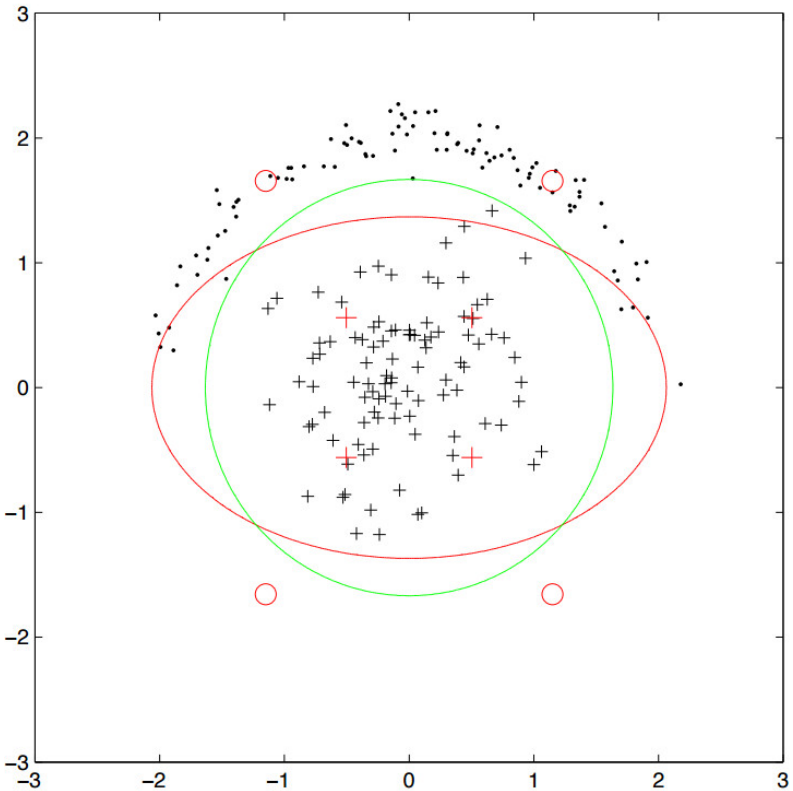
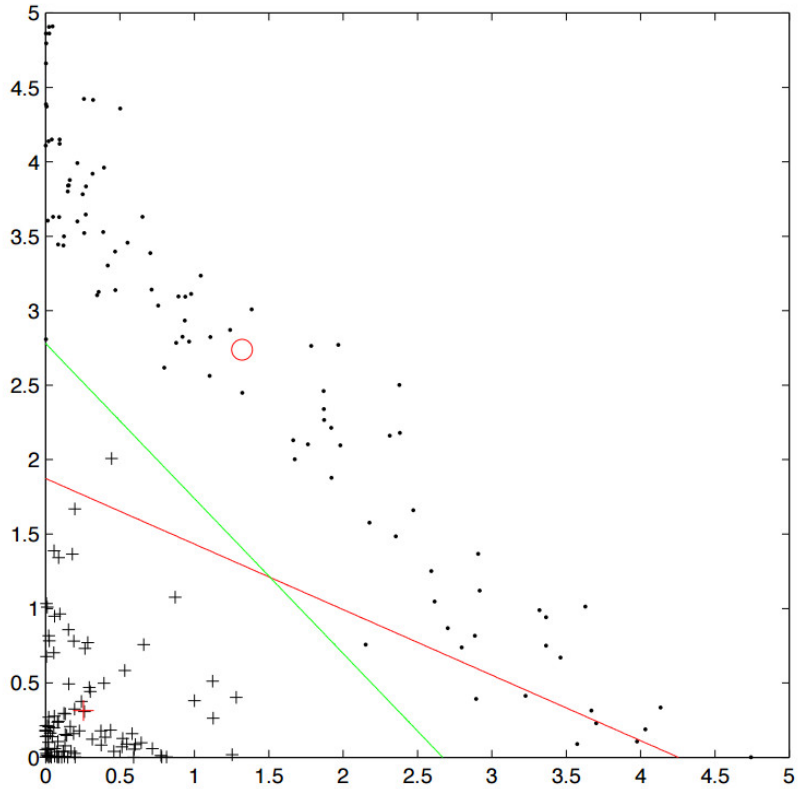
Kernel Methods

Quadratic Decision Boundary





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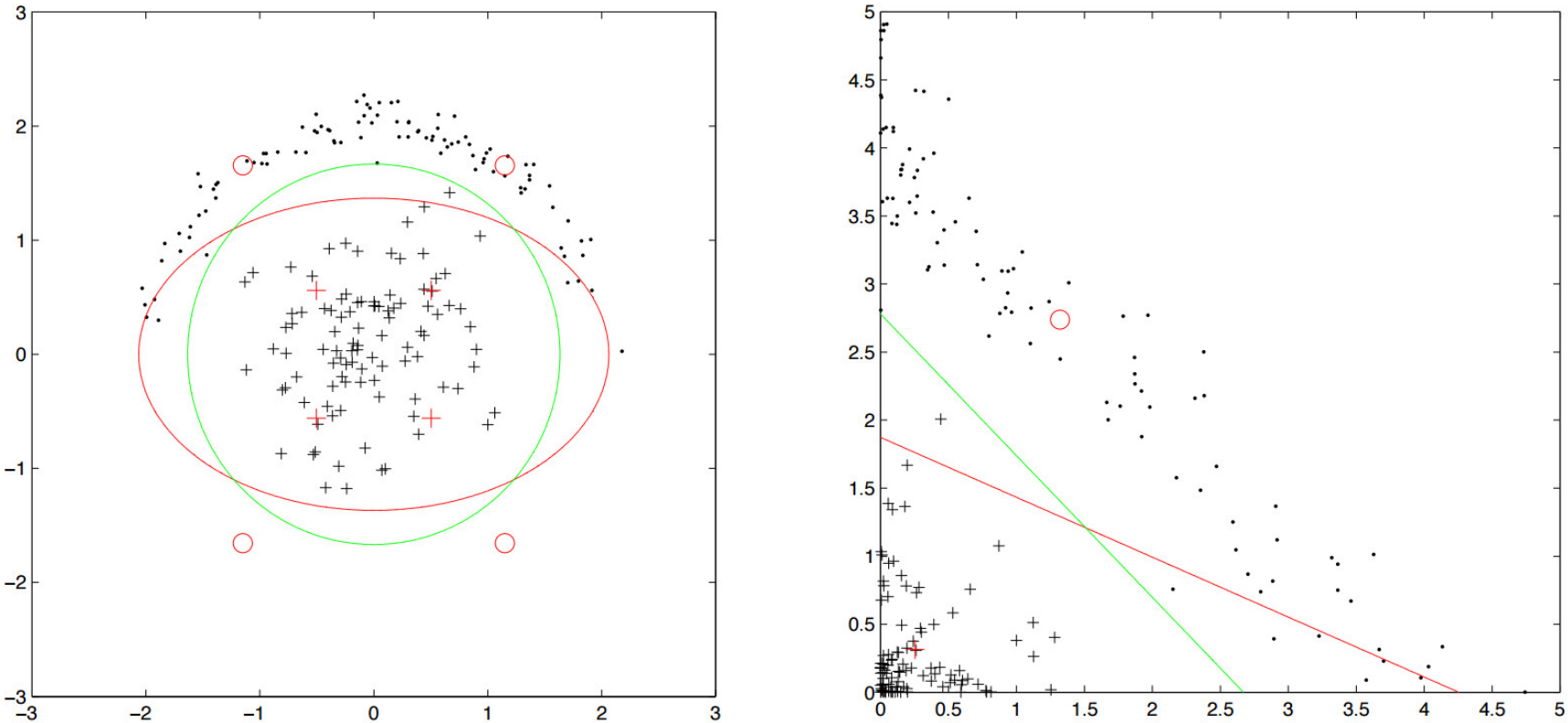

Left: The original set, Right: Transformed using the square of features.

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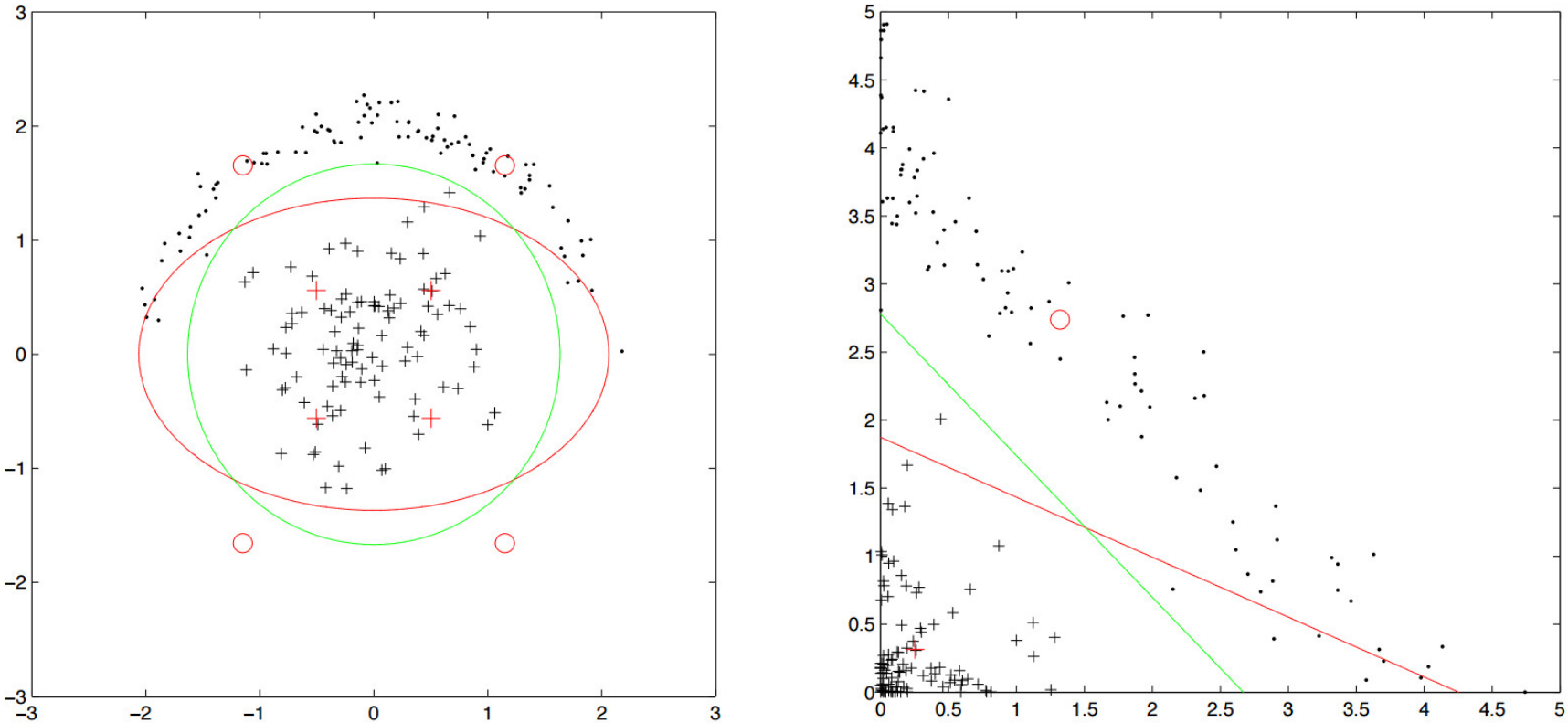

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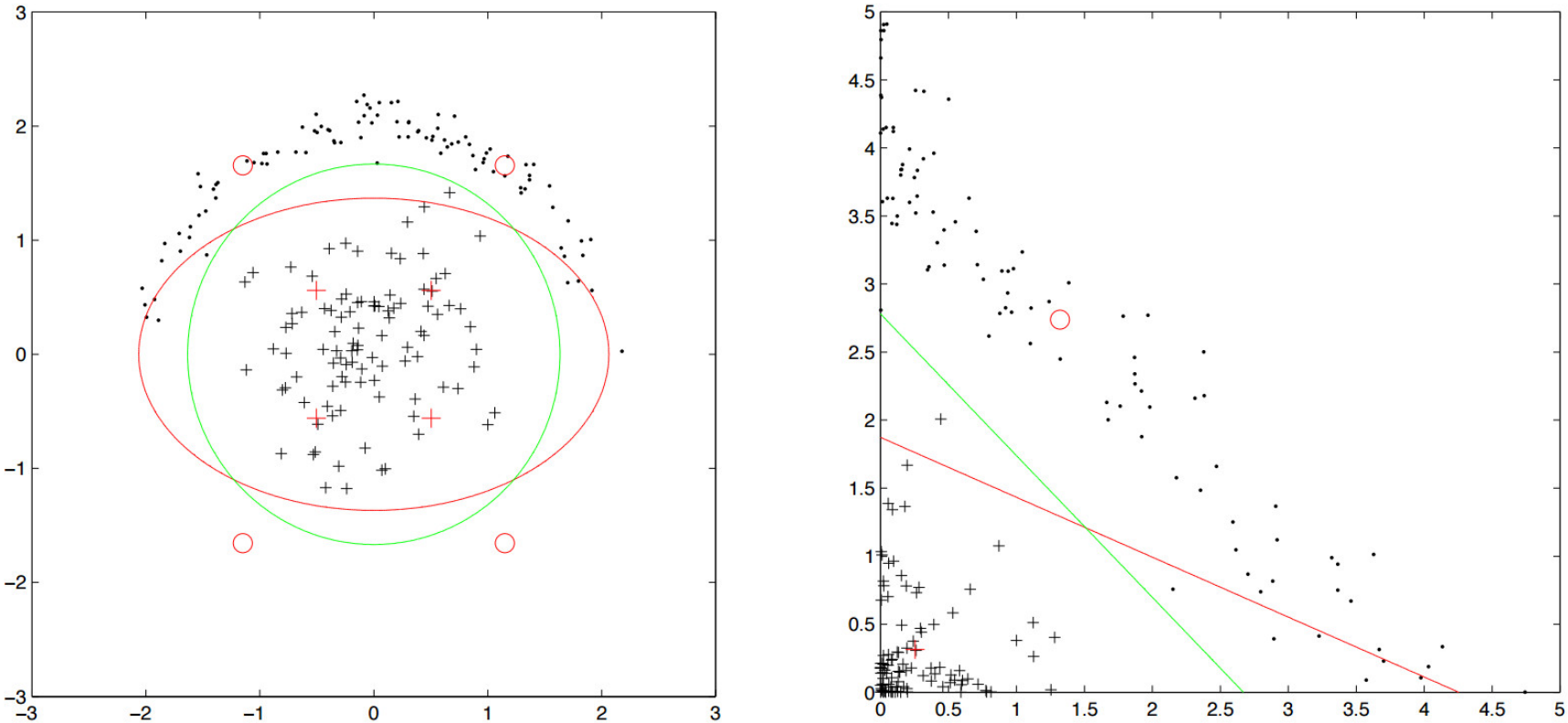

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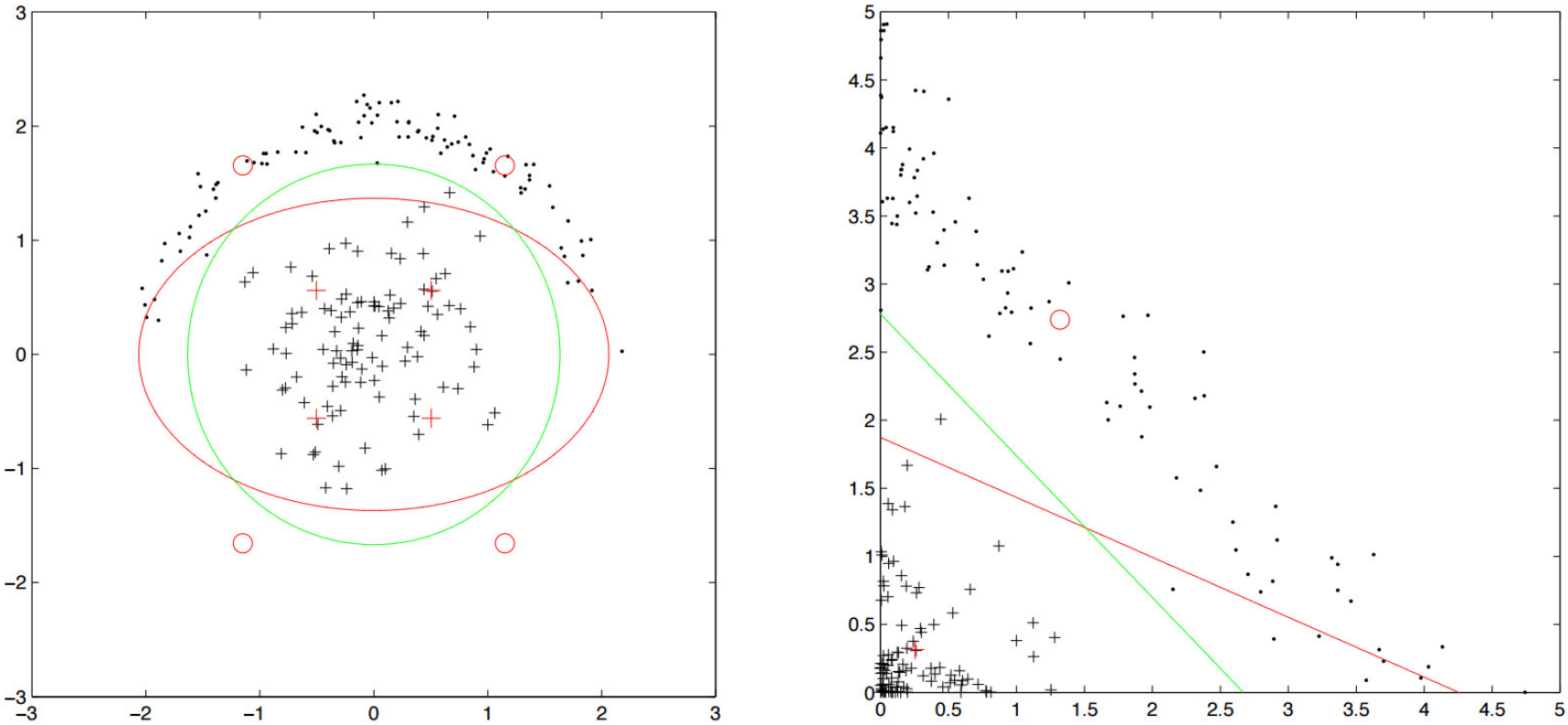

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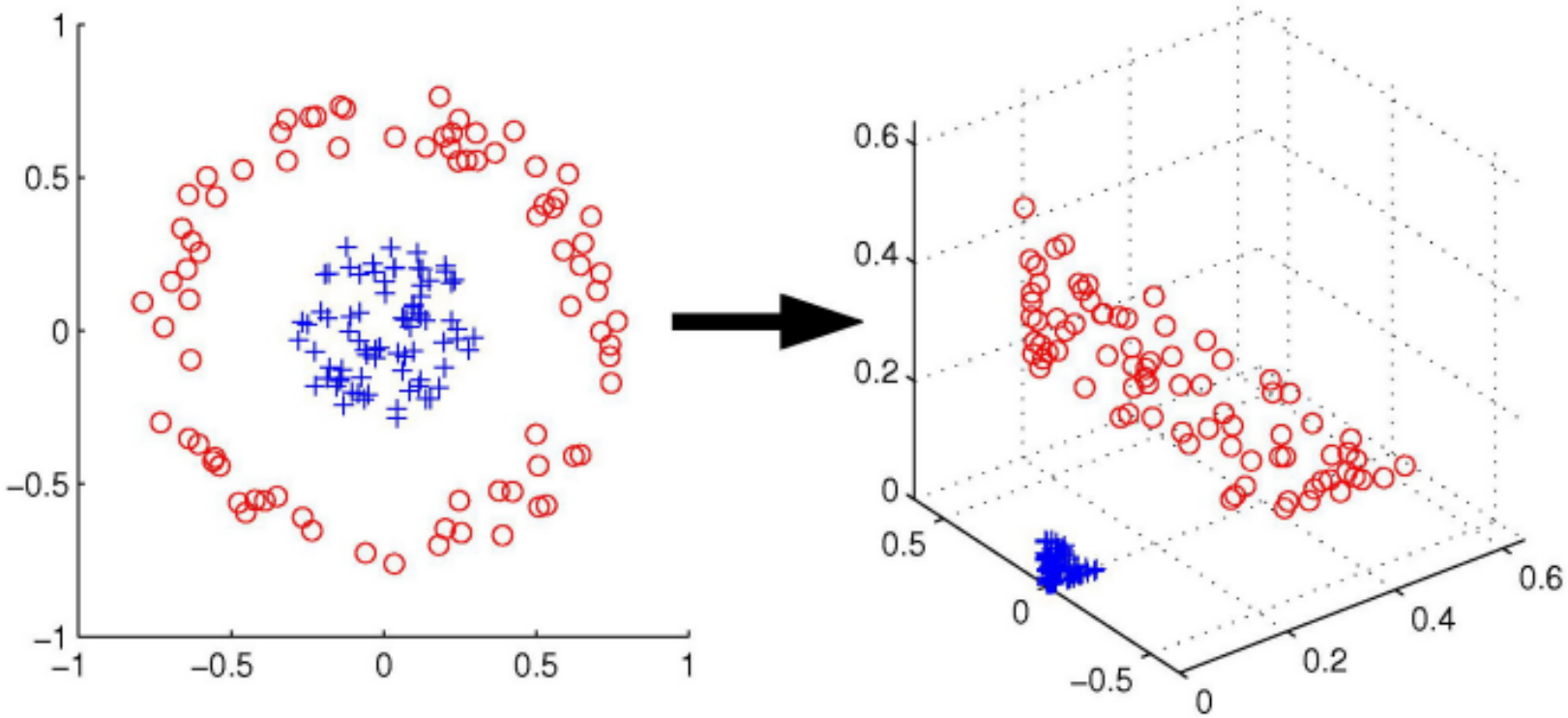
Anothe Solution



Mapping from $\mathbb{R}^2$ to $\mathbb{R}^3$ so that there is "more space" for linear separation.

Do We Need to Map Explicitly?

In general, mapping to (much) higher feature space helps (there are more "degrees of freedom" so linear separability might get a chance).

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To avoid explicit construction of the higher dimensional feature space, we use so called *kernel trick*.

But first we need to *dualize* our learning algorithm.

Linear Regression

- Given a set D of training examples:

$$D = \{(\vec{x}_1, f_1), (\vec{x}_2, f_2), \ldots, (\vec{x}_p, f_p)\}$$

Here $\vec{x}_k = (x_{k1} \ldots, x_{kn}) \in \mathbb{R}^n$ and $f_k \in \mathbb{R}$.

- **Our goal:** Find $\vec{w}$ so that $h[\vec{w}](\vec{x_k}) = \vec{w} \cdot \tilde{\mathrm{x}}_k$ is close to f_k for every $k = 1, \ldots, p$.

Recall that $\tilde{\mathrm{x}}_k = (x_{k0}, x_{k1} \ldots, x_{kn})$ where $x_{k0} = 1$.

- **Squared Error Function:**

$$E(\vec{w}) = \frac{1}{2}\sum_{k=1}^{p}(\vec{w} \cdot \tilde{\mathrm{x}}_k - f_k)^2 = \frac{1}{2}\sum_{k=1}^{p}\left(\sum_{i=0}^{n} w_i x_{ki} - f_k\right)^2$$

Regularized Linear Regression

Regularized Squared Error Function:

$$E(\vec{w}) = \frac{1}{2}\sum_{k=1}^{p}(\vec{w}\cdot\tilde{\mathbf{x}}_k - f_k)^2 + \vec{w}\cdot\vec{w}$$

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The Representer Theorem: The weight vector $\vec{w}^*$ minimizing the regularized squared error function can be written as

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Substituting this expression for weights in E gives

$$E'(\vec{w}) = \frac{1}{2}\sum_{k=1}^{p}\left(\sum_{i=1}^{p}\alpha_i f_i\,\tilde{\mathrm{x}}_i\cdot\tilde{\mathrm{x}}_k - f_k\right)^2 + \sum_{i=1}^{p}\sum_{j=1}^{p}\alpha_i\alpha_j f_i f_j\,\tilde{\mathrm{x}}_i\cdot\tilde{\mathrm{x}}_j$$

and we minimize E' w.r.t. $\alpha_1,\ldots,\alpha_p$. What is this good for??

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Find $\alpha_1, \ldots, \alpha_p$ *minimizing dual regularized squared error*

$$E'(\vec{w}) = \frac{1}{2} \sum_{k=1}^{p} \left(\sum_{i=1}^{p} \alpha_i f_i \, \tilde{\mathrm{x}}_i \cdot \tilde{\mathrm{x}}_k - f_k \right)^2 + \sum_{i=1}^{p} \sum_{j=1}^{p} \alpha_i \alpha_j f_i f_j \, \tilde{\mathrm{x}}_i \cdot \tilde{\mathrm{x}}_j$$

The resulting coefficients $\alpha_1, \ldots, \alpha_p$ give a weight vector

$$\vec{w}^* = \sum_{i=1}^{p} \alpha_i f_i \, \tilde{\mathrm{x}}_i$$

which in turn gives a linear model

$$h[\vec{w}^*](\vec{x}) = \vec{w}^* \tilde{\mathrm{x}} = \sum_{i=1}^{p} \alpha_i f_i \, \tilde{\mathrm{x}}_i \cdot \tilde{\mathrm{x}}$$

Note that all $\tilde{\mathrm{x}}, \tilde{\mathrm{x}}_i, \tilde{\mathrm{x}}_j, \tilde{\mathrm{x}}_k$ occur in dot products with themselves!

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Non-linear model: $h[\vec{\alpha}](\vec{x}) = \sum_{i=1}^{p}\alpha_i f_i\, \kappa(\tilde{x}_i, \tilde{x})$

Here κ is a **kernel function**. But now what is the trick?

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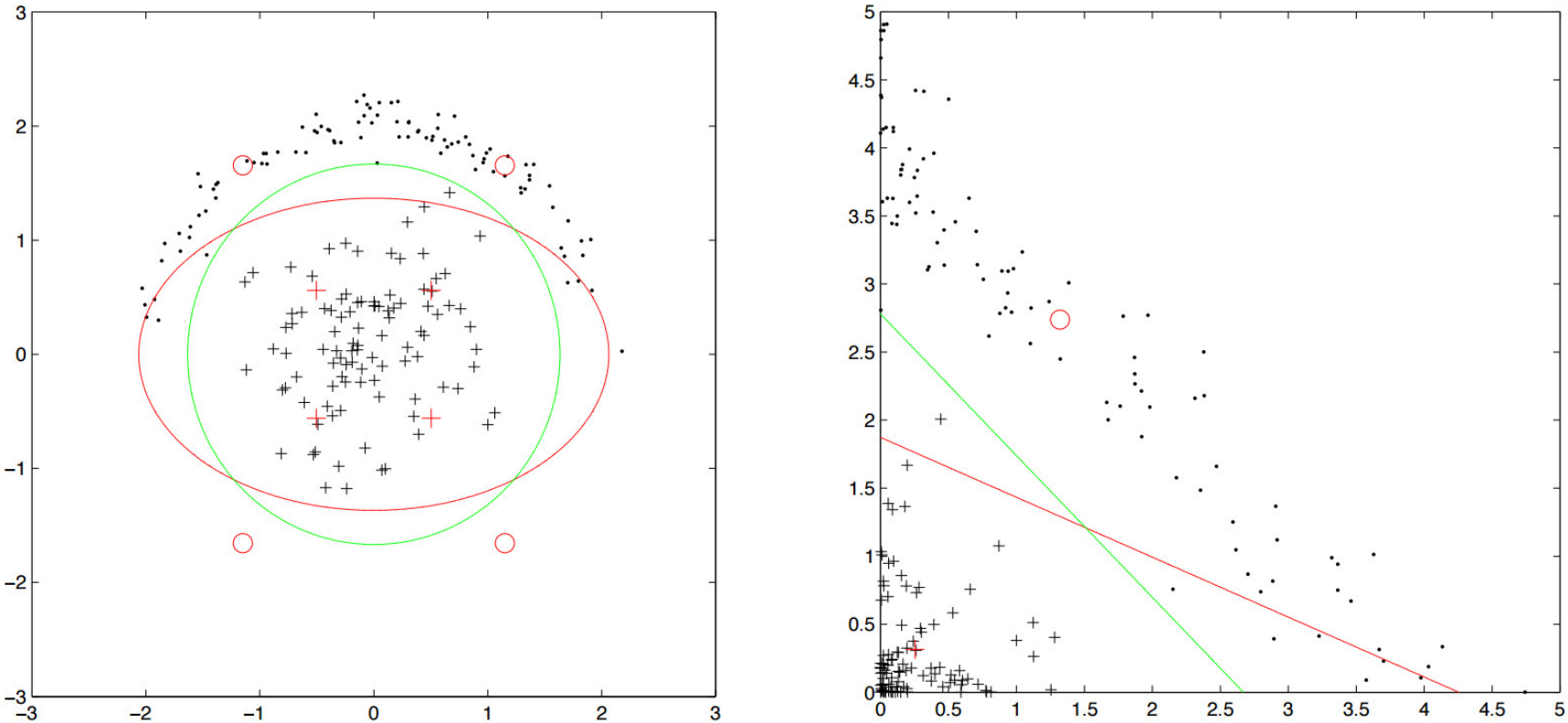
The trick is that suitable kernel functions κ correspond to dot products in transformed spaces!

Recall the Quadratic Decision Boundary



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THE Idea: Using the kernel $\kappa(\tilde{\mathrm{x}}_k, \tilde{\mathrm{x}}_\ell) = (\tilde{\mathrm{x}}_k \cdot \tilde{\mathrm{x}}_\ell)^2$ in the kernel dual regularized squared error corredponds to using the regularized squared error after the transformation ϕ.

Quadratic Decision Boundary

Given a set D of training examples:

$$D = \{(\vec{x}_1, f_1), (\vec{x}_2, f_2), \ldots, (\vec{x}_p, f_p)\}$$

Assume that $f_i \in \{1, -1\}$ indicates the class of $\vec{x}_i$.

Yes, I know that squared error regression should not be used for classification!

Considering $\kappa(\tilde{x}_k, \tilde{x}_\ell) = (\tilde{x}_k \cdot \tilde{x}_\ell)^2$ in our kernel dual regularized squared error we obtain

Find $\vec{\alpha} = \alpha_1, \ldots, \alpha_p$ *minimizing*

$$E'(\vec{w}) = \frac{1}{2} \sum_{k=1}^{p} \left(\sum_{i=1}^{p} \alpha_i f_i \, (\tilde{x}_i \cdot \tilde{x}_k)^2 - f_k \right)^2 + \sum_{i=1}^{p} \sum_{j=1}^{p} \alpha_i \alpha_j f_i f_j \, (\tilde{x}_i \cdot \tilde{x}_j)^2$$

Non-linear classifier: $h[\vec{\alpha}](\vec{x}) = \sum_{i=1}^{p} \alpha_i f_i \, (\tilde{x}_i \cdot \tilde{x})^2$

Intuitively, minimizing E' in $\mathbb{R}^2$ gives a separating hyperplane for the input vectors transformed into $\mathbb{R}^5$. This means, that in $\mathbb{R}^2$ it searches for a quadratic (i.e., non-linear) boundary.

Examples of Kernels

- Linear: $\kappa(\tilde{\mathsf{x}}_\ell, \tilde{\mathsf{x}}_\mathsf{k}) = \tilde{\mathsf{x}}_\ell \cdot \tilde{\mathsf{x}}_\mathsf{k}$

  The corresponding mapping $\phi(\tilde{\mathsf{x}}) = \tilde{\mathsf{x}}$ is identity (no transformation).

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Choosing kernels remains to be black magic of kernel methods. They are usually chosen based on trial and error (of course, experience and additional insight into data helps).

Similar trick can be done with (soft-margin) support vector machines.