Polyhedral Computation

Linear Classifiers & the SVM

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Statistical Inference

- **Statistical**: useful to study random systems...
  - Mutations, environmental changes *etc.*→ **life is random**!
- **Inference**: learn rules using observations assuming some "stationarity".

in this talk: "**yes/no**" rules = "**binary classification**"

- given an image, does it contain the photograph of a human face?
- given a patient's genome, is it safe/effective to give him medecine `XYZ`?
- given a patient's genome, is (s)he at risk of developing Parkinson's disease?
- *etc.*

"**binary classification**" ⇒ **simple 0/1 predictions** for **well-understood problems**

Data

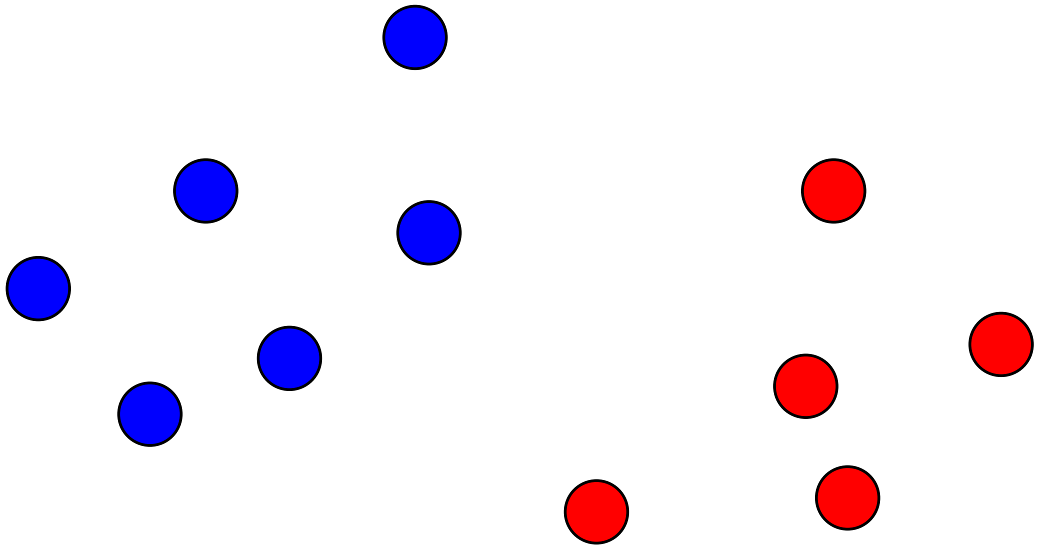
- The **Data** we have: a bunch of vectors $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \cdots, \mathbf{x}_N$.
- Ideally, to infer a "yes/no" rule, we need the **correct answer** for each vector.
- We consider thus a set of **pairs of vector/bit**

$$\text{"training set"} \;=\; \left\{ \left(\mathbf{x}_i = \begin{bmatrix} x_1^i \\ x_2^i \\ \vdots \\ x_d^i \end{bmatrix} \in \mathbb{R}^d,\; \mathbf{y}_i \in \{0,1\} \right)_{i=1..N} \right\}$$

- For illustration purposes **only** we will consider **vectors in the plane**, $d = 2$.
- Points are easier to represent in 2 dimensions than in 20.000...
- The ideas for $d \gg 3$ are **exactly the same**.

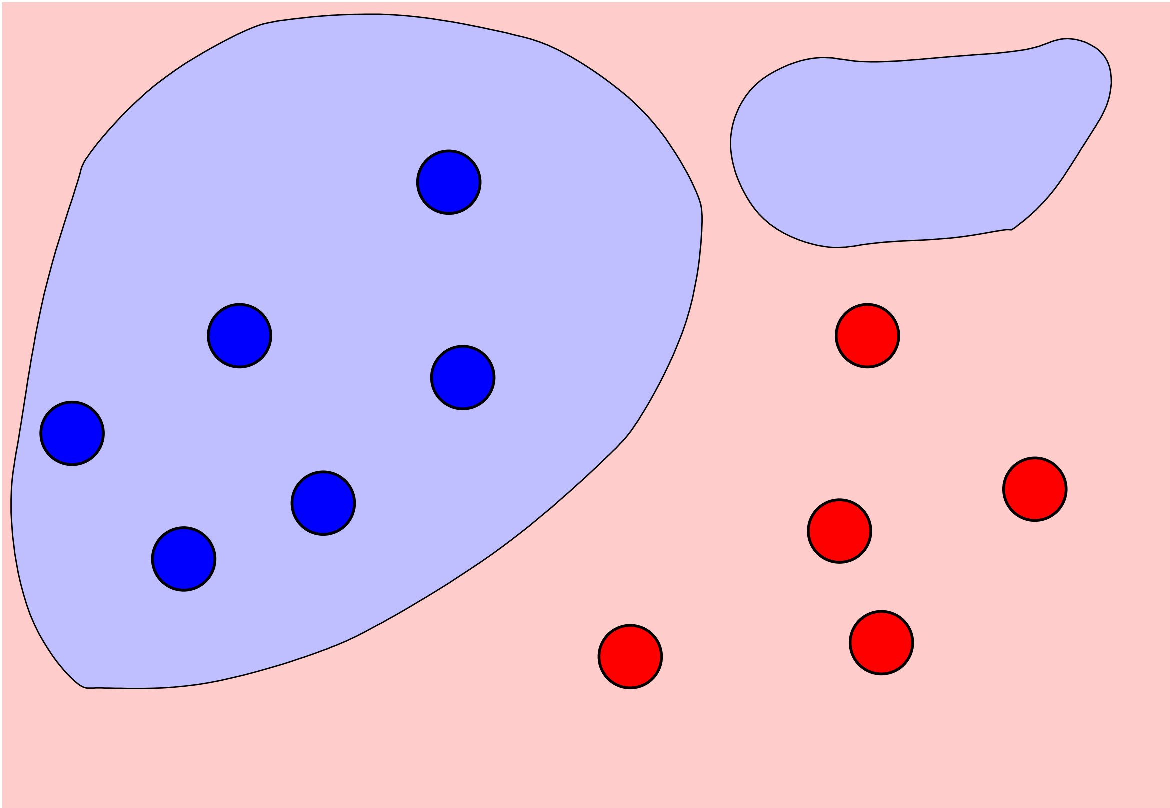
Many thanks to J.P. Vert for some of the following slides

Classification Separation Surfaces for Vectors



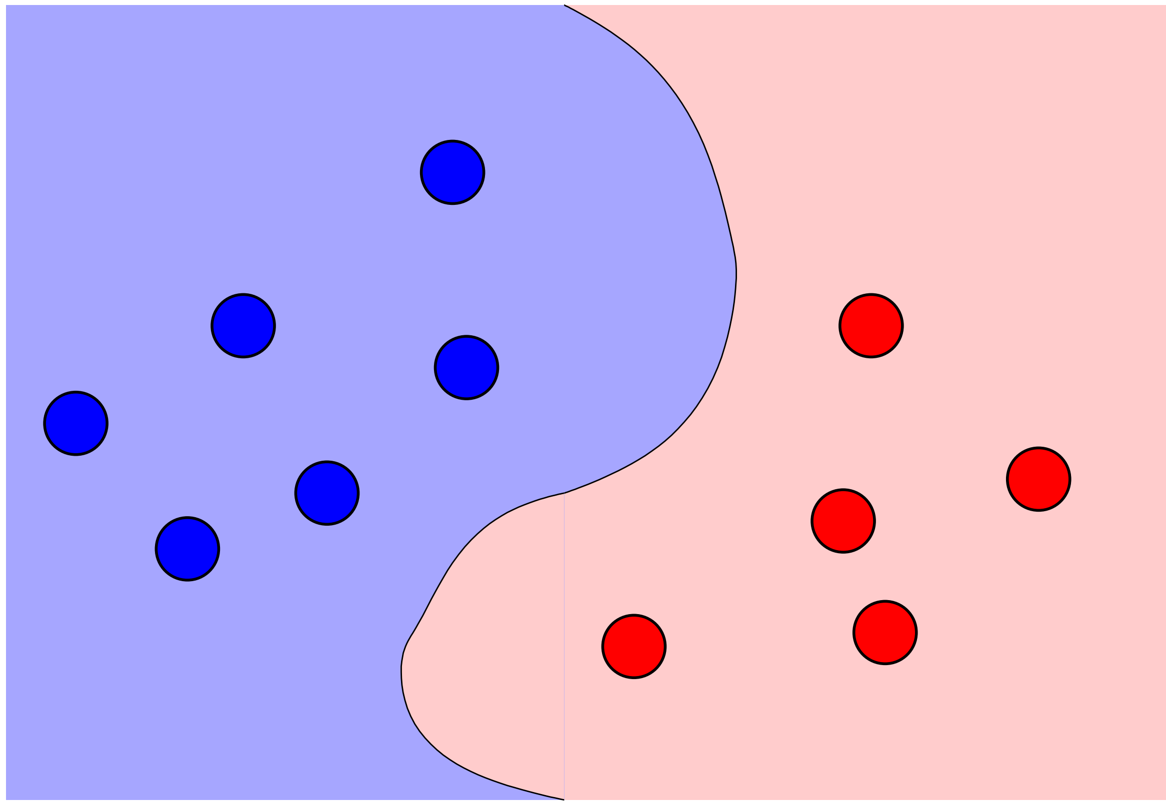
What is a classification rule?

Classification Separation Surfaces for Vectors



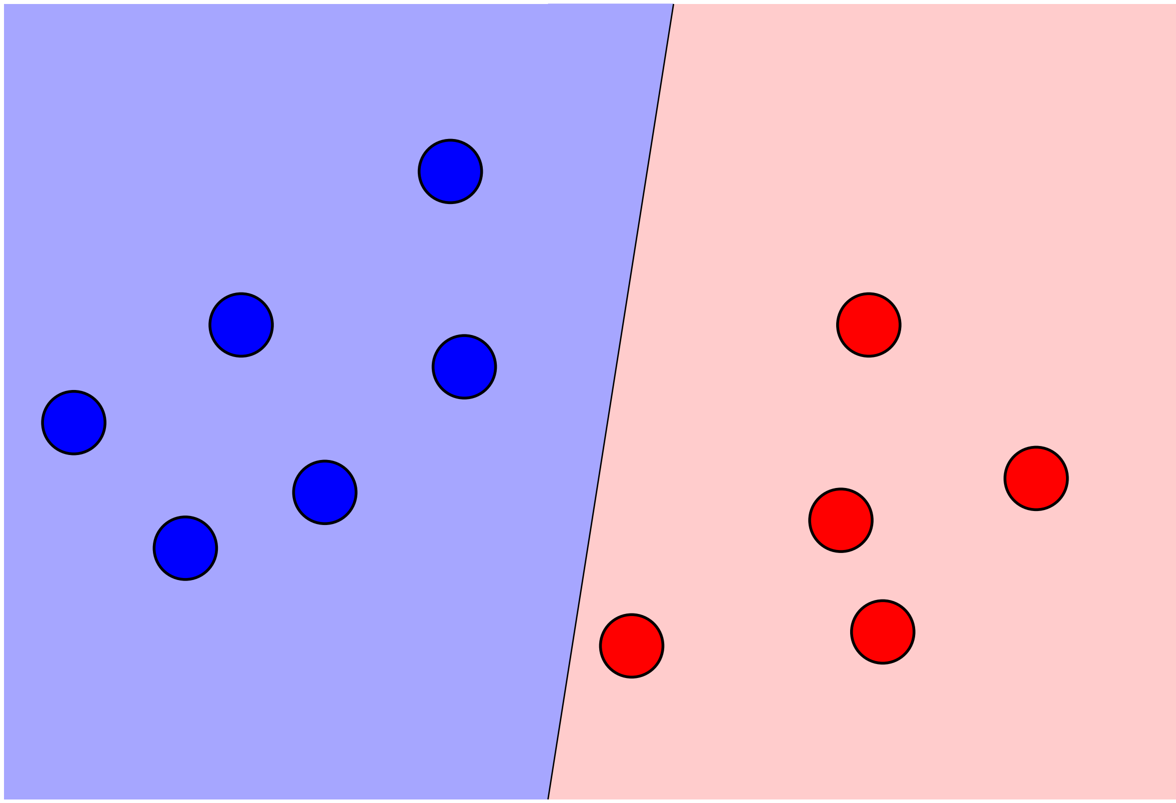
Classification rule = a partition of $\mathbb{R}^d$ into two sets

Classification Separation Surfaces for Vectors



Can be defined by a single surface, *e.g.* a curved line

Classification Separation Surfaces for Vectors



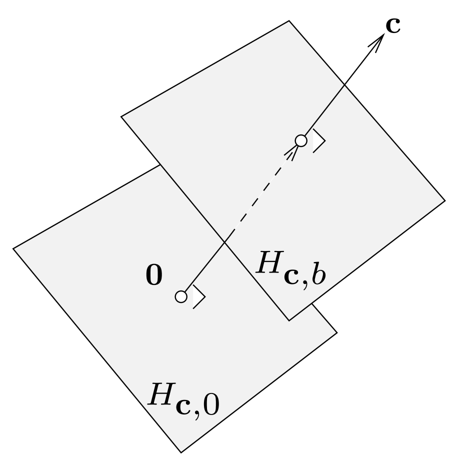
Even more **simple**: using **straight lines** and halspaces.

Linear Classifiers

- **Straight lines** (hyperplanes when $d > 2$) are **the simplest type** of classifiers.
- A hyperplane $H_{\mathbf{c},b}$ is a set in $\mathbb{R}^d$ defined by
  - a normal vector $\mathbf{c} \in \mathbb{R}^d$
  - a constant $b \in \mathbb{R}$. as

$$H_{\mathbf{c},b} = \{\mathbf{x} \in \mathbb{R}^d \,|\, \mathbf{c}^T\mathbf{x} \;=\; b\}$$

- Letting b vary we can "slide" the hyperplane across $\mathbb{R}^d$

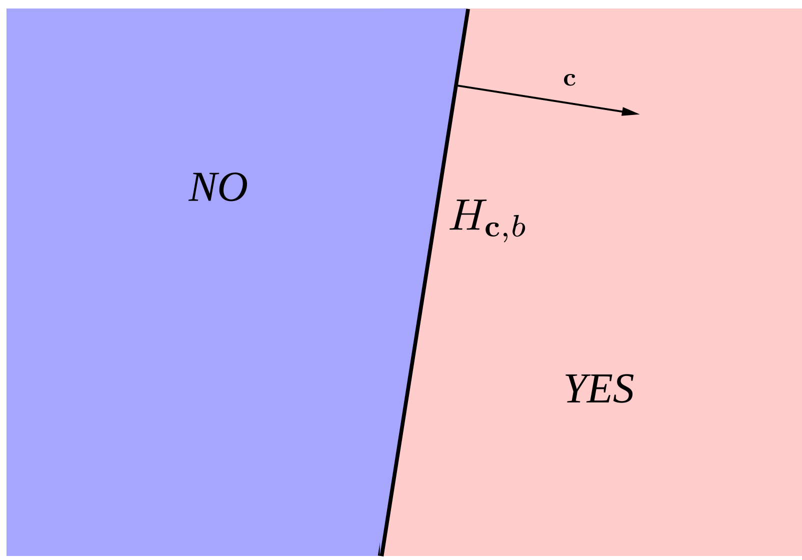


Linear Classifiers

- Exactly like lines in the plane, hypersurfaces **divide** $\mathbb{R}^d$ into **two** halfspaces,

$$\left\{\mathbf{x} \in \mathbb{R}^d \,|\, \mathbf{c}^T\mathbf{x} < b\right\} \cup \left\{\mathbf{x} \in \mathbb{R}^d \,|\, \mathbf{c}^T\mathbf{x} \geq b\right\} = \mathbb{R}^d$$

- Linear classifiers attribute the "yes" and "no" answers given arbitrary $\mathbf{c}$ and b.



- Assuming we only look at halfspaces for the decision surface...

  ...*how to* ***choose*** *the* ***"best"*** $(\mathbf{c}^\star, b^\star)$ *given a* ***training sample****?*

Linear Classifiers

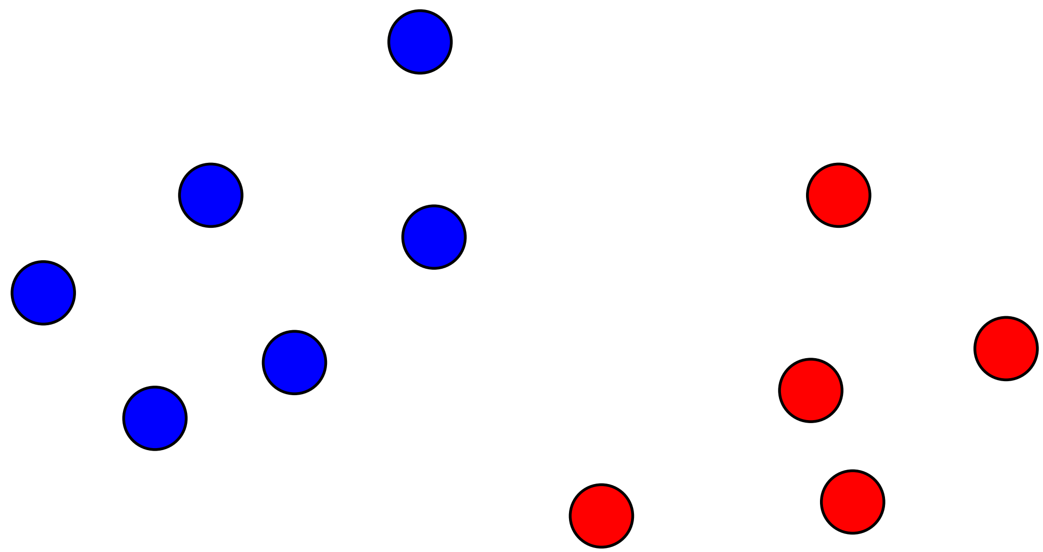
- This specific question,

$$\text{“training set”} \;\left\{\left(\mathbf{x}_i \in \mathbb{R}^d,\ \mathbf{y}_i \in \{0,1\}\right)_{i=1..N}\right\} \xrightarrow{????} \text{“best”}\, \mathbf{c}^\star,\ b^\star$$

  has different answers. Depends on the meaning of “best” [4]:
- **Linear Discriminant Analysis** (or Fisher's Linear Discriminant);
- **Logistic regression** maximum likelihood estimation;
- **Perceptron**, a one-layer neural network;
- *etc.*

$\boxed{\text{Today's focus: the } \textbf{Support vector machine}}$ [5]

Classification Separation Surfaces for Vectors



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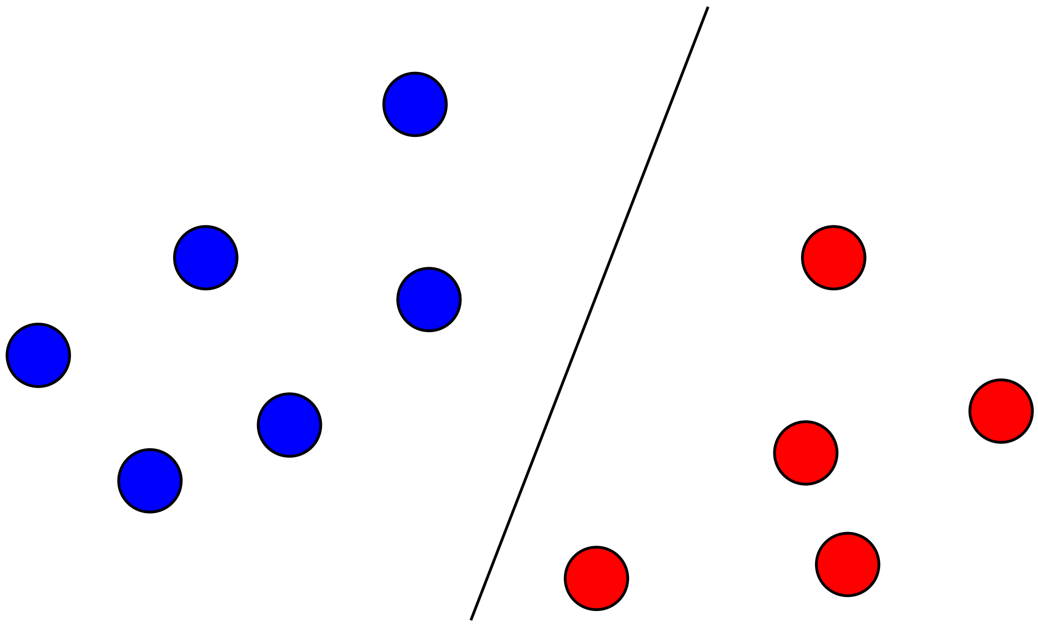

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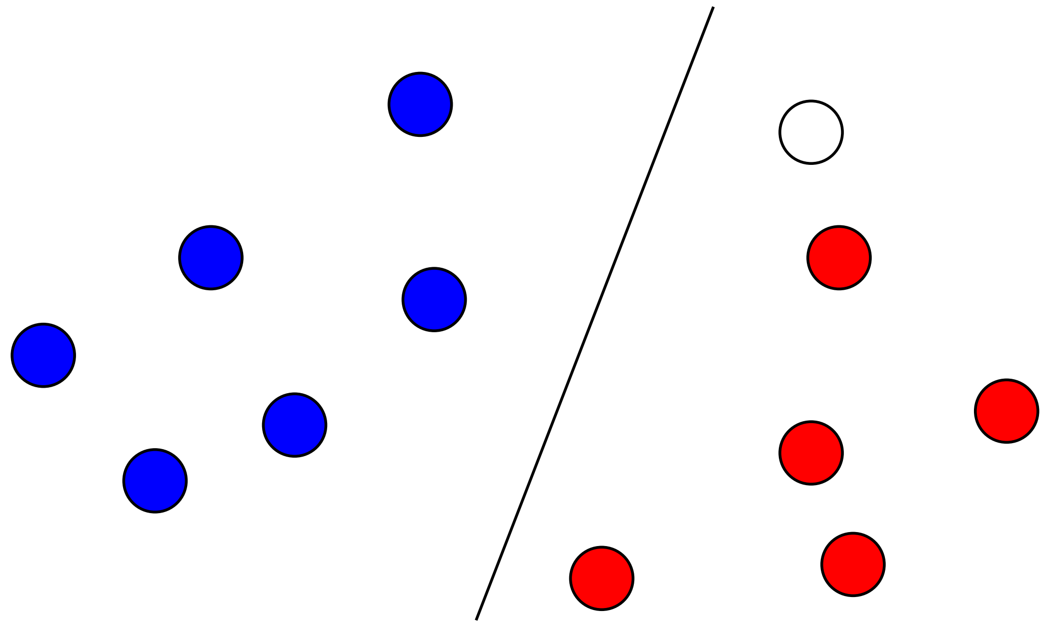

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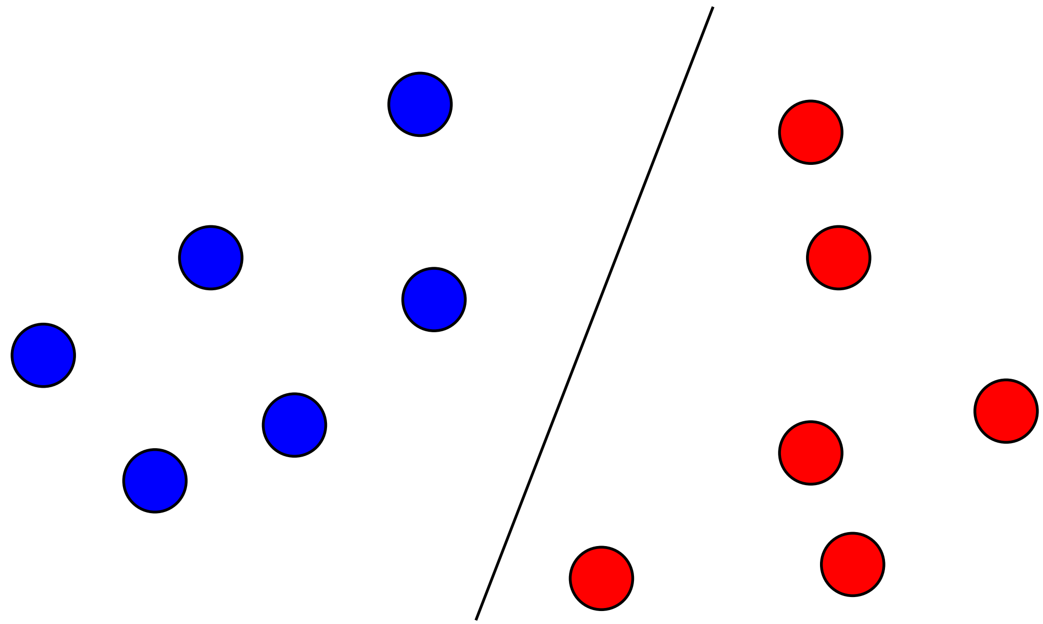
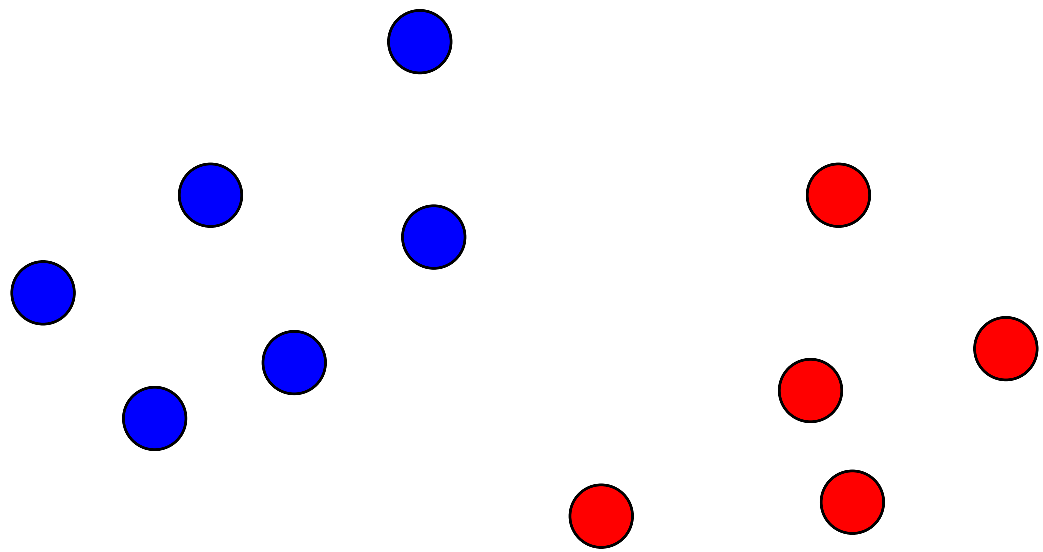


Linear classifier, some degrees of freedom



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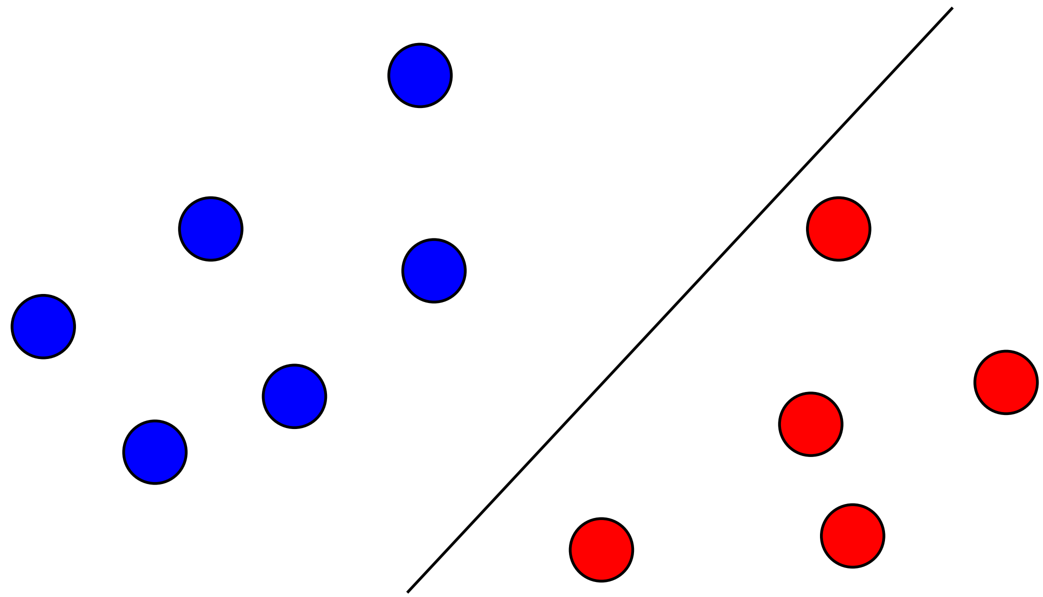

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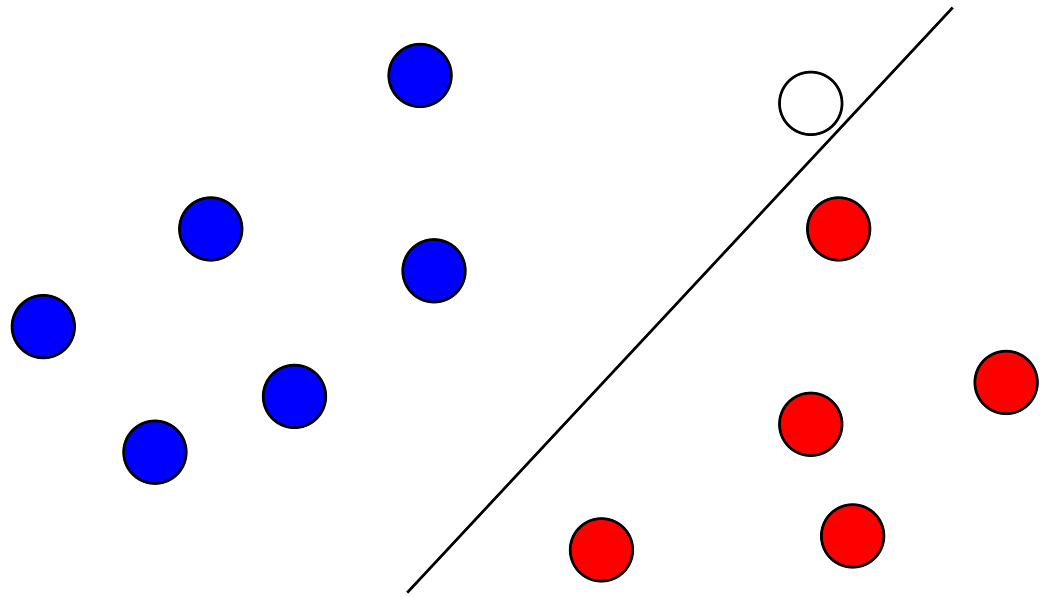

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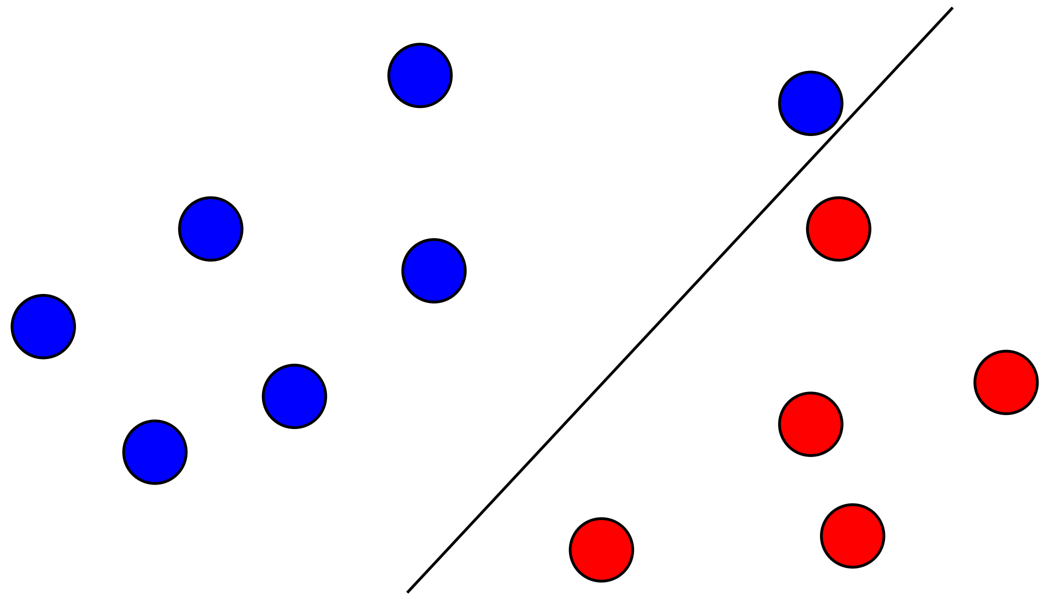
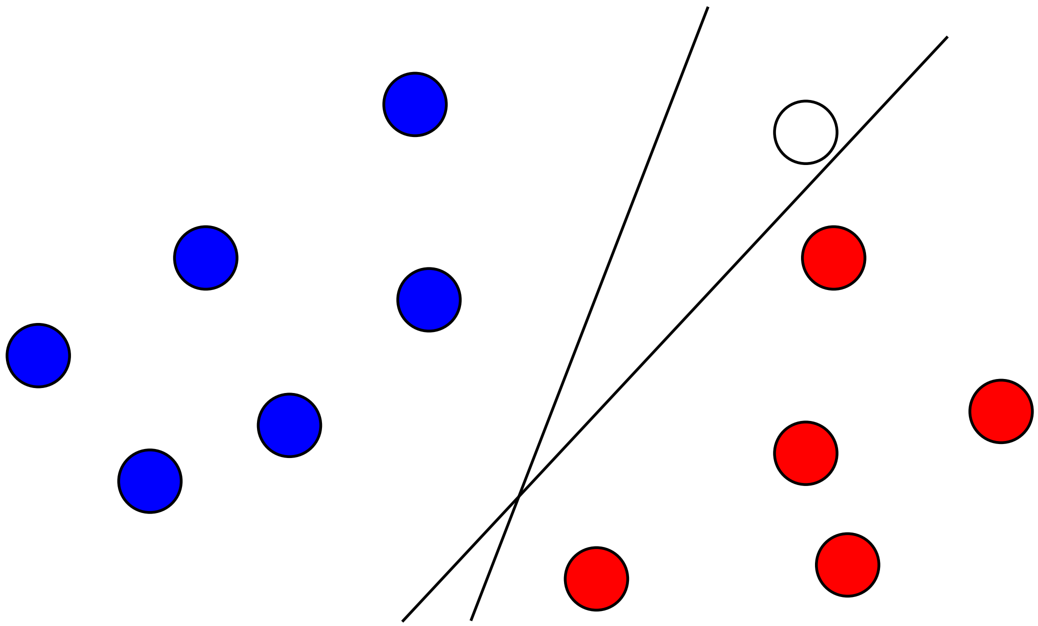
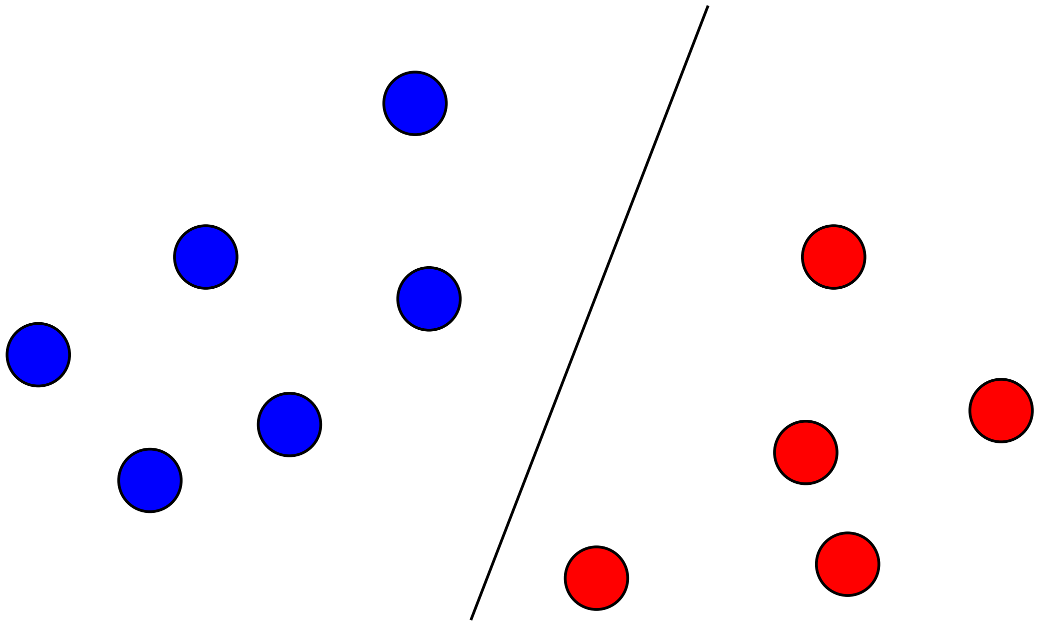


Which one is better?



A criterion to select a linear classifier: the margin [2]



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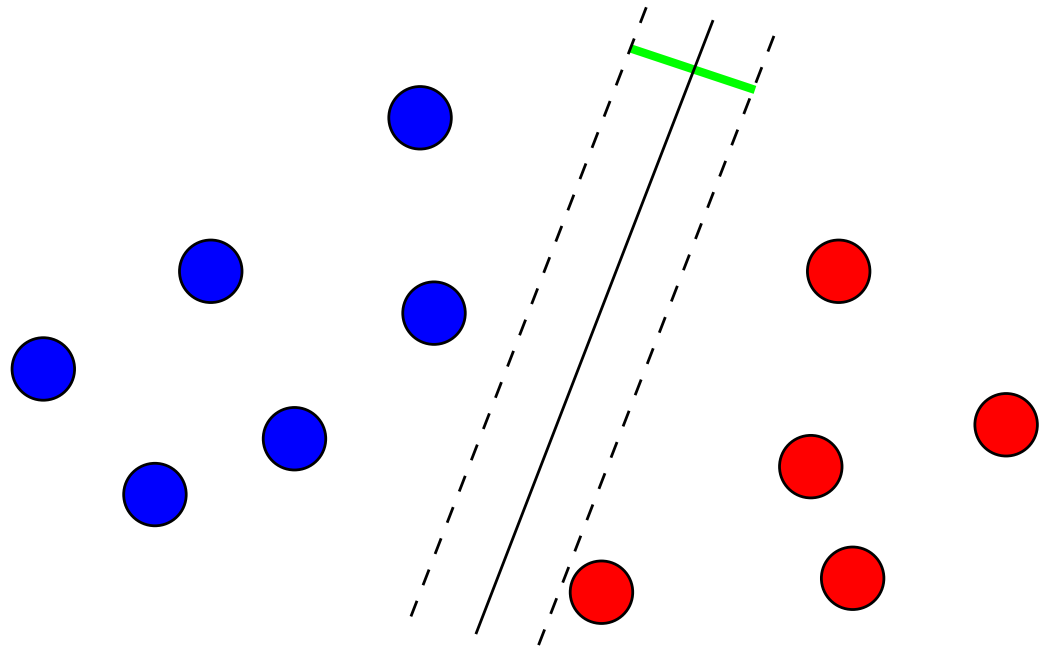

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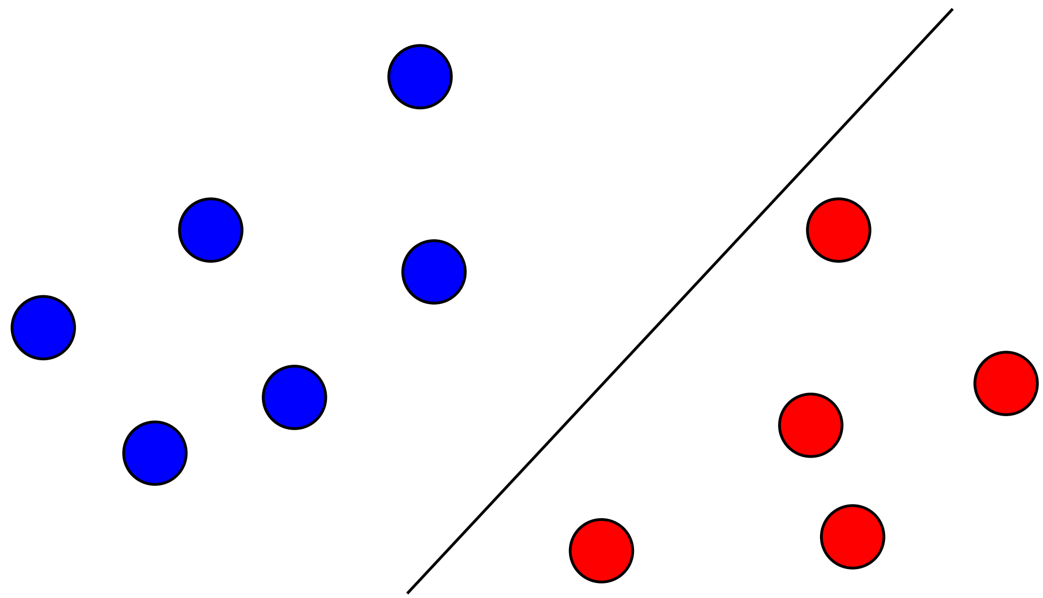

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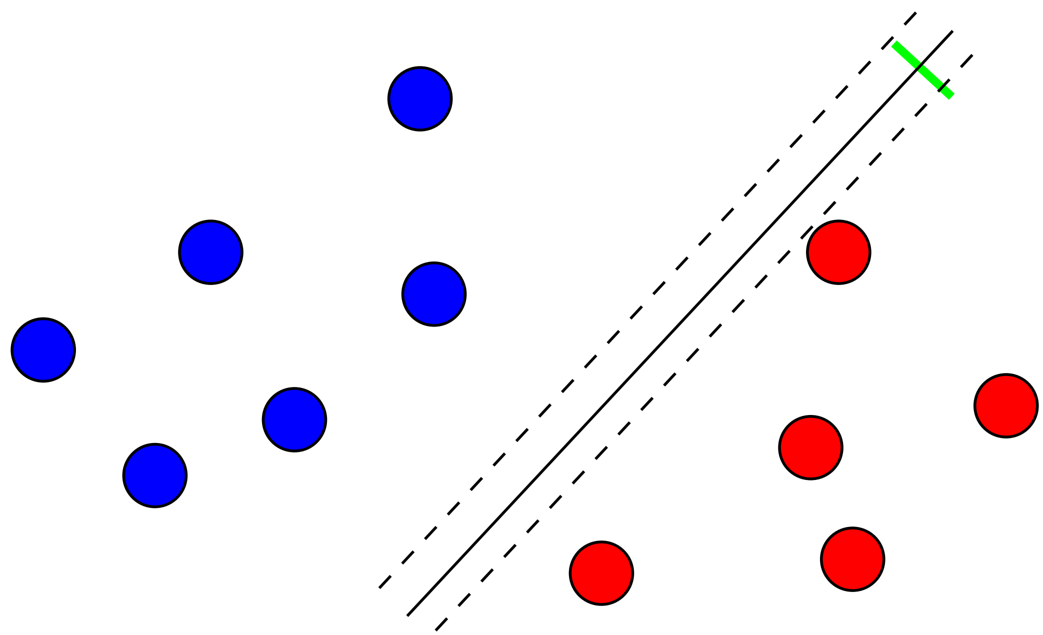

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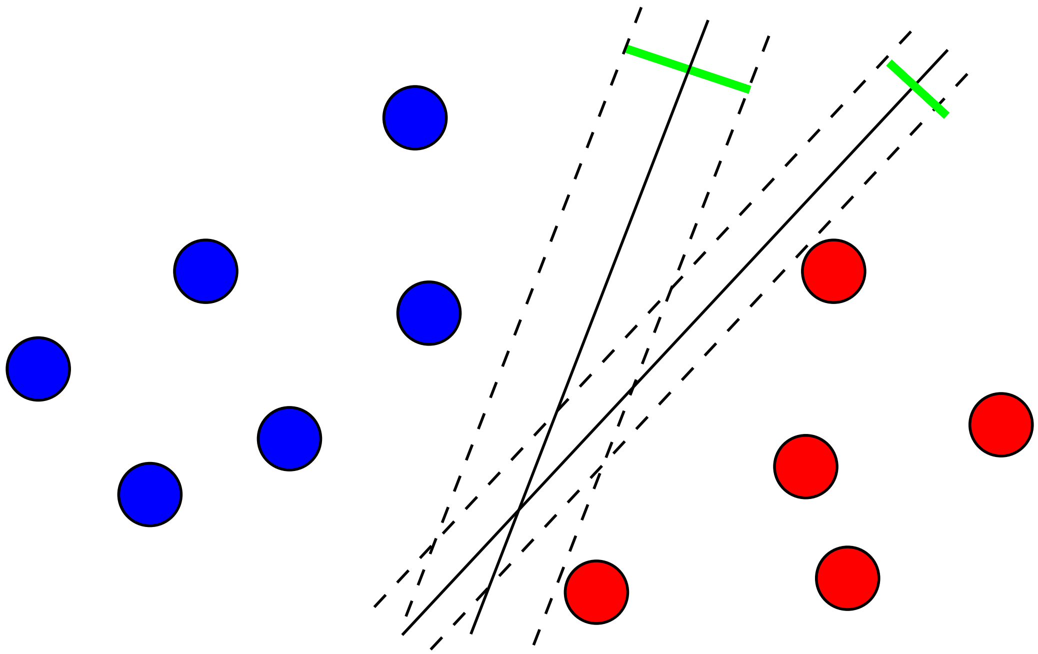
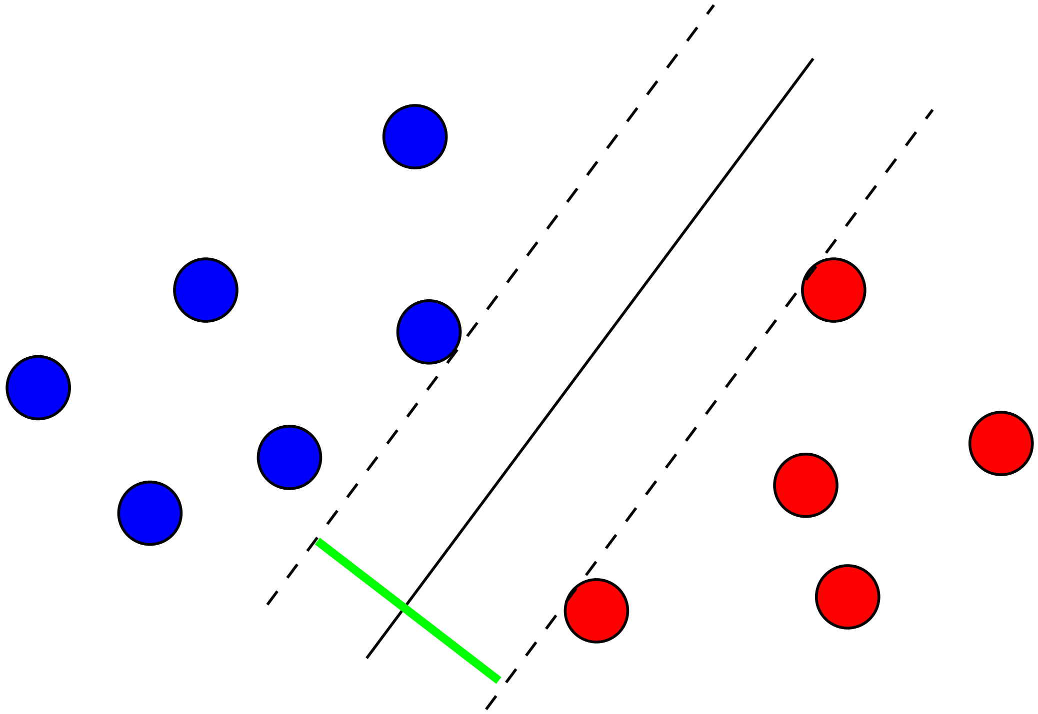
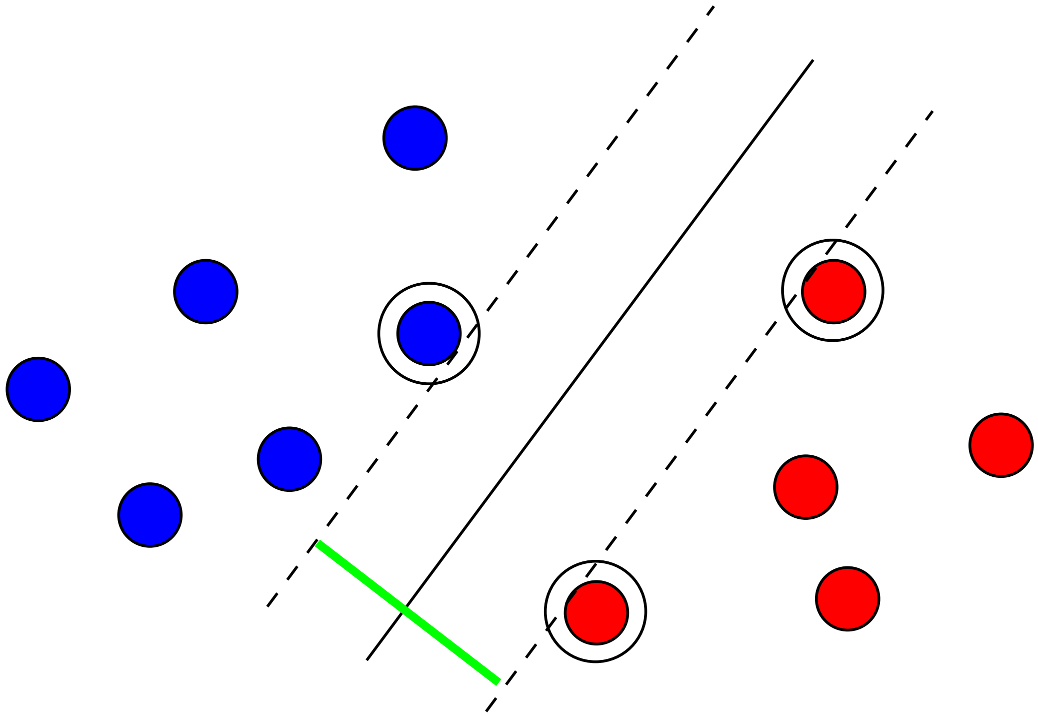


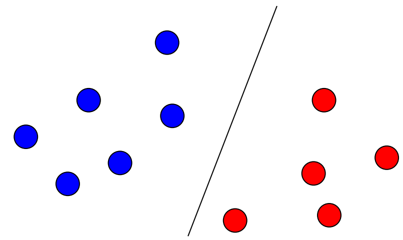
Largest Margin Linear Classifier [2]



Support Vectors with Large Margin



In equations



- We assume (for the moment) that the data are **linearly separable**, i.e., that there exists $(\mathbf{w}, b) \in \mathbb{R}^d \times \mathbb{R}$ such that:

$$\begin{cases} \mathbf{w}^T \mathbf{x}_i + b > 0 & \text{if } \mathbf{y}_i = 1\,, \\ \mathbf{w}^T \mathbf{x}_i + b < 0 & \text{if } \mathbf{y}_i = -1\,. \end{cases}$$

- Next, we give a formula to compute the margin as a function of $\mathbf{w}$.
- Obviously, for any $t \in \mathbb{R}$,

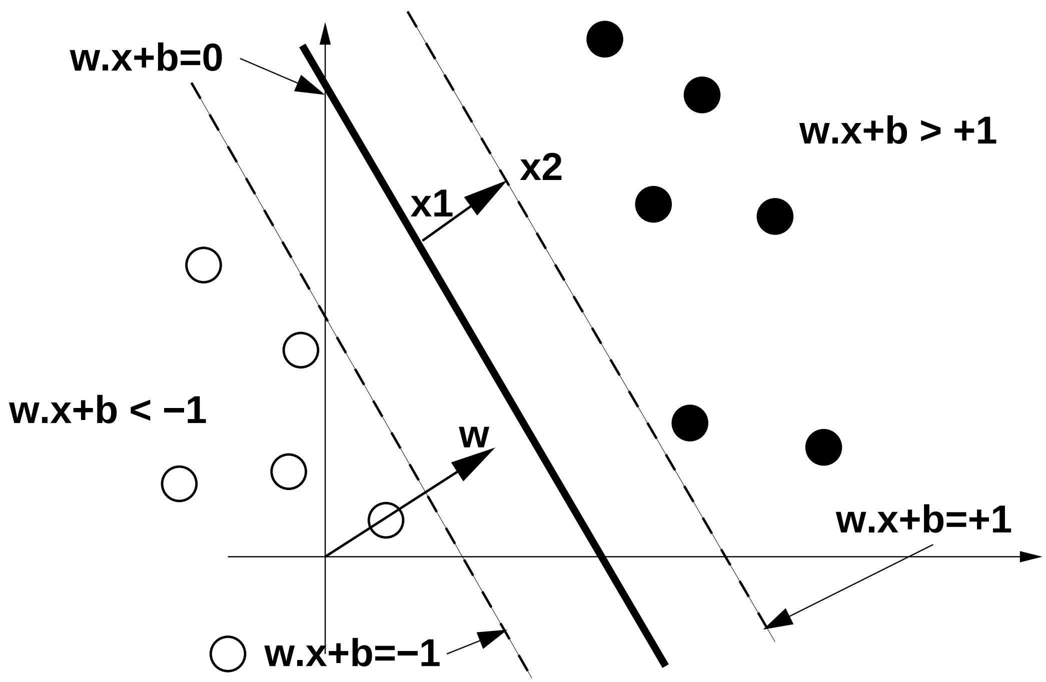
$$H_{\mathbf{w},b} = H_{t\mathbf{w},tb}$$

- Thus $\mathbf{w}$ and b are defined up to a multiplicative constant.
- We need to take care of this in the definition of the margin

How to find the largest separating hyperplane?

For the linear classifier $f(\mathbf{x}) = \mathrm{w}^T\mathbf{x} + b$,
consider the **interstice** defined by the hyperplanes:

- $f(\mathbf{x}) = \mathrm{w}^T\mathbf{x} + b = +1$
- $f(\mathbf{x}) = \mathrm{w}^T\mathbf{x} + b = -1$



- Consider $\mathbf{x}_1$ and $\mathbf{x}_2$ such that $\mathbf{x}_2 - \mathbf{x}_1$ is parallel to w.

The margin is $2/||\mathbf{w}||$

- Margin $= 2/\|\mathbf{w}\|$: the points $\mathbf{x}_1$ and $\mathbf{x}_2$ satisfy:

$$\begin{cases} \mathbf{w}^T\mathbf{x}_1 + b = 0, \\ \mathbf{w}^T\mathbf{x}_2 + b = 1. \end{cases}$$

- By subtracting we get $\mathbf{w}^T(\mathbf{x}_2 - \mathbf{x}_1) = 1$, and therefore:

$$\gamma \stackrel{\text{def}}{=} 2||\mathbf{x}_2 - \mathbf{x}_1|| = \frac{2}{||\mathbf{w}||}.$$

where γ is by definition the **margin**.

All training points should be on the appropriate side

- For positive examples ($y_i = 1$) this means:

$$\mathbf{w}^T \mathbf{x}_i + b \geq 1$$

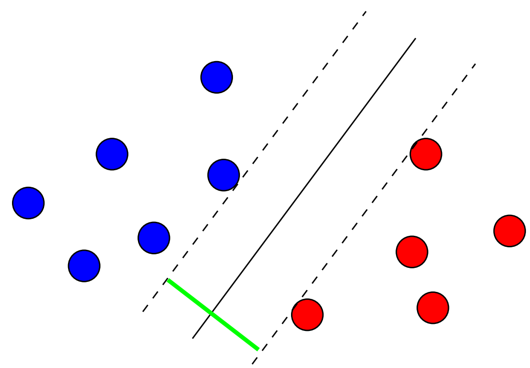
- For negative examples ($y_i = -1$) this means:

$$\mathbf{w}^T \mathbf{x}_i + b \leq -1$$

- in both cases:

$$\forall i = 1, \ldots, n, \qquad \mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b \right) \geq 1$$

Finding the optimal hyperplane



- Find $(\mathbf{w}, b)$ which minimize:

$$\|\mathbf{w}\|^2$$

under the constraints:

$$\forall i = 1, \ldots, n, \qquad \mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) - 1 \geq 0.$$

This is a classical quadratic program on $\mathbb{R}^{d+1}$
linear constraints - **quadratic objective**

Lagrangian

- In order to minimize:

$$\frac{1}{2}||\mathbf{w}||^2$$

under the constraints:

$$\forall i = 1, \ldots, n, \qquad y_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) - 1 \geq 0.$$

- introduce **one dual variable α_i for each constraint**,
- one constraint for **each training point**.
- the **Lagrangian** is, for $\alpha \succeq 0$ (that is for each $\alpha_i \geq 0$)

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2}||\mathbf{w}||^2 - \sum_{i=1}^{n} \alpha_i \left(y_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) - 1\right).$$

The Lagrange dual function

$$g(\alpha) = \inf_{\mathbf{w}\in\mathbb{R}^d, b\in\mathbb{R}} \left\{ \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i \left(y_i \left(\mathbf{w}^T \mathbf{x}_i + b \right) - 1 \right) \right\}$$

is only defined when

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i \mathbf{y}_i \mathbf{x}_i, \quad (\text{ derivating w.r.t } \mathbf{w}) \quad (*)$$

$$0 = \sum_{i=1}^{n} \alpha_i \mathbf{y}_i, \quad (\text{derivating w.r.t } b) \qquad (**)$$

substituting $(*)$ in g, and using $(**)$ as a constraint, get the dual function $g(\alpha)$.

- To solve the dual problem, **maximize** g w.r.t. α.
- Strong duality holds. KKT gives us $\alpha_i(\mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) - 1) = 0$,
  ...*hence*, either $\boldsymbol{\alpha_i = 0}$ or $\boldsymbol{\mathbf{y}_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) = 1}$.
- $\alpha_i \neq 0$ **only** for points on the support hyperplanes $\{(\mathbf{x}, \mathbf{y}) |\, \mathbf{y}_i(\mathbf{w}^T \mathbf{x}_i + b) = 1\}$.

Dual optimum

The dual problem is thus

$$\begin{array}{ll} \text{maximize} & g(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j \\ \text{such that} & \alpha \succeq 0, \sum_{i=1}^{n} \alpha_i \mathbf{y}_i = 0. \end{array}$$

This is a **quadratic program** in $\mathbb{R}^n$, with *box constraints*.
α^* can be computed using optimization software
($e.g.$ built-in `matlab` function)

Recovering the optimal hyperplane

- With α^*, we recover $(\mathbf{w}^T, b^*)$ corresponding to the **optimal hyperplane**.
- $\mathbf{w}^T$ is given by $\mathbf{w}^T = \sum_{i=1}^n y_i \alpha_i \mathbf{x}_i^T$,
- b^* is given by the conditions on the support vectors $\alpha_i > 0$, $\mathbf{y}_i(\mathbf{w}^T \mathbf{x}_i + b) = 1$,

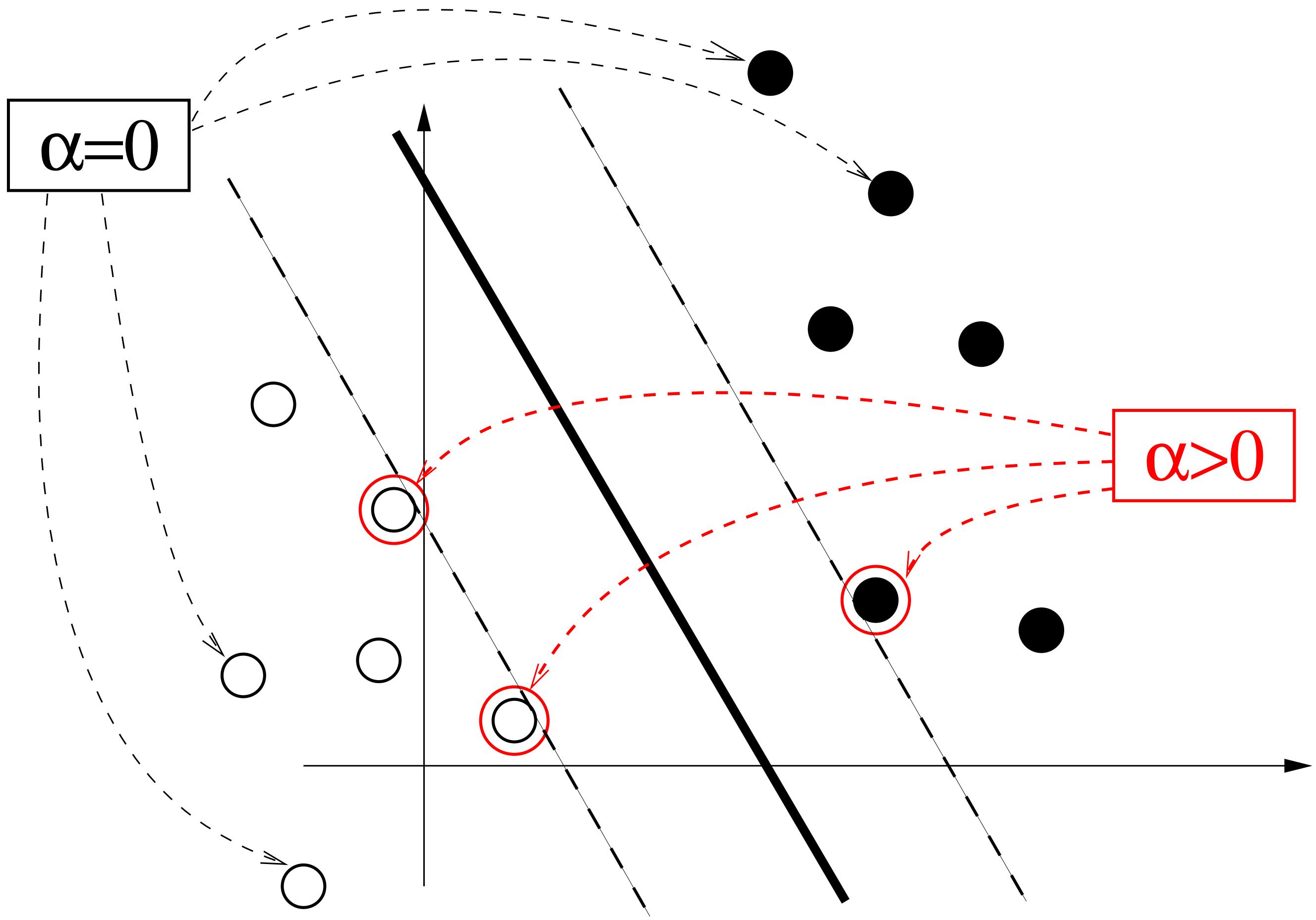
$$b^* = -\frac{1}{2}\left(\min_{\mathbf{y}_i=1,\alpha_i>0}(\mathbf{w}^T\mathbf{x}_i) + \max_{\mathbf{y}_i=-1,\alpha_i>0}(\mathbf{w}^T\mathbf{x}_i)\right)$$

- the **decision function** is therefore:

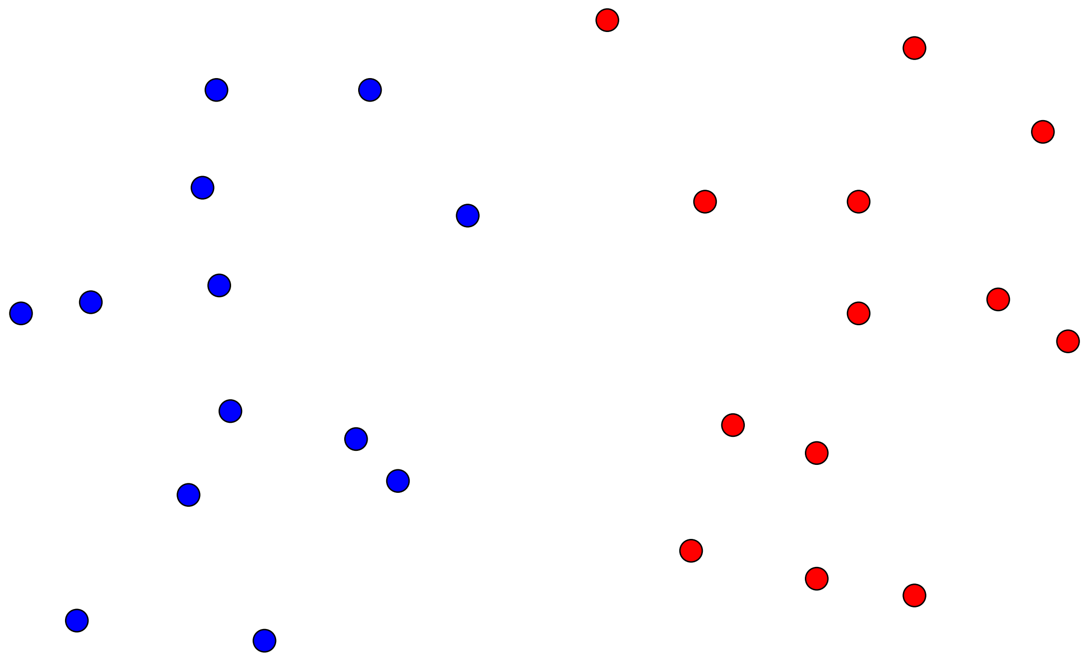
$$\begin{aligned} f^*(\mathbf{x}) &= \mathbf{w}^T\mathbf{x} + b^* \\ &= \sum_{i=1}^n y_i \alpha_i \mathbf{x}_i^T \mathbf{x} + b^*. \end{aligned}$$

- Here the **dual** solution gives us directly the **primal** solution.

Interpretation: support vectors

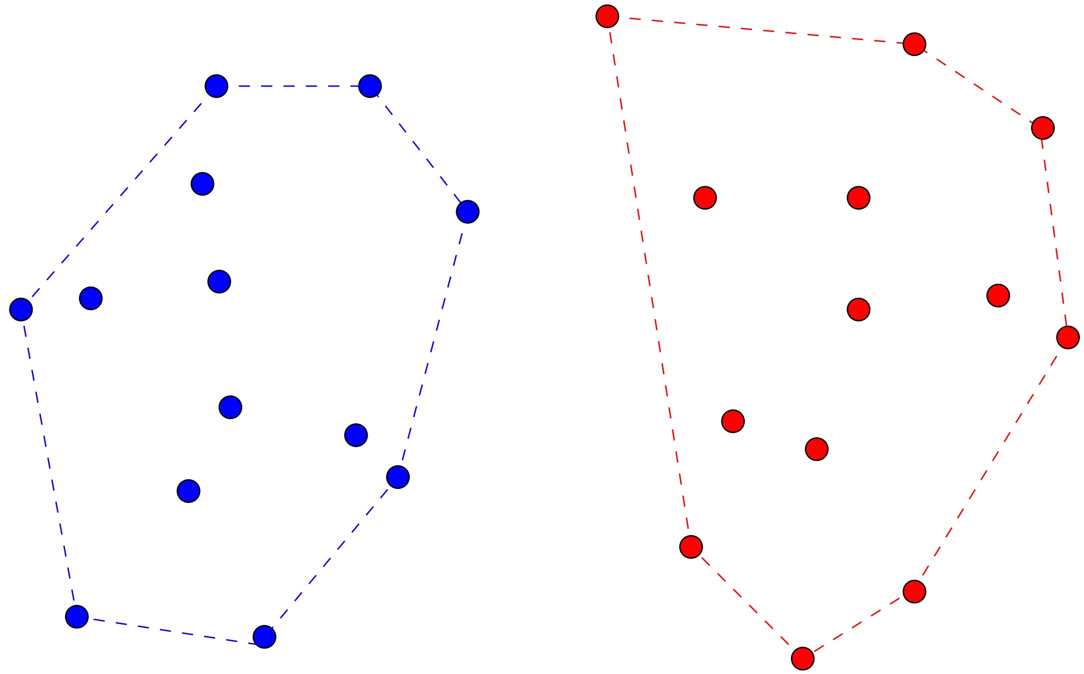


Another interpretation: Convex Hulls [1]



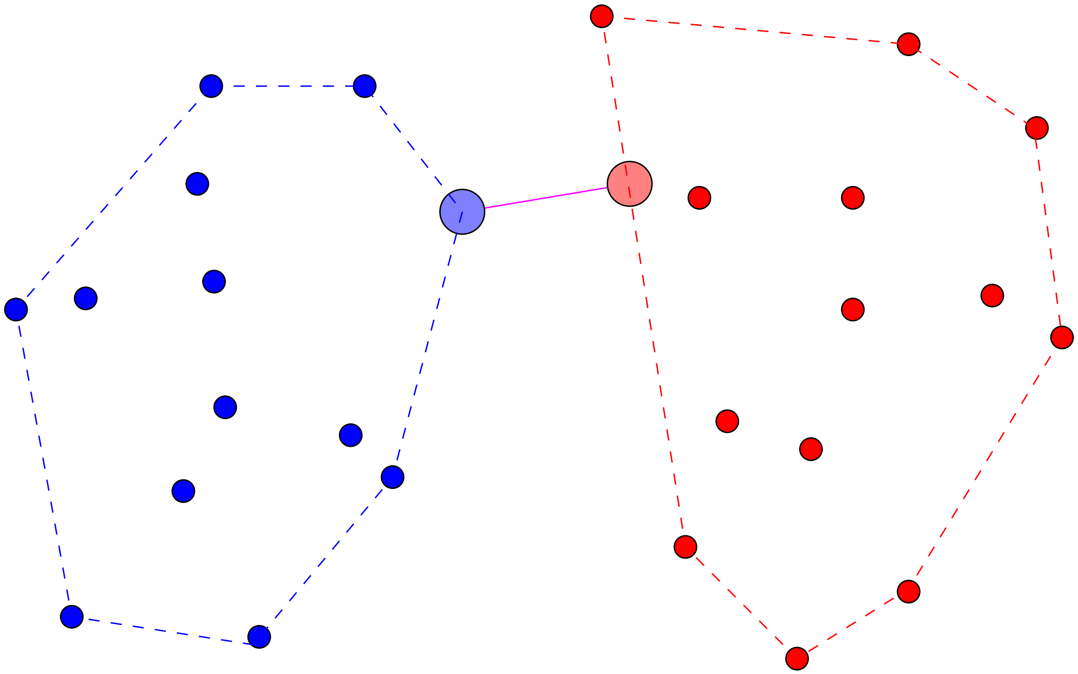
go back to 2 sets of points that are linearly separable

Another interpretation: Convex Hulls



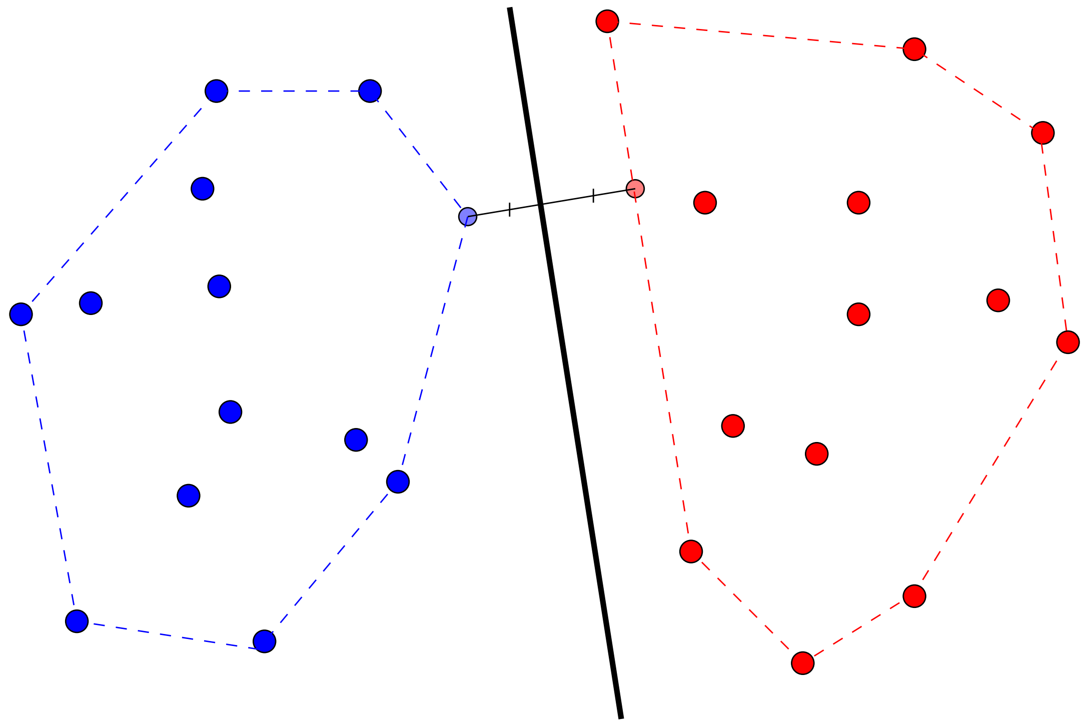
$$\boxed{\text{Linearly separable} = \text{convex hulls do not intersect}}$$

Another interpretation: Convex Hulls



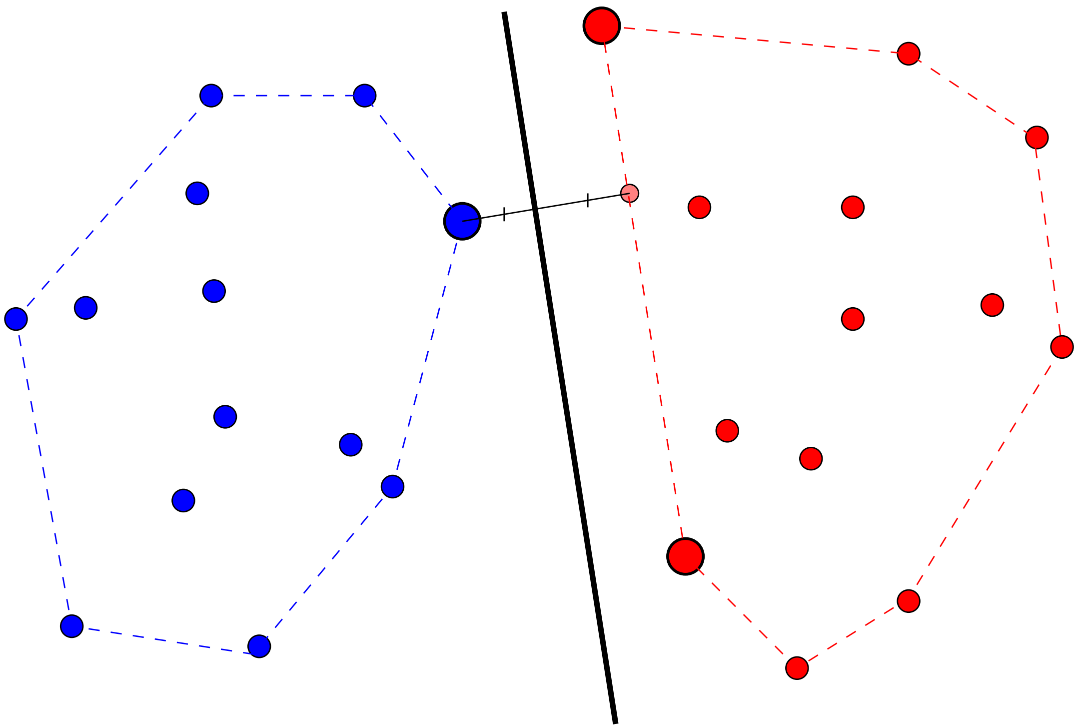
Find two closest points, one in each convex hull

Another interpretation: Convex Hulls



The SVM = bisection of that segment

Another interpretation: Convex Hulls



support vectors = extreme points of the faces on which the two points lie

A brief proof through duality

- Suppose that
  - all the points of the blue set are in a matrix $A \in \mathbb{R}^{d \times n_{-1}}$,
  - all the points of the red set are in a matrix $B \in \mathbb{R}^{d \times n_1}$

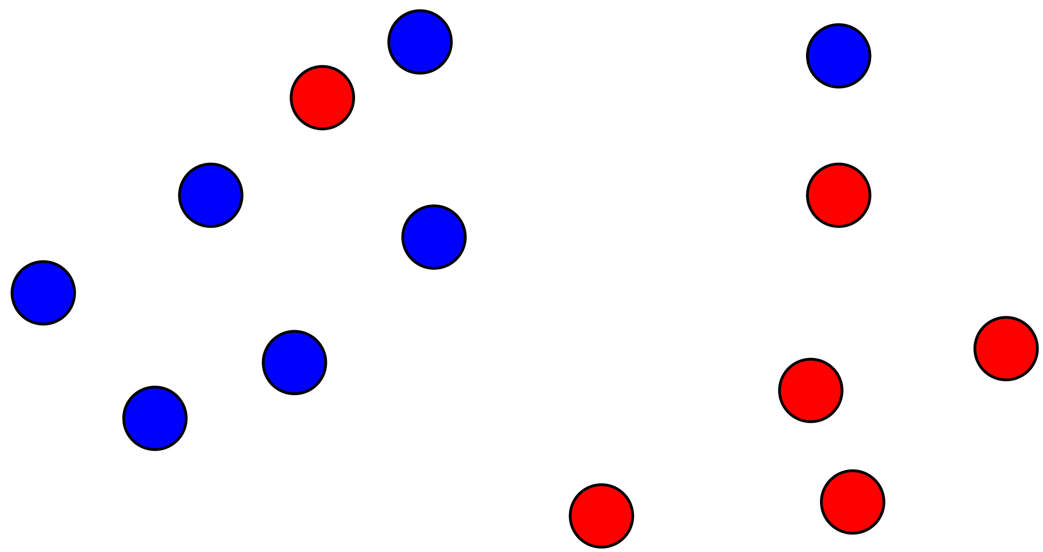
$$\boldsymbol{A} = \begin{bmatrix} \vdots & \cdots & \vdots \\ \boldsymbol{x_1} & \cdots & \boldsymbol{x_{n_{-1}}} \\ \vdots & \cdots & \vdots \end{bmatrix} \in \mathbb{R}^{\boldsymbol{d \times n_{-1}}}, \quad B = \begin{bmatrix} \vdots & \cdots & \vdots \\ x'_1 & \cdots & x'_{n_1} \\ \vdots & \cdots & \vdots \end{bmatrix} \in \mathbb{R}^{d \times n_1}.$$

- Finding the two points in question, and the minimal distance, is given by

$$\begin{array}{ll} \text{minimize} & \|\boldsymbol{A}\mathbf{u} - B\mathbf{v}\|^2 \\ \text{subject to} & \mathbb{1}_{n_{-1}}^T \mathbf{u} = \mathbb{1}_{n_1}^T \mathbf{v} = 1 \\ & 0 \leq \mathbf{u} \in \mathbb{R}^{n_{-1}}, \mathbf{v} \in \mathbb{R}^{n_1} \end{array}$$

- Possible to prove that the primal SVM program, slightly modified, has this dual.
- A bit tedious unfortunately.

What happens when the data is not linearly separable?



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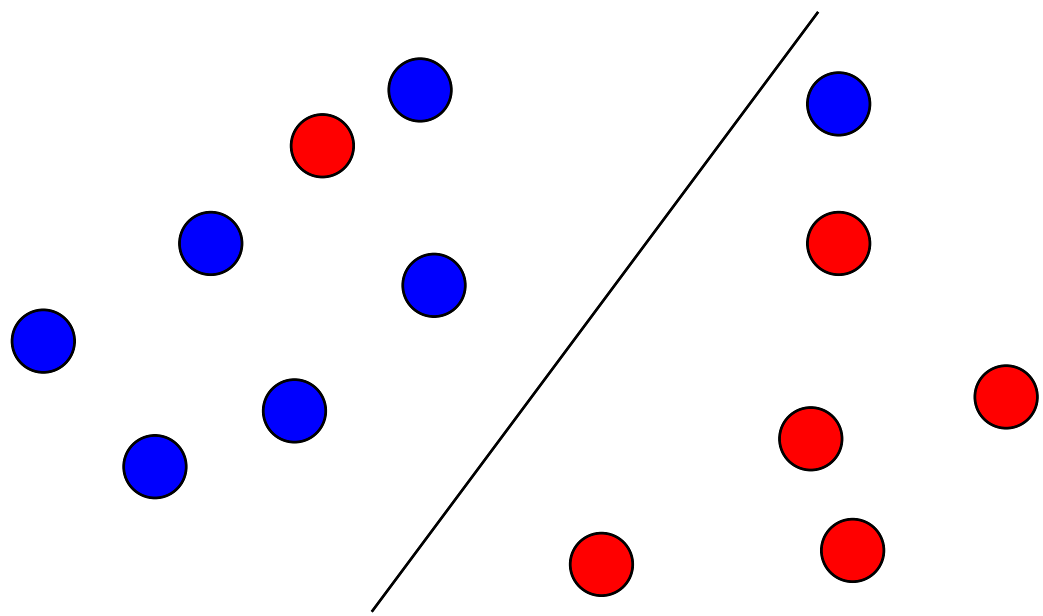

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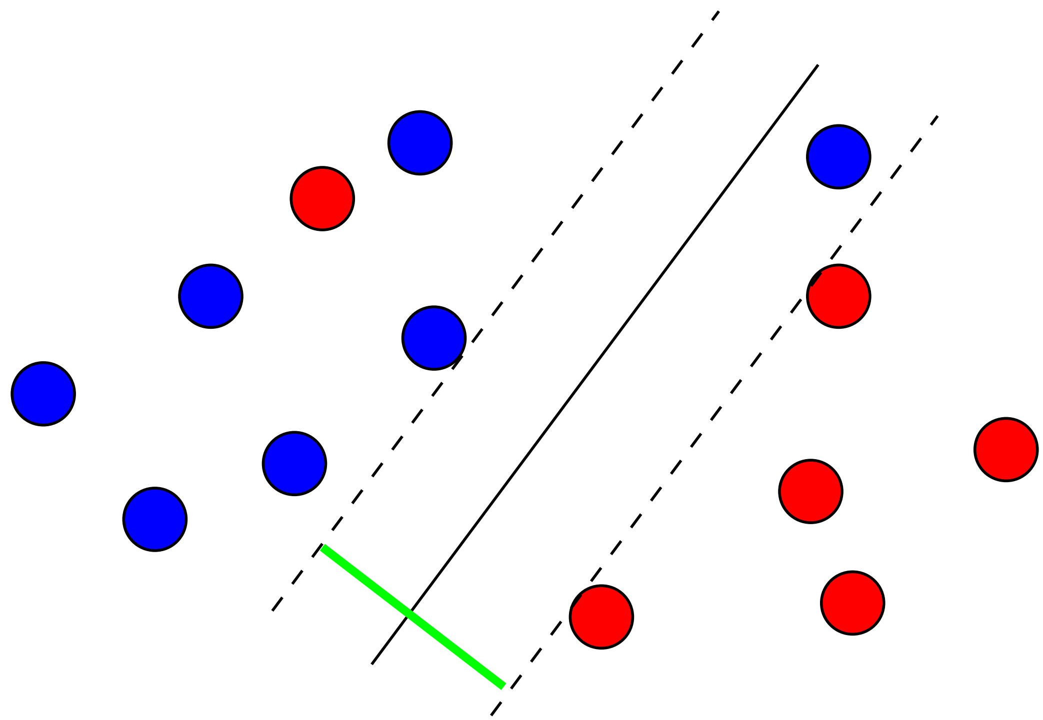

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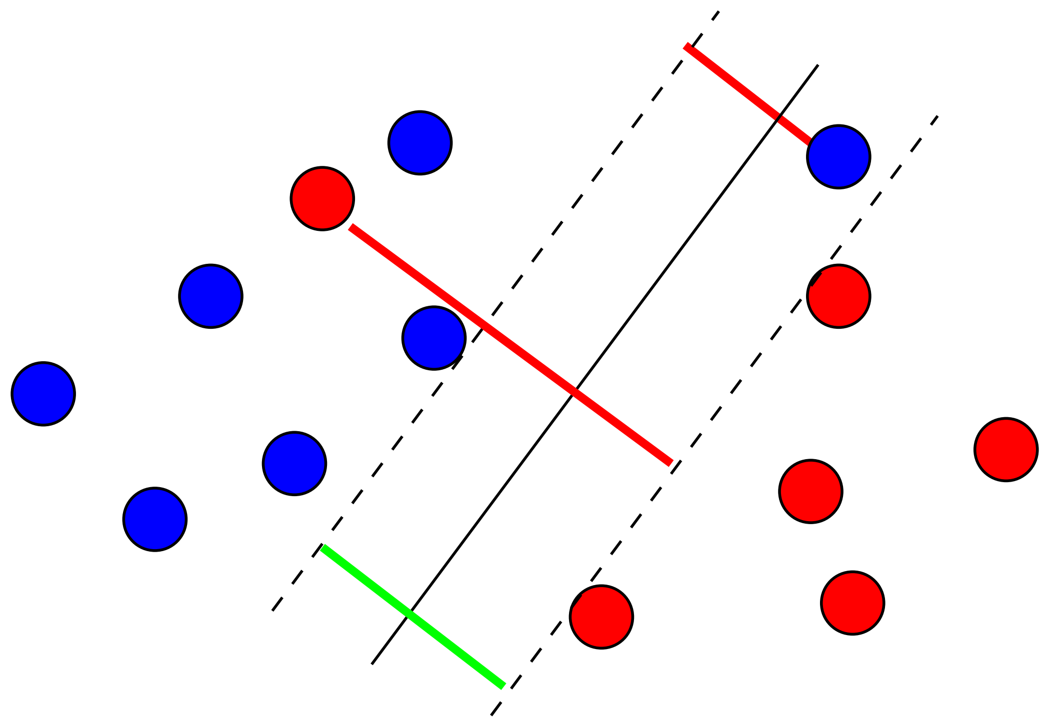
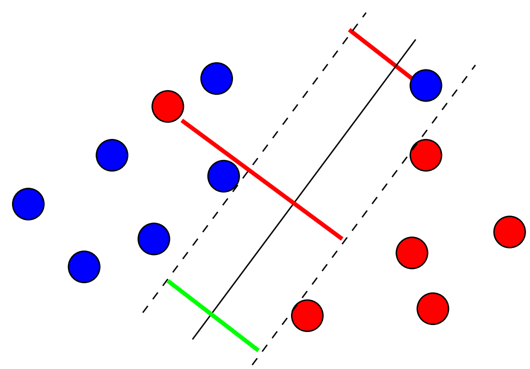


Soft-margin SVM [3]

- Find a trade-off between **large margin** and **few errors**.

- Mathematically:
$$\min_f \left\{ \frac{1}{\text{margin}(f)} + C \times \text{errors}(f) \right\}$$

- C is a parameter



Soft-margin SVM formulation [3]

- The **margin** of a labeled point $(\mathbf{x}, \mathbf{y})$ is

$$\text{margin}(\mathbf{x}, \mathbf{y}) = \mathbf{y}\left(\mathbf{w}^T\mathbf{x} + b\right)$$

- The **error** is
  - 0 if $\text{margin}(\mathbf{x}, \mathbf{y}) > 1$,
  - $1 - \text{margin}(\mathbf{x}, \mathbf{y})$ otherwise.

- The soft margin SVM solves:

$$\min_{\mathbf{w},b}\{\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\max\{0, 1 - \mathbf{y}_i\left(\mathbf{w}^T\mathbf{x}_i + b\right)\}$$

- $c(u, y) = \max\{0, 1 - yu\}$ is known as the **hinge loss**.

- $c(\mathbf{w}^T\mathbf{x}_i + b, \mathbf{y}_i)$ associates a mistake cost to the decision $\mathbf{w}, b$ for example $\mathbf{x}_i$.

Dual formulation of soft-margin SVM

- The soft margin SVM program

$$\min_{\mathbf{w},b}\{\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\max\{0, 1-\mathbf{y}_i\left(\mathbf{w}^T\mathbf{x}_i+b\right)\}$$

can be rewritten as

$$\begin{array}{ll} \text{minimize} & \|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i \\ \text{such that} & \mathbf{y}_i\left(\mathbf{w}^T\mathbf{x}_i+b\right) \geq 1-\xi_i \end{array}$$

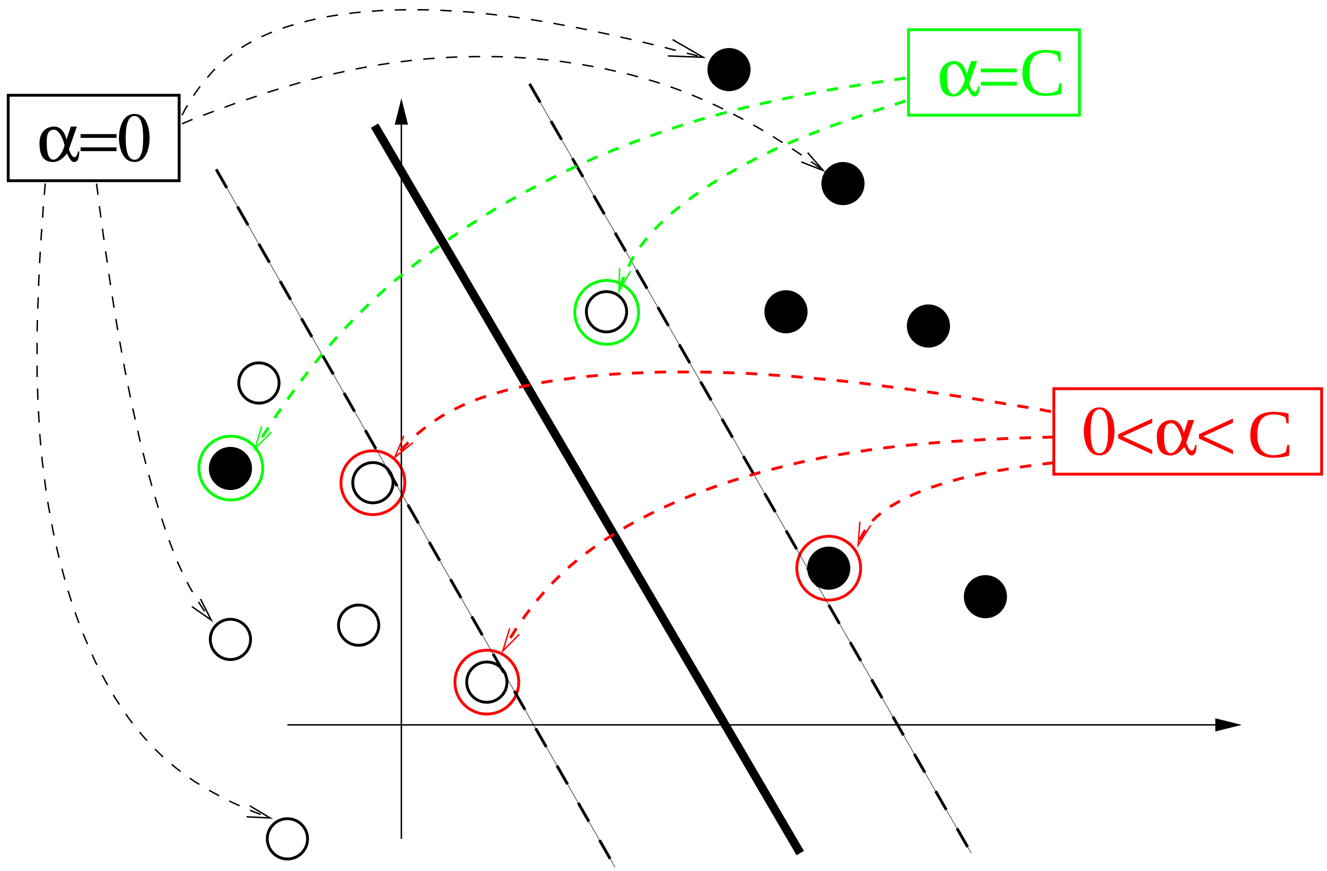
- In that case the dual function

$$g(\alpha) = \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{n}\alpha_i\alpha_j\mathbf{y}_i\mathbf{y}_j\mathbf{x}_i^T\mathbf{x}_j,$$

which is finite under the constraints:

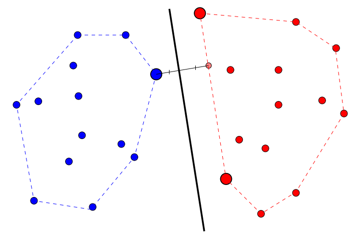
$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1,\dots,n \\ \sum_{i=1}^{n}\alpha_i\mathbf{y}_i = 0. \end{cases}$$

Interpretation: bounded and unbounded support vectors

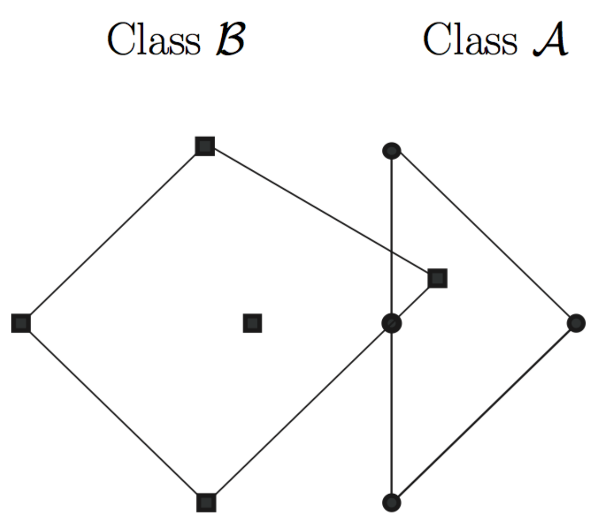


What about the convex hull analogy?

- Remember the separable case



- Here we consider the case where the two sets are not linearly separable, $i.e.$ their convex hulls **intersect.**



What about the convex hull analogy?

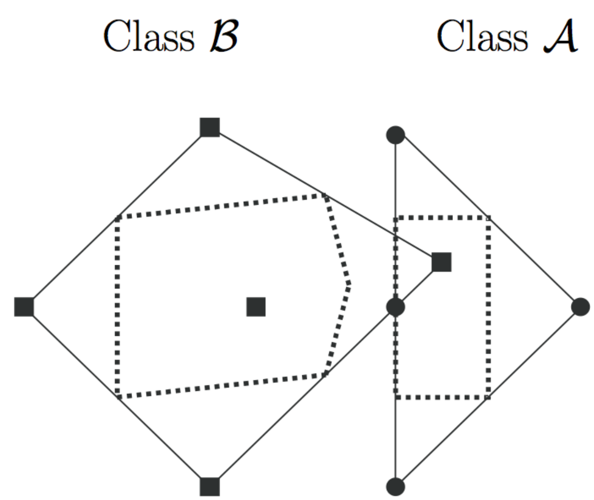
- To follow with the convex hull analogy, consider instead the **reduced** convex hull,

  Definition 1. *Given a set of* n *points* $\mathcal{A}$, *and* $0 \leq C \leq 1$, *the set of finite combinations*

  $$\sum_{i=1}^{n} \lambda_i \mathbf{x}_i, 1 \leq \lambda_i \leq C, \sum_{i=1}^{n} \lambda_i = 1,$$

  is the (C*) reduced convex hull of* $\mathcal{A}$

- Using $C = 1/2$, the reduced convex hulls of $\mathcal{A}$ and $\mathcal{B}$,



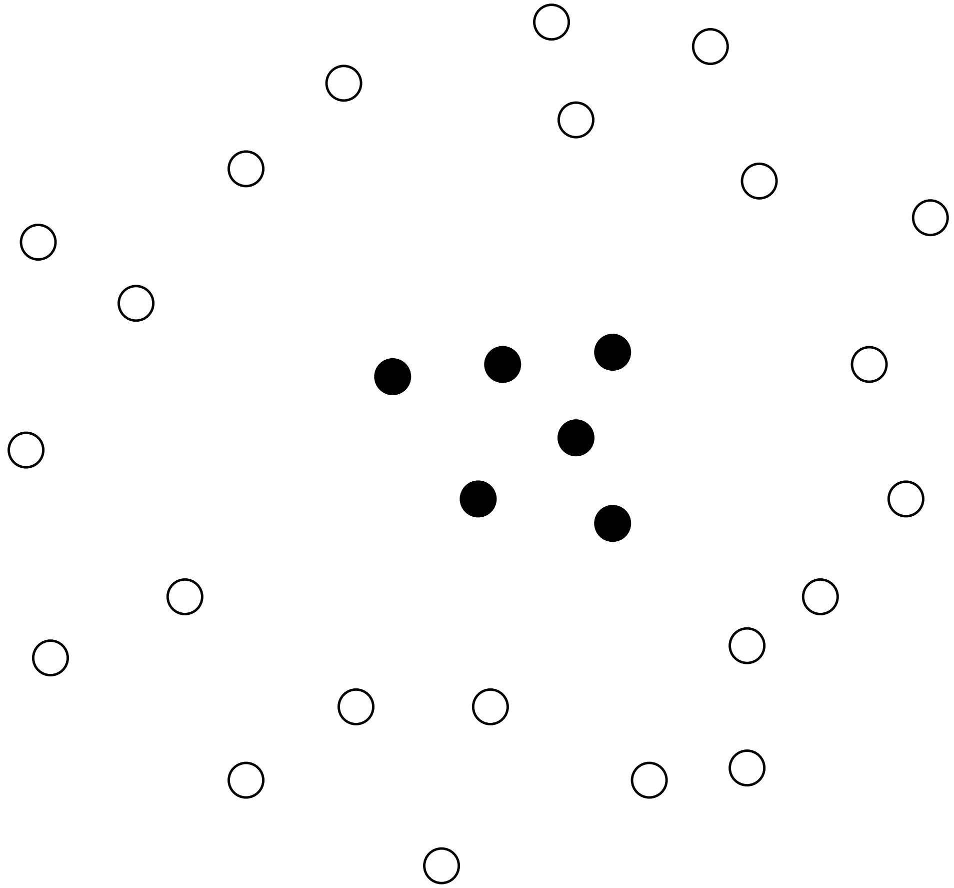
Closest Points in the Reduced Convex Hull

- Idea: find the closest points for the two **reduced** convex hulls

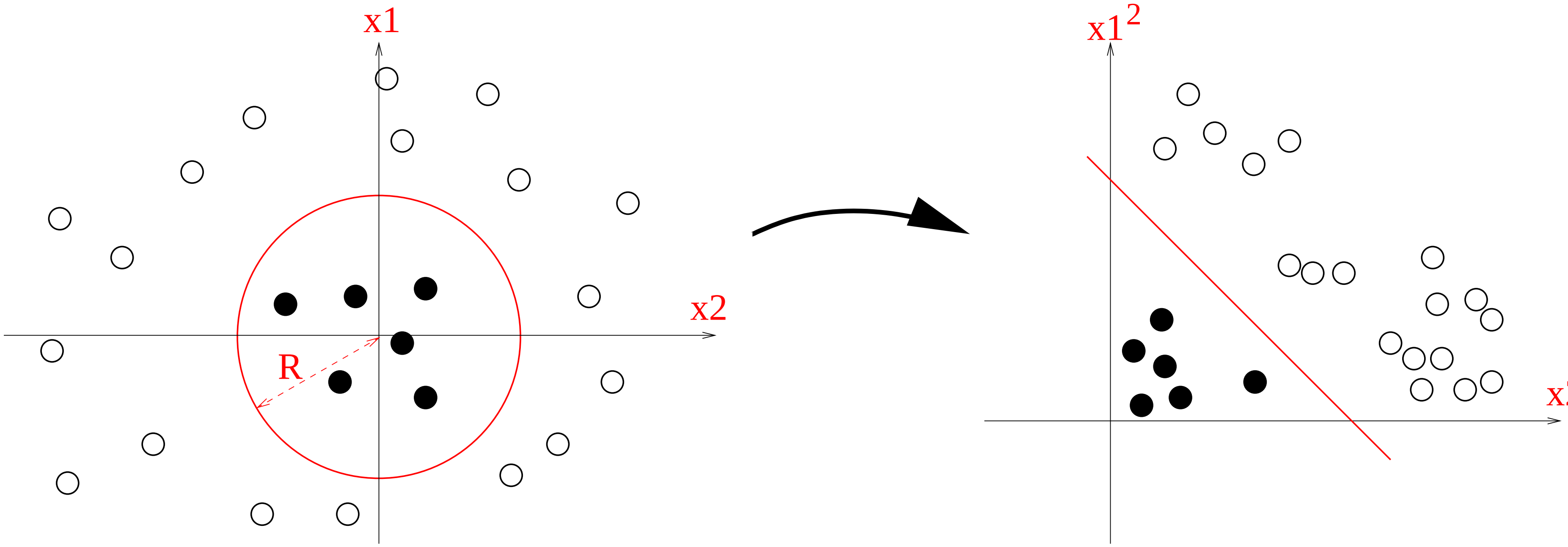
$$
\begin{array}{ll}
\text{minimize} & \|A\mathbf{u} - B\mathbf{v}\|^2 \\
\text{subject to} & \mathbb{1}^T\mathbf{u} = \mathbb{1}^T\mathbf{v} = 1 \\
& \mathbf{u} \leq C\mathbb{1},\ \mathbf{v} \leq C\mathbb{1} \\
& 0 \leq \mathbf{u} \in \mathbb{R}^{n-1}, \mathbf{v} \in \mathbb{R}^{n_1}
\end{array}
$$

- Again, can prove that the soft-margin SVM with C constant accepts as a dual the formulation above.

Sometimes linear classifiers are of little use



Solution: non-linear mapping to a feature space



Let $\phi(\mathbf{x}) = (x_1^2, x_2^2)'$, $\mathbf{w} = (1,1)'$ and $b = 1$. Then the decision function is:

$$f(\mathbf{x}) = x_1^2 + x_2^2 - R^2 = \langle \mathbf{w}, \phi(\mathbf{x}) \rangle + b,$$

Kernel trick for SVM's [3]

- use a mapping ϕ from $\mathcal{X}$ to a feature space,
- which corresponds to the **kernel** k:

$$\forall \mathbf{x}, \mathbf{x}' \in \mathcal{X}, \quad k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$$

- Example: if $\phi(\mathbf{x}) = \phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} x_1^2 \\ x_2^2 \end{bmatrix}$, then

$$k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle = (x_1)^2(x_1')^2 + (x_2)^2(x_2')^2.$$

Training a SVM in the feature space

Replace each $\mathbf{x}^T\mathbf{x}'$ in the SVM algorithm by $\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle = k(\mathbf{x}, \mathbf{x}')$

- **Reminder**: the dual problem is to maximize

$$g(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \, \alpha_j \, y_i \, y_j \, \boldsymbol{k(\mathbf{x}_i, \mathbf{x}_j)},$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \dots, n \\ \sum_{i=1}^{n} \alpha_i \mathbf{y}_i = 0. \end{cases}$$

- The **decision function** becomes:

$$\begin{aligned} f(\mathbf{x}) &= \langle \mathbf{w}, \phi(x) \rangle + b^* \\ &= \sum_{i=1}^{n} y_i \alpha_i \boldsymbol{k(\mathbf{x}_i, \mathbf{x})} + b^*. \end{aligned} \tag{1}$$

The Kernel Trick [5]

The explicit computation of $\phi(\mathbf{x})$ is not necessary.
The kernel $k(\mathbf{x}, \mathbf{x}')$ is enough.

- the SVM optimization for α works **implicitly** in the feature space.
- the SVM is a kernel algorithm: only need to input $\boldsymbol{K}$ and $\mathbf{y}$:

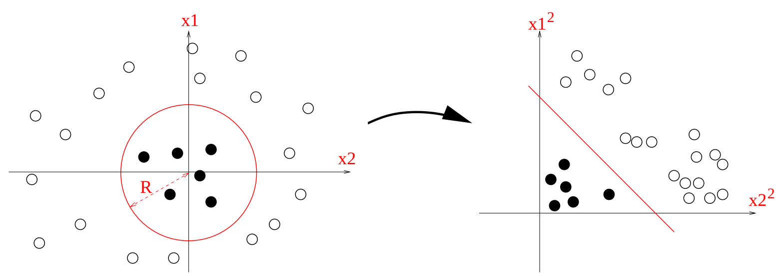
$$\begin{array}{rl} \text{maximize} & g(\alpha) = \alpha^T \mathbf{1} - \frac{1}{2}\alpha^T(\mathbf{y}^T \boldsymbol{K} \mathbf{y})\alpha \\ \text{such that} & 0 \leq \alpha_i \leq C, \quad \text{for } i = 1, \ldots, n \\ & \sum_{i=1}^n \alpha_i \mathbf{y}_i = 0. \end{array}$$

- $\boldsymbol{K}$'s **positive definiten** $\Leftrightarrow$ **problem has an optimum**
- the decision function is $f(\cdot) = \sum_{i=1}^n \alpha_i \boldsymbol{k}(\mathbf{x}_i, \cdot) + b$.

Kernel example: polynomial kernel

- For $\mathbf{x} = (x_1, x_2)^\top \in \mathbb{R}^2$, let $\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$:

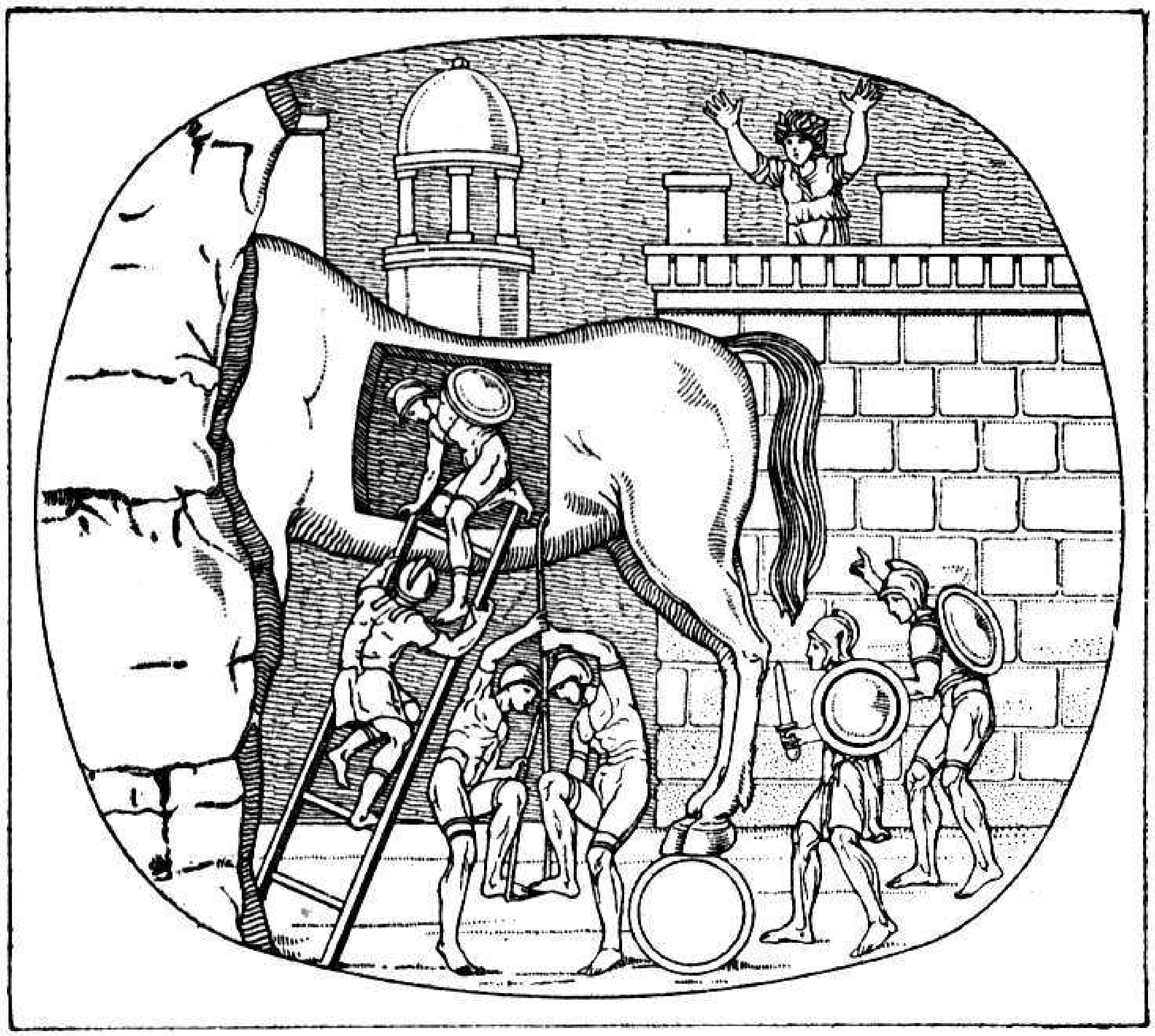
$$\begin{aligned} \boldsymbol{K}(\mathbf{x}, \mathbf{x}') &= x_1^2 x_1'^2 + 2x_1x_2x_1'x_2' + x_2^2x_2'^2 \\ &= \{x_1x_1' + x_2x_2'\}^2 \\ &= \{\mathbf{x}^T\mathbf{x}'\}^2 . \end{aligned}$$



- Many more:

Kernels are Trojan Horses onto Linear Models

- With kernels, complex structures can enter the realm of linear models



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