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Kernel SVM

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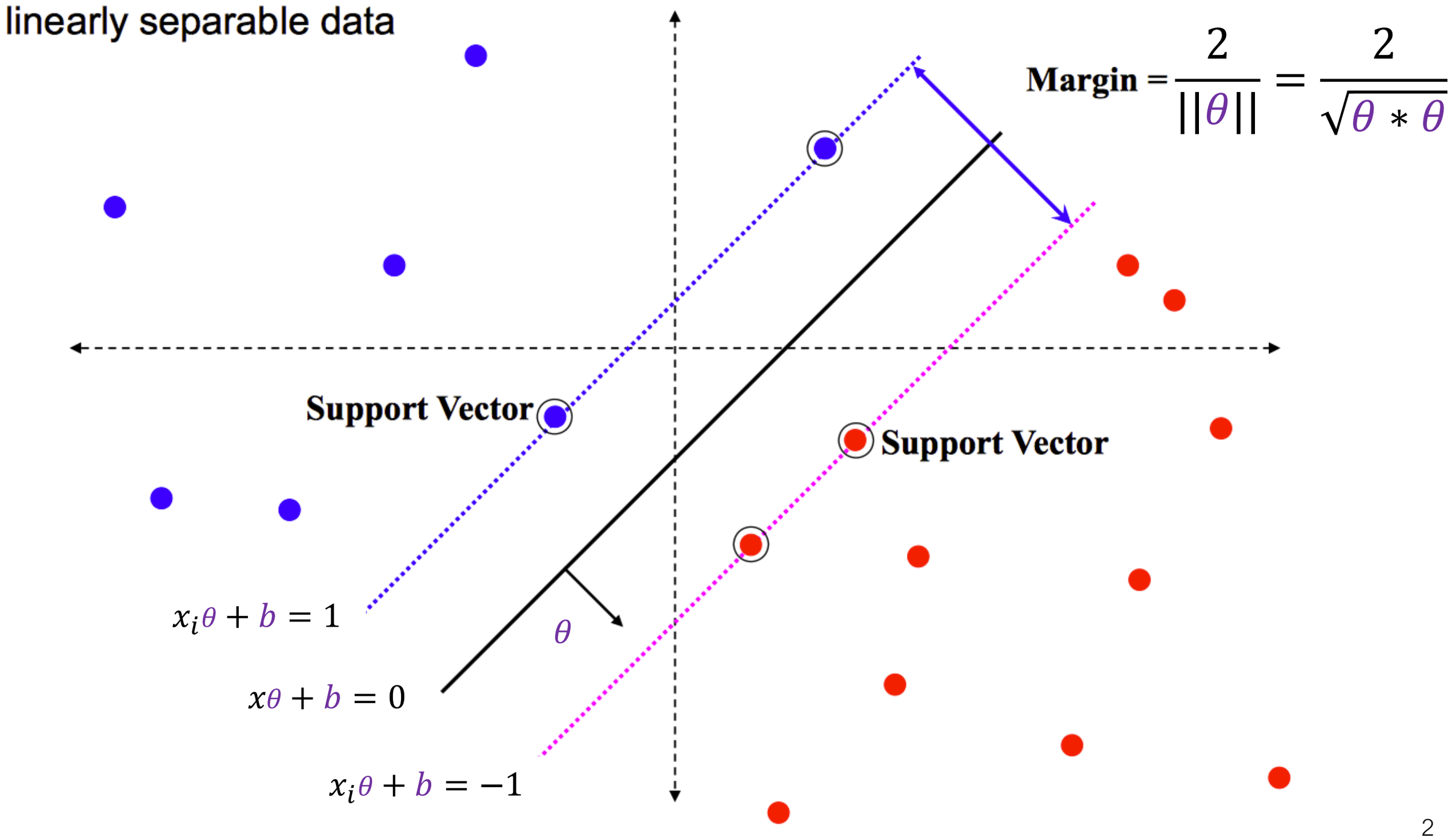
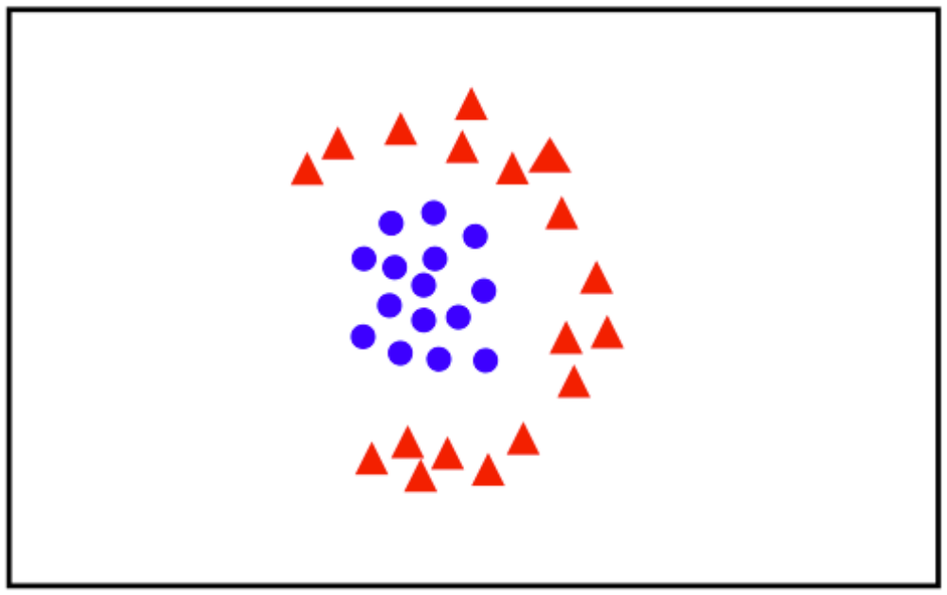
These slides are based on slides from Yaser Mostafa, Le Song, Mahdi Roozbahani and Eric Eaton.

Geometric Interpretation



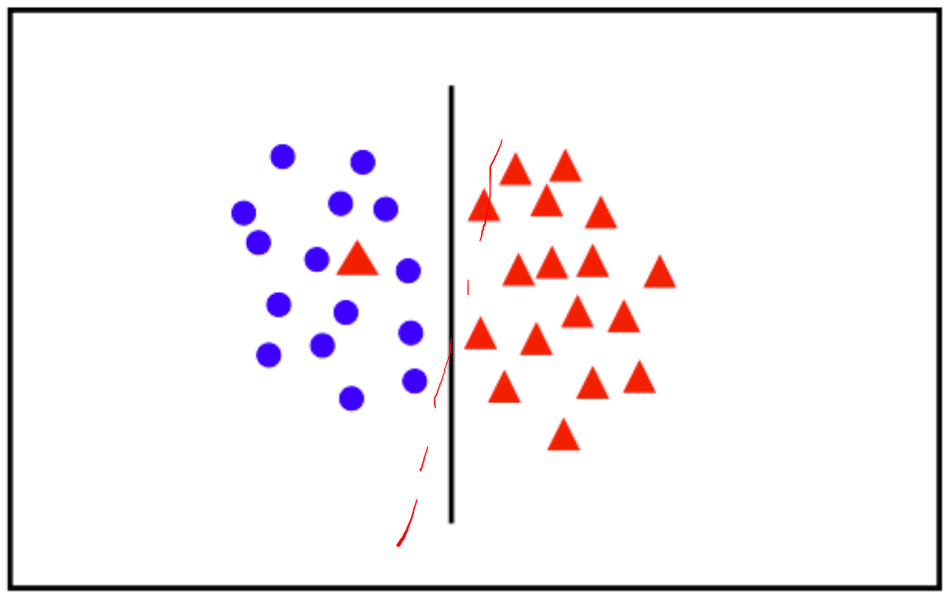
Handling Data that are Not Linearly Separable



- linear classifier not appropriate

??

Kernel trick

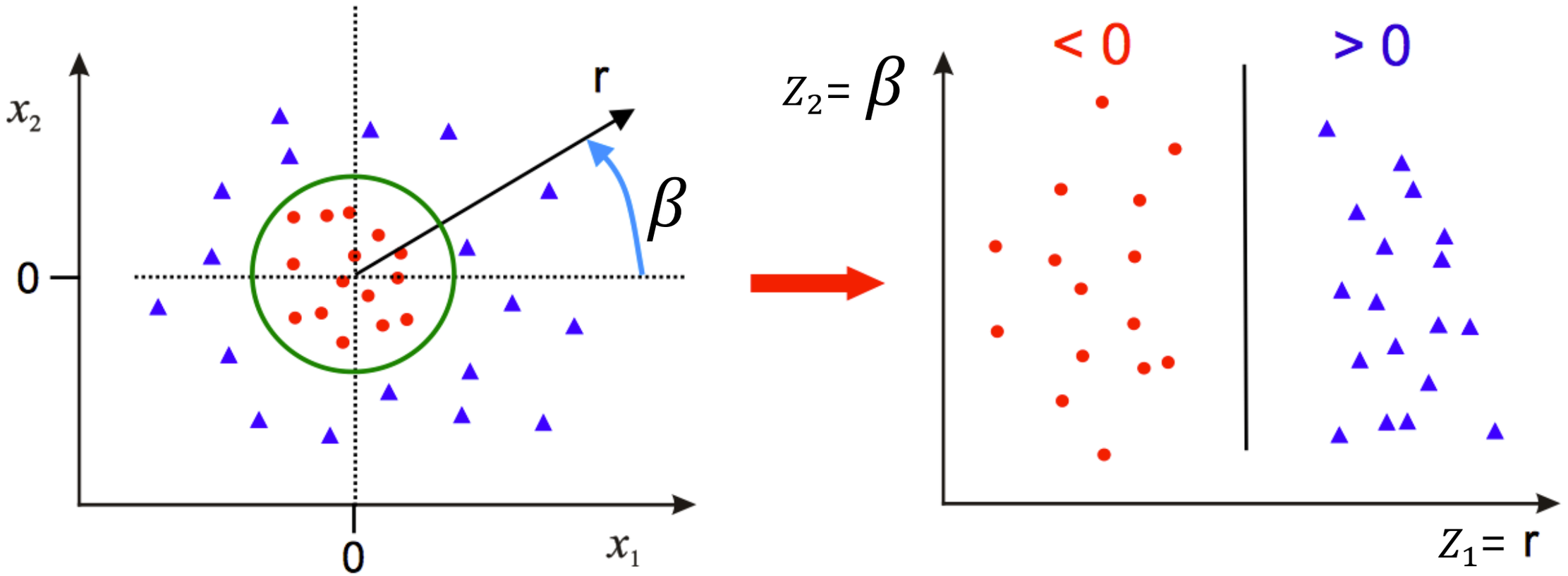


- introduce slack variables

Soft Margin SVM

(allowing ourselves to make errors)

Idea 1: Use Polar Coordinates to go to z space

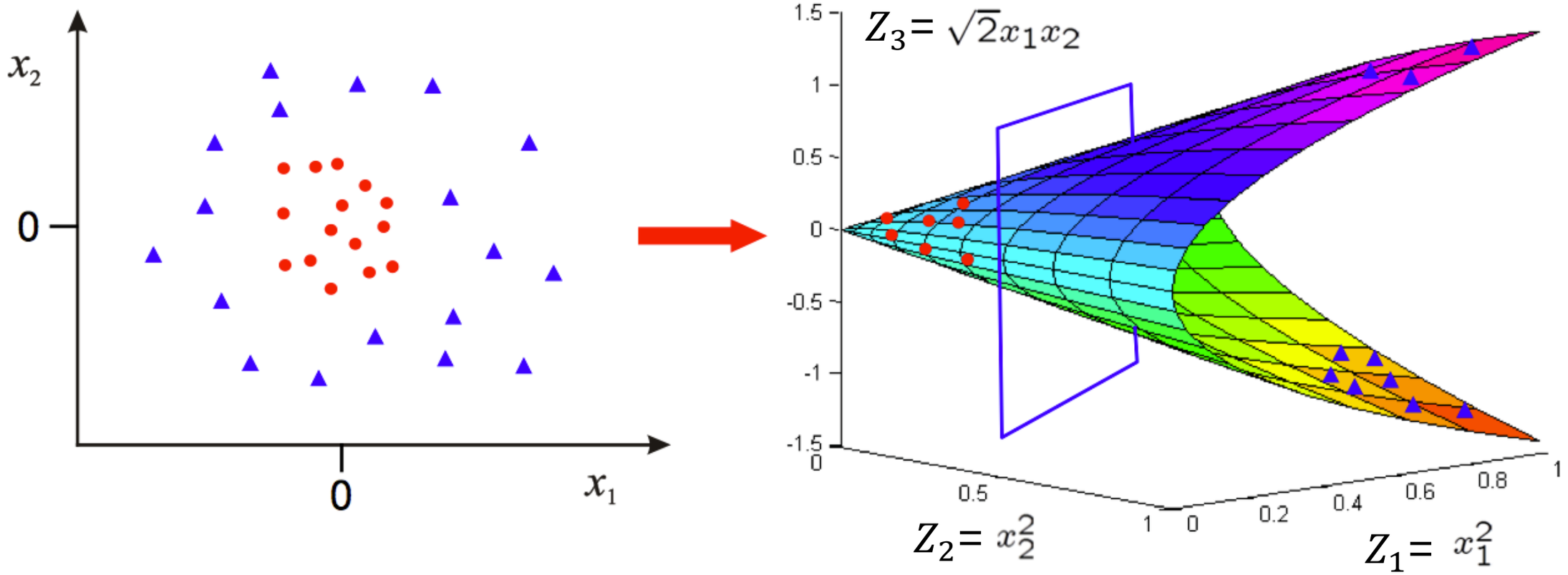


- Data is linearly separable in polar coordinates
- Acts non-linearly in original space

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

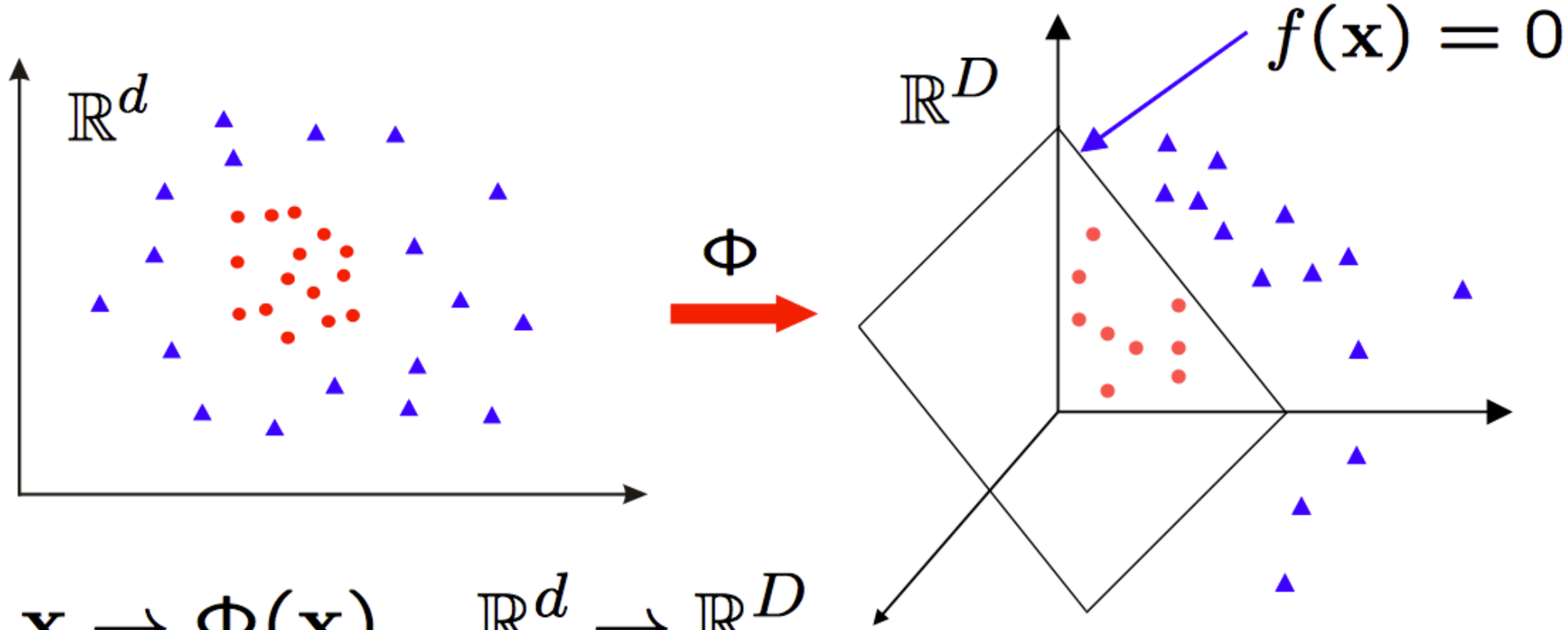
Idea 1: Map Data to Higher Dimension $\mathbb{Z}$ space

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



- 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



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

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:

$$\begin{bmatrix} y_1 y_1 z_1 z_1^T & y_1 y_2 z_1 z_2^T & \cdots & y_1 y_N z_1 z_1^T \\ y_2 y_1 z_2 z_1^T & y_2 y_2 z_2 z_2^T & \cdots & y_2 y_N z_2 z_N^T \\ \cdots & \cdots & \cdots & \cdots \\ y_N y_1 z_N z_1^T & y_N y_2 z_N z_2^T & \cdots & y_N y_N z_N z_N^T \end{bmatrix}$$

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

Example:

$x = (x_1, x_2) \rightarrow 2nd - order\ \Phi$ here x has two dimensions

$z = \Phi(\boldsymbol{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1x_2)$ How many dimensions z has?

$$K(x,x') = z'z^T = 1 + x_1x_1' + x_2x_2' + x_1^2x_1'^2 + x_2^2x_2'^2 + x_1x_1'x_2x_2'$$

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 $x = (1, x_1, x_2)$

Datapoint 2 in x space $x' = (1, x_1', x_2')$

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

Datapoint 1 in z space $\phi(x) = z = (1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2)$

Datapoint 2 in z space $\phi(x') = z' = (1, x_1'^2, x_2'^2, \sqrt{2}x_1', \sqrt{2}x_2', \sqrt{2}x_1'x_2')$

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

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

$z = (1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2)$ $\qquad$ $z' = (1, x_1'^2, x_2'^2, \sqrt{2}x_1', \sqrt{2}x_2', \sqrt{2}x_1'x_2')$

$$K(x, x') = 1 + x_1^2x_1'^2 + x_2^2x_2'^2 + 2x_1x'_1 + 2x_2x'_2 + 2x_1x'_1x_2x'_2$$

$x \rightarrow$ datapoint 1

$x' \rightarrow$ datapoint 2

$$K(x, x') = (1 + x_1x_1' + x_2x_2')^2$$

$x = (1, x_1, x_2)$ $\qquad$ $x' = (1, x_1', x_2')$

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

$c > 0 \rightarrow c\,(1 + x'x^T)^2 \rightarrow$ Inhomogeneous kernel

Example: Let's say we have two datapoints

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

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

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

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

$x = [1 \quad 2]$ $\quad y = cat = +1$

$x' = [-1 \quad 3]$ $\quad y' = dog = -1$

The polynomial kernel

$\mathcal{X} = \mathcal{R}^d \; and \; \Phi: \; \mathcal{X} \; \rightarrow \mathbb{Z}$ 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

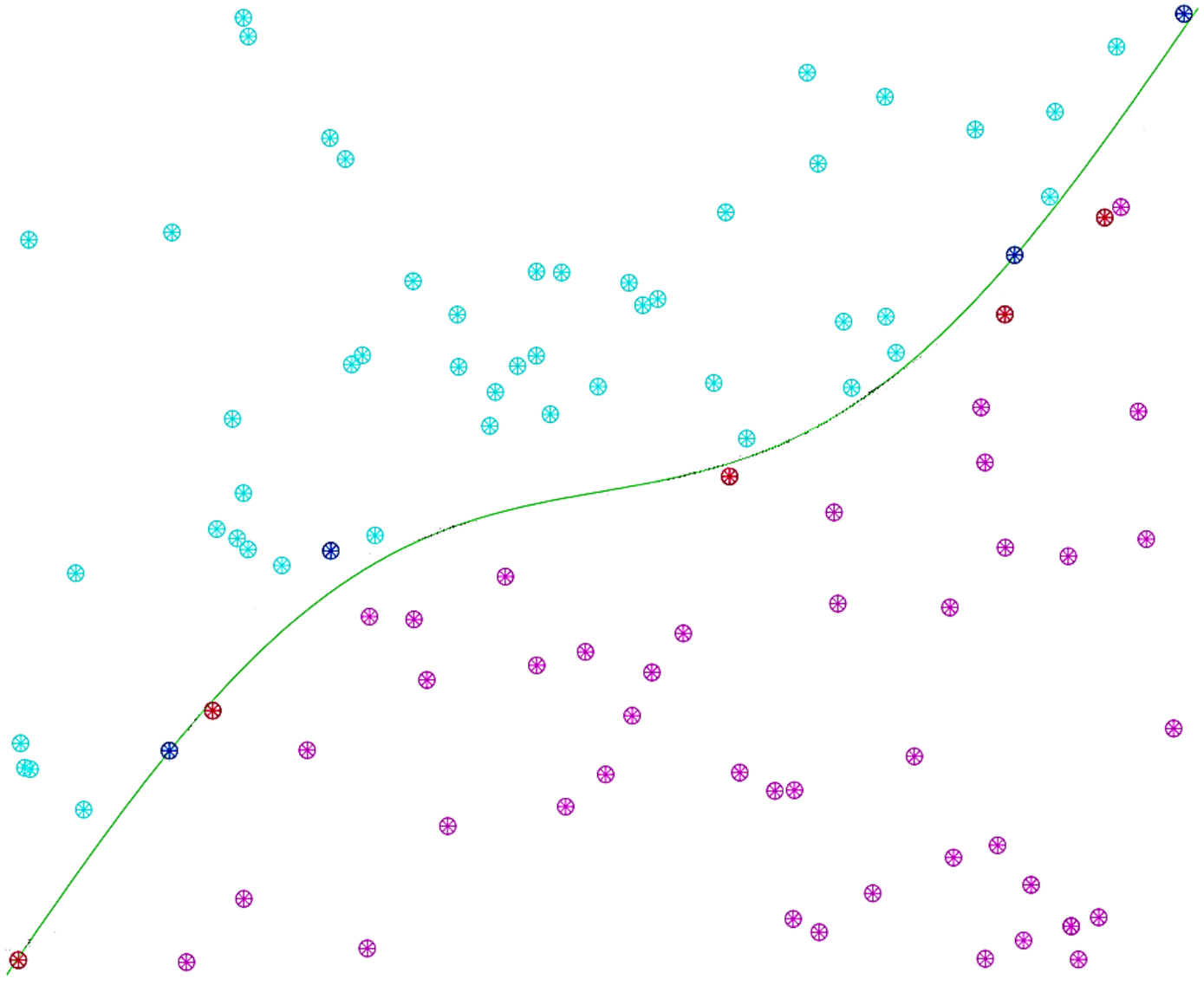
For d and $\gamma = 1 \Rightarrow \quad K(x, x') = \exp(-(x - x')^2)$

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

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

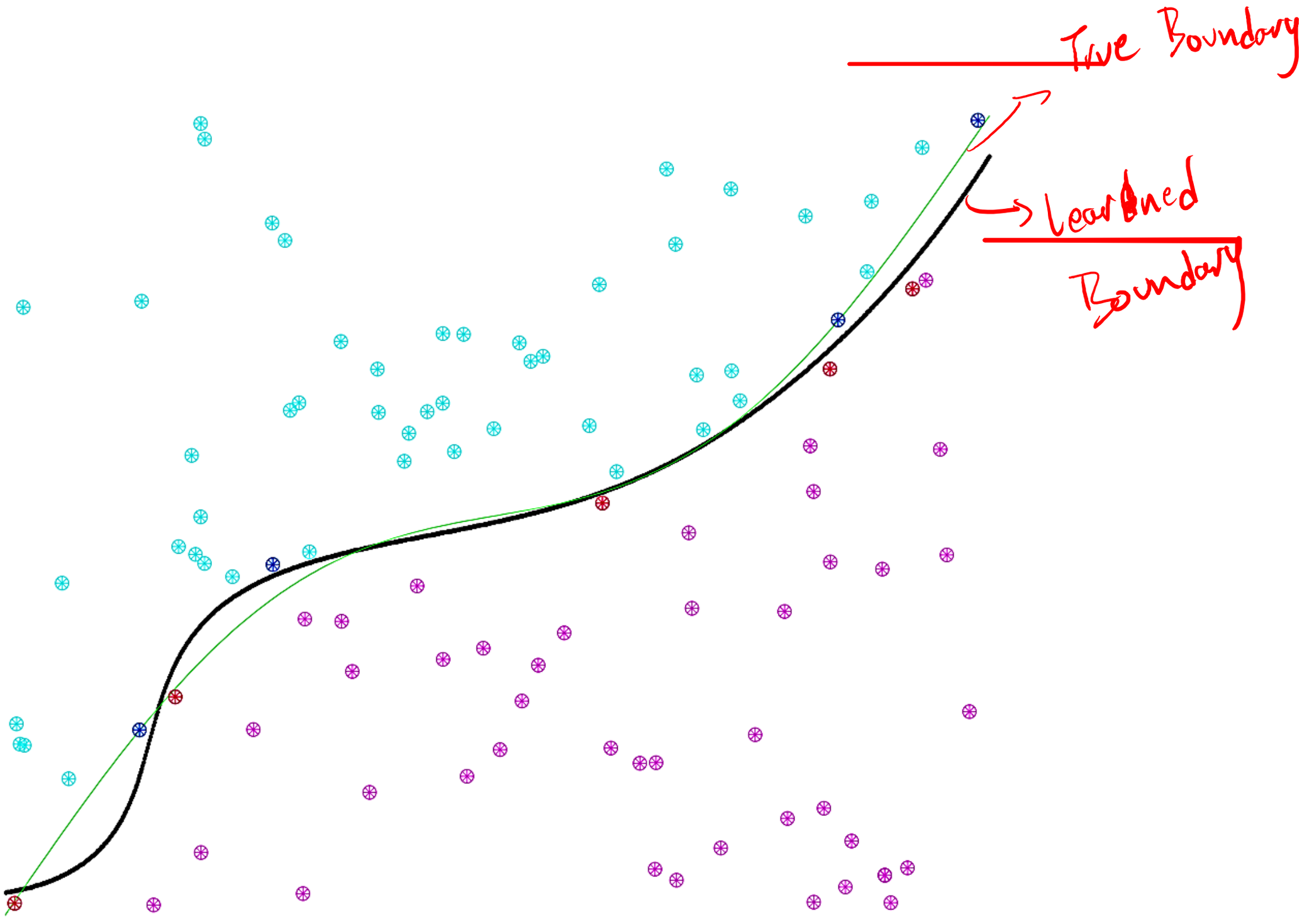
Radial basis kernel in action

Slightly non-linearly separable case for 100 datapoints:



Transforming χ

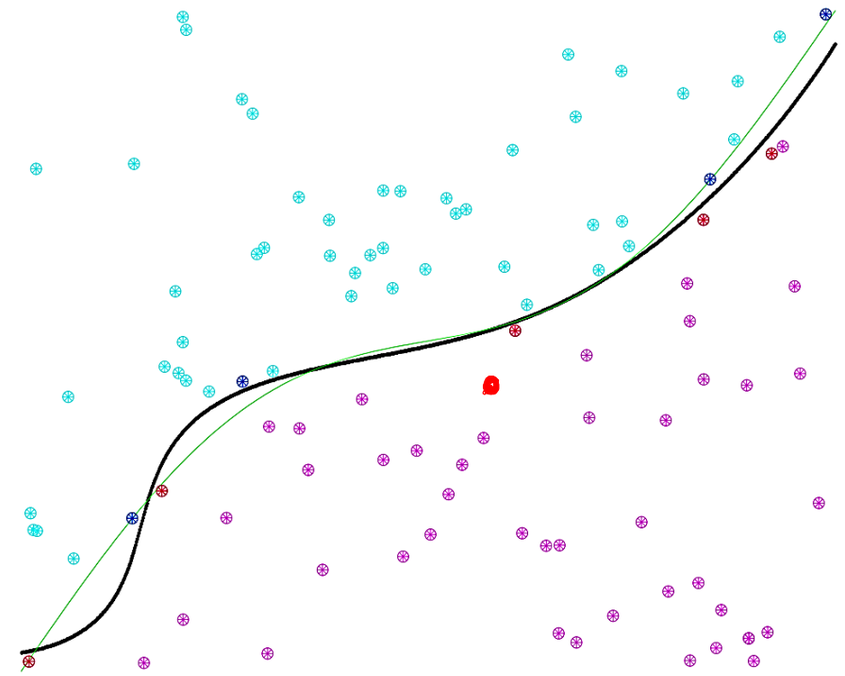
into ∞-dimensional $\mathbb{Z}$ space



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

Expectation — Error — unseen

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

N is number of datapoints

Kernel formulation of SVM

Remember quadratic programming?

$$\begin{bmatrix} y_1 y_1 x_1 x_1^T & y_1 y_2 x_1 x_2^T & \cdots & y_1 y_N x_1 x_1^T \\ y_2 y_1 x_2 x_1^T & y_2 y_2 x_2 x_2^T & \cdots & y_2 y_N x_2 x_N^T \\ \cdots & \cdots & \cdots & \cdots \\ y_N y_1 x_N x_1^T & y_N y_2 x_N x_2^T & \cdots & y_N y_N x_N x_N^T \end{bmatrix}$$

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:

decision boundary

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

in terms of $K(-,-)$

$$where \rightarrow \theta = \sum \alpha_i y_i z_i \rightarrow$$

z_i *in SV*

$$g(x) = sign(\sum \alpha_i y_i z_i z + b)$$

z_i *in SV*

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

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?

Does a z exist?

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

Three approaches:

1. By construction (Polynomial one)
2. Math properties (Mercer's condition)
3. Not worrying about validity of a kernel

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

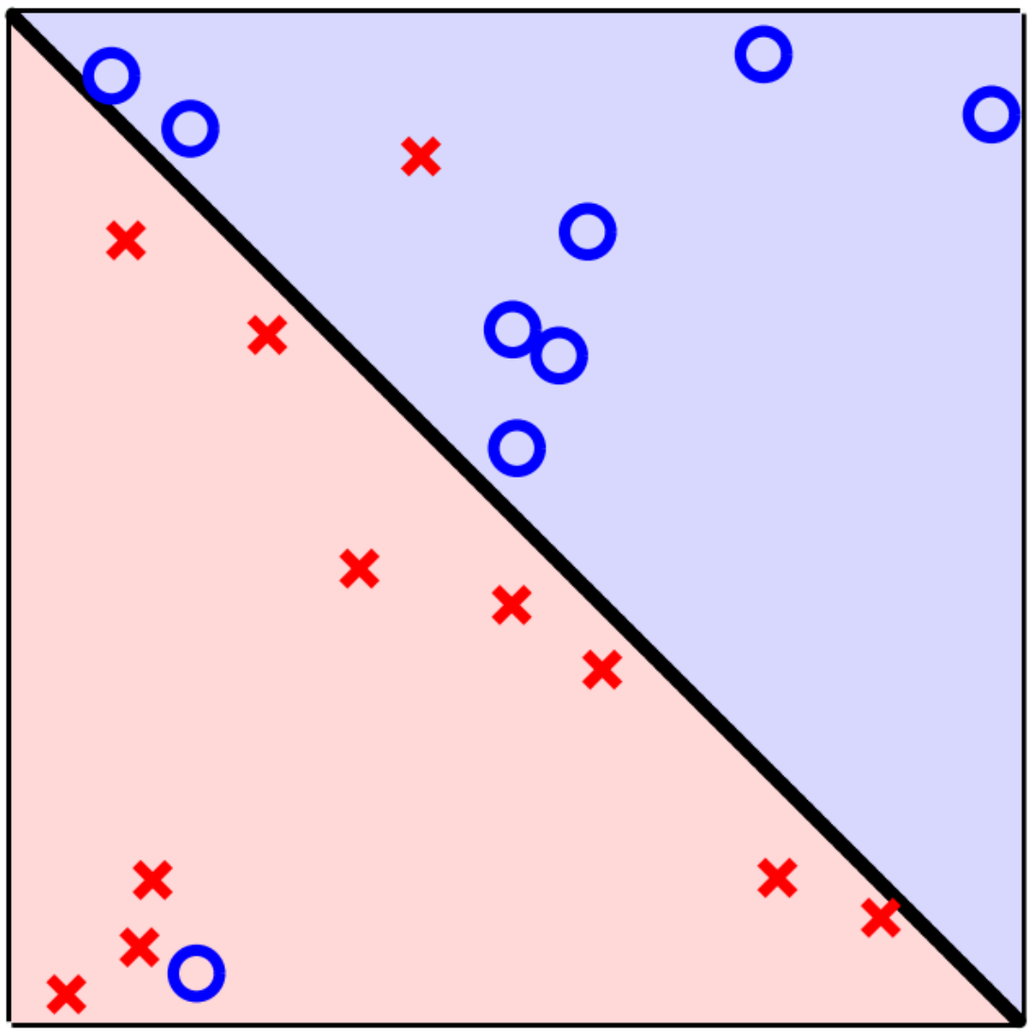
- Linear kernels $k(\mathbf{x}, \mathbf{x}') = x' x^T$
- Polynomial kernels $k(\mathbf{x}, \mathbf{x}') = \left(1 + x' x^T\right)^d$ for any $d > 0$
  - Contains all polynomials terms up to degree d
- Gaussian kernels $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2 / 2\sigma^2\right)$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

Do we need non-linearity for small deviations???

- No!!!!!
- Use Soft-SVM

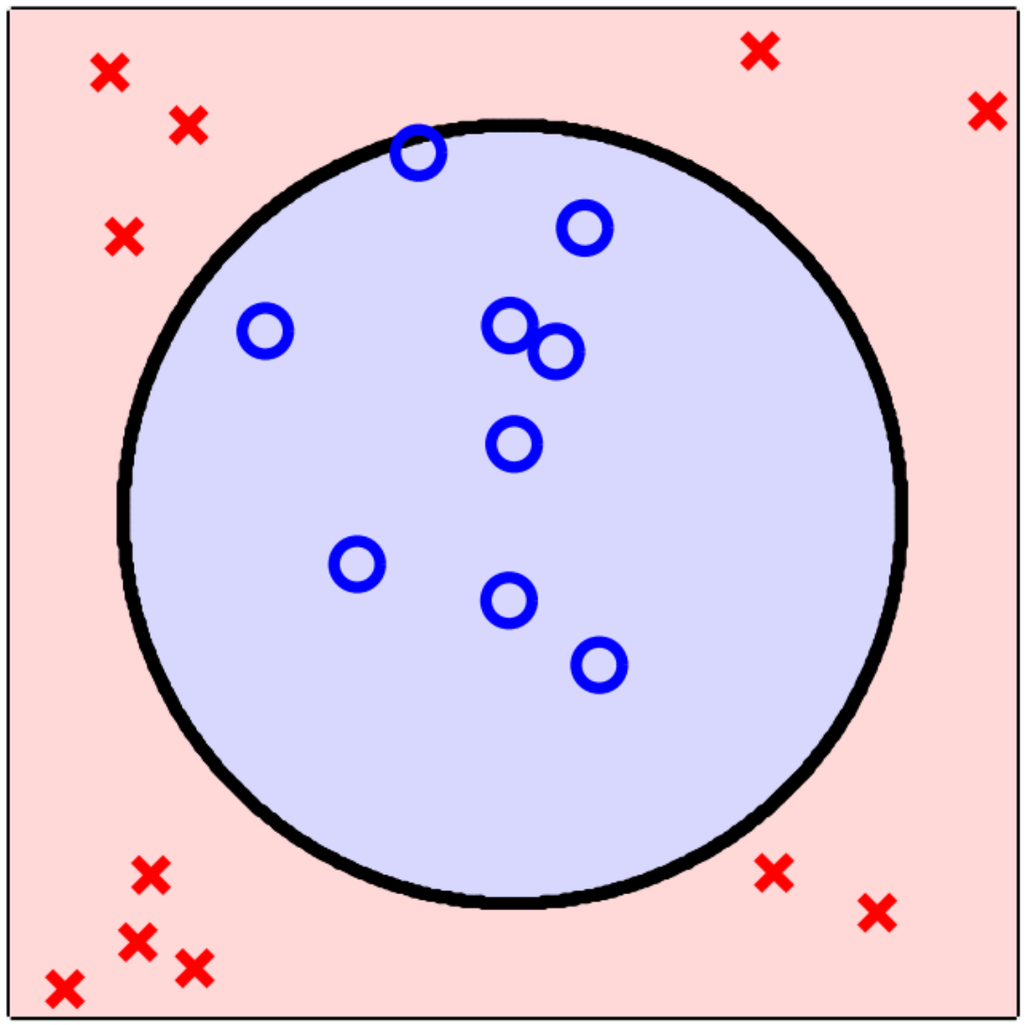
Soft SVM – Two types of non-separable

slightly:



Soft SVM will deal with this

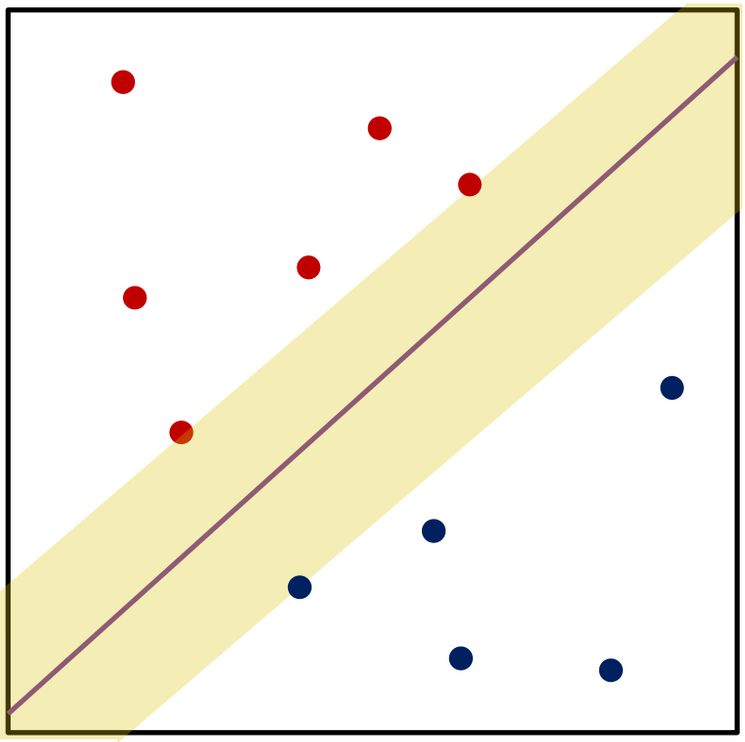
seriously:



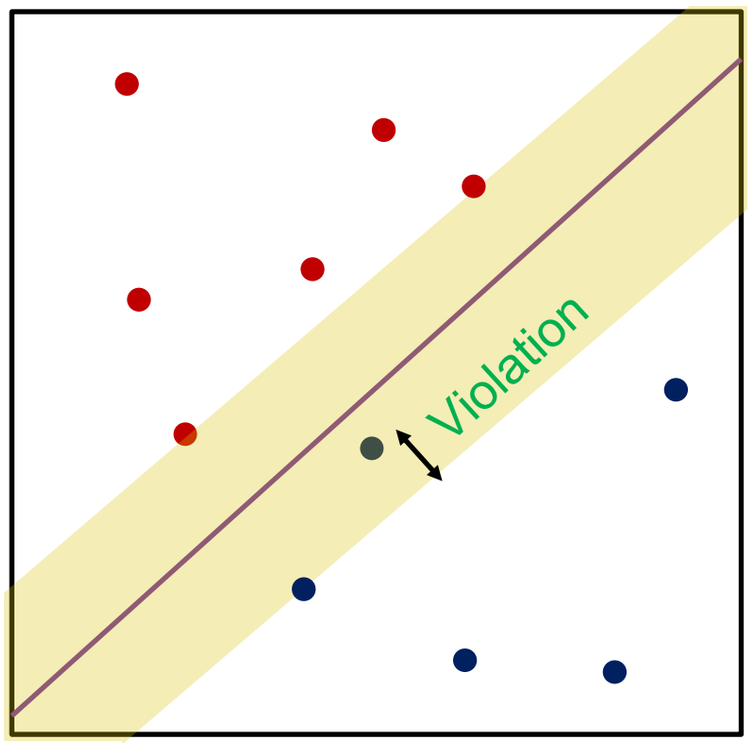
Kernel will deal with this

Error measure

Non-violated case:



Margin violation:



if $y_i(x_i\theta + b) > 1 \Rightarrow$ Non SV

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

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

The new optimization

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 = 0 is equal to Hard SVM

$$s.t. \quad y_i(x_i\theta + b) \geq 1 - \xi_i \qquad \text{for } i = 1, \dots, N$$

$$and\ \xi_i \geq 0 \qquad \text{for } i = 1, \dots, N$$

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

The Lagrange formulation

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

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

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

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

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 $\boldsymbol{\theta}, b, and\ \xi$ and maximize w.r.t $\alpha_i \geq 0\ and\ \beta_i \geq 0$

KKT condition for inequality constraints

Let's do the minimization:

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

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

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

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

The solution

$$\beta_i = C - \alpha_i$$

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

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

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

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

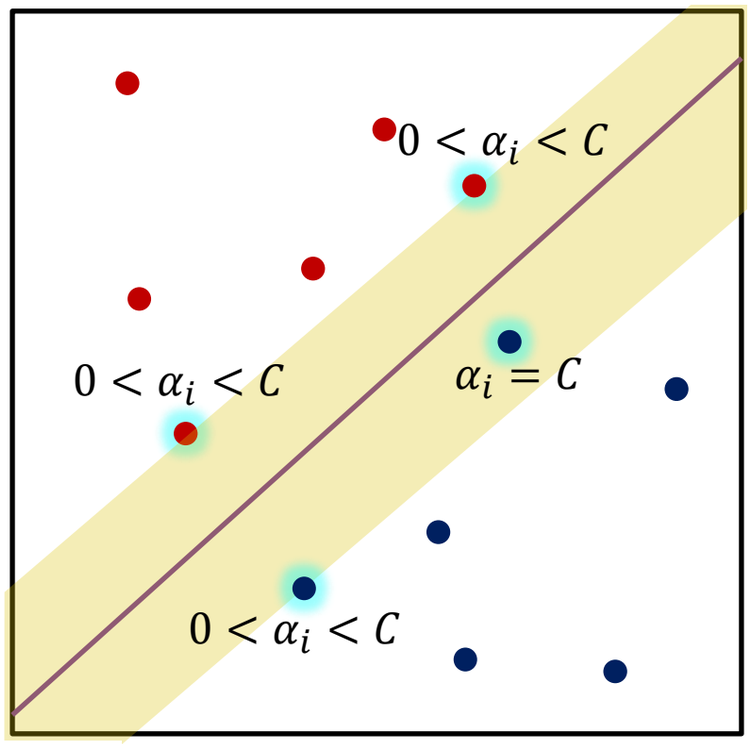
Type of support vectors

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

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

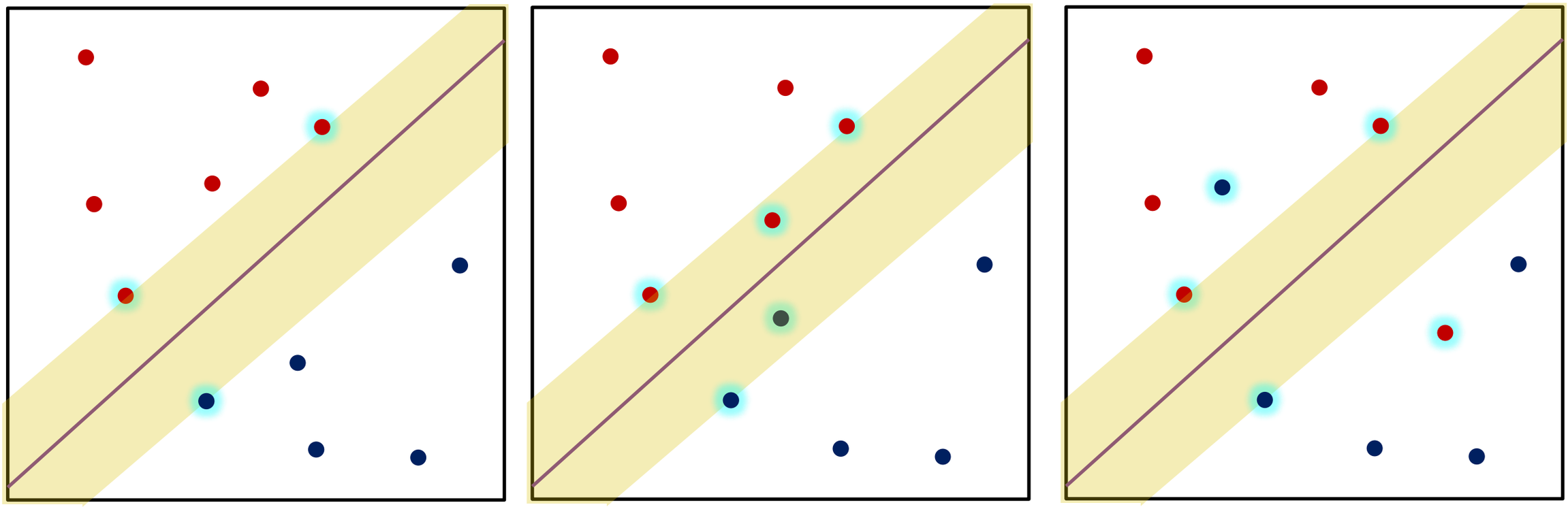
SV on the wrong side

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

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