CZECH TECHNICAL UNIVERSITY IN PRAGUE

Faculty of Electrical Engineering
Department of Cybernetics

Optimal separating hyperplane. Basis expansion. Kernel trick. Support vector machine.

Petr Pošík

Rehearsal

Linear discrimination function

Binary classification of objects $\boldsymbol{x}$ (classification into 2 classes, dichotomy):

- For 2 classes, 1 discrimination function is enough.
- Decision rule:

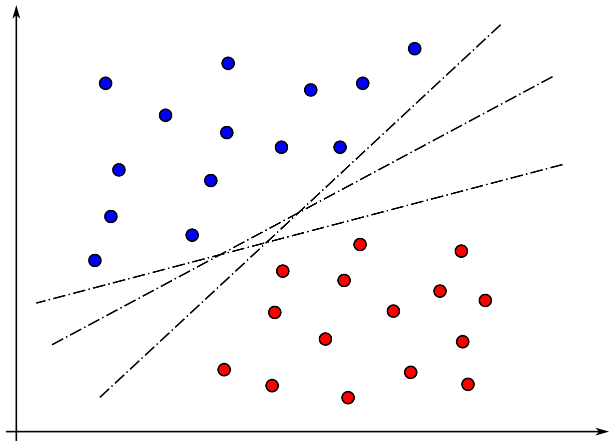
$$\left.\begin{aligned} f(\boldsymbol{x}^{(i)}) > 0 &\Longleftrightarrow \widehat{y}^{(i)} = +1 \\ f(\boldsymbol{x}^{(i)}) < 0 &\Longleftrightarrow \widehat{y}^{(i)} = -1 \end{aligned}\right\} \qquad \text{i.e.} \qquad \widehat{y}^{(i)} = \operatorname{sign}\left(f(\boldsymbol{x}^{(i)})\right)$$

Learning of the linear discrimination function by the *perceptron algorithm*:

- Optimization of

$$J(\boldsymbol{w}, T) = \sum_{i=1}^{|T|} \mathbb{I}\left(y^{(i)} \neq \widehat{y}^{(i)}\right)$$

- The weight vector is a weighted sum of the training points $\boldsymbol{x}^{(i)}$.
- Perceptron finds *any* separating hyperplane, if exists.
- Among the infinite number of separating hyperplanes, which one is the best?



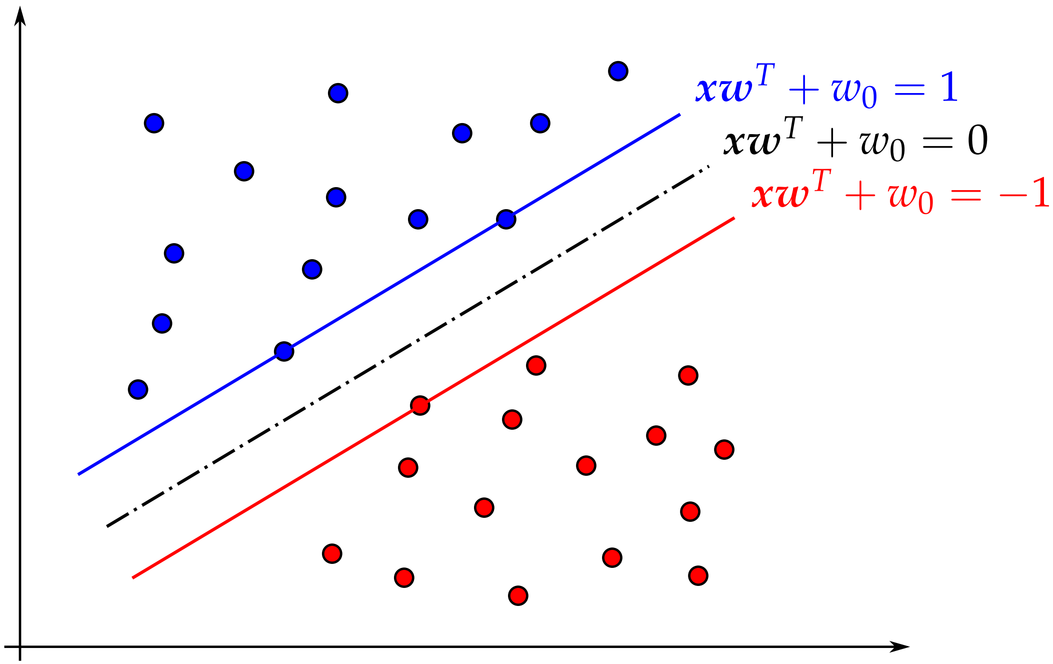
Optimal separating hyperplane

Optimal separating hyperplane

Margin (cz:odstup):

- "The width of the band in which the decision boundary can move (in the direction of its normal vector) without touching any data point."

Maximum margin linear classifier



Plus 1 level: $\{x : \boldsymbol{x}\boldsymbol{w}^T + w_0 = 1\}$
Minus 1 level: $\{x : \boldsymbol{x}\boldsymbol{w}^T + w_0 = -1\}$
Decision boundary: $\{x : \boldsymbol{x}\boldsymbol{w}^T + w_0 = 0\}$

Support vectors:

- Data points $\boldsymbol{x}$ lying at the plus 1 level or minus 1 level.
- Only these points influence the decision boundary!

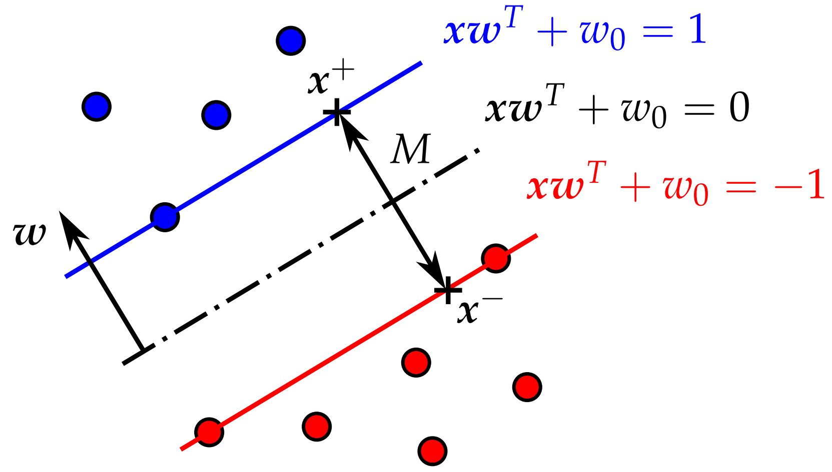
Why we would like to maximize the margin?

- Intuitively, it is safe.
- If we make a small error in estimating the boundary, the classification will likely stay correct.
- The model is invariant with respect to the training set changes, except the changes of support vectors.
- There are sound theoretical results (based on VC dimension) that having a maximum margin classifier is good.
- Maximal margin works well in practice.

Margin size

How to compute the margin M given $\boldsymbol{w} = (w_1, \ldots, w_D)$, w_0?

- Let's choose two points $\boldsymbol{x}^+$ and $\boldsymbol{x}^-$, lying in the plus 1 level and minus 1 level, respectively.
- Let's compute the margin M as their distance.



We know that:

$$\begin{aligned} \boldsymbol{x}^+\boldsymbol{w}^T + w_0 &= 1 \\ \boldsymbol{x}^-\boldsymbol{w}^T + w_0 &= -1 \\ \boldsymbol{x}^- + \lambda\boldsymbol{w} &= \boldsymbol{x}^+ \end{aligned}$$

And we can derive:

$$\begin{aligned} (\boldsymbol{x}^+ - \boldsymbol{x}^-)\boldsymbol{w}^T &= 2 \\ (\boldsymbol{x}^- + \lambda\boldsymbol{w} - \boldsymbol{x}^-)\boldsymbol{w}^T &= 2 \\ \lambda\boldsymbol{w}\boldsymbol{w}^T &= 2 \end{aligned}$$

$$\lambda = \frac{2}{\boldsymbol{w}\boldsymbol{w}^T} = \frac{2}{\|\boldsymbol{w}\|^2}$$

Thus the margin size is

$$M = \|\boldsymbol{x}^+ - \boldsymbol{x}^-\| = \|\lambda\boldsymbol{w}\| = \lambda\|\boldsymbol{w}\| = \frac{2}{\|\boldsymbol{w}\|^2}\|\boldsymbol{w}\| = \frac{2}{\|\boldsymbol{w}\|}$$

Optimal separating hyperplane learning

We want to maximize margin $M = \frac{2}{\|w\|}$ subject to the constraints ensuring correct classification of the training set T. This optimization problem can be formulated as a *quadratic programming* (QP) task.

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- Primary QP task:

$$\text{minimize } \boldsymbol{w}\boldsymbol{w}^T \text{ with respect to } w_1, \ldots, w_D$$

$$\text{subject to } y^{(i)}(\boldsymbol{x}^{(i)}\boldsymbol{w}^T + w_0) \geq 1.$$

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- Dual QP task:

$$\text{maximize } \sum_{i=1}^{|T|} \alpha_i - \frac{1}{2}\sum_{i=1}^{|T|}\sum_{j=1}^{|T|} \alpha_i \alpha_j y^{(i)} y^{(j)} \boldsymbol{x}^{(i)} \boldsymbol{x}^{(j)T} \text{ with respect to } \alpha_1, \ldots, \alpha_{|T|}$$
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- From the solution of the dual task, we can compute the solution of the primal task:

$$\boldsymbol{w} = \sum_{i=1}^{|T|} \alpha_i y^{(i)} \boldsymbol{x}^{(i)}, \qquad w_0 = y^{(k)} - \boldsymbol{x}^{(k)} \boldsymbol{w}^T,$$

where $(\boldsymbol{x}^{(k)}, y^{(k)})$ is any *support vector*, i.e. $\alpha_k > 0$.

Optimal separating hyperplane: concluding remarks

The importance of dual formulation:

- The QP task in dual formulation is easier to solve for QP solvers than the primal formulation.
- New, unseen examples can be classified using function

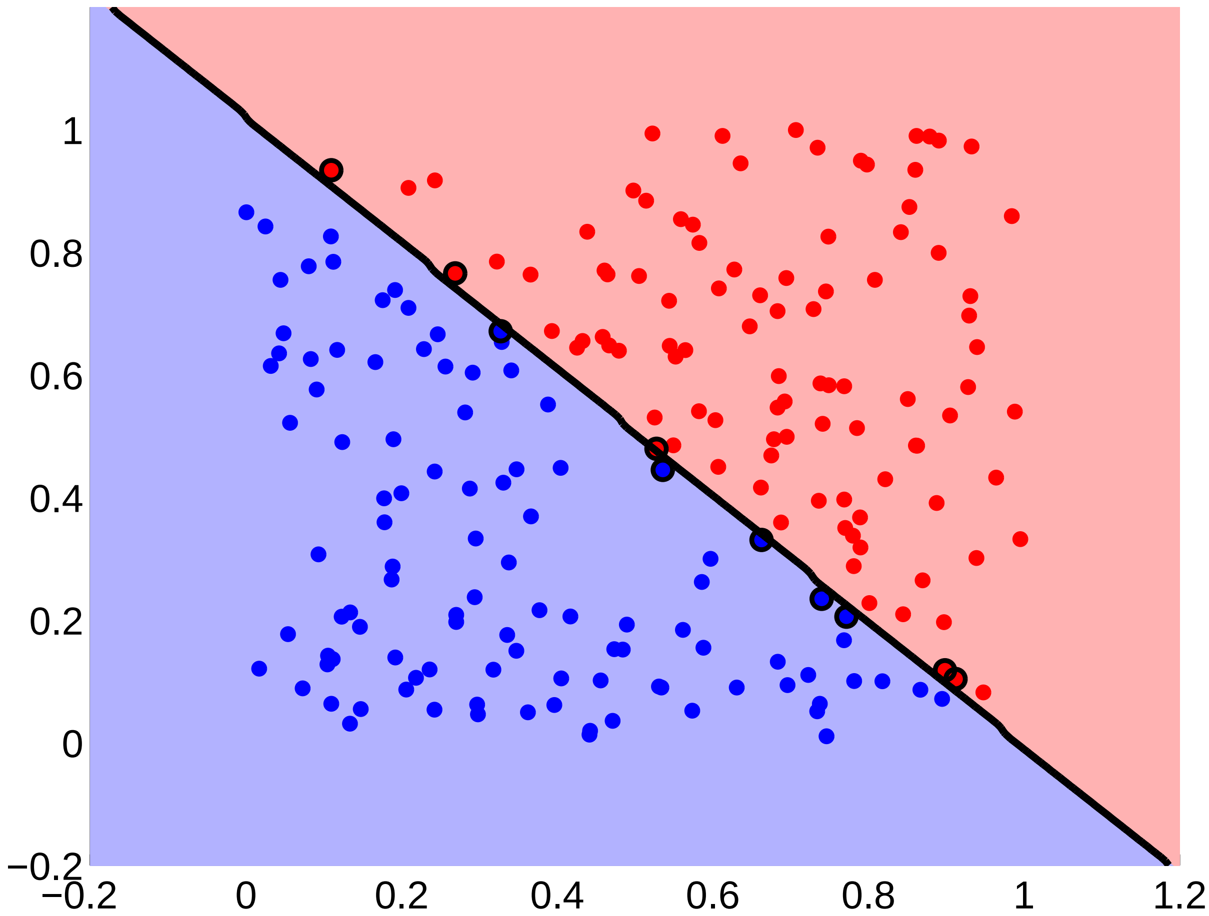
$$f(\boldsymbol{x}, \boldsymbol{w}, w_0) = \operatorname{sign}(\boldsymbol{x}\boldsymbol{w}^T + w_0) = \operatorname{sign}\left(\sum_{i=1}^{|T|} \alpha_i y^{(i)} \boldsymbol{x}^{(i)} \boldsymbol{x}^T + w_0\right),$$

  i.e. the discrimination function contains the examples $\boldsymbol{x}$ only in the form of dot products (which will be useful later).
- The examples with $\alpha_i > 0$ are *support vectors*, thus the sums may be carried out only over the support vectors.
- The dual formulation allows for other tricks which you will learn later.

What if the data are not linearly separable?

- There is a generalization of the QP task formulation for this case (*soft margin*).
- The primal task has double the number of constraints, the task is more complex.
- The results for the QP task with *soft margin* are of the same type as before.

Optimal separating hyperplane: demo



When a linear decision boundary is not enough. . .

Basis expansion

a.k.a. **feature space straightening**.

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Why?

- Linear decision boundary (or linear regression model) may not be flexible enough to perform precise classification (regression).
- The algorithms for fitting linear models can be used to fit *non-linear models*!

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How?

- Let's define a new multidimensional image space F.
- The examples are then tranformed into this image space (new features are derived):

$$\begin{aligned} \boldsymbol{x} \quad &\rightarrow \quad \boldsymbol{z} = \Phi(\boldsymbol{x}), \\ \boldsymbol{x} = (x_1, x_2, \ldots, x_D) \quad &\rightarrow \quad \boldsymbol{z} = (\Phi_1(\boldsymbol{x}), \Phi_2(\boldsymbol{x}), \ldots, \Phi_G(\boldsymbol{x})), \end{aligned}$$

  while usually $D \ll G$.
- In the image space, a linear model is trained. However, this is equivalent to training a non-linear model in the original space.

$$\begin{aligned} f_G(\boldsymbol{z}) &= w_1 z_1 + w_2 z_2 + \ldots + w_G z_G + w_0 \\ f(\boldsymbol{x}) = f_G(\Phi(\boldsymbol{x})) &= w_1 \Phi_1(\boldsymbol{x}) + w_2 \Phi_2(\boldsymbol{x}) + \ldots + w_G \Phi_G(\boldsymbol{x}) + w_0 \end{aligned}$$

Two coordinate systems

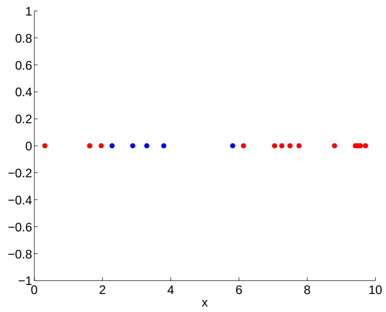
Transformation into a high-dimensional image space

Feature space	Image space
$\boldsymbol{x} = (x_1, x_2, \ldots, x_D)$	$\boldsymbol{z} = (z_1, z_2, \ldots, z_G)$ $z_1 = \log x_1$ $z_2 = x_1^2 x_3$ $z_3 = e^{x_2}$ $\ldots$
$f(\boldsymbol{x}) = w_1 \log x_1 + w_2 x_1^2 x_3 + w_3 e^{x_2} + \ldots + w_0$	$f_G(\boldsymbol{z}) = w_1 z_1 + w_2 z_2 + w_3 z_3 + \ldots + w_0$

Training a linear model in the image space

Non-linear model in the feature space

Two coordinate systems: graphically

Feature space	Image space
	

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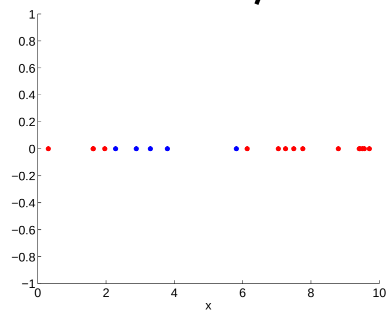	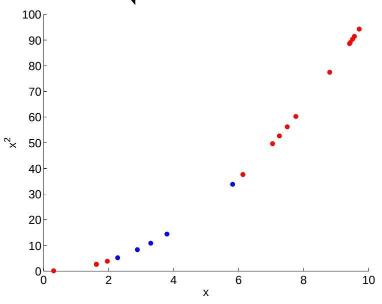

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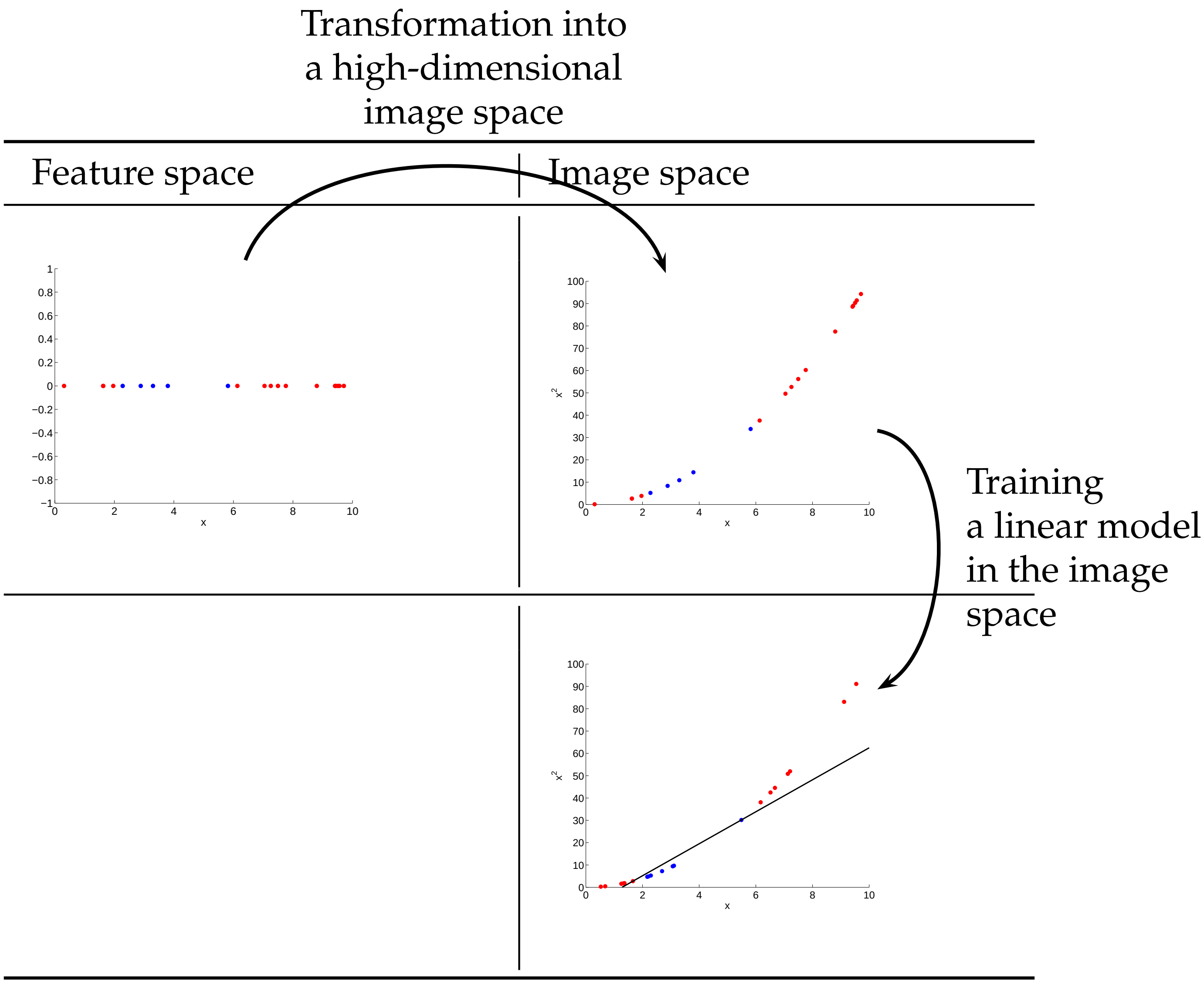

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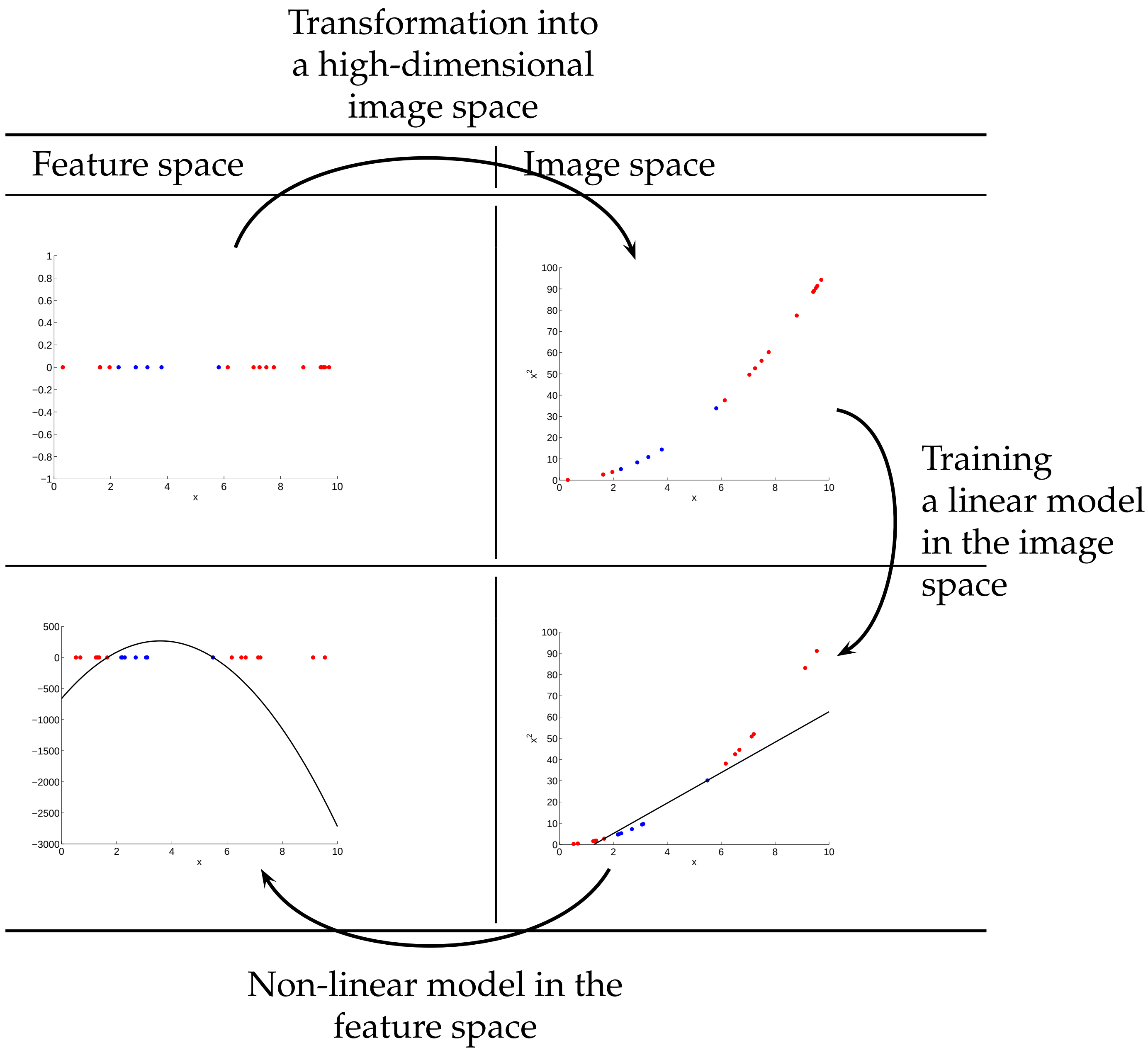

Basis expansion: remarks

Advantages:

- Universal, generally usable method.

Disadvantages:

- We must define what new features shall form the high-dimensional space F.
- The examples must be really transformed into the high-dimensional space F.

For certain type of algorithms, there is a method how to perform the basis expansion withou actually carrying out the mapping!

Support vector machine

Optimal separating hyperplane combined with the basis expansion

To reiterate: when using the optimal separating hyperplane, the examples $\boldsymbol{x}$ occur only in

$$\text{the optimization criterion } \sum_{i=1}^{|T|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|T|} \sum_{j=1}^{|T|} \alpha_i \alpha_j y^{(i)} y^{(j)} \boldsymbol{x}^{(i)} \boldsymbol{x}^{(j)T}$$

$$\text{and in the decision rule } f(\boldsymbol{x}) = \operatorname{sign}\left(\sum_{i=1}^{|T|} \alpha_i y^{(i)} \boldsymbol{x}^{(i)} \boldsymbol{x}^T + w_0 \right).$$

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Application of the basis expansion changes

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What if we use a scalar function $K(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)})$ instead of the dot product in the image space?

$$\text{The optimization criterion: } \sum_{i=1}^{|T|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|T|} \sum_{j=1}^{|T|} \alpha_i \alpha_j y^{(i)} y^{(j)} K(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)})$$

$$\text{The discrimination function: } f(\boldsymbol{x}) = \operatorname{sign}\left(\sum_{i=1}^{|T|} \alpha_i y^{(i)} K(\boldsymbol{x}^{(i)}, \boldsymbol{x}) + w_0 \right).$$

Kernel trick

There are function of 2 vector arguments $K(\boldsymbol{a}, \boldsymbol{b})$ which provide values equal to the dot product $\Phi(\boldsymbol{a})\Phi(\boldsymbol{b})^T$ of the images of the vectors a and b in certain high-dimensional image space. Such functions are called **kernel functions** or **kernels**.

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Kernel trick: Let's have a linear algorithm in which the examples $\boldsymbol{x}$ occur only in dot products.

- Such an algorithm can be made non-linear by replacing the dot products of examples $\boldsymbol{x}$ with *kernels*.
- The result is the same is if the algorithm was trained in some high-dimensional image space with the coordinates given by many non-linear basis functions.
- Thanks to kernels, it is not needed to perform the mapping, the algorithm is much more efficient.

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Frequently used kernels:

Polynomial: $K(\boldsymbol{a}, \boldsymbol{b}) = (\boldsymbol{a}\boldsymbol{b}^T + 1)^d$, where d is the degree of the polynom.

Gaussian (RBF): $K(\boldsymbol{a}, \boldsymbol{b}) = \exp\left(-\frac{|\boldsymbol{a} - \boldsymbol{b}|^2}{\sigma^2}\right)$, where σ^2 is the „width“ of Gaussian.

Support vector machine

Support vector machine

Support vector machine (SVM)

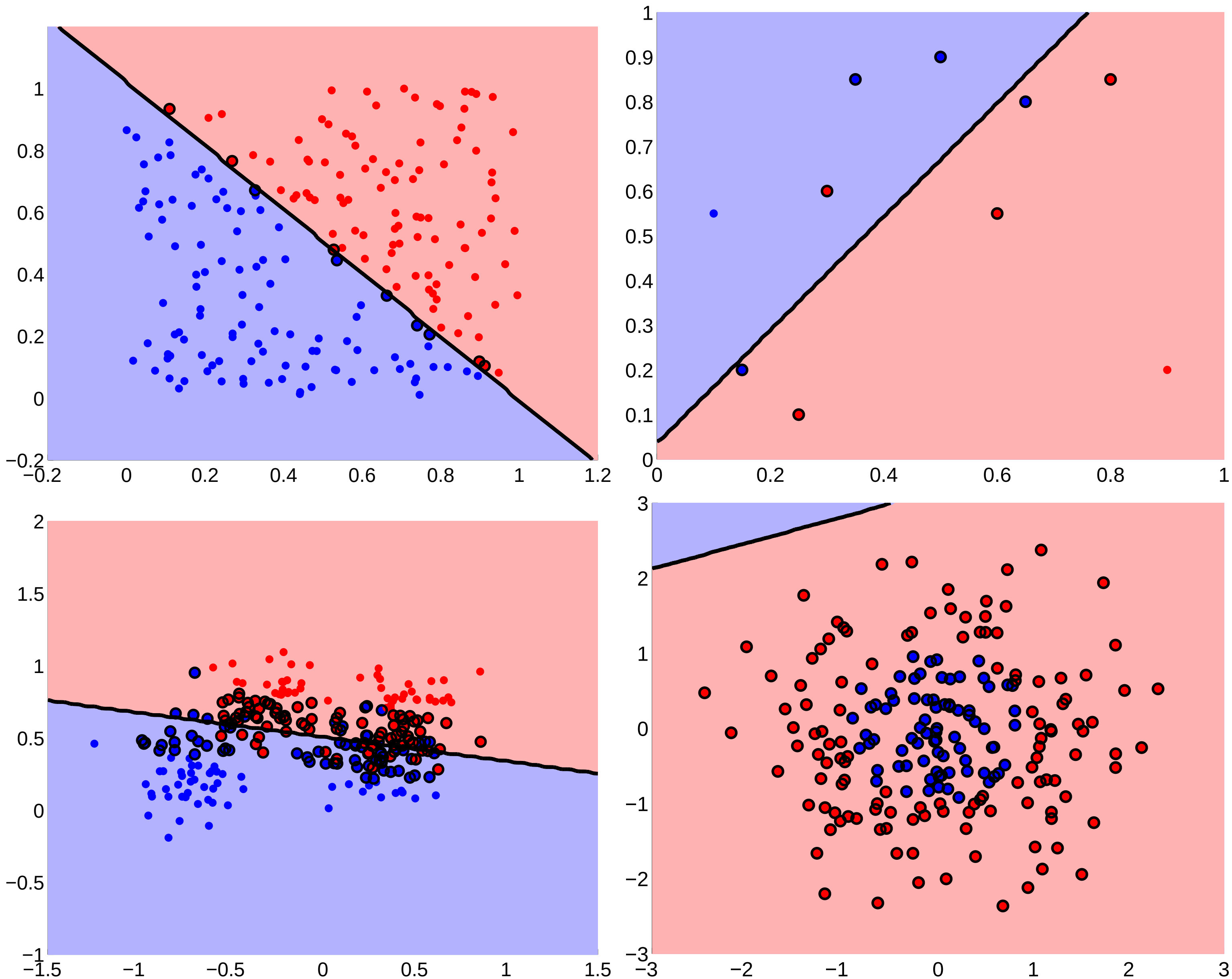
=

optimal separating hyperplane

+

kernel trick

Demo: SVM with linear kernel



Demo: SVM with Gaussian (RBF) kernel