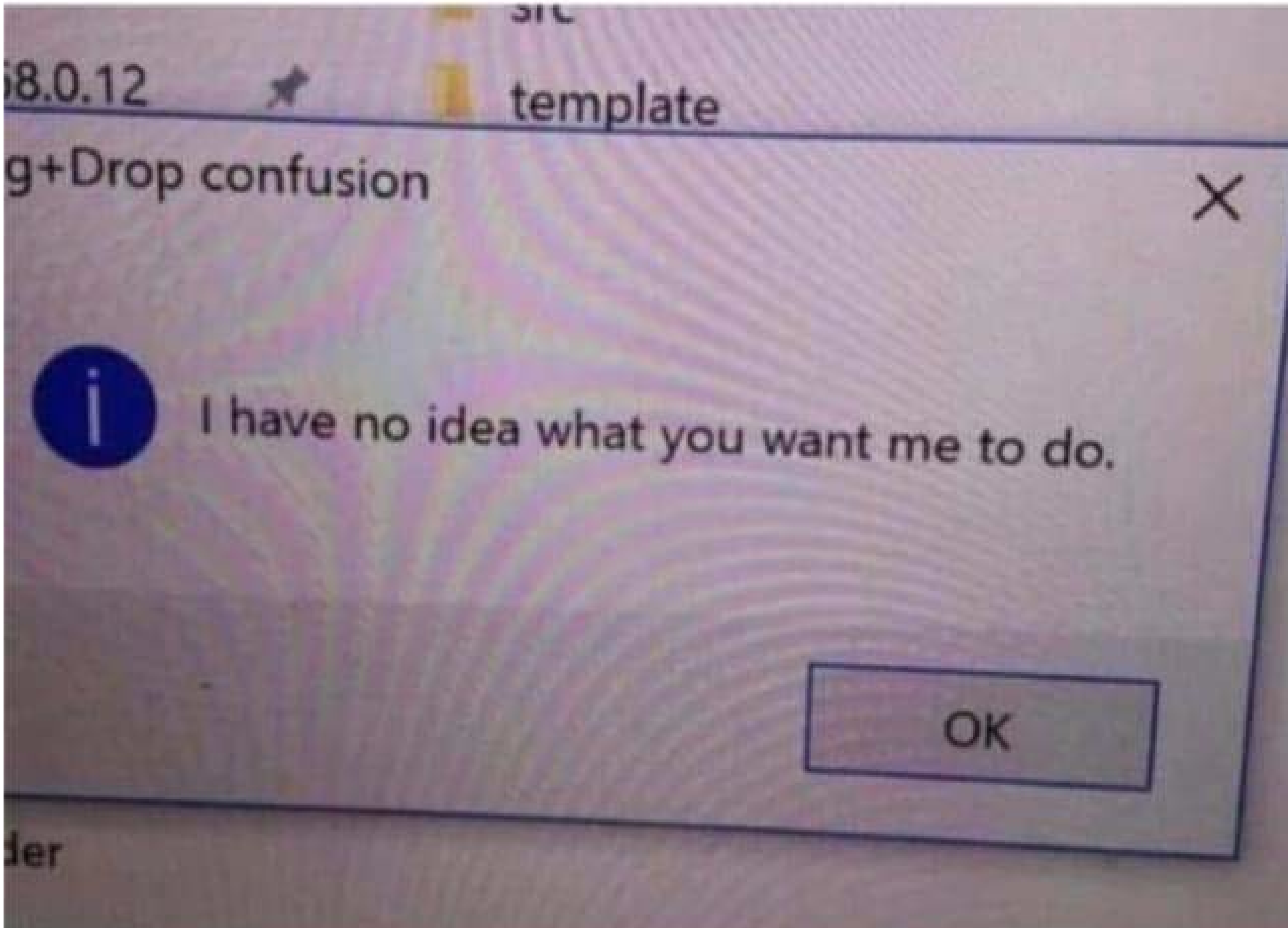
Kernel SVM

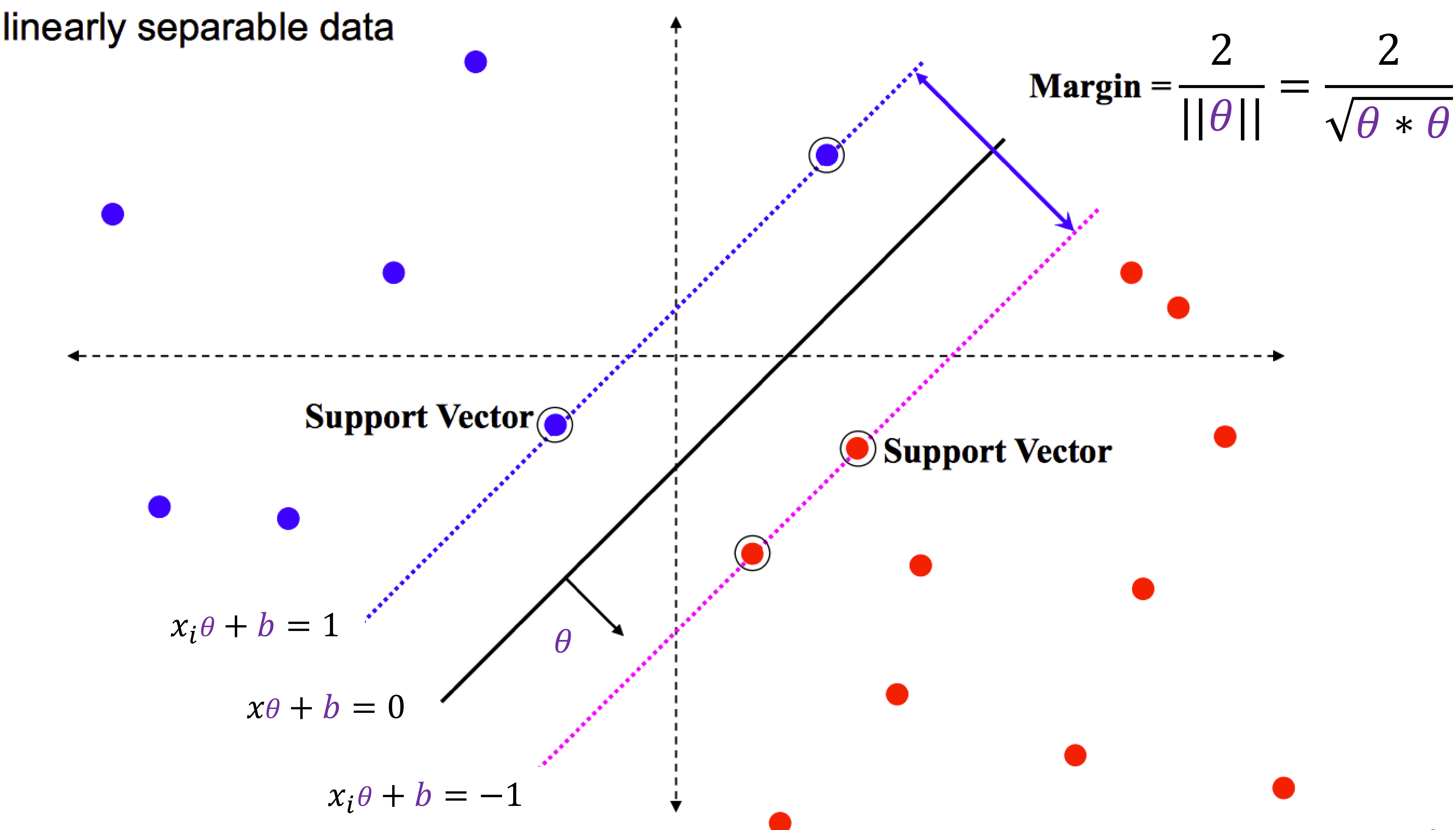
Mahdi Roozbahani
Georgia Tech

These slides are inspired based on slides from Yaser Mostafa, Le Song and Eric Eaton.

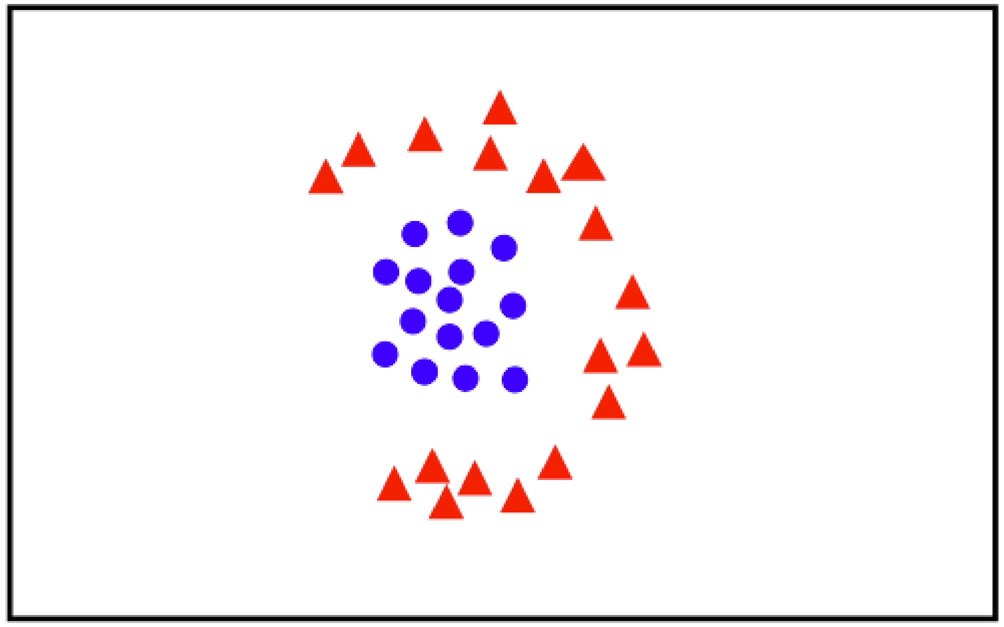
When you get angry at the computer because your code doesn't work



Geometric Interpretation



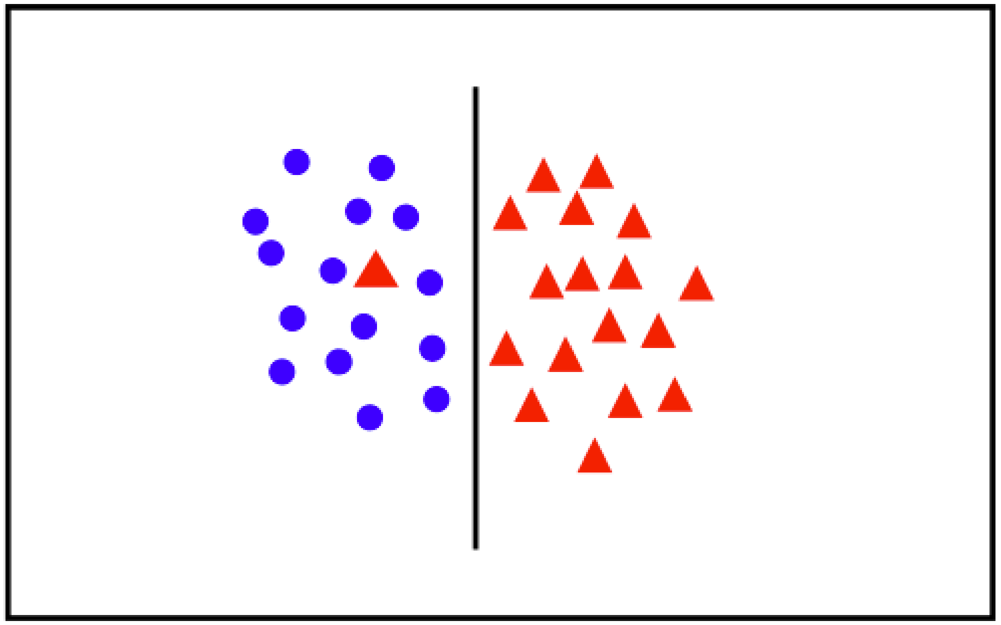
Handling Data that are Not Linearly Separable



- linear classifier not appropriate

??

Kernel trick

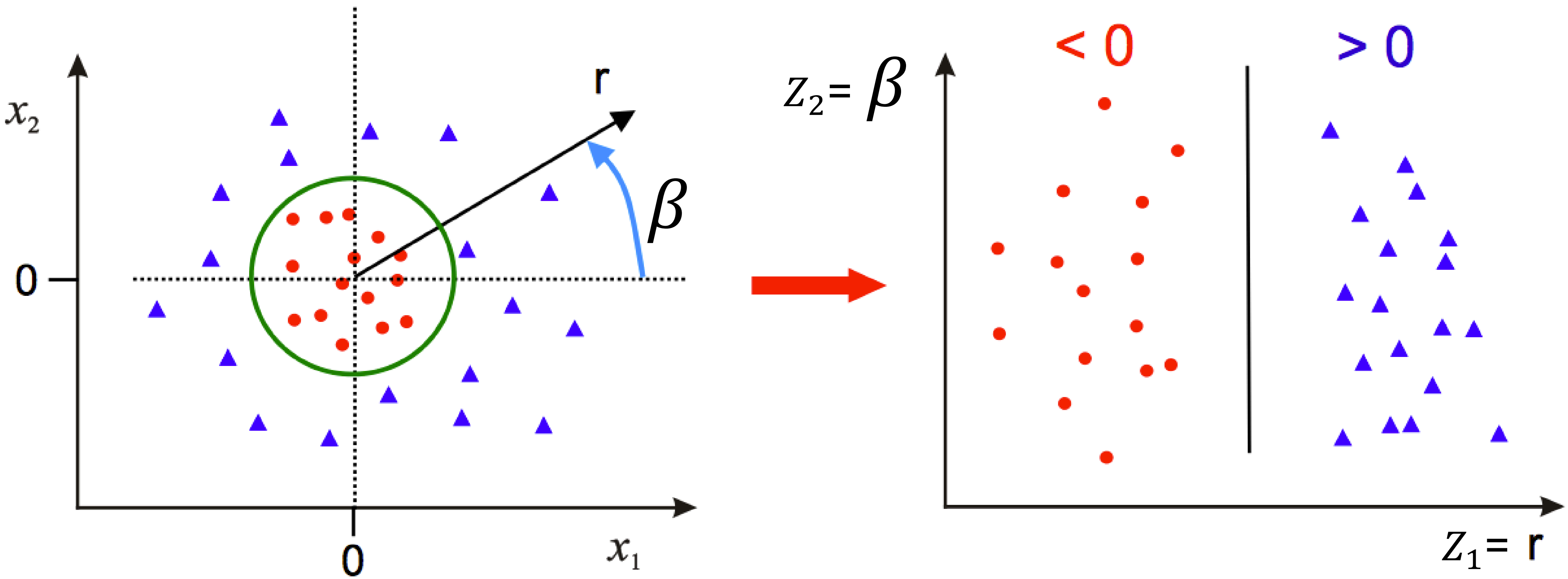


- introduce slack variables

Soft Margin SVM

(allowing ourselves to make errors)

Idea 1: Use Polar Coordinates to go to z space

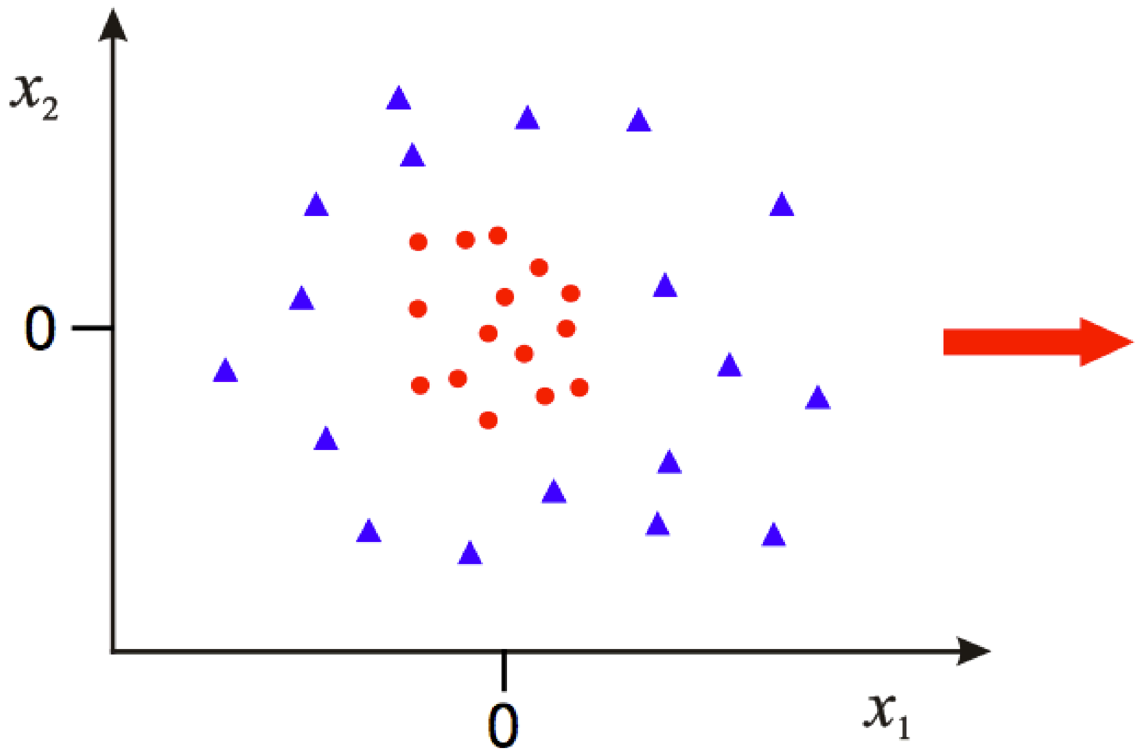


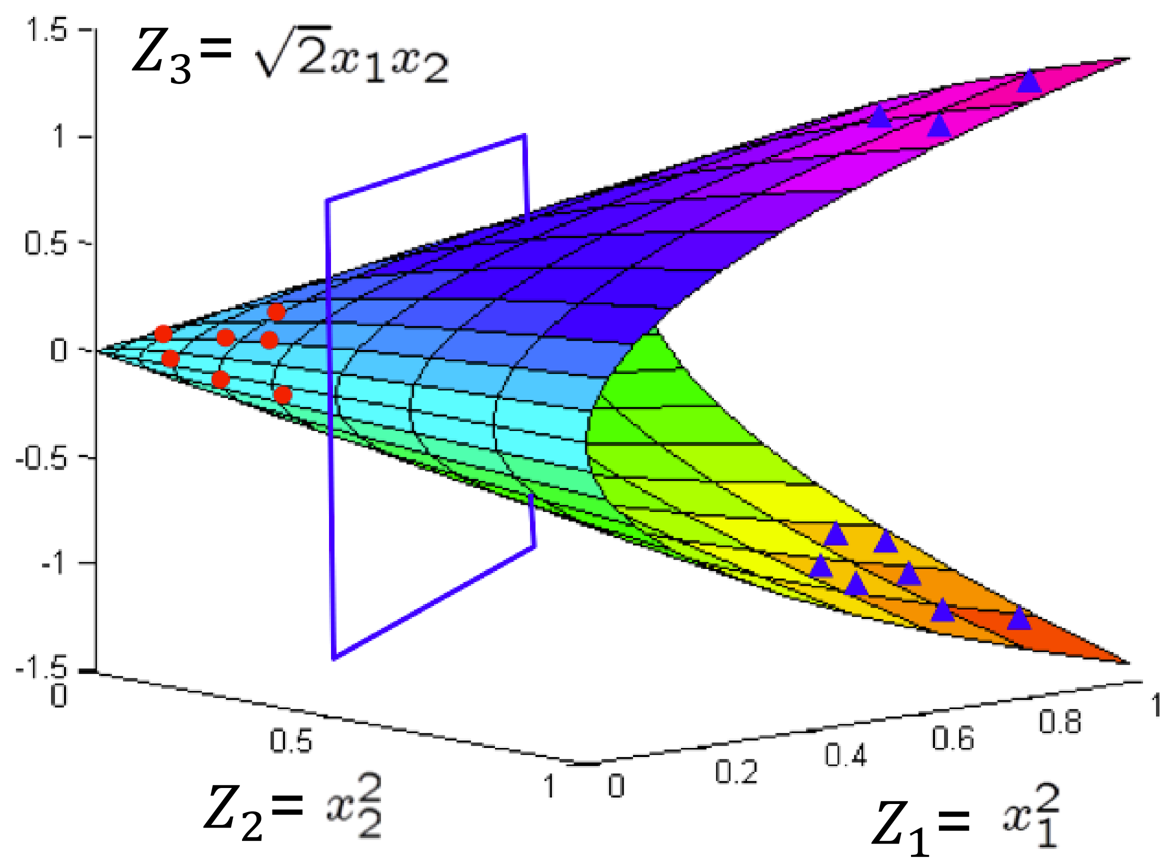
- Data is linearly separable in polar coordinates
- Acts non-linearly in original space

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} r \\ \beta \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^2$$

Idea 1: Map Data to Higher Dimension $\mathbb{Z}$ space

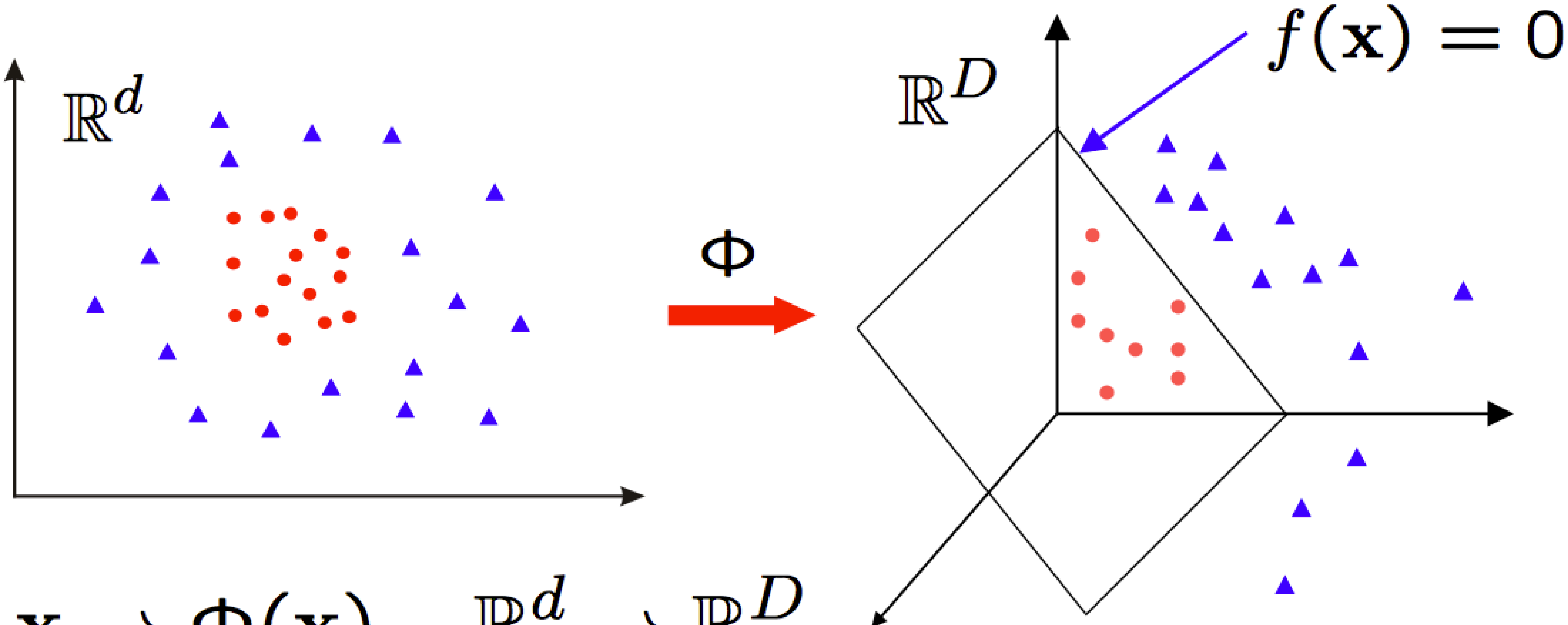
$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$





- Data is linearly separable in 3D
- This means that the problem can still be solved by a linear classifier

SVM in a Transformed Feature Space



$\Phi : \mathbf{x} \to \Phi(\mathbf{x}) \quad \mathbb{R}^d \to \mathbb{R}^D$

Learn classifier linear in $\mathbf{w}$ for $\mathbb{R}^D$:

$$f(x) = \phi(x)\theta + \theta_0 = z\theta + \theta_0$$

$\Phi(\mathbf{x})$ is a feature map

Kernel trick – what do we need from $\mathbb{Z}$ space

$$l(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j z_i z_j^T$$

Inner products

Constraints: $\alpha_i \geq 0$ for $i = 1, \ldots, N$ and $\sum_{i=1}^{N} \alpha_i y_i = 0$

1xD D×1

We already have this:

$$\begin{bmatrix} y_1 y_1 z_1 z_1^T & y_1 y_2 z_1 z_2^T & \ldots & y_1 y_N z_1 z_1^T \\ y_2 y_1 z_2 z_1^T & y_2 y_2 z_2 z_2^T & \ldots & y_2 y_N z_2 z_N^T \\ \ldots & \ldots & \ldots & \ldots \\ y_N y_1 z_N z_1^T & y_N y_2 z_N z_2^T & \ldots & y_N y_N z_N z_N^T \end{bmatrix}_{N \times N}$$

Same result as hard SVM:

Solve α_i using quadratic programming and predict a test data point z in z space➔

$$sign(z\theta + b) = \sum_{z_i in\ SV} \alpha_i y_i z_i z + b$$

Generalized inner product

$k(x,x) = zz^T$ $\quad$ $k(x,x') = zz'^T$

Given **two points** x and x', we need $z'z^T$

$$\begin{bmatrix} yyK(x,x) & yy'K(x,x') \\ y'yK(x',x) & y'y'K(x',x') \end{bmatrix}$$

$k(x',x) = z'z^T$ $\quad$ $k(x',x') = z'z'^T$

Let $K(x,x') = zz'^T$ **The kernel** inner product of x and x'

Example:

$x = (1, h, w) \rightarrow 2nd - order\ \Phi$

$x' = (1, h', w') \rightarrow 2nd - order\ \Phi$

here $x\ and\ x'$ have two dimensions

$z = \Phi(\boldsymbol{x}) = (1, h, w, h^2, w^2, hw)$

$z' = \Phi(\boldsymbol{x}') = (1, h', w', h'^2, w'^2, h'w')$

How many dimensions z has?

$$\underbrace{K(x,x')}_{1\times 1} = zz'^T = 1 + hh' + ww' + h^2h'^2 + w^2w'^2 + hh'ww'$$

We can also calculate: $K(x,x)$ $\quad K(x',x)$ $\quad K(x',x')$

The trick

Can we compute $K(x, x')$ **without** transforming x and x'?

Example:

Datapoint 1 in x space $x = (1, h, w)$

Datapoint 2 in x space $x' = (1, h', w')$

Datapoint 1 and 2 have 2 dimensions in x space and 1 is for the biased term

Datapoint 1 in z space $\phi(x) = z = (1, h^2, w^2, \sqrt{2}h, \sqrt{2}w, \sqrt{2}hw)$

Datapoint 2 in z space $\phi(x') = z' = (1, {h'}^2, {w'}^2, \sqrt{2}h', \sqrt{2}w', \sqrt{2}h'w')$

Datapoint 1 and 2 have 5 dimensions in z space and 1 is for the biased term

We need to calculate the dot product for the kernel

$$K(x, x') = \phi(x)\ \phi(x')^T = zz'^{\mathrm{T}}$$

$z = (1, h^2, w^2, \sqrt{2}h, \sqrt{2}w, \sqrt{2}hw)$ $\quad\quad$ $z' = (1, {h'}^2, {w'}^2, \sqrt{2}h', \sqrt{2}w', \sqrt{2}h'w')$

$$zz'^T = K(x, x') = 1 + h^2h'^2 + w^2w'^2 + 2hh' + 2ww' + 2hh'ww'$$

$$K(x, x') = (1 + hh' + ww')^2$$

$$x = (1, h, w) \qquad x' = (1, h, w)$$

$zz'^T = K(x, x') = (xx'^T)^2$ Homogeneous kernel

Example: Let's say we have two datapoints

We need the build the inner product matrix to optimize SVM parameters.

$$l(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j z_i z_j^T = \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j K(x_i, x_j)$$

$$X = \begin{array}{cc} \text{weight} & \text{Height} \\ \end{array}$$

$$X = \begin{bmatrix} 1 & 2 \\ -1 & 3 \end{bmatrix} \quad Y = \begin{bmatrix} cat \\ dog \end{bmatrix}$$

$$K(x_i, x_j) = \begin{bmatrix} yyK(x,x) & yy'\boxed{K(x,x')} \\ y'yK(x',x) & y'y'K(x',x') \end{bmatrix}$$

$$Z = \begin{array}{c} \\ \\ \end{array}\begin{array}{ccccc} \sqrt{2}w & \sqrt{2}h & \sqrt{2}hw & h^2 & w^2 \end{array}$$

$$Z = \begin{bmatrix} \sqrt{2} & 2\sqrt{2} & 2\sqrt{2} & 4 & 1 \\ -\sqrt{2} & 3\sqrt{2} & -3\sqrt{2} & 9 & 1 \end{bmatrix} \begin{array}{l} z \\ z' \end{array}$$

$$k(x, x') = z z'^T =$$

$$\begin{bmatrix} \sqrt{2} & 2\sqrt{2} & 2\sqrt{2} & 4 & 1 \end{bmatrix} \begin{bmatrix} -\sqrt{2} \\ 3\sqrt{2} \\ -3\sqrt{2} \\ 9 \\ 1 \end{bmatrix} = 8 \checkmark$$

$$(xx')^2 = \left(\begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} -1 \\ 3 \end{bmatrix} \right)^2$$

The polynomial kernel

$\mathcal{X} = \mathcal{R}^{d}$ and Φ: $\mathcal{X} \rightarrow \mathbb{Z}$ is polynomial of order Q

The "equivalent kernel $= K(x, x') = (1 + x^T x')^Q$ Inhomogeneous kernel

$$= (1 + x_1 x_1' + x_2 x_2' + \cdots + x_d x_d')^Q$$

Does it matter if Q is 2 or 1000?

What will happen if we have $d = 10$ and $Q = 100$ and we want to compute the inner product explicitly?

We need to calculate the inner product of two big huge ugly vectors

We only need $\mathbb{Z}$ space to exist

if $K(x, x')$ is an inner product in some space $\mathbb{Z}$, we are doing good

Example:

$$K(x, x') = \exp(-\gamma \|x - x'\|^2)$$ Radial basis kernel

First thing first, this is a function of $x \text{ and } x'$

This function will take us to infinite-dimensional $\mathbb{Z}$ → CONGRATULATIONS

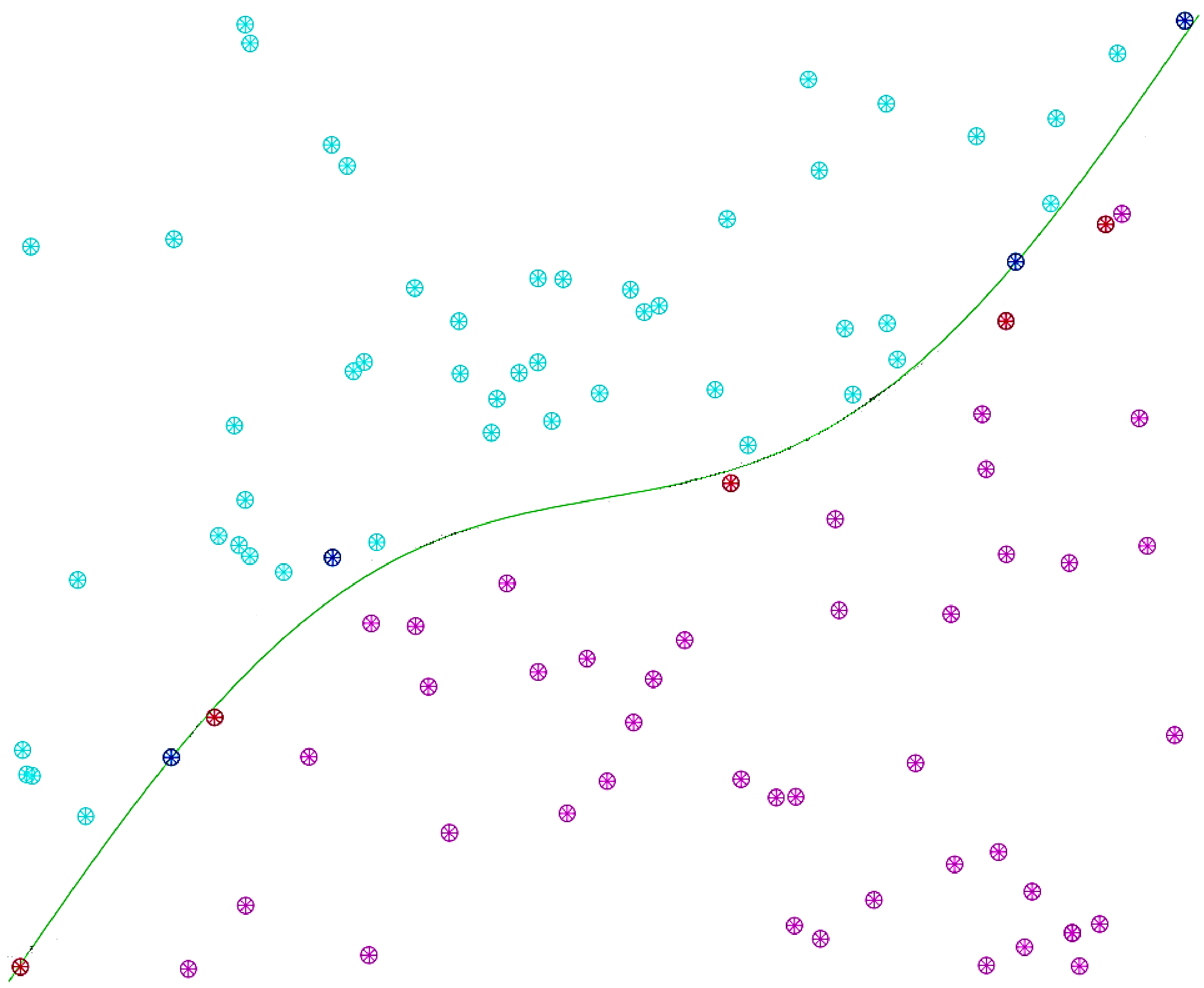
For d and $\gamma = 1 \Rightarrow \quad K(x, x') = \exp(-(x - x')^2)$

$$= \exp(-x^2)\exp(-x'^2) \underbrace{\sum_{k=0}^{\infty} \frac{2^k x^k x'^k}{k!}}$$

exp Taylor expansion for $\exp(2xx')$

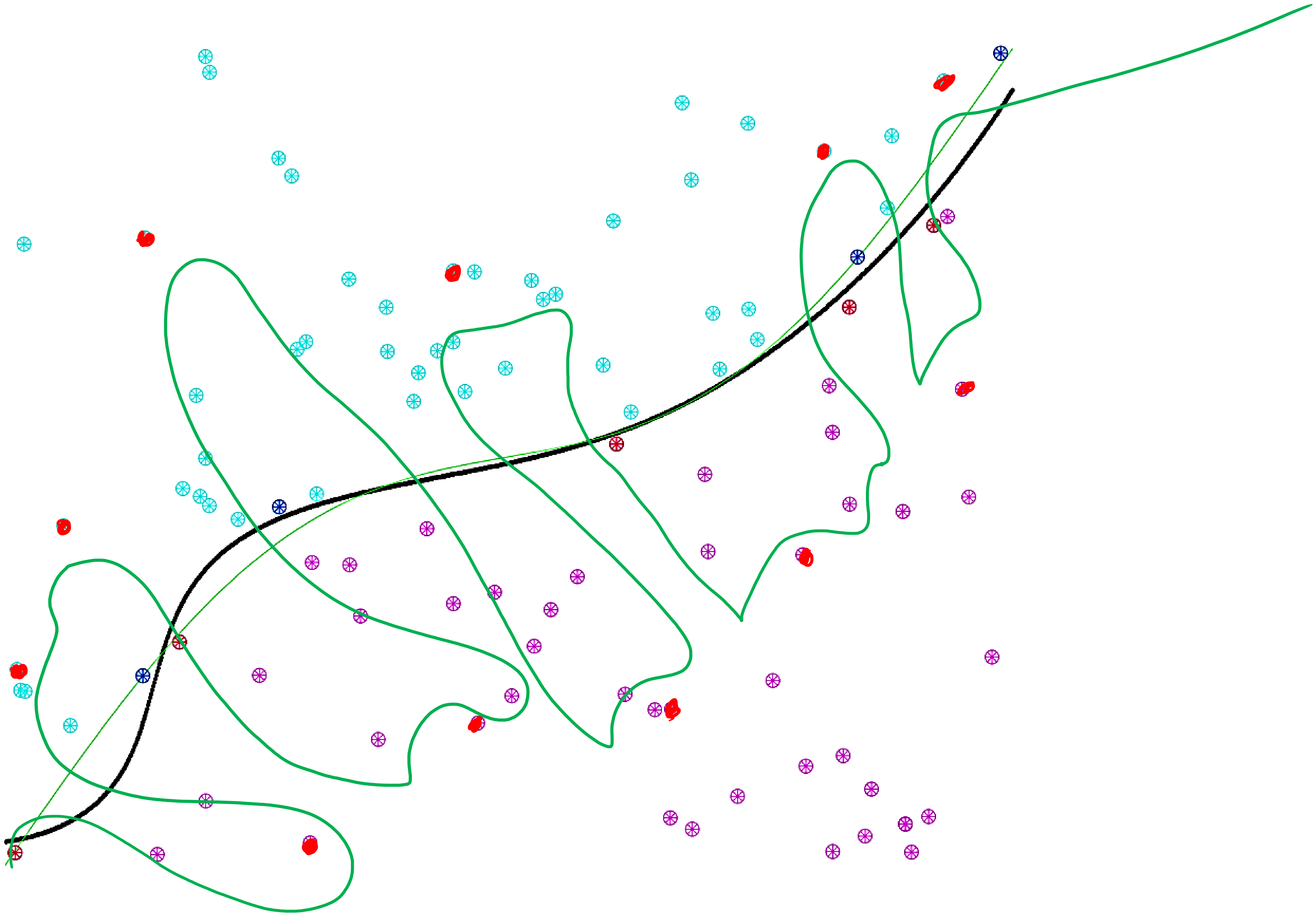
Radial basis kernel in action

Slightly non-linearly separable case for 100 datapoints:



Transforming χ

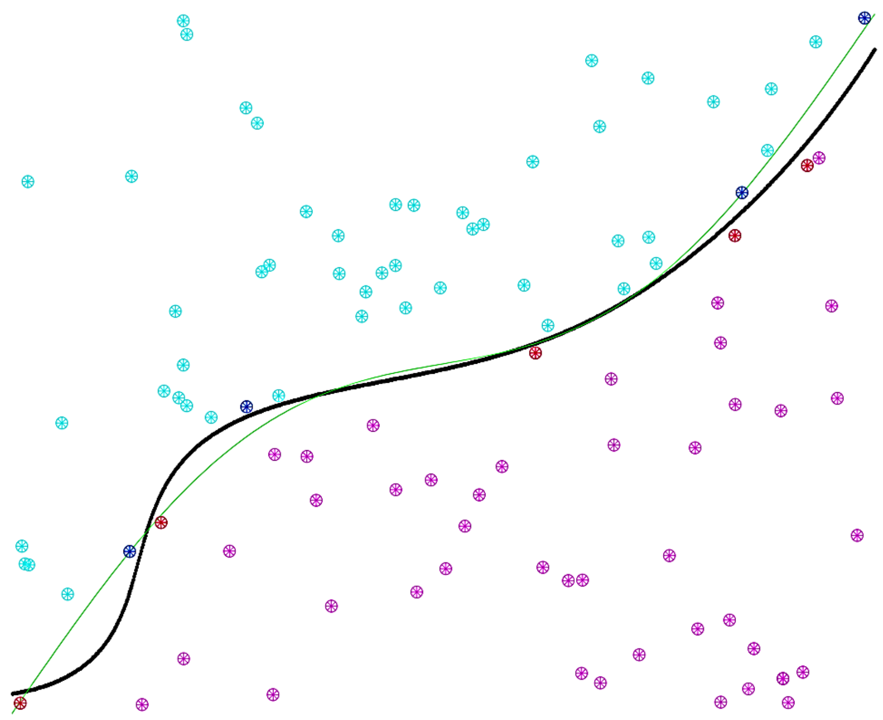
into ∞-dimensional $\mathbb{Z}$ space



Generalization

Are we killing the generalization by going to infinite-dimension? (overfitting)

I am going to answer this with a question. In this, example how many support vectors, we have?



What will happen if we have many support vectors?

The decision boundary line (plane) will be super wiggly ➔ overfitting alarm

$$\mathrm{E}[E_{out}] \leq \frac{\mathrm{E}[Number\ of\ support\ vectors]}{N-1}$$

N is number of datapoints

Kernel formulation of SVM

Remember quadratic programming?

$$\underbrace{\begin{bmatrix} y_1y_1x_1x_1^T & y_1y_2x_1x_2^T & \cdots & y_1y_Nx_1x_1^T \\ y_2y_1x_2x_1^T & y_2y_2x_2x_2^T & \cdots & y_2y_Nx_2x_N^T \\ \cdots & \cdots & \cdots & \cdots \\ y_Ny_1x_Nx_1^T & y_Ny_2x_Nx_2^T & \cdots & y_Ny_Nx_Nx_N^T \end{bmatrix}}_{\text{Quadratic coefficients}}$$

In $\mathbb{Z}$ space, the only thing you need:

$$\begin{bmatrix} y_1y_1K(x_1, x_1) & y_1y_2K(x_1, x_2) & \cdots & y_1y_NK(x_1, x_N) \\ y_2y_1K(x_2, x_1) & y_2y_2K(x_2, x_2) & \cdots & y_2y_1K(x_2, x_N) \\ \cdots & \cdots & \cdots & \cdots \\ y_Ny_1K(x_N, x_1) & y_Ny_2K(x_N, x_2) & \cdots & y_Ny_NK(x_N, x_N) \end{bmatrix}$$

Final stage:

$$g(x) = sign(z\theta + b)$$

$$in\ terms\ of\ K(-,-)$$

$$where \rightarrow \theta = \sum_{z_i\, in\, SV} \alpha_i y_i z_i \rightarrow$$

$$g(x) = sign(\sum_{z_i\, in\, SV} \alpha_i y_i z_i\, z + b)$$

$$g(x) = sign(\sum_{\alpha_i > 0} \alpha_i y_i K(x_i, x) + b)$$

$and\ b$: $$b = y_j - \sum_{\alpha_i > 0, \alpha_j > 0} \alpha_i y_j K(x_i, x_j)$$

$$for\ any\ SV\ \ x_i\ and\ x_j$$

How do we know that the kernel is valid?

$For\ a\ given\ K(x, x') \rightarrow$ We can check the validity

Three approaches:

1. By construction (Polynomial one)

2. Math properties (Mercer's condition)

3. Who cares? ☺

Design your kernel

$K(x, x')$ is valid iff

1. It is symmetric ➔ $K(x, x')$=$K(x', x)$

2. The matrix ➔ $$\begin{bmatrix} y_1 y_1 K(x_1, x_1) & y_1 y_2 K(x_1, x_2) & \dots & y_1 y_N K(x_1, x_N) \\ y_2 y_1 K(x_2, x_1) & y_2 y_2 K(x_2, x_2) & \dots & y_2 y_N K(x_2, x_N) \\ \dots & \dots & \dots & \dots \\ y_N y_1 K(x_N, x_1) & y_N y_2 K(x_N, x_2) & \dots & y_N y_N K(x_N, x_N) \end{bmatrix}$$

is positive-semi definite

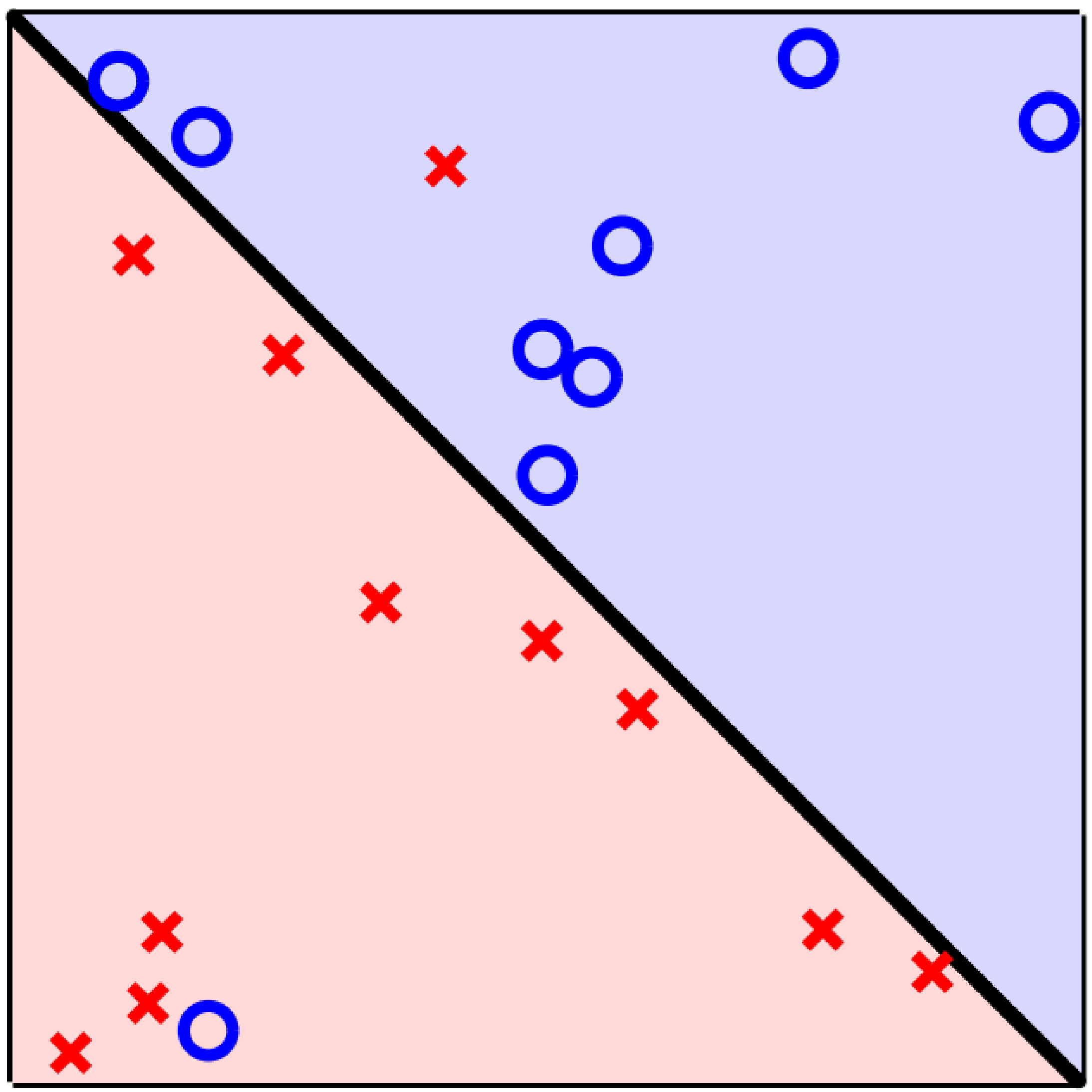
For any $x_1, \dots, x_N$ (Mercer's condition)

Common Kernels

- Linear kernels $k(\mathbf{x}, \mathbf{x}') = xx'^T$
- Polynomial kernels $k(\mathbf{x}, \mathbf{x}') = \left(1 + xx'^T\right)^d$ for any $d > 0$
  - Contains all polynomials terms up to degree d
- Gaussian kernels $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2 / 2\sigma^2\right)$ for $\sigma > 0$
  - Infinite dimensional feature space

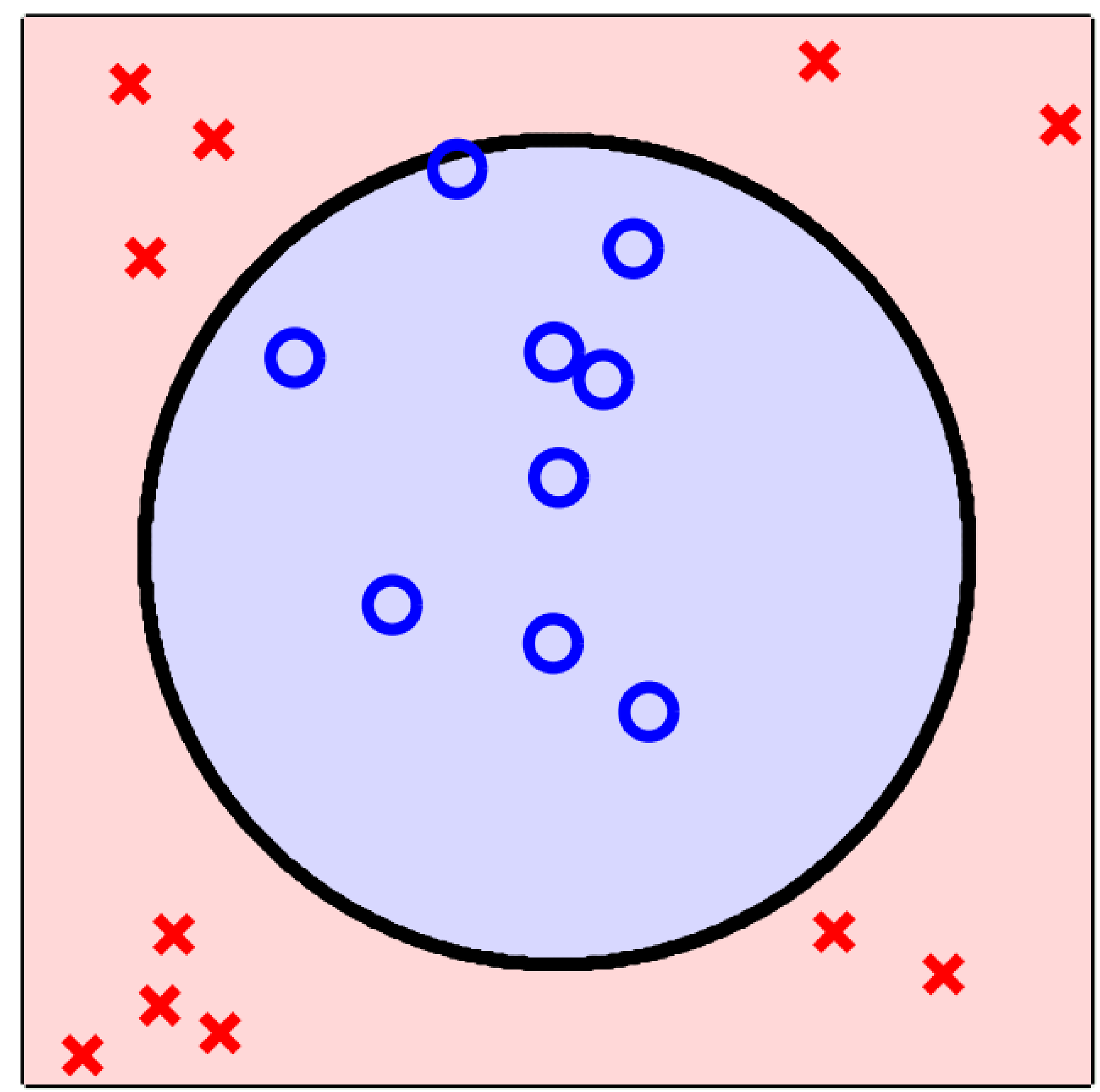
Soft SVM – Two types of non-separable

slightly:



Soft SVM will deal with this

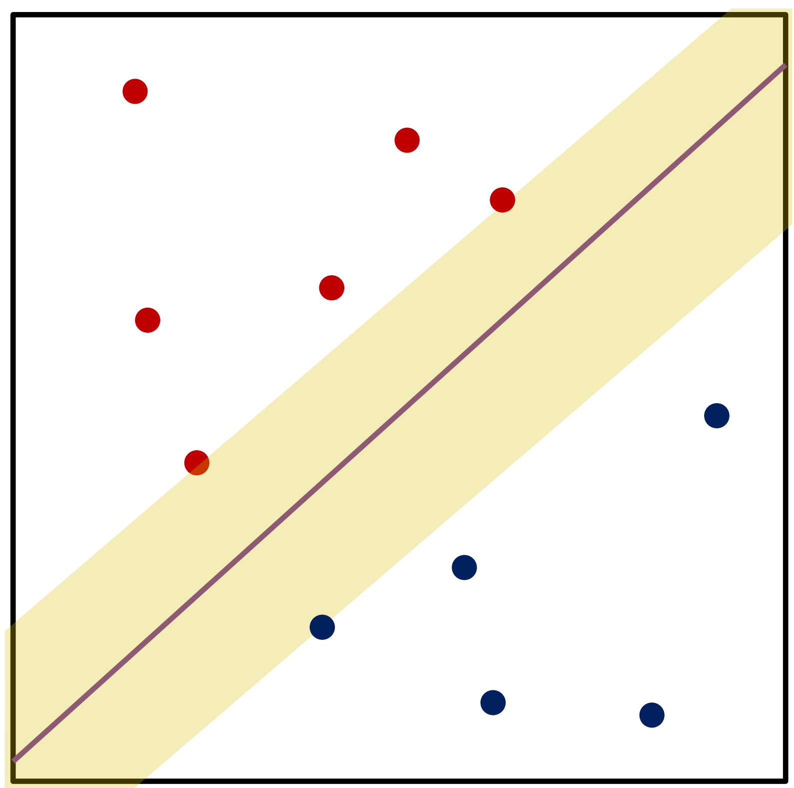
seriously:



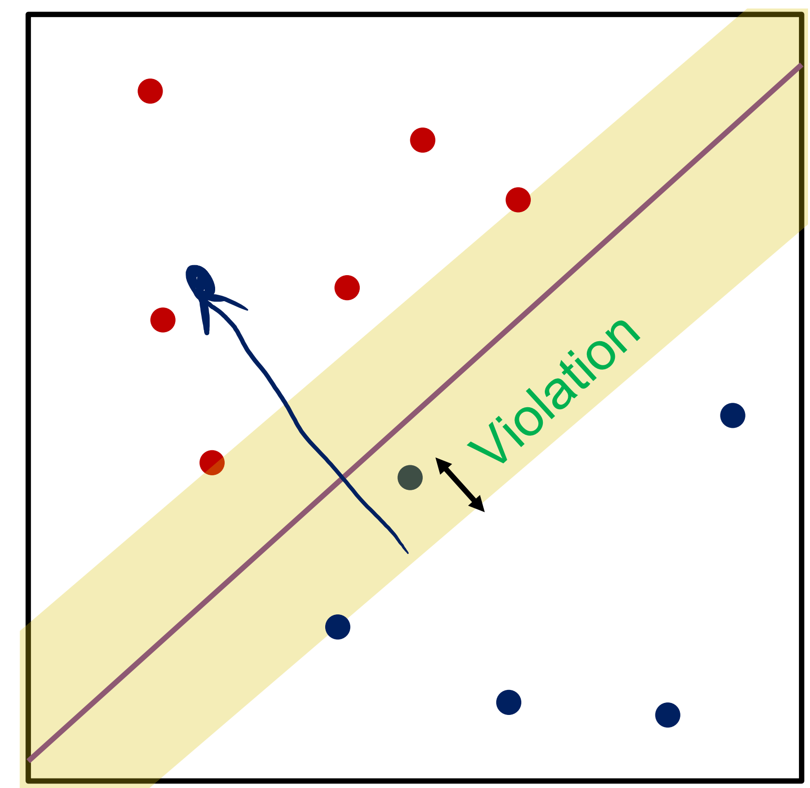
Kernel will deal with this

Error measure

Non-violated case:



Margin violation:



if $\quad y_i(x_i\theta + b) > 1 \Rightarrow \text{Non SV}$

Let's introcduce a slack variable: $\quad y_i(x_i\theta + b) \geq 1 - \xi_i \qquad \xi_i \geq 0$

$$\text{Total violation} = \sum_{i=1}^{N} \xi_i$$

The new optimization

hard SVM

Minimize $\frac{1}{2}\theta\theta^T + C\sum_{i=1}^{N}\xi_i$

C will define the relative importance of the first or second term

$C = inf$ is equal to Hard SVM (will see soon)

$s.t.\quad y_i(x_i\theta + b) \geq 1 - \xi_i$ for $i = 1, \ldots, N$

$and\ \xi_i \geq 0$ for $i = 1, \ldots, N$

$\theta \in \mathbb{R}^d, b \in \mathbb{R}, \xi \in \mathbb{R}^N$

The Lagrange formulation

$f(x)$

s.t $g(x)$

$h(x)$

$L = f(x) - \alpha g(x) - \beta h(x)$

Hard svm: Minimize $\frac{1}{2}\theta\theta^T$ $\quad s.t.\ \ y_i(x_i\theta + b) \geq 1$

$$\mathcal{L}(\theta, b, \alpha) = \frac{1}{2}\theta\theta^T - \sum_{i=1}^{N} \alpha_i(y_i(x_i\theta + b) - 1)$$

Soft svm: Minimize $\frac{1}{2}\theta\theta^T + C\sum_{i=1}^{N} \xi_i$ $\quad s.t.\ \ y_i(x_i\theta + b) \geq 1 - \xi_i$ *and* $\xi_i \geq 0$

$$\mathcal{L}(\theta, b, \xi, \alpha) = \frac{1}{2}\theta\theta^t + C\sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \alpha_i(y_i(x_i\theta + b) - 1 + \xi_i) - \sum_{i=1}^{N} \beta_i\xi_i$$

PLEASE do not scare, terms will be dropping fast

$$\mathcal{L}(\theta, b, \xi, \alpha) = \frac{1}{2}\theta\theta^T + C\sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \alpha_i(y_i(w^T x_i + b) - 1 + \xi_i) - \sum_{i=1}^{N} \beta_i \xi_i$$

Minimize w.r.t $\boldsymbol{\theta}, b, and\ \xi$ $\underbrace{\text{and maximize w.r.t } \alpha_i \geq 0\ and\ \beta_i \geq 0}_{\text{KKT condition for inequality constraints}}$

Let's do the minimization:

$$\nabla_\theta\, \mathcal{L}(\theta, b, \xi, \alpha) = \theta - \sum_{i=1}^{N} \alpha_i y_i x_i = 0$$

$$\nabla_b\, \mathcal{L}(\theta, b, \xi, \alpha) = -\sum_{n=1}^{N} \alpha_i y_i = 0$$

$\beta_i = C - \alpha_i$

$$\nabla_\xi\, \mathcal{L}(\theta, b, \xi, \alpha) = C - \alpha_i - \beta_i = 0$$

If we substitute β_i up there, the whole formulation will get back to hard svm

We should say thank you β_i for the great service

The solution

$\beta_i = C - \alpha_i$

$\beta_i \geqslant 0$ $\quad C - \alpha_i \geqslant 0 \Rightarrow \alpha_i \leqslant C$

$\alpha_i \geqslant 0 \quad 0 \leqslant \alpha_i \leqslant C$

$\beta_i \geq 0$ ➔ $C - \alpha_i \geq 0 \rightarrow 0 \leq \alpha_i \leq C$ for $i = 1, \ldots, N$

$$Maximize \;\; \mathcal{L}(\alpha) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j x_i x_j^T \qquad \text{w.r.t} \quad \alpha$$

$$s.t. \qquad 0 \leq \alpha_i \leq C \quad \text{for } i = 1, \ldots, N \quad \boldsymbol{and} \quad \sum_{i=1}^{N} \alpha_i y_i = 0$$

$\Rightarrow \theta = \sum_{i=1}^{N} \alpha_i y_i x_i$ will minimize $\frac{1}{2}\theta\theta^T + C\sum_{i=1}^{N} \xi_i$

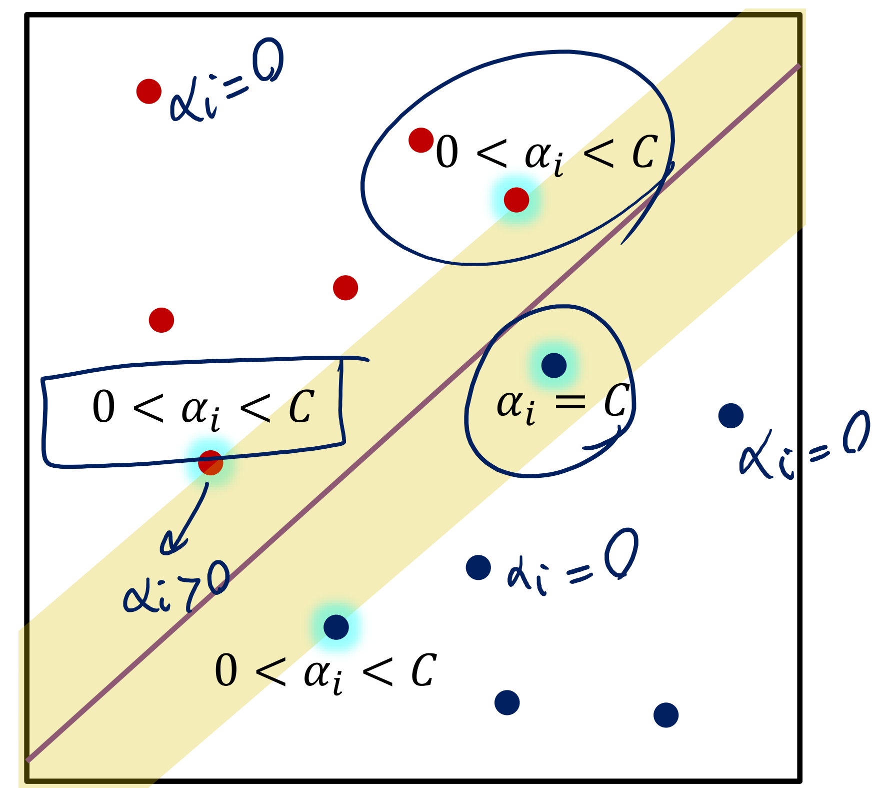
Type of support vectors

We call the three points as **margin** support vectors

$$0 < \alpha_i < C$$

$$\beta_i = C - \alpha_i$$

$y_i(x_i\theta + b) = 1 \Rightarrow \beta_i > 0 \Rightarrow \xi_i = 0$ (KKT condition)



non-margin support vectors ($\alpha_i = C$)

$\beta_i = 0 \Rightarrow \xi_i > 0$ (KKT condition)

$y_i(x_i\theta + b) > 1 - \xi_i$ if $\xi_i > 0$

$$y_i(x_i\theta + b) < 1$$

$$\alpha_i = 0 \Rightarrow y_i(x_i\theta + b) > 1$$

Non SV

$$\alpha_i = C \Rightarrow y_i(x_i\theta + b) < 1$$

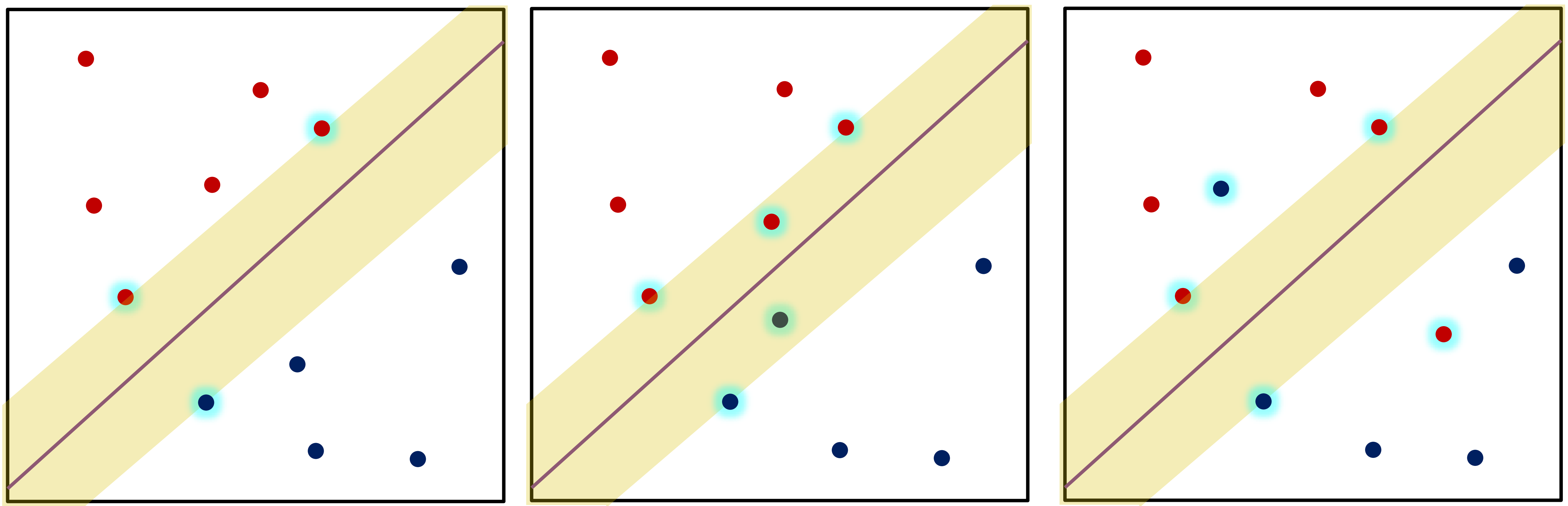
SV on the wrong side

$$0 < \alpha_i < C \Rightarrow y_i(x_i\theta + b) = 1$$

SV on the margin

Any violating points become support vectors

How to choose C?



violating points become
support vectors

How to define the hyper-parameter C: Cross Validation

Primal and Dual Forms of SVM

Primal version of classifier:

$$f(x_{test}) = x_{test}\theta + \theta_0$$

Dual version of classifier:

$$f(x_{test}) = \sum_{x_i \, in \, SV} \alpha_i y_i x_i x_{test}^T + b$$

$k(x, x_{test})$

Soft svm

$\alpha_i > 0$ $0 < \alpha_i < C$

Kernel SVM: Summary

• Classifiers can be learnt for high dimensional features spaces, without actually having to map the points into the high dimensional space

• Data may be linearly separable in the high dimensional space, but not linearly separable in the original feature space

• Kernels can be used for an SVM because of the scalar product in the dual form, but can also be used elsewhere – they are not tied to the SVM formalism