Loss Function: Solve Lagrange Function Using Gradient Decent Optimization

1. Margin:
2. Noise: Add error team to avoid overfitting problem.
3. Activation Function: From lower dimension to higher dimension
4. Supported Vector Weight: for important features

Supported Vector Machine

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0.1 Homogenous Coordinates

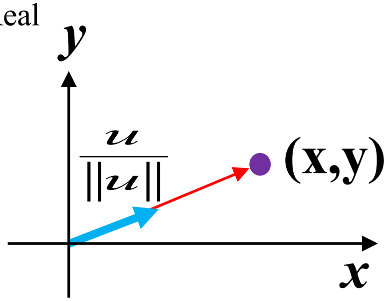
Homogenous Matrix *A*, *b=Ax*

Linear Combination y=w1*x1+w2*x2+b =

$$f(x) = a_0 + \sum_{n=1}^{\infty}\left(a_n \cos\frac{n\pi x}{L} + b_n \sin\frac{n\pi x}{L}\right)$$

Point or sample in high dimension: 20x20 pixels face image is a point/sample/vector in 400 dimensions

- **A simplistic view**
  - Homogenous coordinates (matrix) are a mechanism that allows us to associate points and vectors in space with vectors in R Real



- **Location/Point *u* = Unit vector * Amplitude = $\frac{u}{||u||}$ * $||u||$**
  = direction = scaling
  = rotation

- **SVD: $(A-m) = UWV^T$; $(A-m)V=UW$; Gaussian Model $N(m,\sigma^2)$**
  where translation $\frac{u}{|u|}$
  ***U*: Orthonormal Matrix, Eigenvector, rotation**
  ***W*: Scale Matrix, Eigenvalue, Standard Deviation**
  V: Rotation (Orthonormal) Matrix

Camera Model

0.2 Advantage of Homogenous Matrix: Ax=b

Solution/Optimization of Homogenous Matrix

-Local optimization (0 moment): 1 and 2 =>
-Global optimization: 3 => 1) LM 2) EM 3) SGD (Stochastic Gradient Decent)

1. **Closed-Form Solution:**
   $Ax = 0$ => A^tA = Covariance Matrix =SVD =UWU^T: Smallest eigenvalue >0 ➔ eigenvector
2. **Pseudo Inverse:**
   $Ax = b$, $x=(A^TA)^{-1} * A^Tb$

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3. **Sum of Squared Difference:** (max likelihood – exponential term)
   $\min \; E = \sum [Ax - b]^2$

Deep Learning: Stochastic Gradient Decent

   3.1 $Ax = b'$: estimation value. b: ground truth, $E = \sum [b' - b]^2$
   - a. Initial value estimation => Pseudo Inverse (linear approach)
   - b. L-M (Levenberg-Marquardt Algorithm: non-linear approach)
     - b.1 First order Taylor series expansion
     - b.2 2nd order Taylor series expansion (sensitive to noise)

Machine learning for prediction

   3.2 $Ax = b'$: estimation value. b'': estimation value, $E = \sum [b' - b'']^2$
   - a. EM (Expected-Maximization), initial b' = average value

Unsupervised Learning
Use at Reinforcement Learning for Reward r

4. **Lagrange Approach (outlier) with constraint**
   $\min \; E = \sum [Ax - b]^2 + \lambda (x^2+y^2)^2$

Constraint: GAN …

0.3 GPT - GAN for Loss Constraint (Regulation) Term and Prediction

GAN: Generative Adversarial Network

◻ Metrics - Lagrange multiplier method

岭回归(Ridge Regression)是在平方误差的基础上增加正则项

λ called Lagrange Multiplier

$$\text{Loss } L = \sum_{i=1}^{n}\Big(\overset{\text{G.T.}}{y_i} - \sum_{j=0}^{p} w_j x_{ij}\Big)^2 + \boxed{\boxed{\lambda}\sum_{j=0}^{p} w_j^2} \quad \text{With } \lambda\text{=1000}$$

This is for bias optimization

This is for variance optimization

通过确定λ的值可以使得在方差和偏差之间达到平衡：随着λ的增大，模型方差减小而偏差增大。

variance bias

对w求导，结果为

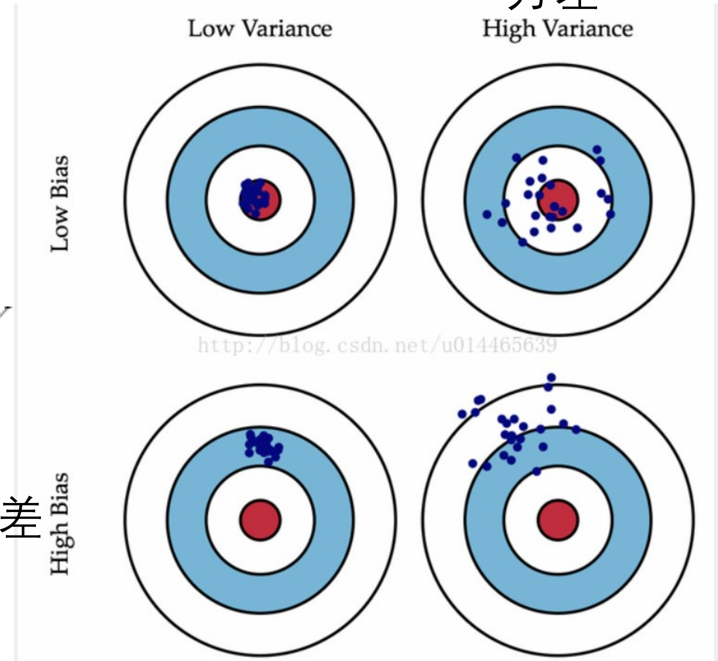
$$\frac{\partial L}{\partial w} = 2X^T(Y - XW) - 2\lambda W$$

令其为0，可求得w的值：

$$\hat{w} = (X^TX + \lambda I)^{-1}X^TY$$

方差

偏差



Low variance is better

- GAN for loss constraint (regulation) term and prediction
  - ➔ Regulation term to improve the recall/precision and stability
  - ➔ But training process is not easy convergence, so need pre-training

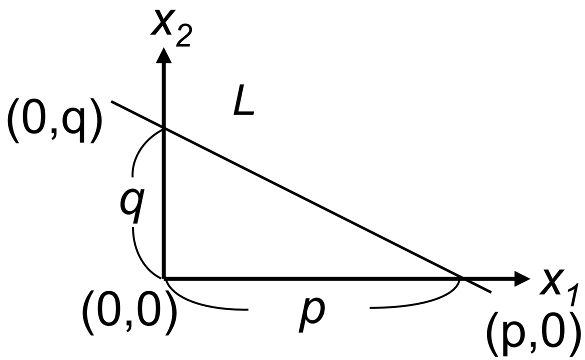
Outline

1. Basic Concept

- Introduction
  - SVM is a classifier derived from statistical learning theory by Vapnik and Cortes (1995).
  - Relatively easy to use.
  - Suitable for pattern classification or nonlinear regression problems.

1.1 Background Knowledge: Linear Equation (1/3)

- Linear Equation Representation



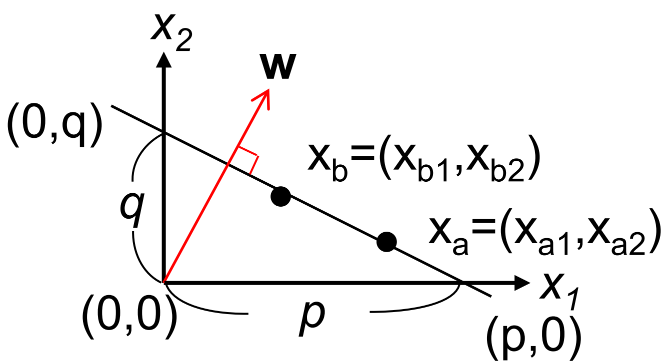
  - Assume a line *L* passing two axes at (p,0) and (0,q).
  - This line could be represented by $\frac{x_1}{p}+\frac{x_2}{q}=1$
  - Reformulate:

$$\frac{x_1}{p}+\frac{x_2}{q}=1 \Rightarrow qx_1+px_2-pq=0$$

$$\Rightarrow [q \quad p]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}-pq=0 \Rightarrow \mathrm{w}^T\mathrm{x}+b=0$$

1.1 Background Knowledge: Linear Equation (2/3)

- Normal vector



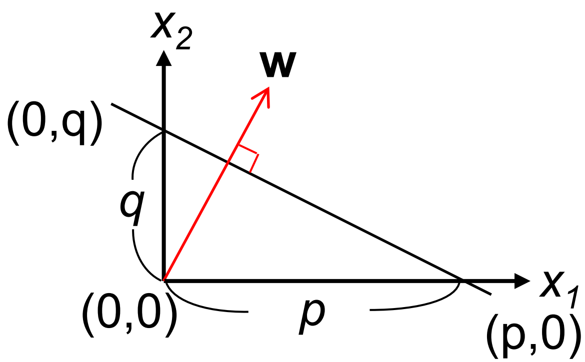
- Assume two points x_a and x_b at the line.
- So we have a vector (x_a-x_b)

$$\left.\begin{aligned} w^T x_a + b = 0 \\ w^T x_b + b = 0 \end{aligned}\right\} \Rightarrow w^T x_a - w^T x_b = 0 \Rightarrow w^T(x_a - x_b) = 0$$

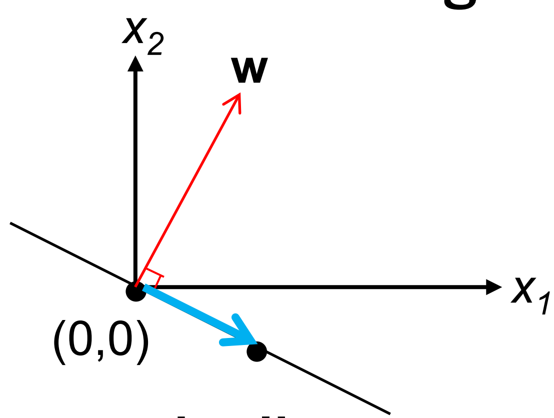
- w is the normal vector of line equation.

1.1 Background Knowledge: Linear Equation (3/3)

- How about b = 0?



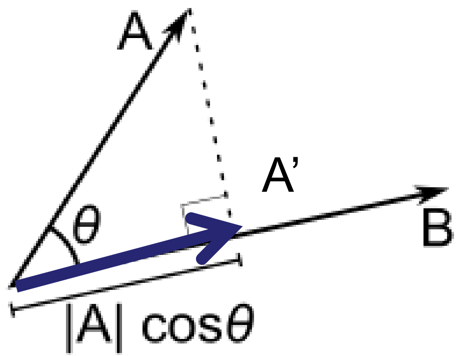
  - Assume b=0, so we get $\mathbf{w}^T\mathbf{x} + b = 0 \Rightarrow \mathbf{w}^T\mathbf{x} = 0 \Rightarrow \mathbf{w}^T(\mathbf{x} - \vec{0}) = 0$
  - It means that x is origin or that x $\perp$ w



  - b=0 $\Longrightarrow$ the line passes through origin

1.1 Background Knowledge: Inner Product

- **Inner Product**



$$< A, B > = A^T B = \|A\| \cdot \|B\| \cos\theta$$

projection

$$\Rightarrow \|A\| \cos\theta = \frac{A^T B}{\|B\|}$$

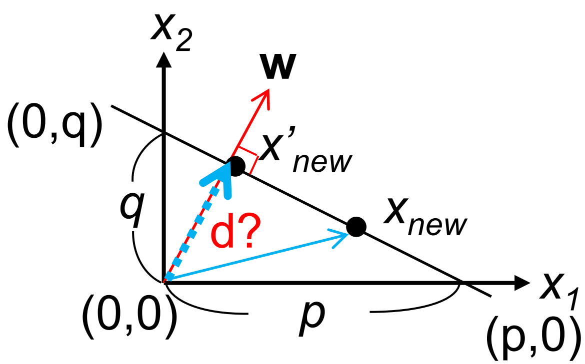
– **The length of projected vector A' is** $\frac{A^T B}{\|B\|} = A^T \frac{B}{\| B \|}$

A向量在 B 向量上的分量=投影量

1. || A || = ((x-x0)^2 + (y-y0)^2) ^ ½, normalization term as standard deviation?
2. cos_theta = (A B) / |A| |B| as NCC

1.1 Background Knowledge: Distance to Origin

- What is the distance to the origin?



  - Assume there is a point x_{new} at this line
  - We know the length of projected point x'_{new} along w is d= $\frac{\mathbf{w}^T\mathbf{x}_{new}}{\|\mathbf{w}\|}$
  - And x_{new} satisfies the equation: $\mathbf{w}^T\mathbf{x}_{new} + b = 0$
  - Combine two terms:

$$\mathbf{w}^T\mathbf{x}_{new} + b = 0 \Rightarrow \frac{\mathbf{w}^T\mathbf{x}_{new} + b}{\|\mathbf{w}\|} = 0 \Rightarrow \frac{\mathbf{w}^T\mathbf{x}_{new}}{\|\mathbf{w}\|} = \frac{-b}{\|\mathbf{w}\|}$$

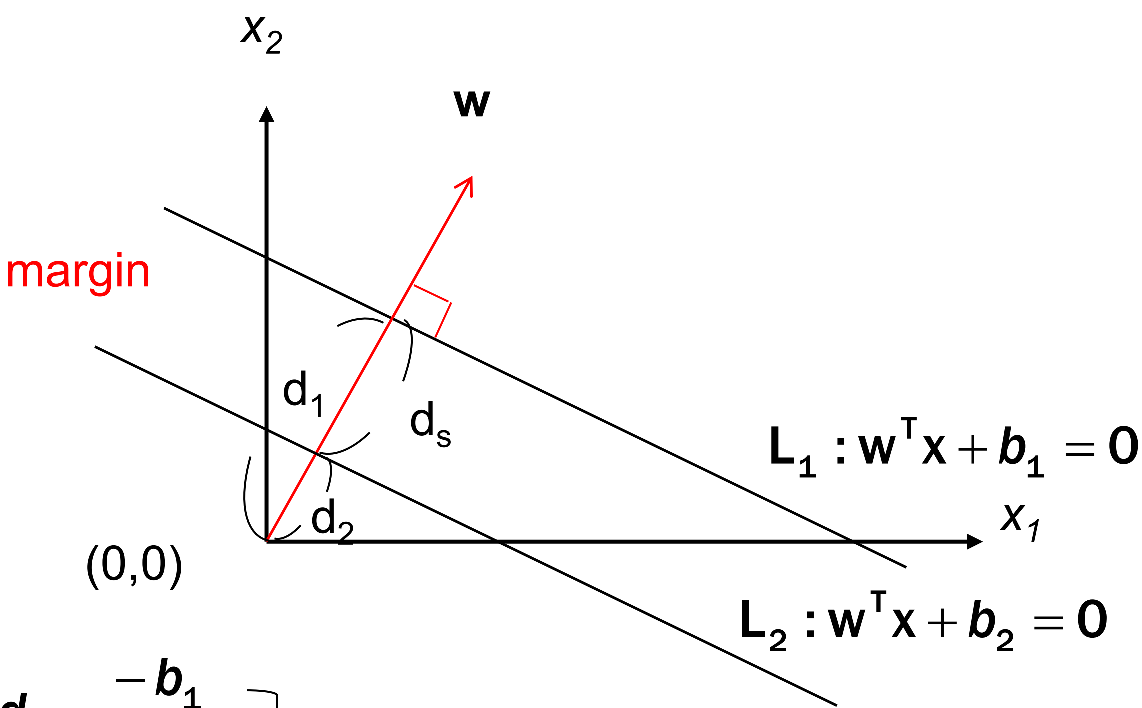
Distance from origin (0,0) to line L

$$\mathbf{d} = \frac{-b}{\|\mathbf{w}\|} = \frac{\mathbf{w}^T\mathbf{x}_{new}}{\|\mathbf{w}\|}$$

d= {(w1,w2) * (0,0) + b} / ||w||

1.1 Background Knowledge: Distance between Parallel Lines

- What is the distance d_s between two lines L_1 and L_2?

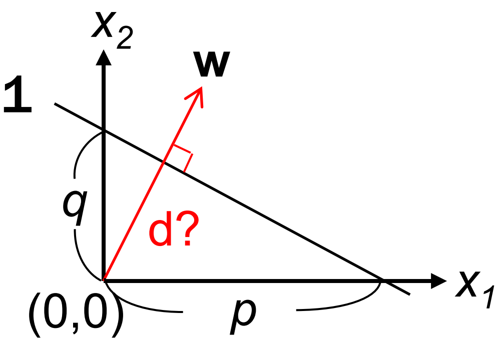


$$\left.\begin{aligned} d_1 &= \frac{-b_1}{\|w\|} \\ d_2 &= \frac{-b_2}{\|w\|} \end{aligned}\right\} \Rightarrow \boxed{d_s = d_1 - d_2 = \frac{-b_1}{\|w\|} - \frac{-b_2}{\|w\|} = \frac{-(b_1 - b_2)}{\|w\|}}$$

1.1 Background Knowledge

- **Linear Equation**

Linear equation: $\frac{x_1}{p} + \frac{x_2}{q} = 1$



James:
W: scaling and rotation
b: translation
b=0?
W: rotation, Scaling = 1,

*W=w/||w|| * ||w||*

Unit vector = direction   magnitude

d=??

$$\frac{x_1}{p} + \frac{x_2}{q} = 1 \Rightarrow qx_1 + px_2 - pq = 0$$

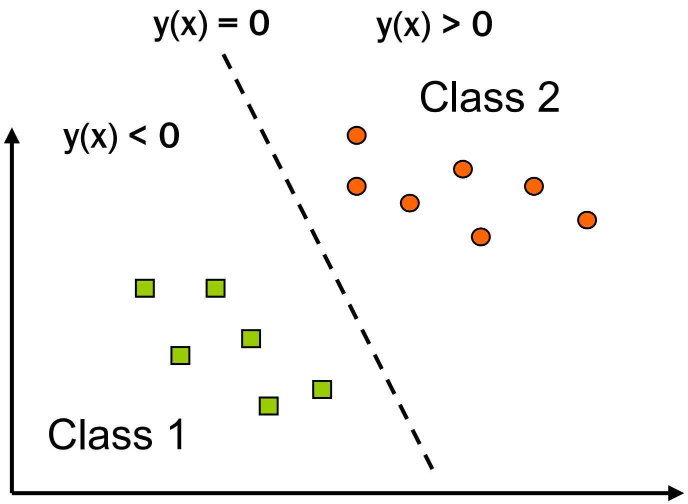
$$\Rightarrow \begin{bmatrix} q & p \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - pq = 0$$

$$\Rightarrow \mathbf{w}^T\mathbf{x} - b = 0$$

where w = [*q p*]^T, x = [x_1 x_2]^T, and *b* = *pq*.

1.2 Classification Problem

- Classification Problem
  - Assume two classes of data: circles and squares
  - Find a hyperplane (dim>2) to separate two classes



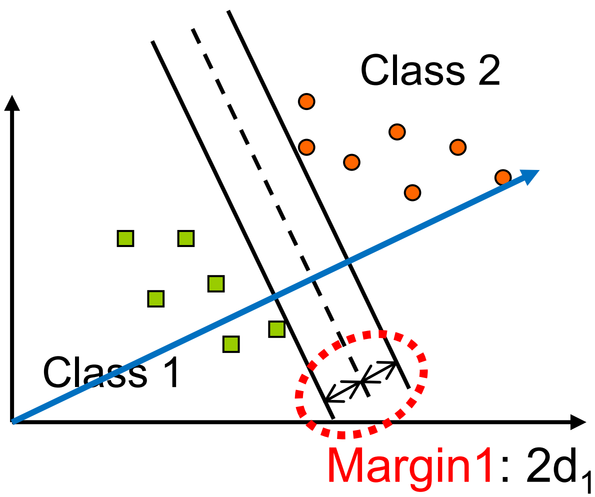
  - A separating hyperplane: $y(x) = w^T x + b = 0$

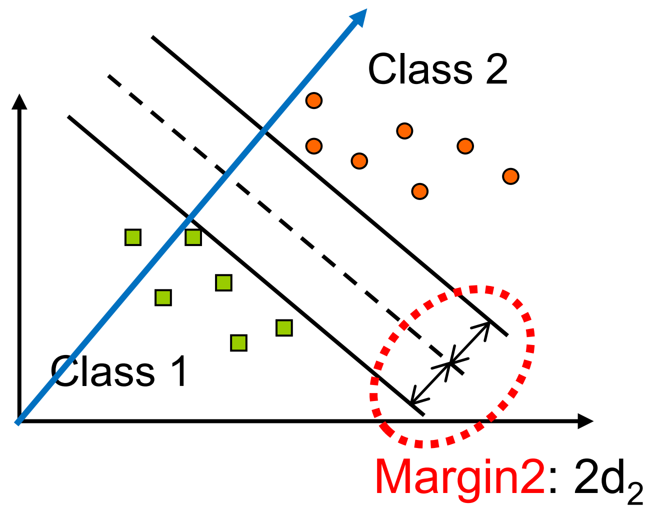
    $(w^T x_i) + b > 0$ if x_i is of class 2

    $(w^T x_i) + b < 0$ if x_i is of class 1

1.2 Classification Problem: Optimal Separating Plane (1/2)

- **Optimal Separating Plane**





  - **Which is a better classifier?**
  - **James: Why?**

$d_2>d_1$

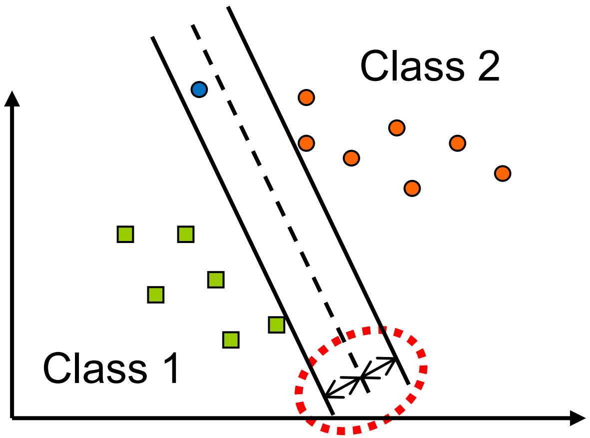
Margin 2d=? Margin 2d'=?

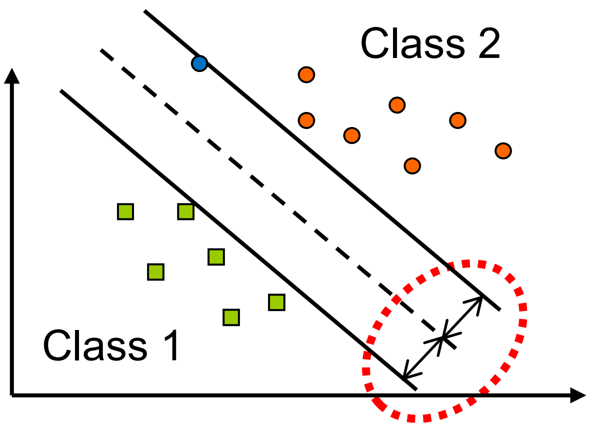
$W^Tx+b=0$ => $w'^Tx+b'=0$
$W^Tx+b=a$ => $w'^Tx+b'=1$
$W^Tx+b=-a$ => $w'^Tx-b'=-1$

Because of scaling and merge into w and b to become w' and b'

1.2 Classification Problem: Optimal Separating Plane (2/2)

- Consider the outlier data
  - A new point: Blue circle

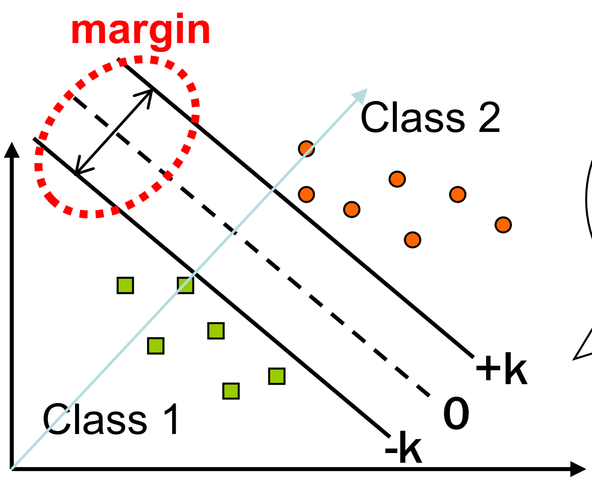




- The margin provides the potential tolerance to outlier data. Therefore margin2 is better than magin1

1.2 Classification Problem: Margin Classifier (1/2)

- Margin Classifier
  - Consider the margin



$$w^T x + b = \begin{bmatrix} +k \\ 0 \\ -k \end{bmatrix}$$

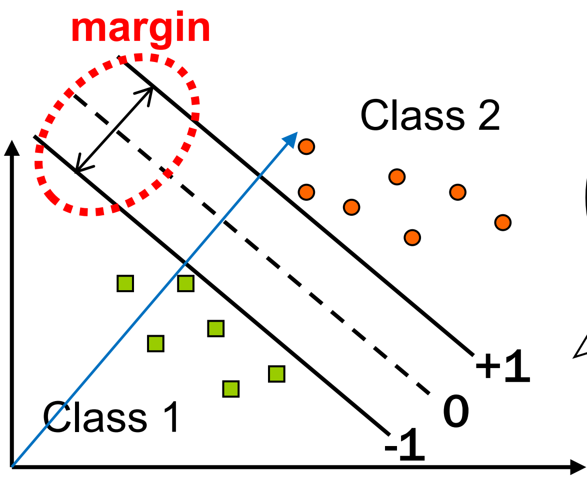
  - Reformulate:

$$w^T x + b = k \Rightarrow \frac{w^T x + b}{k} = 1 \Rightarrow (\frac{w}{k})^T x + \frac{b}{k} = 1 \Rightarrow w'^T x + b' = 1$$

$$where\ \mathrm{w}' = \frac{\mathrm{w}}{\mathrm{k}}\ \mathrm{and}\ \mathrm{b}' = \frac{\mathrm{b}}{\mathrm{k}}$$

1.2 Classification Problem: Margin Classifier (2/2)

- Margin Classifier



$$w^T x + b = \begin{bmatrix} +1 \\ 0 \\ -1 \end{bmatrix}$$

$$w^T x + b = 1 \Rightarrow w^T x + b - 1 = 0$$

$$w^T x + b = -1 \Rightarrow w^T x + b + 1 = 0$$

$$\Rightarrow d_s = d_1 - d_2 = \frac{-b_1}{\|w\|} - \frac{-b_2}{\|w\|}$$

$$\Rightarrow \frac{-(b-1)}{\|w\|} - \frac{-(b+1)}{\|w\|} = \frac{-(-2)}{\|w\|}$$

  - Training vectors: x_i, $i = 1, \ldots, l$

    Define an indicator/labeling vector **y**

$$y_i = \begin{cases} 1 & \text{, if } x_i \text{ in class 2} \\ -1 & \text{, if } x_i \text{ in class 1} \end{cases}$$

  - A separating hyperplane: $w^T x + b = 0$

$$\begin{cases} (w^T x_i) + b > 0 & \text{if } y_i = 1 \\ (w^T x_i) + b < 0 & \text{if } y_i = -1 \end{cases}$$

Brief Conclusion:

w: Rotation (+ scaling) of decision line

b: Translation of decision line

RetinaNet??

1.2 Classification Problem: Maximal Margin

- Maximal Margin
  - Width of the margin between $w^T x + b = 1$ and -1:

Margin 2d'=? $2/\|w\| = 2/\sqrt{w^T w}$ → max

  - The decision boundary L should classify all data correctly.

$$\Rightarrow y_i(w^T x_i + b) \geq 1$$

yi= +1 or -1

  - The first SVM formula: a constrained optimization problem [Boser et al., 1992]

$$\max 2/\|w\| = 2/\sqrt{w^T w}$$

$$\Rightarrow \max 4/w^T w$$

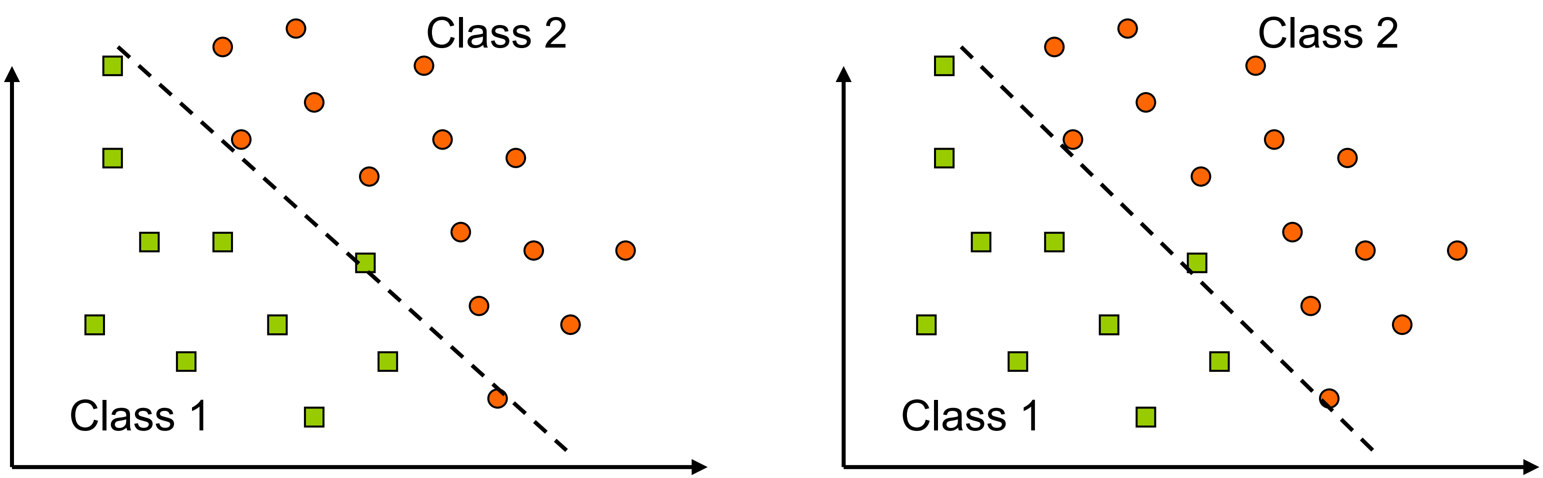
$$\Rightarrow \min w^T w$$

$$\boxed{\begin{array}{l} \min_{w,b} \frac{1}{2} w^T w \\ \text{subject to } y_i(w^T x_i + b) \geq 1,\ i = 1, \ldots, l \end{array}}$$

RetinaNet??

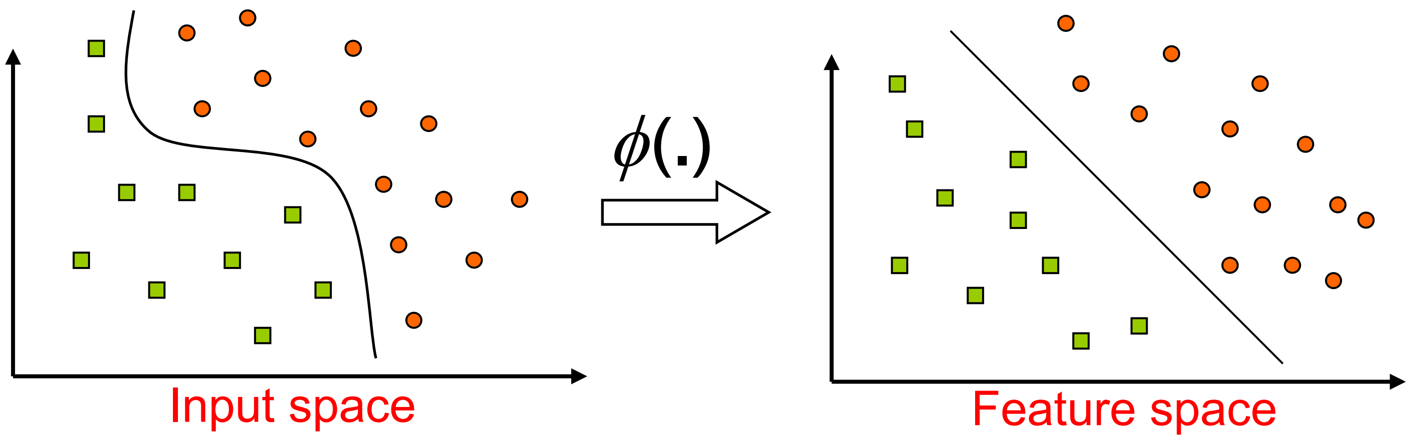
1.3 Nonlinearly Separable Data

- **Nonlinearly Separable Data**
  - No linear plane could separate data perfectly



  - **Solution**
    1) Nonlinear transformation => (james:)
       1.1) To higher dimension $\phi(.)$ via kernel function and then linear separation
       1.2) Or transfer to, for example, inside circle and outside circle. That is, decision boundary is nonlinear??
    2) Soft margin => allow training error, i.e, ERR != 0, occurs

1.3 Nonlinearly Separable Data: Nonlinear Transformation (1/2)



- Why nonlinear transform $\phi(.)$?
  1) Data are more easily separated in higher dimensional (maybe infinite) feature space .
  2) Linear operation in the feature space is equivalent to nonlinear operation in input space.
- Ex:

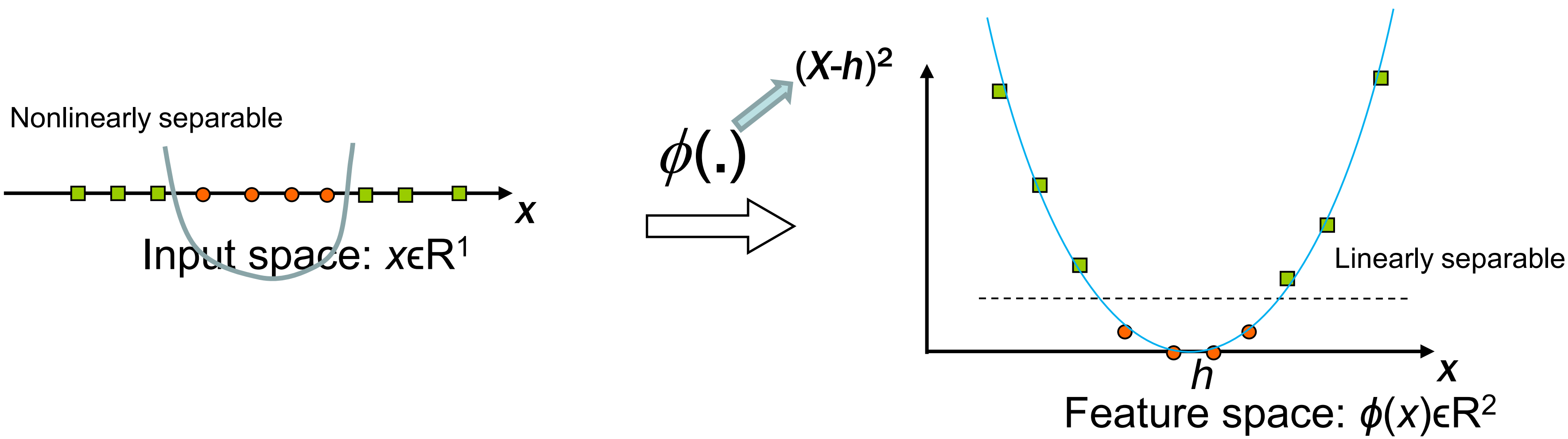
$$x \in R^3 \quad \phi(x) \in R^{10}$$

$$\phi(x) = (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_3, x_1^2, x_2^2, x_3^2, \sqrt{2}x_1x_2, \sqrt{2}x_1x_3, \sqrt{2}x_2x_3)$$

(x_1, x_2, x_3)

1.3 Nonlinearly Separable Data: Nonlinear Transformation (2/2)

- Example



  - The circle points spread between the square points.
  - After the nonlinear mapping, there explicitly exists a linear plane separating circle points from square points.

1.3 Nonlinearly Separable Data: Kernel Function

- Kernel Function
  - The relationship between the kernel function *K* and the mapping $\phi(.)$ is

$$K(x,y) = \langle \phi(x), \phi(y) \rangle = \phi(x)^T \phi(y)$$

  - In practice, we **specify *K*** instead of choosing $\phi(.)$ directly.
  - Intuitively, *K*(x,y) represents the similarity of ϕ(x) and ϕ(y) as we desired.

J: Inner product is kind of similarity measure

  - *K*(x,y) needs to satisfy ***Mercer's Condition*** (described later) to make sure that $\phi(.)$ exists.
- SVM solves two issues simultaneously
  - Nonlinear transformation using kernels
  - Minimize $\|w\|$

1.3 Nonlinearly Separable Data: Typical Kernel Function

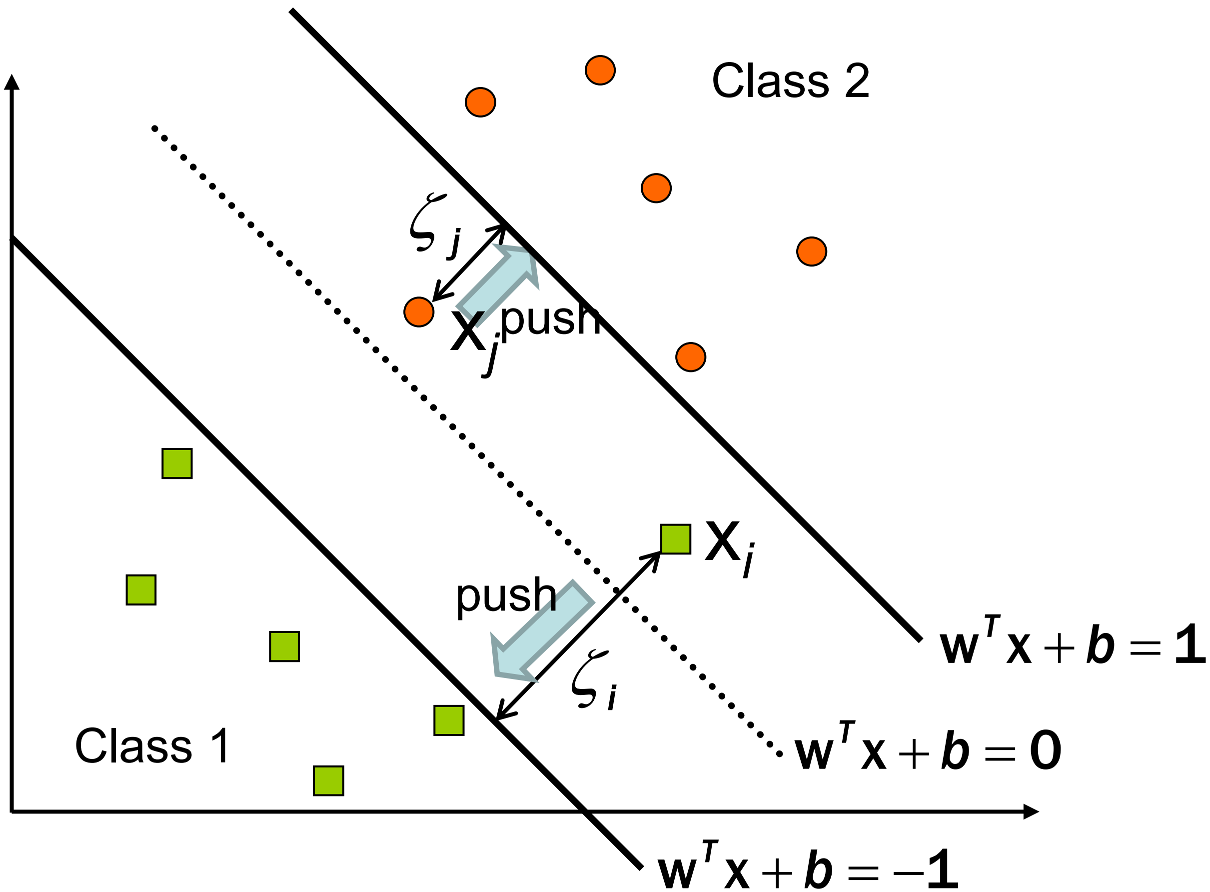
Similar to activation function at deep learning

- Typical Kernel Function
  1) Polynomial kernel
     $K(\mathrm{x},\mathrm{y}) = (\mathrm{x}^T\mathrm{y}+1)^d$, *d:* degree
  2) Radial basis function (Gaussian kernel)
     $$K(\mathrm{x},\mathrm{y}) = \exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right),\ \sigma: \text{width}$$
  3) Sigmoid function
     $K(\mathrm{x},\mathrm{y}) = \tanh(\kappa\mathrm{x}^T\mathrm{y}+\theta),\quad \kappa,\theta: \text{parameters}$

  – The choice of different kernel functions is problem-dependent.

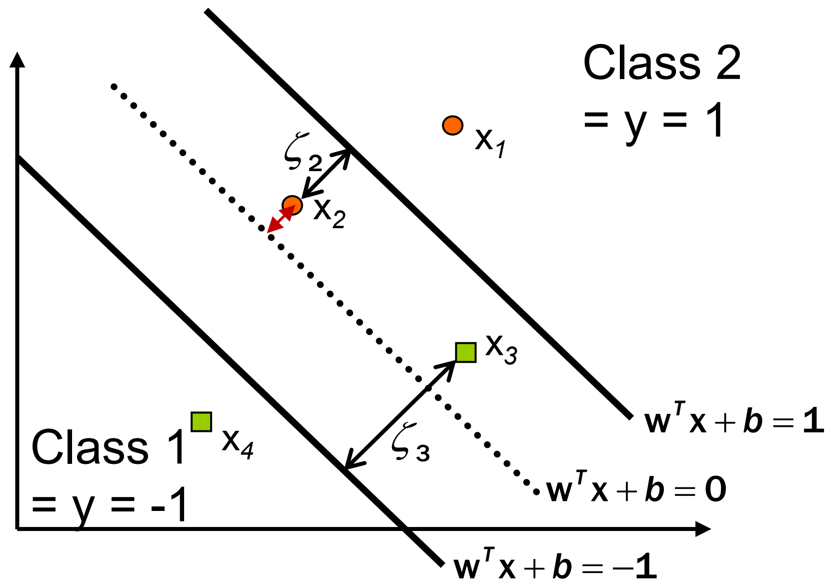
1.3 Nonlinearly Separable Data: Soft Margin Hyperplane (1/3)

- Soft Margin Hyperplane
  - To avoid overfitting, we allow "training errors" ζ_i in classification



1.3 Nonlinearly Separable Data: Soft Margin Hyperplane (2/3)

- The Inequality Constraint $y_i(w^T x_i + b) \geq 1 - \zeta_i$
  - Consider four points x_1, x_2, x_3, and x_4



Class = G.T.

x_1: $y_1 = 1$, $(w^Tx_1+b)>1$ (ex: 1.5), so $y_1(w^Tx_1+b)>1$ (ex: 1.5), and then $\zeta_1 = 0$ (no error)
satisfy constraint

x_2: $y_2 = 1$, $1>(w^Tx_2+b)>0$ (ex: 0.5), so $1>y_2(w^Tx_2+b)>0$ (ex: 0.5), and then $1>\zeta_2> 0$ (ex: 0.5)

x_3: $y_3 = -1$, $1>(w^Tx_3+b)>0$ (ex: 0.5), so $0>y_3(w^Tx_3+b)>-1$ (ex: -0.5), and then $2> \zeta_3> 1$ (ex: 1.5)

x_4: $y_4 = -1$, $(w^Tx_4+b)<-1$ (ex: -1.5), so $y_4(w^Tx_4+b)>1$ (ex: 1.5), and then $\zeta_4 = 0$ (no error)
satisfy constraint

1.3 Nonlinearly Separable Data: Soft Margin Hyperplane (3/3)

- Soft Margin Optimization Problem
  - Include an additional term of training errors $\sum_{i=1}^{l} \zeta_i$
  - Combine with margin term by multiplying a scalar C
  - Reformulate:

$$\min_{w,b,\zeta} \quad \frac{1}{2} w^T w + C \sum_{i=1}^{l} \zeta_i$$

$$\text{subject to } y_i(w^T x_i + b) \geq 1 - \zeta_i, \zeta_i \geq 0, \text{for } i = 1, \cdots, l$$

1.4 Standard SVM ??

w: Line Rotation + Scaling
=> Line Rotation

- Standard SVM [Vapnik and Cortes, 1995]
  - Key Idea
    1) Higher dimensional feature space
    2) Allow training errors
  - Constrained Optimization Problem

Margin Term: Find the best rotation factor by margin w

Training Error Term: Min Sum of ζ_i : Min sum of all training errors

C: Bigger C, margin??? If linear margin, the total training errors are big. If nonlinear margin such as curve, then the total training errors will reduce.

J + Carl: Cause nonlinear margin occur

$$\min_{\mathbf{w},b,\zeta} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{l}\zeta_i$$

subject to $y_i(\mathbf{w}^T\phi(x_i)+b) \geq 1-\zeta_i,\ \ \zeta_i \geq 0,\ i = 1, \ldots, l$

C: Tradeoff parameters between training error and margin *w* (need to tune)

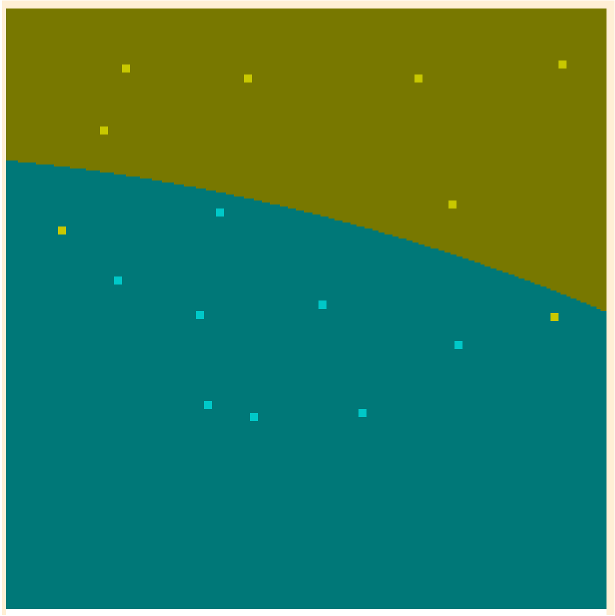
- **w:** a vector in high dimensional space

$\Rightarrow$ maybe infinite variables. Difficult to solve

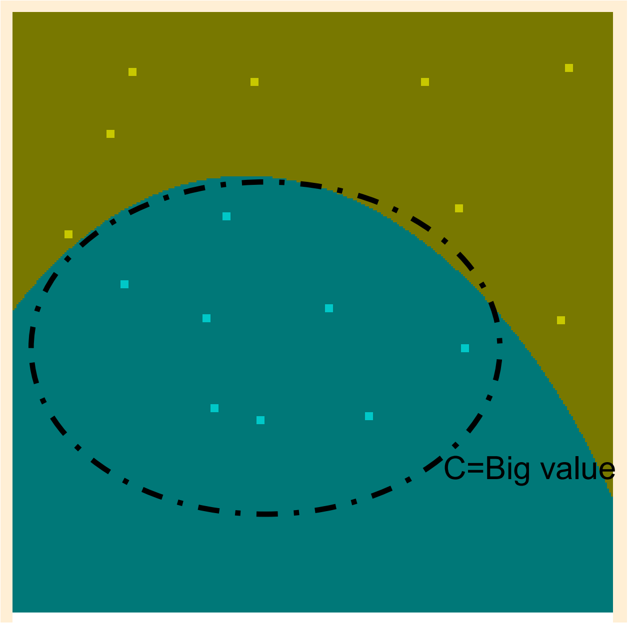
1.4 Standard SVM: Effect of Tradeoff Parameter

- Effect of Tradeoff Parameter
  - The effect of C can be observed using the SVM Toy on the libsvm webpage:
  - http://www.csie.ntu.edu.tw/~cjlin/libsvm/

C=1



C=100



1.4 Standard SVM: Duality

$$L(w,b,\alpha)=\frac{1}{2}w^T w-\sum_{i=1}^{l}\alpha_i\left[y_i(w^T x_i+b)-1\right]$$

$$\frac{\partial L}{\partial w}=w-\sum_{i=1}^{l}\alpha_i y_i x_i=0 \Rightarrow w=\sum_{i=1}^{l}\alpha_i y_i x_i,\ \alpha_i\geq 0$$

- Duality
  - Transform the primal problem to the dual problem

$$\min L(w,b,\alpha)=\max_{\alpha\geq 0}(\min_{w,b} L(w,b,\alpha))$$

- The Dual Problem

A finite problem: # variables = #training data

$$\boxed{\min_{\alpha}\ \frac{1}{2}\alpha^T Q\alpha-e^T\alpha}$$

$$L(w,b,\alpha) \Leftarrow (w=\sum_{i=1}^{l}\alpha_i y_i x_i)$$

x: sample position

subject to $0\leq\alpha_i\leq C,\ i=1,\ldots,l,\ \ y^T\alpha=0$

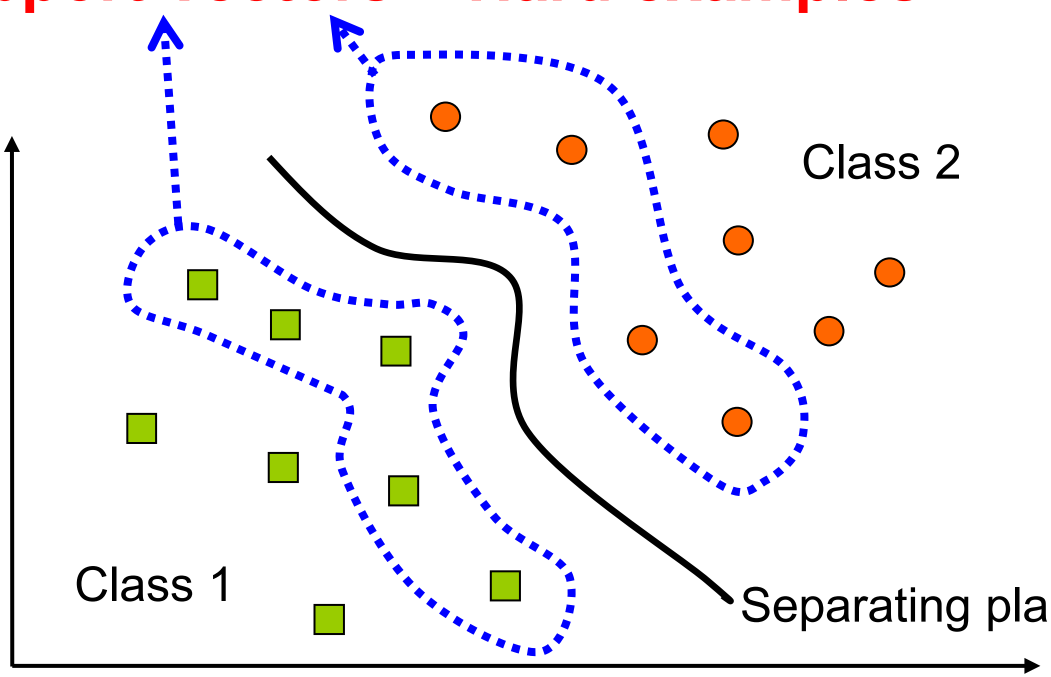
where $Q_{ij}=y_i y_j \phi(x_i)^T\phi(x_j)$ and $e=[1,\ldots,1]^T$

  - At optimum, w is recovered as $w=\sum_{i=1}^{l}\alpha_i y_i\phi(x_i)$
  - The only difference with the linearly separable case is the upper bound C on α_i
  - A quadratic programming solver can be applied to find α_i

1.4 Standard SVM: Support Vectors

- Support Vectors
  - The support vectors are a subset of training data closest to the separating plane and therefore the most difficult to classify.

Support Vectors = Hard examples



1.4 Standard SVM: Decision Function

$$L(w,b,\alpha)=\frac{1}{2}w^Tw-\sum_{i=1}^{l}\alpha_i\left[y_i(w^Tx_i+b)-1\right]$$

$$\frac{\partial L}{\partial w}=w-\sum_{i=1}^{l}\alpha_i y_i x_i=0 \;\Rightarrow\; w=\sum_{i=1}^{l}\alpha_i y_i x_i,\ \ \alpha_i\ge 0$$

- Decision Function
  - At optimum, w is recovered as $w=\sum_{i=1}^{l}\alpha_i y_i\phi(x_i)$
  - Let $\phi(x)$ be the testing data, then decision function

$$w^T\phi(x)+b$$

$$=\sum_{i=1}^{l}\alpha_i y_i \underline{\phi(x_i)^T\phi(x)}+b$$

$$=\sum_{i=1}^{l}\alpha_i y_i \underline{K(x_i,x)}+b$$

  - By using the dual variable α_i, it is no need to write down w.
  - Very often, α_i is optimized to zero. In other words, x_i with non-zero α_i are so-called support vectors which determine the decision boundary.

1.4 Standard SVM: Mercer's Condition

- Mercer's Condition [1903]
  - What kind of K_{ij} can be represented as $\phi(x_i)^T \phi(x_j)$?
  - $K(x, y) = \phi(x)^T \phi(y)$ if and only if $\forall g$ s.t.

$$\int g(x)^2 dx \text{ finite} \Rightarrow \int K(x, y) g(x) g(y) dx dy \geq 0$$

  - It is useful for some kernel. However, still not easy to check.

2. Dual SVM Derivation

- Duality
  - Transform the primal problem to the dual problem

$$\min L(w,b,\alpha) = \max_{\alpha \geq 0}(\min_{w,b} L(w,b,\alpha))$$

Lagrange:

$$L(\mathrm{w},b,\alpha) = \frac{1}{2}\mathrm{w}^T\mathrm{w} - \sum_{i=1}^{l}\alpha_i\left[y_i(\mathrm{w}^T x_i + b) - 1\right]$$

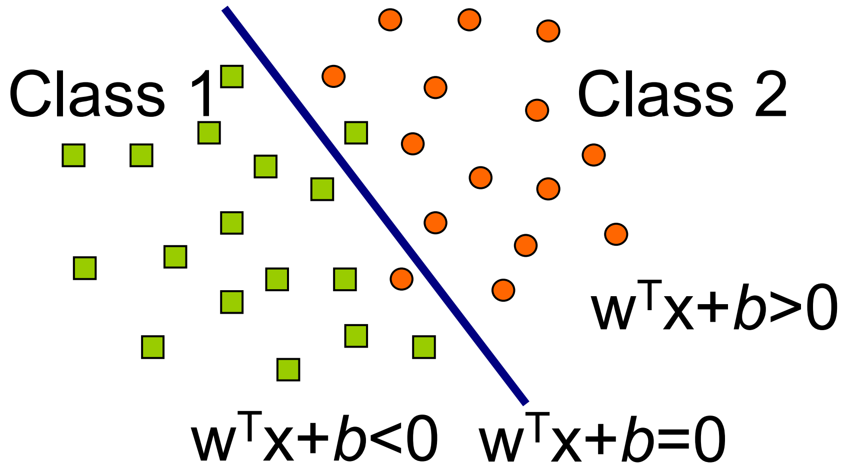
Derivation of w and b

Max(Lamda):

$$\tilde{L}(\alpha) = \sum_{i=1}^{l}\alpha_i - \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j y_i y_j x_i^T x_j$$

2.1 SVMs Reminder

- **Original SVM Problem**



  - **Consider the problem without ζ_i and C**

$$\min_{\mathrm{w,b}} \frac{1}{2}\mathrm{w}^T\mathrm{w}$$

subject to $y_i(\mathrm{w}^T x_i + b) \geq 1$, i = 1, ..., l

  - **A constrained optimization problem: Use lagrange multiplier method to solve**

2.2 Lagrange Multiplier Method

- Constrained Optimization Problem
  - Find x=[x_1 x_2 ... x_n] which minimizes f(x) subject to the inequality constraints: $g_j(x) \leqq 0$, j=1, 2, ..., *m.*

- Lagrange Function
  - Transform the inequality constraints to equality constraints by using $G_j(x,y)=g_j(x)+y_j^2=0$, where y=[y_1 y_2 ... y_m] is the vector of slack variables.
  - Lagrange function: $L(x,y,\lambda)=f(x)+\Sigma_j \lambda_j G_j(x,y)$

2.2 Lagrange Multiplier Method

- Lagrange Function
  - The solution of L is given by solving

$$\begin{cases} \dfrac{\partial L}{\partial x_i} = \dfrac{\partial f}{\partial x_i} + \sum_{j=1}^{m} \lambda_j \dfrac{\partial g_j}{\partial x_i} = 0,\ i = 1,2,\ldots,n \\ \dfrac{\partial L}{\partial \lambda_j} = g_j(x) + y_j^2 = 0,\ \ j = 1,2,\ldots,m \\ \dfrac{\partial L}{\partial y_j} = 2\lambda_j y_j = 0,\ \ j = 1,2,\ldots,m \end{cases}$$

2.3 The Linearly Separable Case (1/2)

- The Primal Problem

$$\min_{\mathbf{w},b} \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

subject to $y_i(\mathbf{w}^T x_i + b) \geq 1$, $i = 1, \ldots, l$

- The Lagrange function

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{l}\alpha_i\left[y_i(\mathbf{w}^T x_i + b) - 1\right]$$

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{l}\alpha_i y_i x_i = 0 \Rightarrow \mathbf{w} = \sum_{i=1}^{l}\alpha_i y_i x_i, \quad \alpha_i \geq 0$$

where α_i is the weight of data point x_i.

2.3 The Linearly Separable Case (2/2)

- Notice the value of α_i:
  - $\alpha_i = 0$, don't care about the constraints!
  - $\alpha_i > 0$, the i-th point x_i is close to the hyperplane.

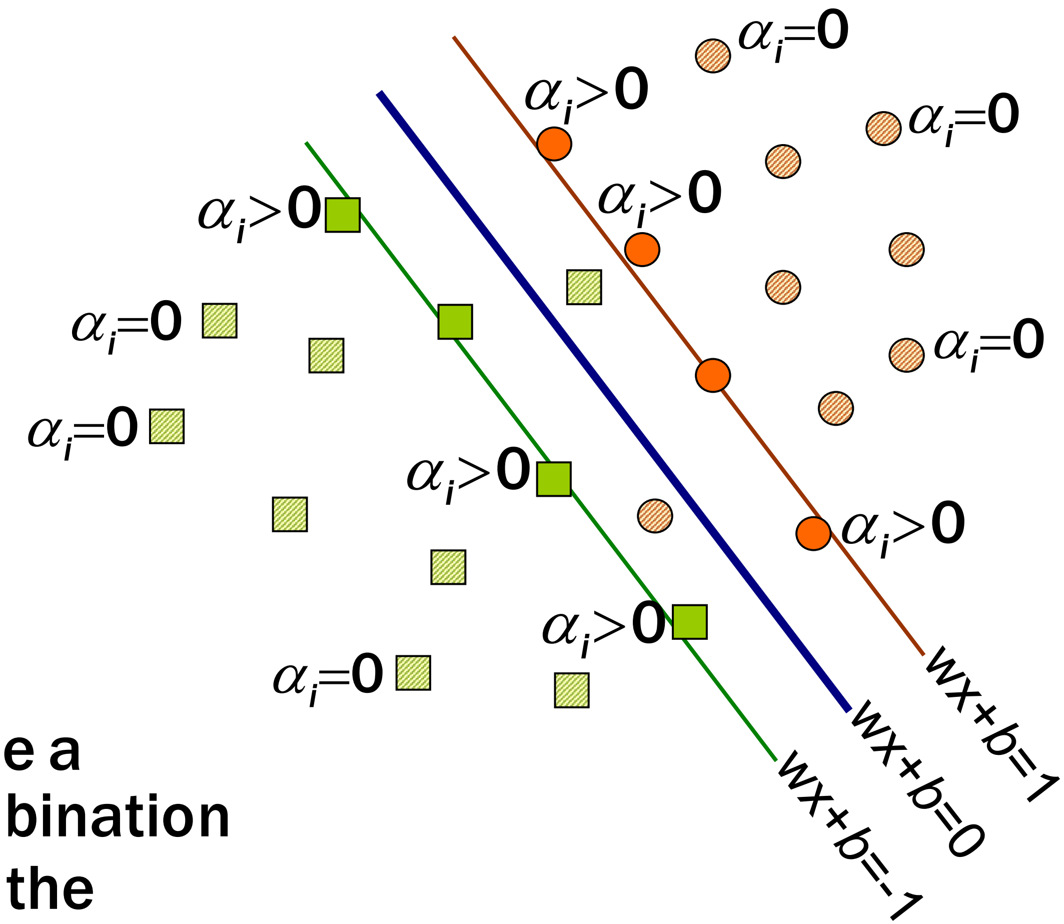
    Support vector

    At optimum, $\frac{\partial L}{\partial \alpha_i} = y_i(w^T x_i + b) - 1 = 0$

    $$y_i(w^T x_i + b) = 1 \;\Rightarrow\; b = \frac{1}{y_i} - w^T x_i$$

    notice $y_i = 1 / y_i, \;\; y_i = \{-1, +1\}$
- Therefore, we can obtain b by $b = y_i - w^T x_i$, for any i where $\alpha_i > 0$.
  (Average b over all points where $\alpha_i > 0$)

2.3 The Linearly Separable Case: Dual SVM Interpretation



$$\mathbf{w} = \sum_{i=1}^{l} \alpha_i y_i \mathbf{x}_i,$$

w is going to be a weighted combination of points near the hyperplane.

2.3 The Linearly Separable Case: Dual Problem (1/2)

- Dual Problem
  - Substitute $\mathbf{w}=\sum_{i=1}^{l}\alpha_i y_i \mathbf{x}_i$ into $L(\mathbf{w},b,\alpha)$ to get $\tilde{L}(\alpha)$

$$\tilde{L}(\alpha)$$

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

$$=\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i y_i \mathbf{x}_i^T\alpha_j y_j \mathbf{x}_j-\sum_{i=1}^{l}\alpha_i y_i\Big(\sum_{j=1}^{l}\alpha_j y_j \mathbf{x}_j\Big)^T\mathbf{x}_i \qquad \text{hint}: \sum_{i=1}^{l}\alpha_i y_i=0$$

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

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

2.3 The Linearly Separable Case: Dual Problem (2/2)

- Dual Problem
  - Reformulate $\tilde{L}(\alpha)$ to a quadratic programming problem

$$\min_{\alpha} \frac{1}{2}\alpha^T Q\alpha - e^T\alpha$$

subject to $\alpha_i \geq 0$ for i=1,...,l and $y^T\alpha = 0$

where $Q \in R^{l\times l}$, $Q_{ij} = y_i y_j x_i{}^T x_j$, $e = [1 \quad \cdots \quad 1]^T \in R^{l\times 1}$

, $\alpha = [\alpha_1 \quad \ldots \quad \alpha_l]^T \in R^{l\times 1}$, and $y = [y_1 \quad \ldots \quad y_l]^T \in R^{l\times 1}$

  - We can apply quadratic programming solver to find α

$$k(x_i, x_j) = x_i{}^T x_j$$

  - Use kernel tricks to find decision function…Substitute support vectors to get b, without knowing w

2.3 The Linearly Separable Case: Dual SVM Formulation

- Lagrange function has to be

$$L(\mathrm{w},b,\alpha)=\frac{1}{2}\mathrm{w}^{\mathrm{T}}\mathrm{w}-\sum_{i=1}^{l}\alpha_i\left[y_i(\mathrm{w}^T x_i+b)-1\right]$$

- Dual problem is given by

$$\min_{\alpha\geq 0}\text{Primal}=\max_{\alpha\geq 0}\ \min_{\mathrm{w},b} L(\mathrm{w},b,\alpha)$$

- Solution is given by

$$\alpha=\arg\min_{\alpha}\sum_{i=1}^{l}\alpha_i-\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j y_i y_j x_i^T x_j,\ \sum_{i=1}^{l}\alpha_i y_i=0,\ \alpha_i\geq 0$$

- Thus w and b can be obtained by

$$\mathrm{w}=\sum_{i=1}^{l}\alpha_i y_i x_i$$

$$b=y_i-\mathrm{w}^{\mathrm{T}}x_i,\ \text{for any } k \text{ where } \alpha_k\geq 0$$

Q: Why should $\Sigma_i \alpha_i y_i = 0$?

A:

- If $\sum_{i=1}^{l} \alpha_i y_i \neq 0$, move b to ∞, then $-b\sum_{i=1}^{l} \alpha_i y_i$ will be −∞. That is, $L(\mathrm{w}, b, \boldsymbol{\alpha})$ decreases to −∞.

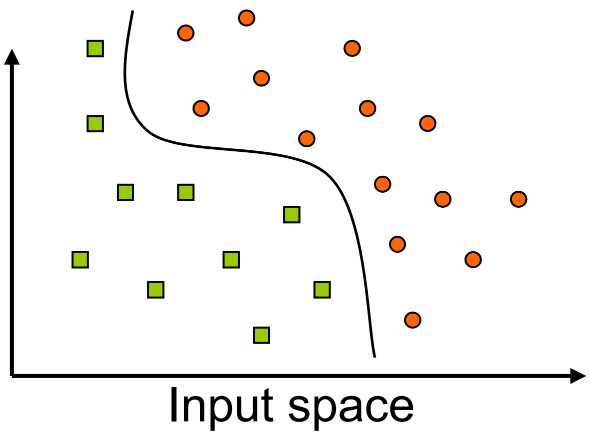
- $\min_{\mathrm{w},b} L(\mathrm{w}, b, \alpha) =$

$$\begin{cases} -\infty & \text{if } \sum_{i=1}^{l} \alpha_i y_i \neq 0 \\ \min_{\mathrm{w}} \frac{1}{2}\mathrm{w}^T\mathrm{w} - \sum_{i=1}^{l} \alpha_i \left[y_i \mathrm{w}^T x_i - 1 \right] & \text{if } \sum_{i=1}^{l} \alpha_i y_i = 0 \end{cases}$$

- Hence, we have w only when $\sum_{i=1}^{l} \alpha_i y_i = 0$.

2.4 The Nonlinearly Separable Case

- Nonlinearly Separable Data
  - More Often than not, the data could not separated by a linear plane



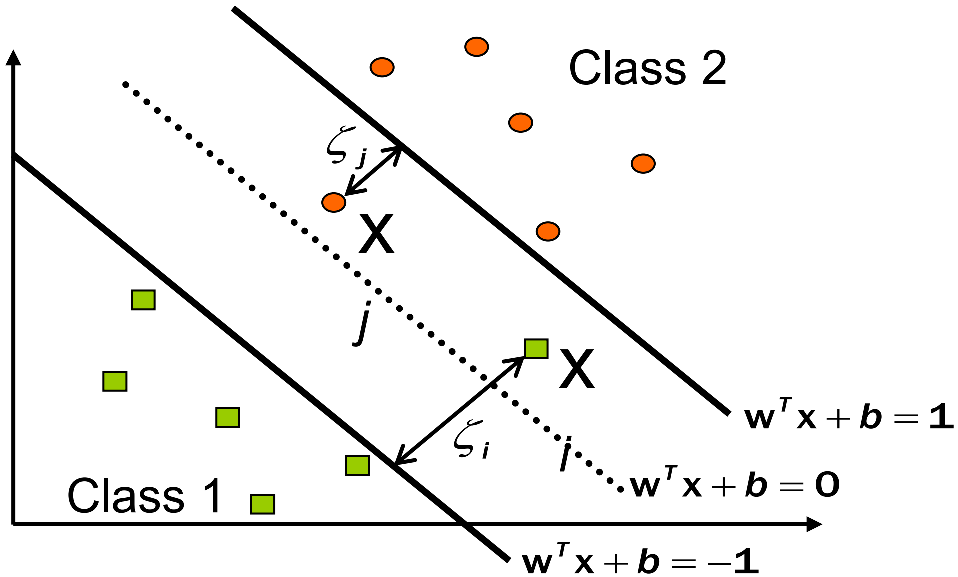
  - Solution for nonlinearly separable case

    1) Soft Margin

    2) Nonlinear Mapping to High dimensional space

2.4.1 Soft Margin (1/2)

- Soft Margin
  - Allow training error ζ_i



- Primal problem:

$$\min_{w,b} \ \frac{1}{2} w^T w + C \sum_{i=1}^{l} \zeta_i$$

subject to $y_i(w^T x_i + b) \geq 1 - \zeta_i, \ \ \zeta_i \geq 0$

2.4.1 Soft Margin (2/2)

- **Lagrange function:**

$$L(\mathrm{w}, b, \alpha, \zeta_i) = \frac{1}{2}\mathrm{w}^{\mathrm{T}}\mathrm{w} + C\sum_{i=1}^{l}\zeta_i - \sum_{i=1}^{l}\alpha_i\left[y_i(\mathrm{w}^T x_i + b) - 1)\right] + \sum_{i=1}^{l}\mu_i(\zeta_i - 0)$$

$$\frac{\partial L}{\partial \mathrm{w}} = \mathrm{w} - \sum_{i=1}^{l}\alpha_i y_i x_i = 0 \;\Rightarrow\; \mathrm{w} = \sum_{i=1}^{l}\alpha_i y_i x_i,\;\; \alpha_i \geq 0$$

$$\frac{\partial L}{\partial b} = -\sum_{i=1}^{l}\alpha_i y_i = 0 \Rightarrow \sum_{i=1}^{l}\alpha_i y_i = 0$$

$$\frac{\partial L}{\partial \zeta_i} = C - \alpha_i + \mu_i = 0 \Rightarrow \alpha_i = C - \mu_i$$

2.4.1 Soft Margin: Dual Problem (1/2)

- **Dual Problem:**

$$\tilde{L}(\alpha)$$

$$= \frac{1}{2}(\sum_{i=1}^{l}\alpha_i y_i x_i)^T(\sum_{j=1}^{l}\alpha_j y_j x_j) + C\sum_{i=1}^{l}\zeta_i - \sum_{i=1}^{l}\alpha_i\left\{y_i[(\sum_{j=1}^{l}\alpha_j y_j x_j)^T x_i + b] - 1 + \zeta_i\right\} - \sum_{i=1}^{l}\mu_i\zeta_i$$

$$= \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j y_i y_j x_i^T x_j + \sum_{i=1}^{l}C\zeta_i - \sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i y_i \alpha_j y_j x_j^T x_i \boxed{-\sum_{i=1}^{l}\alpha_i y_i b} + \sum_{i=1}^{l}\alpha_i - \sum_{i=1}^{l}\alpha_i\zeta_i - \sum_{i=1}^{l}\mu_i\zeta_i$$

$$= \sum_{i=1}^{l}\alpha_i - \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j y_i y_j x_i^T x_j + \boxed{\sum_{i=1}^{l}(C-\mu_i)}\zeta_i - \sum_{i=1}^{l}\alpha_i\zeta_i$$

hint: $\sum_{i=1}^{l}\alpha_i y_i = 0$

hint: $\alpha_i = C - \mu_i$

$$= \sum_{i=1}^{l}\alpha_i - \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j y_i y_j x_i^T x_j + \boxed{\sum_{i=1}^{l}(\alpha_i)}\zeta_i - \sum_{i=1}^{l}\alpha_i\zeta_i$$

$$= \sum_{i=1}^{l}\alpha_i - \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j y_i y_j x_i^T x_j$$

2.4.1 Soft Margin: Dual Problem (2/2)

- Dual Problem
  - $\alpha_i = C - \mu_i$ with $\mu_i \geq 0$ implies $C \geq \alpha_i$
  - Combine $C \geq \alpha_i$ and $\alpha_i \geq 0 \Rightarrow C \geq \alpha_i \geq 0$
  - Reformulate $\tilde{L}(\alpha)$ to a quadratic programming problem

$$\min_{\alpha} \frac{1}{2}\alpha^T Q\alpha - e^T\alpha$$

subject to $C \geq \alpha_i \geq 0$ for i=1,…,l and $y^T\alpha = 0$

where $Q \in R^{l\times l}$, $Q_{ij} = y_i y_j x_i^T x_j$, $e = [1 \quad \cdots \quad 1]^T \in R^{l\times 1}$

, $\alpha = [\alpha_1 \quad \ldots \quad \alpha_l]^T \in R^{l\times 1}$, and $y = [y_1 \quad \ldots \quad y_l]^T \in R^{l\times 1}$

  - We can apply quadratic programming solver to find α

2.4.2 Nonlinear Mapping (1/2)

- Project data onto high dimensional space $\phi(x_i)$
  - The hard margin case

$$\min_{\alpha} \frac{1}{2}\alpha^T Q\alpha - e^T\alpha, \text{ subject to } \boxed{\alpha_i \geq 0} \text{ for } i = 1,\cdots,l \text{ and } y^T\alpha = 0$$

$$\text{where } Q \in R^{l\times l}, Q_{ij} = y_i y_j \phi(x_i)^T \phi(x_j), e = [1 \quad \cdots \quad 1]^T \in R^{l\times 1}$$

$$, \alpha = [\alpha_1 \quad \cdots \quad \alpha_l]^T \in R^{l\times 1} \text{ and } y = [y_1 \quad \cdots \quad y_l]^T \in R^{l\times 1}$$

  - The soft margin case

$$\min_{\alpha} \frac{1}{2}\alpha^T Q\alpha - e^T\alpha, \text{ subject to } \boxed{C \geq \alpha_i \geq 0} \text{ for } i = 1,\cdots,l \text{ and } y^T\alpha = 0$$

$$\text{where } Q \in R^{l\times l}, Q_{ij} = y_i y_j \phi(x_i)^T \phi(x_j), e = [1 \quad \cdots \quad 1]^T \in R^{l\times 1}$$

$$, \alpha = [\alpha_1 \quad \cdots \quad \alpha_l]^T \in R^{l\times 1} \text{ and } y = [y_1 \quad \cdots \quad y_l]^T \in R^{l\times 1}$$

2.4.2 Nonlinear Mapping (2/2)

- Kernel Trick
  - Because the dimension of $\phi(\mathrm{x}_i)$ may be infinity, we have problem on calculating the inner product of two points in the high dimensional space.
  - We define $K(x_i,x_j)=\phi(x_i)^T\phi(x_j)$ as kernel function.
  - Use the kernel function (ex: $K(\mathrm{x},\mathrm{y})=\exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right)$), we can get the inner product value directly without computing the mapping $\phi(\mathrm{x}_i)$.
- The decision function would be reformulated:

$$\mathrm{w}^T\phi(\mathrm{x})+b=\sum_{i=1}^{l}\alpha_i \mathrm{y}_i \underline{\phi(\mathrm{x}_i)^T\phi(\mathrm{x})}+b=\sum_{i=1}^{l}\alpha_i \mathrm{y}_i \underline{K(\mathrm{x}_i,\mathrm{x})}+b$$

3. Training Linear and Nonlinear SVMs

- Training Nonlinear SVMs Technique
  - Save storage
  - Speedup
    1) Caching
    2) Shrinking

- Training Linear SVMs Technique
  - Decomposition
  - Approximation

3.1 Training Nonlinear SVM

- Training Nonlinear SVM
  - The dual

$$\min_{\alpha} \quad \frac{1}{2}\alpha^T Q\alpha - e^T\alpha$$

subject to $0 \le \alpha_i \le C,\ i = 1,\ldots,l,\ y^T\alpha = 0$

where $Q_{ij} = y_i y_j \phi(x_i)^T \phi(x_j)$ and $e = [1,\ldots,1]^T$

  - $Q_{ij} \neq 0$, Q: an *l* by *l* symmetric and fully dense matrix.

    In practice, 30,000 training data: 30,000 variables

    $\Rightarrow$ size(Q) = $30{,}000^2 * 8/2$ = 3GB, cause storage problem!
  - Traditional methods such as Newton and Quasi-Newton are hard to be applied.

3.1 Training Nonlinear SVM: Decomposition Method

- Decomposition Method
  - B: selected working set, N: the remaining set
  - B^k: B in k-th iteration
  - Sub-problem in each iteration

$$\min_{\alpha_B} \frac{1}{2}\begin{bmatrix}\alpha_B^T & (\alpha_N^k)^T\end{bmatrix}\begin{bmatrix}Q_{BB} & Q_{BN} \\ Q_{NB} & Q_{NN}\end{bmatrix}\begin{bmatrix}\alpha_B \\ \alpha_N^k\end{bmatrix}$$

$$-\begin{bmatrix}\mathbf{e}_B^T & (\mathbf{e}_N^k)^T\end{bmatrix}\begin{bmatrix}\alpha_B \\ \alpha_N^k\end{bmatrix}$$

subject to $0 \le \alpha_t \le C, \ \ t \in B, \ \ y_B^T\alpha_B = -y_N^T\alpha_N^k$

where α_B is the only variable related to **B.**

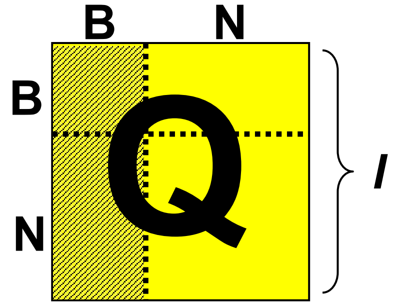
3.1.1 Avoid Storage Problem (1/3)

- Avoid Storage Problem
  - Consider min only with respect to α_B

    $\Rightarrow$ Remove several terms related to α_N
  - The new objective function

$$\frac{1}{2}\alpha_B^T Q_{BB}\alpha_B + (-e_B + Q_{BN}\alpha_N^k)^T \alpha_B + \text{const}$$

    the part out of working set is regarded as constant.



  - To avoid the storage problem, *B* columns of *Q* are stored only when needed

3.1.1 Avoid Storage Problem (2/3)

- How Does It Work?
  - It converges slowly compared to some optimization methods, e.g. Newton and Quasi-Newton.
  - The decision function

$$\operatorname{sgn}\left(\sum_{i=1}^{l} \alpha_i y_i K(x_i, x) + b\right)$$

  - It is no need to obtain accurate α

    $\Rightarrow$ It is also no need to apply many iterations.
  - If #support vectors << #training data, training will be fast.
  - α is usually initialized to be 0.

3.1.1 Avoid Storage Problem (3/3)

- Example
  - An example of training 50,000 data using LIBSVM on a Pentium M 1.4G laptop.
  - Converge in 5m1.456s, while calculating Q may have taken more than 5 minutes.
  - #SVs = 3,370 << 50,000 = #training data
  - We can observe that it is a good case where many remain zero all the time.

3.1.2 Speedup Decomposition (1/3)

- Speedup Decomposition
  - Caching [Joachims, 1998]

    Store recently used kernel columns as the real computer cache.

  - Ex. (in LIBSVM)

    100K cache: 11.463s

    40M cache: 7.817s
  - Note that SVM is a quadratic optimization problem, so the size of cache is not proportional to the converging time.

3.1.2 Speedup Decomposition (2/3)

- Speedup Decomposition
  - Shrinking [Joachims, 1998]

    Some bounded elements do not change anymore until the end. Thus we can heuristically resize it to a smaller problem by removing these elements.
  - After certain iterations, most bounded elements are identified and do not change anymore. [Lin, 2002]

- Caching and shrinking are useful.

3.1.2 Speedup Decomposition (3/3)

- Caching: Issues
  - Goal: minimize the total number of calculating columns among *k* iterations
  - A simple way:

    Store recently used columns
  - A better usage of cache:

    Deliberately select those in cache
  - Idea: The columns in cache have been calculated, so it is no need to spend more effort to calculate new kernel columns.

3.2 Training Linear SVMs

- Training Linear SVMs
  - Linear kernel:

$$\min_{\mathbf{w},b,\zeta} \frac{1}{2}\mathbf{w}^{T}\mathbf{w} + C\sum_{i=1}^{l}\zeta_i$$

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

  - An optimum

$$\zeta_i = \max(0, 1 - y_i(\mathbf{w}^{T}\mathbf{x}_i + b))$$

3.2 Training Linear SVMs

- Training Linear SVMs
  - Remaining variable: **w**, *b*

$$\min_{\mathbf{w},b} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{l}\max(0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b))$$

  - The maximum term is not differentiable
  - #variables = #features + 1
  - Traditional optimization methods can be applied.
  - Although data set is large, if #features is small, it is easier to solve.
  - It is challenging if #features and #data is large.

3.2.1 Decomposition Methods for SVMs

- Decomposition Methods
  - Upper bounded components are related to training errors.
  - When C is large enough, **w** does not change anymore. [Keerthi and Lin, 2003]
  - Recall $\mathbf{w} = \sum_{i=1}^{l} \alpha_i y_i \mathbf{x}_i \in R^n, \quad b \in R^1$

    $$\#(0 < \alpha_i < C) \le n + 1$$
  - Starting from small C, faster convergence [Kao et al., 2004]
  - Using C = 1, 2, 4, 8, ...

3.2.2 Approximations (1/2)

- Approximations
  - Solving the dual is difficult when #data is large and using nonlinear kernels.
  - A simple and effective way: subsampling (e.g. k-NN or hierarchical settings)
  - Incremental way:

    Randomly separate data into 10 parts

    Train 1^{st} part $\Rightarrow SV^1$, then train ($SV^1 + 2^{nd}$ part), ... until 10 parts are trained
  - Select good points, i.e. remove some unnecessary points first: k-NN
  - Goal: process smaller data set at the same time

3.2.2 Approximations (2/2)

- How to select B?
  - Random [Lee and Mangasarian, 2001]
  - Incremental [Keerthi et al., 2006]: starting from a small subset then add points to it in each iteration
- In machine learning, it is very often to balance between simplification and performance

4. Conclusion

- Conclusion
  - SVM could find a hyperplane which separate the different classes of data.
  - In the nonlinearly separable case, we can use the soft margin and/or nonlinear mapping to solve this problem.
  - Using the kernel trick, we can avoid the complex computation in high dimensional space.

- More Problem
  - How about multiclasses?

5. Reference (1/3)

- Chistianini and Shawe-Taylor, 2000
- Scholkopf and Smola, 2002
- www.csie.ntu.edu.tw/~cjlin/ (or lecture of Lin's talk in MLSS2006 pp.4-17)
- www.kernel-machines.org/phpbb/
- svm.cs.rhul.ac.uk/pagesnew/GPat.shtml

5. Reference (2/3)

- Lecture of Lin's talk in MLSS2006 pp.19-25
- Lecture of C. Guestrin, Machine Learning of CMU

5. Reference (3/3)

- Lecture of Lin's talk in MLSS2006 pp.28-48
- SVM Applet
  www.site.uottawa.ca/%7Egcaron/applets.htm