

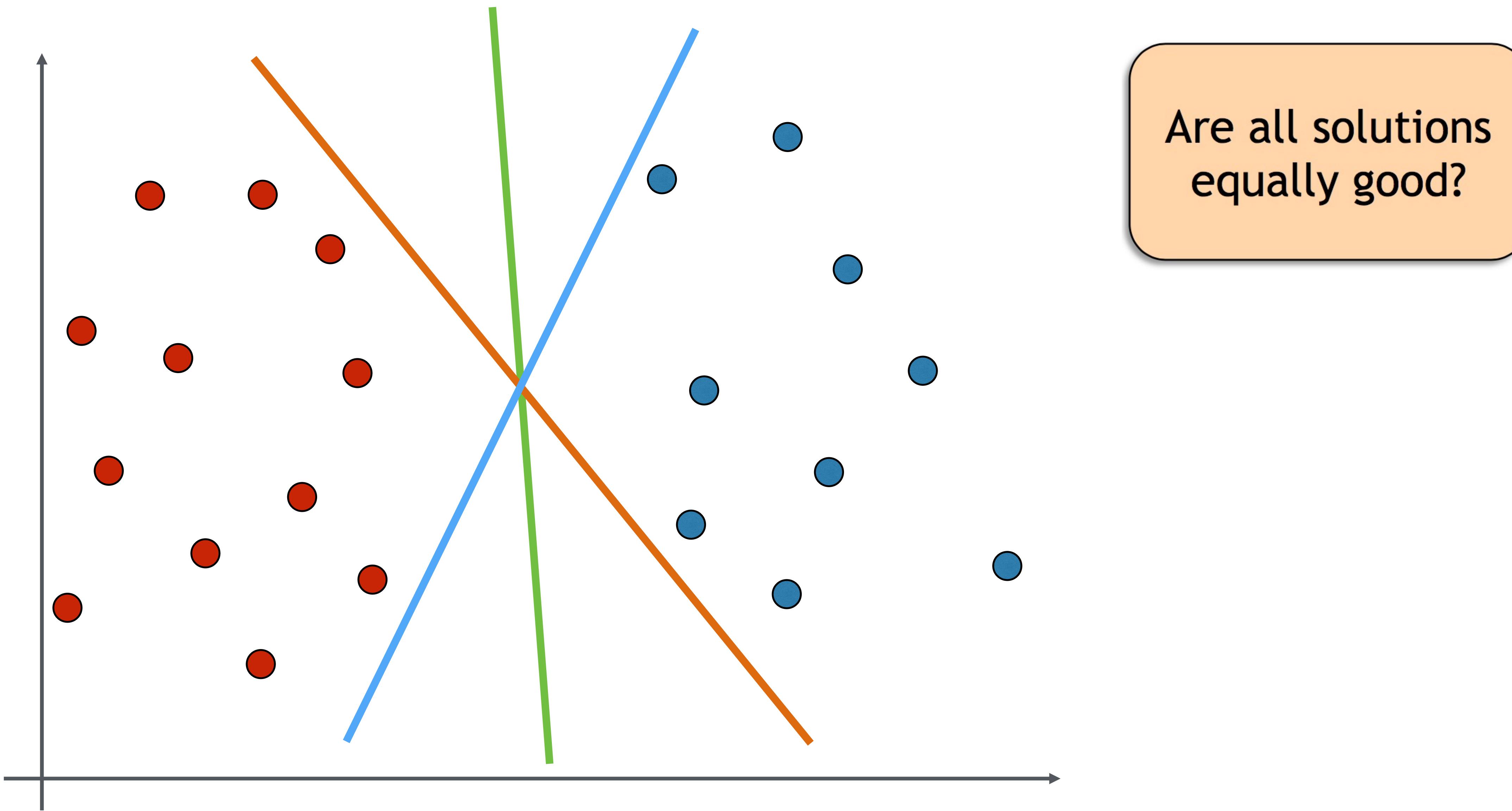
Statistical Methods in AI (CSE 471)

SVM

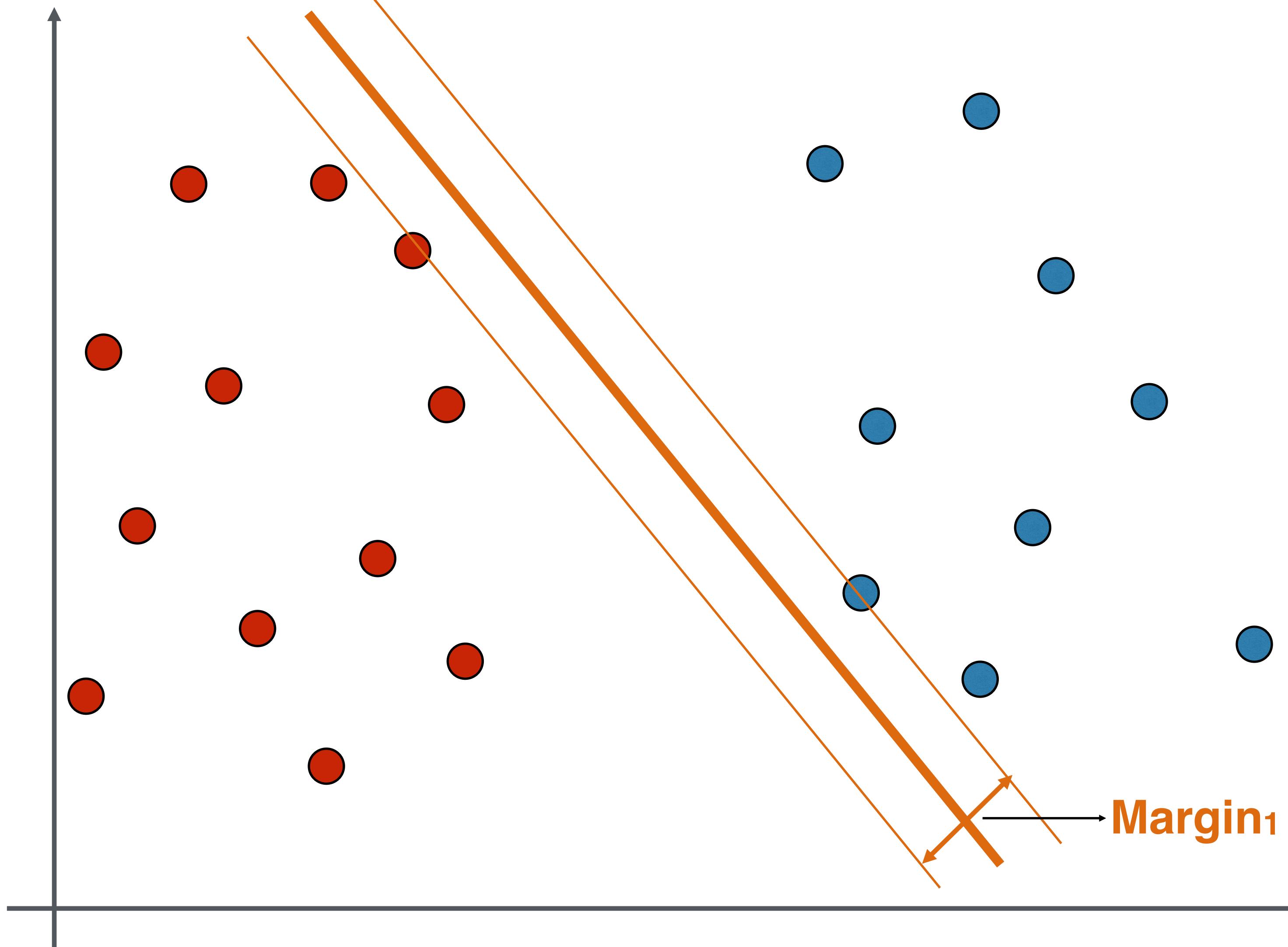
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Multiple solutions exist for linearly separable data



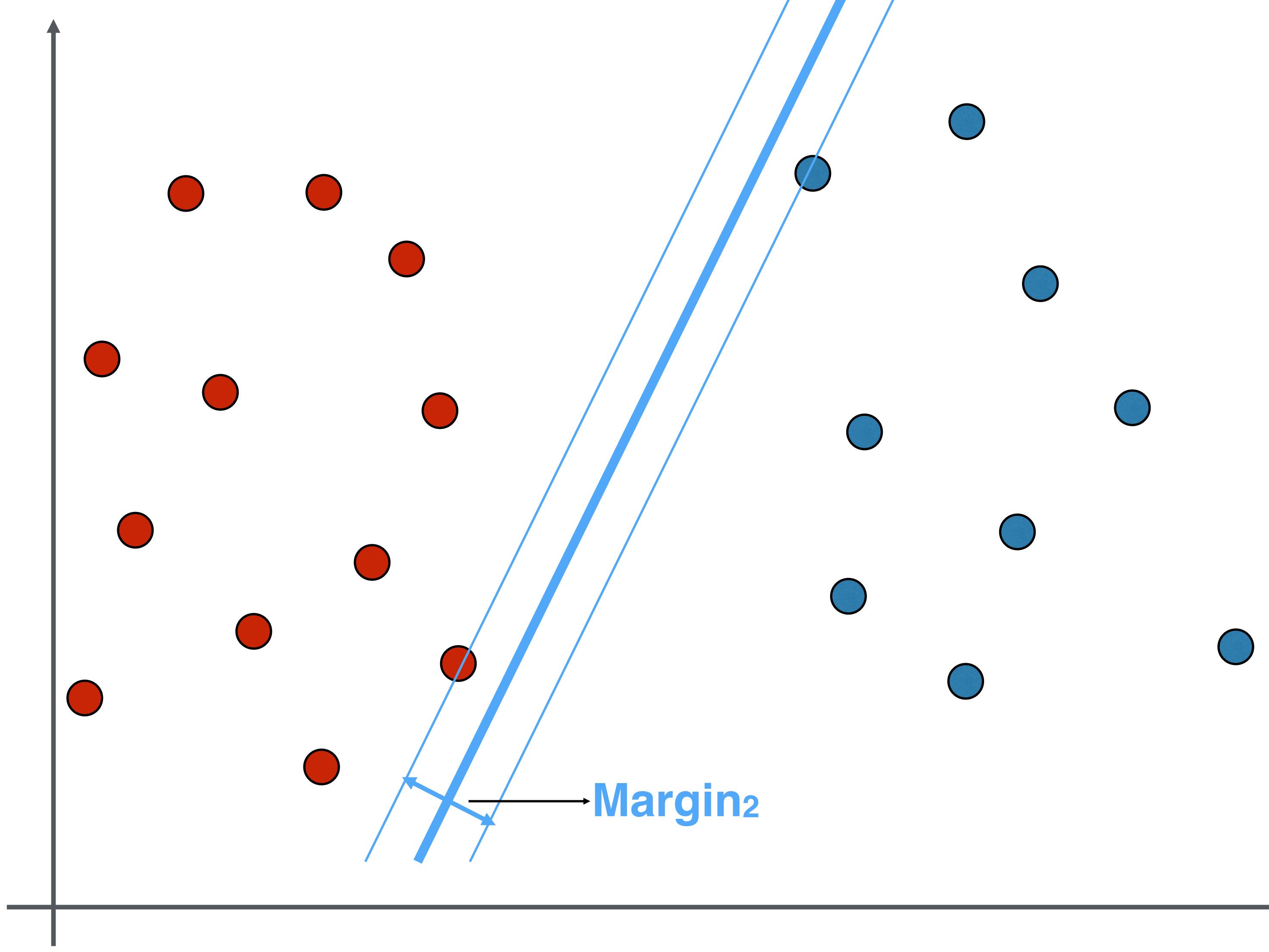
Margin: No-mans Band



Margin: Width of a band around
decision boundary without any
training samples

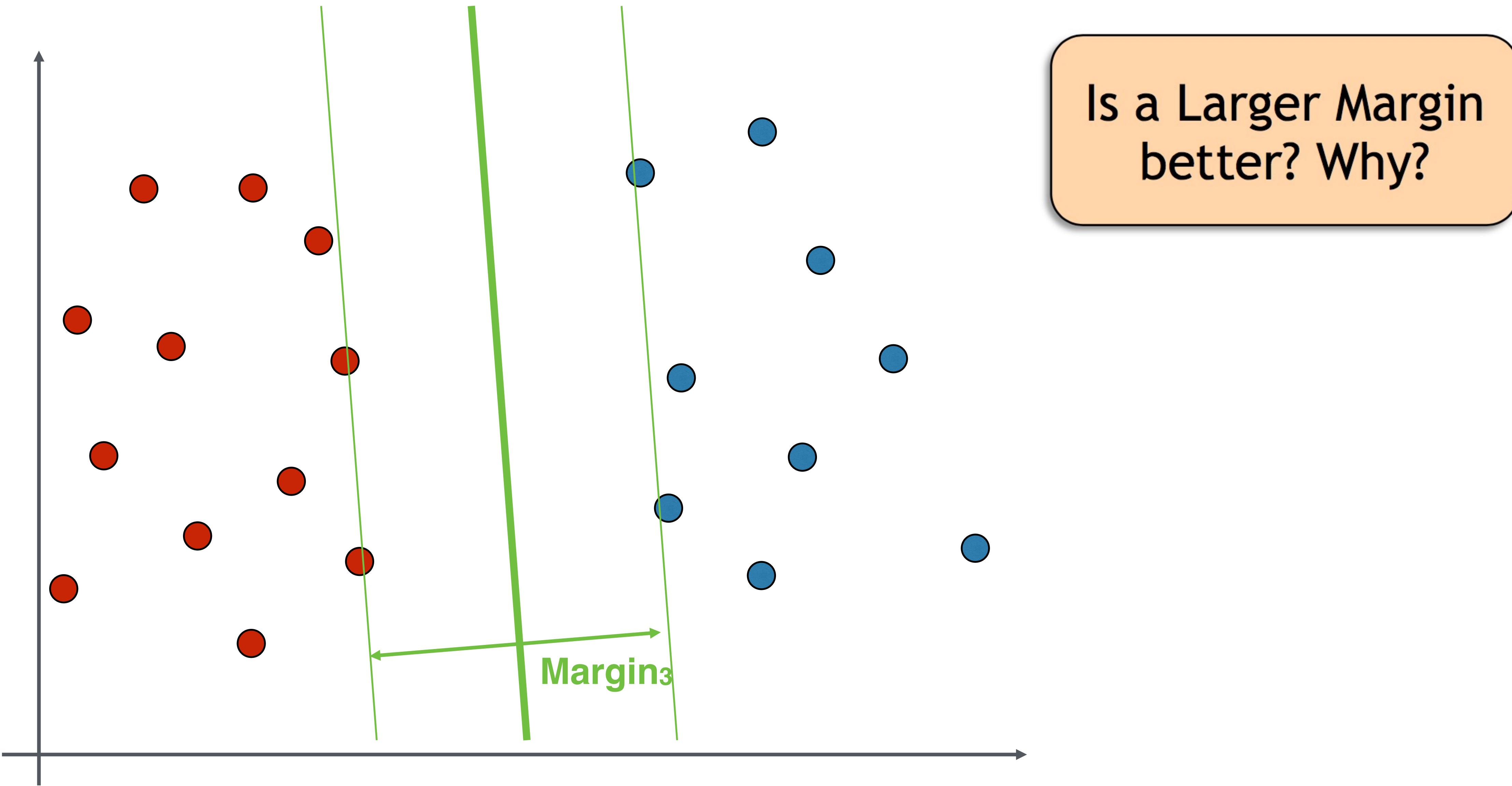
Margin_1

Multiple solutions exist for linearly separable data

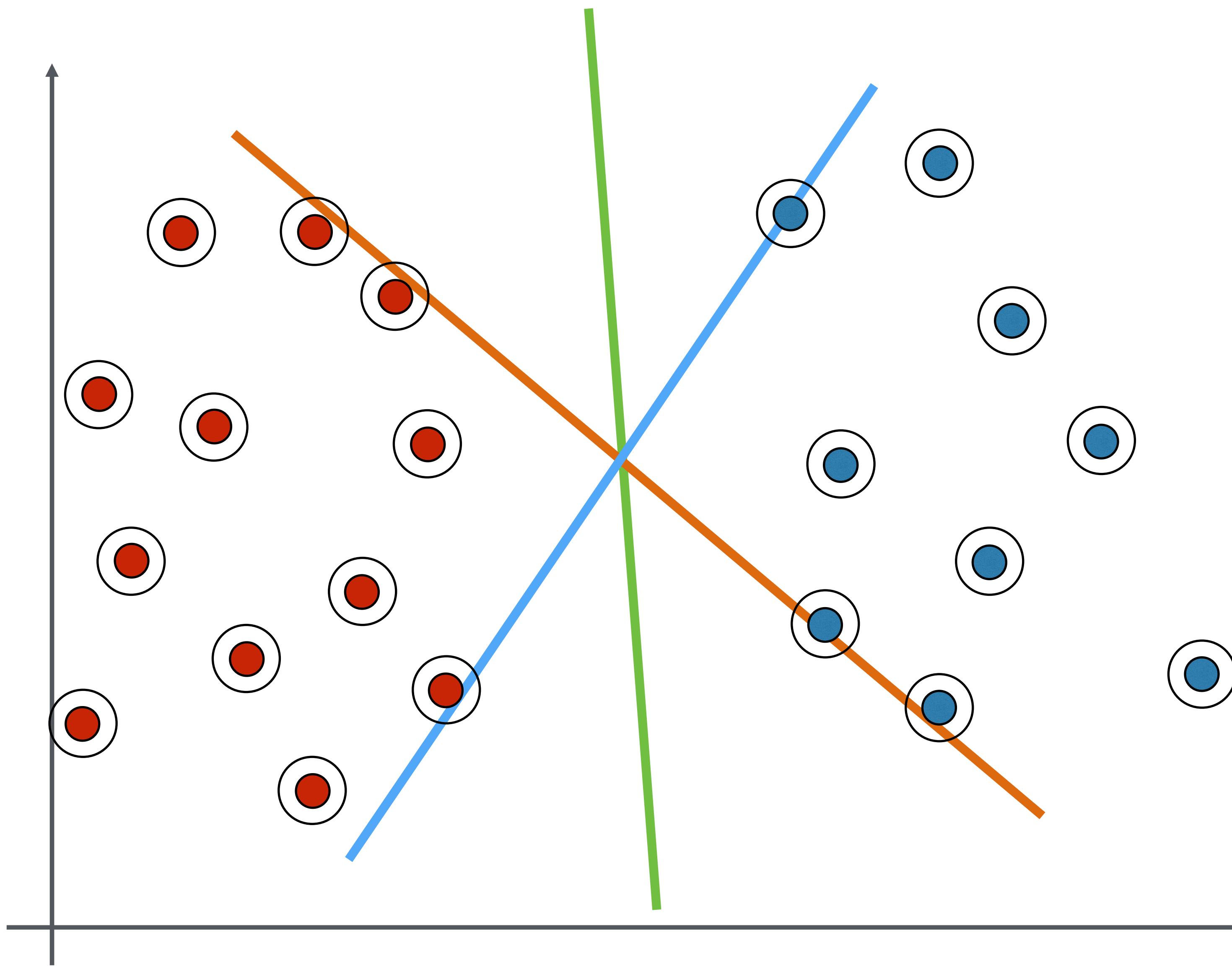


Margin: Width of a band around
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Multiple solutions exist for linearly separable data

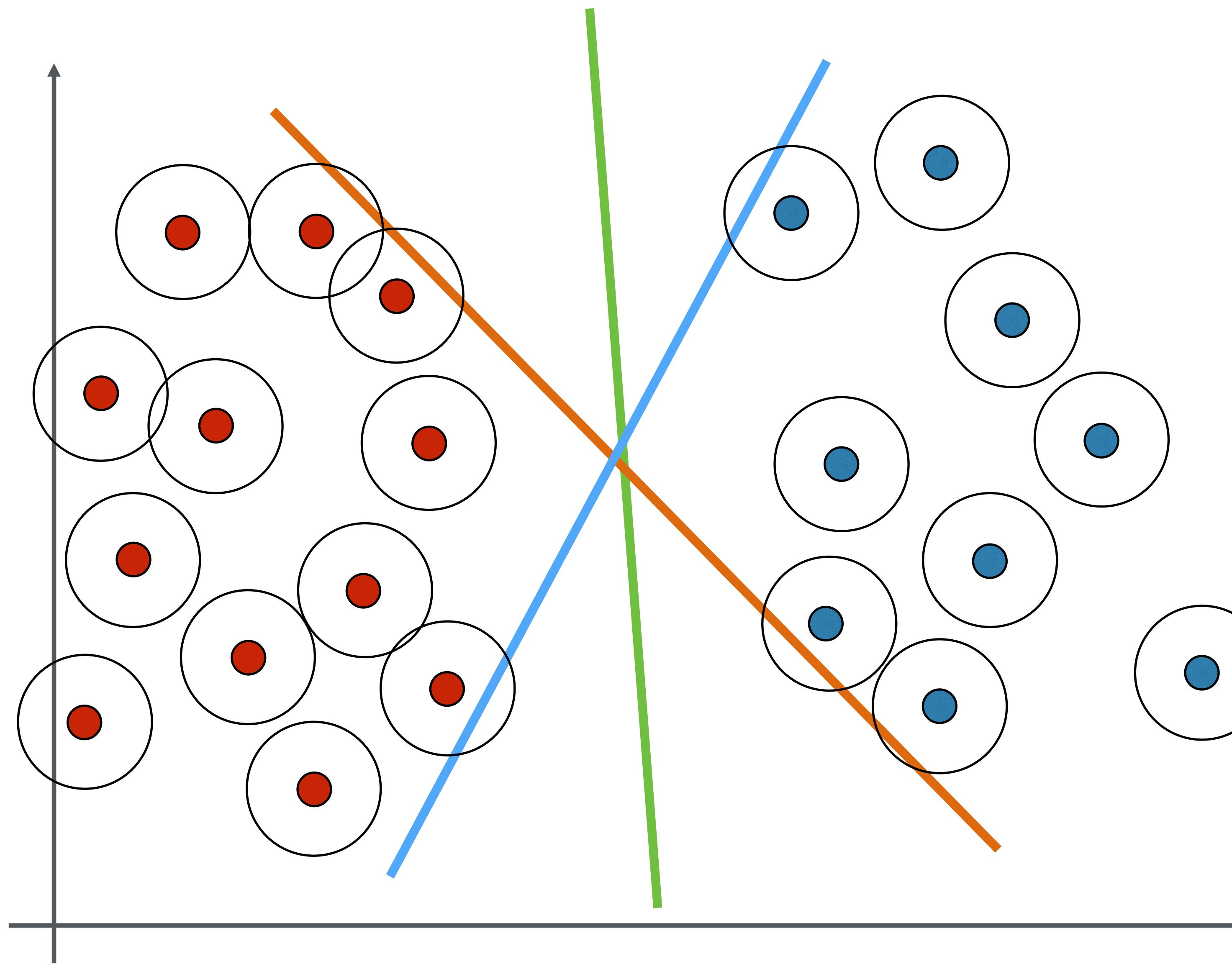


Margin: Bubbles around samples



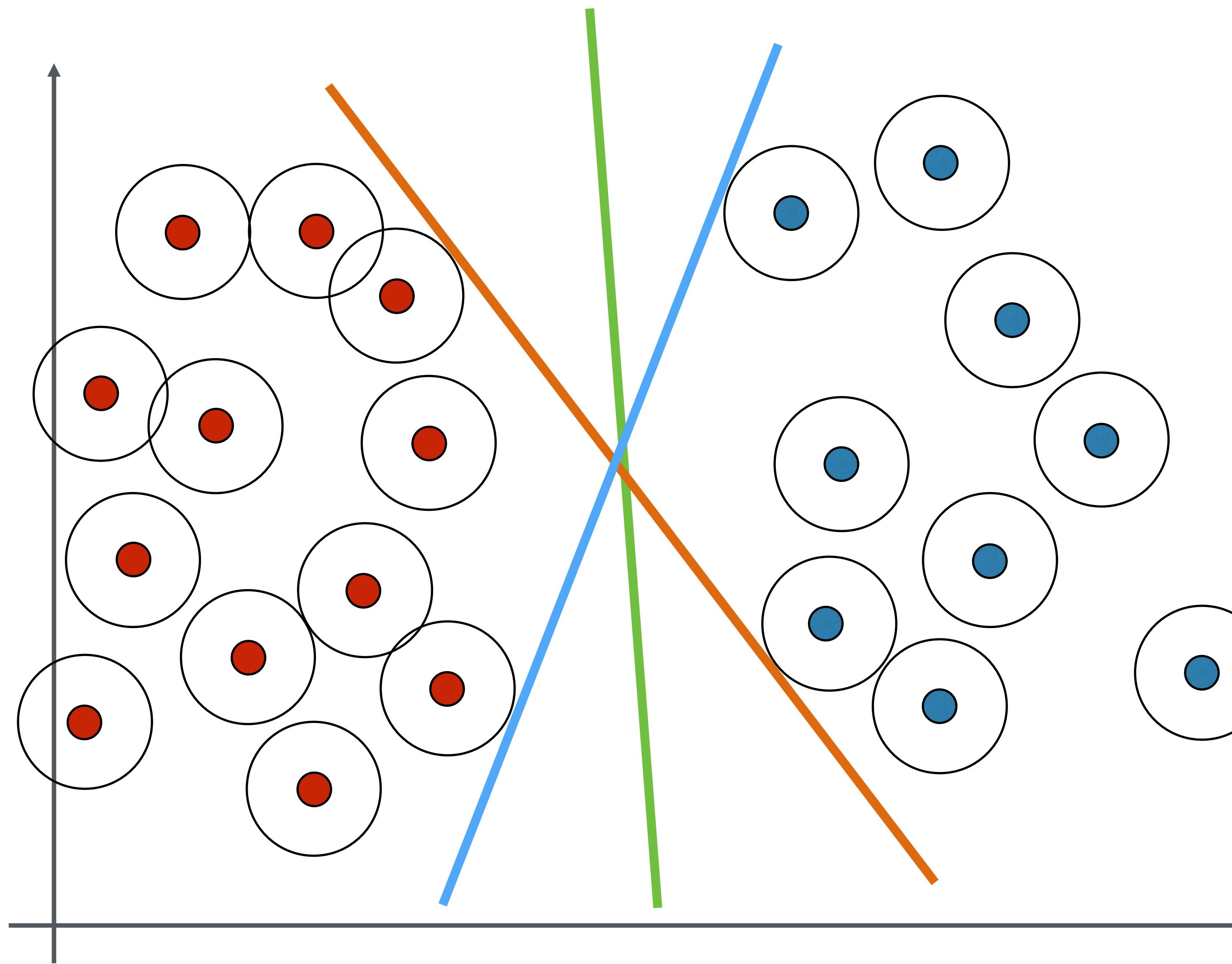
Margin: Radius of a region
around each training sample,
through which the decision
boundary cannot pass

Margin: Bubbles around samples



Margin: Radius of a region around each training sample, through which the decision boundary cannot pass

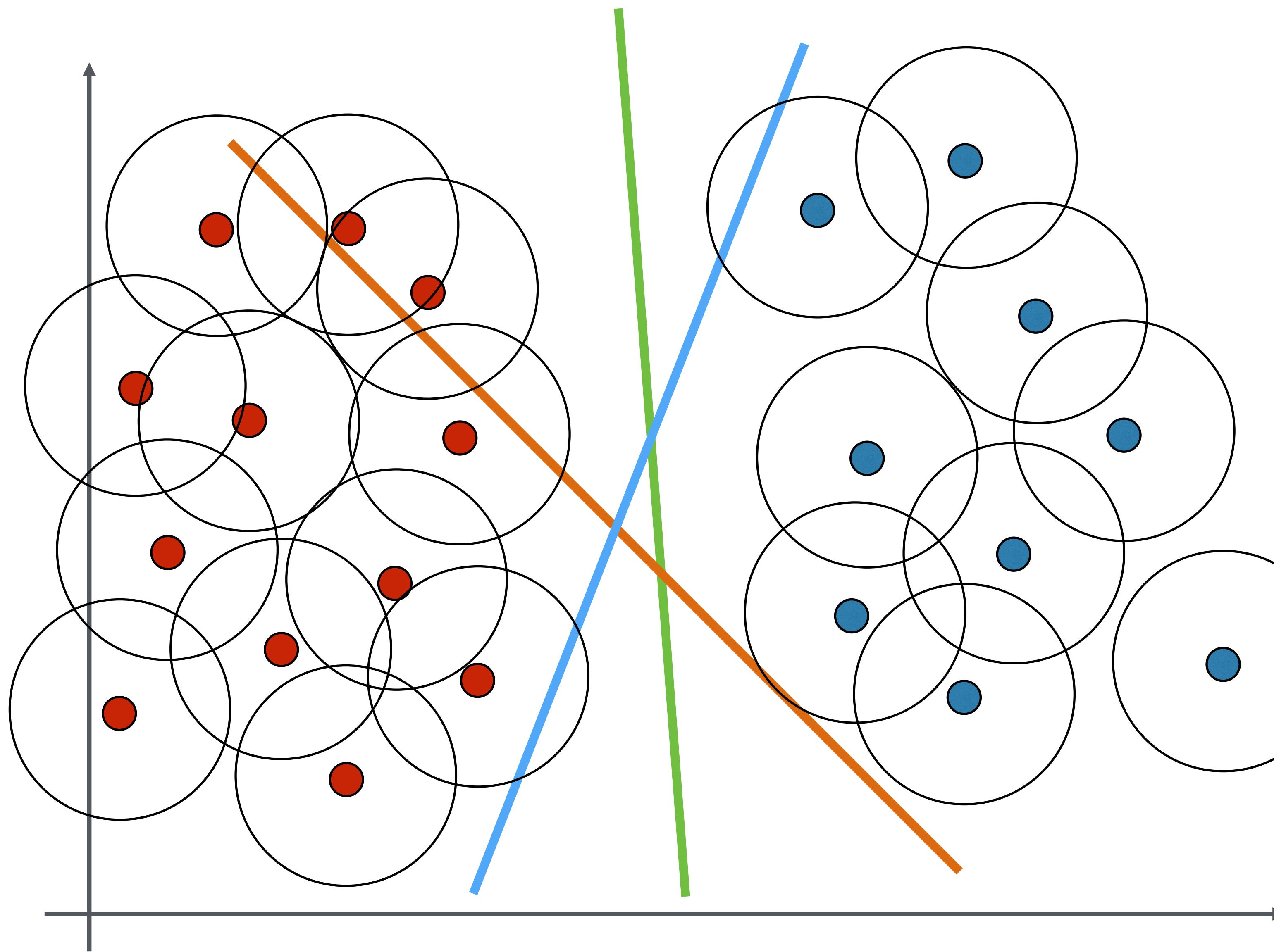
Margin: Bubbles around samples



Margin: Radius of a region around each training sample, through which the decision boundary cannot pass

As the margin increases, the feasible region reduces

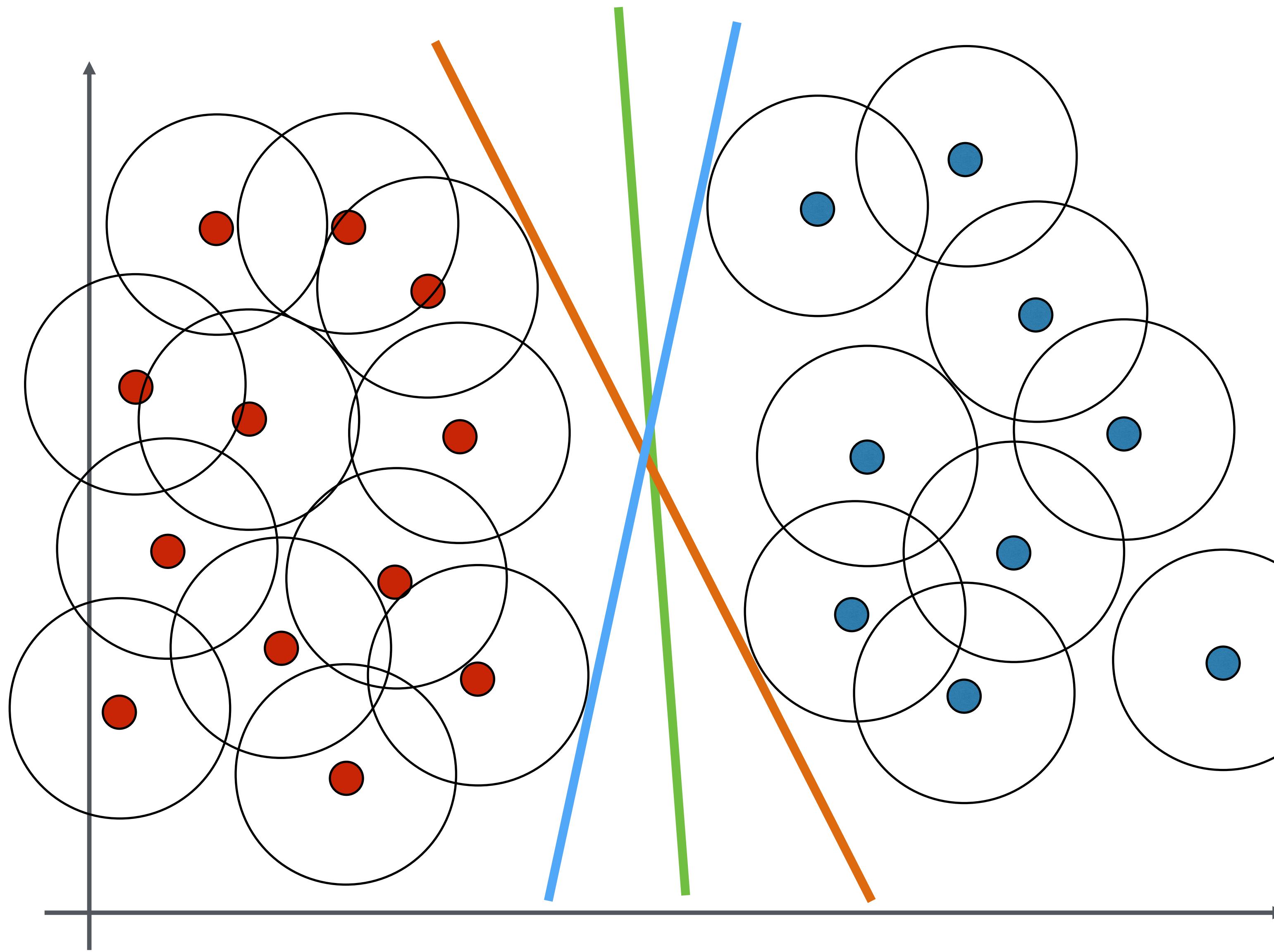
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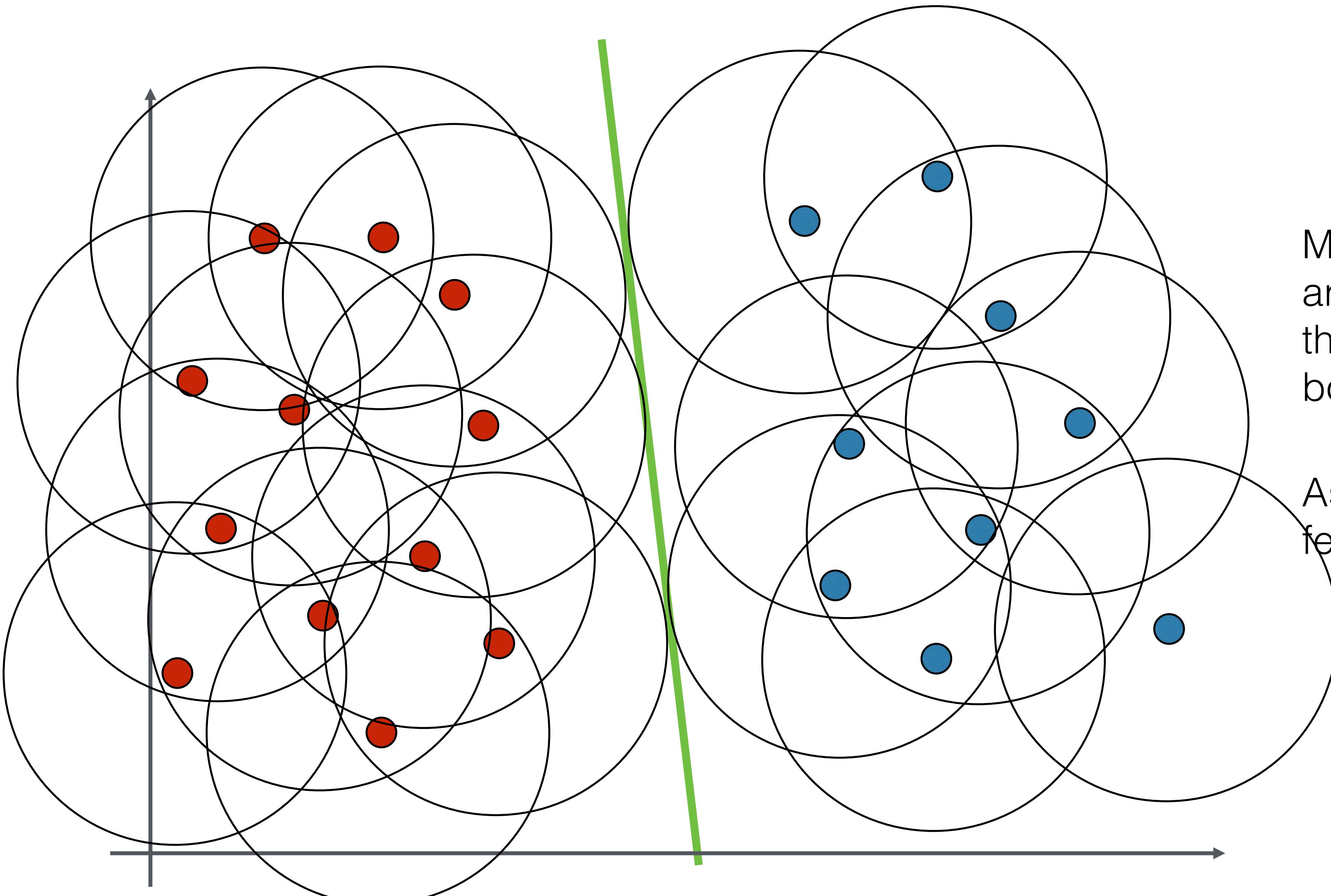
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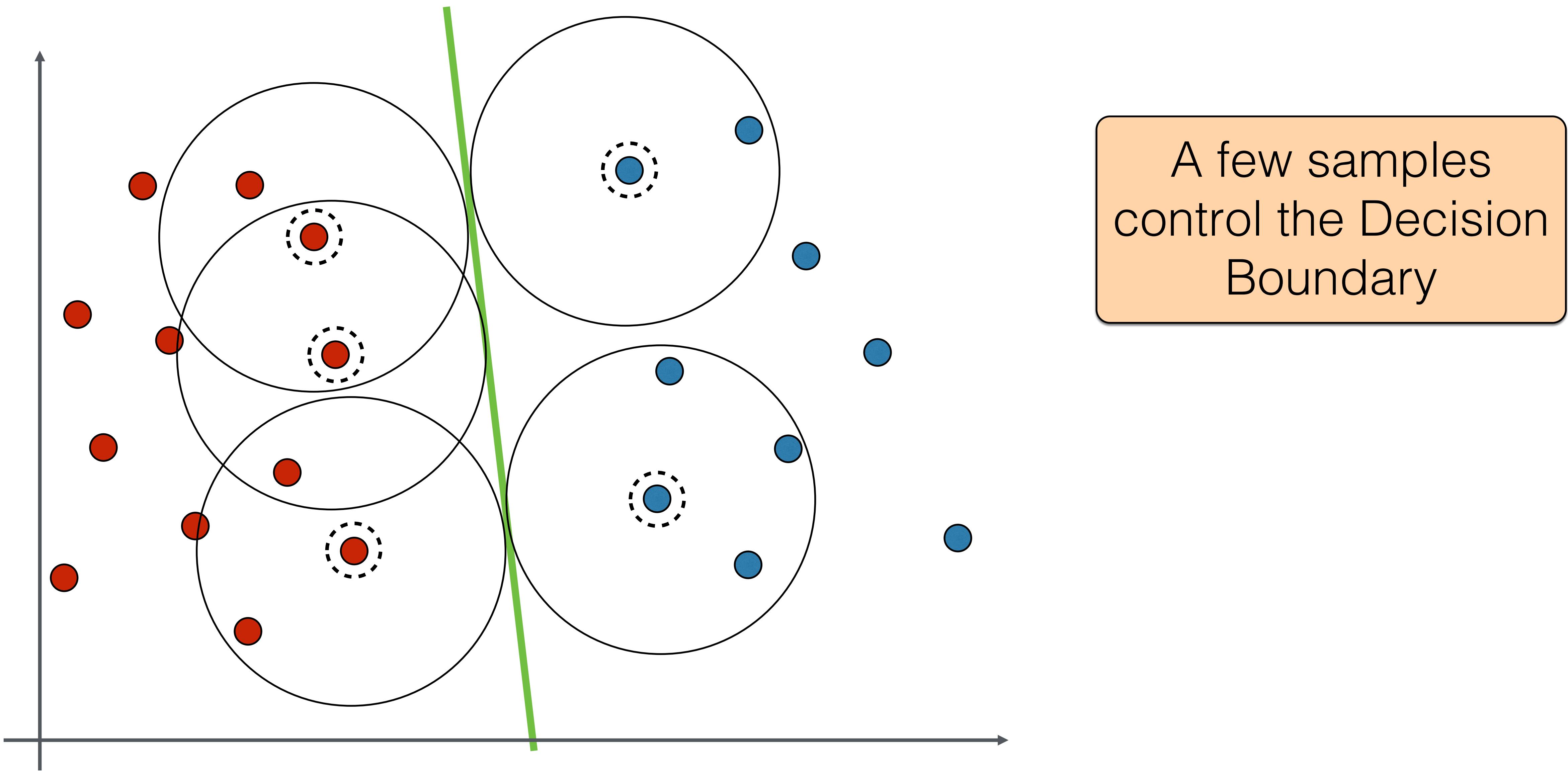
Margin: Bubbles around samples



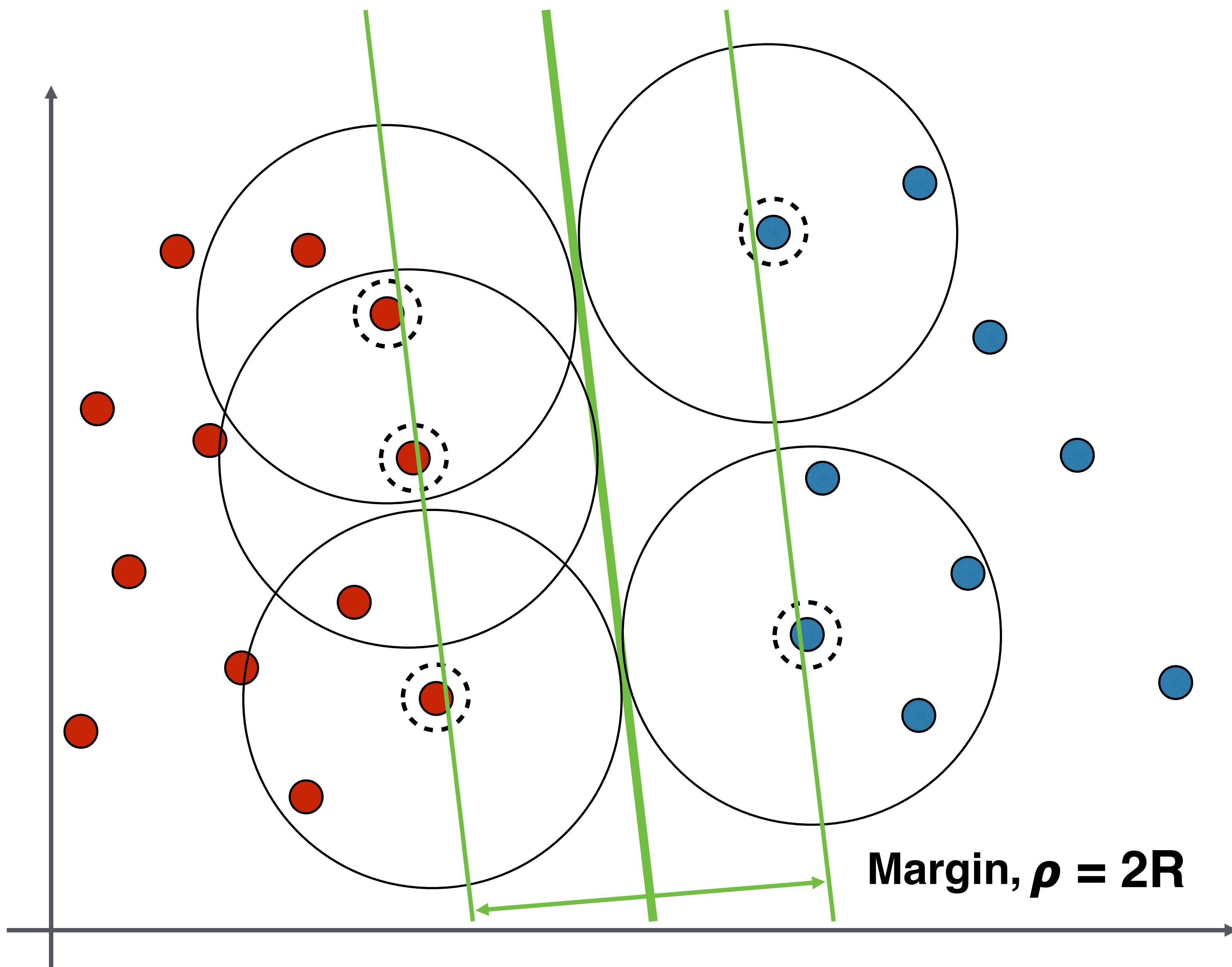
Margin: Radius of a region around each training sample, through which the decision boundary cannot pass

As the margin increases, the feasible region reduces

Margin: Bubbles around samples



Band vs. Bubbles

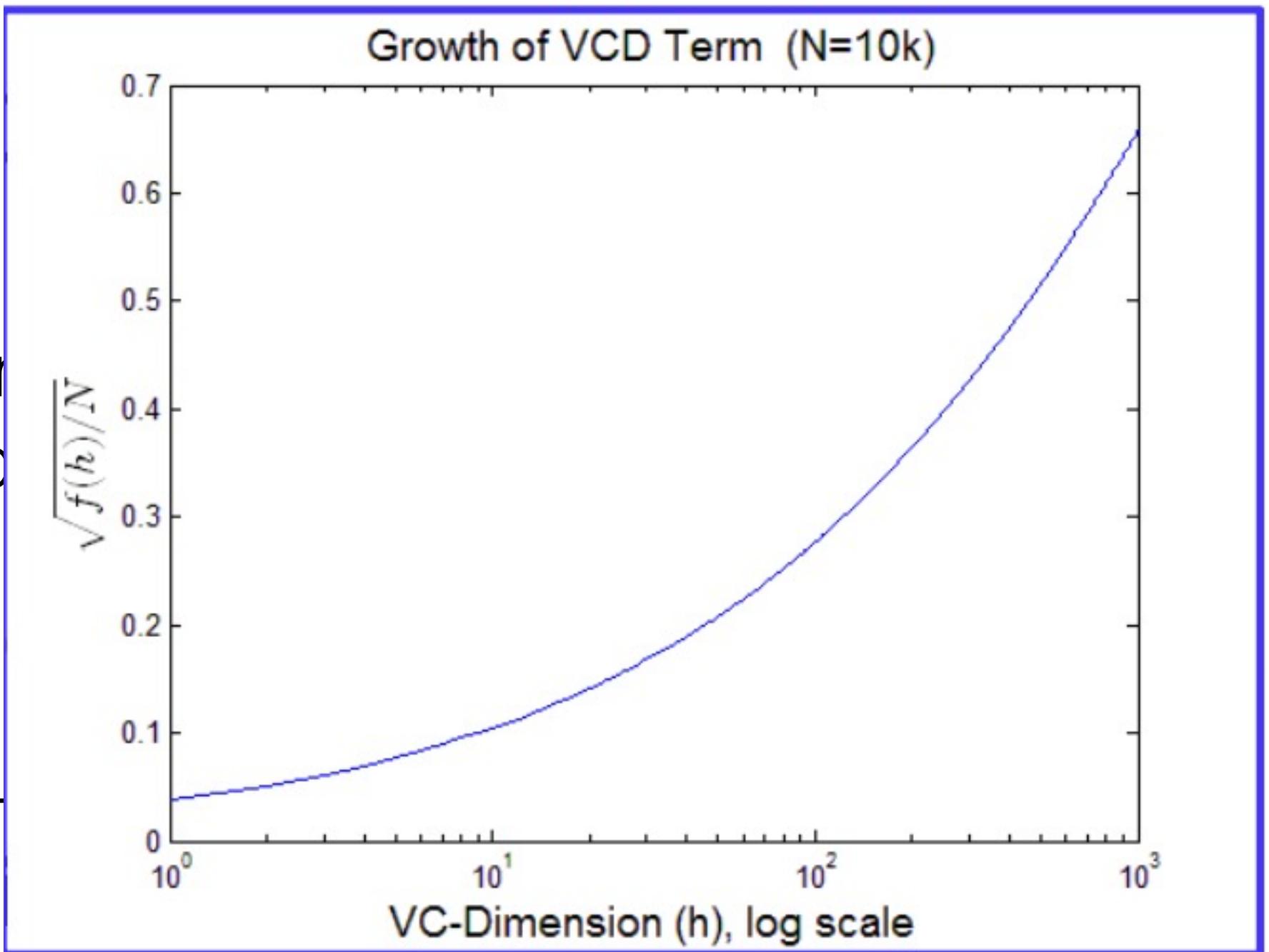


Samples that support the boundary are called **Support Vectors**

Both interpretations lead to the same decision boundary

Breakthrough work from Vapnik

1. Vapnik, Vladimir N., and A. Ya Chervonenkis. "On the uniform convergence of relative frequencies of events to their probabilities." Measures of Complexity and Structure in Recursion Theory. Sov. Mat. Primenen., 1971, Volume 16, Issue 2, Pages 264–279
2. Vapnik, Vladimir N., Estimation of Dependences Based on Empirical Data, Springer, Berlin, 1982.
3. Vapnik, Vladimir N., The Nature of Statistical Learning Theory, Springer, Berlin, 1995.



Bound on expected loss:

$$R(\alpha) \leq R_{train}(\alpha) + \sqrt{\frac{f(h)}{N}}$$

h is the VC dimension, and $f(h)$ is given by:

$$f(h) = h + h \log(2N) - h \log(h) - c$$

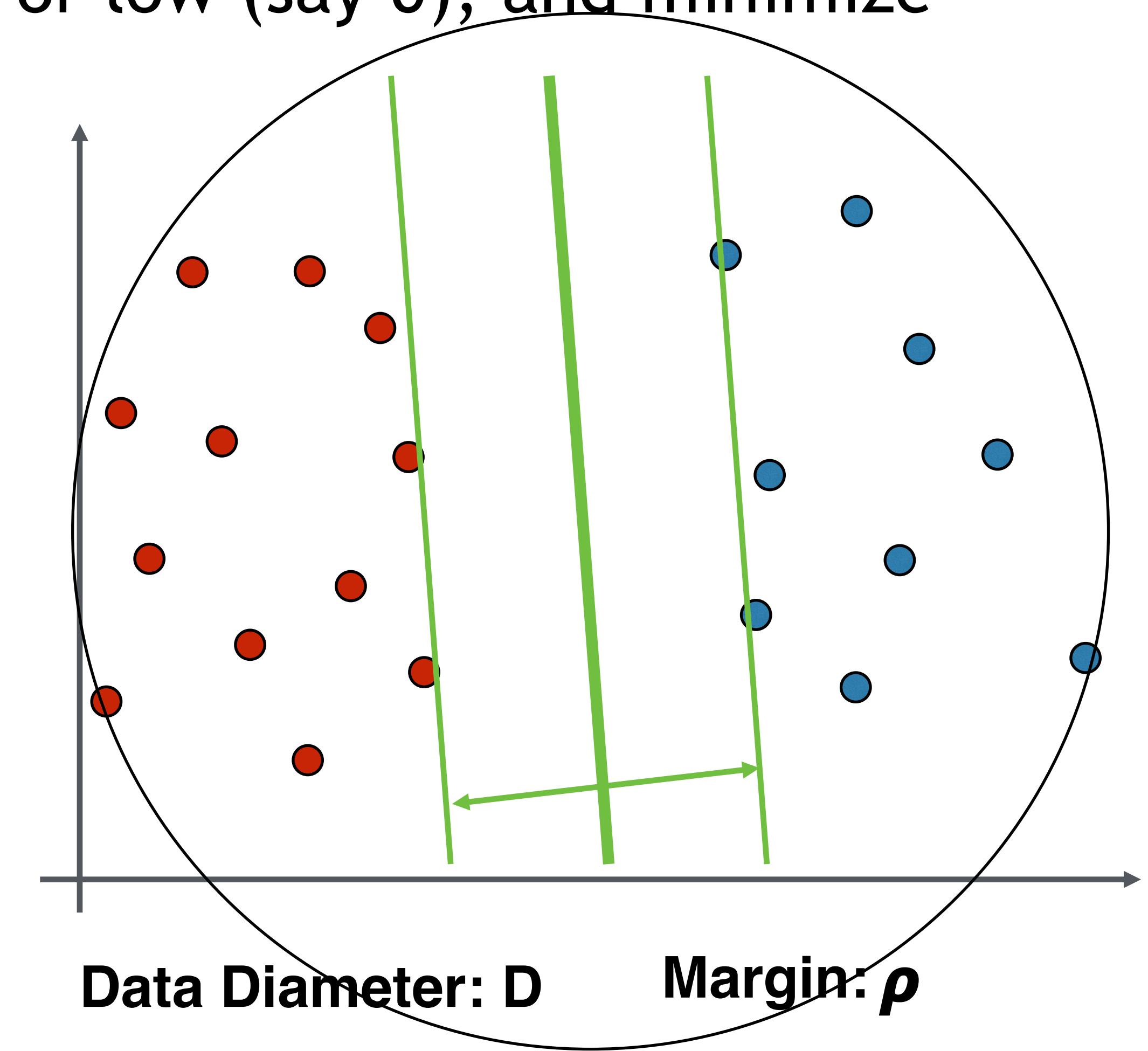
Why maximise the margin?

- To reduce test error, keep training error low (say 0), and minimize the ∇

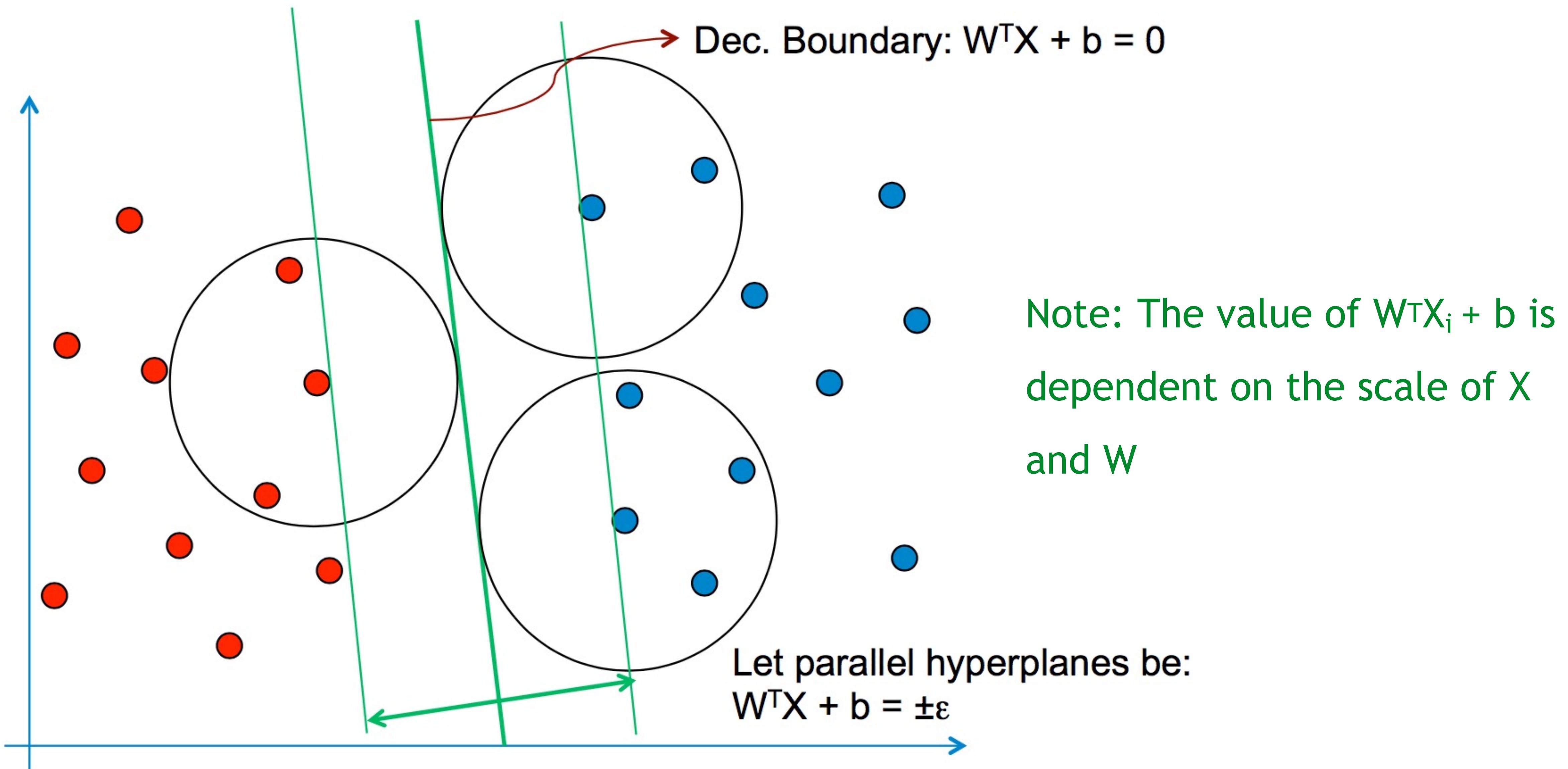
Relative Margin: $\frac{\rho}{D}$

$$\text{VC-D, } h \leq \min\left\{d, \left\lceil \frac{D^2}{\rho^2} \right\rceil\right\} + 1$$

- Maximizing margin improves generalization.
- h can be made independent of the dimensionality: d .

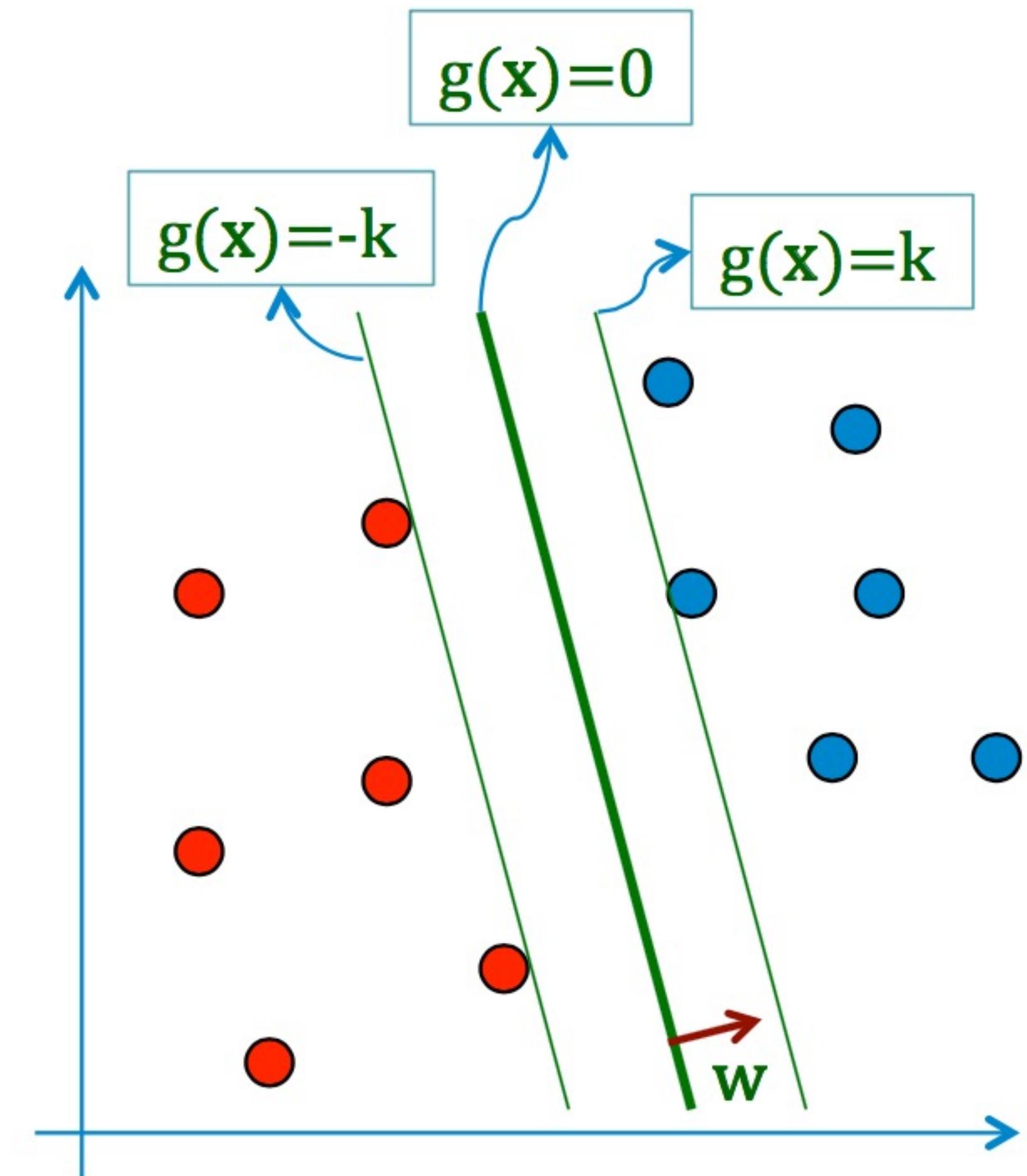


Formalizing the margin



Formulation

- Let $g(x) = w^T x + b$.
- We want to maximize k such that:
 - $w^T x_i + b \geq k$ for $d_i=1$
 - $w^T x_i + b \leq -k$ for $d_i=-1$
- Value of $g(x)$ depends on $\|w\|$:
 1. Keep $\|w\|=1$, and maximize $g(x)$, or
 2. Let $g(x) \geq 1$, and minimize $\|w\|$.
- We use approach (2) and formulate the problem as:
 - Minimize: $\frac{1}{2} w^T w$
 - Subject to: $d_i(w^T x_i + b) \geq 1$, for $i=1..N$



Optimization

Minimize: $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w}$

Subject to: $d_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \geq 0 \quad \forall i$

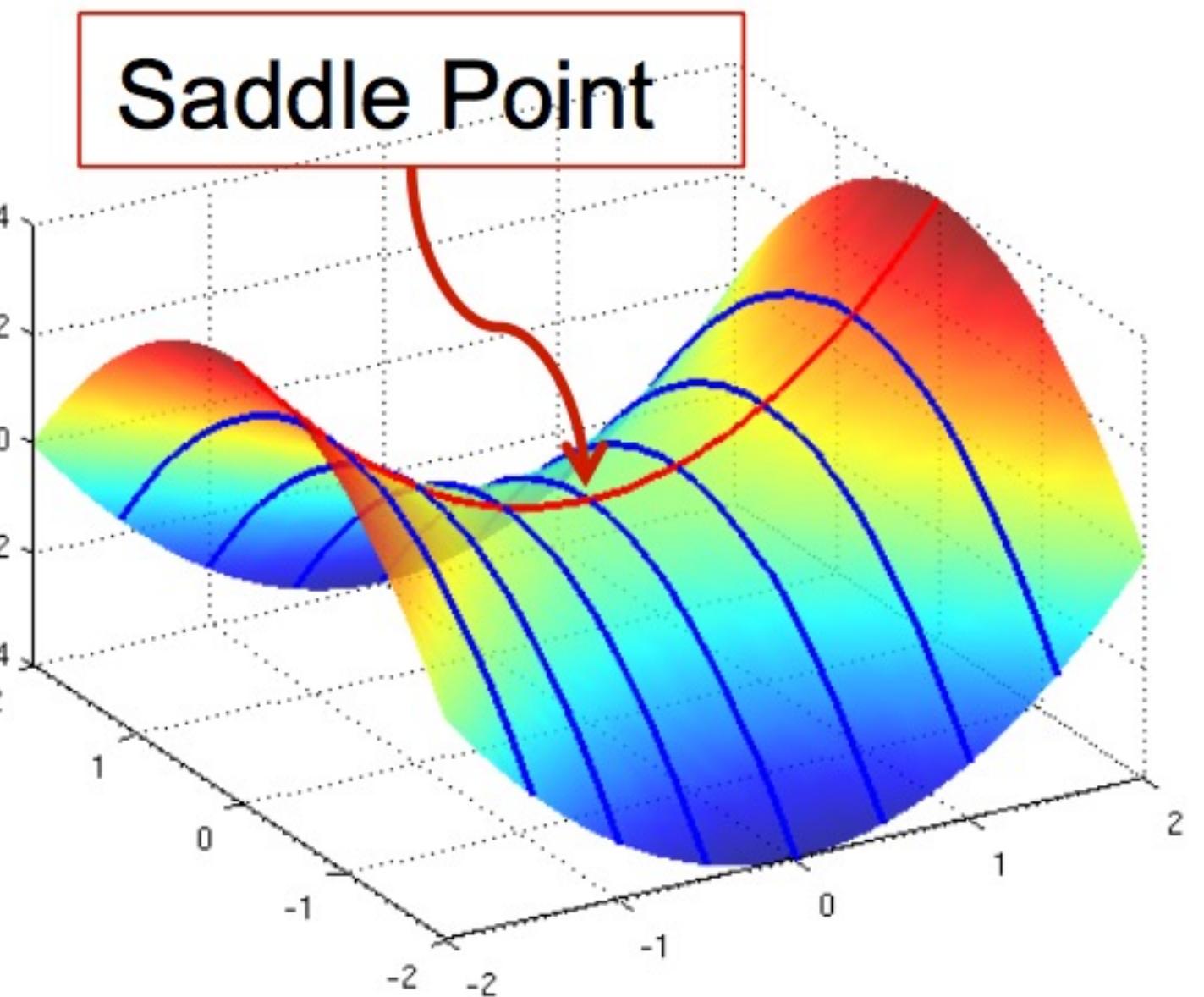
Quadratic function: QP solvers

Lagrangian form:

Minimize: $J(\mathbf{w}, b, \alpha) = \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{i=1}^N \alpha_i d_i(\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^N \alpha_i$

Subject to: $\alpha_i \geq 0 \quad \forall i$

Minimize J with respect to w and b, and maximize with respect to α .



Converting to Dual form

Objective: $J(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{i=1}^N \alpha_i d_i (\mathbf{w}^T \mathbf{x}_i + b) + \sum_{i=1}^N \alpha_i$

At the optimum:

$$1: \frac{\partial J}{\partial \mathbf{w}} = 0$$

and

$$2: \frac{\partial J}{\partial b} = 0$$

$$1: \mathbf{w}_o = \sum_{i=1}^N \alpha_i d_i \mathbf{x}_i$$

$$2: \sum_{i=1}^N \alpha_i d_i = 0$$

$$3: \alpha_i [d_i (\mathbf{w}_o^T \mathbf{x}_i + b_o) - 1] = 0$$

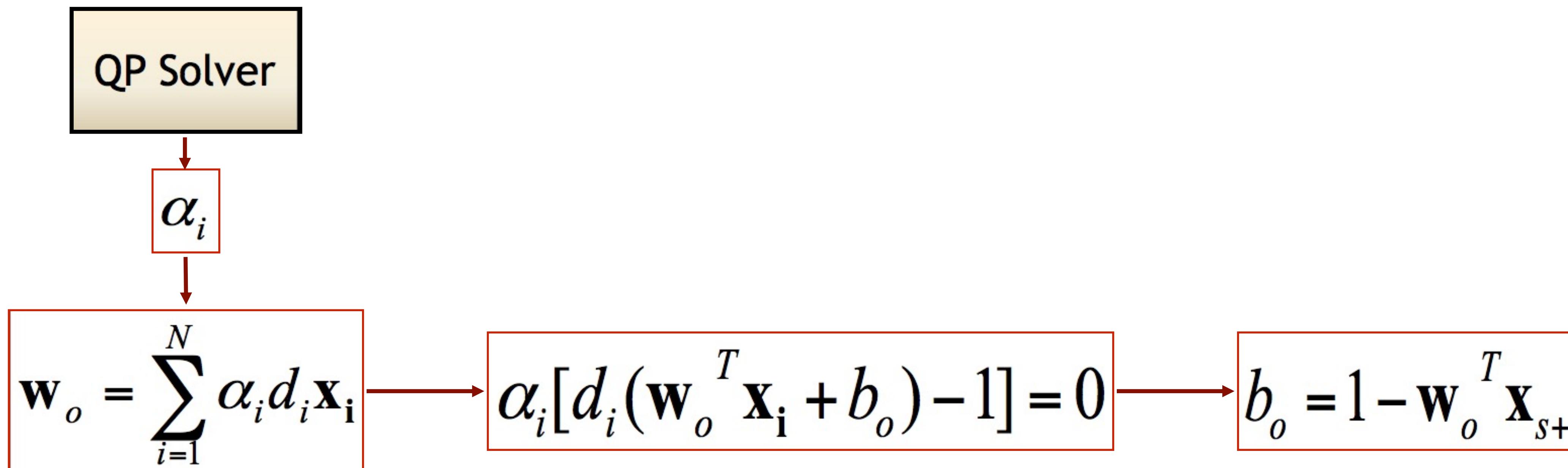
Obj: $J(\mathbf{w}, b, \mathbf{a}) = \sum_{i=1}^N \alpha_i + \frac{1}{2} \mathbf{w}^T \mathbf{w} - \mathbf{w}^T \sum_{i=1}^N \alpha_i d_i \mathbf{x}_i - b \sum_{i=1}^N \alpha_i d_i$

$$Q(\mathbf{a}) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \mathbf{x}_i^T \mathbf{x}_j$$

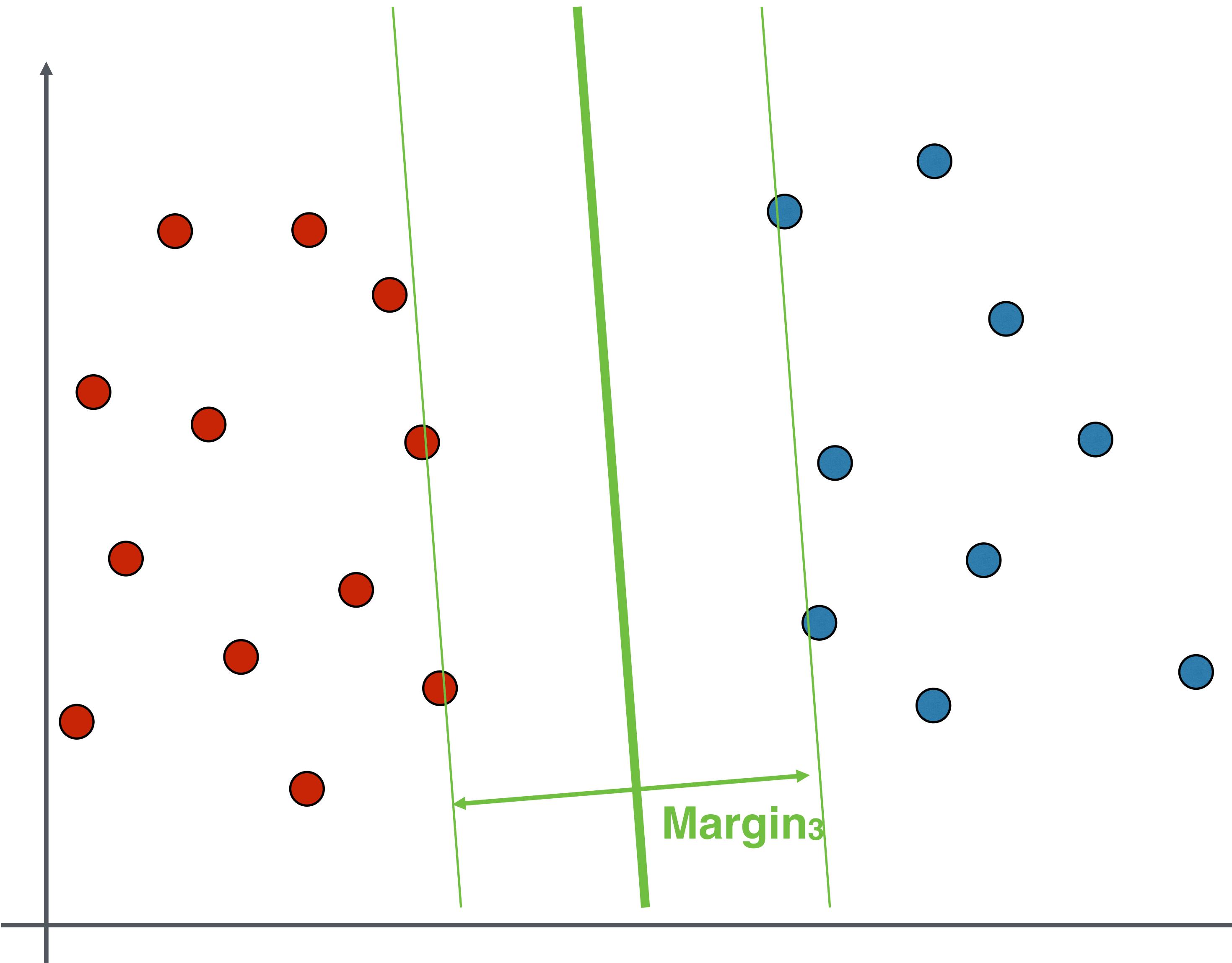
Solving the Dual form

$$Q(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \mathbf{x}_i^T \mathbf{x}_j$$

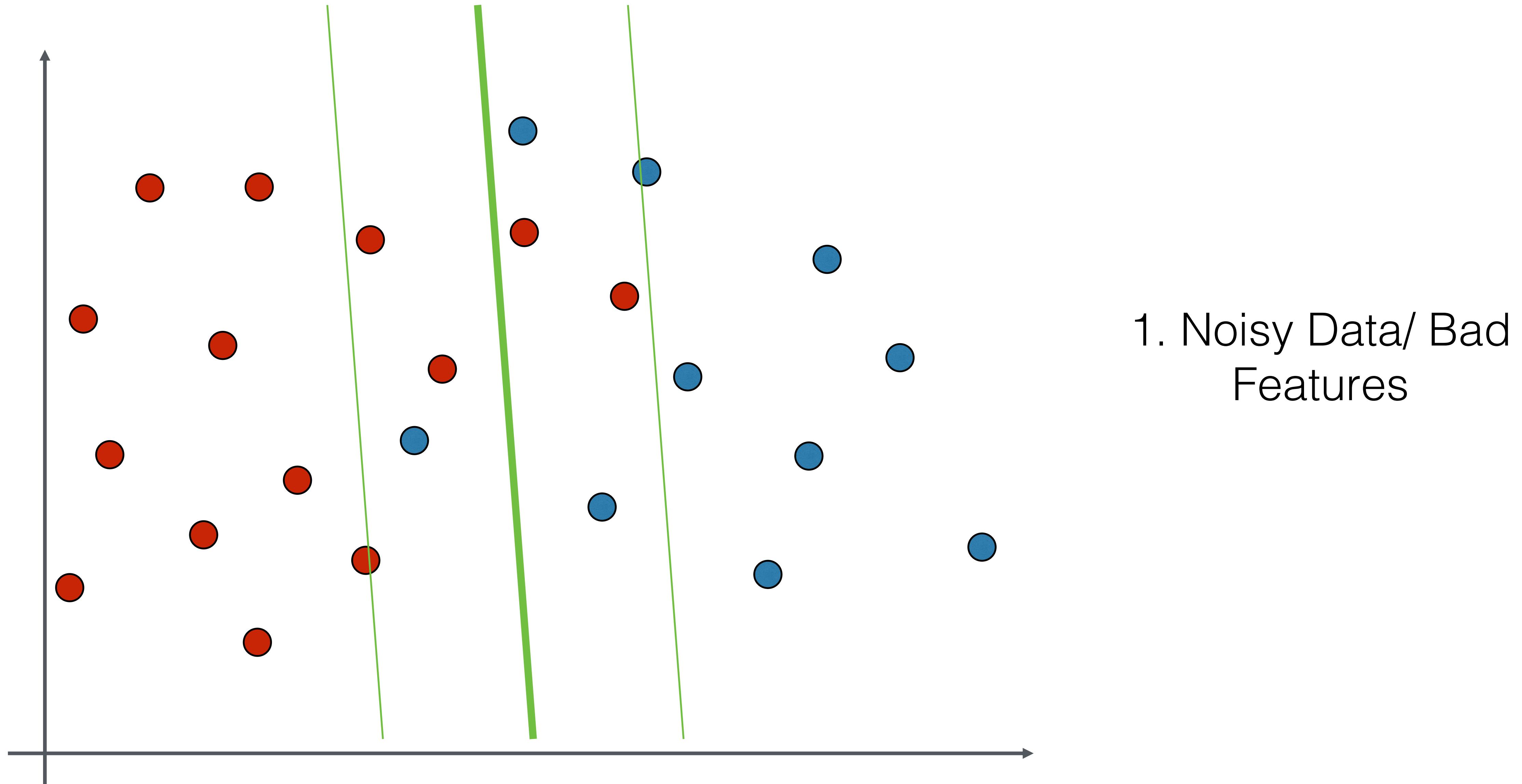
Subject to $\alpha_i \geq 0 \quad \forall i$ and $\sum_{i=1}^N \alpha_i d_i = 0$



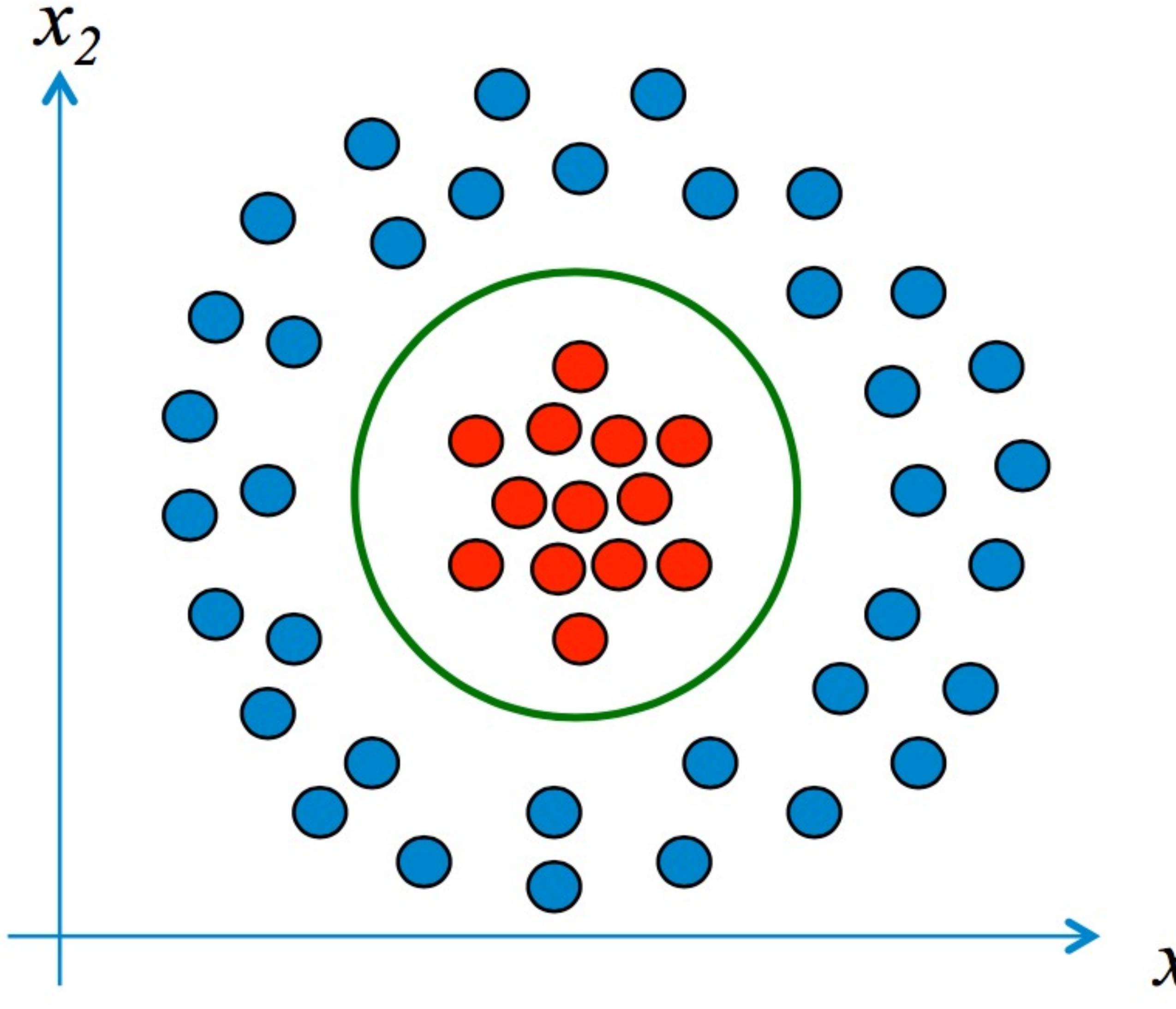
Non Separable Data



Non Separable Data

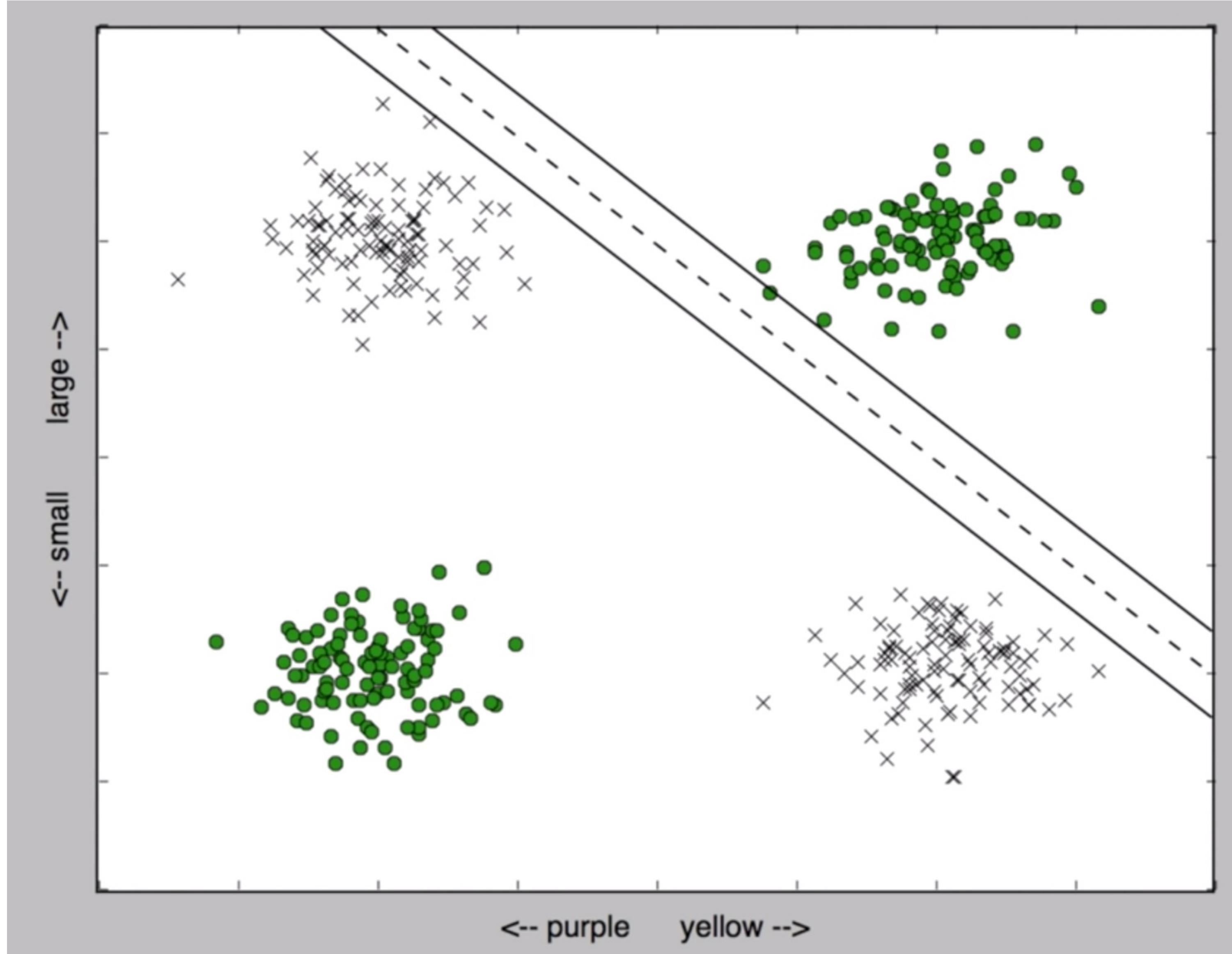


Non Separable Data



2. Non Linear Boundary

Non Separable Data



SVM with Noisy data

$$\text{Minimize: } \Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

$$\text{Subject to: } d_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 \quad \forall i$$

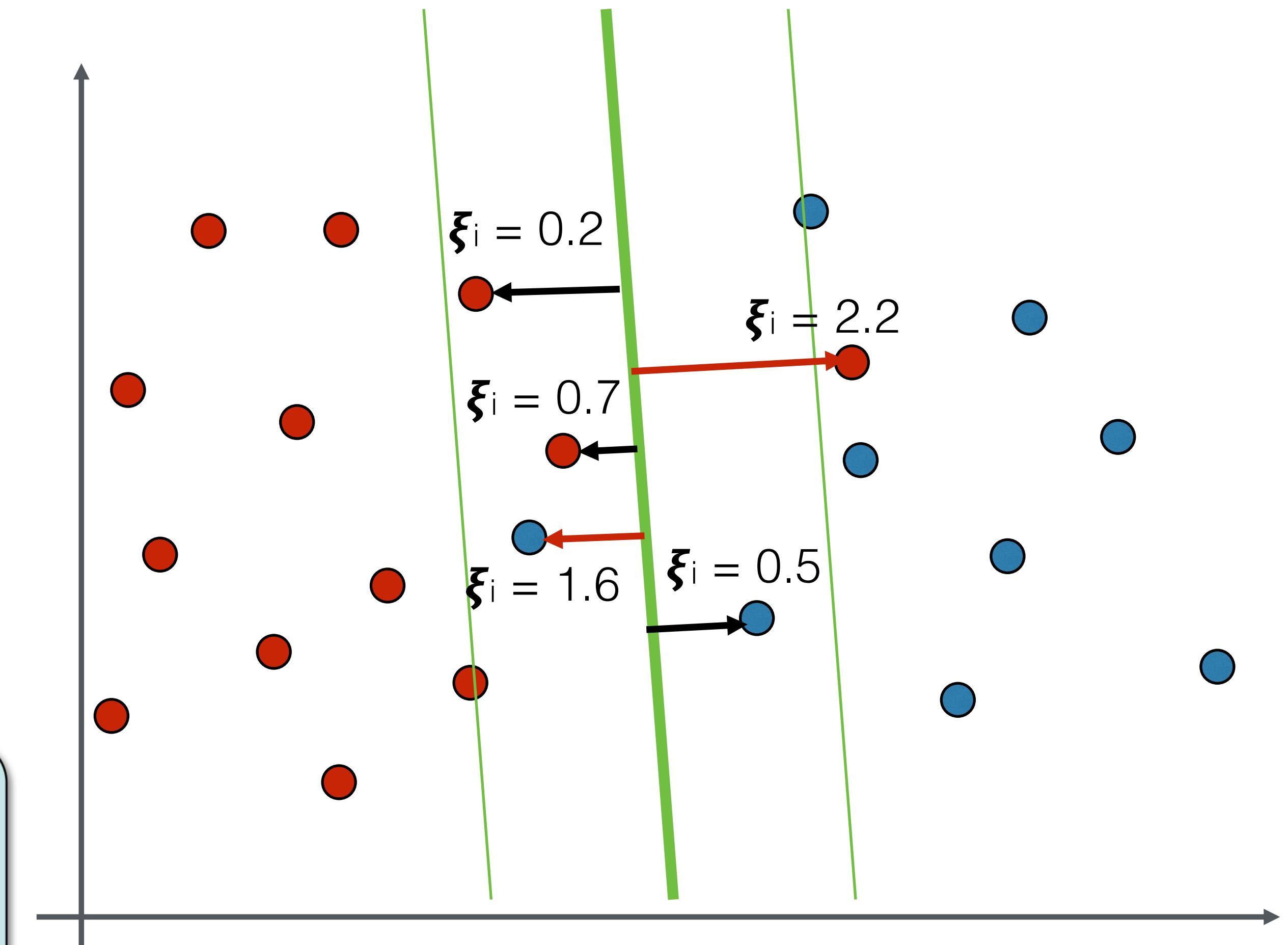
↓
Introduce slack variables $\xi_i \geq 0$

$$\text{Minimize: } \Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

$$\text{Subject to: } d_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \xi_i \quad \forall i$$

$$\text{Minimize: } \Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi_i$$

$$\text{Subject to: } d_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \xi_i ; \quad \xi_i \geq 0 , \quad \forall i$$



Dual Form with Slack variables

$$Q(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \mathbf{x}_i^T \mathbf{x}_j$$

Subject to $\alpha_i \geq 0 \quad \forall i$ and $\sum_{i=1}^N \alpha_i d_i = 0$



$$Q(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \mathbf{x}_i^T \mathbf{x}_j$$

Subject to $0 \leq \alpha_i \leq C \quad \forall i$ and $\sum_{i=1}^N \alpha_i d_i = 0$

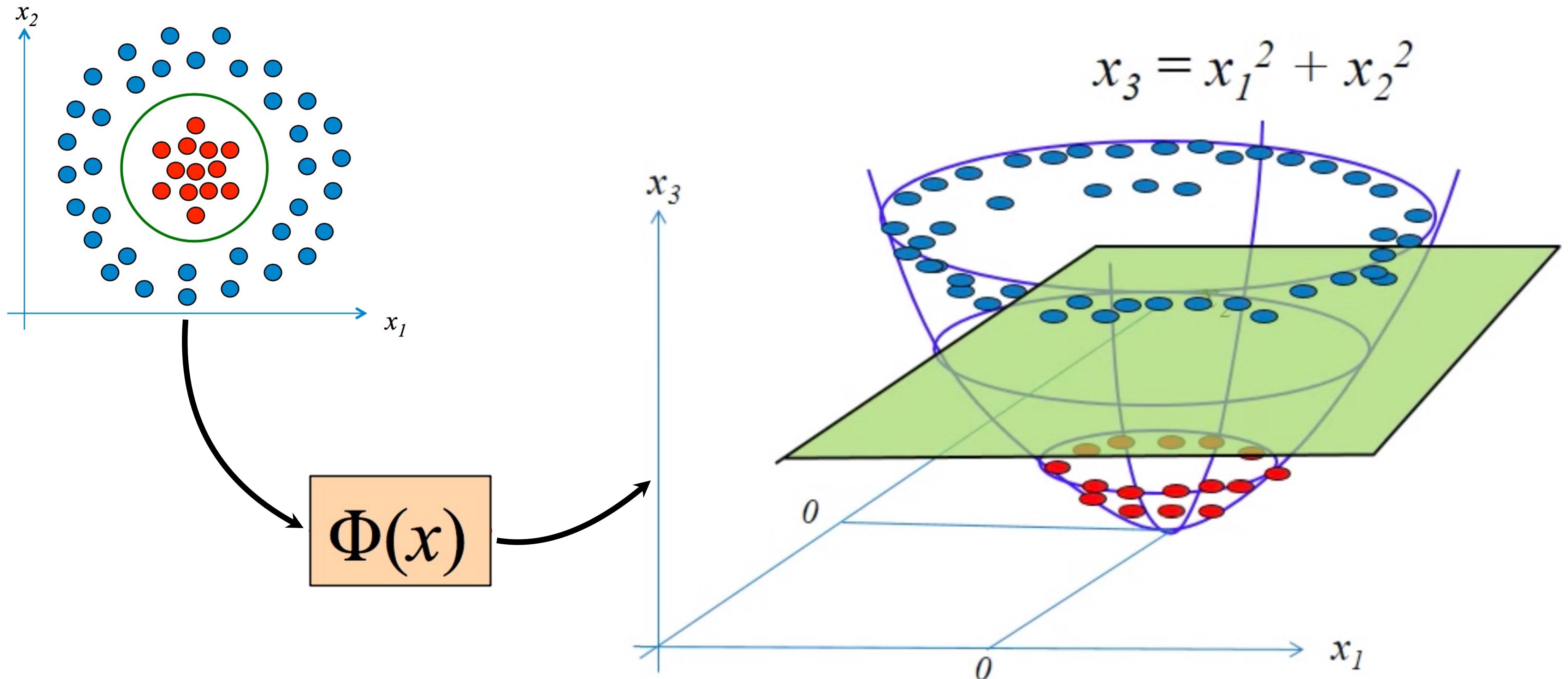
Dual Form with Slack variables

$$Q(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \mathbf{x}_i^T \mathbf{x}_j$$

Subject to $0 \leq \alpha_i \leq C \quad \forall i$ and $\sum_{i=1}^N \alpha_i d_i = 0$

- Note that neither the slack variables, nor their Lagrange multipliers appear in the dual
- The only change is the additional constraint on α_i
- The parameter C controls the relative weight between training error and the VC dimension

Non Linear Boundaries



Non linear mapping from into a higher dimensional space

SVM post mapping

$$Q(\mathbf{a}) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j \Phi(\mathbf{x}_i) \bullet \Phi(\mathbf{x}_j)$$

Training

$$\text{Subject to } 0 \leq \alpha_i \leq C \quad \forall i \quad \text{and} \quad \sum_{i=1}^N \alpha_i d_i = 0$$

$$\text{Label} = sign (\mathbf{w}_o \bullet \Phi(\mathbf{x}_{\text{test}}) + b_o)$$

$$\mathbf{w}_o = \sum_{i=1}^N \alpha_i d_i \Phi(\mathbf{x}_i)$$

$$\therefore \text{Label} = sign \left(\sum_{i=1}^N (\alpha_i d_i \Phi(\mathbf{x}_i) \bullet \Phi(\mathbf{x}_{\text{test}})) + b_o \right)$$

Testing

SVM post mapping

- Data vectors occur only as dot products in SVM-learning and testing
- If we can find a function $K(X, Y)$, which is equivalent to $\Phi(X) \cdot \Phi(Y)$, we can avoid explicit mapping to high dimensions.

$$Q(\mathbf{a}) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j d_i d_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{Label} = sign \left(\sum_{i=1}^N (\alpha_i d_i K(\mathbf{x}_i, \mathbf{x}_{\text{test}})) + b_o \right)$$

What do we gain by using K?

$$\text{Let } \Phi(\mathbf{X}) = \Phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_2 x_1 \\ x_2 x_2 \end{bmatrix}$$

$$\text{Let } K(\mathbf{X}, \mathbf{Y}) = \Phi(\mathbf{X}) \bullet \Phi(\mathbf{Y}) = \begin{bmatrix} x_1^2 \\ x_1 x_2 \\ x_2 x_1 \\ x_2^2 \end{bmatrix} \bullet \begin{bmatrix} y_1^2 \\ y_1 y_2 \\ y_2 y_1 \\ y_2^2 \end{bmatrix}$$

$$= x_1^2 y_1^2 + 2x_1 x_2 y_1 y_2 + x_2^2 y_2^2 = (x_1 y_1 + x_2 y_2)^2 = (\mathbf{X} \bullet \mathbf{Y})^2$$

We can compute $K(\mathbf{X}, \mathbf{Y}) = (\mathbf{X} \bullet \mathbf{Y})^2$ instead of mapping with Φ explicitly and then computing dot product.

What do we gain by using K?

- Original Space: 2-dimensional

Let $K(\mathbf{X}, \mathbf{Y}) = (\mathbf{X} \cdot \mathbf{Y})^3 = (x_1 y_1 + x_2 y_2)^3$

$$\Phi(\mathbf{X}) = \Phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} x_1^3 \\ x_1^2 x_2 \\ x_1 x_2^2 \\ x_2^3 \end{bmatrix}$$

What do we gain by using K?

- Original Space: 3-dimensional

$$\text{Let } K(\mathbf{X}, \mathbf{Y}) = (\mathbf{X} \cdot \mathbf{Y})^3 = (x_1y_1 + x_2y_2 + x_3y_3)^3$$

$$\Phi(\mathbf{X}) = \Phi\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}\right) = \begin{bmatrix} x_1^3 \\ x_2^3 \\ x_3^3 \\ x_1^2 x_2 \\ x_1 x_2^2 \\ x_1^2 x_3 \\ x_1 x_3^2 \\ x_2^2 x_3 \\ x_2 x_3^2 \\ x_1 x_2 x_3 \end{bmatrix}$$

A Generic Polynomial Kernel

- Adding two Kernels gives you a new Kernel:

$$K(\mathbf{X}, \mathbf{Y}) = K_1(\mathbf{X}, \mathbf{Y}) + K_2(\mathbf{X}, \mathbf{Y}) \quad : \quad \Phi(\mathbf{X}) = \begin{bmatrix} \Phi_1(\mathbf{X}) \\ \Phi_2(\mathbf{X}) \end{bmatrix}$$

$$K(\mathbf{X}, \mathbf{Y}) = \Phi(\mathbf{X}) \bullet \Phi(\mathbf{Y}) = \Phi_1(\mathbf{X}) \bullet \Phi_1(\mathbf{Y}) + \Phi_2(\mathbf{X}) \bullet \Phi_2(\mathbf{Y})$$

$$K_p(\mathbf{X}, \mathbf{Y}) = (1 + \mathbf{X} \bullet \mathbf{Y})^p = 1 + \mathbf{X} \bullet \mathbf{Y} + (\mathbf{X} \bullet \mathbf{Y})^2 + \dots + (\mathbf{X} \bullet \mathbf{Y})^p$$

Just adding a 1 and raising to the power of p maps the input vector into a space containing all original dimensions, all 2-products, 3-products,..,p-products.

Mercer's Theorem

- Using Kernels, we avoid explicit mapping with Φ
- In fact, we do not even have to know what Φ is as long as we are sure there exists a valid Φ
- Mercer's Theorem:

Any given kernel can be expanded as a series :

$$K(\mathbf{X}, \mathbf{Y}) = \sum_{i=1}^{\infty} \lambda_i \Phi_i(\mathbf{X}) \cdot \Phi_i(\mathbf{Y}), \quad \lambda_i > 0; \text{ iff}$$

$K(\mathbf{X}, \mathbf{Y})$ satisfies the Mercer's conditions

(symmetric, continuous, positive semi - definite)

Popular Kernels

- Polynomial:

$$K_p(\mathbf{X}, \mathbf{Y}) = (1 + \mathbf{X} \cdot \mathbf{Y})^p$$

- Radial Basis Function (RBF) or Gaussian:

$$K_r(\mathbf{X}, \mathbf{Y}) = e^{-\frac{1}{2\sigma^2} \|\mathbf{X} - \mathbf{Y}\|_2^2}$$

- Hyperbolic Tangent:

$$K_s(\mathbf{X}, \mathbf{Y}) = \tanh(\beta_0 \mathbf{X} \cdot \mathbf{Y} + \beta_1)$$