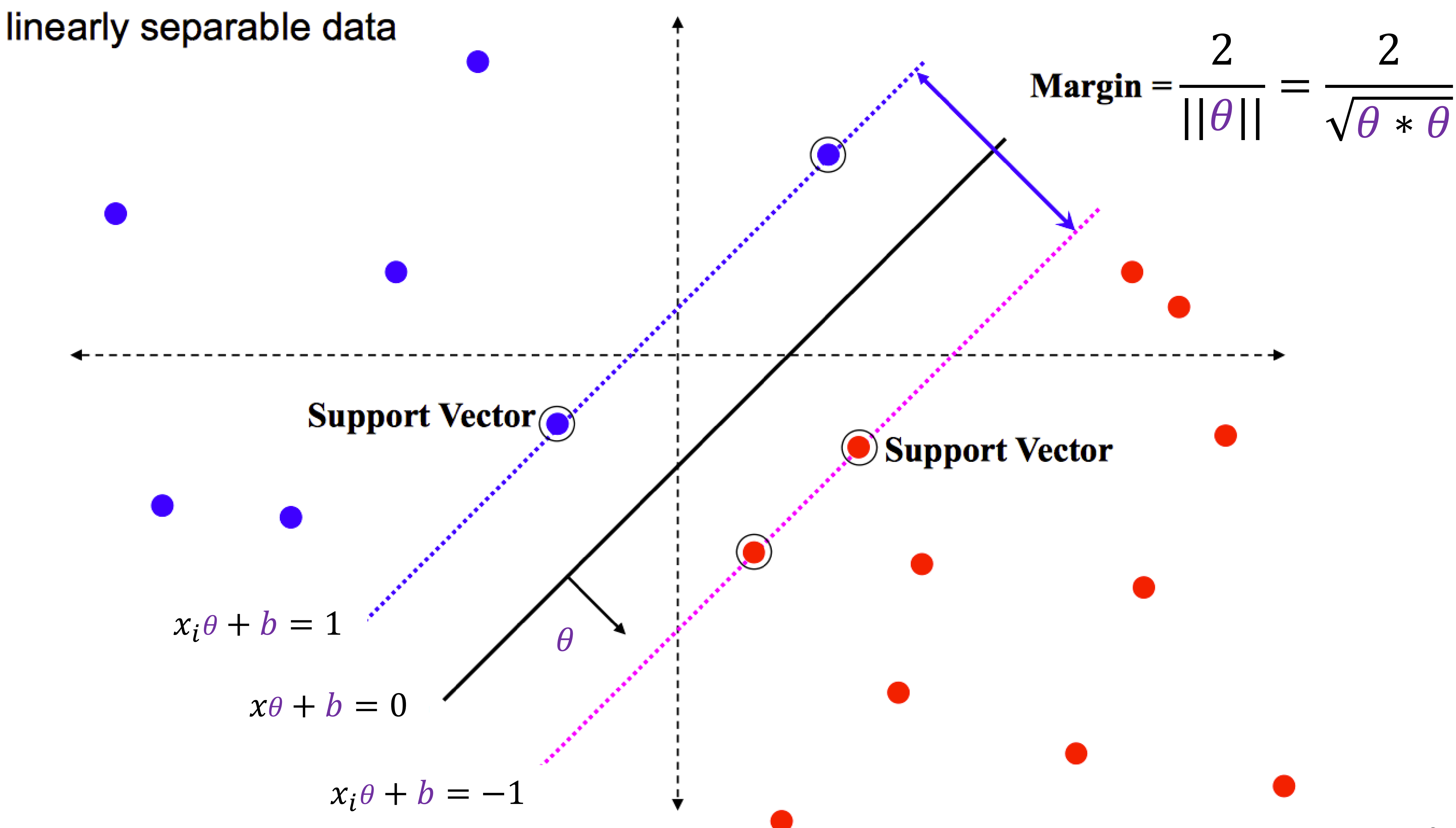
Kernel SVM

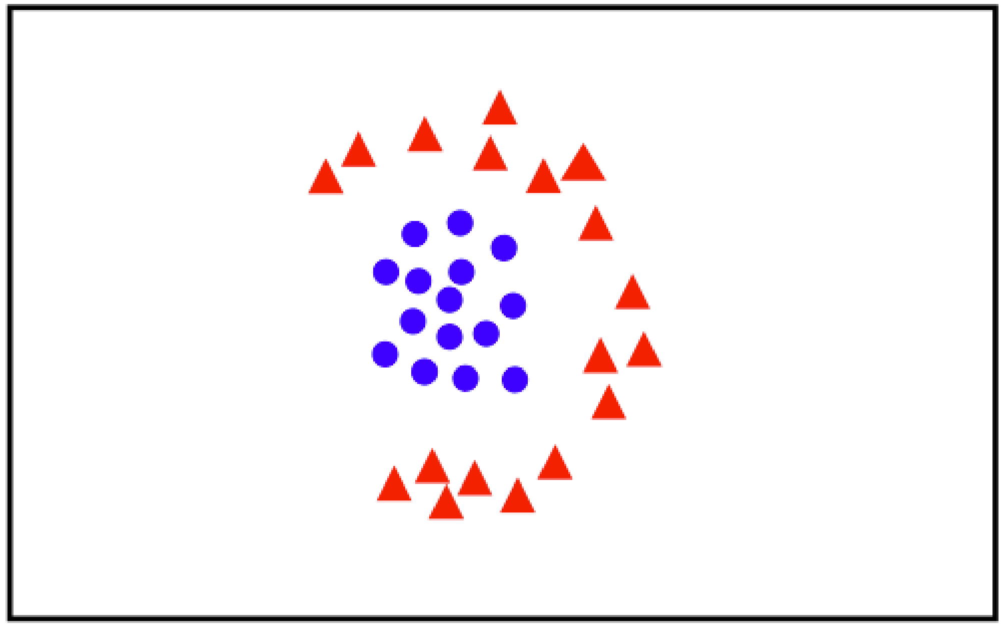
Mahdi Roozbahani
Georgia Tech

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

Geometric Interpretation



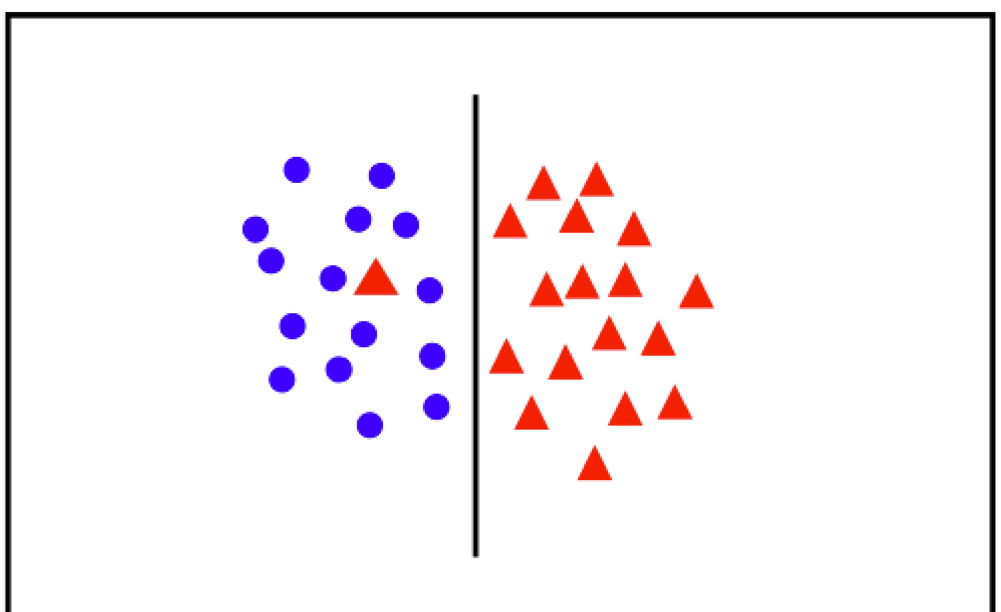
Handling Data that are Not Linearly Separable



- linear classifier not appropriate

??

Kernel trick

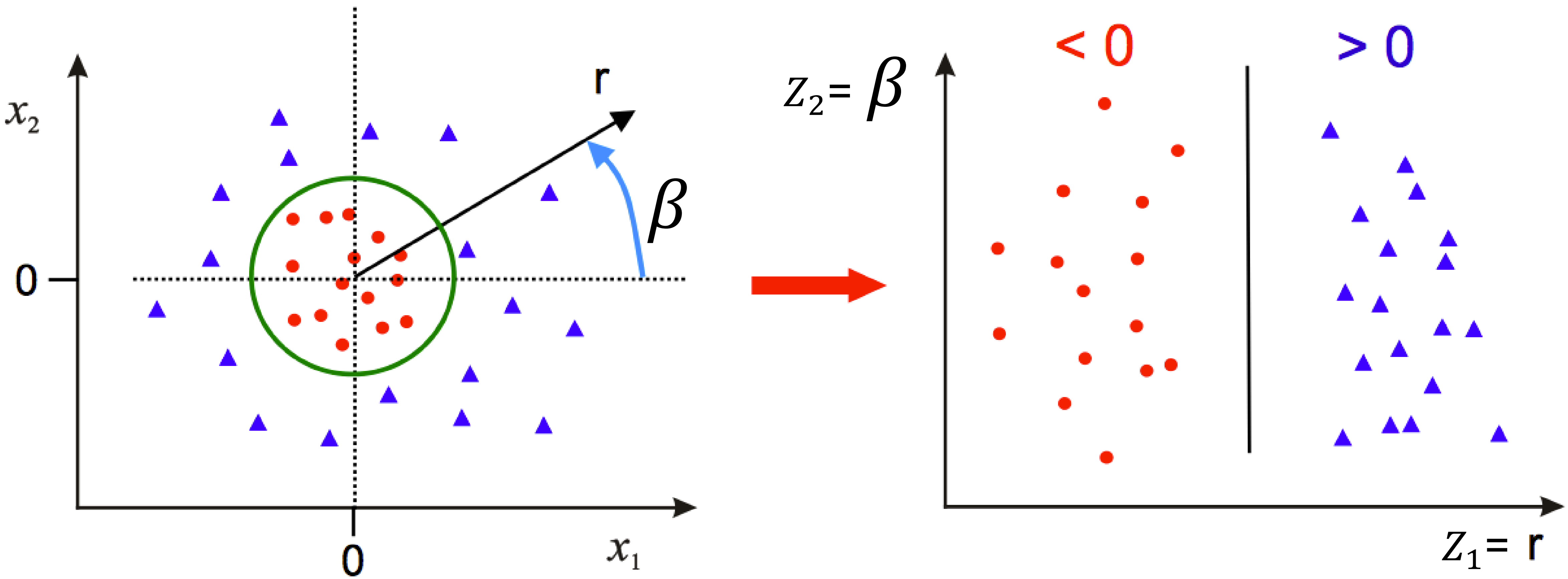


- introduce slack variables

Soft Margin SVM

(allowing ourselves to make errors)

Idea 1: Use Polar Coordinates to go to z space

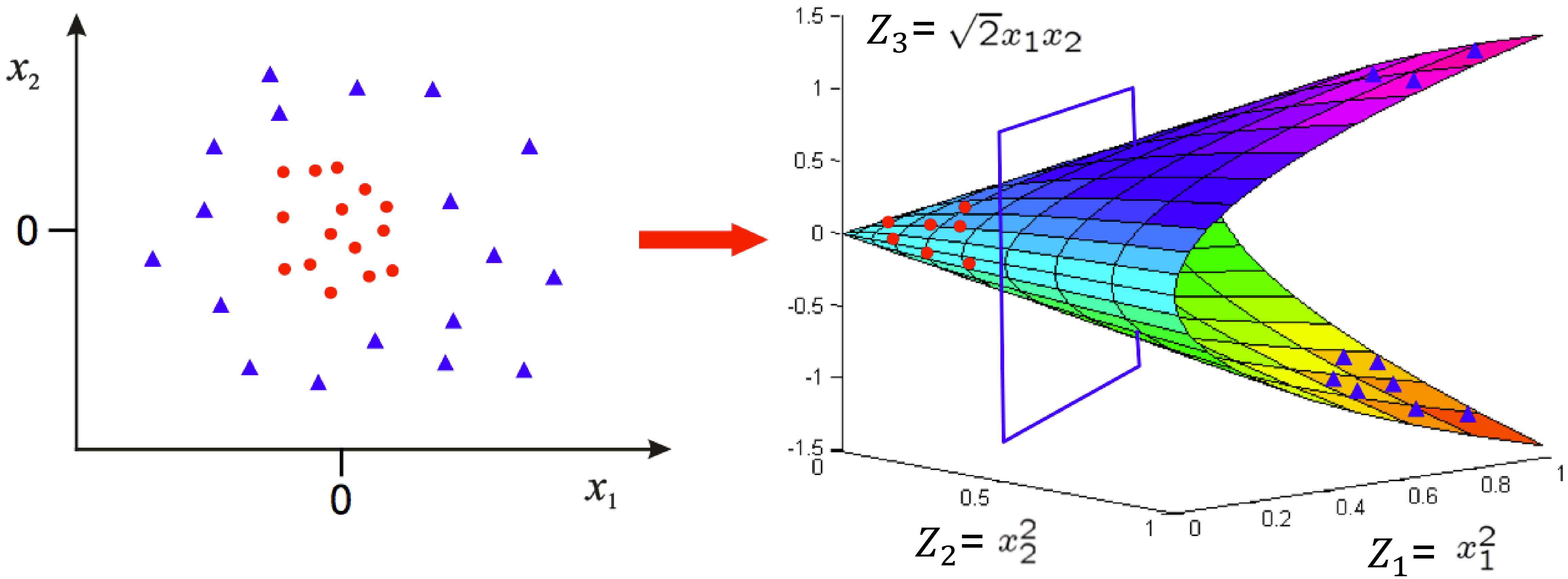


- Data is linearly separable in polar coordinates
- Acts non-linearly in original space

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

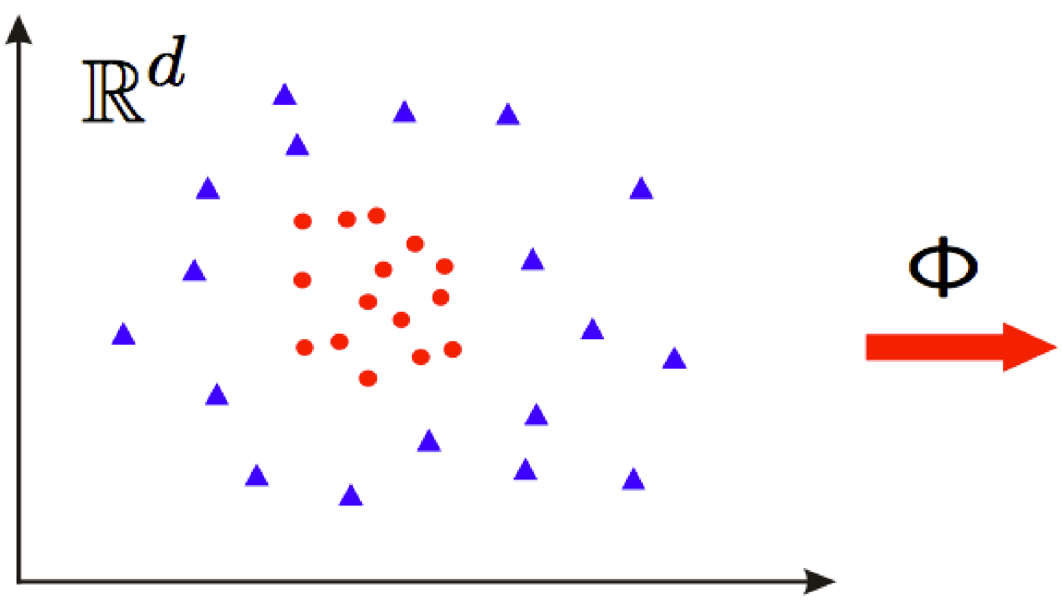
Idea 1: Map Data to Higher Dimension $\mathbb{Z}$ space

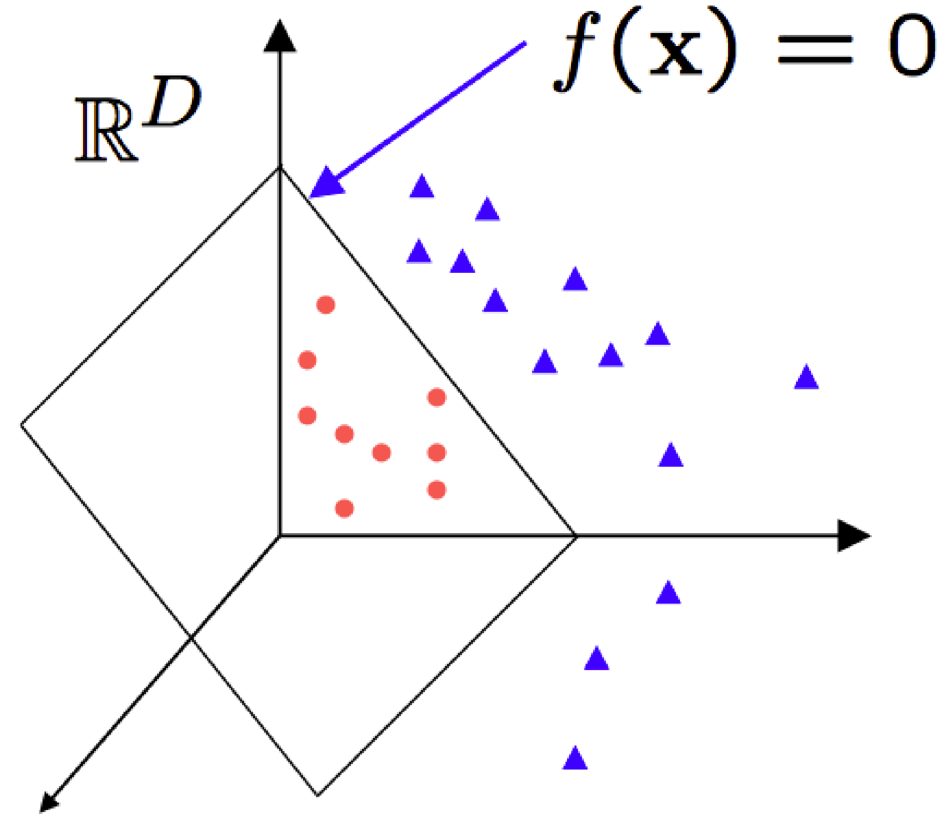
$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$



- 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 $\sum_{i=1}^{N} \alpha_i y_i = 0$

We already have this:
$$\begin{bmatrix} y_1 y_1 z_1 z_1^T & y_1 y_2 z_1 z_2^T & \ldots & y_1 y_N z_1 z_1^T \\ y_2 y_1 z_2 z_1^T & y_2 y_2 z_2 z_2^T & \ldots & y_2 y_N z_2 z_N^T \\ \ldots & \ldots & \ldots & \ldots \\ y_N y_1 z_N z_1^T & y_N y_2 z_N z_2^T & \ldots & y_N y_N z_N z_N^T \end{bmatrix}$$

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

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

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

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

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

How many dimensions z has?

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

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

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

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

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

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

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

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

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

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

Example: Let's say we have two datapoints

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

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

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

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

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

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 $x \; and \; x'$

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

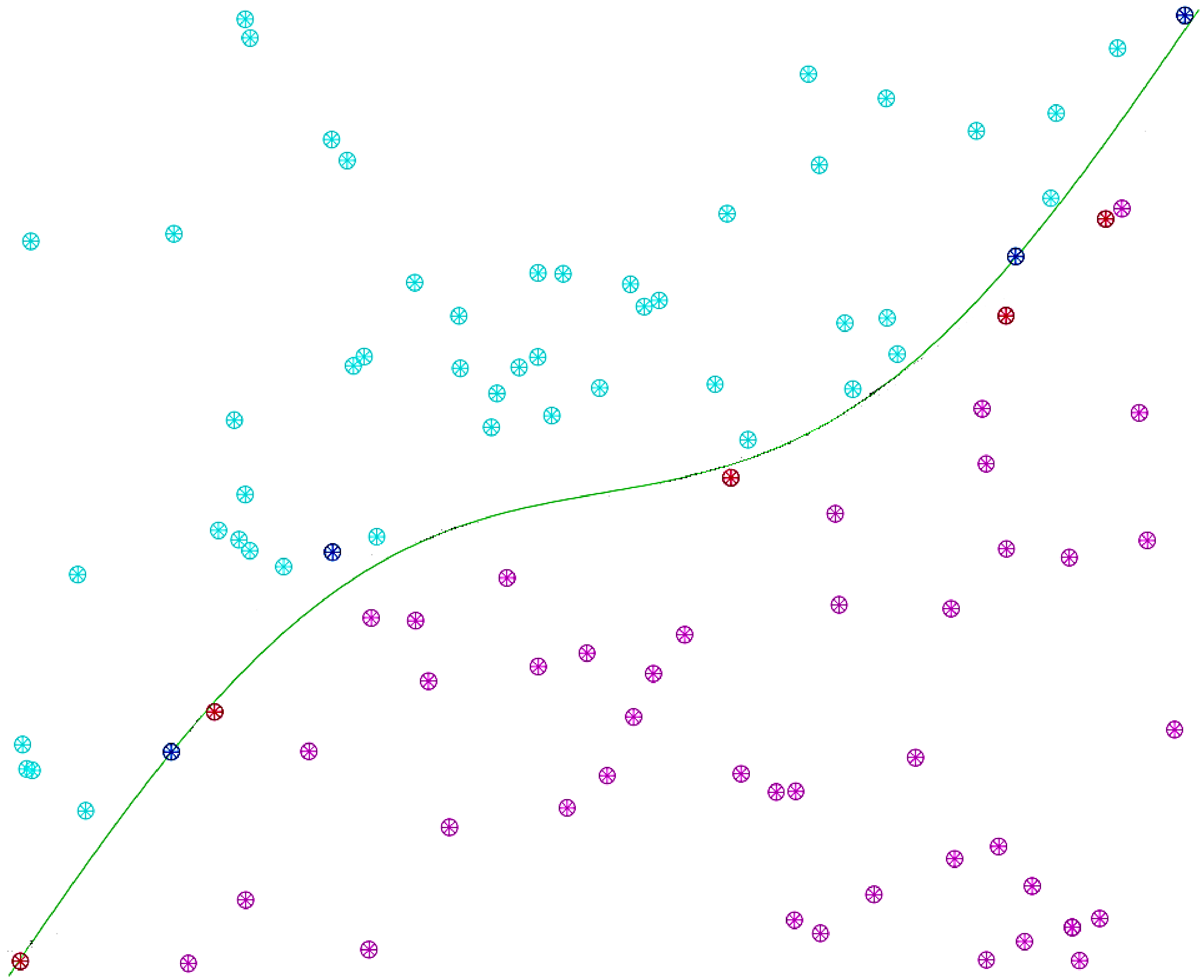
For d and $\gamma = 1 \Rightarrow \quad K(x, x') = \exp(-(x - x')^2)$

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

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

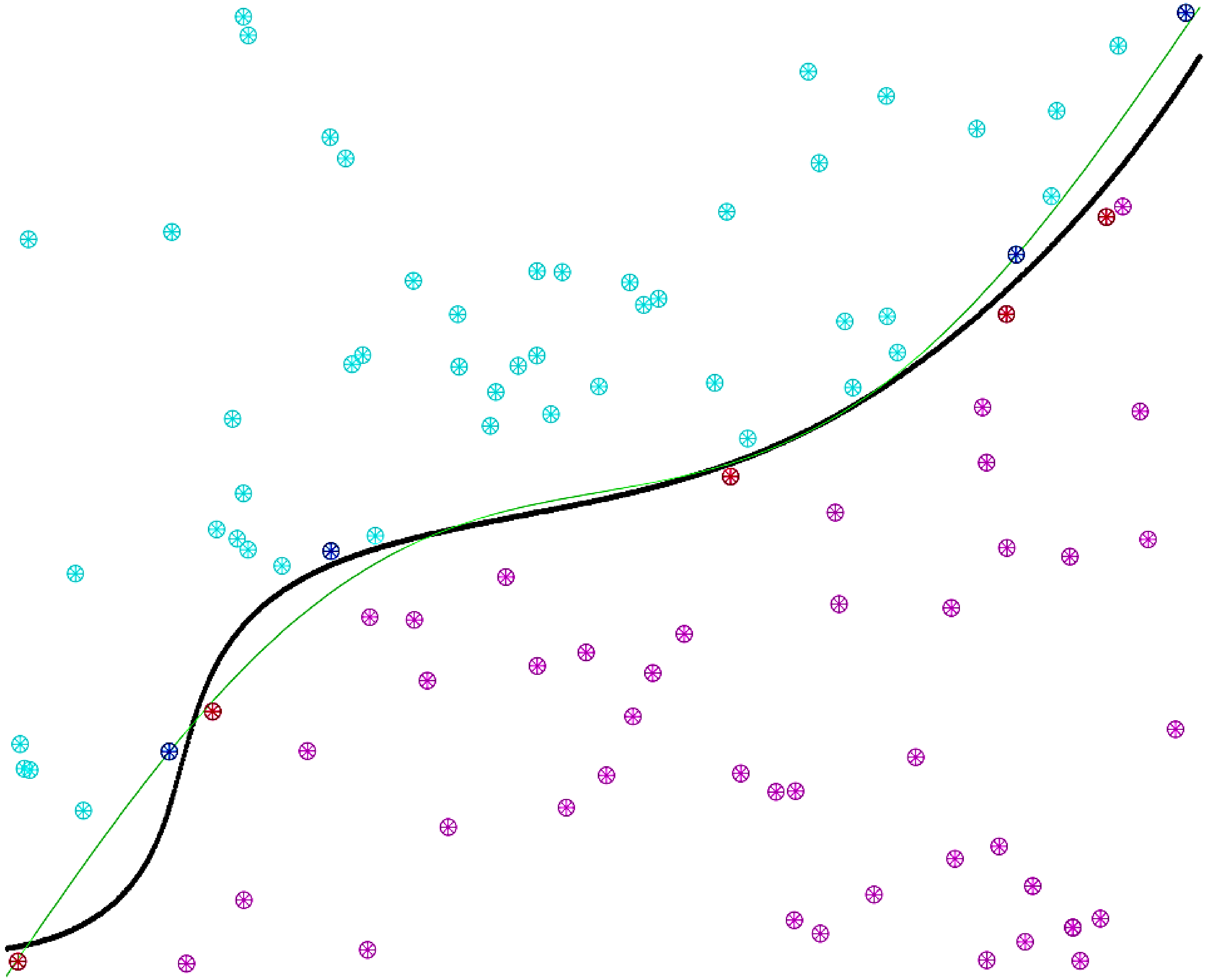
Radial basis kernel in action

Slightly non-linearly separable case for 100 datapoints:



Transforming χ

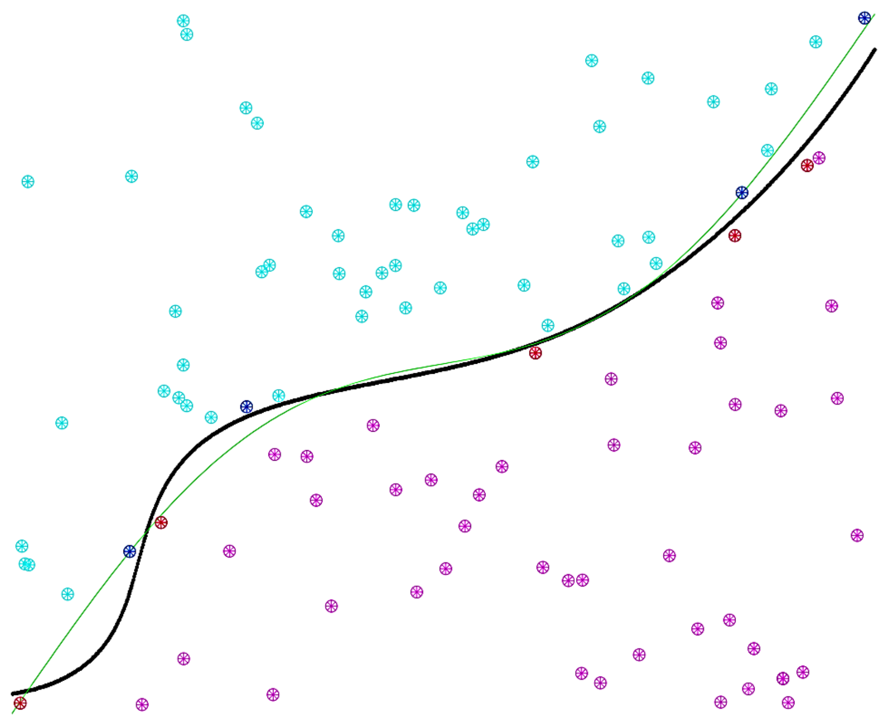
into ∞-dimensional $\mathbb{Z}$ space



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?

$$\underbrace{\begin{bmatrix} y_1 y_1 x_1 x_1^T & y_1 y_2 x_1 x_2^T & \cdots & y_1 y_N x_1 x_1^T \\ y_2 y_1 x_2 x_1^T & y_2 y_2 x_2 x_2^T & \cdots & y_2 y_N x_2 x_N^T \\ \cdots & \cdots & \cdots & \cdots \\ y_N y_1 x_N x_1^T & y_N y_2 x_N x_2^T & \cdots & y_N y_N x_N x_N^T \end{bmatrix}}_{\text{Quadratic coefficients}}$$

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

$$\begin{bmatrix} y_1 y_1 K(x_1, x_1) & y_1 y_2 K(x_1, x_2) & \cdots & y_1 y_N K(x_1, x_N) \\ y_2 y_1 K(x_2, x_1) & y_2 y_2 K(x_2, x_2) & \cdots & y_2 y_1 K(x_2, x_N) \\ \cdots & \cdots & \cdots & \cdots \\ y_N y_1 K(x_N, x_1) & y_N y_2 K(x_N, x_2) & \cdots & y_N y_N K(x_N, x_N) \end{bmatrix}$$

Final stage:

$g(x) = sign(z\theta + b)$ $\qquad$ $in\ terms\ of\ K(-,-)$

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

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

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

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

How do we know that the kernel is valid?

$For\ a\ given\ K(x, x')$ → 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 ➔ $$\begin{bmatrix} y_1y_1K(x_1,x_1) & y_1y_2K(x_1,x_2) & \cdots & y_1y_NK(x_1,x_N) \\ y_2y_1K(x_2,x_1) & y_2y_2K(x_2,x_2) & \cdots & y_2y_NK(x_2,x_N) \\ \cdots & \cdots & \cdots & \cdots \\ y_Ny_1K(x_N,x_1) & y_Ny_2K(x_N,x_2) & \cdots & y_Ny_NK(x_N,x_N) \end{bmatrix}$$

is positive-semi definite

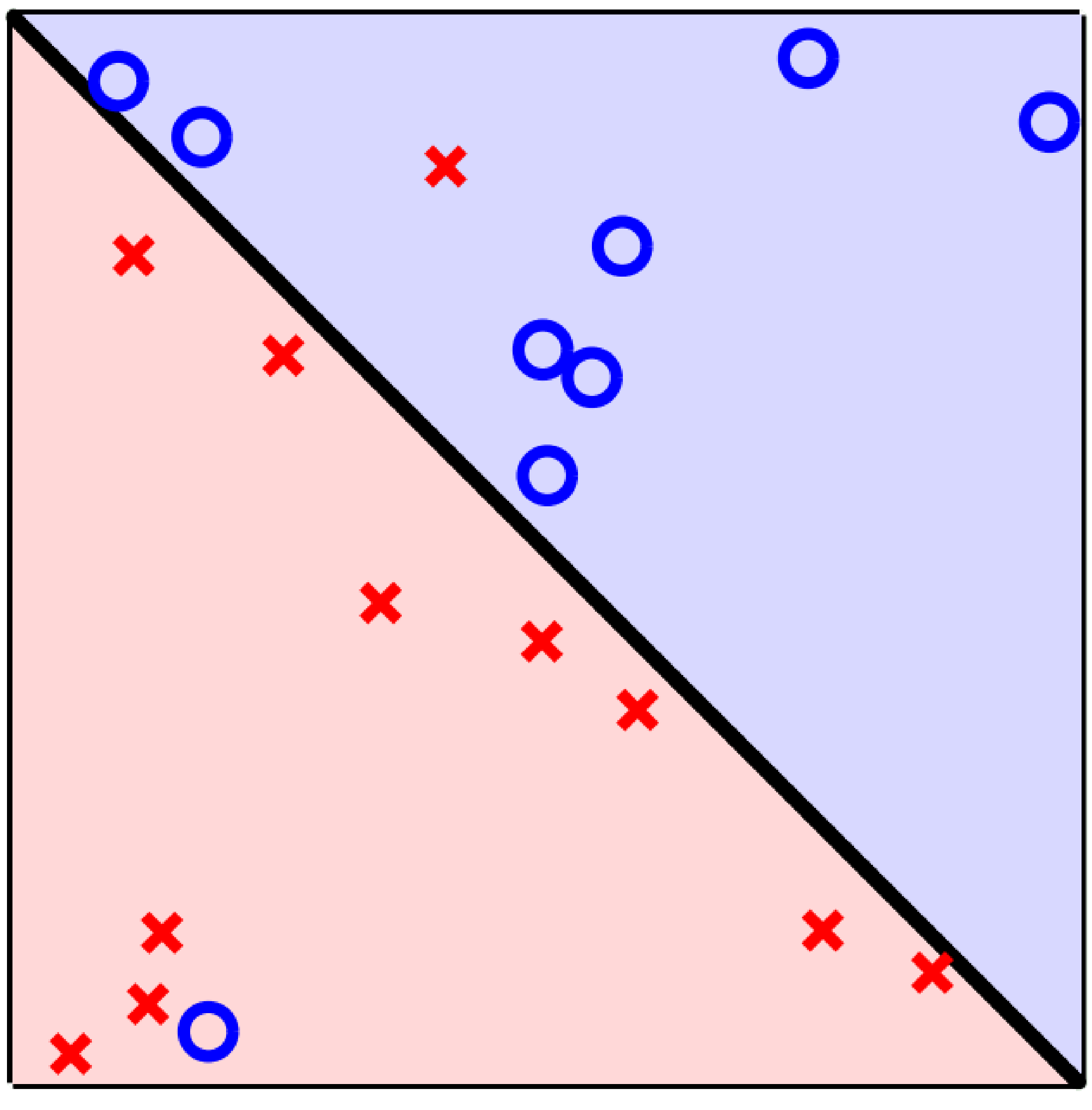
For any $x_1, \ldots, x_N$ (Mercer's condition)

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

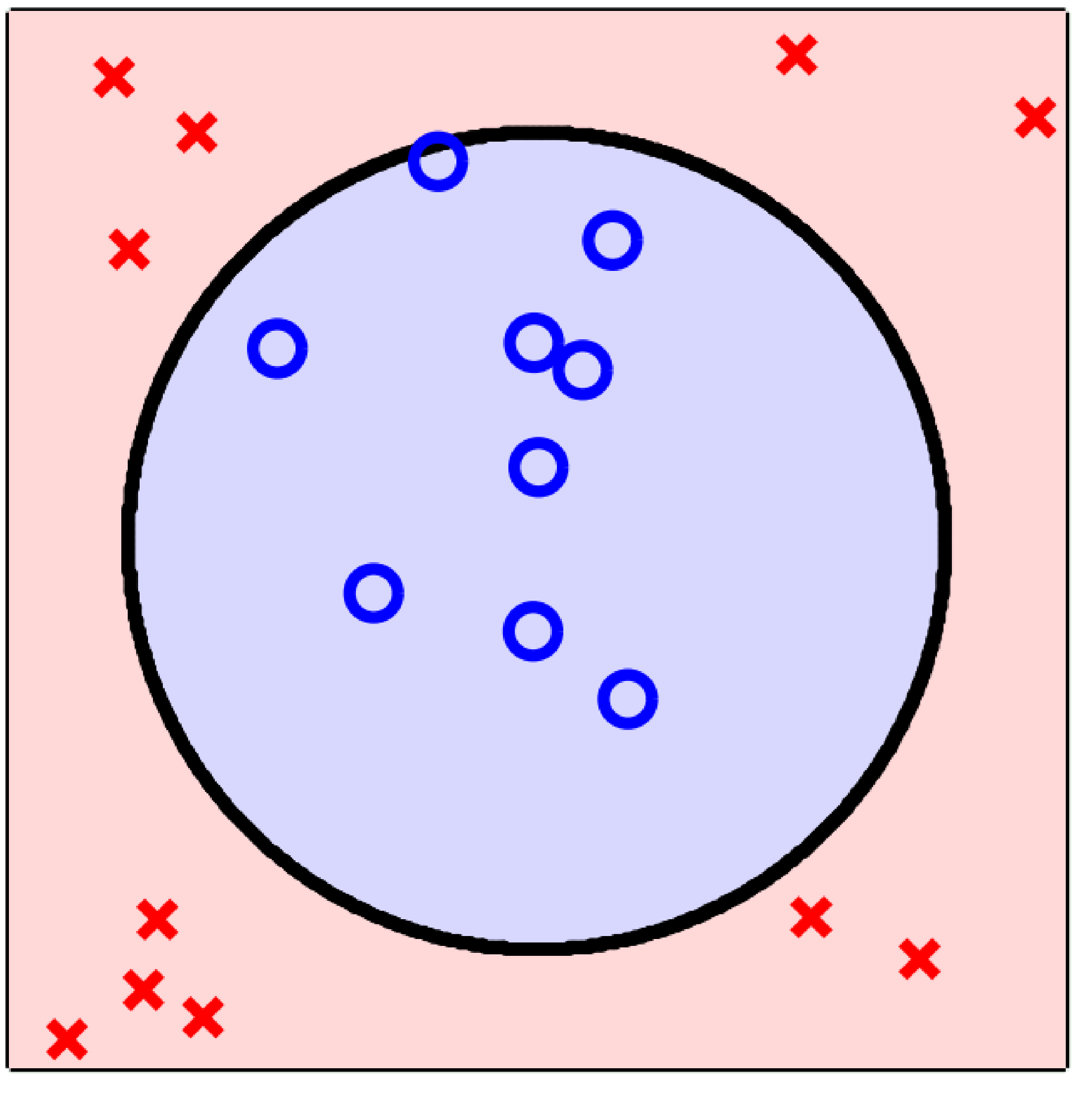
Soft SVM – Two types of non-separable

slightly:



Soft SVM will deal with this

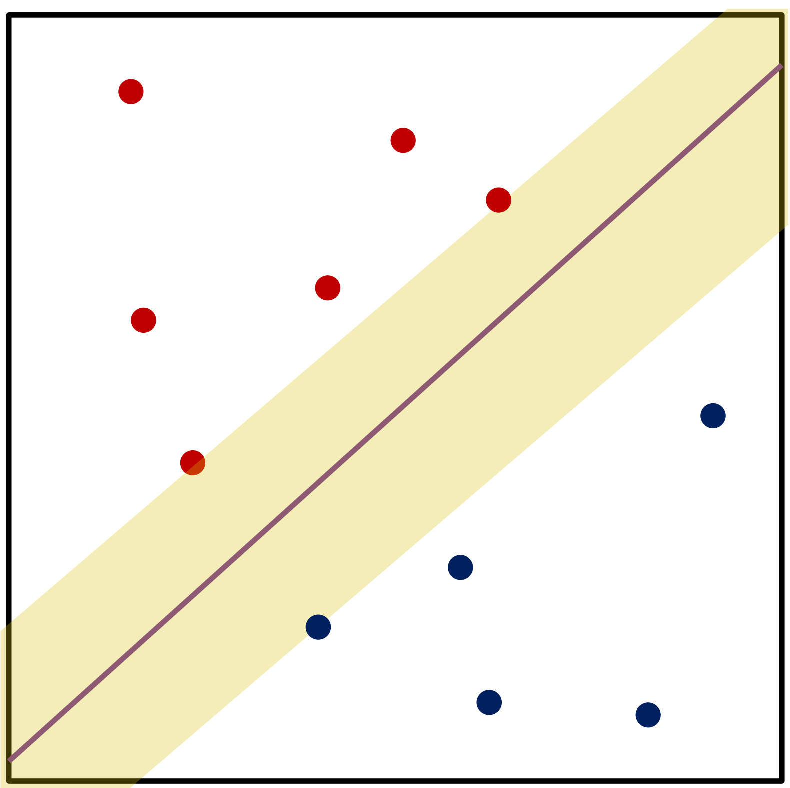
seriously:



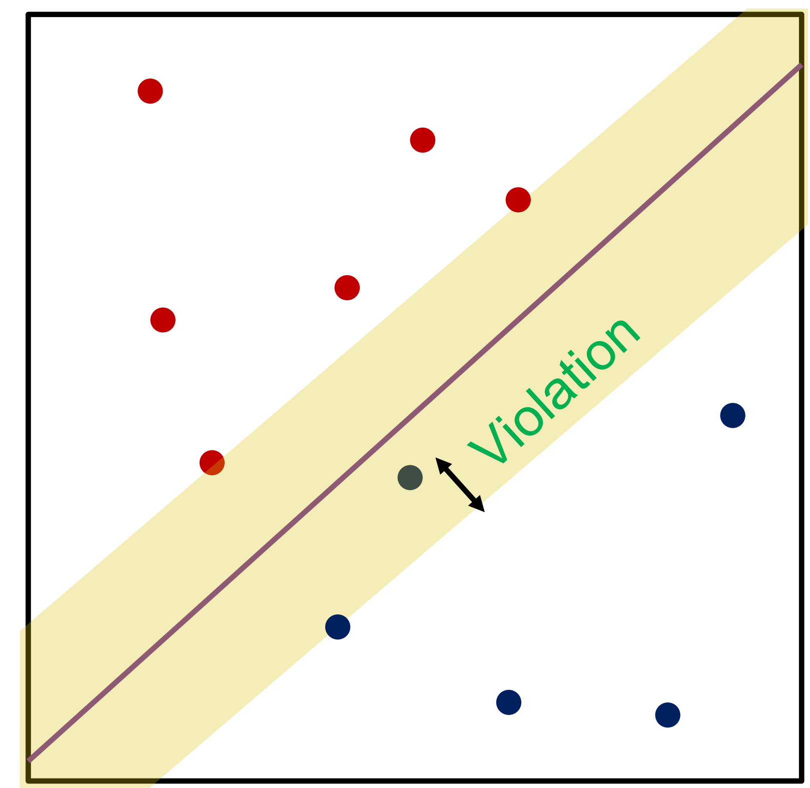
Kernel will deal with this

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

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

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

$\mathrm{C} = inf$ 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

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

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

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

Let's do the minimization:

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

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

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

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

$$\beta_i = C - \alpha_i$$

$$\beta_i \geq 0 \quad \Rightarrow \quad C - \alpha_i \geq 0 \rightarrow 0 \leq \alpha_i \leq C \qquad \text{for } i = 1, \dots, N$$

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

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

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

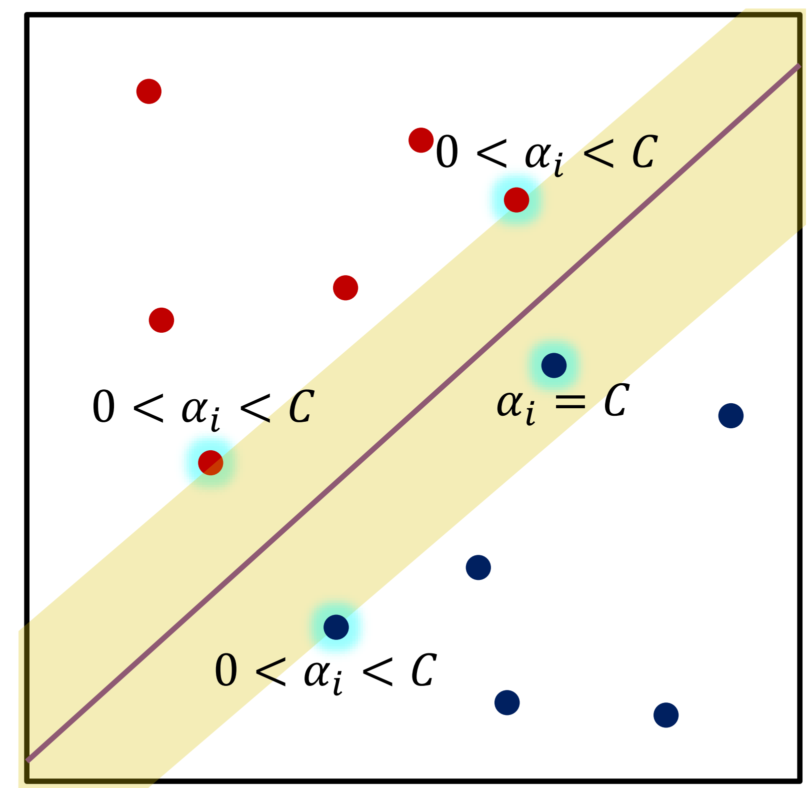
Type of support vectors

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

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

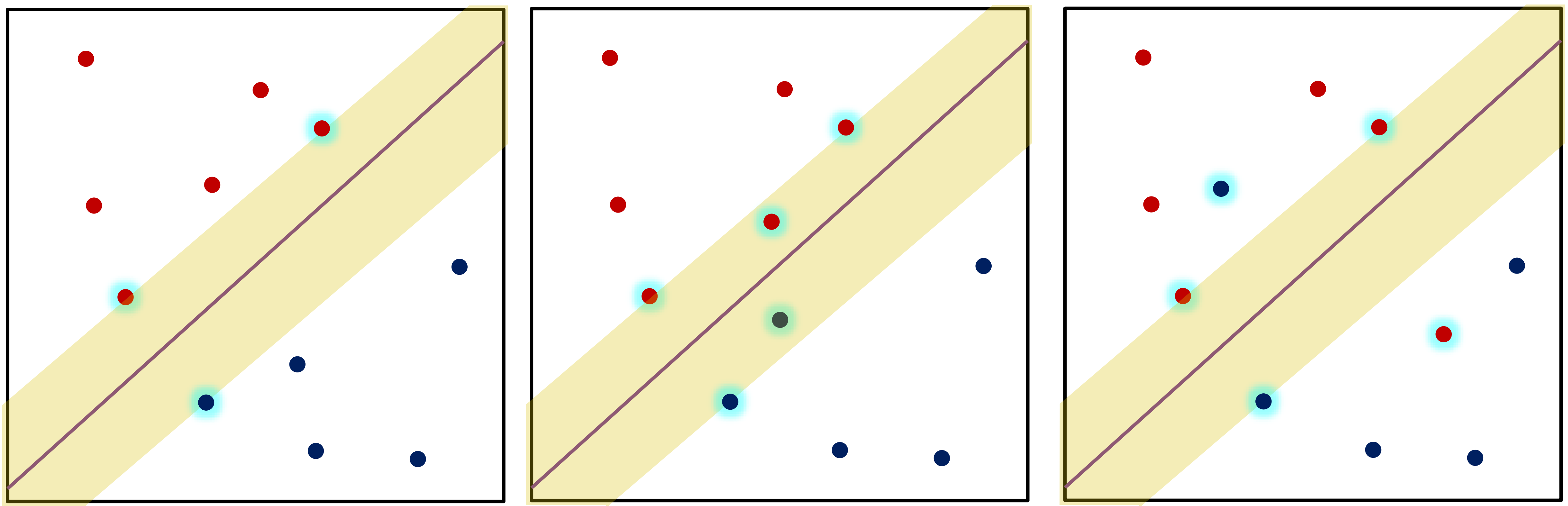
SV on the wrong side

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

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:

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

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