Machine learning

Support Vector Machines

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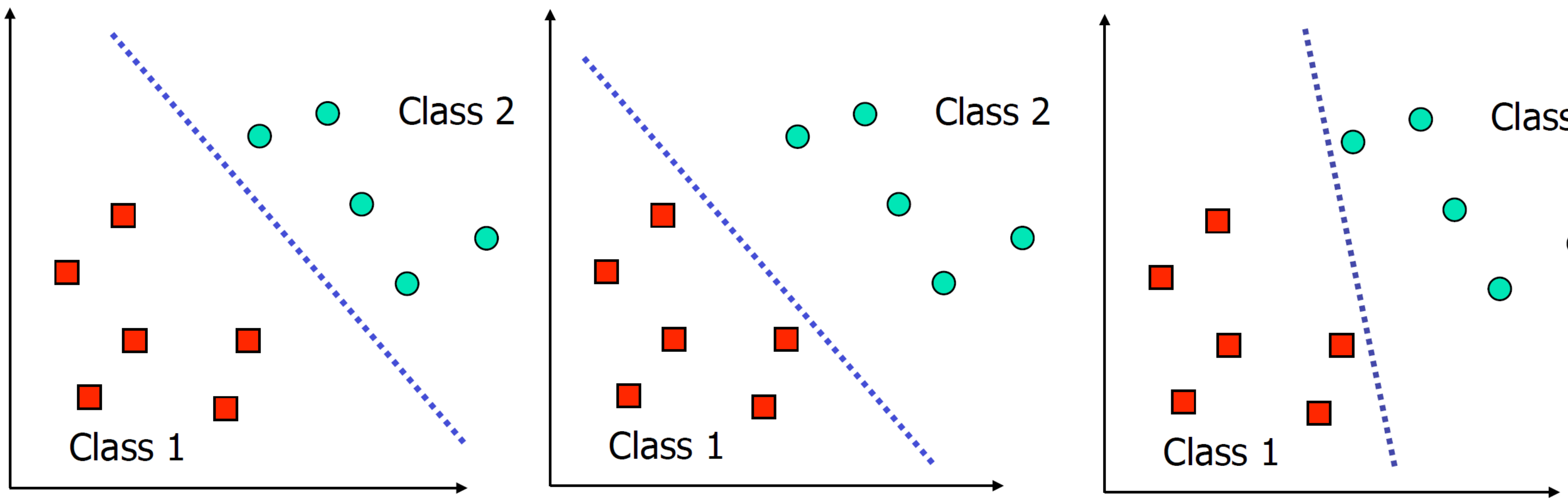
History of SVM

- SVM is related to **statistical learning theory** [3]
- SVM was first introduced in 1992 [1]
- SVM becomes popular because of its success in **handwritten** digit recognition
  - 1.1% test error rate for SVM. This is the same as the error rates of a carefully constructed neural network, LeNet 4.
- SVM is now regarded as an important example of "**kernel methods**", one of the key area in machine learning
  - Note: the meaning of "kernel" is different from the "kernel" function for **Parzen windows**

What is a good Decision Boundary?

- Are all decision boundaries **equally good**?



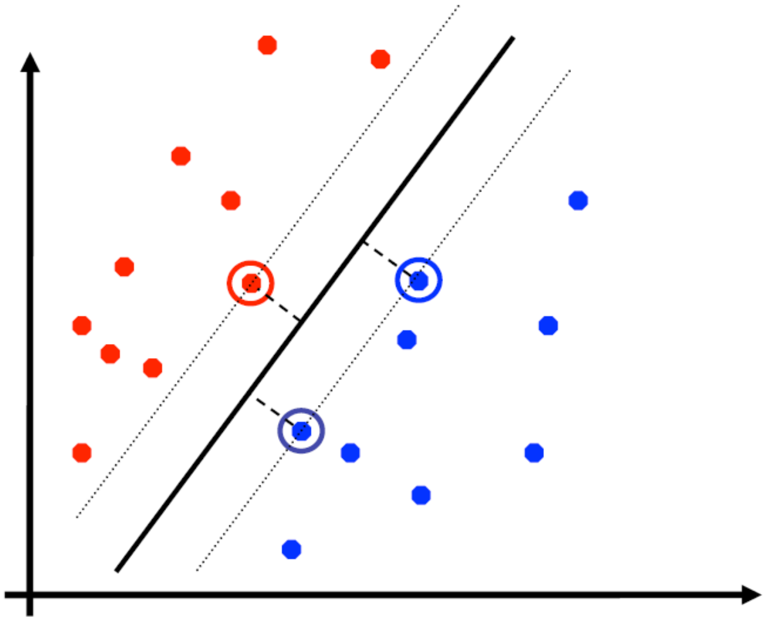
- The decision boundary should be **as far away** from the data of **both classes** as possible
  - We should maximize the **margin**, **m**

The maximum margin linear classifier is the

- SVMs (Vapnik, 1990's) choose the linear separator with the **largest margin**
- The simplest kind of SVM (Called an LSVM)

V. Vapnik

- **Support Vectors** are those data points that the **margin pushes** up against
  - These are **the most difficult samples** to classify.
- SVM is **good** according to **intuition**, **theory (VC dimension)**, **practice**



Linear model for classification bias-variance trade off

- Given a set of **training patterns** and class labels as $(\mathbf{x}_1, \mathbf{y}_1), \ldots,$ $(\mathbf{x}_n, \mathbf{y}_n) \in R^d \times \{\pm 1\}$, the goal is to find a classifier function $f: R^d \to \{\pm 1\}$ such that $f(x) = y$ will **correctly classify** new patterns.

- Support vector machines are based on the class of **hyperplanes**

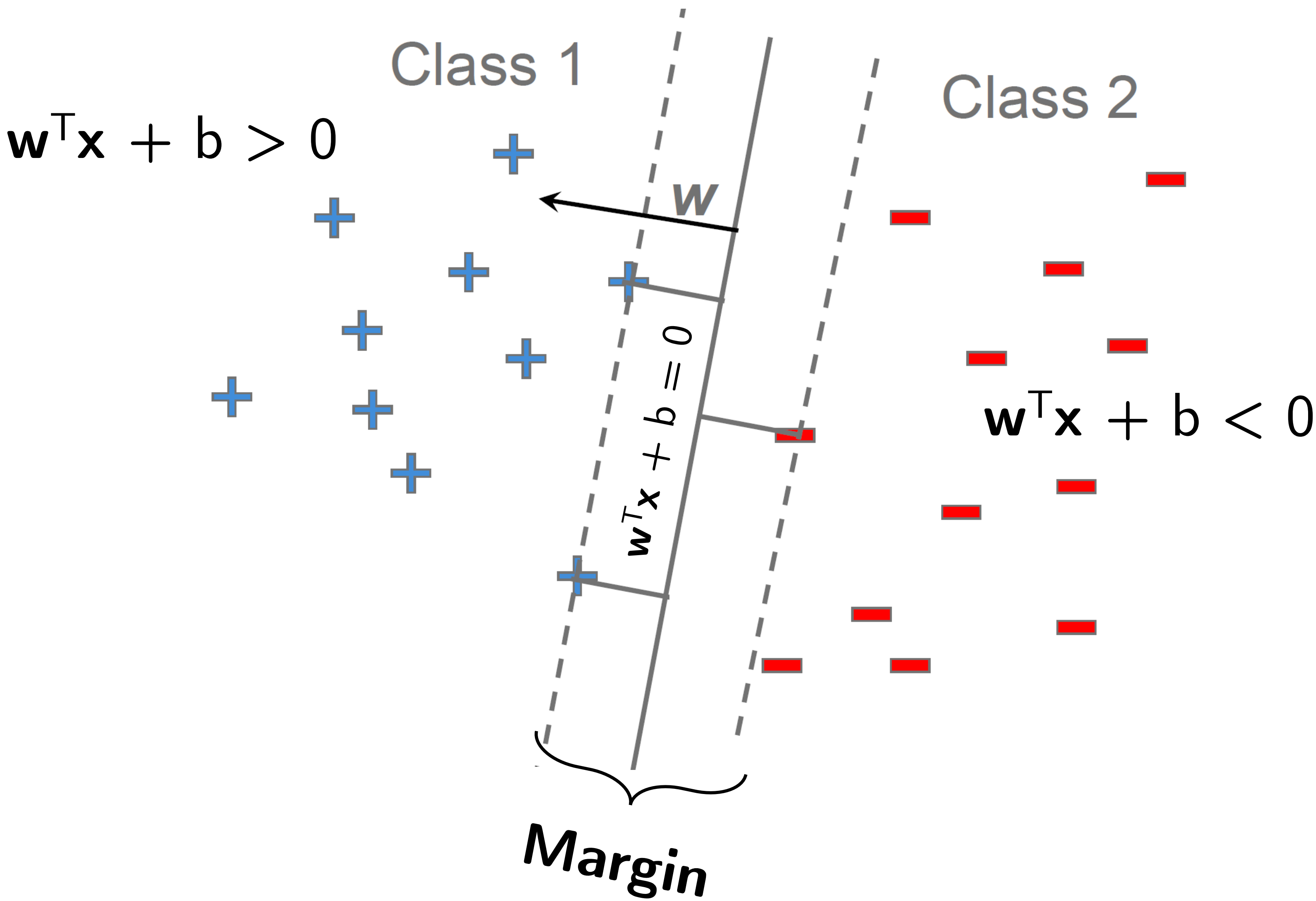
$$(\mathbf{w}^T \cdot \mathbf{x}) + b = 0, \quad \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}$$

- Corresponding to **decision functions**

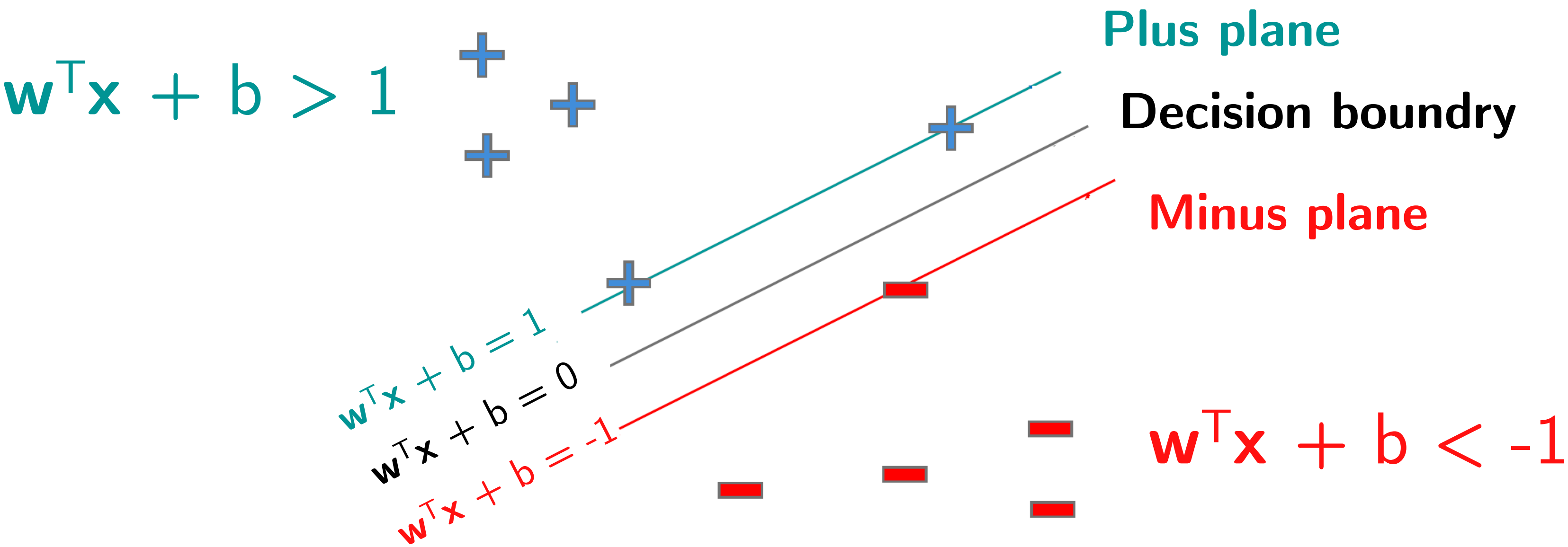
$$f(\mathbf{x}) = \mathrm{sign}((\mathbf{w}^T \cdot \mathbf{x}) + b)$$

- Note that the decision boundary is **unaffected** by the **scaling** of the parameters $(\mathbf{w}, b) \to (\alpha\mathbf{w}, \alpha b)$.

Pick the one with the largest margin



Scaling



- Classification rule:
  - Classify as: $+1$ if $\mathbf{w}^T\mathbf{x} + b \geq 1$

    -1 if $\mathbf{w}^T\mathbf{x} + b \leq -1$
- **Goal**: Find the maximum margin classifier

The Primal Hard SVM

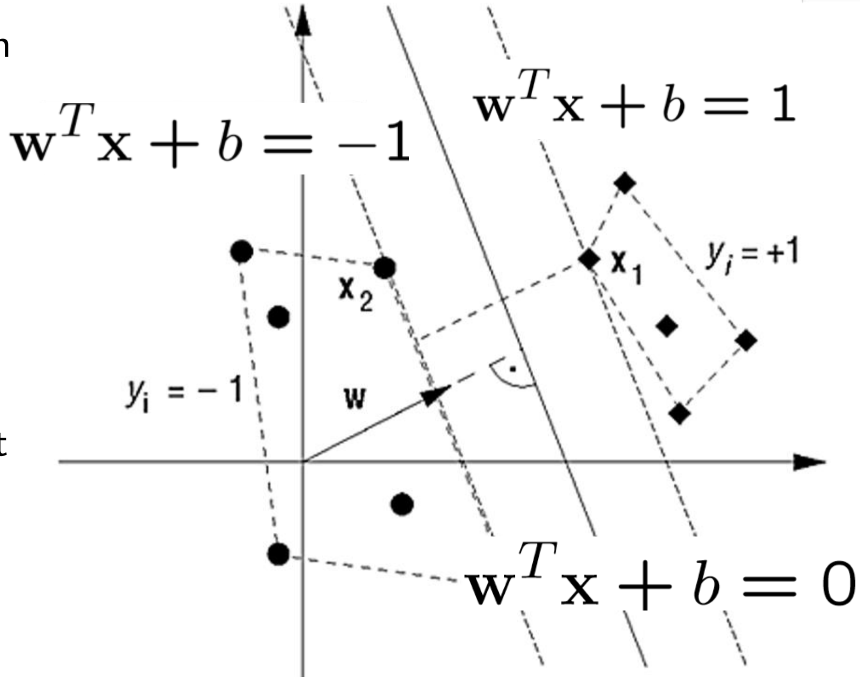
- A binary classification problem of separating **balls** from **diamonds**.
- The optimal hyperplane is orthogonal to the **shortest line** connecting the **convex hulls** of the two classes (dotted), and **intersects it half** way between the two classes.
- There is a weight vector **w** and a threshold b such that the points closest to the **hyperplane** satisfy

$$|(\mathbf{w}^T \cdot \mathbf{x}_i) + b| = 1$$

- corresponding to

$$y_i((\mathbf{w}^T \cdot \mathbf{x}_i) + b) \geq 1.$$

- The **margin**, measured perpendicularly to the hyperplane, equals $\boxed{\frac{2}{||\mathbf{w}||}}$
- **Distance** between the **origin** and the line $\mathbf{w}^t\mathbf{x}=k$ is $k/||\mathbf{w}||$



Note:

$$(\mathbf{w}^t \cdot \mathbf{x}_1) + b = +1$$
$$(\mathbf{w}^t \cdot \mathbf{x}_2) + b = 1$$
$$\Rightarrow (\mathbf{w}^t \cdot (\mathbf{x}_1 - \mathbf{x}_2)) = 2$$
$$\Rightarrow \left(\frac{\mathbf{w}}{||\mathbf{w}||} \cdot (\mathbf{x}_1 - \mathbf{x}_2)\right) = \frac{2}{||\mathbf{w}||}$$

Finding the Decision Boundary

- The decision boundary can be found by solving the following **constrained optimization problem**

$$\boxed{\text{Minimize } \frac{1}{2}||\mathbf{w}||^2}$$

$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 \qquad \forall i$$

- This is a constrained optimization problem. Solving it requires **some new tools**
  - This is a **QP** problem (Quadratic cost function, linear constraints)
- The analytical solution of this equation provide great reduction in complexity (Vapnik works)

Unconstrained Minimization

- **Assume**:
  - Let f : $\Omega \to$ R be a continuously differentiable function.
- Necessary and sufficient conditions for a local minimum: x* is a local minimum of f(x) if and only if
  1. f has zero **gradient** at x*:

$$\nabla_{\mathbf{x}} f(\mathbf{x}^*) = \mathbf{0}$$

  2. and the Hessian of f at x* is **positive semi-definite**

$$\mathbf{v}^t \left(\nabla^2 f(\mathbf{x}^*)\right) \mathbf{v} \geq \mathbf{0}, \ \forall \mathbf{v} \in \mathbb{R}^n$$

where

$$\nabla^2 f(\mathbf{x}) = \begin{pmatrix} \frac{\partial^2 f(\mathbf{x})}{\partial x_1^2} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f(\mathbf{x})}{\partial x_n^2} \end{pmatrix}$$

Recall: Constrained Optimization: Equality Constraints

- The constrained **optimization** problem is

$$\min_{\mathbf{x} \in \mathbb{R}^{\mathrm{d}}} f(\mathbf{x}) \text{ subject to } h_i(\mathbf{x}) = 0 \text{ for } i = 1, \ldots, l$$

- Construct the **Lagrangian** (introduce a multiplier for each constraint)

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\mu}) = f(\mathbf{x}) + \textstyle\sum_{i=1}^{l} \mu_i h_i(\mathbf{x}) = f(\mathbf{x}) + \boldsymbol{\mu}^t \mathbf{h}(\mathbf{x})$$

- Then x^* a local **minimum** $\iff$ there exists a unique $\boldsymbol{\mu}^*$ s.t.

$$\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}^*, \boldsymbol{\mu}^*) = \mathbf{0}$$

$$\nabla_{\boldsymbol{\mu}} \mathcal{L}(\mathbf{x}^*, \boldsymbol{\mu}^*) = \mathbf{0}$$

$$\mathbf{y}^t (\nabla^2_{\mathbf{xx}} \mathcal{L}(\mathbf{x}^*, \mu^*)) \mathbf{y} \geq 0 \quad \forall \mathbf{y} \text{ s.t. } \nabla_{\mathbf{x}} h(\mathbf{x}^*)^t \mathbf{y} = 0$$

Positive definite **Hessian** tells us we have a local minimum

Constrained Optimization

Inequality Constraints (Karush–Kuhn–Tucker (KKT) conditions)

- Given the **optimization** problem

$$\boxed{\min_{\mathbf{x}\in\mathbb{R}^{\mathrm{d}}} f(\mathbf{x}) \ \text{ subject to } \ g_j(\mathbf{x}) \leq 0 \text{ for } j = 1, \ldots, m}$$

- Dene the **Lagrangian** as

$$\boxed{\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \textstyle\sum_{j=1}^{m} \lambda_j \, g_j(\mathbf{x}) = f(\mathbf{x}) + \boldsymbol{\lambda}^t \, \mathbf{g}(\mathbf{x})}$$

- Then x* a local **minimum** $\Longleftrightarrow$ there exists a unique **λ*** s.t.

$$\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}^*, \boldsymbol{\lambda}^*) = \mathbf{0}$$

$$\lambda_j^* \geq 0 \text{ for } j = 1, \ldots, m$$

$$\lambda_j^* \, g(\mathbf{x}^*) = 0 \text{ for } j = 1, \ldots, m$$ **Complementary slackness**

$$g_j(\mathbf{x}^*) \leq 0 \text{ for } j = 1, \ldots, m$$

Plus positive definite constraints on $\nabla_{\mathbf{xx}} \mathcal{L}(\mathbf{x}^*, \boldsymbol{\lambda}^*)$.

Back to the Original Problem

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$

$$\text{subject to } 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b) \leq 0 \qquad \text{for } i = 1, \ldots, n$$

- The **Lagrangian** is

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

- Note that $||\mathbf{w}||^2 = \mathbf{w}^T\mathbf{w}$
- Setting the gradient of $\mathcal{L}$ w.r.t. **w** and b to zero, we have

$$\nabla_w \mathcal{L}(w, b, \alpha) = \mathbf{w} + \sum_{i=1}^{n} \alpha_i(-y_i)\mathbf{x}_i = \mathbf{0} \quad \boxed{\Rightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i}$$

$$\frac{\partial}{\partial b}\mathcal{L}(w, b, \alpha) = \boxed{\sum_{i=1}^{n} \alpha_i y_i = 0}$$

The Dual Problem

- If we substitute $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$ to $\mathcal{L}$, we have

$$\mathcal{L} = \frac{1}{2} \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i^T \sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \left(\sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i + b \right) \right)$$

$$= \boxed{\frac{1}{2}} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i \underbrace{- \sum_{i=1}^{n} \alpha_i y_i \sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i}_{} - b \sum_{i=1}^{n} \alpha_i y_i \quad 0$$

$$= \boxed{-\frac{1}{2}} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i$$

- Note that $\sum_{i=1}^{n} \alpha_i y_i = 0$
- This is a function of α_i **only**

The Dual Problem

Dot product

Scalar

$$\boxed{\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j}$$

- Subject to:

$$\alpha_i \geq 0 \quad \text{and} \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

- **Matrix notation**:

$$\boxed{\hat{\boldsymbol{\alpha}} = \arg\max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \boldsymbol{\alpha}^T \mathbf{1}_n - \tfrac{1}{2} \boldsymbol{\alpha}^T \boldsymbol{Y} \boldsymbol{G} \boldsymbol{Y} \boldsymbol{\alpha}}$$

$$\boldsymbol{Y} \doteq diag(y_1, \ldots, y_n), \;\; y_i \in \{-1, 1\}^n$$

$$\boldsymbol{G} \in \mathbb{R}^{n \times n} \doteq \{G_{ij}\}_{i,j}^{n,n}, \text{ where } G_{ij} \doteq \langle \mathbf{x}_i, \mathbf{x}_j \rangle \text{ Gram matrix}$$

- This is a **quadratic programming** (QP) problem and a global maximum of α_i can always be found

Why is it called Support Vector Machine?

$$\mathcal{L} = \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right)$$

- Based on **complementary slackness in** KKT conditions we have

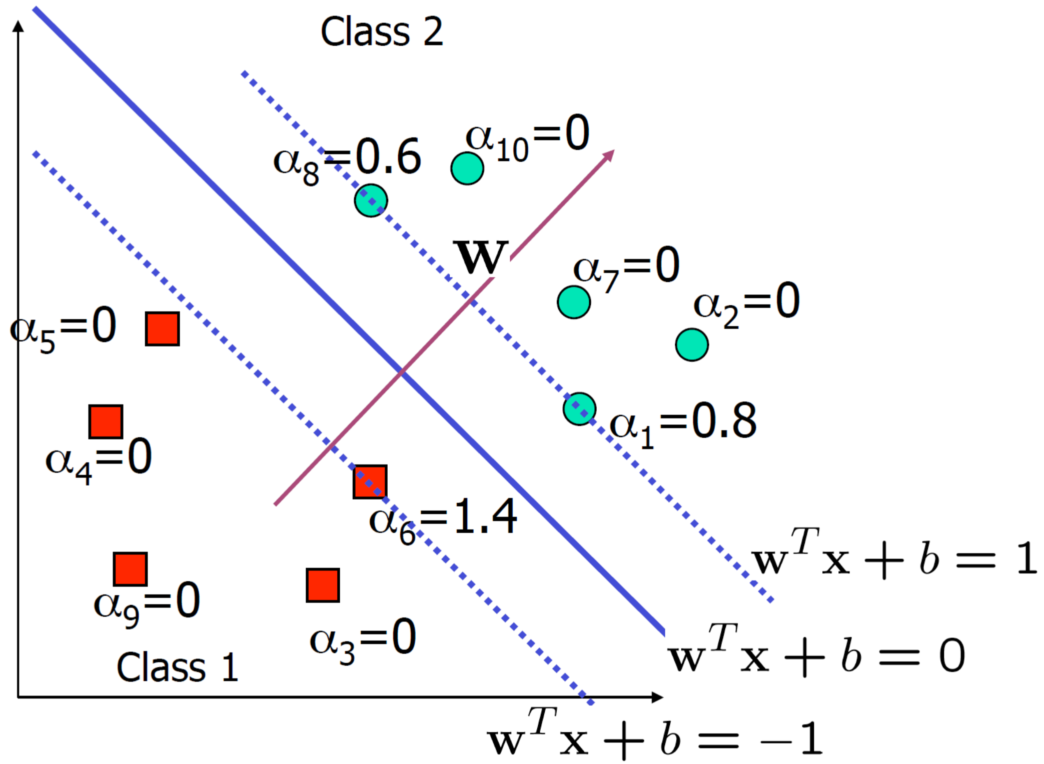
$\lambda_j^* g(\mathbf{x}^*) = 0$ for $j = 1, \ldots, m$

$$\alpha_i \left(1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right) = 0$$

- Sinc $\alpha_i \geq 0$, either $\alpha_i = 0$ or $(1 - y_i(\mathbf{W}^t\mathbf{x}_i + b)) = 0$
- Only if $\mathbf{x}_i$ is on the **margin line** (**support vectors**) the $(1 - y_i(\mathbf{W}^t\mathbf{x}_i + b))$ will be zero
- So, many of the α_i are **zero and** $\mathbf{x}_i$ with non-zero α_i are called support vectors (SV)

A Geometrical Interpretation

- The decision boundary is **determined only** by the **SV**
- Let t_j ($j=1, \ldots, s$) be the indices of the s support vectors.



$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

Finding w and b

- The optimal value of w states in terms of the optimal **value** of α_i, **w** can be recovered by

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j} \Rightarrow \mathbf{w} = \sum_{i=1}^{s} \alpha_i y_i \mathbf{x}_i$$

- The value of b can be computed as the solution of

$$\alpha_i (y_i ((\mathbf{w} \cdot \mathbf{x}_i) + b) - 1) = 0$$

- using any of the **support vectors** but it is numerically **safer** to take the **average value** of b resulting from all such equations.

The Quadratic Programming Problem and Final Solution

- For SVM, **sequential minimal optimization** (SMO) seems to be the most popular:
  - A QP with **two variables** is trivial to solve
  - Each iteration of SMO picks a **pair of** (α_i,α_j) and solve the QP with these two variables; Repeat until convergence

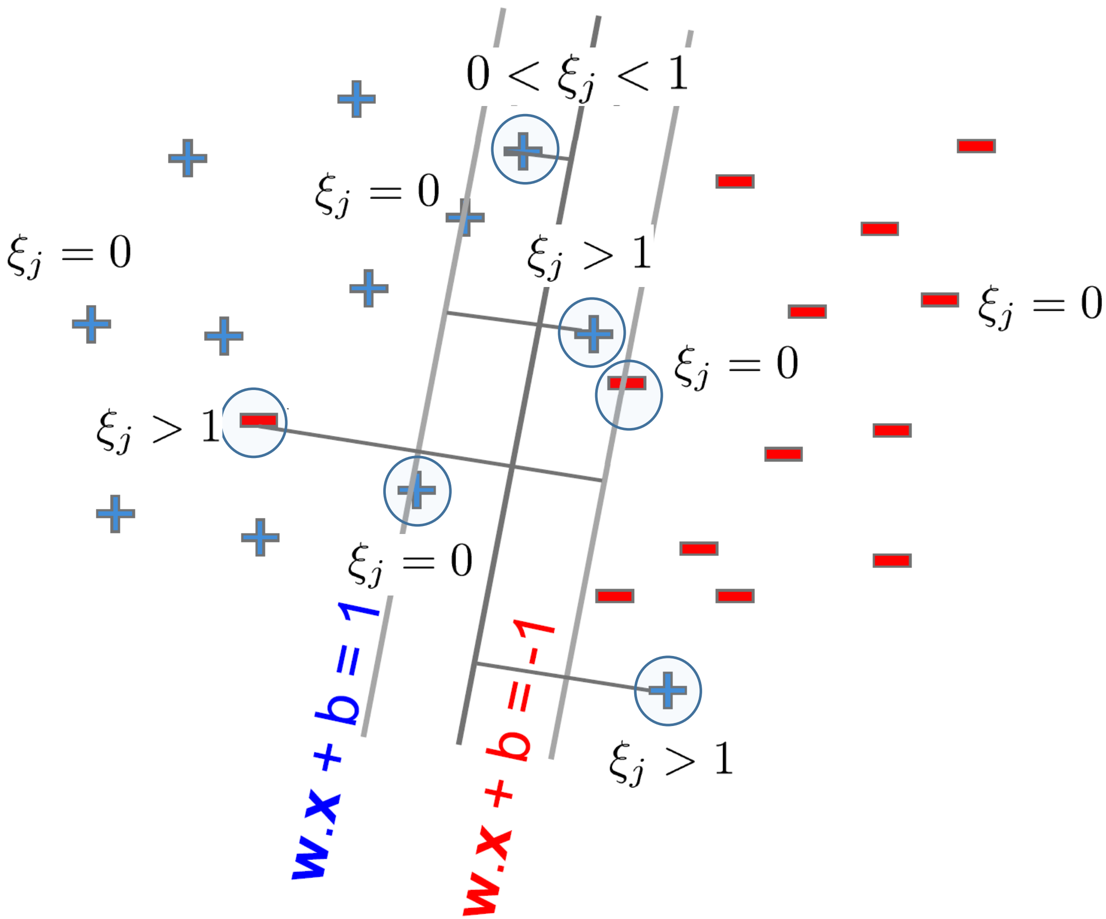
$$\boxed{\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j}$$

- Both the quadratic programming problem and the final decision function depend only **on the dot products between patterns**
- For **testing** with a new data **z**

$$f(\mathbf{x}) = \operatorname{sign}\left(\sum_{j=1}^{s} \alpha_{t_j} y_{t_j} (\mathbf{x}_{t_j}^T \mathbf{z}) + b\right)$$

Non-linearly Separable Problems (Soft SVM)

- We allow "**error**" ξ_i in classification; it is **based on the output** of the discriminant function $\mathbf{w}^T\mathbf{x}+b$



If we minimize $\sum_i \xi_i$, ξ_i can be computed by

$$\begin{cases} \mathbf{w}^T\mathbf{x}_i + b \geq 1 - \xi_i & y_i = 1 \\ \mathbf{w}^T\mathbf{x}_i + b \leq -1 + \xi_i & y_i = -1 \\ \xi_i \geq 0 & \forall i \end{cases}$$

- ξ_i are "**slack** variables" in optimization
- Note that ξ_i=0 if there is no error for **xi**
- ξ_i is an **upper bound** of the number of errors

- ξi **named slack variable**

Soft Margin Hyperplane

- We want to **minimize**

$$\frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i$$

C : **tradeoff parameter** between **error** and **margin**

- The optimization problem becomes

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i$$

$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$$

- We can form the **Lagrangian** (α_i's and r_i's are our Lagrange multipliers):

$$\mathcal{L}(w,b,\xi,\alpha,r) = \frac{1}{2}w^Tw + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i\left[y_i\ (x^Tw+b) - 1 + \xi_i\right] - \sum_{i=1}^{n}r_i\xi_i.$$

The Dual Soft SVM

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

- **w** is recovered as:

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

- This is very **similar** to the optimization problem in the linear separable case, except that there is an **upper bound C on α_i now**
- Once again, a QP solver can be used to find α_i

sequential minimal optimization (SMO) coordinate ascent

- We've already seen two optimization algorithms, **gradient ascent** and **Newton's method**.
- The new algorithm is called **coordinate ascent**:

Loop until convergence: {

For $i = 1, \ldots, n$, {

$$\alpha_i := \arg\max_{\hat{\alpha}_i} W(\alpha_1, \ldots, \alpha_{i-1}, \hat{\alpha}_i, \alpha_{i+1}, \ldots, \alpha_n).$$

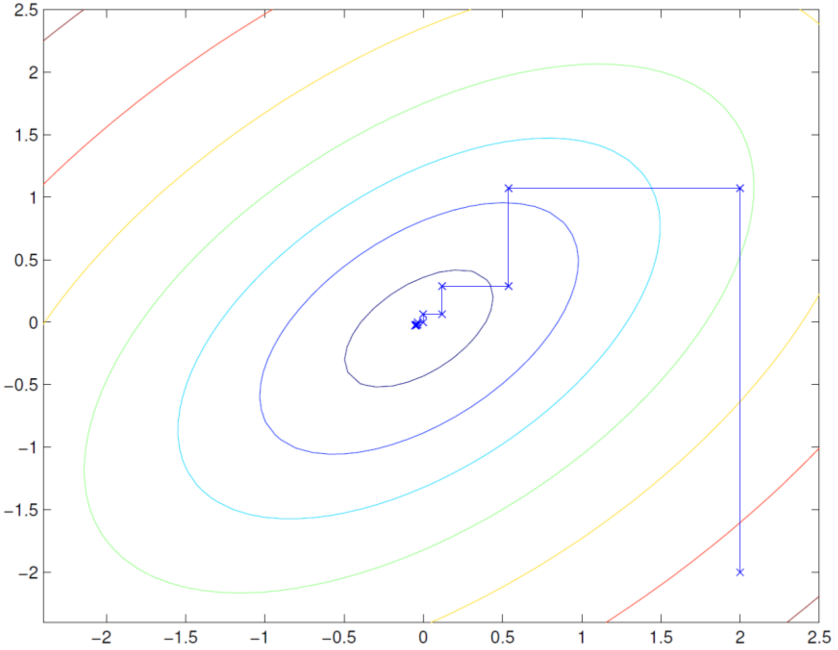
}

}

- We will **hold** all the **variables except** for some α_i fixed, and **reoptimize** W with respect to just the parameter α_i.
- The inner-loop **reoptimizes** the variables in order $\alpha_1, \alpha_2, \ldots, \alpha_n, \alpha_1, \alpha_2, \ldots$.
- More **sophisticated** version might choose other orderings; (choose the next variable to update according to which one we expect to allow us to make the **largest increase** in $W(\alpha)$.)

Coordinate ascent

- The **ellipses** in the figure are the contours of a **quadratic function**
- Coordinate ascent was initialized at (2,−2),
- Notice that on each step, coordinate ascent takes a step that's **parallel to one** of the axes, since **only one variable** is being optimized at a time.



SMO algorithm for SVM

- Dual optimization problem that we want to solve:

$$\max_\alpha \quad W(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y_i y_i \alpha_i \alpha_j \langle x_i, x_j \rangle.$$
$$\text{s.t.} \quad 0 \le \alpha_i \le C, \quad i = 1, \ldots, n$$
$$\sum_{i=1}^{n} \alpha_i y_i = 0.$$

- If we want to update some subject of the α_i's, we must update **at least two of them** simultaneously
  - If **we fixed** α_1, we **can't make** any change to α_1

$$\sum_{i=1}^{n} \alpha_i y_i = 0. \Rightarrow \alpha_1 y_1 = -\sum_{i=2}^{n} \alpha_i y_i \Rightarrow \alpha_1 = -y_1 \sum_{i=2}^{n} \alpha_i y_i$$

SMO algorithm for SVM

- Repeat till convergence
  1. Select some pair α_i and α_j to update next
  2. Reoptimize $W(\alpha)$ with respect to α_i and α_j , while holding all the other α_k's ($k \neq i, j$) fixed.
- We've decided to hold $\alpha_3, \ldots, \alpha_n$ **fixed**:

$$\alpha_1 y_1 + \alpha_2 y_2 = -\sum_{i=3}^{n} \alpha_i y_i$$

- right hand side is fixed, we can just let it be denoted by some **constant** ζ:

$$\alpha_1 y_1 + \alpha_2 y_2 = \zeta.$$

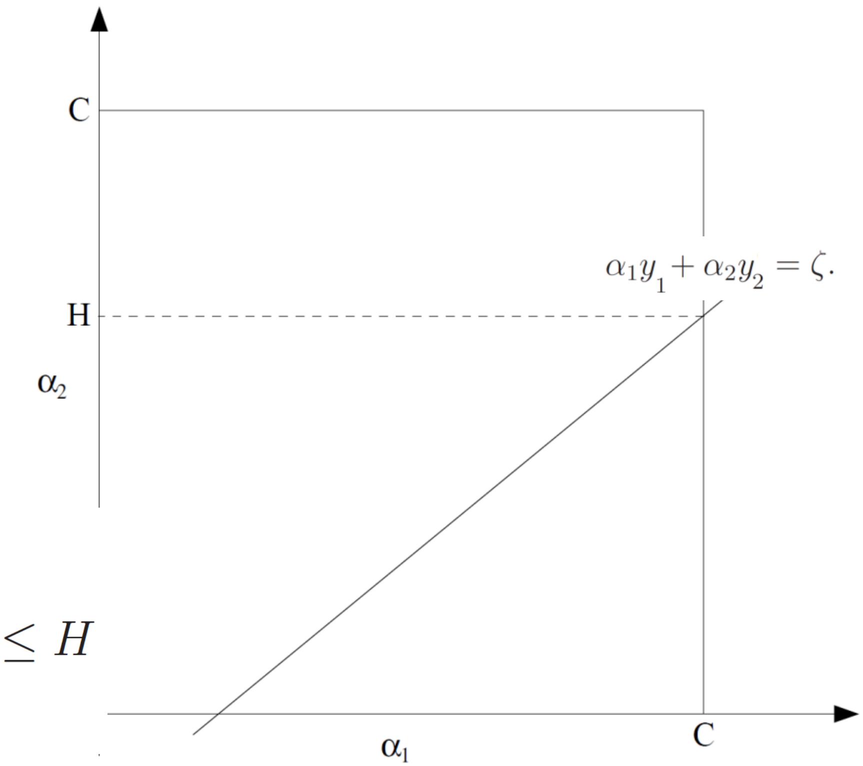
$$\alpha_1 = (\zeta - \alpha_2 y_2) y_1$$

$$W(\alpha_1, \alpha_2, \ldots, \alpha_n) = W((\zeta - \alpha_2 y_2) y_1, \alpha_2, \ldots, \alpha_n).$$

This can also be **expressed** in the form

$$a\alpha_2^2 + b\alpha_2 + c$$

We can **find** the resulting value optimal simply by taking α_2^{new}, and "**clipping**" it to lie in the [L,H] interval



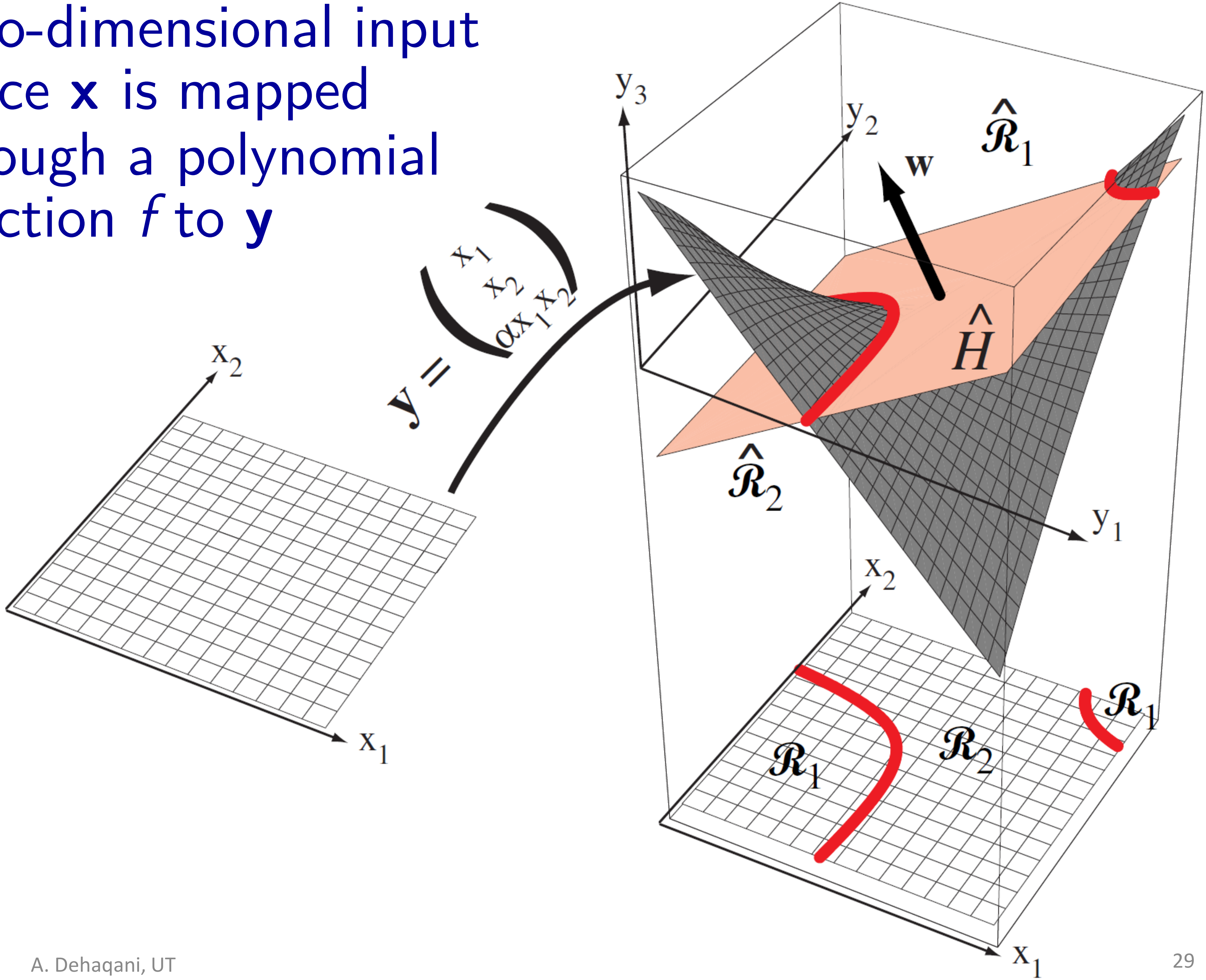
$$\alpha_2^{new} = \begin{cases} H & \text{if } \alpha_2^{new,unclipped} > H \\ \alpha_2^{new,unclipped} & \text{if } L \le \alpha_2^{new,unclipped} \le H \\ L & \text{if } \alpha_2^{new,unclipped} < L \end{cases}$$

We can compute α_1^{new} by first equation

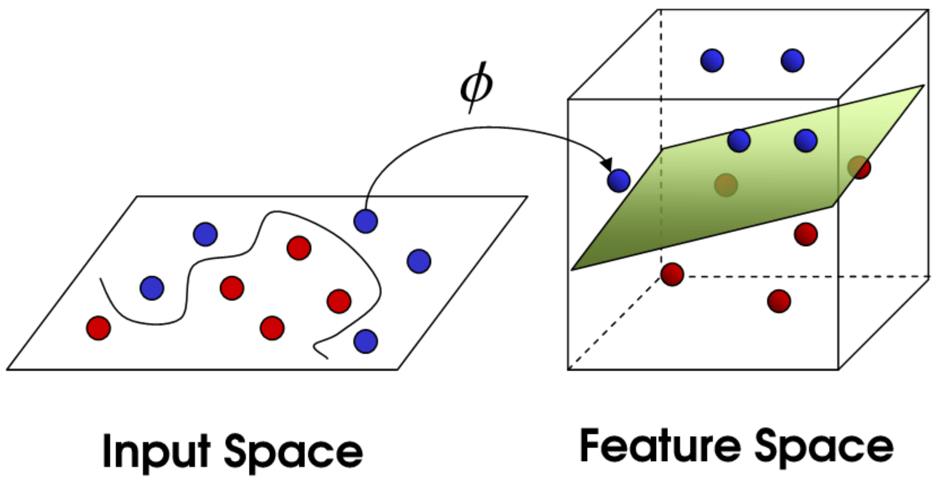
Extension to Non-linear Decision Boundary

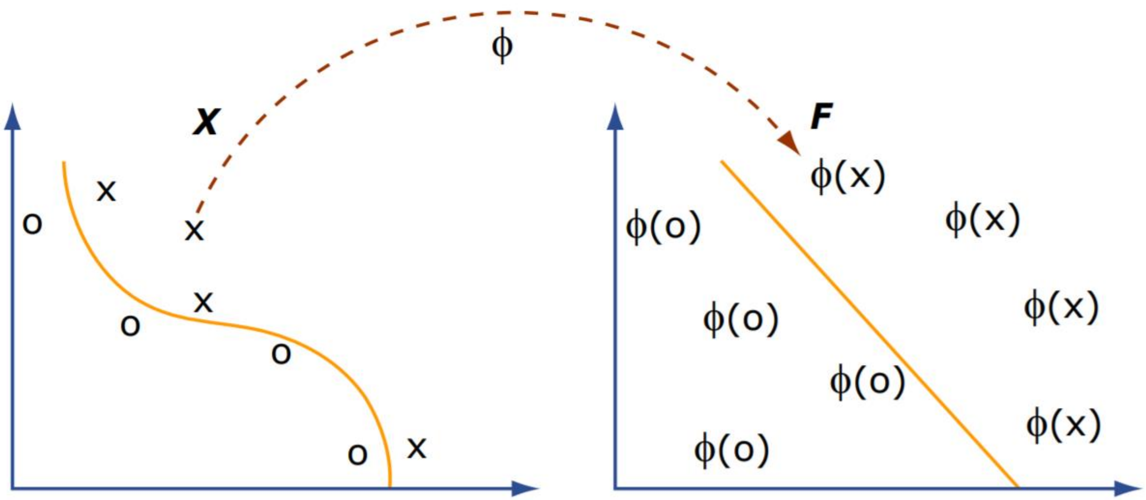
- So far, we have only considered large-margin classifier with a **linear decision boundary (correspond with equal variance Gaussian)**
- How to **generalize** it to become **nonlinear**?
- Key idea: transform $\mathbf{x}_i$ to a **higher dimensional** space to "**make life easier**"
  - **Input** space: the space the point $\mathbf{x}_i$ are located
  - **Feature** space: the space of $\varphi(\mathbf{x}_i)$ after transformation
- Linear operation in the feature space is **equivalent** to **nonlinear** operation in input space

Two-dimensional input space **x** is mapped through a polynomial function *f* to **y**



Transforming the Data





- **Feature space** is of **higher dimension** than the **input space** in practice
- Computation in the feature space can be **costly** because it is high dimensional
  - The **kernel trick** comes to rescue

The Kernel Trick

- Recall the SVM **optimization problem**

$$\max.\ \ W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } C \geq \alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i y_i = 0$$

- The data points only appear as **inner product**
- As long as we can calculate the **inner product in the feature space**, we **do not** need the **mapping explicitly**
- Many common **geometric operations** (angles, distances) can be expressed by **inner products**
- Define the **kernel function** K by $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$

$$\boxed{\max.\ \ W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)}$$

Testing the new data

- For testing, the new data **z** is classified as class 1 if f≥0, and as class 2 if f<0

Original
$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$
$$f = \mathbf{w}^T \mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}^T \mathbf{z} + b$$

- With kernel function (change all **inner products** to **kernel** functions)

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \phi(\mathbf{x}_{t_j})$$
$$f = \langle \mathbf{w}, \phi(\mathbf{z}) \rangle + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} K(\mathbf{x}_{t_j}, \mathbf{z}) + b$$

kernel trick

- Suppose φ(.) is given as follows

$$\phi(\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

- An **inner product** in the feature space is

$$\langle \phi(\left[\begin{smallmatrix} x_1 \\ x_2 \end{smallmatrix}\right]), \phi(\left[\begin{smallmatrix} y_1 \\ y_2 \end{smallmatrix}\right]) \rangle = (1 + x_1y_1 + x_2y_2)^2$$

- So, if we define the kernel function as follows, there is no need to **carry out φ(.) explicitly**

$$K(\mathbf{x}, \mathbf{y}) = (1 + x_1y_1 + x_2y_2)^2$$

- This use of kernel function to **avoid carrying out** φ(.) **explicitly** is known as the kernel trick

Kernel Functions

- In practical use of SVM, the user **specifies** the kernel function; the **transformation** φ(.) is **not explicitly stated**
  - Given a kernel function $K(\mathbf{x}_i, \mathbf{x}_j)$, the **transformation** φ(.) is given by its **eigenfunctions** (a concept in functional analysis)
  - Eigenfunctions can be difficult to construct explicitly
- This is why people **only** specify the **kernel** function **without** worrying about the **exact transformation**
- Another view: kernel function, being an inner product, is really a **similarity measure** between the objects

Examples of Kernel Functions

- **Polynomial** kernel with **degree** d

$$K(\mathbf{x},\mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^d$$

- **Gaussian kernel** with width σ

$$K(\mathbf{x},\mathbf{y}) = \exp(-||\mathbf{x}-\mathbf{y}||^2/(2\sigma^2))$$

  - Closely related to **radial basis function** **neural networks**
  - The feature space is **infinite-dimensional** (it still be written as a dot product in a new feature space $k(\mathbf{x}, \mathbf{x}_0) = \Phi(\mathbf{x}) * \Phi(\mathbf{x}_0)$, only with an **infinite number of dimensions**)

- **Sigmoid** with parameter κ and θ

$$K(\mathbf{x},\mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y} + \theta)$$

  - It does not satisfy the **Mercer condition** on all κ and θ

More on Kernel Functions

- Since the training of SVM **only** requires the value of $K(\mathbf{x}_i,\mathbf{x}_j)$, there is **no restriction** of the **form** of $\mathbf{x}_i$ and $\mathbf{x}_j$
  - $\mathbf{x}_i$ can be a **sequence or a tree**, instead of a feature vector
- $K(\mathbf{x}_i, \mathbf{x}_j)$ is just a **similarity measure** comparing **x**i and **x**j
- For a test object **z**, the **discriminant function** essentially is a weighted sum of the **similarity between z and a** preselected set of objects (the support vectors)

$$f(\mathbf{z}) = \sum_{\mathbf{x}_i \in \mathcal{S}} \alpha_i y_i K(\mathbf{z}, \mathbf{x}_i) + b$$

$\mathcal{S}$: the set of support vectors

Necessary conditions for valid kernels.

- **Kernel matrix**:
  - A square, n-by-n matrix K be defined so that its (i,j)-entry is given by $K_{ij} = K(\mathbf{x}_i,\mathbf{x}_j)$
- K must be **symmetric**.
- Theorem (**Mercer**). Let $K : R^d \times R^d \rightarrow R$ be given. Then for K to be a valid (Mercer) kernel, it is **necessary** and **sufficient** that for any $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, $(n < \infty)$, the corresponding **kernel matrix** is symmetric pos-itive semi-definite
- Theorem (Mercer). If we have a kernel K(x,z) that is positive, we can expand K in terms of **eigenfunctions** and **eigenvalues**
  - K is **positive**; which here means

$$\forall f \in L_2(\mathcal{X}), \quad \int_{\mathcal{X}\times\mathcal{X}} k(\mathbf{x},\mathbf{z}) f(\mathbf{x}) f(\mathbf{z}) d\mathbf{x} d\mathbf{z} \geq 0,$$

  - we can expand K(x,z)

$$k(\mathbf{x},\mathbf{z}) = \sum_{j=1}^{\infty} \lambda_j \psi_j(\mathbf{x}) \psi_j(\mathbf{z}).$$

  - $\psi_j \in L_2(\mathcal{X})$ **eigenfunctions** and $\lambda_j > 0$ **eigenvalues**

K in the finite states (finding feature map)

- **Eigendecomposition** takes this form

$$\mathbf{K} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{\mathrm{T}}$$

$$\mathrm{K}= \begin{array}{c c} & \begin{array}{ccc} 1 & j & m \end{array} \\ \begin{array}{c} m \\ i \\ 1 \end{array} & \left[\begin{array}{ccc} & & \\ & k(x_i, x_j) & \\ & & \end{array} \right] \end{array}$$

- Consider this **feature map**:

$$\boldsymbol{\Phi}(x_i) = [\sqrt{\lambda_1} v_1^{(i)}, \ldots, \sqrt{\lambda_t} v_t^{(i)}, \ldots, \sqrt{\lambda_m} v_m^{(i)}].$$

- writing it for $\mathbf{x}_j$ too

$$\boldsymbol{\Phi}(x_j) = [\sqrt{\lambda_1} v_1^{(j)}, \ldots, \sqrt{\lambda_t} v_t^{(j)}, \ldots, \sqrt{\lambda_m} v_m^{(j)}].$$

- With this choice, k is just a **dot product** in R^m

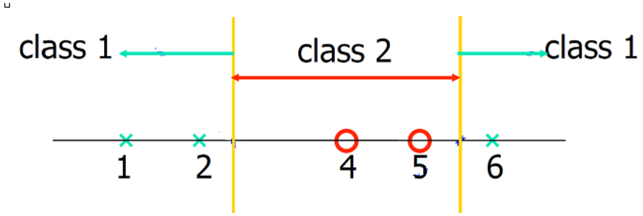
$$\langle \boldsymbol{\Phi}(x_i), \boldsymbol{\Phi}(x_j) \rangle_{\mathbf{R}^m} = \sum_{t=1}^{m} \lambda_t v_t^{(i)} v_t^{(j)} = (\mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{\mathrm{T}})_{ij} = K_{ij} = k(x_i, x_j).$$

More on Kernel Functions

- **Not** all similarity measure can be used as kernel function, however
  - The kernel function needs to satisfy the Mercer function,
    - i.e., the function is "**positive-definite**"
    - This implies that the n by n **kernel matrix**, in which the (i,j)-th entry is the $K(\mathbf{x}_i, \mathbf{x}_j)$, is always **positive definite**
- This also means that the **QP is convex** and can be solved in **polynomial** time
- The learning algorithm that you can write in terms of **only inner products** between **input feature vectors**, then by replacing this with $K(x, y)$ where K is a kernel, you can "magically" work efficiently in the **high dimensional feature space** corresponding to K.
- **linear regression** and SVMs are two well known examples

Example

- Suppose we have 5 1D data points
  - $x_1=1$, $x_2=2$, $x_3=4$, $x_4=5$, $x_5=6$, with 1, 2, 6 as class 1 and 4, 5 as class 2
  - $\Rightarrow y_1=1$, $y_2=1$, $y_3=-1$, $y_4=-1$, $y_5=1$



- We use the polynomial **kernel** of degree 2
  - $K(x,y) = (xy+1)^2$
  - C is set to 100
- We first **find** α_i (i=1, …, 5) by

$$\text{max.} \quad \sum_{i=1}^{5} \alpha_i - \frac{1}{2} \sum_{i=1}^{5} \sum_{j=1}^{5} \alpha_i \alpha_j y_i y_j (x_i x_j + 1)^2$$

$$\text{subject to } 100 \geq \alpha_i \geq 0, \sum_{i=1}^{5} \alpha_i y_i = 0$$

Example

- By using a QP solver, we get
  - $\alpha_1=0$, $\alpha_2=2.5$, $\alpha_3=0$, $\alpha_4=7.333$, $\alpha_5=4.833$
  - Note that the **constraints** are indeed **satisfied**
- The **support vectors** are $\{x_2=2, x_4=5, x_5=6\}$
- The **discriminant function** is

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \phi(\mathbf{x}_{t_j})$$

$$f = \langle \mathbf{w}, \phi(\mathbf{z}) \rangle + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} K(\mathbf{x}_{t_j}, \mathbf{z}) + b$$

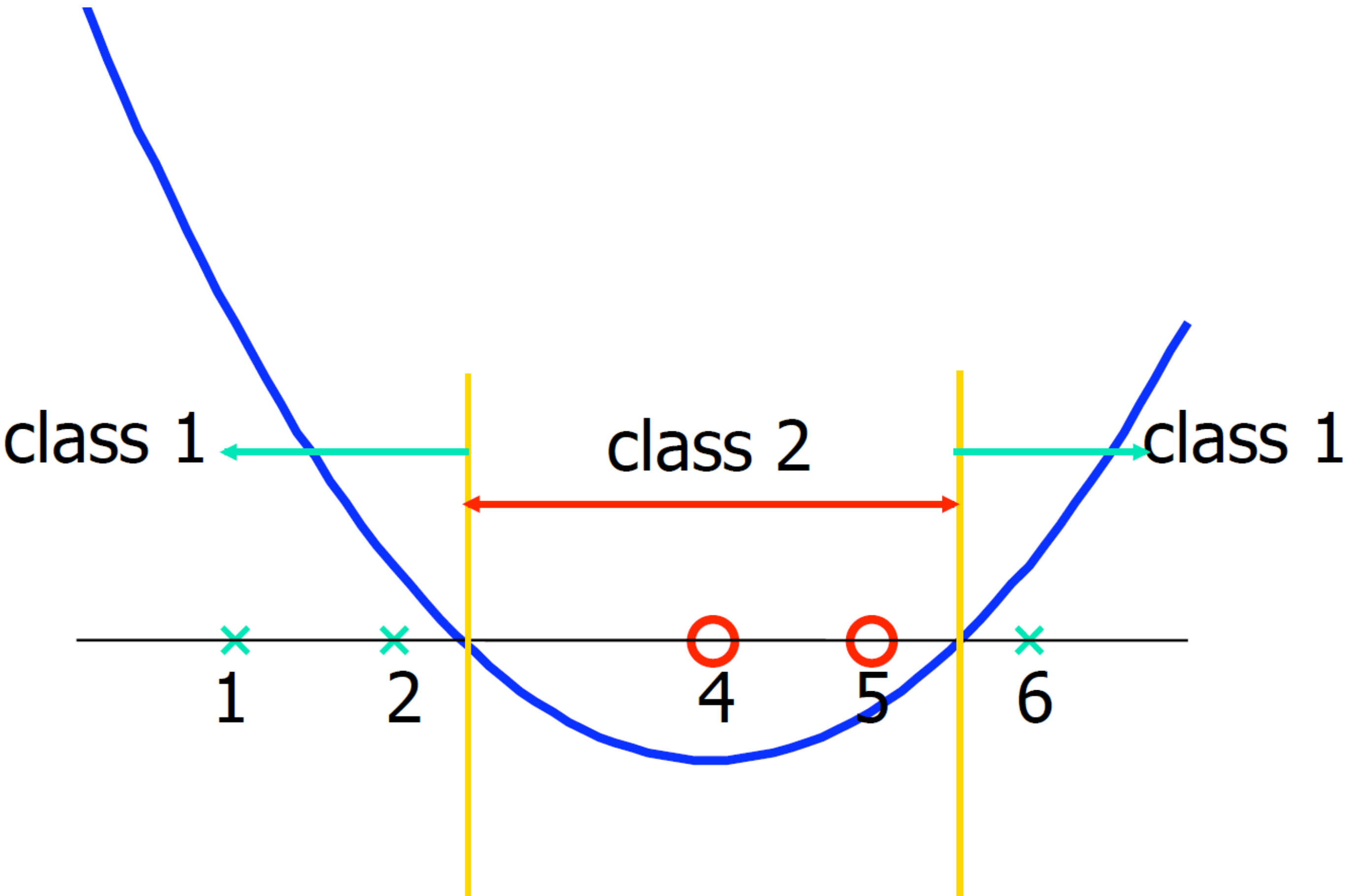
$$f(z) = 2.5(1)(2z+1)^2 + 7.333(-1)(5z+1)^2 + \underbrace{4.833}_{\alpha_5}\underbrace{(1)}_{y_5}\underbrace{(6z+1)^2}_{K(z,x_5)} + b$$

$$= 0.6667z^2 - 5.333z + b$$

- b is recovered by solving f(2)=1 or by f(5)=-1 or by f(6)=1,

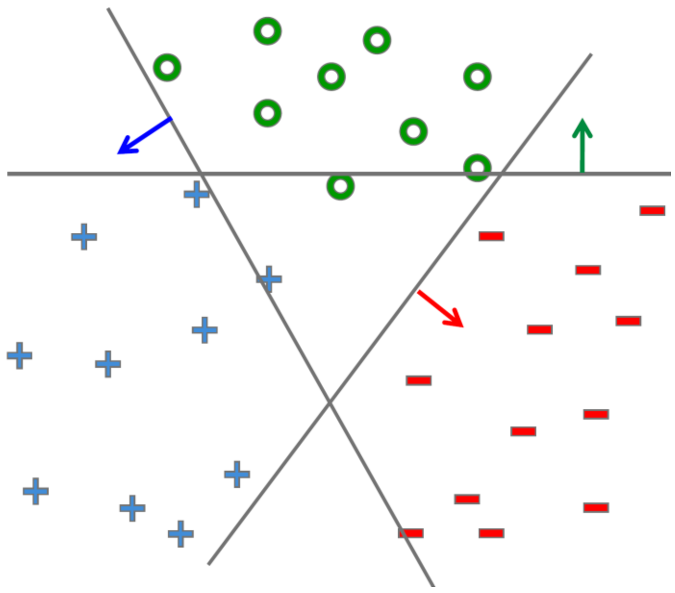
$$f(z) = 0.6667z^2 - 5.333z + 9$$

Value of discriminant function



What about multiple classes?

- One against all
  - **Learn 3 classifiers separately**:
    - Class k vs. rest
  - $(\mathbf{w}_k, b_k)_{k=1,2,3}$
  - $y = \arg\max_k \mathbf{w}_k x + b_k$
  - Disadvantages: ambiguous area
- In each step, **remove one class**:
  - Problem: sensitive to order
- One against one:
  - **Majority voting**



Multi-class SVM

- Simultaneously learn **3 sets of weights**
  - **Need new constraints** : (The "**score**" of the correct class **must be better** than the "score" of-wrong lasses)

$$\text{minimize}_{\mathbf{w},b} \quad \sum_y \mathbf{w}^{(y)} \cdot \mathbf{w}^{(y)}$$

Margin: gap between **correct class** and nearest other class

$$\mathbf{w}^{(y_j)} \cdot \mathbf{x}_j + b^{(y_j)} \geq \mathbf{w}^{(y')} \cdot \mathbf{x}_j + b^{(y')} + 1, \ \forall y' \neq y_j, \ \forall j$$

- Introducing **slack variables** and **maximize margin** (joint optimization):

$$\text{minimize}_{\mathbf{w},b} \quad \sum_y \mathbf{w}^{(y)} \cdot \mathbf{w}^{(y)} + C \sum_j \sum_{y \neq y_j} \xi_j^{(y)}$$

$$\mathbf{w}^{(y_j)} \cdot \mathbf{x}_j + b^{(y_j)} \geq \mathbf{w}^{(y)} \cdot \mathbf{x}_j + b^{(y)} + 1 - \xi_j^{(y)}, \ \forall y \neq y_j, \ \forall j$$

$$\xi_j^{(y)} \geq 0$$

- **Finally** we select class:

$$y = \arg\max_k \mathbf{w}^{(k)} \cdot x + b^{(k)}$$

- Usually the **binary classification** works **better**

Epsilon Support Vector Regression (ε-SVR)

- Given: a data set $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ with target values $\{u_1, \ldots, u_n\}$, we want to do **ε**-SVR
- The **optimization** problem is

$$MIN \ \frac{1}{2}||\boldsymbol{w}||^2 + C\sum_{i=1}^{n}|\xi_i|$$

Subject to

$$|y_i - w_i x_i| \ \leq \ \varepsilon + |\xi_i|$$

Ordinary Least Squares (OLS)

$$MIN \ \sum_{i=1}^{n}(y_i - w_i x_i)^2$$

- The error term is instead **handled** in the constraints
- SVR gives us the **flexibility** to define how much error is acceptable in our model

Epsilon Support Vector Regression (ε-SVR)

- C is a parameter to **control** the amount of **influence of** the error
- The $\frac{1}{2}||\mathbf{w}||^2$ term serves as **controlling** the **complexity** of the **regression** function
  - This is similar to **ridge regression (**a technique for **regression** data that suffer from multicollinearity.)

$$\hat{\beta}^{ridge} = \underset{\beta \in \mathbb{R}}{argmin} \|y - XB\|_2^2 + \lambda \|B\|_2^2$$

- After training (solving the QP), we get values of α_i and α_i^*, which are both zero if **xi** does not contribute to the **error function**
- For a new data **z**,

$$f(\mathbf{z}) = \sum_{j=1}^{s} (\alpha_{t_j} - \alpha_{t_j}^*) K(\mathbf{x}_{t_j}, \mathbf{z}) + b$$

ε-insensitive loss function