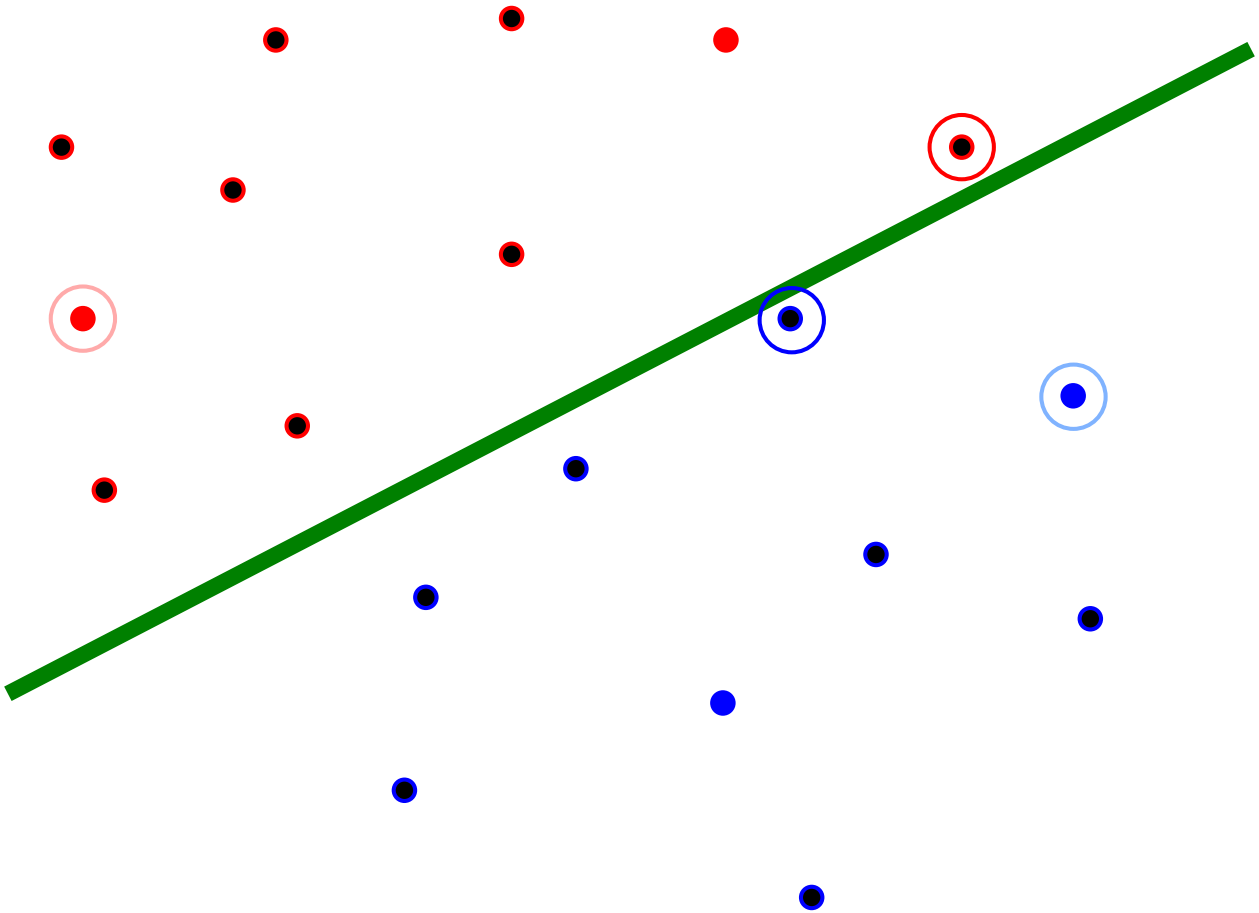
Active learning example : ask for labels of the 2 closest



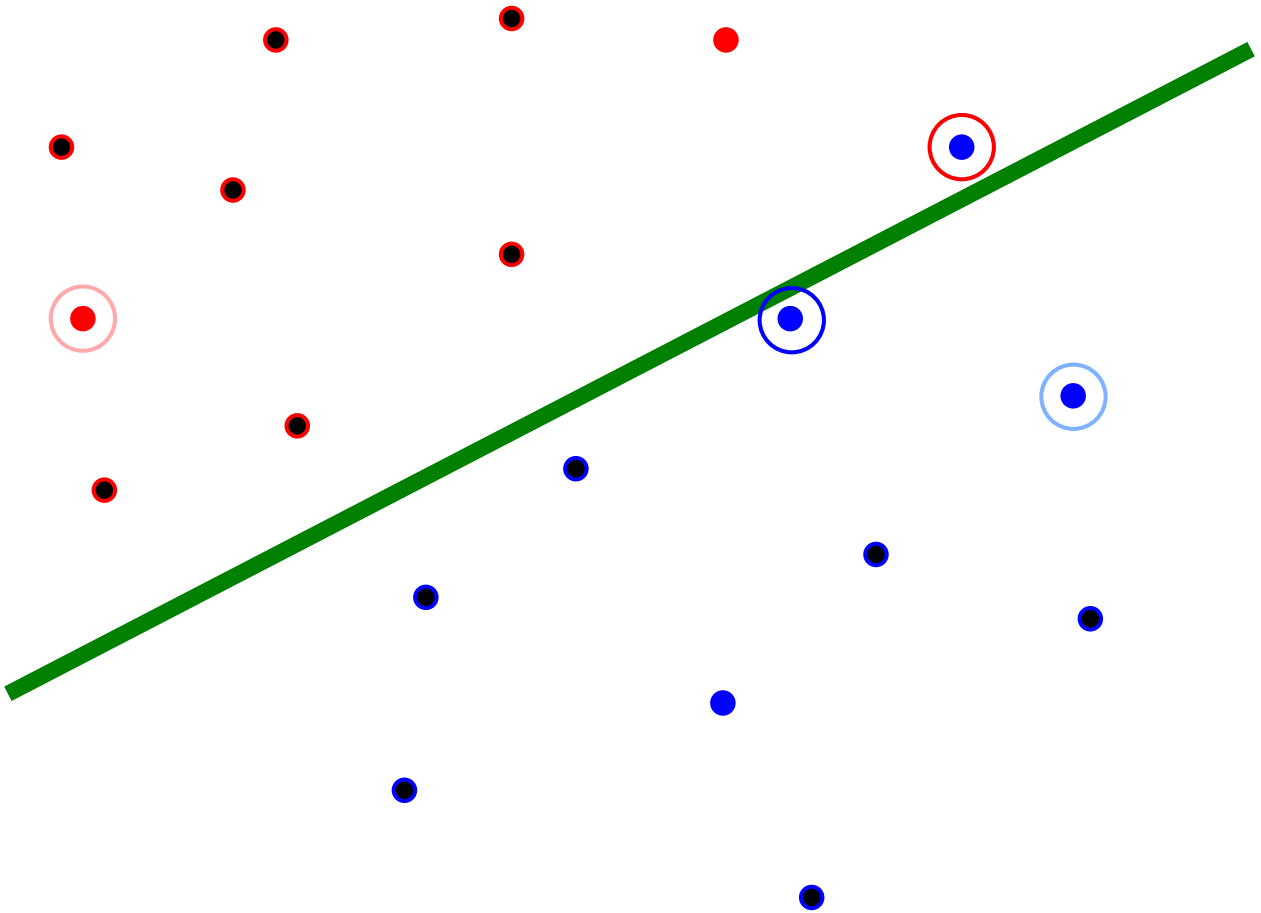
Active learning example : recompute linear SVM and labels



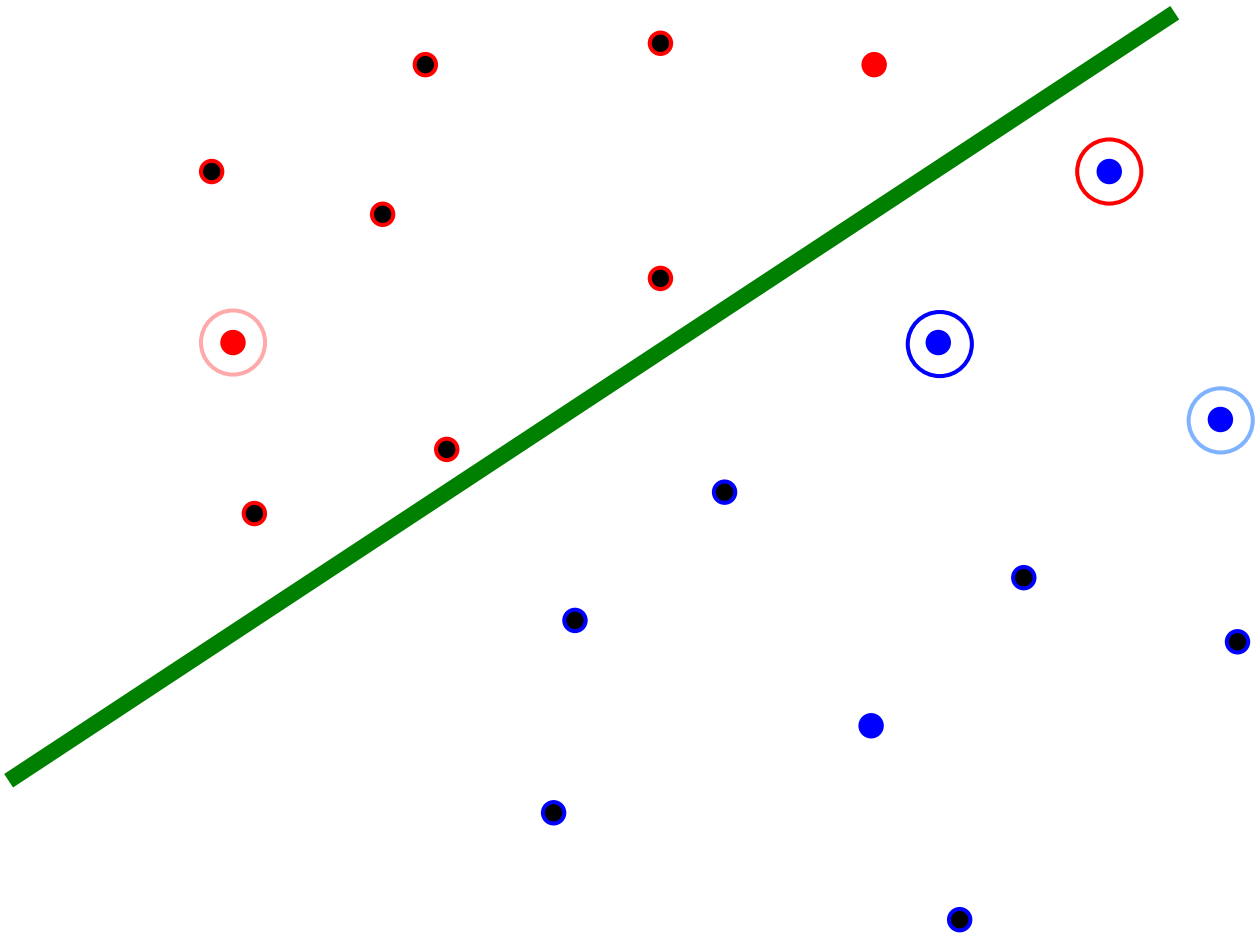
Active learning example : ask for labels of the 2 closest



Active learning example : correct one label

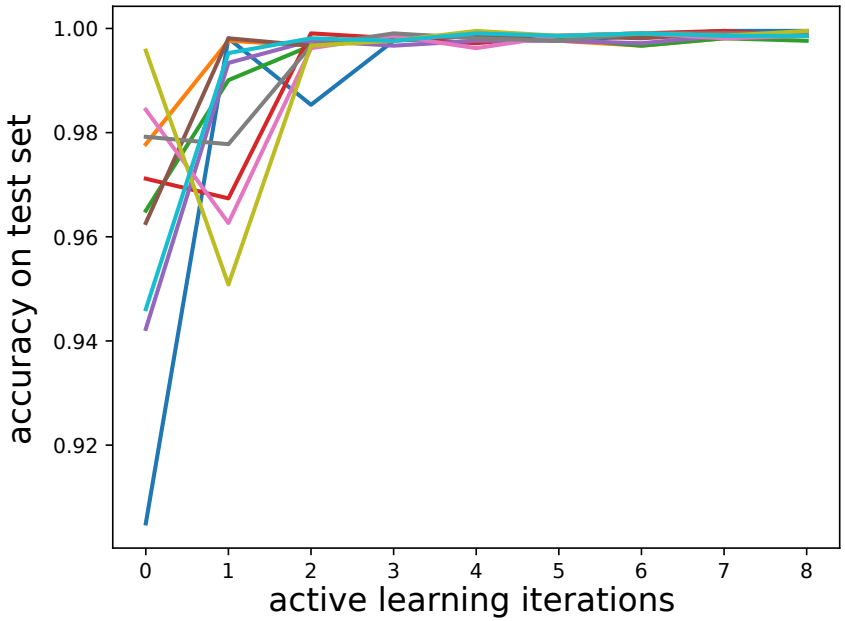


Active learning example : recompute linear SVM



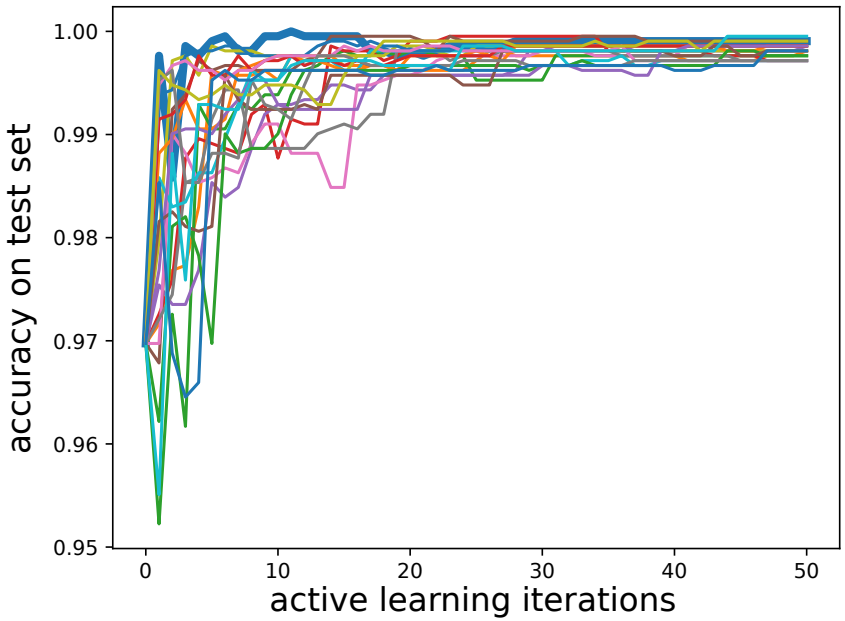
Active learning example : MNIST classes '0' and '1'

- Start randomly with 2 samples from class '0' and 2 samples from class '1'.
  - Each curve corresponds to a new random start (10 curves).
- Add 4 new annotated samples at each iteration. The new annotated samples are chosen as the closest to the boundary.
  - Fast convergence even for the worse starts
  - With all data : 0.99905



Active learning example : MNIST classes '0' and '1'

- Start with 2 samples from class '0' and 2 samples from class '1'
  - the same start for all the curves
- Add 4 new annotated samples at each iteration.
- In bold : the new annotated samples are chosen as the closest to the boundary.
- Other curves : new annotated samples are randomly chosen (each curve corresponds to different trials). **Longer to converge !**



Support Vector Machines

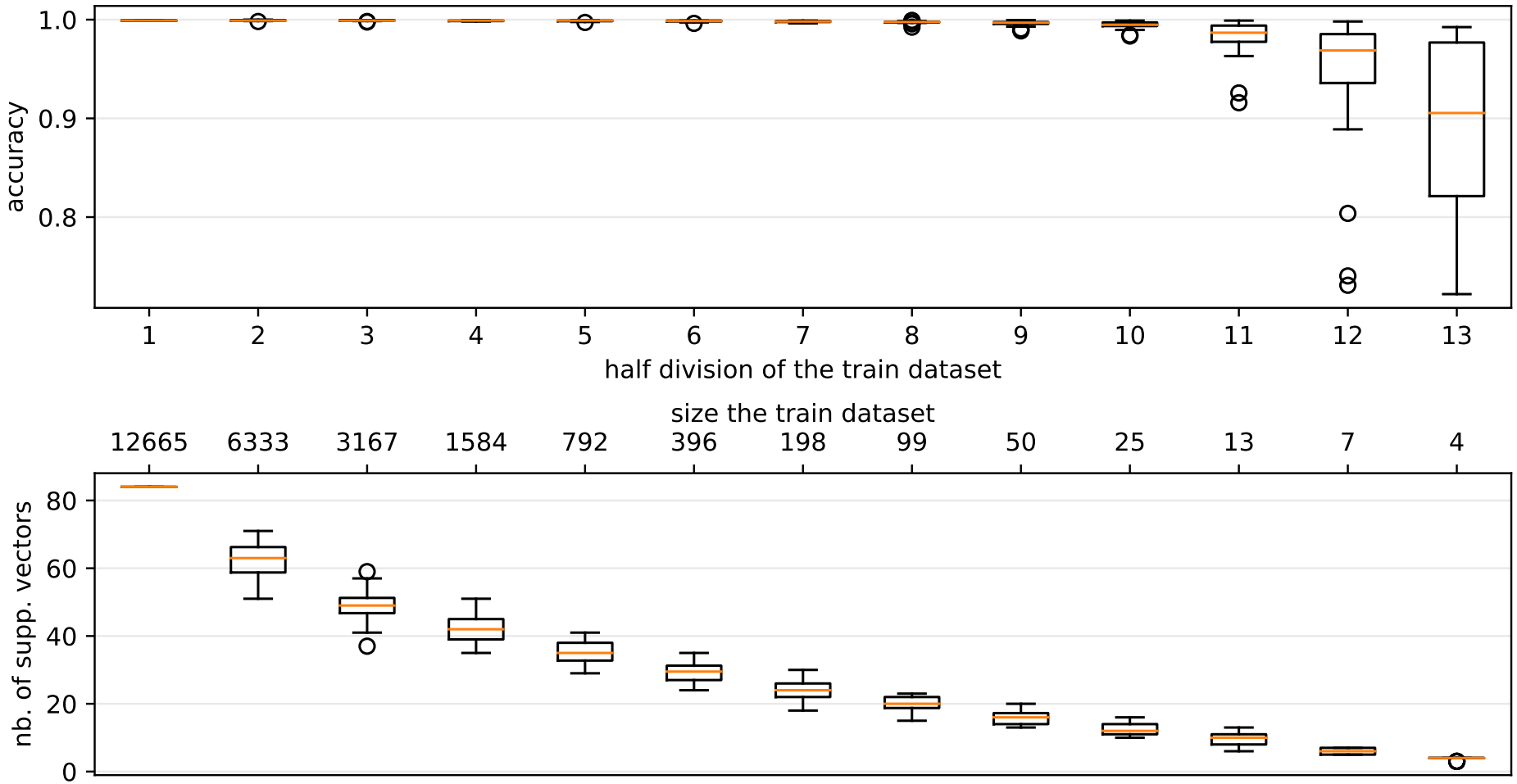
- SVMs are important because of theoretical reasons :
  - Robust to very large number of variables
  - Produce sparse models that are defined only by a small subset of training points ("support vectors")
  - Can learn both simple and highly complex classification models (by using the "kernel trick")
  - Do not require direct access to data and can work with only dot-products of data points/
  - Employ sophisticated mathematical principles to avoid overfitting with internal capacity control (regularization)

Support Vector Machines

- SVMs are important because of superior empirical results
  - Do not have more free parameters than the number of support vectors, irrespective of the number of variables in the dataset
  - Require solution of a convex QP optimization problem that has a global minimum and can be solved efficiently. Thus optimizing the SVM model parameters is not subject to heuristic optimization failures that plague other machine learning methods (e.g. neural networds, decision trees, ...)

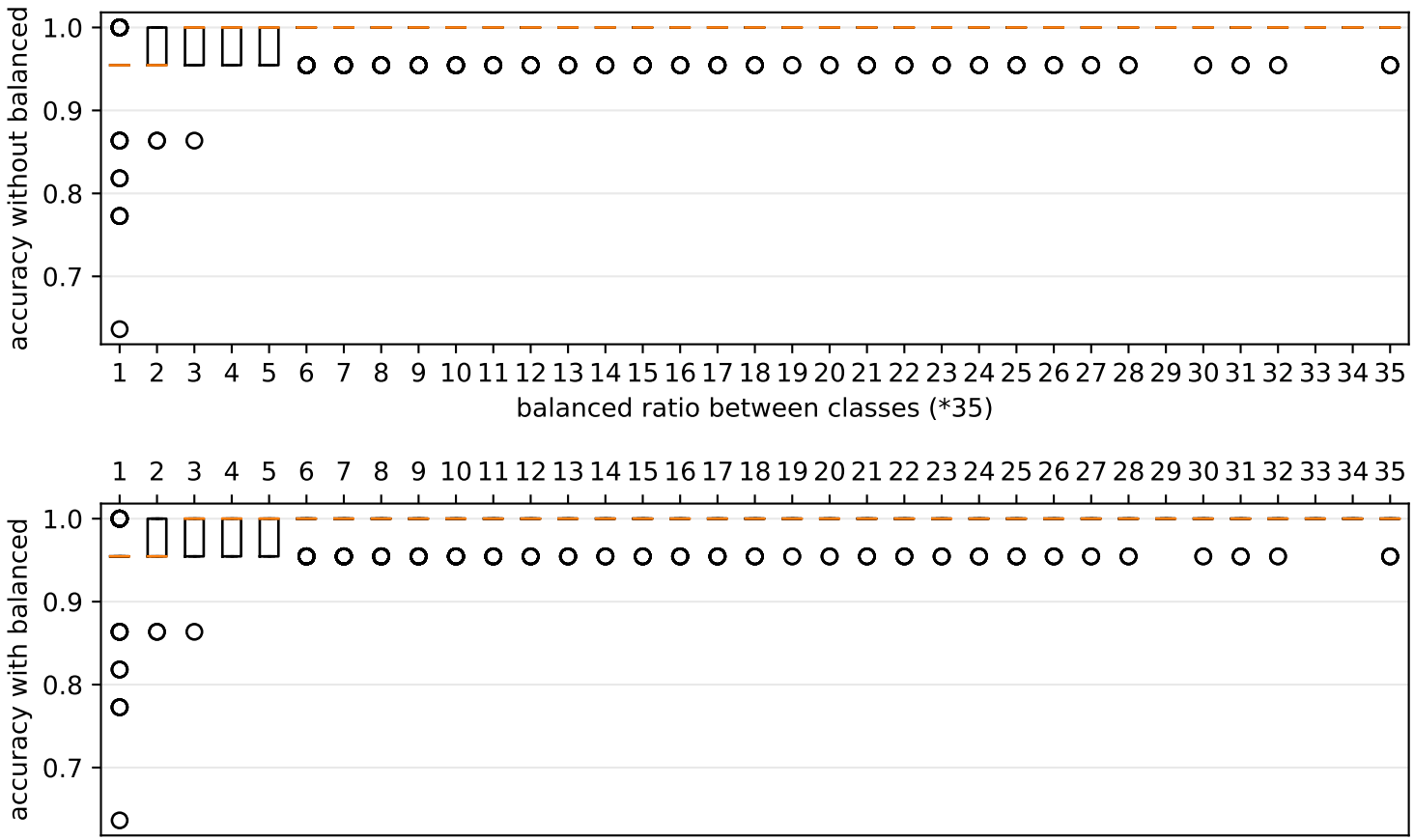
Experimenting the size reduction of train data

- MNIST data set (2 classes : '0' and '1', 12665 data, 784 features)
- linear SVM using default parameter (C=1)
- recursive division by 2 of the train dataset (not the test !)
- 24 trials for each set of parameters (data shuffled)



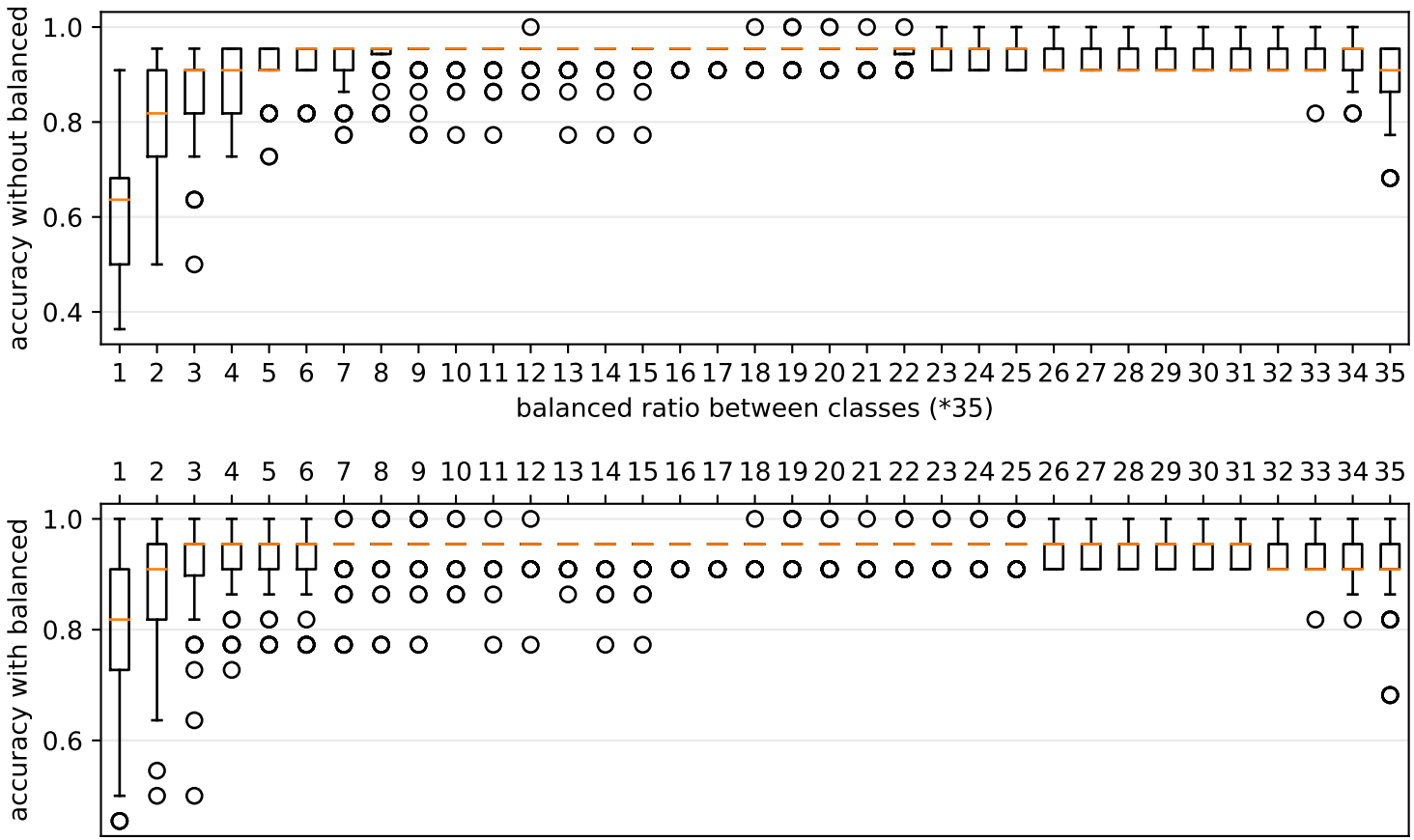
Unbalanced data

- Iris dataset (3 classes, 150 data, 4 features).
- linear SVM using default parameters. 2nd experiment using balanced weights.
- constant size of train dataset :35. Varying ratio of class sizes.
- 100 trials for each set of parameters (data shuffled)



Unbalanced data

- Iris dataset (3 classes, 150 data, **2** features).
- linear SVM using default parameters. 2nd experiment using balanced weights.
- constant size of train dataset :35. Varying ratio of class sizes.
- 100 trials for each set of parameters (data shuffled)



Unbalanced data

- MNIST data set (2 classes : '0' and '1', 12665 data, 784 features)
- linear SVM using default parameters. 2nd experiment using balanced weights.
- constant size of train dataset : 5923. Varying ratio of class sizes.
- 24 trials for each set of parameters (data shuffled)