732A99/TDDE01 Machine Learning

Lecture 3a Block 1: Kernel Methods

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Contents

Literature

- Main source
  - Bishop, C. M. *Pattern Recognition and Machine Learning*. Springer, 2006. Sections 2.5 and 6.1-6.2.
- Additional source
  - Devroye, L., Györfi, L. and Lugosi, G. *A Probabilistic Theory of Pattern Recognition*. Springer, 1996. Sections 6.4 and 10.0.
  - Hastie, T., Tibshirani, R. and Friedman, J. *The Elements of Statistical Learning*. Springer, 2009. Chapter 6.

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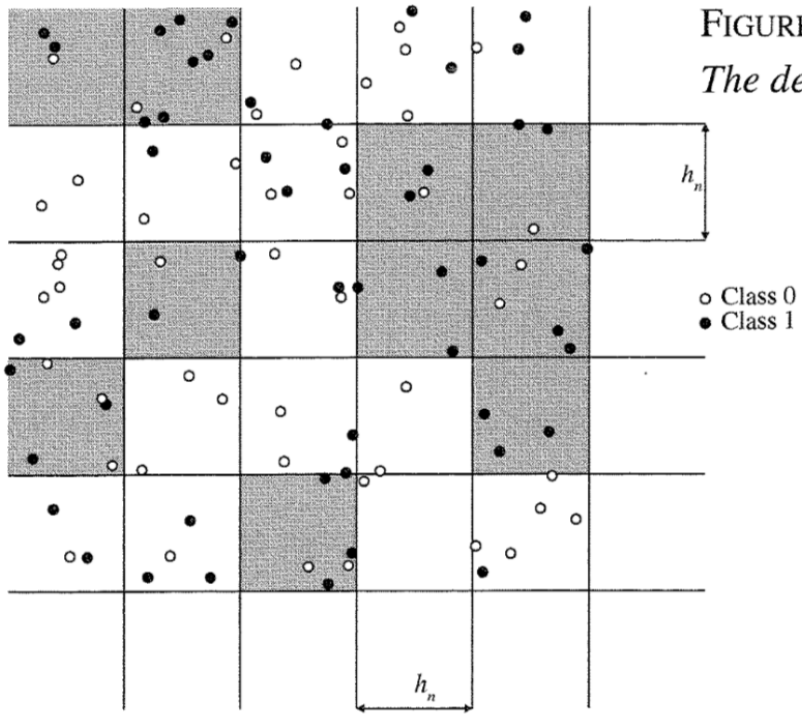

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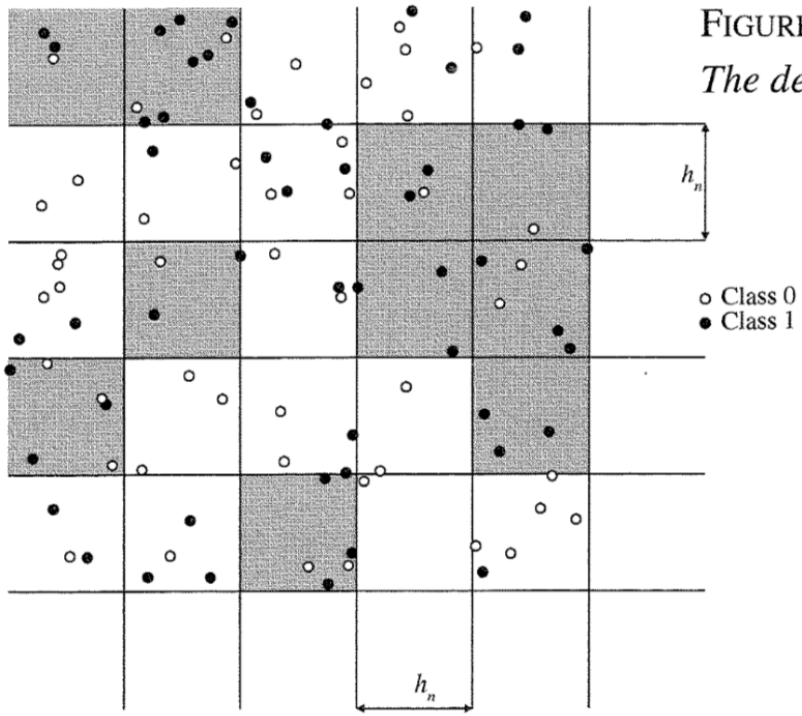

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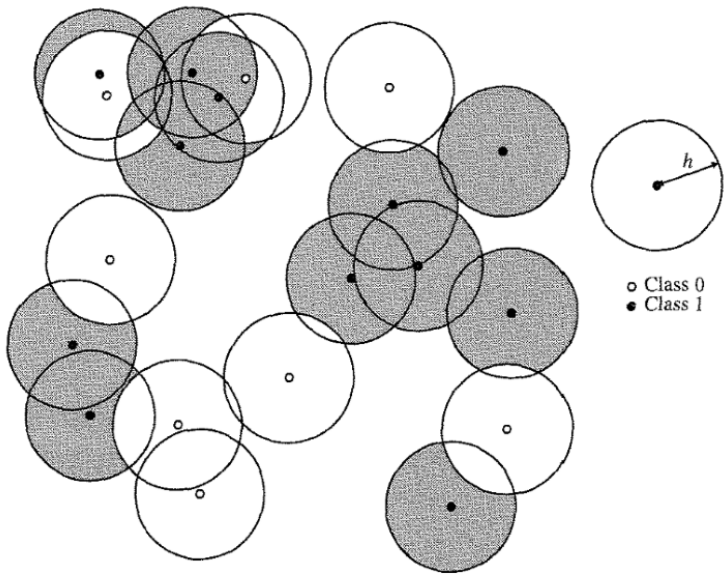

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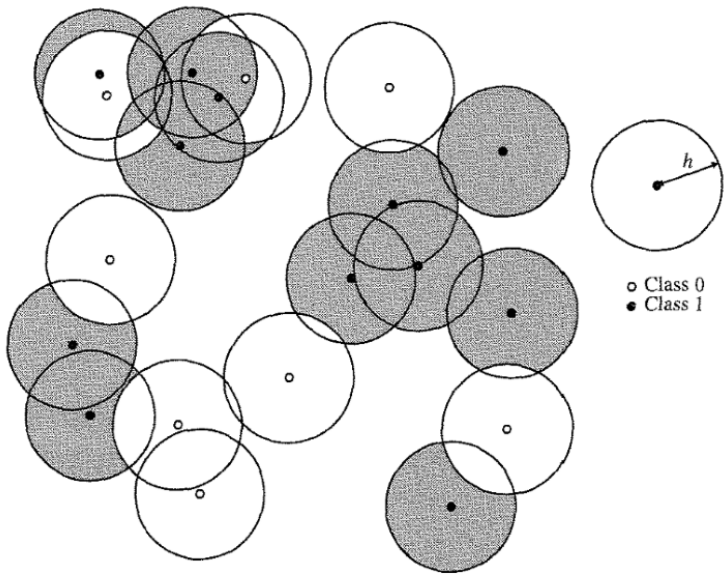

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where $S(\boldsymbol{x}, h)$ is a D-dimensional closed ball of radius h centered at $\boldsymbol{x}$.

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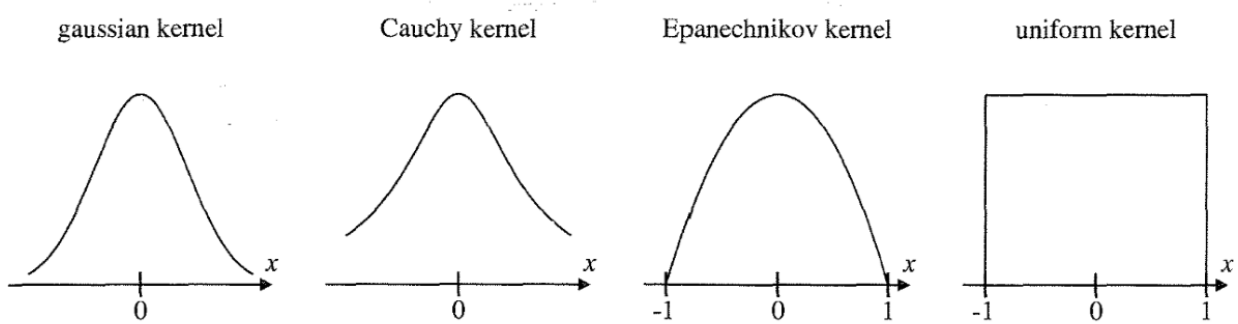

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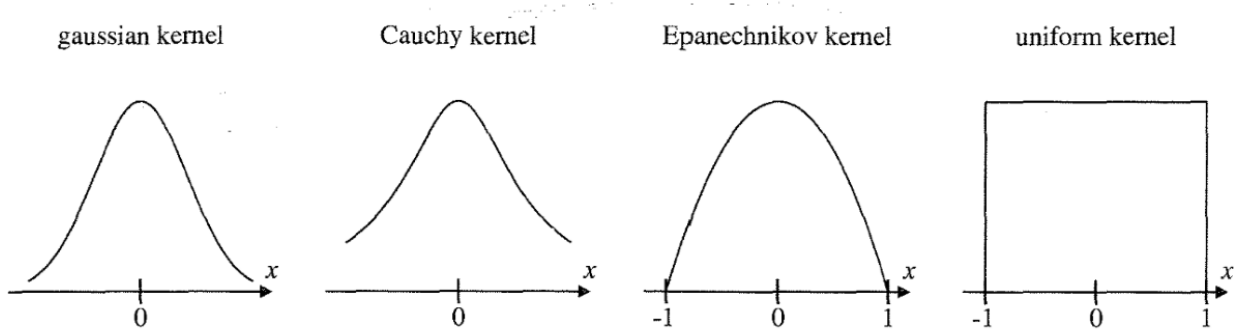

FIGURE 10.3. *Various kernels on $\mathcal{R}$.*

- Gaussian kernel: $k(u) = exp(-||u||^2)$ where $||\cdot||$ is the Euclidean norm.
- Cauchy kernel: $k(u) = 1/(1 + ||u||^{D+1})$
- Epanechnikov kernel: $k(u) = (1 - ||u||^2)\mathbf{1}_{\{||u||\leq 1\}}$
- Moving window kernel: $k(u) = \mathbf{1}_{\{u \in S(0,1)\}}$

Kernel Classification

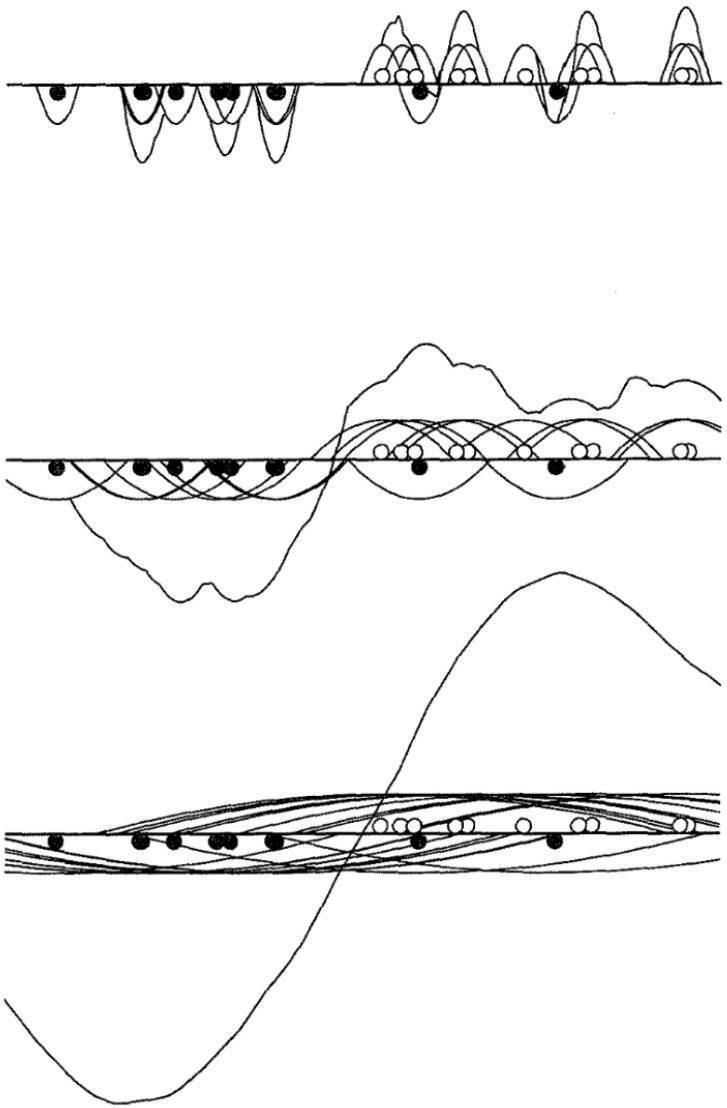

FIGURE 10.2. *Kernel rule on the real line. The figure shows* $\sum_{i=1}^{n}(2Y_i-1)K((x-X_i)/h)$ *for* $n = 20$, $K(u) = (1-u^2)I_{\{|u|\le 1\}}$ *(the Epanechnikov kernel), and three smoothing factors* h. *One definitely undersmooths and one oversmooths. We took* $p = 1/2$, *and the class-conditional densities are* $f_0(x) = 2(1-x)$ *and* $f_1(x) = 2x$ *on* $[0, 1]$.

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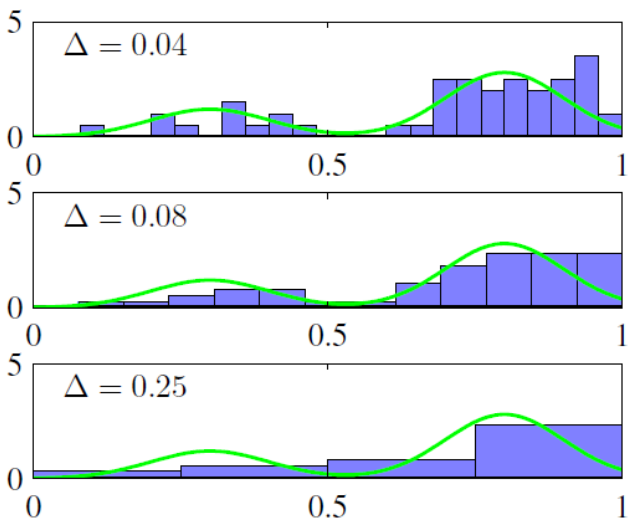
or

$$p_k(\boldsymbol{x}) = \frac{1}{N} \sum_n k\Big(\frac{\boldsymbol{x} - \boldsymbol{x}_n}{h}\Big)$$

assuming that $k(u) \geq 0$ for all u and $\int k(u) du = 1$.

Histogram, Moving Window, and Kernel Density Estimation

Figure 2.24 An illustration of the histogram approach to density estimation, in which a data set of 50 data points is generated from the distribution shown by the green curve. Histogram density estimates, based on (2.241), with a common bin width Δ are shown for various values of Δ.



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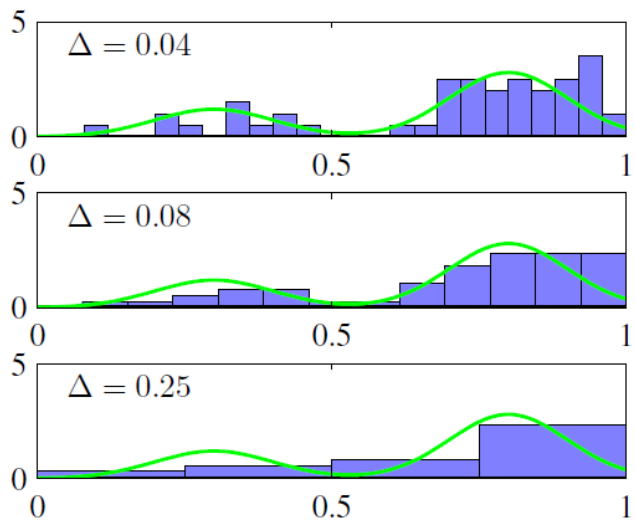
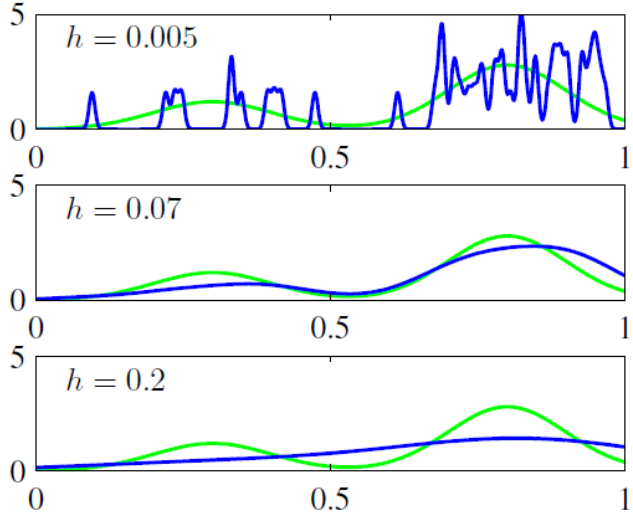


Figure 2.25 Illustration of the kernel density model (2.250) applied to the same data set used to demonstrate the histogram approach in Figure 2.24. We see that h acts as a smoothing parameter and that if it is set too small (top panel), the result is a very noisy density model, whereas if it is set too large (bottom panel), then the bimodal nature of the underlying distribution from which the data is generated (shown by the green curve) is washed out. The best density model is obtained for some intermediate value of h (middle panel).



Histogram, Moving Window, and Kernel Density Estimation

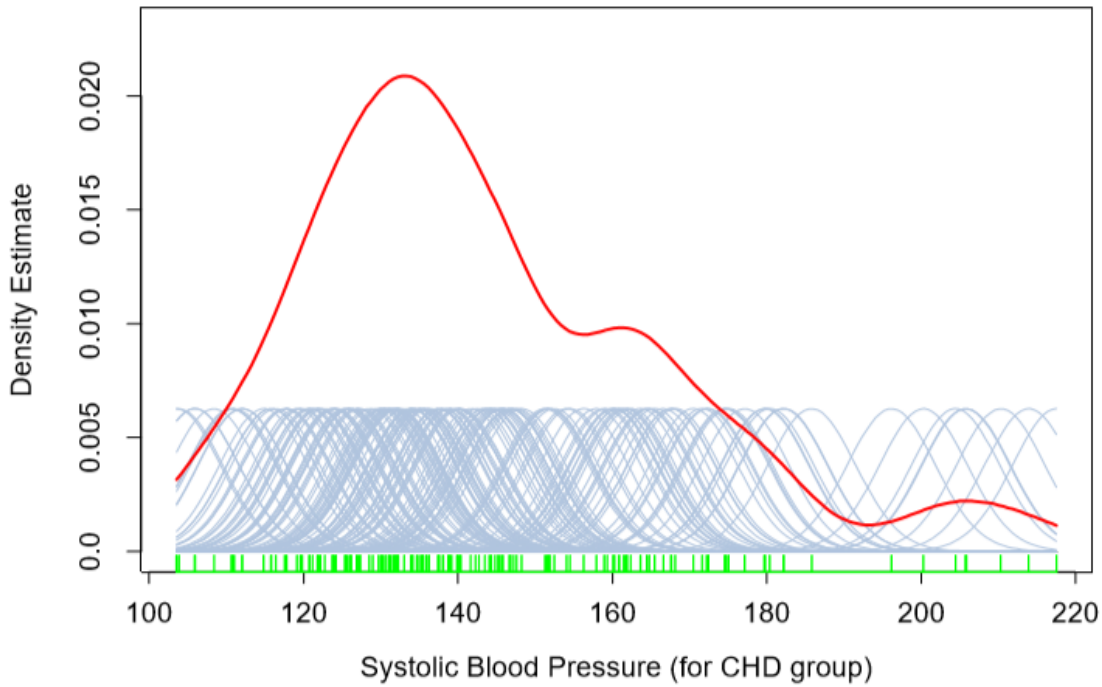


FIGURE 6.13. *A kernel density estimate for systolic blood pressure (for the CHD group). The density estimate at each point is the average contribution from each of the kernels at that point. We have scaled the kernels down by a factor of 10 to make the graph readable.*

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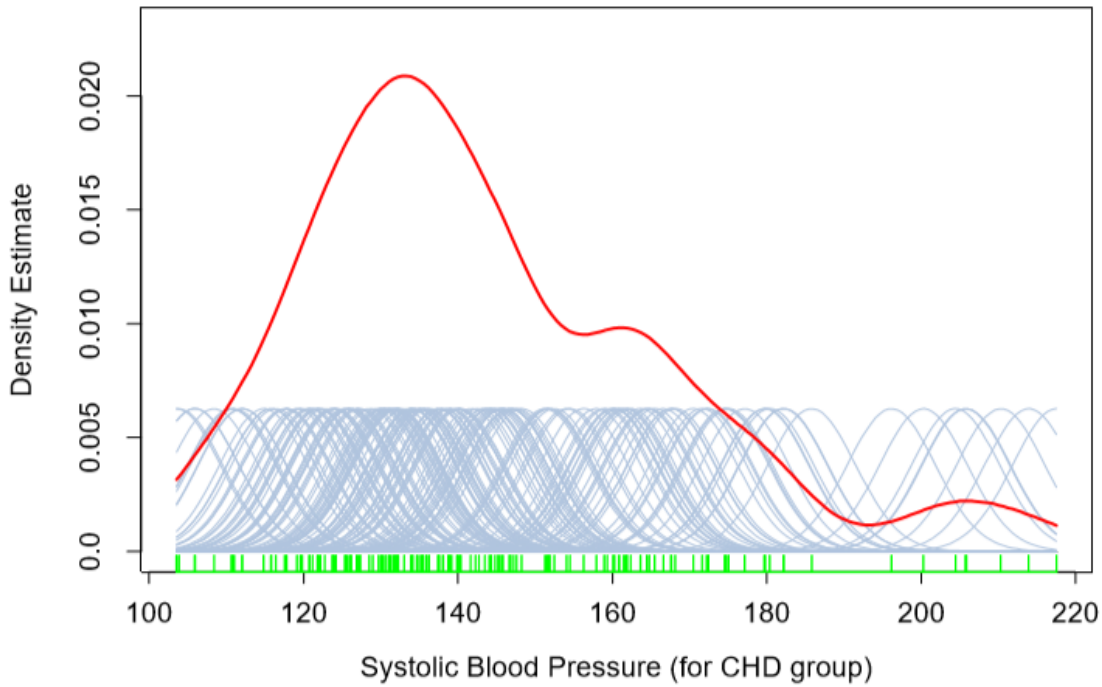

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- From kernel density estimation to kernel classification:
  1. Estimate $p(\boldsymbol{x}|y=0)$ and $p(\boldsymbol{x}|y=1)$ using the methods just seen.
  2. Estimate $p(y)$ as class proportions.
  3. Compute $p(y|\boldsymbol{x}) \propto p(\boldsymbol{x}|y)p(y)$ by Bayes theorem.

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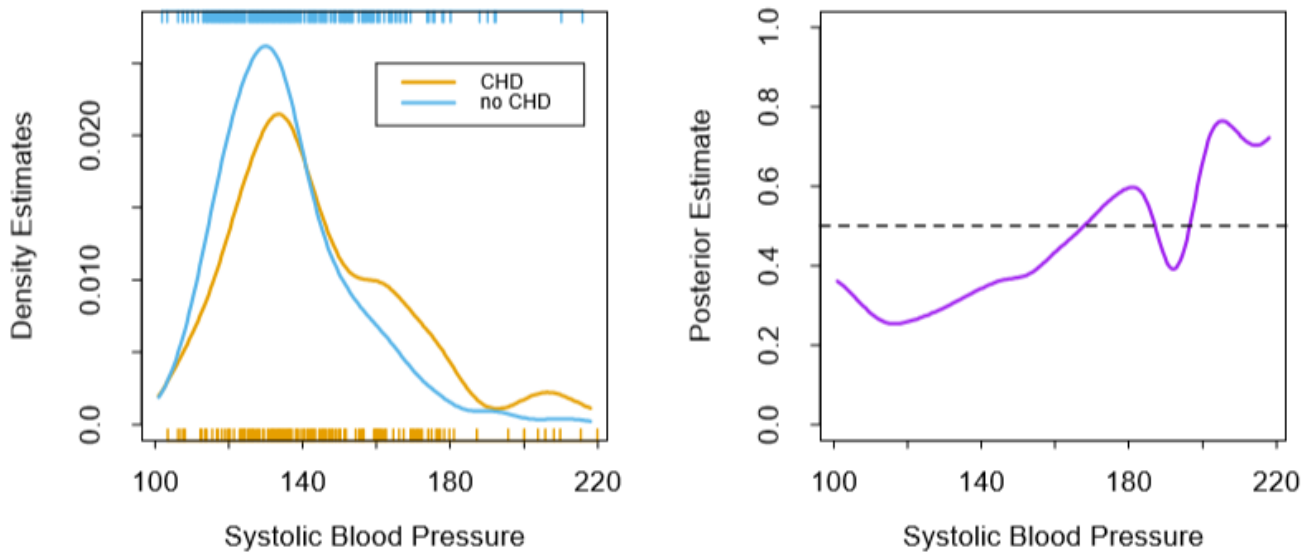

FIGURE 6.14. *The left panel shows the two separate density estimates for systolic blood pressure in the CHD versus no-CHD groups, using a Gaussian kernel density estimate in each. The right panel shows the estimated posterior probabilities for CHD, using (6.25).*

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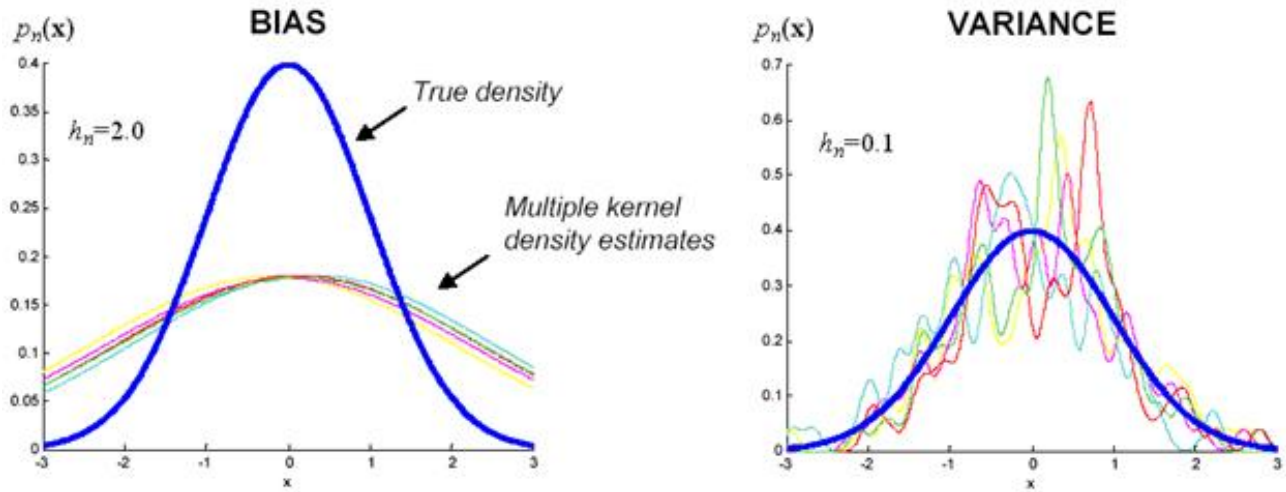
- What does "right" mean ? E.g., minimize loss function.
- Note that the width of the kernel corresponds to a bias-variance trade-off.



- Small width implies considering few points. So, the variance will be large (similar to the variance of a single point). The bias will be small since the points considered are close to $\boldsymbol{x}$.
- Large width implies considering many points. So, the variance will be small and the bias will be large.

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- Cross-validation is a technique to estimate the prediction error of a model.

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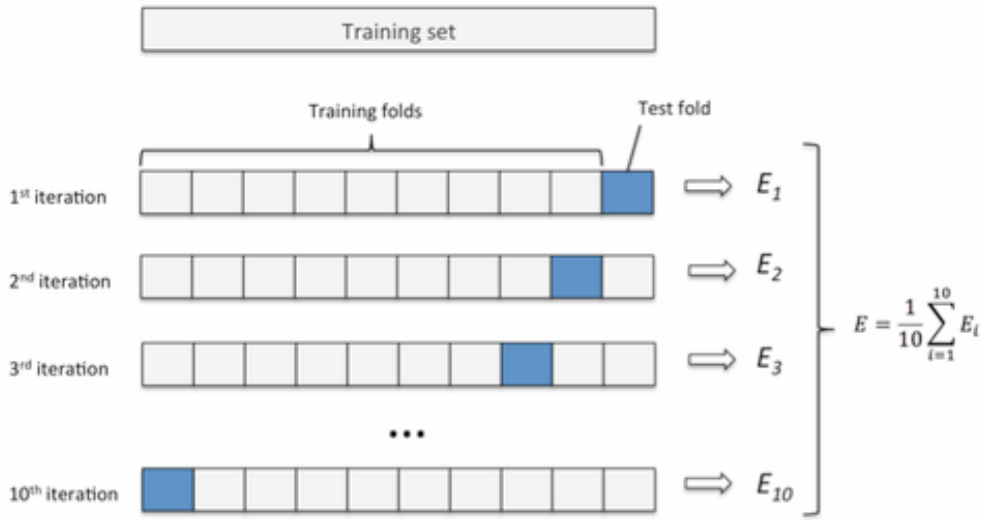

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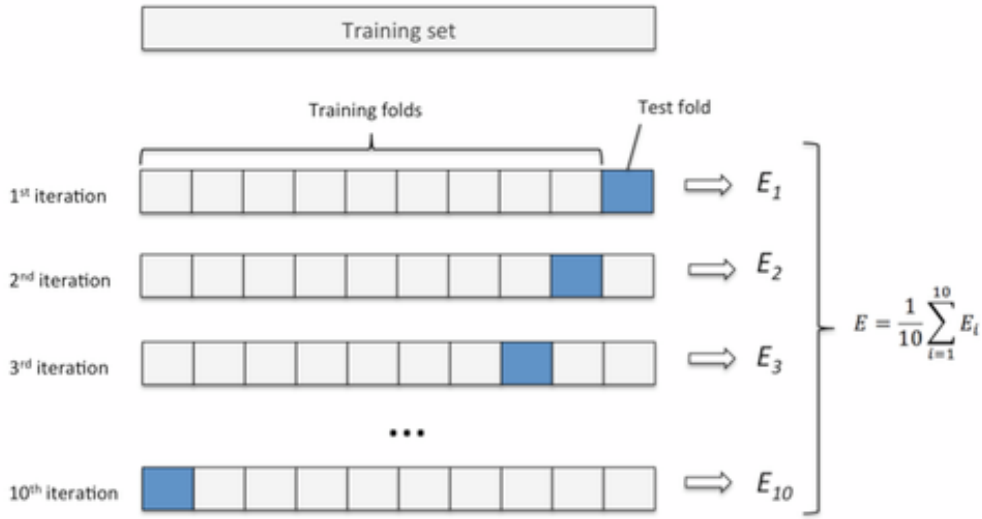

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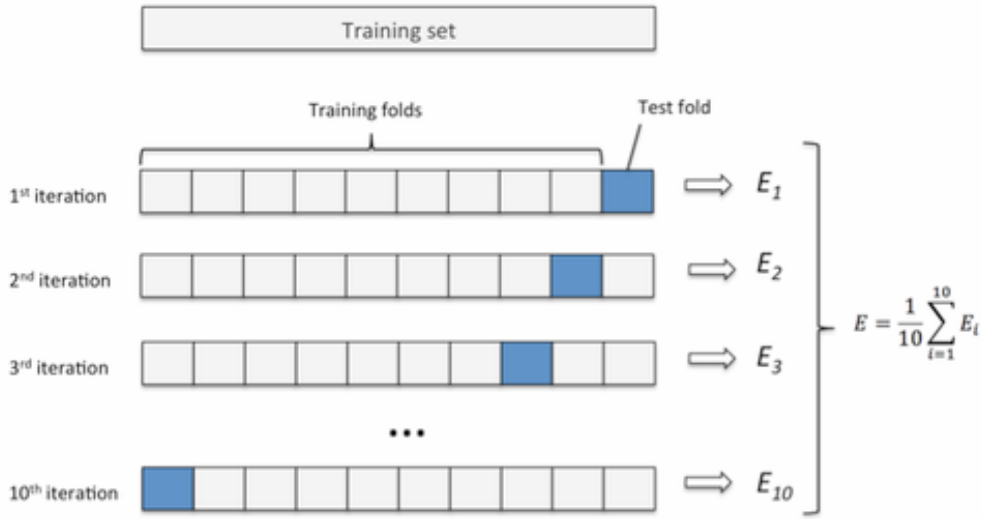

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- Typically, $K = 5, 10$ works well.

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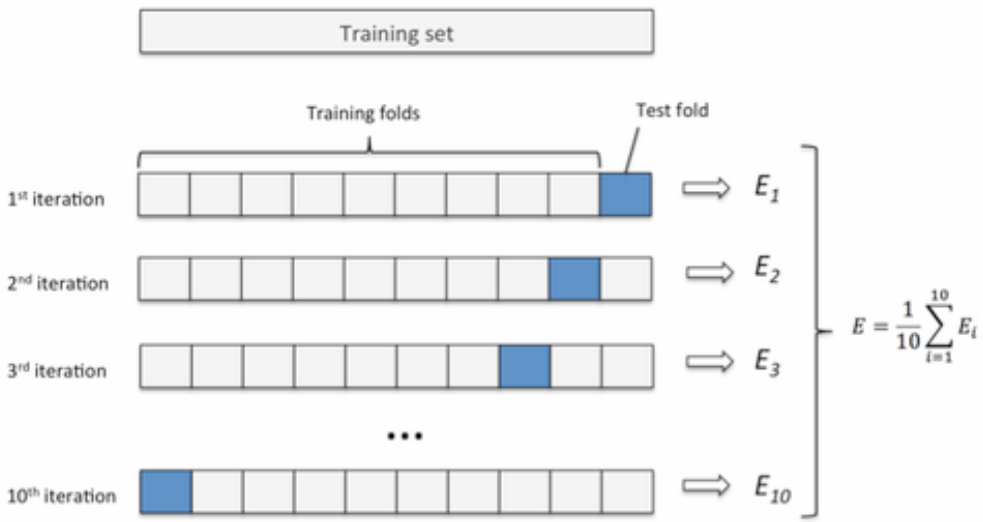
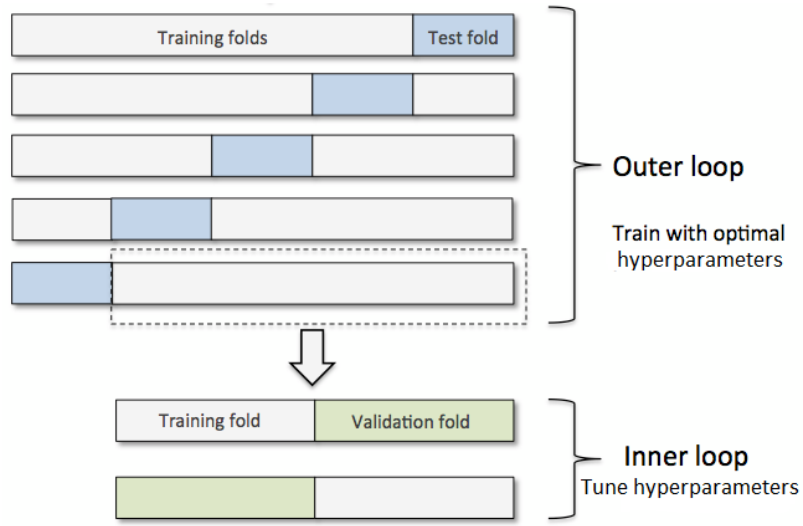
Cross-validation for estimating model prediction error



Nested cross-validation for estimating model **selection** prediction error



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- Model: For example, ridge regression with a given value for the penalty factor λ. Only the parameters (weights) need to be determined (closed-form solution).
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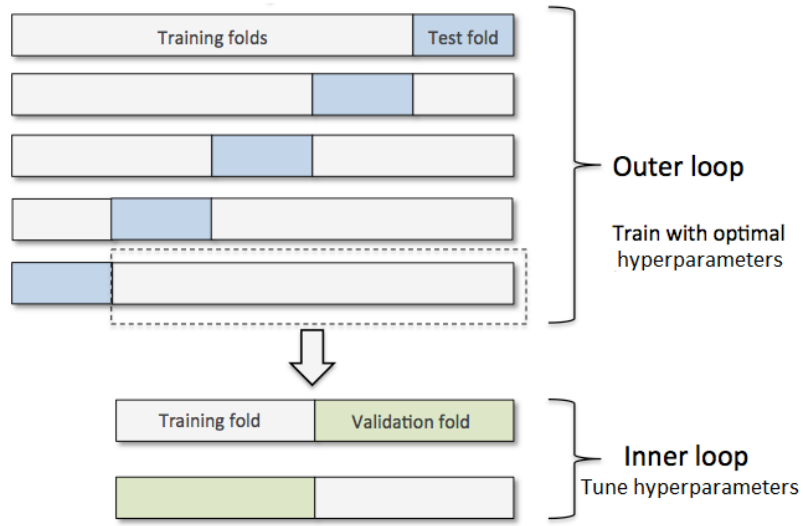

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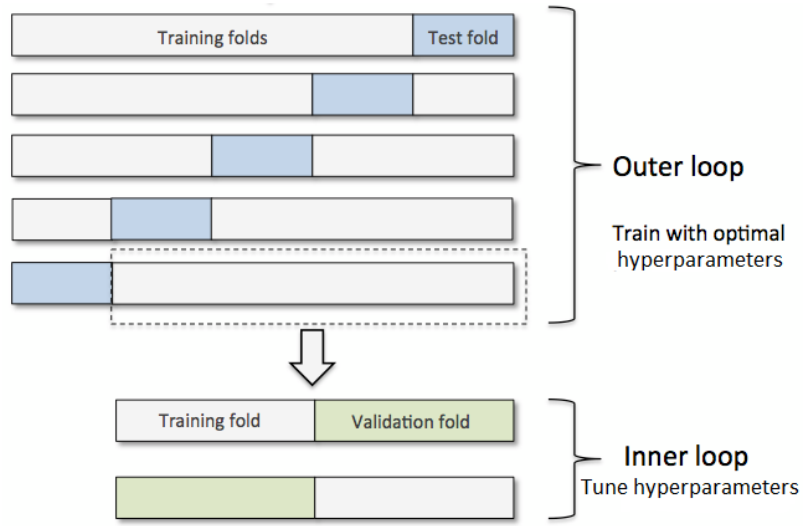

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- Which is the fitted model returned by nested cross-validation ?

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- The kernel function $k\left(\frac{x-x'}{h}\right)$ is invariant to translations, and it can be generalized as $k(\boldsymbol{x}, \boldsymbol{x}')$. For instance,
  - Polynomial kernel: $k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^T \boldsymbol{x}' + c)^M$
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  is symmetric and positive semi-definite for all choices of $\{\boldsymbol{x}_n\}$, then $k(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T \phi(\boldsymbol{x}')$ where $\phi(\cdot)$ is a mapping from the input space to the feature space.

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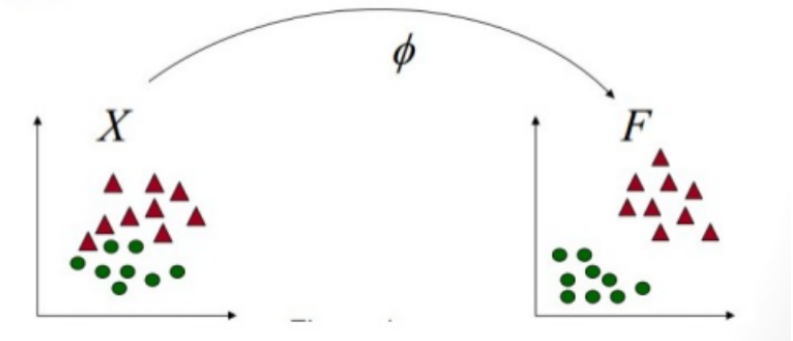

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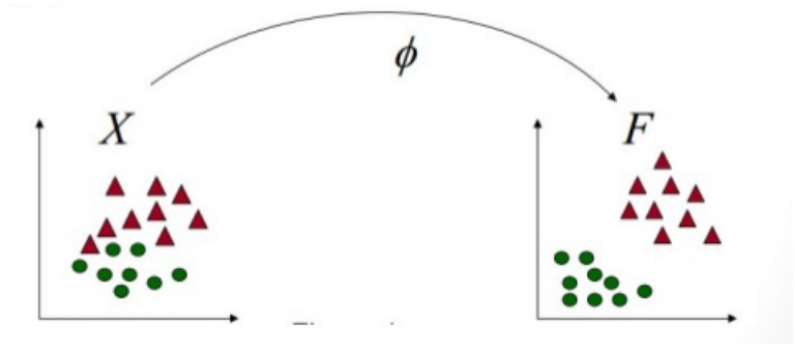

- The feature space may be non-linear and even infinite dimensional. For instance,

$$\phi(\boldsymbol{x}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2c}x_1, \sqrt{2c}x_2, c)$$

  for the polynomial kernel with $M = D = 2$.

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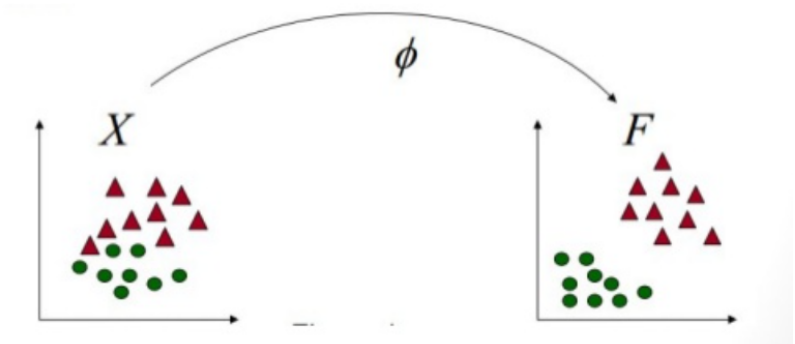

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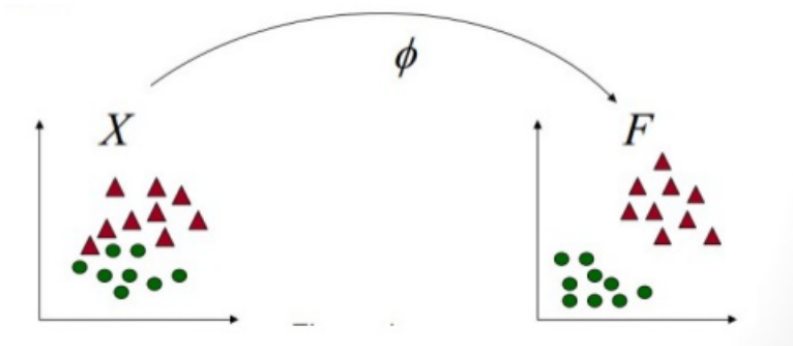

- Note that we do not need to compute $\phi(\boldsymbol{x})$ and $\phi(\boldsymbol{x}_n)$.

Kernel Trick

- Two alternatives for building $k(\boldsymbol{x}, \boldsymbol{x}')$:
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Techniques for Constructing New Kernels.

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= c k_1(\mathbf{x}, \mathbf{x}') && (6.13)\\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') && (6.14)\\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.15)\\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.16)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') && (6.17)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}') && (6.18)\\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) && (6.19)\\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}' && (6.20)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}_a') + k_b(\mathbf{x}_b, \mathbf{x}_b') && (6.21)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}_a') k_b(\mathbf{x}_b, \mathbf{x}_b') && (6.22)
\end{aligned}
$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

Summary

- Kernel methods: Smoothing models.
- Model selection: Nested cross-validation.
- Kernel trick: It allows to work in the feature space without constructing it.