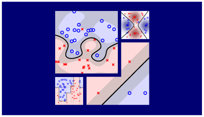
Machine Learning Techniques
(機器學習技法)



Lecture 3: Kernel Support Vector Machine

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Roadmap

1. Embedding Numerous Features: Kernel Models

Lecture 2: Dual Support Vector Machine

dual SVM: another **QP** with **valuable geometric messages** and almost **no dependence on $\tilde{d}$**

Lecture 3: Kernel Support Vector Machine

- Kernel Trick
- Polynomial Kernel
- Gaussian Kernel
- Comparison of Kernels

2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models

Dual SVM Revisited

goal: SVM **without dependence on $\tilde{d}$**

half-way done:

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \frac{1}{2}\boldsymbol{\alpha}^T \mathrm{Q_D} \boldsymbol{\alpha} - \mathbf{1}^T \boldsymbol{\alpha} \\ \text{subject to} \quad & \mathbf{y}^T \boldsymbol{\alpha} = 0; \\ & \alpha_n \geq 0, \text{for } n = 1, 2, \ldots, N \end{aligned}$$

- $q_{n,m} = y_n y_m \mathbf{z}_n^T \mathbf{z}_m$: inner product in $\mathbb{R}^{\tilde{d}}$

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can we do so?

Fast Inner Product for $\mathbf{\Phi}_2$

2nd order polynomial transform

$$\mathbf{\Phi}_2(\mathbf{x}) = (1, x_1, x_2, \ldots, x_d, x_1^2, x_1x_2, \ldots, x_1x_d, x_2x_1, x_2^2, \ldots, x_2x_d, \ldots, x_d^2)$$

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—include both x_1x_2 & x_2x_1 for '**simplicity**' **:-)**

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$$\mathbf{\Phi}_2(\mathbf{x})^T \mathbf{\Phi}_2(\mathbf{x}') \quad = \quad 1 + \sum_{i=1}^{d} \qquad + \sum_{i=1}^{d} \sum_{j=1}^{d}$$

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$$\mathbf{\Phi}_2(\mathbf{x})^T\mathbf{\Phi}_2(\mathbf{x}') = 1 + \sum_{i=1}^{d} x_i x_i' + \sum_{i=1}^{d}\sum_{j=1}^{d} x_i x_j x_i' x_j'$$

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\end{aligned}$$

for $\boldsymbol{\Phi}_2$, transform + inner product can be carefully done in $O(d)$ instead of $O(d^2)$

Kernel: Transform + Inner Product

transform $\boldsymbol{\Phi} \Longleftrightarrow$ **kernel function**: $K_{\boldsymbol{\Phi}}(\mathbf{x}, \mathbf{x}') \equiv \boldsymbol{\Phi}(\mathbf{x})^T \boldsymbol{\Phi}(\mathbf{x}')$

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$$b = y_s - \mathbf{w}^T \mathbf{z}_s$$

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$$g_{\text{SVM}}(\mathbf{x}) = \text{sign}\left(\mathbf{w}^T \mathbf{\Phi}(\mathbf{x}) + b\right)$$

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kernel trick: plug in **efficient kernel function**
to avoid dependence on $\tilde{d}$

Kernel SVM with QP

Kernel Hard-Margin SVM Algorithm

1. $q_{n,m} = y_n y_m K(\mathbf{x}_n, \mathbf{x}_m)$; $\mathbf{p} = -\mathbf{1}_N$; $(\mathrm{A}, \mathbf{c})$ for equ./bound constraints

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4. return SVs and their α_n as well as b such that for new $\mathbf{x}$,

$$g_{\mathrm{SVM}}(\mathbf{x}) = \mathrm{sign}\left(\sum_{\text{SV indices } n} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b \right)$$

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- (1): time complexity $O(N^2) \cdot$ (kernel evaluation)

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- (1): time complexity $O(N^2) \cdot$ (kernel evaluation)
- (2): QP with N variables and $N + 1$ constraints

Kernel SVM with QP

Kernel Hard-Margin SVM Algorithm

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- (1): time complexity $O(N^2) \cdot$ (kernel evaluation)
- (2): QP with N variables and $N + 1$ constraints
- (3) & (4): time complexity $O(\#\text{SV}) \cdot$ (kernel evaluation)

Kernel SVM with QP

Kernel Hard-Margin SVM Algorithm

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kernel SVM:
use computational shortcut to avoid $\tilde{d}$ & predict with SV only

Fun Time

Consider two examples $\mathbf{x}$ and $\mathbf{x}'$ such that $\mathbf{x}^T\mathbf{x}' = 10$. What is $K_{\mathbf{\Phi}_2}(\mathbf{x}, \mathbf{x}')$?

1. 1
2. 11
3. 111
4. 1111

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Reference Answer: ③

Using the derivation in previous slides, $K_{\mathbf{\Phi}_2}(\mathbf{x}, \mathbf{x}') = 1 + \mathbf{x}^T\mathbf{x}' + (\mathbf{x}^T\mathbf{x}')^2$.

General Poly-2 Kernel

$$\Phi_2(\mathbf{x}) = (1, x_1, \ldots, x_d, x_1^2, \ldots, x_d^2) \quad \Leftrightarrow \quad K_{\Phi_2}(\mathbf{x}, \mathbf{x}') = 1 + \mathbf{x}^T\mathbf{x}' + (\mathbf{x}^T\mathbf{x}')^2$$

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$$K_2(\mathbf{x}, \mathbf{x}') = (1 + \gamma\mathbf{x}^T\mathbf{x}')^2 \text{ with } \gamma > 0$$

- K_2: somewhat '**easier**' to calculate than K_{Φ_2}

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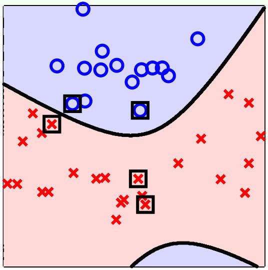
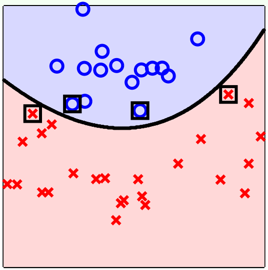
K_2 commonly used

Poly-2 Kernels in Action

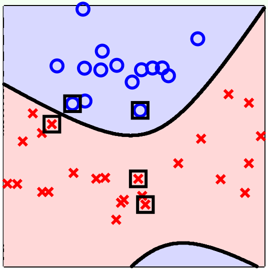


$1 + \mathbf{x}^T\mathbf{x}' + (\mathbf{x}^T\mathbf{x}')^2$

Poly-2 Kernels in Action



$(1 + 0.001\mathbf{x}^T\mathbf{x}')^2$



$1 + \mathbf{x}^T\mathbf{x}' + (\mathbf{x}^T\mathbf{x}')^2$

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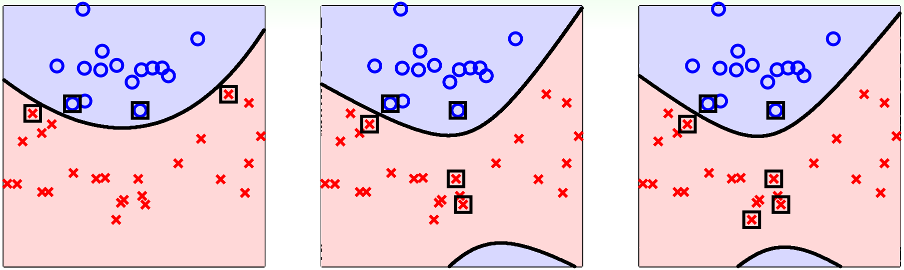

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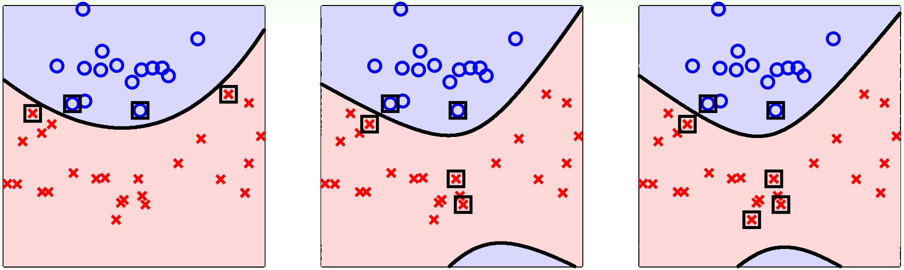

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- g_{SVM} **different**, SVs **different**
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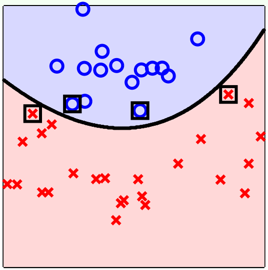

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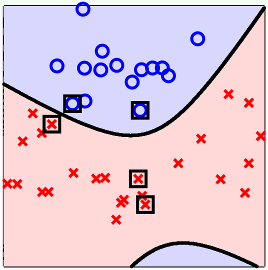

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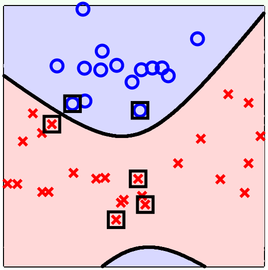

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- change of kernel $\Leftrightarrow$ change of **margin definition**

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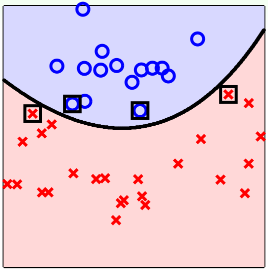

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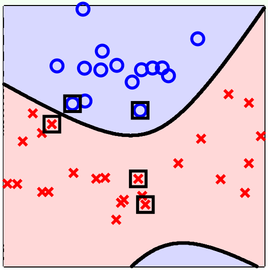

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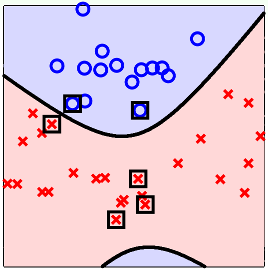

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need selecting K, just like selecting $\boldsymbol{\Phi}$

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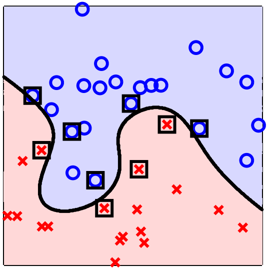

10-th order polynomial
with margin 0.1

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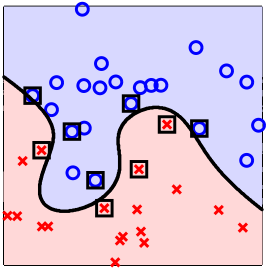
SVM + Polynomial Kernel: Polynomial SVM



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Special Case: Linear Kernel

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Special Case: Linear Kernel

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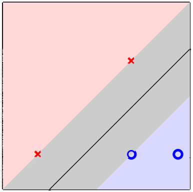

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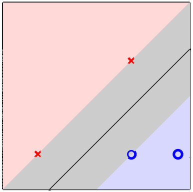

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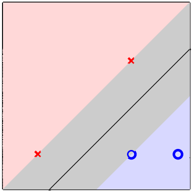

linear first, remember? :-)

Fun Time

Consider the general 2-nd polynomial kernel $K_2(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma \mathbf{x}^T \mathbf{x}')^2$. Which of the following transform can be used to derive this kernel?

1. $\mathbf{\Phi}(\mathbf{x}) = (1, \sqrt{2\gamma}x_1, \ldots, \sqrt{2\gamma}x_d, \gamma x_1^2, \ldots, \gamma x_d^2)$
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Reference Answer: 4

We need to have ζ^2 from the 0-th order terms, $2\gamma\zeta\mathbf{x}^T\mathbf{x}'$ from the 1-st order terms, and $\gamma^2(\mathbf{x}^T\mathbf{x}')^2$ from the 2-nd order terms.

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$= \mathbf{\Phi}(x)^T \mathbf{\Phi}(x')$

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&= \exp(-(x)^2)\exp(-(x')^2)\exp(2xx') \\
&= \mathbf{\Phi}(x)^T \mathbf{\Phi}(x')
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more generally, **Gaussian kernel**
$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\gamma\|\mathbf{x}-\mathbf{x}'\|^2\right)$ with $\gamma > 0$

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Gaussian SVM:
find α_n to combine Gaussians centered at $\mathbf{x}_n$
& achieve large margin in infinite-dim. space

Support Vector Mechanism

	large-margin hyperplanes + higher-order transforms with kernel trick
#	not many
boundary	sophisticated

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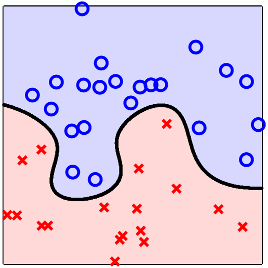
new possibility by Gaussian SVM:
infinite-dimensional linear classification, with generalization 'guarded by' large-margin **:-)**

Gaussian SVM in Action



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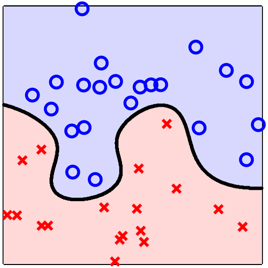

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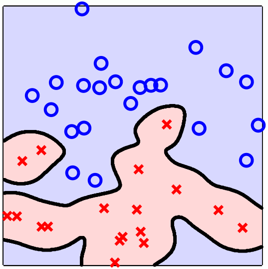

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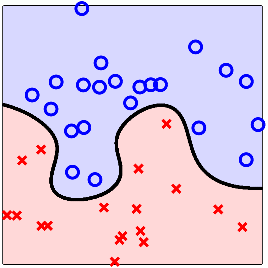

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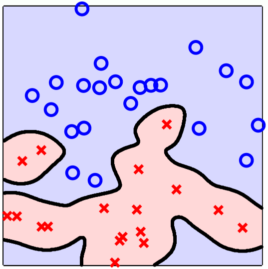

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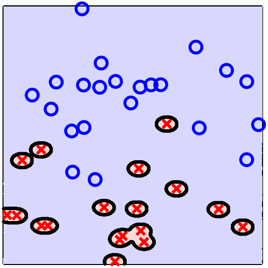

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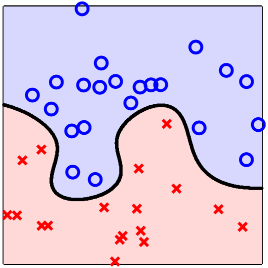

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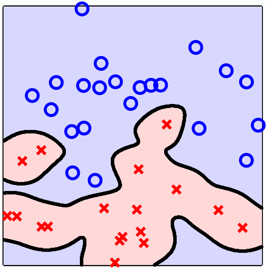

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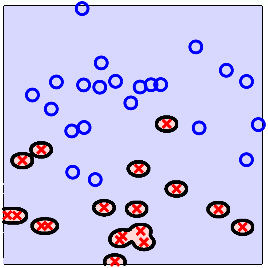

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- large $\gamma \Longrightarrow$ sharp Gaussians $\Longrightarrow$ 'overfit'?

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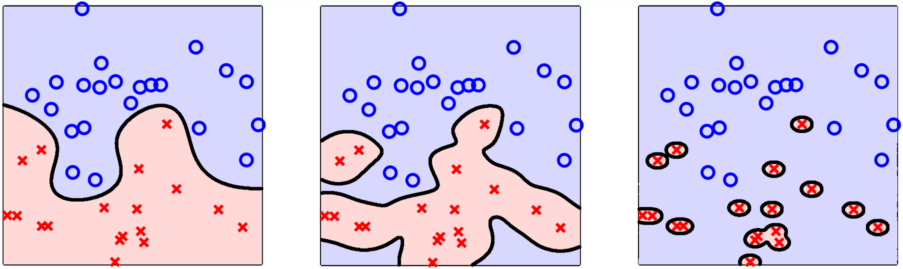

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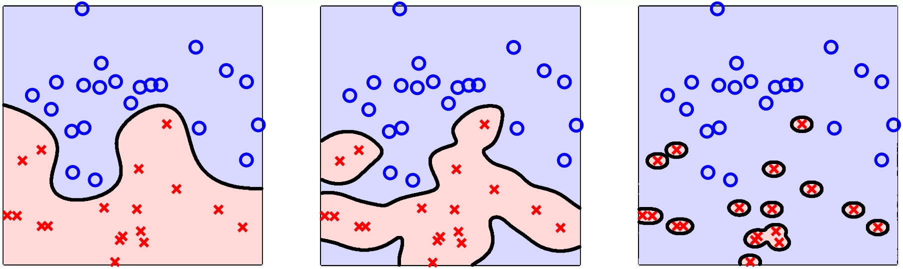

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Gaussian SVM: need careful selection of γ

Fun Time

Consider the Gaussian kernel $K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma\|\mathbf{x} - \mathbf{x}'\|^2)$. What function does the kernel converge to if $\gamma \to \infty$?

1. $K_{\text{lim}}(\mathbf{x}, \mathbf{x}') = 0$
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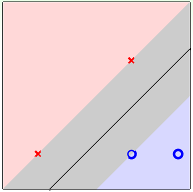
Reference Answer: (2)

If $\mathbf{x} = \mathbf{x}'$, $K(\mathbf{x}, \mathbf{x}') = 1$ regardless of γ. If $\mathbf{x} \neq \mathbf{x}'$, $K(\mathbf{x}, \mathbf{x}') = 0$ when $\gamma \to \infty$. Thus, K_{lim} is an impulse function, which is an extreme case of how the Gaussian gets sharper when $\gamma \to \infty$.

Linear Kernel: Cons and Pros



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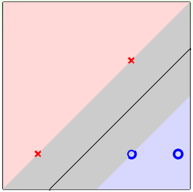

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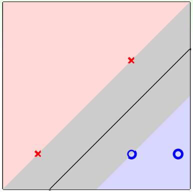

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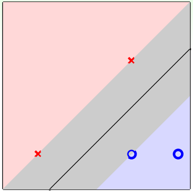

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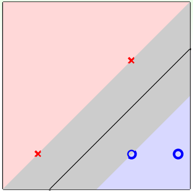

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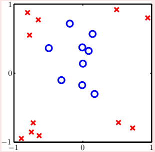

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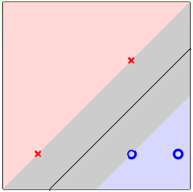

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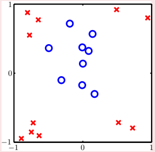

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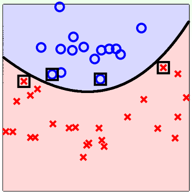
linear kernel: an important **basic** tool

Polynomial Kernel: Cons and Pros



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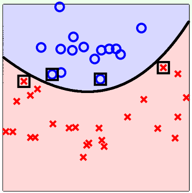

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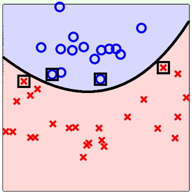

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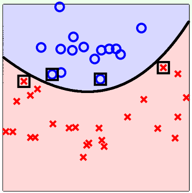

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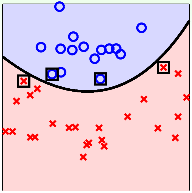

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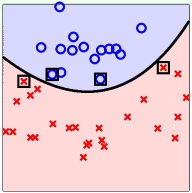

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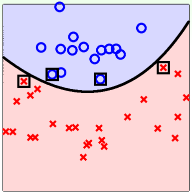

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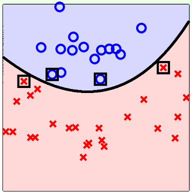

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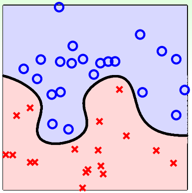
—sometimes efficiently done by **linear on $\mathbf{\Phi}_Q(\mathbf{x})$**

Gaussian Kernel: Cons and Pros



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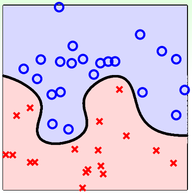

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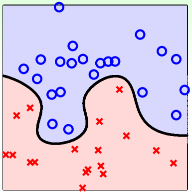
Pros

- **more powerful than linear/poly.**

Gaussian Kernel: Cons and Pros



$$K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$$

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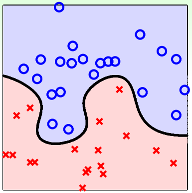

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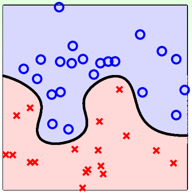

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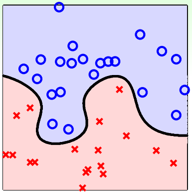

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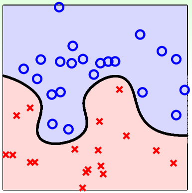

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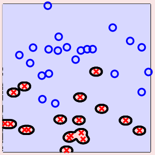

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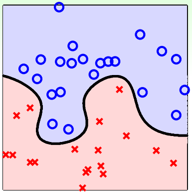

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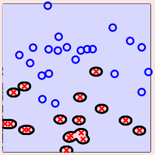

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Gaussian kernel: **one of most popular** but shall **be used with care**

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$= \mathrm{Z}\mathrm{Z}^T$ must **always** be **positive semi-definite**

define your own kernel: possible, **but hard**

Fun Time

Which of the following is not a valid kernel? (*Hint: Consider two 1-dimensional vectors* $\mathbf{x}_1 = (1)$ *and* $\mathbf{x}_2 = (-1)$ *and check Mercer's condition.*)

1. $K(\mathbf{x}, \mathbf{x}') = (-1 + \mathbf{x}^T\mathbf{x}')^2$
2. $K(\mathbf{x}, \mathbf{x}') = (0 + \mathbf{x}^T\mathbf{x}')^2$
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Reference Answer: (1)

The kernels in (2) and (3) are just polynomial kernels. The kernel in (4) is equivalent to the kernel in (3). For (1), the matrix K formed from the kernel and the two examples is not positive semi-definite. Thus, the underlying kernel is not a valid one.

Summary

1. Embedding Numerous Features: Kernel Models

Lecture 3: Kernel Support Vector Machine

- Kernel Trick
  kernel as shortcut of transform + inner product
- Polynomial Kernel
  embeds specially-scaled polynomial transform
- Gaussian Kernel
  embeds infinite dimensional transform
- Comparison of Kernels
  linear for efficiency or Gaussian for power

- **next: avoiding overfitting in Gaussian (and other kernels)**

2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models