Random Matrices Meet Machine Learning: A Large Dimensional Analysis of LS-SVM

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In this work:

- new random matrix approach to linearize kernels
- asymptotic analysis of LS-SVM for $n, p \to \infty$
- new insights

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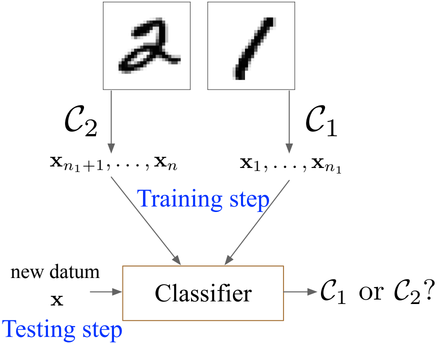

- **Training**:
  Training set: $\mathbf{x}_1,\ldots,\mathbf{x}_{n_1} \in \mathcal{C}_1$, $\mathbf{x}_{n_1+1},\ldots,\mathbf{x}_n \in \mathcal{C}_2$.
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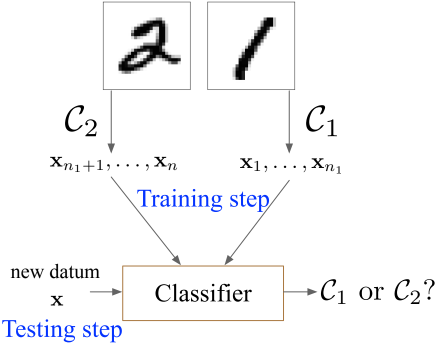
Binary Classification Problem



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- **Testing**:
  New datum $\mathbf{x} \Rightarrow$ which class?

Least Squares Support Vector Machines (1)

When $\mathcal{C}_1, \mathcal{C}_2$ are linearly separable.

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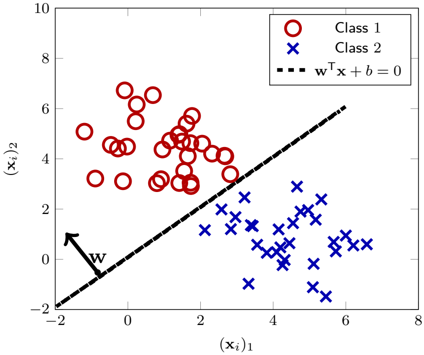
Optimization problem: find separating hyperplane

$$\arg\min_{\mathbf{w}} \quad J(\mathbf{w}, e) = \|\mathbf{w}\|^2 + \frac{\gamma}{n} \sum_{i=1}^{n} e_i^2$$

$$\text{such that} \quad y_i = \mathbf{w}^\mathsf{T} \mathbf{x}_i + b + e_i$$
$$\text{for } i = 1, \ldots, n$$



Least Squares Support Vector Machines (2)

When no linear separability:
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To solve the optimization problem:

$$\arg\min_{\mathbf{w}} \quad J(\mathbf{w}, e) = \|\mathbf{w}\|^2 + \frac{\gamma}{n} \sum_{i=1}^{n} e_i^2$$

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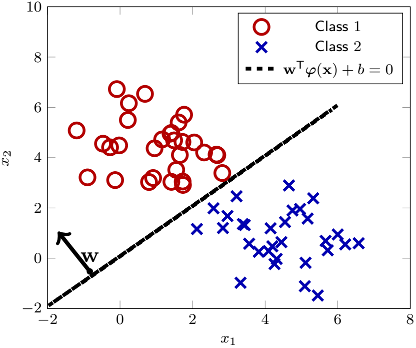

Least Squares Support Vector Machines (3)

- **Training**: Solution given by $\mathbf{w} = \sum_{i=1}^{n} \alpha_i \boldsymbol{\varphi}(\mathbf{x}_i)$, where

$$\begin{cases} \boldsymbol{\alpha} & = \mathbf{S}\left(\mathbf{I}_n - \frac{\mathbf{1}_n \mathbf{1}_n^\mathsf{T} \mathbf{S}}{\mathbf{1}_n^\mathsf{T} \mathbf{S} \mathbf{1}_n}\right)\mathbf{y} = \mathbf{S}\left(\mathbf{y} - b\mathbf{1}_n\right) \\ b & = \frac{\mathbf{1}_n^\mathsf{T} \mathbf{S} \mathbf{y}}{\mathbf{1}_n^\mathsf{T} \mathbf{S} \mathbf{1}_n} \end{cases} \tag{1}$$

with $\mathbf{S} \equiv \left(\mathbf{K} + \frac{n}{\gamma}\mathbf{I}_n\right)^{-1}$ resolvent of kernel matrix:

$$\mathbf{K} \equiv \left\{\boldsymbol{\varphi}(\mathbf{x}_i)^\mathsf{T} \boldsymbol{\varphi}(\mathbf{x}_j)\right\}_{i,j=1}^{n} = \left\{ f\left(\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{p}\right)\right\}_{i,j=1}^{n} \tag{2}$$

for some *translation invariant* kernel function $f : \mathbb{R}_+ \mapsto \mathbb{R}_+$, $\mathbf{y} \equiv [y_1, \ldots, y_n]^\mathsf{T}$ and $\boldsymbol{\alpha} \equiv [\alpha_1, \ldots, \alpha_n]^\mathsf{T}$.

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- **bing**: Decision for new $\mathbf{x}$

$$g(\mathbf{x}) = \boldsymbol{\alpha}^\mathsf{T} \mathbf{k}(\mathbf{x}) + b \tag{3}$$

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Advantage

Explicit form, as opposed to SVM $\Rightarrow$ easier to analyze.

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  - **Key Notation**: $\tau \equiv \frac{2}{p} \operatorname{tr} C^\circ$

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Recall

- kernel matrix $\mathbf{K}$: $\mathbf{K}_{i,j} = f\left(\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{p}\right)$
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For $\mathbf{x}_i \in \mathcal{C}_a$ and $\mathbf{x}_j \in \mathcal{C}_b$

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$$= \frac{1}{p}\operatorname{tr}\mathbf{C}_a + \frac{1}{p}\operatorname{tr}\mathbf{C}_b + O\left(\frac{1}{\sqrt{n}}\right) = \underbrace{\frac{2}{p}\operatorname{tr}\mathbf{C}^\circ}_{\equiv\tau=O(1)} + \underbrace{\frac{1}{p}\operatorname{tr}(\mathbf{C}_a - \mathbf{C}^\circ) + \frac{1}{p}\operatorname{tr}(\mathbf{C}_b - \mathbf{C}^\circ)}_{O(n^{-1/2})} + O\left(\frac{1}{\sqrt{n}}\right)$$

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  - $\|\mathbf{C}_a\| = O(1)$ and $\operatorname{tr}(\mathbf{C}_2 - \mathbf{C}_1) = O(\sqrt{n})$
- Gaussian data: $\mathbf{x}_i \sim \mathcal{N}(\boldsymbol{\mu}_a, \mathbf{C}_a)$ or $\mathbf{x}_i = \boldsymbol{\mu}_a + \mathbf{w}_i$ where $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \mathbf{C}_a)$

For $\mathbf{x}_i \in \mathcal{C}_a$ and $\mathbf{x}_j \in \mathcal{C}_b$

$$\frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_j\|^2 = \frac{1}{p}\|\mathbf{w}_i - \mathbf{w}_j\|^2 + \underbrace{\frac{1}{p}\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\|^2}_{O(n^{-1})} + \underbrace{\frac{2}{\sqrt{p}}(\boldsymbol{\mu}_a - \boldsymbol{\mu}_b)^\mathsf{T}(\mathbf{w}_i - \mathbf{w}_j)}_{O(n^{-1})}$$

$$= \frac{\mathbb{E}[\|\mathbf{w}_i\|^2] + \mathbb{E}[\|\mathbf{w}_j\|^2]}{p} + \underbrace{\frac{\|\mathbf{w}_i\|^2 - \mathbb{E}[\|\mathbf{w}_i\|^2]}{p} + \frac{\|\mathbf{w}_j\|^2 - \mathbb{E}[\|\mathbf{w}_j\|^2]}{p} - \frac{2}{p}\mathbf{w}_i^\mathsf{T}\mathbf{w}_j}_{O(n^{-1/2})} + O(\frac{1}{n})$$

$$= \frac{1}{p}\operatorname{tr}\mathbf{C}_a + \frac{1}{p}\operatorname{tr}\mathbf{C}_b + O(\frac{1}{\sqrt{n}}) = \underbrace{\frac{2}{p}\operatorname{tr}\mathbf{C}^\circ}_{\equiv\tau=O(1)} + \underbrace{\frac{1}{p}\operatorname{tr}(\mathbf{C}_a - \mathbf{C}^\circ) + \frac{1}{p}\operatorname{tr}(\mathbf{C}_b - \mathbf{C}^\circ)}_{O(n^{-1/2})} + O(\frac{1}{\sqrt{n}})$$

$$\Rightarrow \frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_j\|^2 = \tau + O(n^{-1/2})$$

Kernel linearization (2)

Recall: kernel matrix

$$\mathbf{K}_{i,j} = f\left(\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{p}\right)$$

For $\mathbf{x}_i \in \mathcal{C}_a$ and $\mathbf{x}_j \in \mathcal{C}_b$: $\frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_j\|^2 = \tau + O(n^{-1/2})$, thus for $\mathbf{K}_{i,j}$

$$\mathbf{K}_{i,j} = f\left(\tau + O(n^{-1/2})\right) = f(\tau) + f'(\tau)[\ldots] + f''(\tau)[\ldots]\ldots$$

or in matrix form

$$\mathbf{K} = f(\tau)\mathbf{1}_n\mathbf{1}_n^\mathsf{T} + f'(\tau)[\ldots] + f''(\tau)[\ldots] + \ldots$$

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Consequence

Asymptotic statistics of $\mathbf{K}$, thus of

$$g(\mathbf{x}) = \boldsymbol{\alpha}^\mathsf{T}\mathbf{k}(\mathbf{x}) + b$$

Asymptotic Behavior of the Decision Function

Theorem

Under previous assumptions, for $\mathbf{x} \in \mathcal{C}_a$, $a \in \{1, 2\}$

$$n\left(g(\mathbf{x}) - G_a\right) \xrightarrow{d} 0$$

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Simulations on Gaussian data

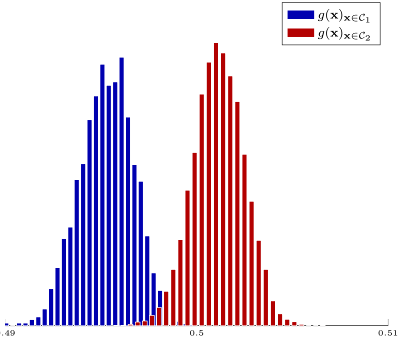
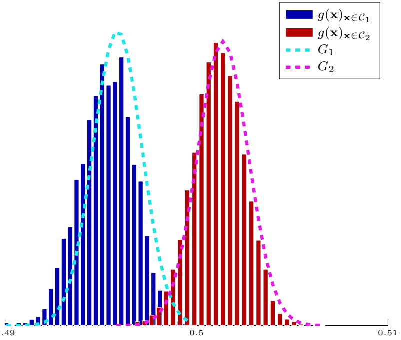


Figure: Gaussian approximation of $g(\mathbf{x})$, $n = 256, p = 512$, $c_1 = 1/4, c_2 = 3/4$, $\gamma = 1$, Gaussian kernel with $\sigma^2 = 1$, $\mathbf{x} \in \mathcal{N}(\boldsymbol{\mu}_a, \mathbf{C}_a)$ with $\boldsymbol{\mu}_a = [\mathbf{0}_{a-1}; 3; \mathbf{0}_{p-a}]$, $\mathbf{C}_1 = \mathbf{I}_p$ and $\{\mathbf{C}_2\}_{i,j} = .4^{|i-j|}(1 + \frac{5}{\sqrt{p}})$.



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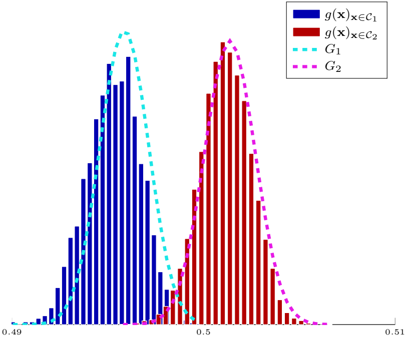
Simulations on Gaussian data



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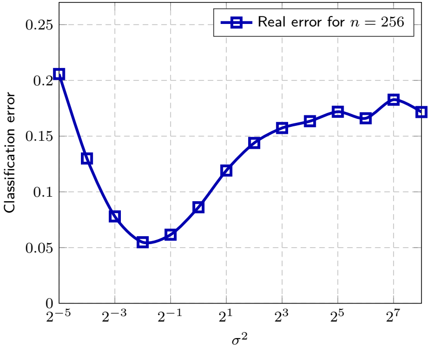
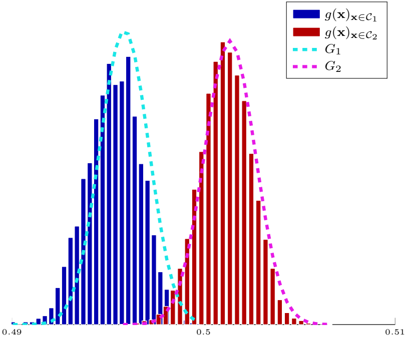


Figure: Performance of LS-SVM, $c_0 = 2$, $c_1 = c_2 = 1/2$, $\gamma = 1$, Gaussian kernel $f(x) = \exp(\frac{x}{2\sigma^2})$. $\mathbf{x} \in \mathcal{N}(\boldsymbol{\mu}_a, \mathbf{C}_a)$, with $\boldsymbol{\mu}_a = [\mathbf{0}_{a-1}; 2; \mathbf{0}_{p-a}]$, $\mathbf{C}_1 = \mathbf{I}_p$ and $\{\mathbf{C}_2\}_{i,j} = .4^{|i-j|}(1 + \frac{4}{\sqrt{p}})$.



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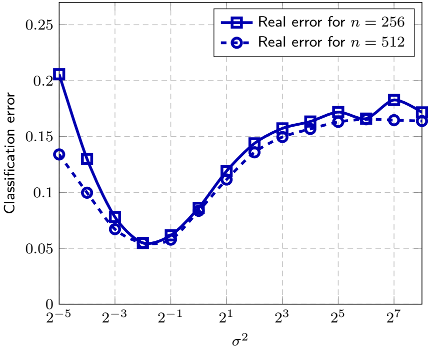

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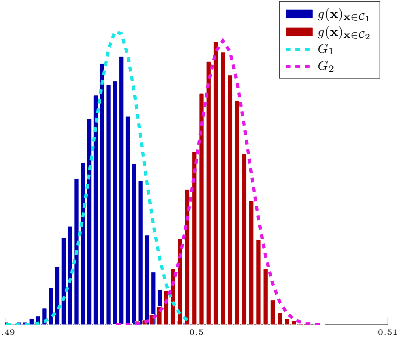
Simulations on Gaussian data



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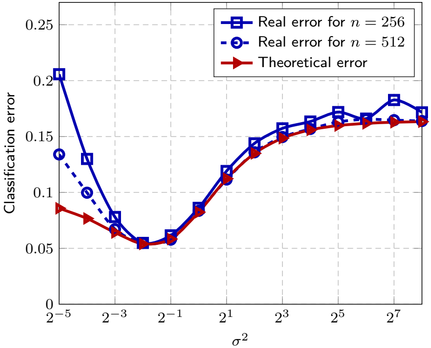

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Simulations on MNIST data

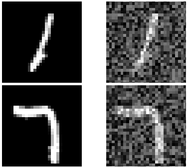
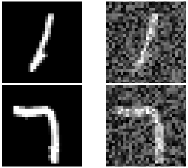


Figure: Samples from the MNIST database, without and with 0dB noise.

Simulations on MNIST data



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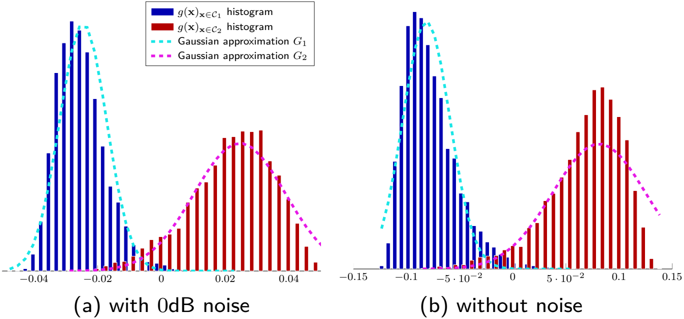

Figure: Gaussian approximation of $g(\mathbf{x})$, $n = 256, p = 784$, $c_1 = c_2 = 1/2$, $\gamma = 1$, Gaussian kernel with $\sigma^2 = 1$, MNIST data (numbers 1 and 7) without and with 0dB noise.

Discussion

Some consequences:

1. imbalanced training data: $c_2 - c_1 \neq 0$
   $\Rightarrow$ Decision boundary $c_2 - c_1$ instead of 0!

Theorem

$n\left(g(\mathbf{x}) - G_a\right) \xrightarrow{d} 0$ *and* $G_a \sim \mathcal{N}(\mathrm{E}_a, \mathrm{Var}_a)$ *with*

$$\mathrm{E}_a = \begin{cases} c_2 - c_1 - 2c_2 \cdot c_1 c_2 \gamma \mathfrak{D} \ , & a = 1 \\ c_2 - c_1 + 2c_1 \cdot c_1 c_2 \gamma \mathfrak{D} \ , & a = 2 \end{cases}$$

$$\mathrm{Var}_a = 8\gamma^2 c_1^2 c_2^2 \left(\mathcal{V}_1^a + \mathcal{V}_2^a + \mathcal{V}_3^a\right)$$

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   $\Rightarrow f'(\tau) < 0$ and $f''(\tau) > 0$

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2. $\mathfrak{D}$ as large as possible: conditions of f
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3. influence of γ:
   $\Rightarrow$ (asymptotically) not important!
4. dominant difference in means
   $\Rightarrow$ irrelevant kernel choice!

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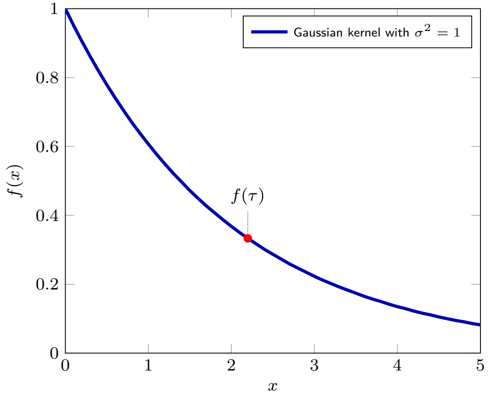
Kernel comparison[1]



Recall: kernel matrix

$$\mathbf{K}_{i,j} = f\left(\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{p}\right)$$

Table: Performance of different kernels

Kernel	Success rate
▬	91.4%

[1]Gaussian mixture data with $\boldsymbol{\mu}_a = \left[\mathbf{0}_{a-1}; 2; \mathbf{0}_{p-a}\right]$, $\mathbf{C}_1 = \mathbf{I}_p$ and $\{\mathbf{C}_2\}_{i,j} = .4^{|i-j|}(1 + \frac{4}{\sqrt{p}})$. $n_{\text{test}} = n = 256$, $p = 512$, $\gamma = 1$.

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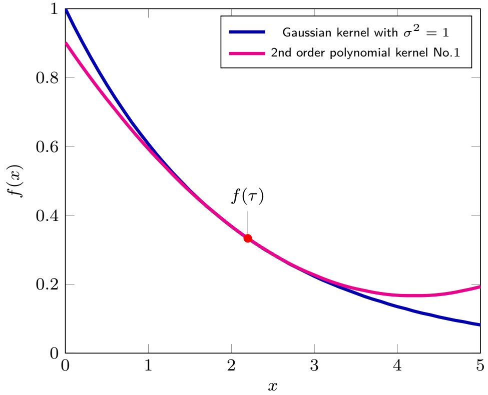

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Table: Performance of different kernels

Kernel	Success rate
(blue: Gaussian)	91.4%
(magenta: polynomial No.1)	91.2%

- No.1: same $f(\tau)$, $f'(\tau)$, $f''(\tau)$ as Gaussian kernel.

[1] Gaussian mixture data with $\boldsymbol{\mu}_a = \left[\mathbf{0}_{a-1}; 2; \mathbf{0}_{p-a}\right]$, $\mathbf{C}_1 = \mathbf{I}_p$ and $\{\mathbf{C}_2\}_{i,j} = .4^{|i-j|}(1 + \frac{4}{\sqrt{p}})$. $n_{\text{test}} = n = 256$, $p = 512$, $\gamma = 1$.

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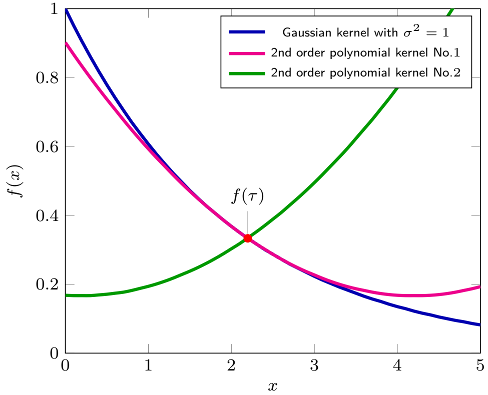

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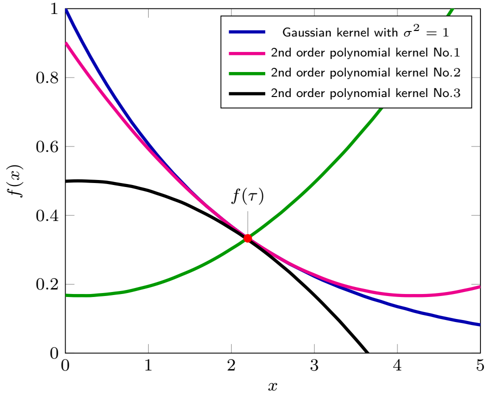
Table: Performance of different kernels

Kernel	Success rate
blue (Gaussian)	91.4%
magenta (No.1)	91.2%
green (No.2)	33.6%

- No.1: same $f(\tau)$, $f'(\tau)$, $f''(\tau)$ as Gaussian kernel.
- No.2: same $f(\tau)$ and $f''(\tau)$, while $f'(\tau)$ of opposite sign.

[1] Gaussian mixture data with $\boldsymbol{\mu}_a = \left[\mathbf{0}_{a-1}; 2; \mathbf{0}_{p-a}\right]$, $\mathbf{C}_1 = \mathbf{I}_p$ and $\{\mathbf{C}_2\}_{i,j} = .4^{|i-j|}(1 + \frac{4}{\sqrt{p}})$. $n_{\text{test}} = n = 256$, $p = 512$, $\gamma = 1$.

Kernel comparison[1]



Recall: kernel matrix

$$\mathbf{K}_{i,j} = f\left(\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{p}\right)$$

Table: Performance of different kernels

Kernel	Success rate
(blue)	91.4%
(magenta)	91.2%
(green)	33.6%
(black)	67.1%

- No.1: same $f(\tau)$, $f'(\tau)$, $f''(\tau)$ as Gaussian kernel.
- No.2: same $f(\tau)$ and $f''(\tau)$, while $f'(\tau)$ of opposite sign.
- No.3: same $f(\tau)$ and $f'(\tau)$, while $f''(\tau)$ of opposite sign.

[1] Gaussian mixture data with $\boldsymbol{\mu}_a = \left[\mathbf{0}_{a-1}; 2; \mathbf{0}_{p-a}\right]$, $\mathbf{C}_1 = \mathbf{I}_p$ and $\{\mathbf{C}_2\}_{i,j} = .4^{|i-j|}(1 + \frac{4}{\sqrt{p}})$. $n_{\text{test}} = n = 256$, $p = 512$, $\gamma = 1$.

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References:

- Z. Liao, R. Couillet, "**A Large Dimensional Analysis of Least Squares Support Vector Machines**", (submitted to) Journal of Machine Learning Research, 2016.
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Thank you!