Weka(2) & SVM

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Data format for Weka (.ARFF)

Header

```
@relation heart-disease-simplified

@attribute age numeric
@attribute sex { female, male}
@attribute chest_pain_type { typ_angina, asympt, non_anginal, atyp_angina}
@attribute cholesterol numeric
@attribute exercise_induced_angina { no, yes}
@attribute class { present, not_present}

@data
63,male,typ_angina,233,no,not_present
```

Data
(CSV format)

```
67,male,asympt,286,yes,present
67,male,asympt,229,yes,present
38,female,non_anginal,?,no,not_present
```

Note: You can easily generate ‘arff’ file by adding a header to a usual CSV text file

How to Evaluate the Performance? (1/2)

- Usually, build a Confusion Matrix out of given data
- Evaluation Metrics
  - Accuracy (percent correct)
  - Precision
  - Recall
  - Many other metrics: F-measure, Kappa score, etc.
- For fare evaluation, the ‘cross-validation’ scheme is used

How to Evaluate the Performance? (2/2)

- Confusion Matrix

Real / Prediction	Positive	Negative	
Positive	**TP**	**FP**	**All with positive Test**
Negative	**FN**	**TN**	**All with Negative Test**
	All with Disease	**All without Disease**	**Everyone**

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}$$

$$\text{Precision} = \frac{TP}{TP + FP} \qquad \text{Recall} = \frac{TP}{TP + FN}$$

As **recall** ↑ **precision** ↓

conversely:

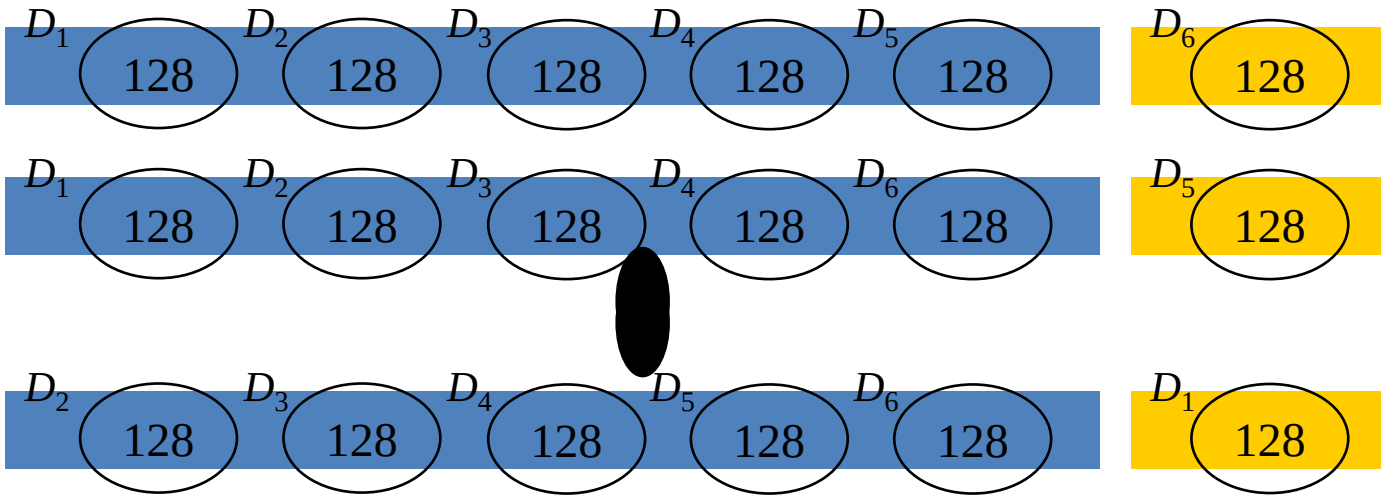
As **recall** ↓ **precision** ↑

Evaluation Method - Cross Validation

- *K*-fold Cross Validation
  - The data set is randomly divided into *k* subsets.
  - One of the *k* subsets is used as the 'test set' and the other *k*-1 subsets are put together to form a 'training set'.

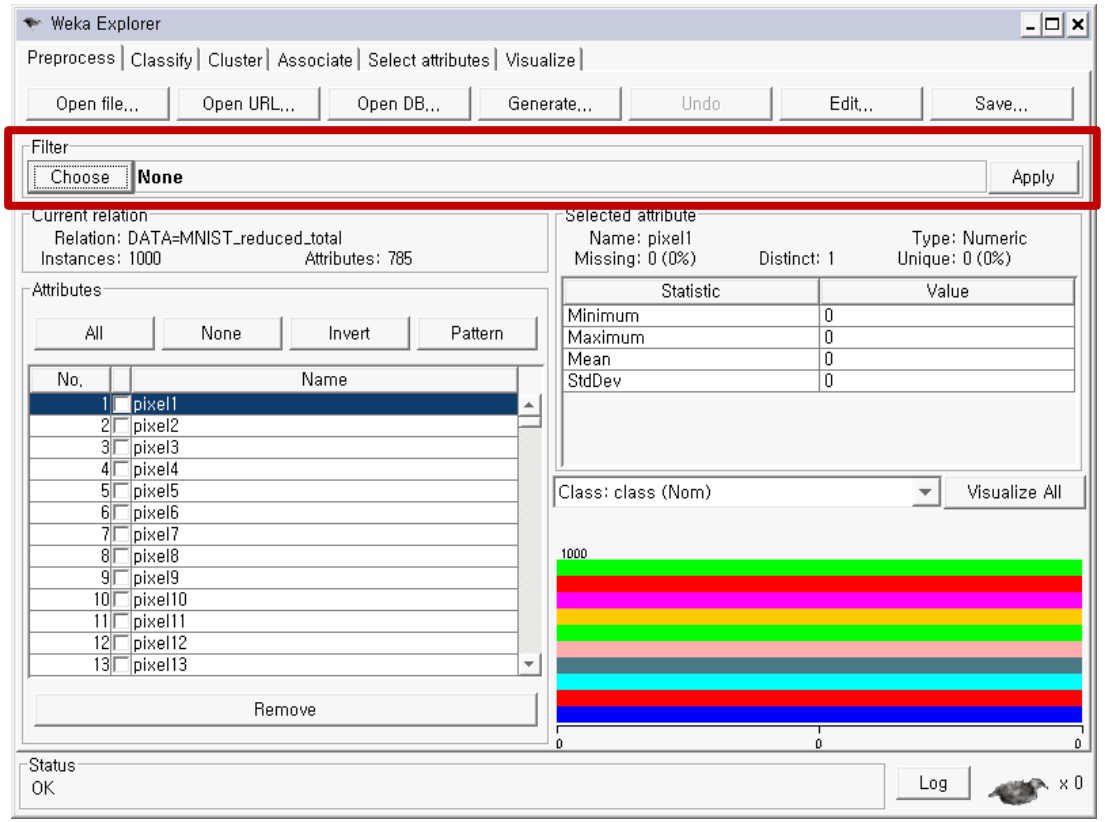
$$Error = \frac{1}{k}\sum_{i=1}^{k} Error_i$$

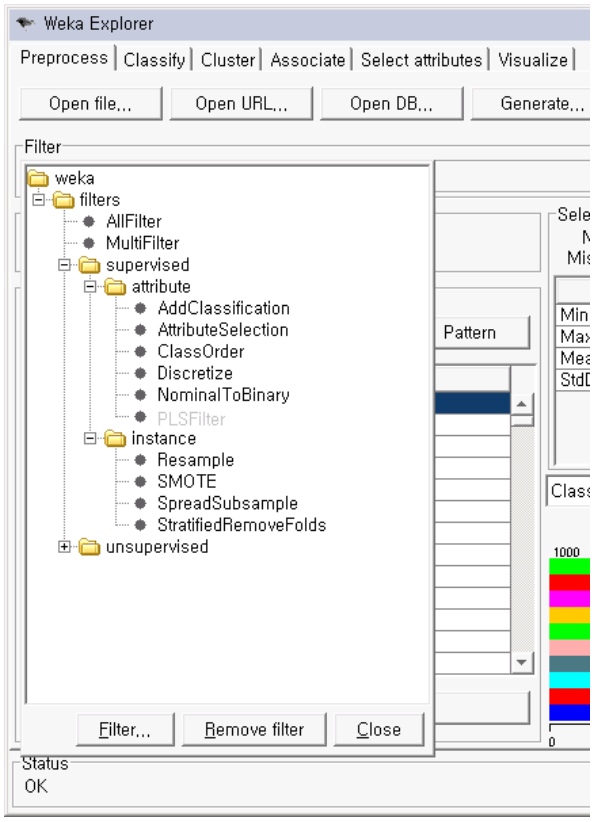
6-fold cross validation



Data Manipulation with Filter in Weka

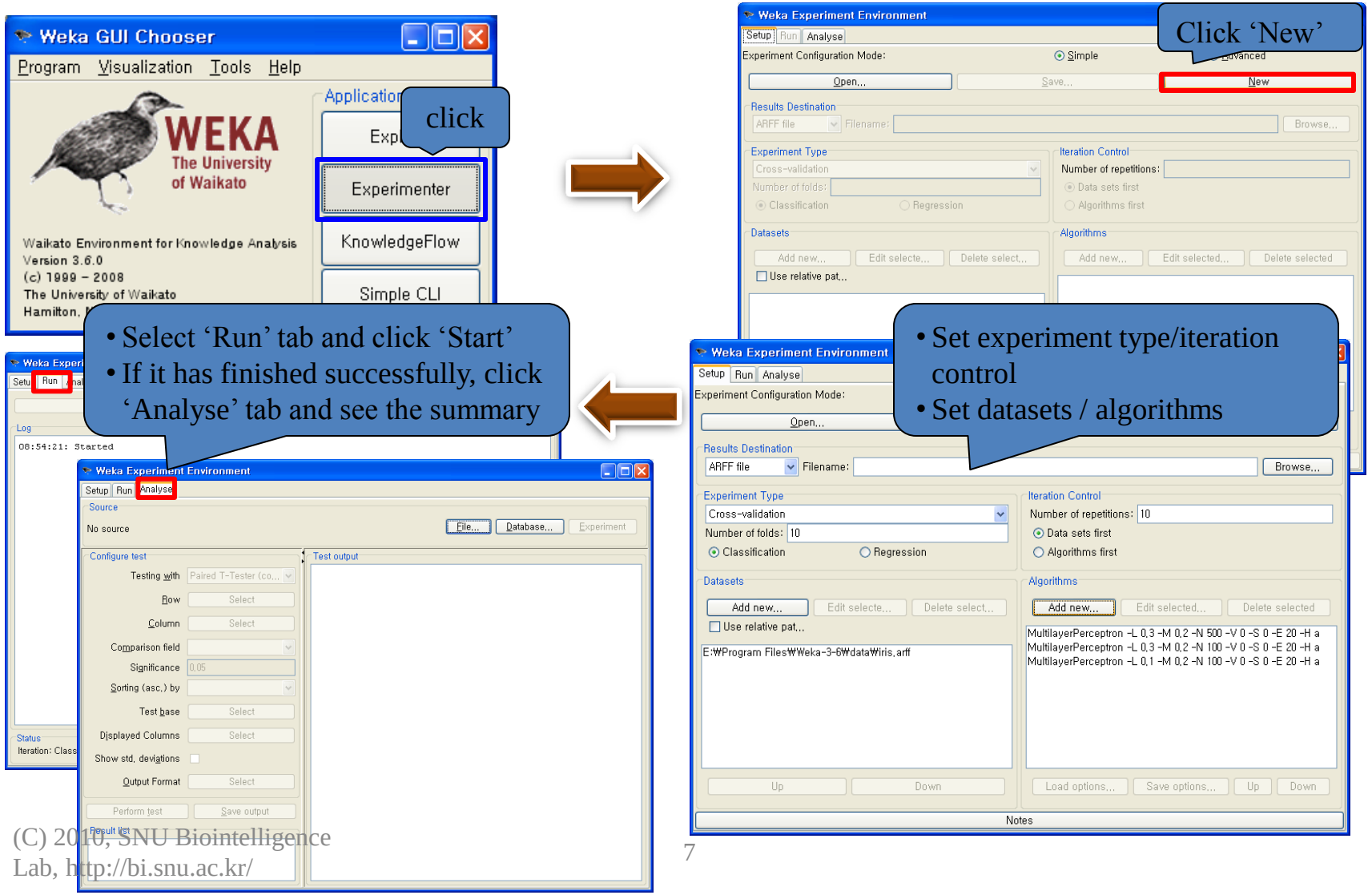
- Attribute
  - Selection, discretize
- Instance
  - Re-sampling, selecting specified folds





Using Experimenter in Weka

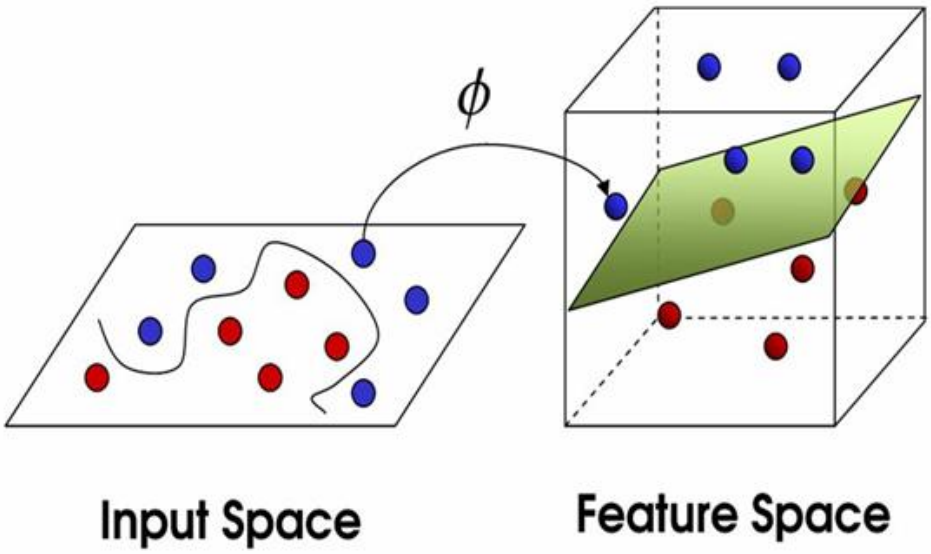
- Tool for ‘Batch’ experiments

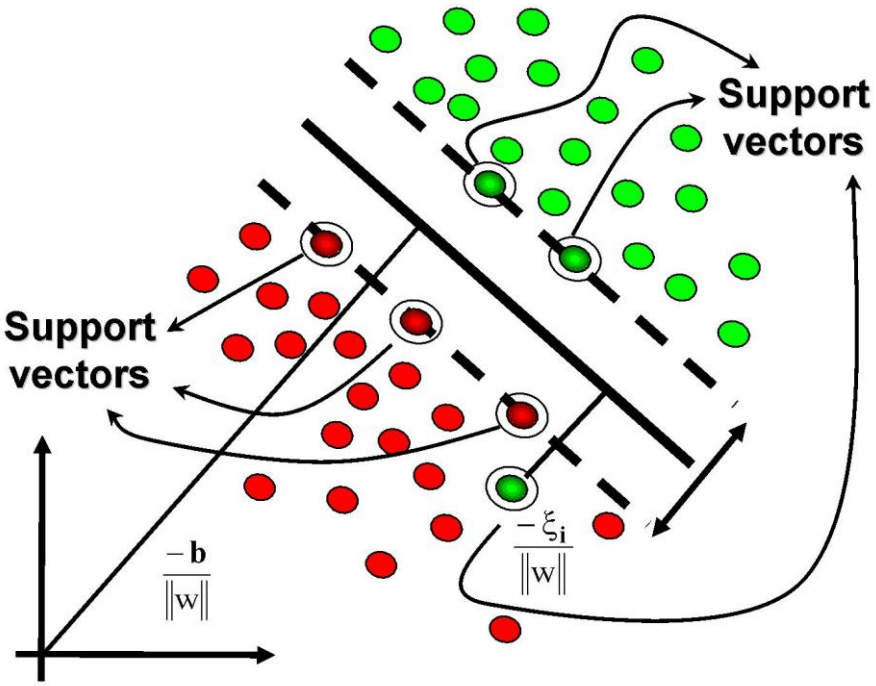


SVM

Support Vector Machines

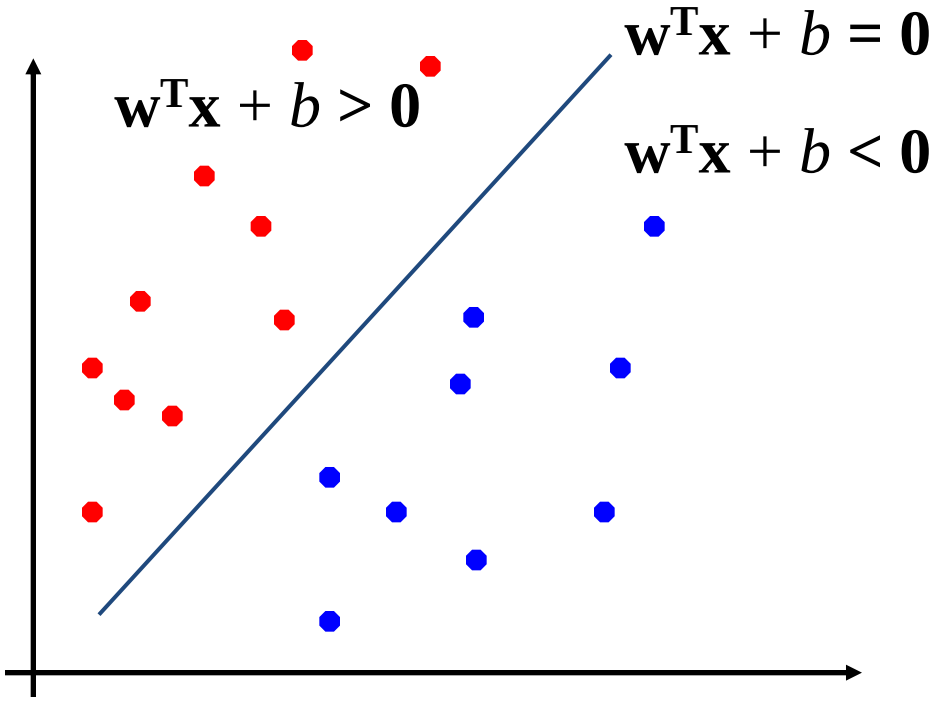
- SMO (sequential minimal optimization) for training SVM
  - In Weka, classifiers-functions-SMO





Perceptron Revisited: Linear Separators

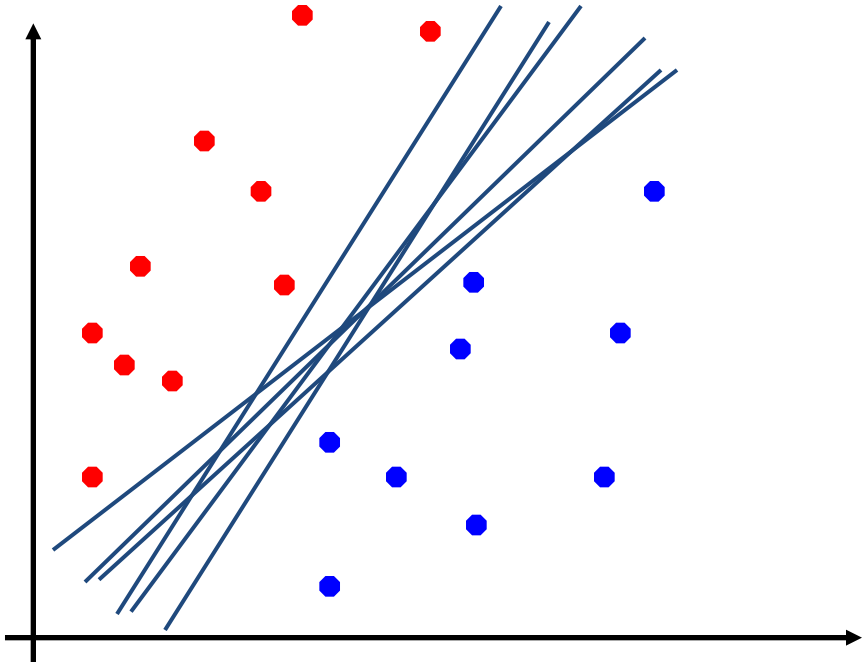
- Binary classification can be viewed as the task of separating classes in feature space:



$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$$

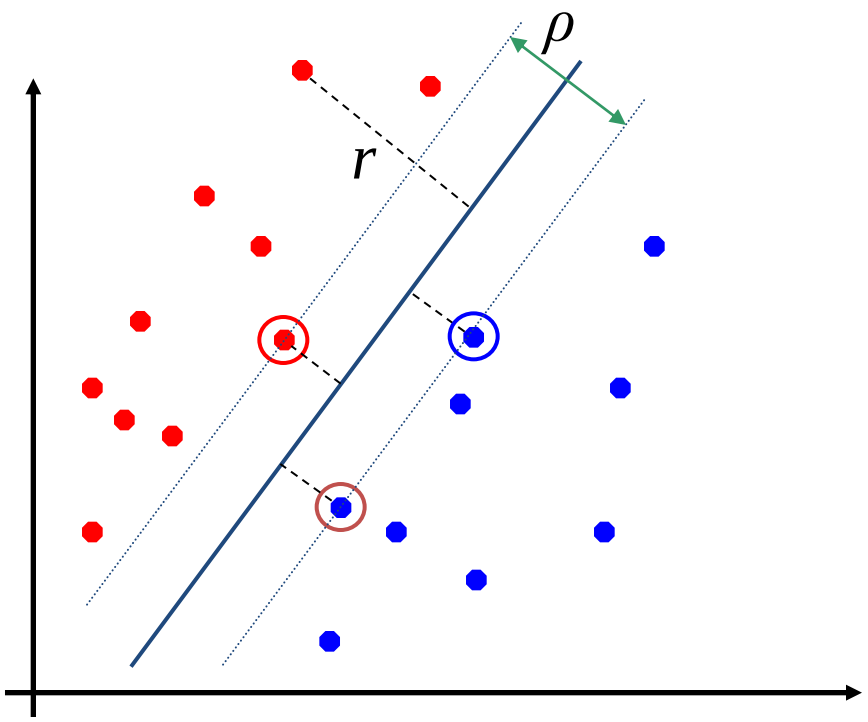
Linear Separators

- Which of the linear separators is optimal?



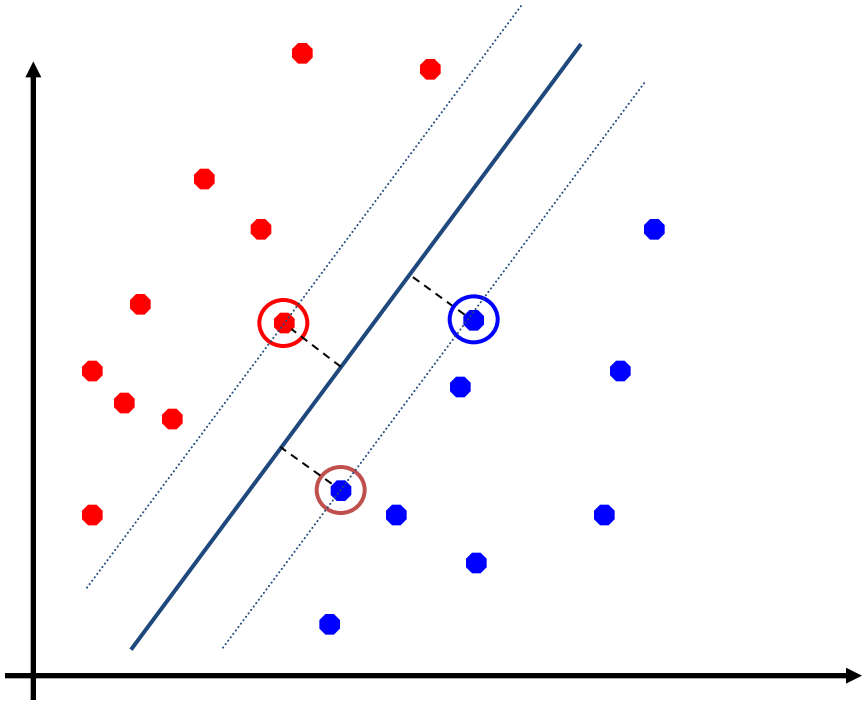
Classification Margin

- Distance from example $\mathbf{x}_i$ to the separator is $r = \dfrac{\mathbf{w}^T\mathbf{x}_i + b}{\|\mathbf{w}\|}$
- Examples closest to the hyperplane are ***support vectors***.
- ***Margin*** ρ of the separator is the distance between support vectors.



Maximum Margin Classification

- Maximizing the margin is good according to intuition and PAC theory.
- Implies that only support vectors matter; other training examples are ignorable.



Linear SVM Mathematically

- Let training set $\{(\mathbf{x}_i, y_i)\}_{i=1..n}$, $\mathbf{x}_i \in \mathbf{R}^d$, $y_i \in \{-1, 1\}$ be separated by a hyperplane with margin ρ. Then for each training example $(\mathbf{x}_i, y_i)$:

$$\begin{aligned} &\mathbf{w}^T\mathbf{x}_i + b \leq -\rho/2 \quad \text{if } y_i = -1 \\ &\mathbf{w}^T\mathbf{x}_i + b \geq \rho/2 \quad \text{if } y_i = 1 \end{aligned} \quad \Leftrightarrow \quad y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq \rho/2$$

- For every support vector $\mathbf{x}_s$ the above inequality is an equality. After rescaling $\mathbf{w}$ and b by $\rho/2$ in the equality, we obtain that distance between each $\mathbf{x}_s$ and the hyperplane is $r = \frac{y_s(\mathbf{w}^T\mathbf{x}_s + b)}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}$

- Then the margin can be expressed through (rescaled) $\mathbf{w}$ and b as:

$$\rho = 2r = \frac{2}{\|\mathbf{w}\|}$$

Linear SVMs Mathematically (cont.)

- Then we can formulate the *quadratic optimization problem:*

Find $\mathbf{w}$ and b such that

$\rho = \frac{2}{\|\mathbf{w}\|}$ is maximized

and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

Which can be reformulated as:

Find $\mathbf{w}$ and b such that

$\mathbf{\Phi}(\mathbf{w}) = \|\mathbf{w}\|^2 = \mathbf{w}^T\mathbf{w}$ is minimized

and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i (\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

Solving the Optimization Problem

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^T\mathbf{w}$ is minimized
and for all $(\mathbf{x}_i, y_i)$, $i=1..n$: $y_i (\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

- Need to optimize a *quadratic* function subject to *linear* constraints.
- Quadratic optimization problems are a well-known class of mathematical programming problems for which several (non-trivial) algorithms exist.
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every inequality constraint in the primal (original) problem:

Find $\alpha_1 \ldots \alpha_n$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2} \Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

The Optimization Problem Solution

- Given a solution $\alpha_1 \ldots \alpha_n$ to the dual problem, solution to the primal is:

$$\mathbf{w} = \Sigma \alpha_i y_i \mathbf{x}_i \qquad b = y_k - \Sigma \alpha_i y_i \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_k \quad \text{for any } \alpha_k > 0$$

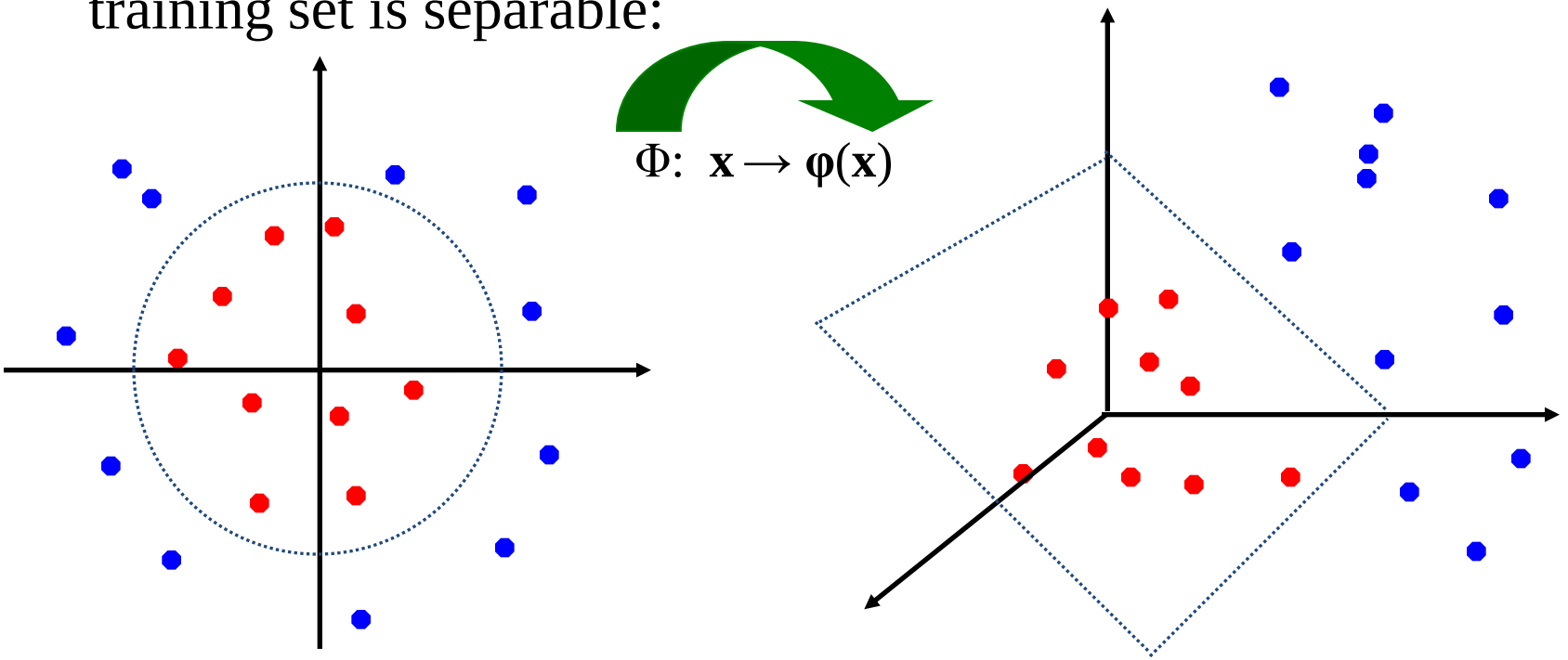
- Each non-zero α_i indicates that corresponding $\mathbf{x}_i$ is a support vector.
- Then the classifying function is (note that we don't need **w** explicitly):

$$f(\mathbf{x}) = \Sigma \alpha_i y_i \mathbf{x}_i^{\mathrm{T}} \mathbf{x} + b$$

- Notice that it relies on an *inner product* between the test point **x** and the support vectors $\mathbf{x}_i$ – we will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products $\mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j$ between all training points.

Non-linear SVMs: Feature spaces

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



Some Notes on the Parameter Setting

- Parameter Setting = Car Tuning
  - need much experience or many times of trial
  - you may get worse results if you are unlucky

- Multilayer Perceptron (MLP)
  - Main parameters for learning: hiddenLayers, learningRate, momentum, trainingTime (epoch), seed

- J48
  - Main parameters: unpruned, numFolds, minNumObj
  - Many parameters are for controlling the size of the result tree, i.e. confidenceFactor, pruning

- SMO (SVM)
  - Main parameters: c (complexity parameter), kernel, kernel parameters

Practice

- Basic
  - Comparing the performances of algorithms
    - MultilayerPerceptron vs. J48 vs. SVM
    - Checking the trained model (structure & parameter)
  - Tuning parameters to get better models
  - Understanding 'Test options' & 'Classifier output' in Weka

- Advanced
  - Building committee machines using 'meta' algorithms for classification
  - Preprocessing / data manipulation – applying 'Filter'
  - Batch experiment with 'Experimenter'
  - Design & run a batch process with 'KnowledgeFlow'