Kernel Methods in Statistics
Past, Present and Future

Soham Sarkar

LIKE 2022

10 January 2022

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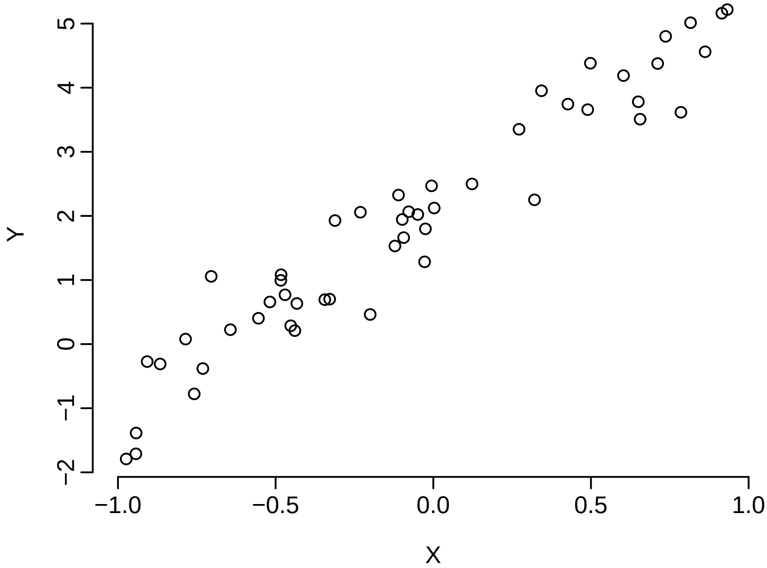

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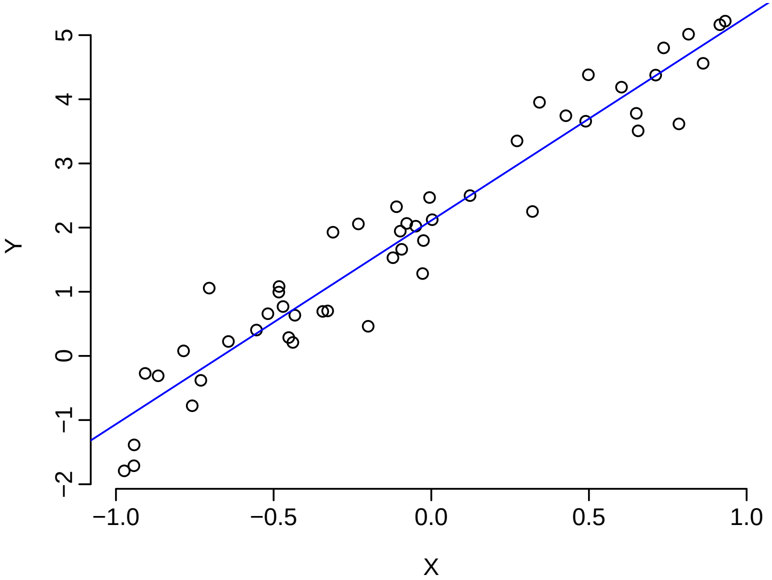

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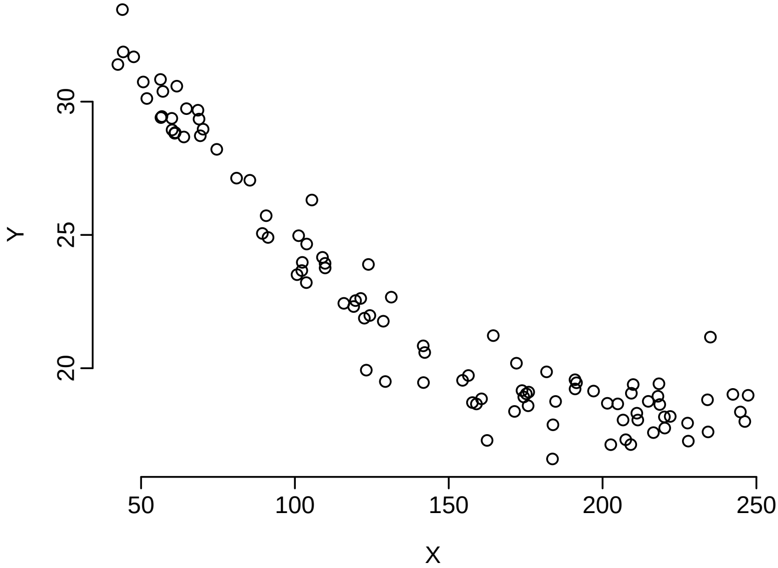

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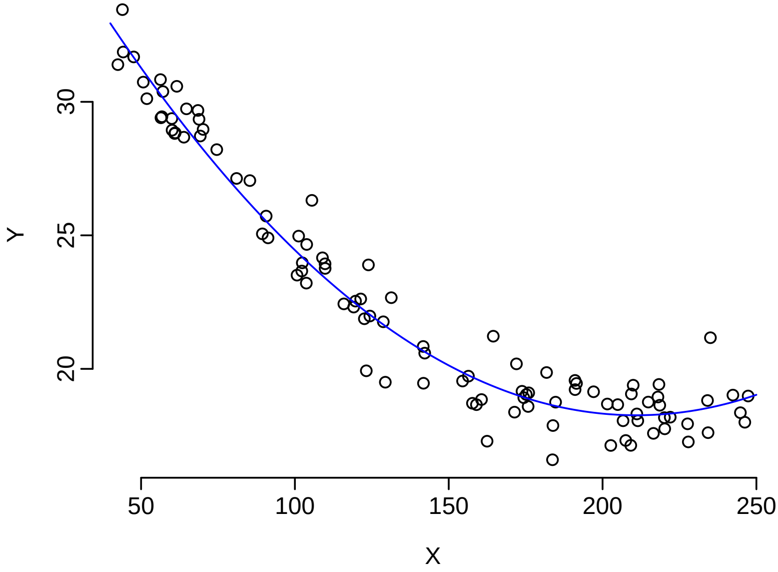

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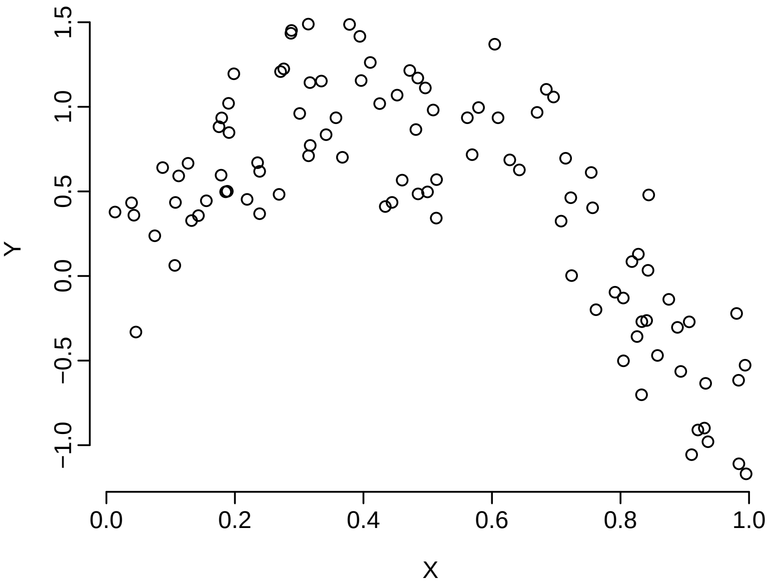

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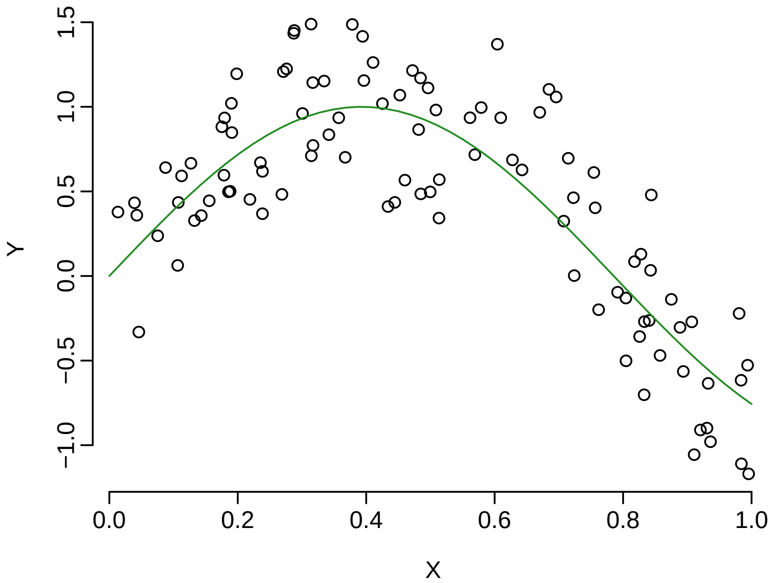

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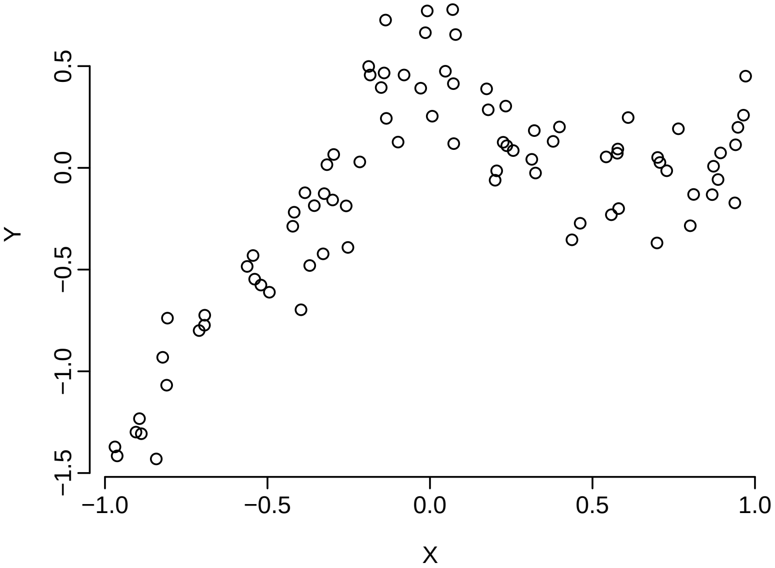

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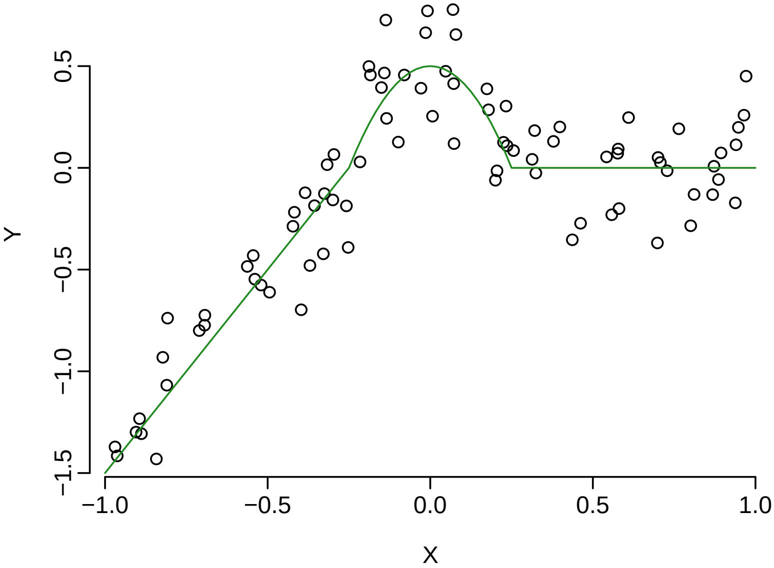

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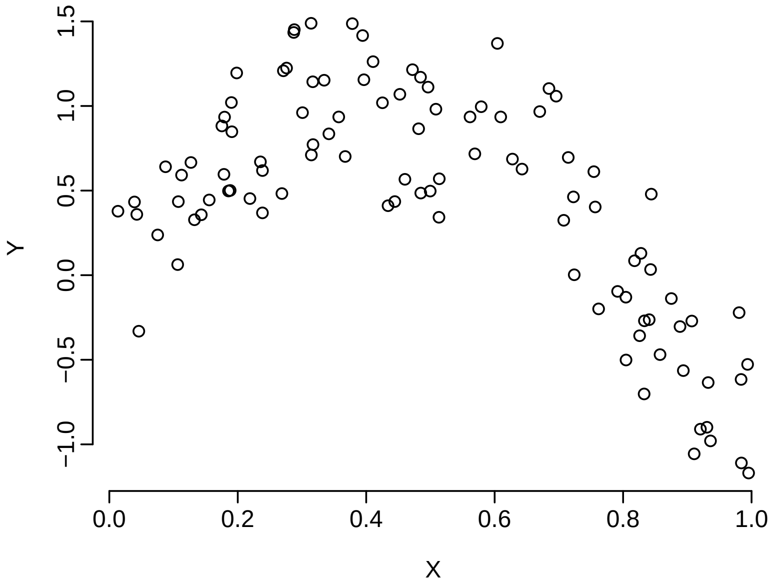

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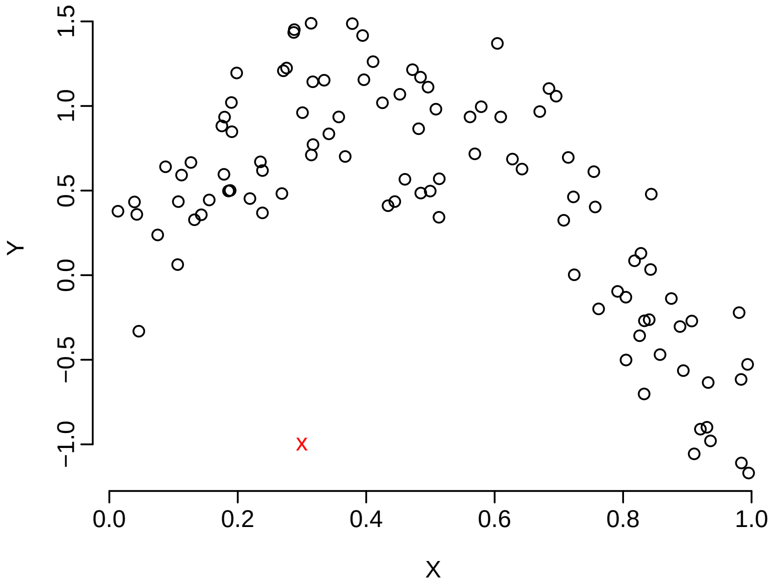

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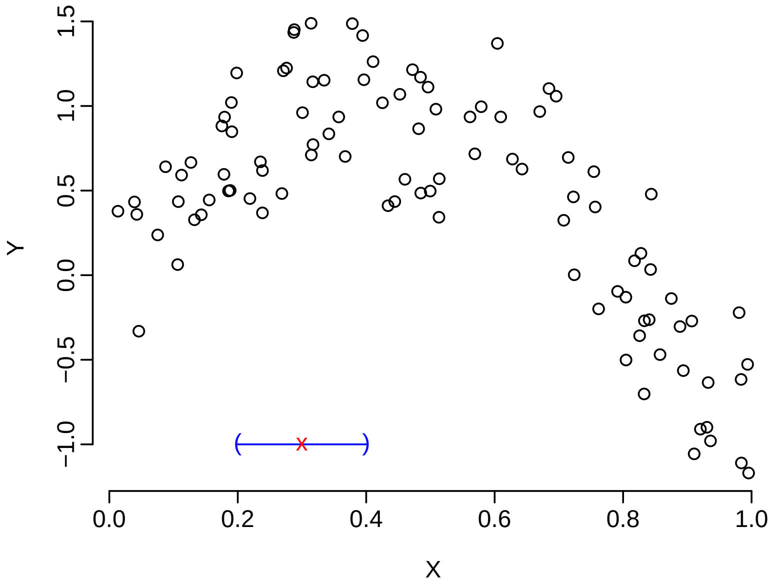

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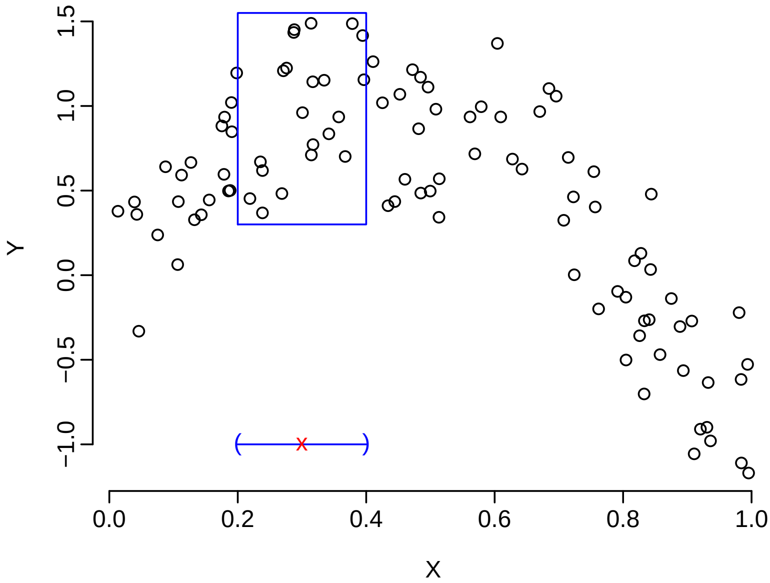

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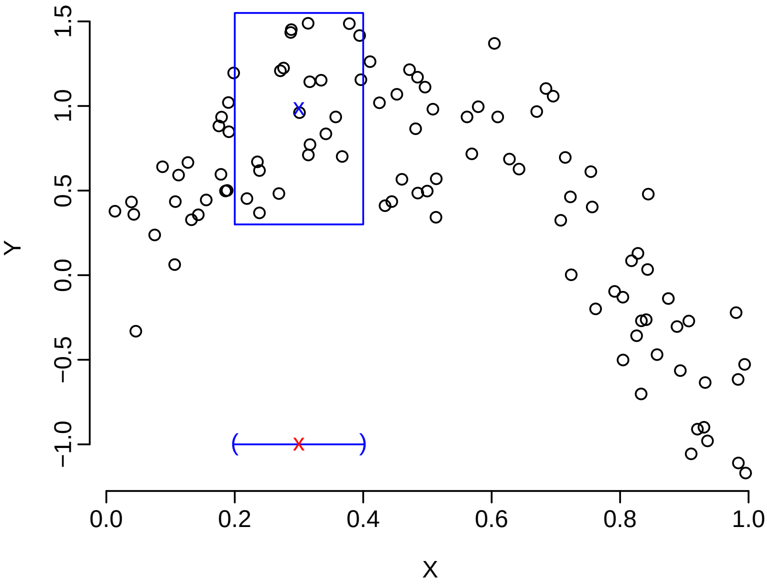

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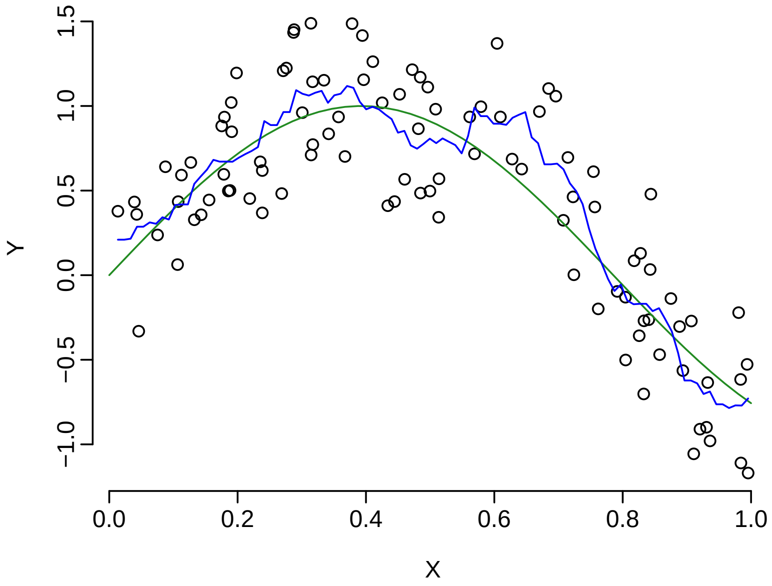

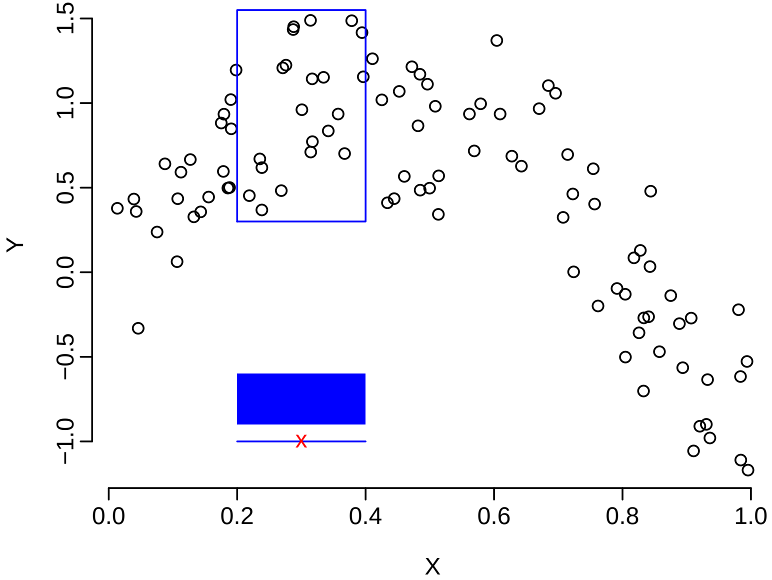
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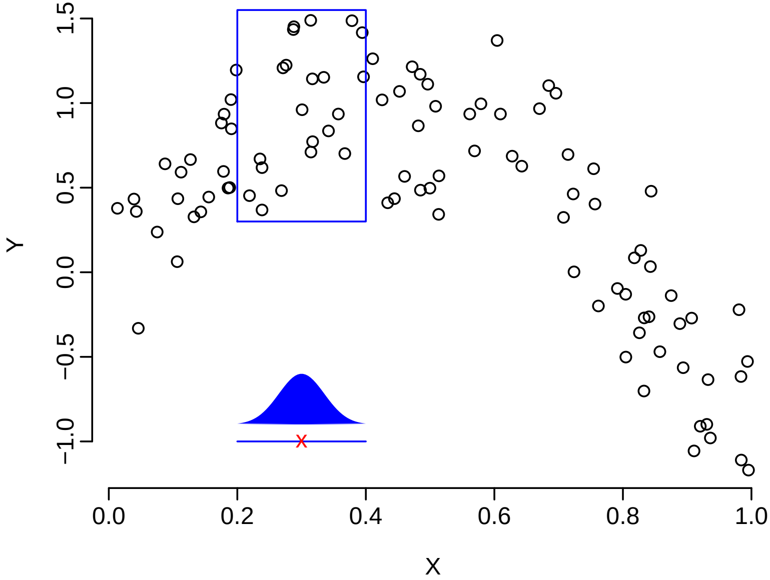
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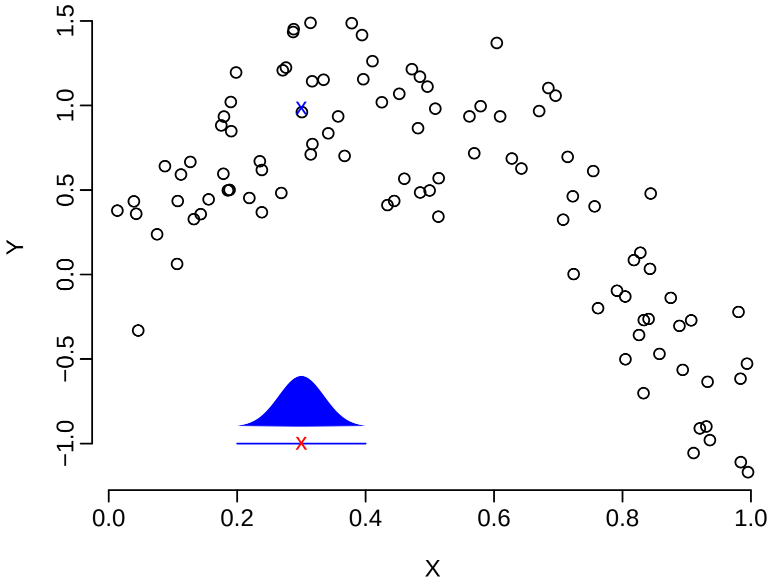
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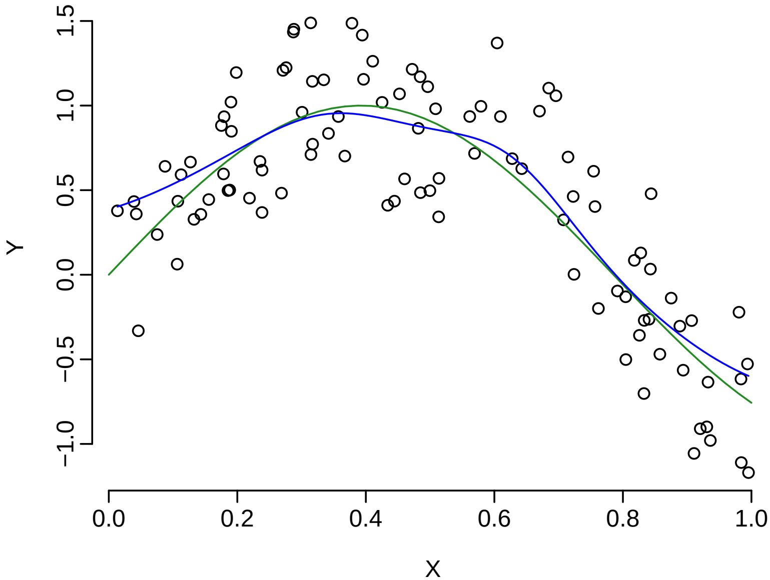
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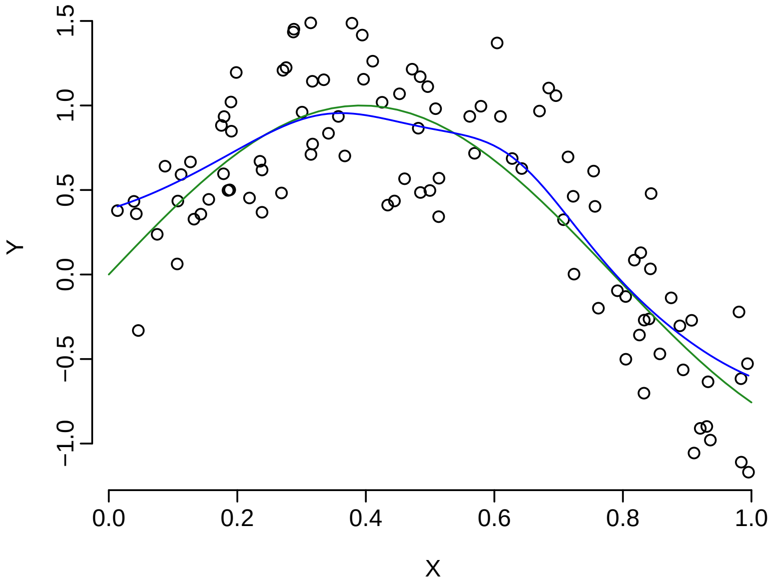

$$\widehat{f}(x) = \frac{\sum_{i=1}^{n} y_i K\left(\frac{x-x_i}{h}\right)}{\sum_{i=1}^{n} K\left(\frac{x-x_i}{h}\right)}$$ — the Nadaraya-Watson estimator (1964).

K is a kernel. Usually: $\int K(u)\,\mathrm{d}u = 1, \int uK(u)\,\mathrm{d}u = 0, \int u^2 K(u)\,\mathrm{d}u < \infty.$

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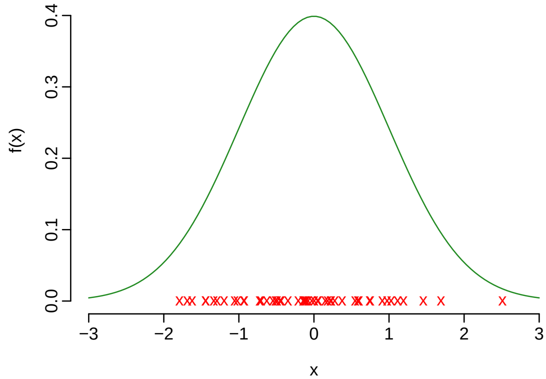

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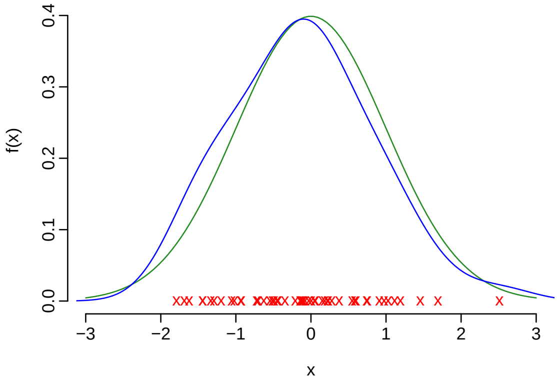

Kernel density estimator: $$\widehat{f}(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)$$

— Rosenblatt (1956), Parzen (1962)

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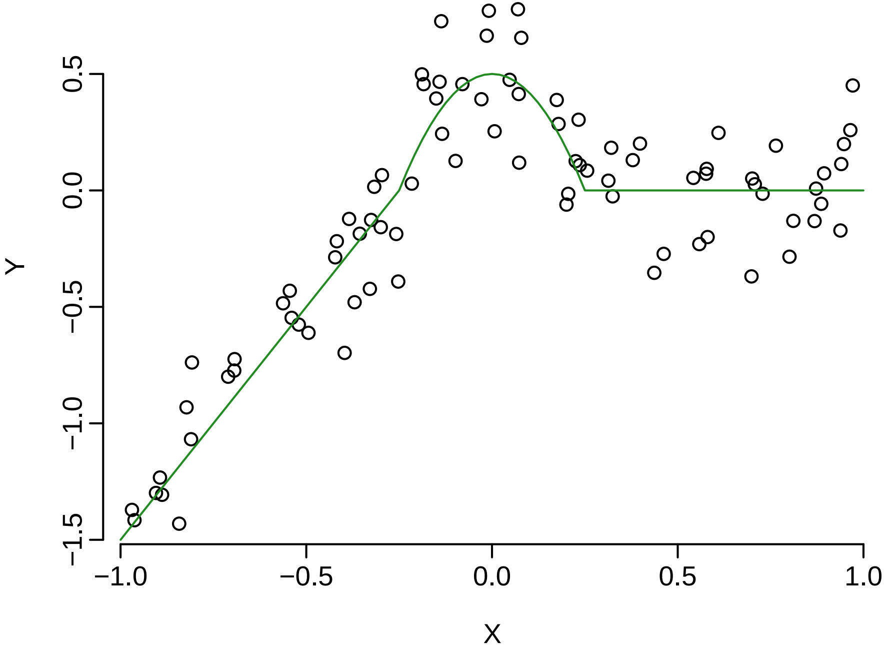

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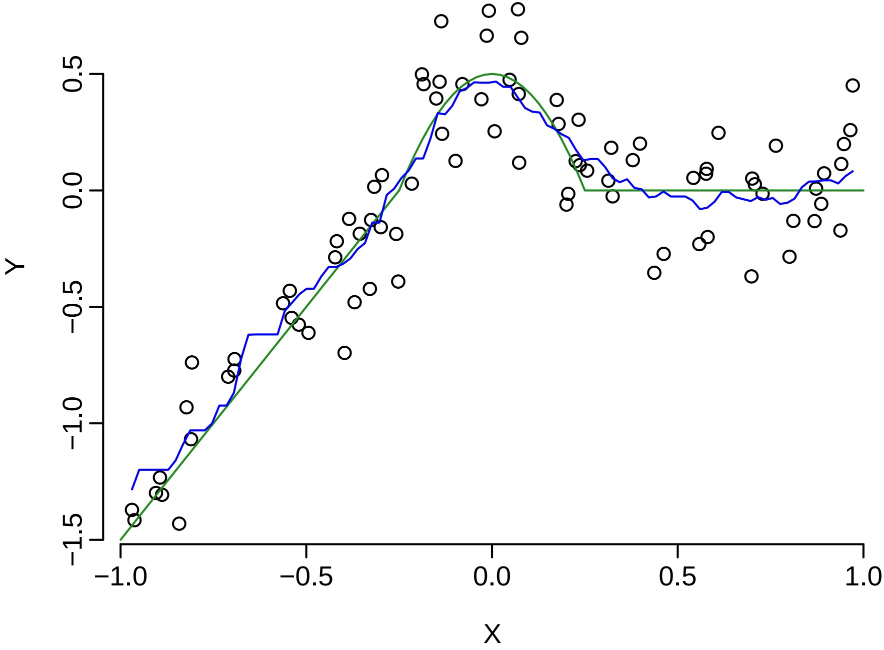

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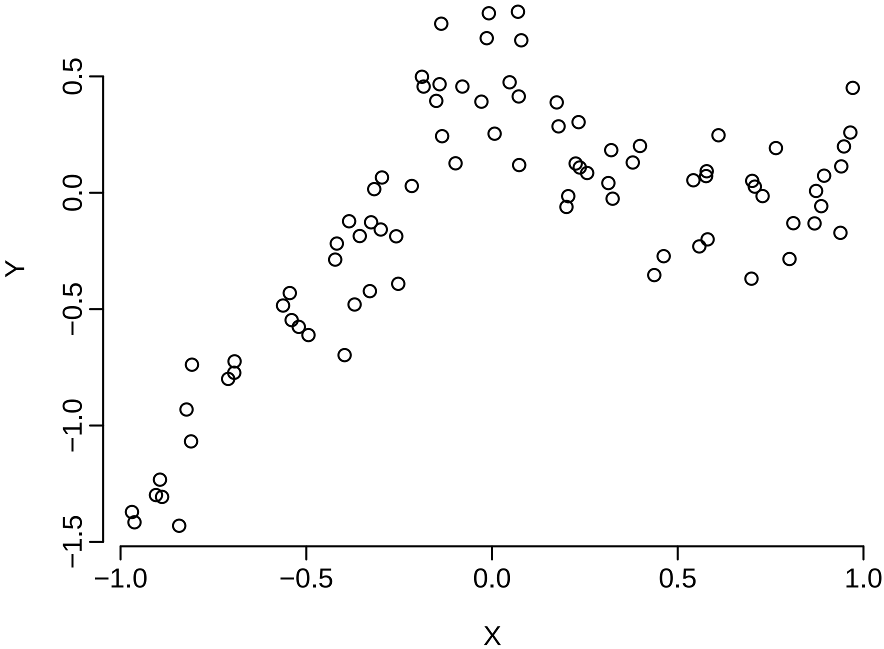

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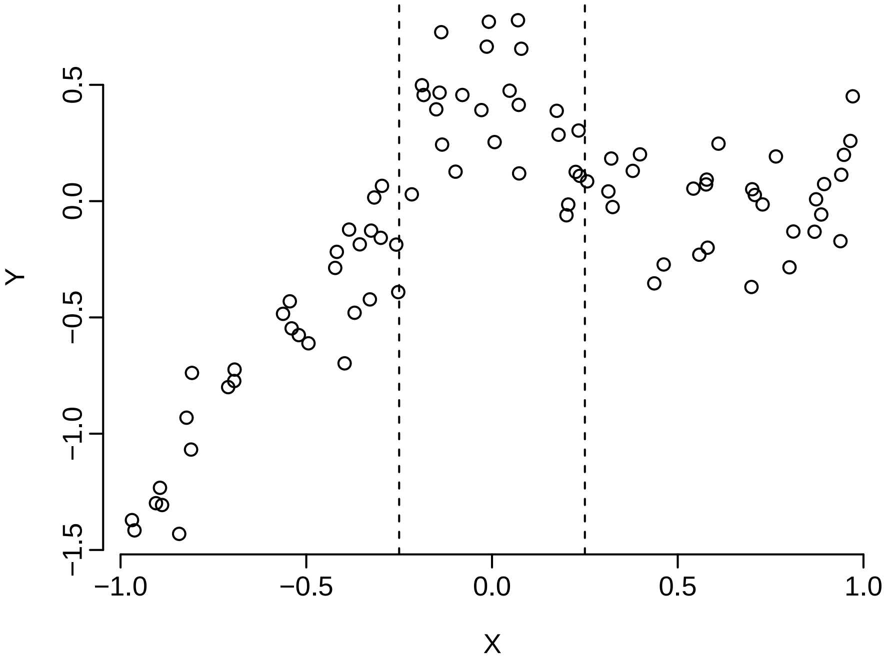

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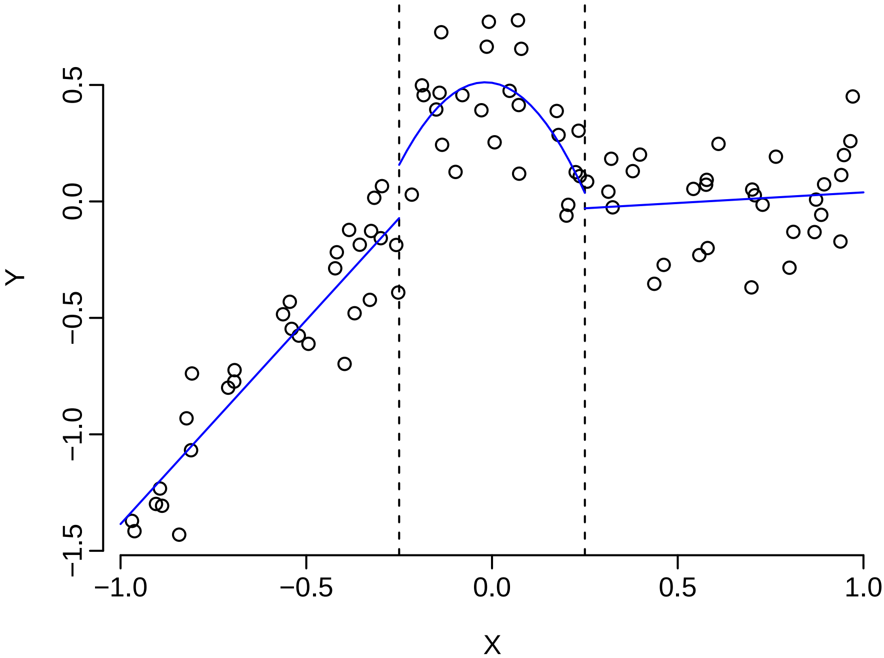

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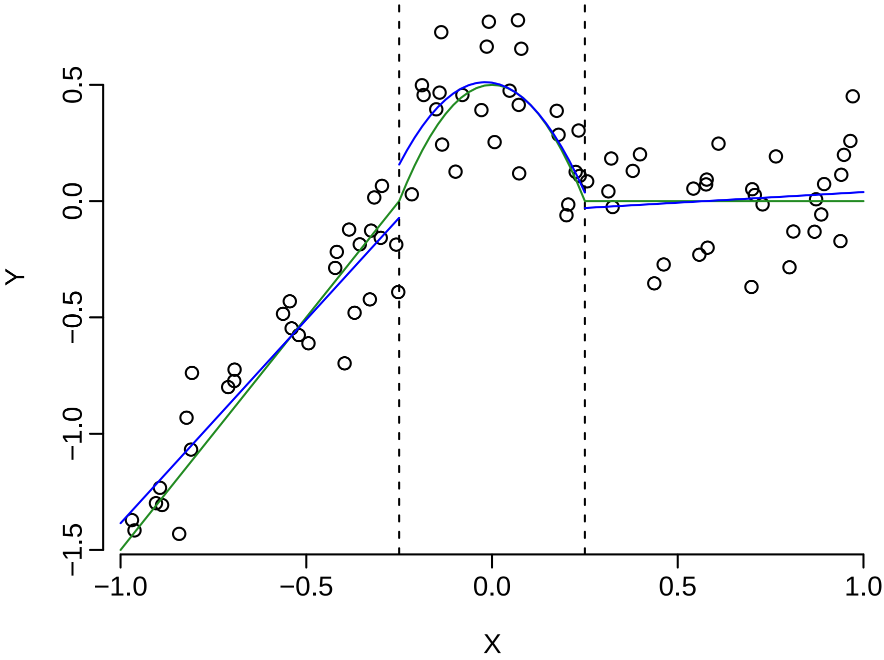

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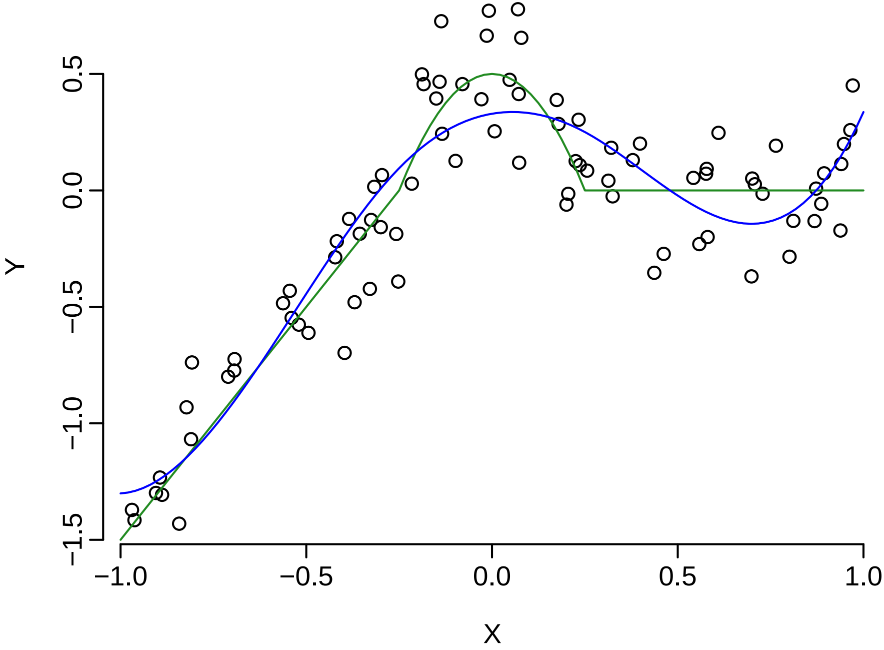

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Cubic spline f with knots $\xi_1, \ldots, \xi_K$: f continuous, f', f'' continuous at $\xi_1, \ldots, \xi_K$

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Remarkably, the solution exists and is given by a cubic spline with knots at $x_1, \ldots, x_n$.

— Representer theorem. Kimeldorf & Wahba (1971)

The solution can be obtained in a closed form.

Modern kernels

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$$K(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle_{\mathcal{H}}, \qquad \forall \mathbf{x}, \mathbf{y} \in \mathcal{X}.$$

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- A kernel induces and is induced by an inner-product. Has important consequences.

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- $K(\mathbf{x}, \mathbf{y}) = e^{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{\sigma^2}}, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^d.$ Gaussian/RBF kernel

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- For $f = \sum_{i=1}^{m} \alpha_i K(\cdot, \mathbf{x}_i)$ and $g = \sum_{j=1}^{n} \beta_j K(\cdot, \mathbf{y}_j)$, $\langle f, g \rangle_{\mathscr{H}} = \sum_{i=1}^{m} \sum_{j=1}^{n} \alpha_i \beta_j K(\mathbf{x}_i, \mathbf{y}_j)$.

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Let $\mathscr{H}$ be an RKHS with kernel K. Consider the following problem:

$$\text{minimize} \sum_{i=1}^{n} L(y_i, f(\mathbf{x}_i)) + \lambda \|f\|_{\mathscr{H}}^2 \quad \text{w.r.t. } f \in \mathscr{H}.$$

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Can show: $\displaystyle\int (f''(t))^2 \, \mathrm{d}t = \|f\|_{\mathscr{H}}^2$ in an appropriate RKHS $\mathscr{H}$. This leads to our previous result.

Kernel As A Tool for Dimension Augmentation

In regression spline, we did the following:

- From the given feature $x \in \mathbb{R}$, derive new features $x, x^2, (x - x_1)_+^3, \dots, (x - x_n)_+^3$.
- Perform linear regression with the derived features.

In essence, we augment the feature dimension and use linear methods in the augmented space!

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The problem may not be linear at the **x**-level ... but may be linear at a higher dimension!!

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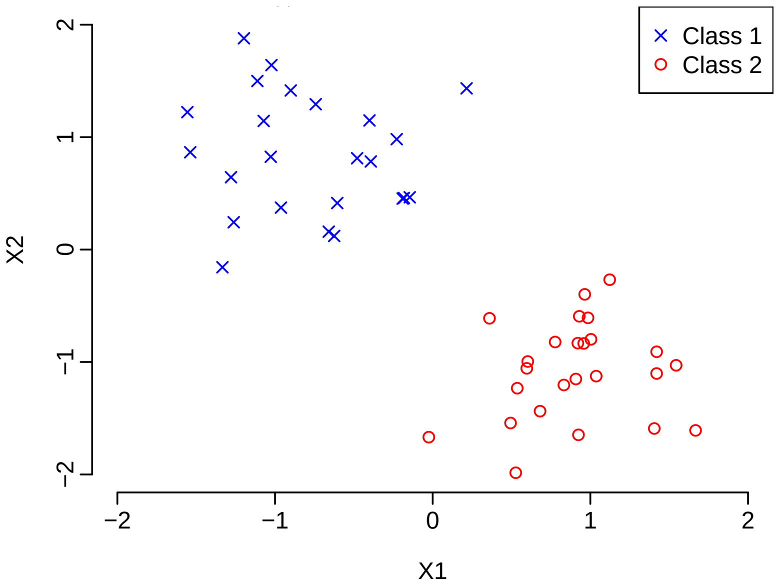

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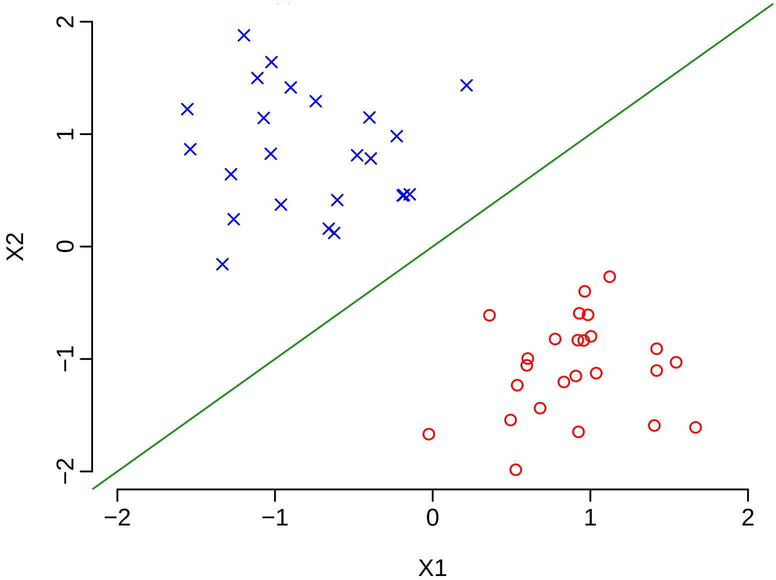
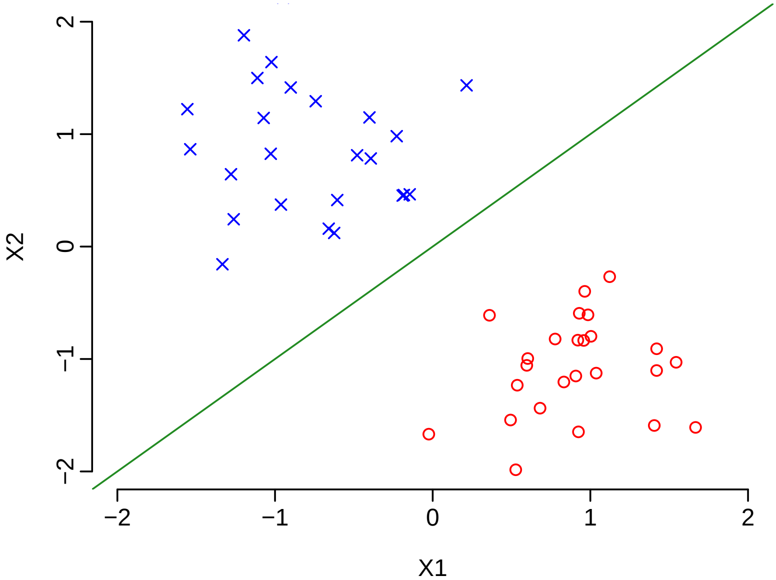
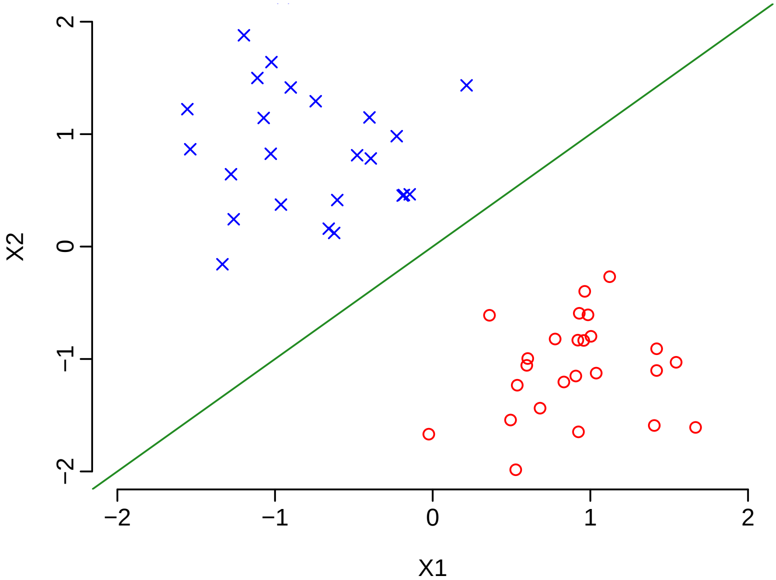


Classification



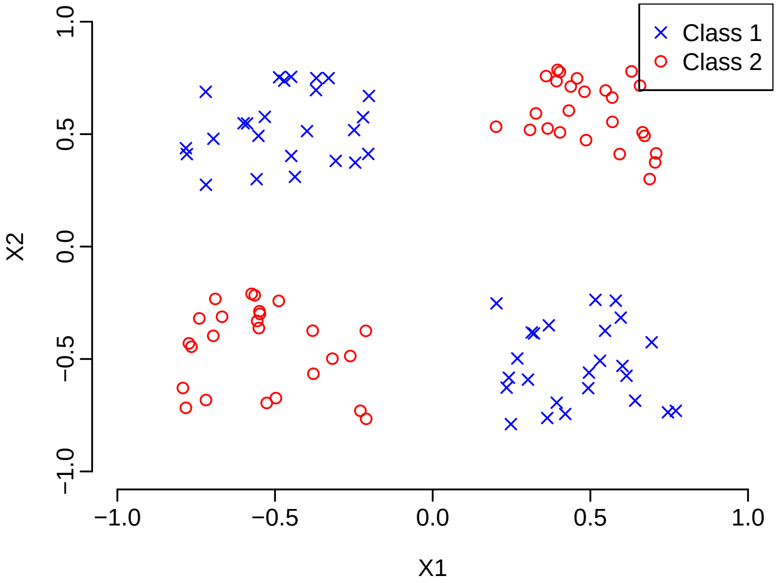
Linear classifier: $\delta(x_1, x_2) = \begin{cases} 1 & \text{if } \beta_1 x_1 + \beta_2 x_2 > \alpha \\ 2 & \text{otherwise} \end{cases}$

Classification

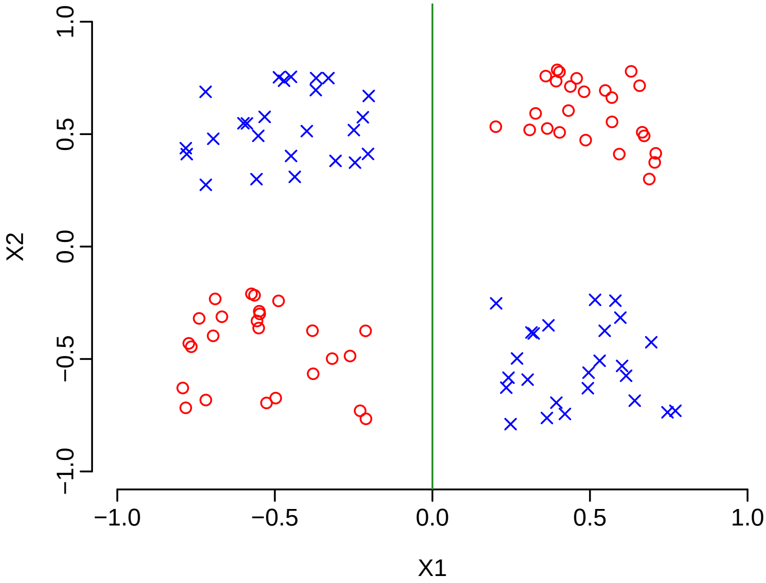


In general, Linear classifier: $\delta(\mathbf{x}) = \begin{cases} 1 & \text{if } \boldsymbol{\beta}^\top \mathbf{x} > \alpha \\ 2 & \text{otherwise} \end{cases}$

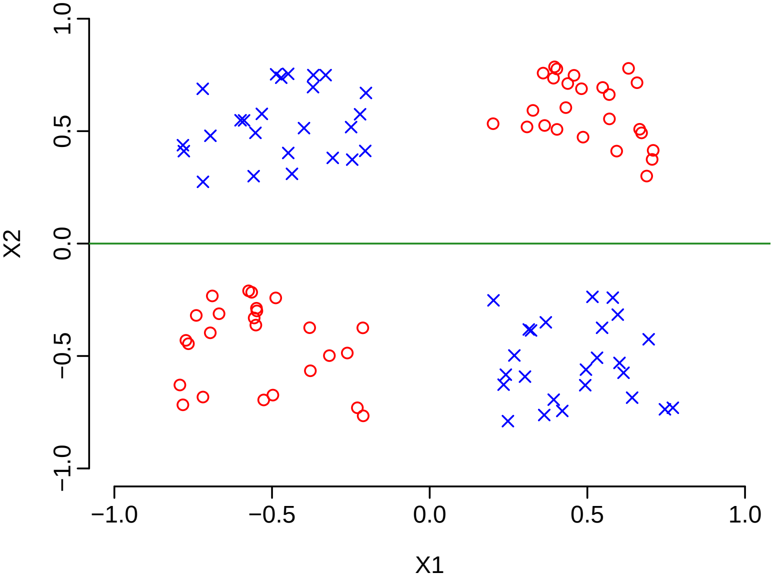
Another Example



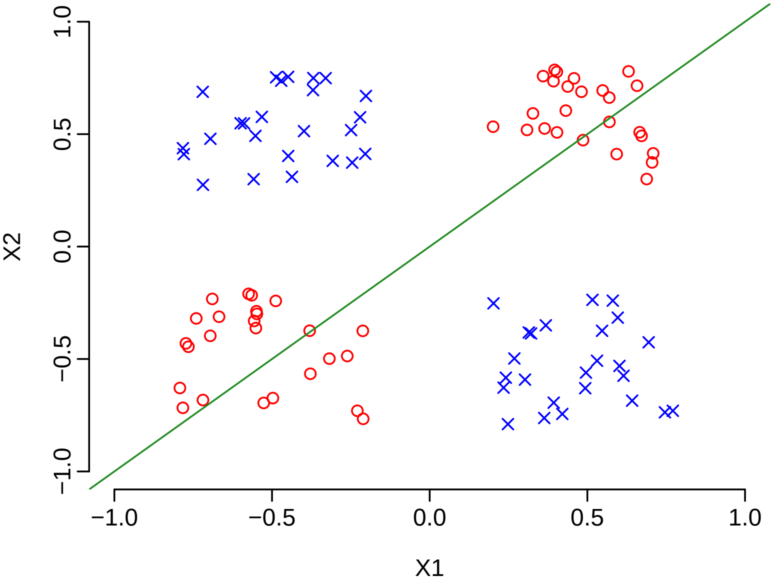
Another Example



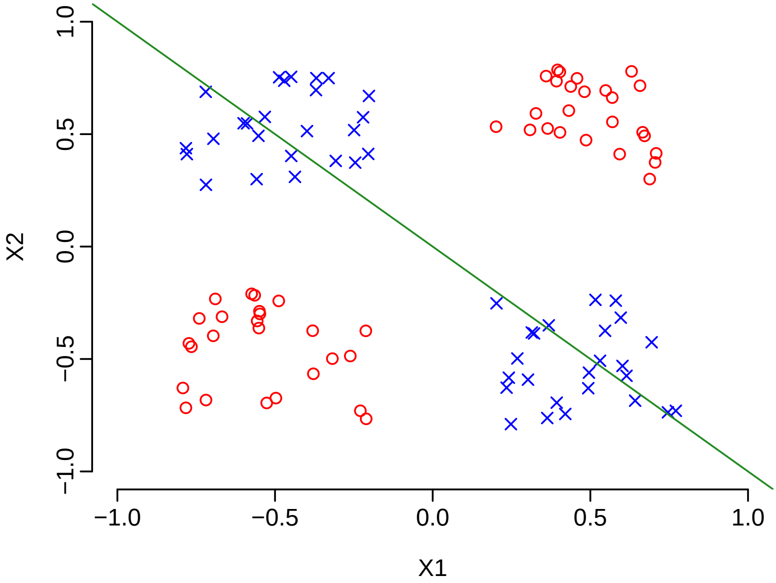
Another Example



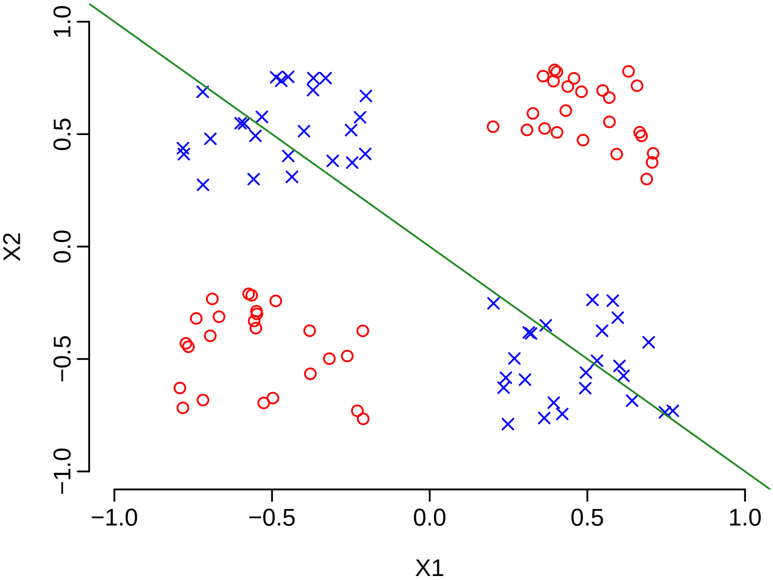
Another Example



Another Example

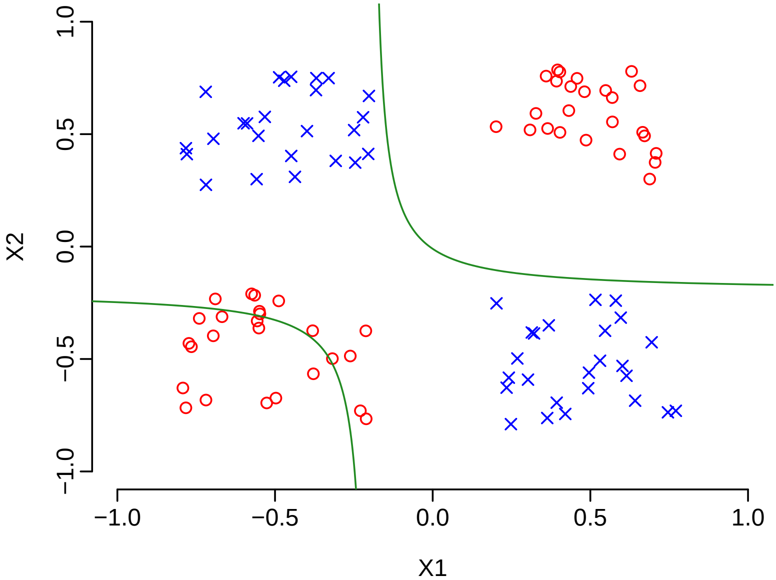


Another Example



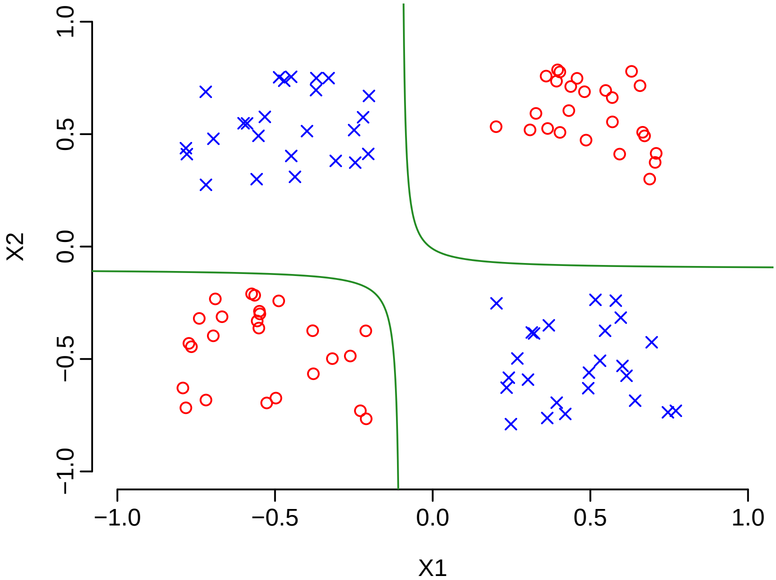
Linear classifier does not work in this case.

Another Example



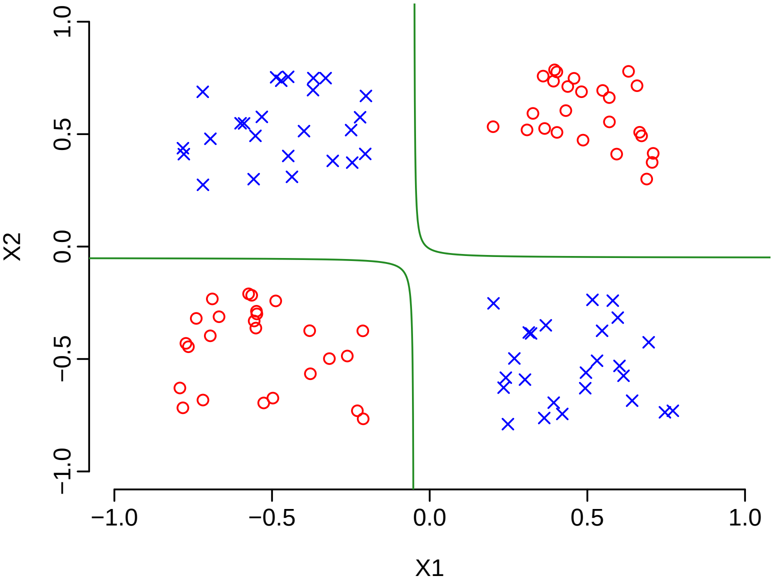
$$\delta(x_1, x_2) = \begin{cases} 1 & \text{if } x_1 + x_2 + 5x_1x_2 > 0.01 \\ 2 & \text{otherwise} \end{cases}$$

Another Example



$$\delta(x_1, x_2) = \begin{cases} 1 & \text{if } x_1 + x_2 + 10x_1x_2 > 0.01 \\ 2 & \text{otherwise} \end{cases}$$

Another Example



$$\delta(x_1, x_2) = \begin{cases} 1 & \text{if } x_1 + x_2 + 20x_1x_2 > 0.01 \\ 2 & \text{otherwise} \end{cases}$$

The problem is not linearly solvable in (x_1, x_2).

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Transform: $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \mapsto \begin{pmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{pmatrix}$

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Transform: $\underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} \mapsto \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{pmatrix}}_{\phi(\mathbf{x})}$

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The problem is linearly solvable in the transformed variable $\phi(\mathbf{x})$.

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But how does that help?

The problem is not linearly solvable in (x_1, x_2).

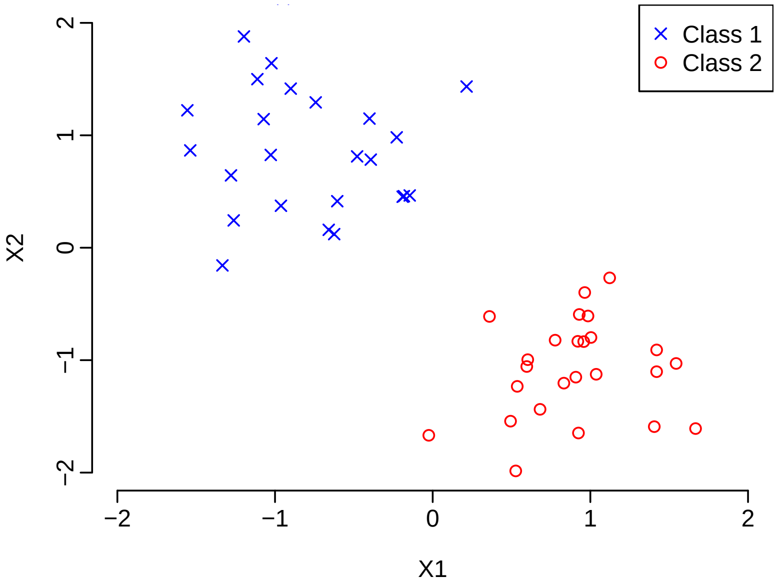
Transform: $\underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{\mathbf{x}} \mapsto \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{pmatrix}}_{\phi(\mathbf{x})}$

The problem is linearly solvable in the transformed variable $\phi(\mathbf{x})$.

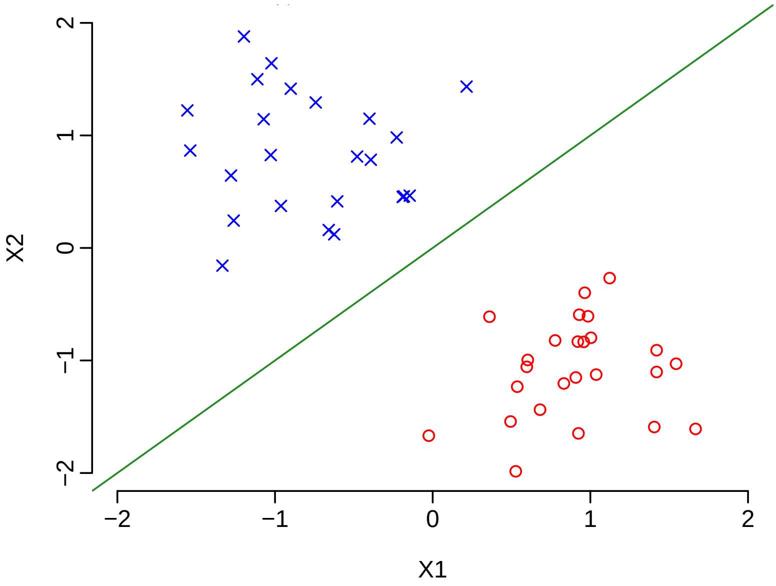
But how does that help?

For that, need to see how linear classifiers work.

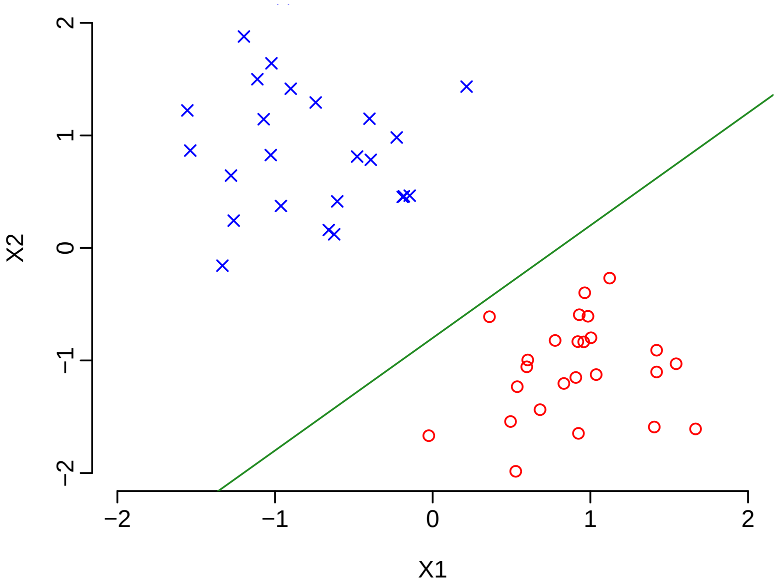
Back to the Linear Problem



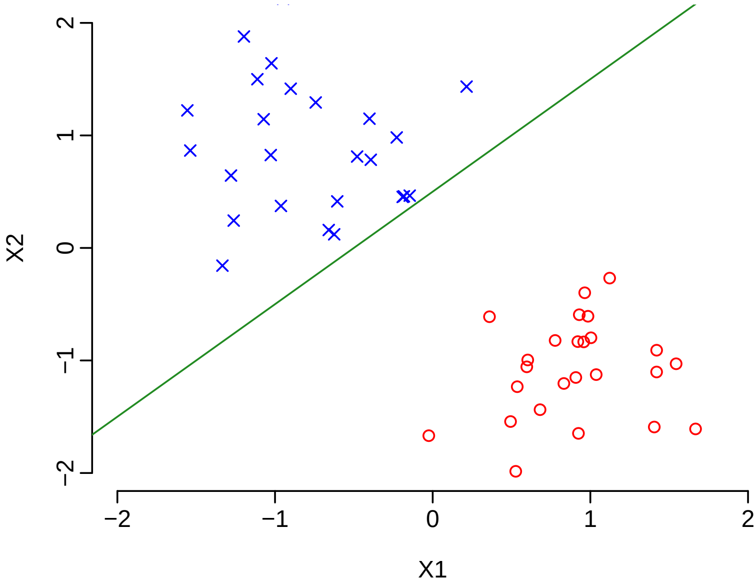
Back to the Linear Problem



Back to the Linear Problem



Back to the Linear Problem



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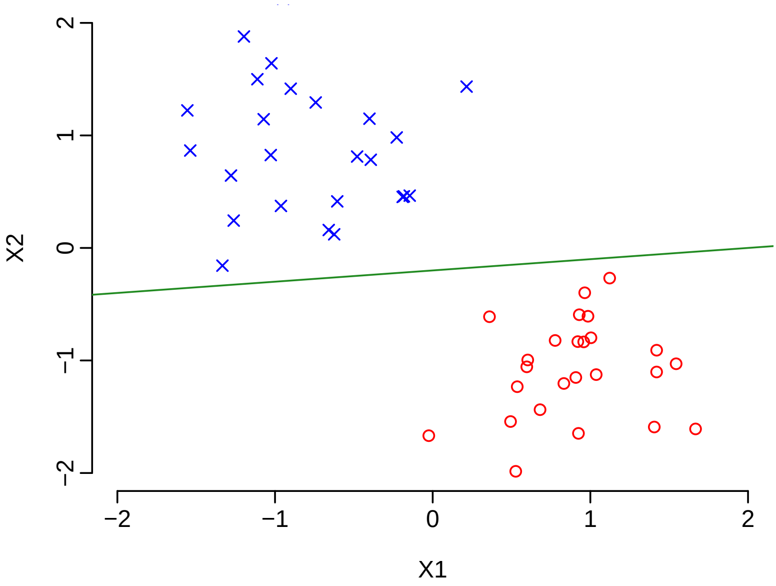

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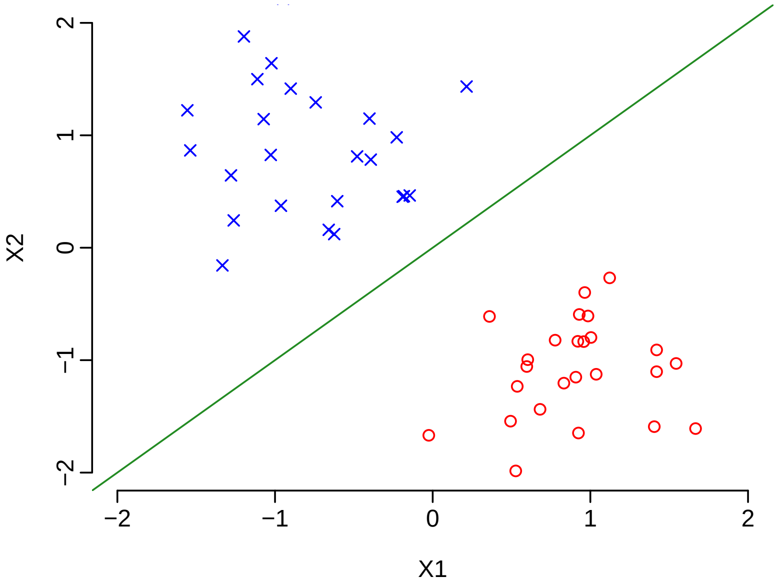
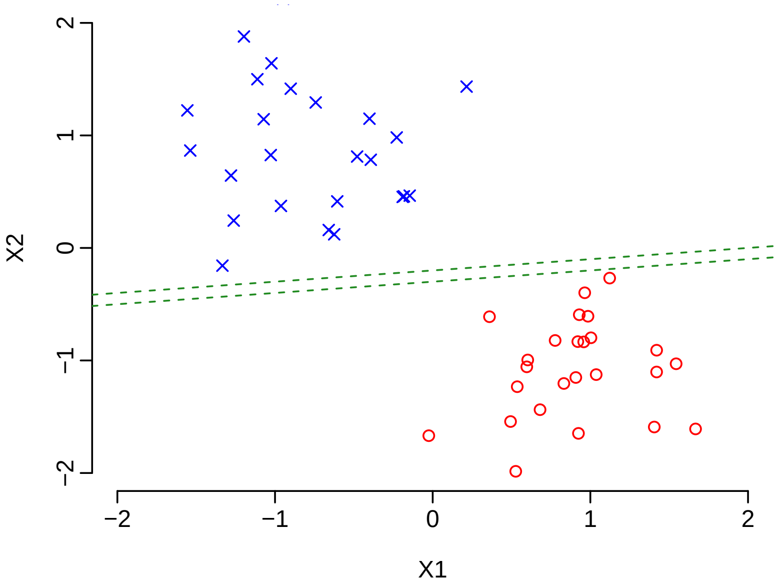


Margin

Margin



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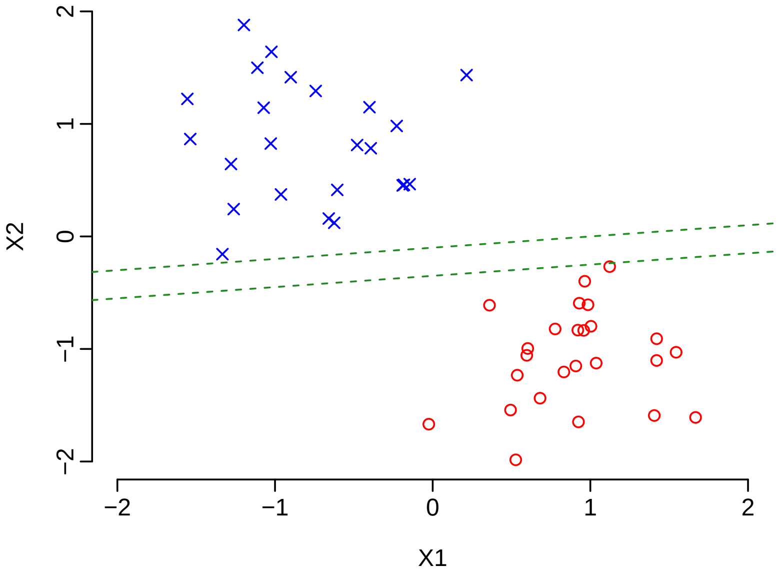

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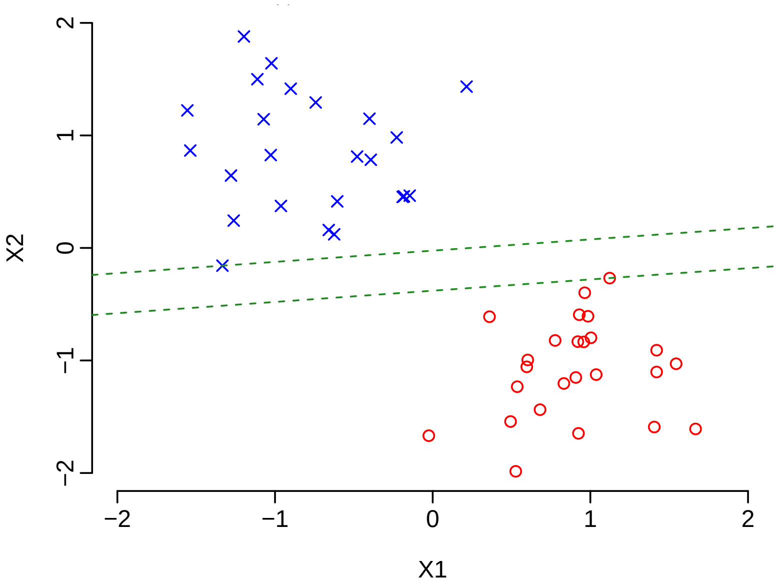

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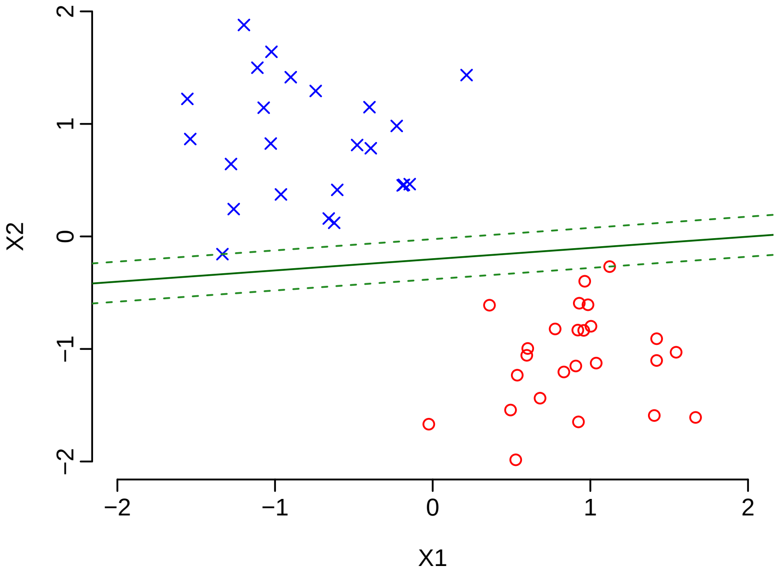

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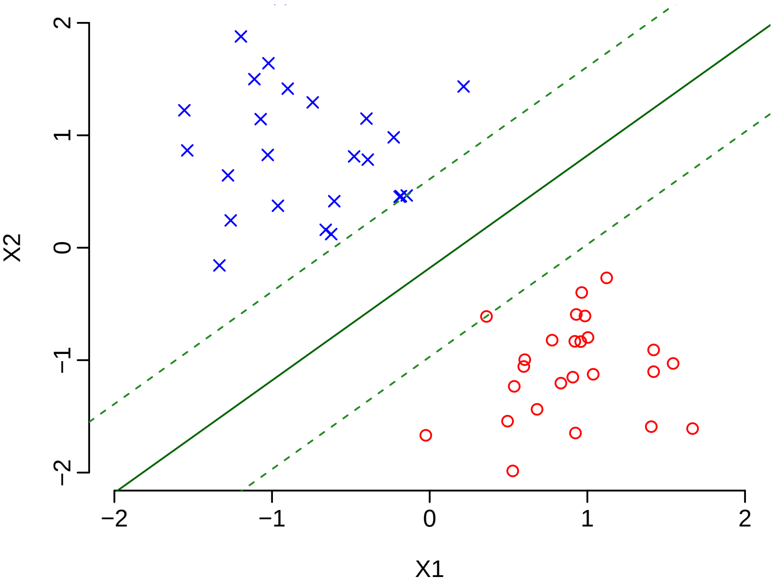

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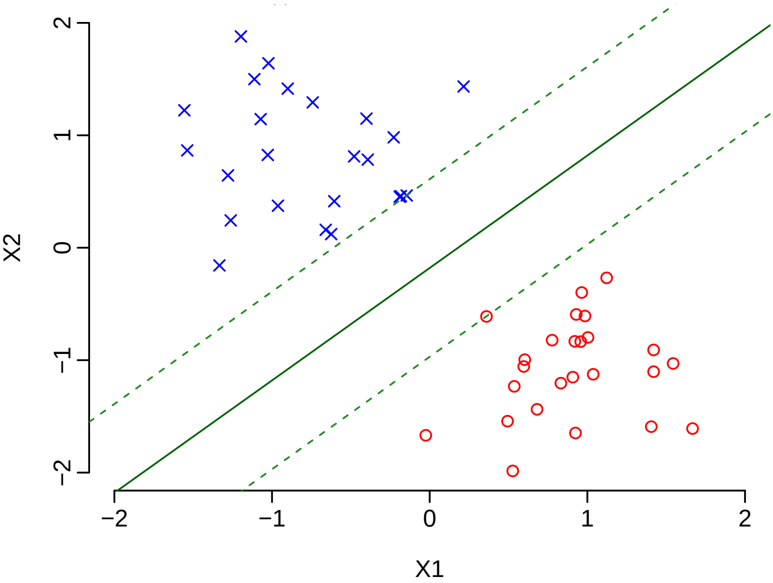

We prefer the direction which leads to the largest margin.

Mathematically ...

Let $y = \begin{cases} +1 & \text{if from Class 1} \\ -1 & \text{if from Class 2} \end{cases}$

Our classifier is: $\delta(\mathbf{x}) = \begin{cases} \text{Class 1} & \text{if } \boldsymbol{\beta}^\top \mathbf{x} + \beta_0 > 0 \\ \text{Class 2} & \text{if } \boldsymbol{\beta}^\top \mathbf{x} + \beta_0 < 0 \end{cases}$

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Correct decision if: $\begin{cases} \boldsymbol{\beta}^\top \mathbf{x} + \beta_0 > 0 & \text{when } \mathbf{x} \text{ comes from Class 1} \\ \boldsymbol{\beta}^\top \mathbf{x} + \beta_0 < 0 & \text{when } \mathbf{x} \text{ comes from Class 2} \end{cases}$

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Find $\boldsymbol{\beta}, \beta_0$ such that

$$y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) > 0 \; \forall\, i = 1, \ldots, n.$$

Mathematically ...

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Too many possibilities!!

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Too many possibilities!!

Make the gap as large as possible.

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Find $\boldsymbol{\beta}, \beta_0$ such that

$$y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) > 0 \; \forall \, i = 1, \ldots, n.$$

Too many possibilities!!

Impose $y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M$ and make M as large as possible.

Mathematically ...

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$$y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M \; \forall \, i = 1, \ldots, n \quad \text{and} \quad M \text{ is as large as possible.}$$

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Too many possibilities!!

Impose $y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M$ and make M as large as possible.

Find $\boldsymbol{\beta}, \beta_0$ such that

$$y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M \ \forall\, i = 1, \ldots, n \quad \text{and} \quad \underbrace{M \text{ is as large as possible}}_{\text{maximizing the margin}}.$$

$$\underset{\boldsymbol{\beta},\beta_0,\|\boldsymbol{\beta}\|=1}{\text{maximize}} \; M \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M \; \forall \, i = 1, \ldots, n$$

$$
\begin{aligned}
&\underset{\boldsymbol{\beta},\beta_0,\|\boldsymbol{\beta}\|=1}{\text{maximize}} \;\; M \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M \;\forall\, i = 1, \ldots, n \\
\Leftrightarrow \quad &\underset{\boldsymbol{\beta},\beta_0}{\text{maximize}} \;\; M \quad \text{s.t.} \quad \frac{1}{\|\boldsymbol{\beta}\|} y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M \;\forall\, i = 1, \ldots, n
\end{aligned}
$$

$$\underset{\boldsymbol{\beta},\beta_0,\|\boldsymbol{\beta}\|=1}{\text{maximize}} \; M \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M \; \forall\, i = 1, \ldots, n$$

$$\Leftrightarrow \quad \underset{\boldsymbol{\beta},\beta_0}{\text{maximize}} \; M \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M\|\boldsymbol{\beta}\| \; \forall\, i = 1, \ldots, n$$

$$
\begin{aligned}
& \underset{\boldsymbol{\beta},\beta_0,\|\boldsymbol{\beta}\|=1}{\text{maximize}} \; M \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M \;\forall\, i = 1,\dots,n \\
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\Leftrightarrow \quad & \underset{\boldsymbol{\beta},\beta_0}{\text{maximize}} \; \frac{1}{\|\boldsymbol{\beta}\|} \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq 1 \;\forall\, i = 1,\dots,n \qquad \big(\text{rescale by setting } M\|\beta\| = 1\big)
\end{aligned}
$$

$$
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& \underset{\boldsymbol{\beta},\beta_0,\|\boldsymbol{\beta}\|=1}{\text{maximize}} \;\; M \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M \; \forall\, i = 1, \ldots, n \\
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$$

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\Leftrightarrow \;\; & \underset{\boldsymbol{\beta},\beta_0}{\text{maximize}} \;\; M \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq M\|\boldsymbol{\beta}\| \; \forall\, i = 1,\ldots,n \\
\Leftrightarrow \;\; & \underset{\boldsymbol{\beta},\beta_0}{\text{maximize}} \;\; \frac{1}{\|\boldsymbol{\beta}\|} \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq 1 \; \forall\, i = 1,\ldots,n \qquad \big(\text{rescale by setting } M\|\beta\| = 1\big) \\
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\Leftrightarrow \;\; & \underset{\boldsymbol{\beta},\beta_0}{\text{minimize}} \;\; \frac{1}{2}\|\boldsymbol{\beta}\|^2 \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq 1 \; \forall\, i = 1,\ldots,n
\end{aligned}
$$

$$\underset{\boldsymbol{\beta},\beta_0}{\text{minimize}} \;\; \frac{1}{2}\|\boldsymbol{\beta}\|^2 \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq 1 \;\forall\, i = 1, \ldots, n.$$

$$\underset{\boldsymbol{\beta},\beta_0}{\text{minimize}} \quad \frac{1}{2}\|\boldsymbol{\beta}\|^2 \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq 1 \ \forall\, i = 1, \ldots, n.$$

Primal:

$$L_P(\boldsymbol{\beta}, \beta_0) = \frac{1}{2}\|\boldsymbol{\beta}\|^2 - \sum_{i=1}^{n} \lambda_i \{y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) - 1\}.$$

$$\underset{\boldsymbol{\beta},\beta_0}{\text{minimize}} \quad \frac{1}{2}\|\boldsymbol{\beta}\|^2 \quad \text{s.t.} \quad y_i(\boldsymbol{\beta}^\top \mathbf{x}_i + \beta_0) \geq 1 \;\forall\, i = 1, \ldots, n.$$

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Set the derivatives to zero:

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— Optimal separating hyperplane. Vapnik & Chervonenkis (1974)

Transform: $\mathbf{x} \to \phi(\mathbf{x})$

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— Boser, Guyon & Vapnik (1992)

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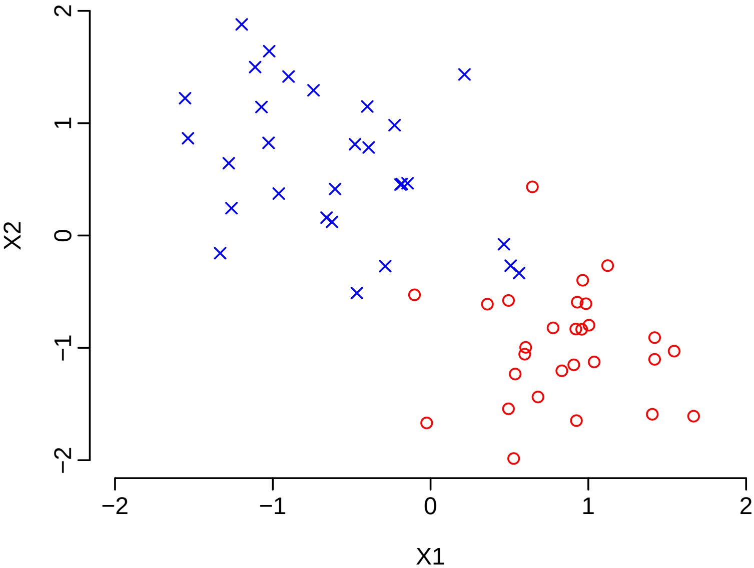

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1. Transform the feature: $\mathbf{x} \to \phi(\mathbf{x})$
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  E.g. SVM with Gaussian RBF: $\exp\left(-\dfrac{\|\mathbf{x}-\widetilde{\mathbf{x}}\|^2}{\sigma^2}\right)$ has been very successful.

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$$\boldsymbol{\beta}_l = \underset{\|\boldsymbol{\beta}\|=1, \boldsymbol{\beta}^\top \boldsymbol{\beta}_1 = \cdots = \boldsymbol{\beta}^\top \boldsymbol{\beta}_{l-1} = 0}{\arg\max} \frac{1}{n} \sum_{i=1}^n \left(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle\right)^2 = \underset{\|\boldsymbol{\beta}\|=1, \boldsymbol{\beta}^\top \boldsymbol{\beta}_1 = \cdots = \boldsymbol{\beta}^\top \boldsymbol{\beta}_{l-1} = 0}{\arg\max} \quad \widehat{\operatorname{var}}\left(\langle \boldsymbol{\beta}, \mathbf{X} \rangle\right)$$

Turns out: $\displaystyle \frac{1}{n} \sum_{i=1}^n \left(\langle \boldsymbol{\beta}, \mathbf{x}_i \rangle\right)^2 = \boldsymbol{\beta}^\top \mathbf{S} \boldsymbol{\beta}, \qquad \mathbf{S} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top$ — sample covariance matrix.

Kernel PCA

$\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$. Assumed centered, $\sum_{i=1}^n \mathbf{x}_i = 0$ (W.l.o.g.!).

Usual PCA: Find directions with largest variation.

$$\boldsymbol{\beta}_1 = \operatorname*{arg\,max}_{\|\boldsymbol{\beta}\|=1} \frac{1}{n}\sum_{i=1}^n \big(\langle \boldsymbol{\beta}, \mathbf{x}_i\rangle\big)^2 = \operatorname*{arg\,max}_{\|\boldsymbol{\beta}\|=1} \widehat{\operatorname{var}}\big(\langle \boldsymbol{\beta}, \mathbf{X}\rangle\big)$$

$$\boldsymbol{\beta}_2 = \operatorname*{arg\,max}_{\|\boldsymbol{\beta}\|=1, \boldsymbol{\beta}^\top\boldsymbol{\beta}_1=0} \frac{1}{n}\sum_{i=1}^n \big(\langle \boldsymbol{\beta}, \mathbf{x}_i\rangle\big)^2 = \operatorname*{arg\,max}_{\|\boldsymbol{\beta}\|=1, \boldsymbol{\beta}^\top\boldsymbol{\beta}_1=0} \widehat{\operatorname{var}}\big(\langle \boldsymbol{\beta}, \mathbf{X}\rangle\big)$$

$$\vdots$$

$$\boldsymbol{\beta}_l = \operatorname*{arg\,max}_{\|\boldsymbol{\beta}\|=1, \boldsymbol{\beta}^\top\boldsymbol{\beta}_1=\cdots=\boldsymbol{\beta}^\top\boldsymbol{\beta}_{l-1}=0} \frac{1}{n}\sum_{i=1}^n \big(\langle \boldsymbol{\beta}, \mathbf{x}_i\rangle\big)^2 = \operatorname*{arg\,max}_{\|\boldsymbol{\beta}\|=1, \boldsymbol{\beta}^\top\boldsymbol{\beta}_1=\cdots=\boldsymbol{\beta}^\top\boldsymbol{\beta}_{l-1}=0} \widehat{\operatorname{var}}\big(\langle \boldsymbol{\beta}, \mathbf{X}\rangle\big)$$

Turns out: $\displaystyle \frac{1}{n}\sum_{i=1}^n \big(\langle \boldsymbol{\beta}, \mathbf{x}_i\rangle\big)^2 = \boldsymbol{\beta}^\top \mathbf{S}\boldsymbol{\beta}$, $\displaystyle \mathbf{S} = \frac{1}{n}\sum_{i=1}^n \mathbf{x}_i\mathbf{x}_i^\top$ — sample covariance matrix.

The PC directions are given by the eigenvectors of $\mathbf{S}$: $\mathbf{S}\boldsymbol{\beta}_l = \lambda_l \boldsymbol{\beta}_l$.

$$\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^\top. \quad \mathbf{S}\boldsymbol{\beta} = \lambda\boldsymbol{\beta} \quad \Rightarrow \quad \boldsymbol{\beta} \in \mathrm{span}\{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \quad \Rightarrow \quad \boldsymbol{\beta} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i.$$

$$\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i\mathbf{x}_i^\top. \quad \mathbf{S}\boldsymbol{\beta} = \lambda\boldsymbol{\beta} \quad \Rightarrow \quad \boldsymbol{\beta} \in \operatorname{span}\{\mathbf{x}_1, \dots, \mathbf{x}_n\} \quad \Rightarrow \quad \boldsymbol{\beta} = \sum_{i=1}^{n}\alpha_i\mathbf{x}_i.$$

$$\boldsymbol{\beta}^\top\boldsymbol{\beta} = \sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j\langle\mathbf{x}_i, \mathbf{x}_j\rangle$$

$$\boldsymbol{\beta}^\top\widetilde{\boldsymbol{\beta}} = \sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\widetilde{\alpha}_j\langle\mathbf{x}_i, \mathbf{x}_j\rangle$$

$$\boldsymbol{\beta}^\top\mathbf{S}\boldsymbol{\beta} = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{j'=1}^{n}\alpha_j\alpha_{j'}\langle\mathbf{x}_i, \mathbf{x}_j\rangle\langle\mathbf{x}_i, \mathbf{x}_{j'}\rangle$$

$$\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^\top. \quad \mathbf{S}\boldsymbol{\beta} = \lambda\boldsymbol{\beta} \quad \Rightarrow \quad \boldsymbol{\beta} \in \operatorname{span}\{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \quad \Rightarrow \quad \boldsymbol{\beta} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i.$$

$$\boldsymbol{\beta}^\top \boldsymbol{\beta} = \sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle = \boldsymbol{\alpha}^\top \mathbf{K} \boldsymbol{\alpha}$$

$$\boldsymbol{\beta}^\top \widetilde{\boldsymbol{\beta}} = \sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \widetilde{\alpha}_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle = \boldsymbol{\alpha}^\top \mathbf{K} \widetilde{\boldsymbol{\alpha}}$$

$$\boldsymbol{\beta}^\top \mathbf{S} \boldsymbol{\beta} = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{j'=1}^{n} \alpha_j \alpha_{j'} \langle \mathbf{x}_i, \mathbf{x}_j \rangle \langle \mathbf{x}_i, \mathbf{x}_{j'} \rangle = \boldsymbol{\alpha}^\top \mathbf{K}^2 \boldsymbol{\alpha}$$

$$\mathbf{K} = \Big(\big(\langle \mathbf{x}_i, \mathbf{x}_j \rangle \big) \Big)_{1 \le i,j \le n}, \quad \boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^\top.$$

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$$\dots$$

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$$\boldsymbol{\beta}^\top\mathbf{S}\boldsymbol{\beta} = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{j'=1}^{n}\alpha_j\alpha_{j'}\langle\mathbf{x}_i, \mathbf{x}_j\rangle\langle\mathbf{x}_i, \mathbf{x}_{j'}\rangle = \boldsymbol{\alpha}^\top\mathbf{K}^2\boldsymbol{\alpha}$$

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For a new observation $\mathbf{x}$, the l-th PC score: $\langle\boldsymbol{\beta}_l, \mathbf{x}\rangle = \sum_{i=1}^{n}\alpha_{l,i}\langle\mathbf{x}_i, \mathbf{x}\rangle$

$$\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i\mathbf{x}_i^\top. \quad \mathbf{S}\boldsymbol{\beta} = \lambda\boldsymbol{\beta} \quad \Rightarrow \quad \boldsymbol{\beta} \in \operatorname{span}\{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \quad \Rightarrow \quad \boldsymbol{\beta} = \sum_{i=1}^{n} \alpha_i \mathbf{x}_i.$$

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- Obtaining the PC's depend on the inner-product matrix $\mathbf{K}$.
- Obtaining PC scores for a new observation depends on inner-product.

Kernel PCA algorithm: Schölkopf, Smola & Müller (1998)

- Take a kernel K. Define the kernel matrix $\mathbf{K} = \big(\big(K(\mathbf{x}_i, \mathbf{x}_j)\big)\big)_{1 \le i,j \le n}$.
- For $l = 1, 2, \ldots$, find:

$$\boldsymbol{\alpha}_l = \arg\max_{\boldsymbol{\alpha}} \;\; \boldsymbol{\alpha}^\top \mathbf{K}^2 \boldsymbol{\alpha} \quad \text{s.t.} \quad \boldsymbol{\alpha}^\top \mathbf{K} \boldsymbol{\alpha} = 1, \boldsymbol{\alpha}^\top \mathbf{K} \boldsymbol{\alpha}_1 = \cdots = \boldsymbol{\alpha}^\top \mathbf{K} \boldsymbol{\alpha}_{l-1} = 0.$$

The l-th kernel PC is: $\displaystyle\sum_{i=1}^{n} \alpha_{l,i} K(\cdot, \mathbf{x}_i)$.

For an observation $\mathbf{x}$, the l-th PC score is: $\displaystyle\sum_{i=1}^{n} \alpha_{l,i} K(\mathbf{x}, \mathbf{x}_i)$.

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  For an observation $\mathbf{x}$, the l-th PC score is: $\displaystyle\sum_{i=1}^{n} \alpha_{l,i} K(\mathbf{x}, \mathbf{x}_i)$.

At a conceptual level:

- Transform $\mathbf{x} \to \phi(\mathbf{x}) = K(\cdot, \mathbf{x})$.
- Perform PCA in the transformed space.
- Linear in the transformed space $\Rightarrow$ Non-linear in the actual space.

Kernel PCA algorithm: Schölkopf, Smola & Müller (1998)

- Take a kernel K. Define the kernel matrix $\mathbf{K} = \big(\big(K(\mathbf{x}_i, \mathbf{x}_j)\big)\big)_{1 \le i,j \le n}$.
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  The l-th kernel PC is: $\displaystyle\sum_{i=1}^n \alpha_{l,i} K(\cdot, \mathbf{x}_i).$

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No need to form the transformation ever. All calculations involve kernel evaluations only.

Kernel PCA algorithm: Schölkopf, Smola & Müller (1998)

- Take a kernel K. Define the kernel matrix $\mathbf{K} = \big((K(\mathbf{x}_i, \mathbf{x}_j))\big)_{1 \le i,j \le n}$.
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  For an observation $\mathbf{x}$, the l-th PC score is: $\displaystyle\sum_{i=1}^{n} \alpha_{l,i} K(\mathbf{x}, \mathbf{x}_i)$.

At a conceptual level:

- Transform $\mathbf{x} \to \phi(\mathbf{x}) = K(\cdot, \mathbf{x})$.
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- Linear in the transformed space $\Rightarrow$ Non-linear in the actual space.

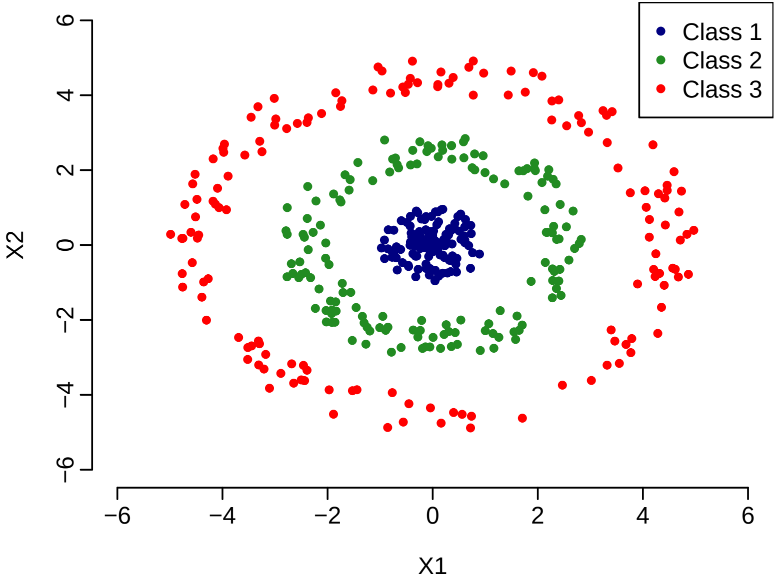
No need to form the transformation ever. All calculations involve kernel evaluations only.

⋆ We assumed centered observations.

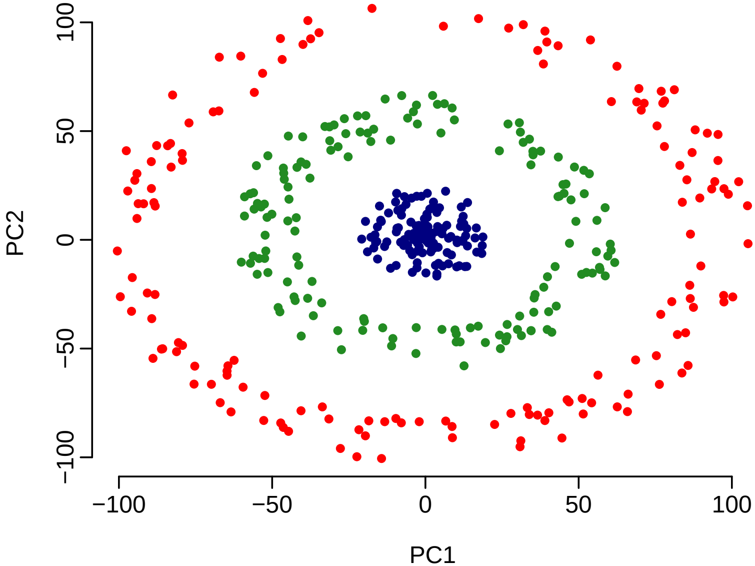
In general, need to use the double centered kernel matrix:

$$\widetilde{\mathbf{K}} = (\mathbf{I} - \mathbf{H})\mathbf{K}(\mathbf{I} - \mathbf{H}), \quad \mathbf{H} = \tfrac{1}{n}\mathbf{1}\mathbf{1}^\top$$

An Example

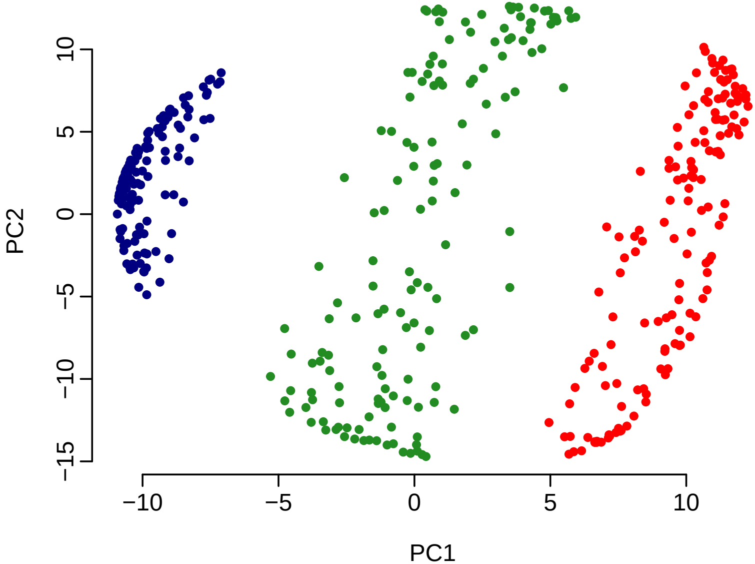


An Example



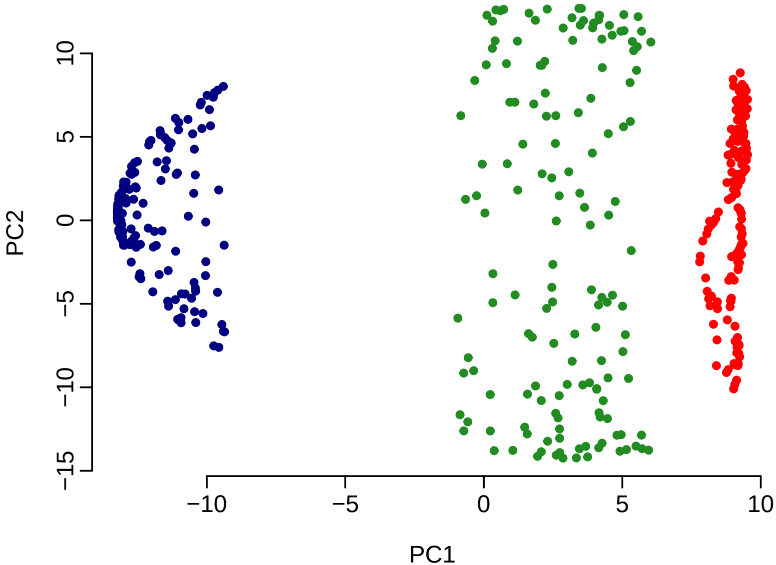
Usual PCA

An Example



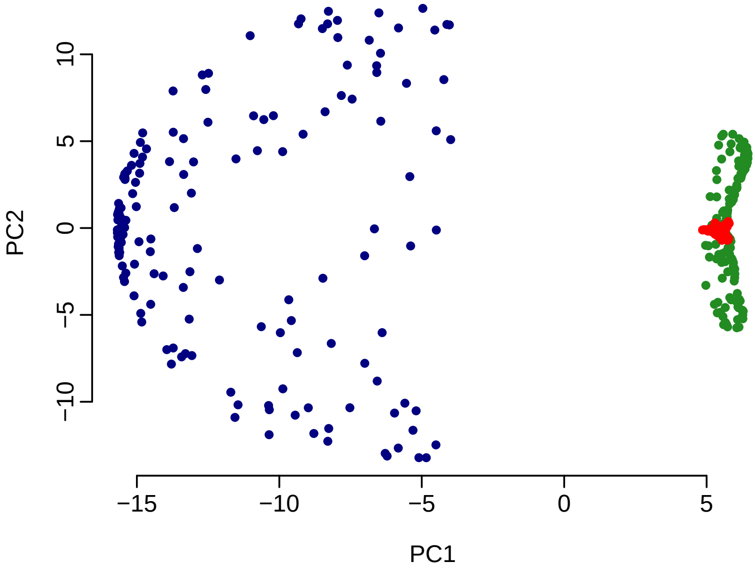
Kernel PCA with RBF kernel ($\sigma = 10$).

An Example



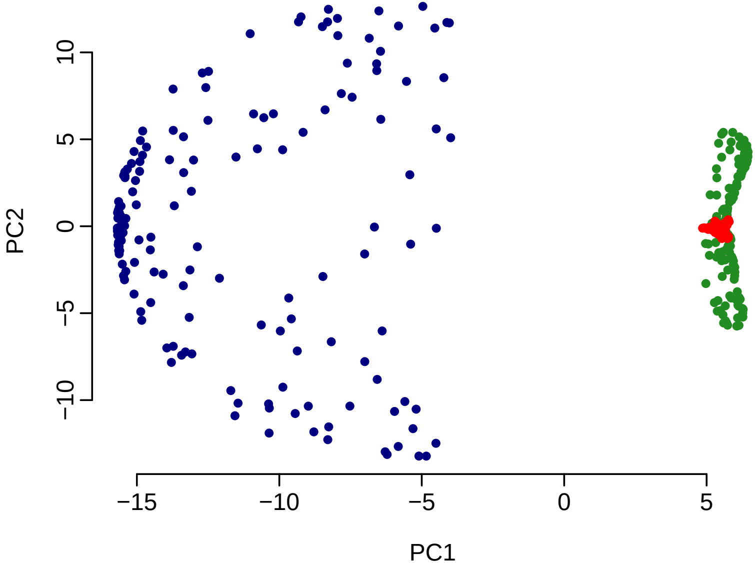
Kernel PCA with RBF kernel ($\sigma = 5$).

An Example



Kernel PCA with RBF kernel ($\sigma = 1$).

An Example



Kernel PCA with RBF kernel ($\sigma = 1$).

Choice of hyper-parameter is crucial

Kernel Two-sample Test

Two sets of observations: $\mathbf{x}_1, \ldots, \mathbf{x}_m \sim \mathbf{X}$, $\mathbf{y}_1, \ldots, \mathbf{y}_n \sim \mathbf{Y}$.

Want to check if they have the same distribution — $\mathcal{H}_0 : \mathbf{X} \overset{\mathcal{D}}{=} \mathbf{Y}$ against $\mathcal{H}_a : \mathbf{X} \overset{\mathcal{D}}{\neq} \mathbf{Y}$.

Kernel Two-sample Test

Two sets of observations: $\mathbf{x}_1, \ldots, \mathbf{x}_m \sim \mathbf{X}$, $\mathbf{y}_1, \ldots, \mathbf{y}_n \sim \mathbf{Y}$.

Want to check if they have the same distribution — $\mathcal{H}_0 : \mathbf{X} \stackrel{\mathcal{D}}{=} \mathbf{Y}$ against $\mathcal{H}_a : \mathbf{X} \stackrel{\mathcal{D}}{\neq} \mathbf{Y}$.

- Can use: $T = \left\|\bar{\mathbf{x}} - \bar{\mathbf{y}}\right\|^2$ for the test.

  Corresponds to checking: $\mathbb{E}(\mathbf{X}) = \mathbb{E}(\mathbf{Y})$ against $\mathbb{E}(\mathbf{X}) \neq \mathbb{E}(\mathbf{Y})$
  - A location alternative.
  - $\mathbf{X}$ and $\mathbf{Y}$ are well separated.

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  - A location alternative.
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- Transform the data: $\mathbf{x} \to \phi(\mathbf{x})$.

  Hope that the sets are well separated in the transformed space.

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Two sets of observations: $\mathbf{x}_1, \ldots, \mathbf{x}_m \sim \mathbf{X}$, $\mathbf{y}_1, \ldots, \mathbf{y}_n \sim \mathbf{Y}$.

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$$T = \left\| \frac{1}{m} \sum_{i=1}^{m} \phi(\mathbf{x}_i) - \frac{1}{n} \sum_{j=1}^{n} \phi(\mathbf{y}_j) \right\|^2.$$

Kernel Two-sample Test

Two sets of observations: $\mathbf{x}_1, \ldots, \mathbf{x}_m \sim \mathbf{X}$, $\mathbf{y}_1, \ldots, \mathbf{y}_n \sim \mathbf{Y}$.

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$$T = \left\| \frac{1}{m} \sum_{i=1}^{m} \phi(\mathbf{x}_i) - \frac{1}{n} \sum_{j=1}^{n} \phi(\mathbf{y}_j) \right\|^2.$$

$$= \frac{1}{m^2} \sum_{i=1}^{m} \sum_{j=1}^{m} \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle + \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \langle \phi(\mathbf{y}_i), \phi(\mathbf{y}_j) \rangle - \frac{2}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} \langle \phi(\mathbf{x}_i), \phi(\mathbf{y}_j) \rangle$$

Kernel Two-sample Test

Two sets of observations: $\mathbf{x}_1, \ldots, \mathbf{x}_m \sim \mathbf{X}$, $\mathbf{y}_1, \ldots, \mathbf{y}_n \sim \mathbf{Y}$.

Want to check if they have the same distribution — $\mathcal{H}_0 : \mathbf{X} \stackrel{\mathcal{D}}{=} \mathbf{Y}$ against $\mathcal{H}_a : \mathbf{X} \stackrel{\mathcal{D}}{\neq} \mathbf{Y}$.

- Can use: $T = \left\|\bar{\mathbf{x}} - \bar{\mathbf{y}}\right\|^2$ for the test.

  Corresponds to checking: $\mathbb{E}(\mathbf{X}) = \mathbb{E}(\mathbf{Y})$ against $\mathbb{E}(\mathbf{X}) \neq \mathbb{E}(\mathbf{Y})$
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$$
\begin{aligned}
T &= \left\| \frac{1}{m}\sum_{i=1}^{m}\phi(\mathbf{x}_i) - \frac{1}{n}\sum_{j=1}^{n}\phi(\mathbf{y}_j) \right\|^2. \\
&= \frac{1}{m^2}\sum_{i=1}^{m}\sum_{j=1}^{m}\langle\phi(\mathbf{x}_i), \phi(\mathbf{x}_j)\rangle + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\langle\phi(\mathbf{y}_i), \phi(\mathbf{y}_j)\rangle - \frac{2}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}\langle\phi(\mathbf{x}_i), \phi(\mathbf{y}_j)\rangle \\
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Kernel Two-sample Test

Two sets of observations: $\mathbf{x}_1, \ldots, \mathbf{x}_m \sim \mathbf{X}$, $\mathbf{y}_1, \ldots, \mathbf{y}_n \sim \mathbf{Y}$.

Want to check if they have the same distribution — $\mathcal{H}_0 : \mathbf{X} \overset{\mathcal{D}}{=} \mathbf{Y}$ against $\mathcal{H}_a : \mathbf{X} \overset{\mathcal{D}}{\neq} \mathbf{Y}$.

- Can use: $T = \left\|\bar{\mathbf{x}} - \bar{\mathbf{y}}\right\|^2$ for the test.

  Corresponds to checking: $\mathbb{E}(\mathbf{X}) = \mathbb{E}(\mathbf{Y})$ against $\mathbb{E}(\mathbf{X}) \neq \mathbb{E}(\mathbf{Y})$
  - A location alternative.
  - $\mathbf{X}$ and $\mathbf{Y}$ are well separated.
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- For suitable choices of K, this test is exact.

  — viable against the general alternative: $\mathbf{X} \overset{\mathcal{D}}{\neq} \mathbf{Y}$.

  More on this from other speakers!

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    – vectors, matrices, images, texts etc.

  All we need is to be able to evaluate the kernel.

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- Some other methods:
  - Kernel ridge regression.
  - Kernel logistic regression.
  - Kernel nearest neighbor.
  - Kernel canonical correlation analysis (CCA).
  - Kernel K-means clustering.

A look into the future

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- Large scale problems.
  - For n observations, need at least n^2 computations for the kernel matrix.
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- Large scale problems.
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- Learning the kernel.
  - The choice of K is crucial for kernel methods.
  - How to select a good kernel from the data?

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