Foundations of Machine Learning (ST510)

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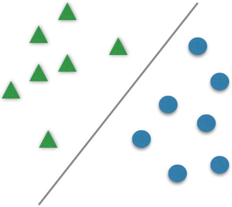
LSE

Motivating examples

Example-1: non-linear (large-margin) classification

- Given: $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, $y_i \in \{-1, 1\}$.
- Goal: find an f classifier such that $f(\mathbf{x}) \approx y$.



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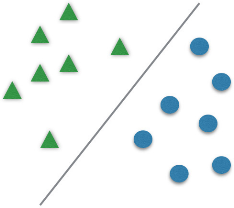

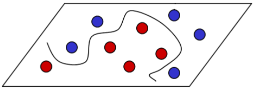

Input Space

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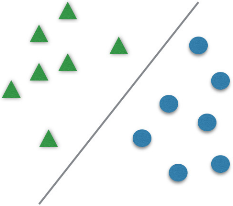
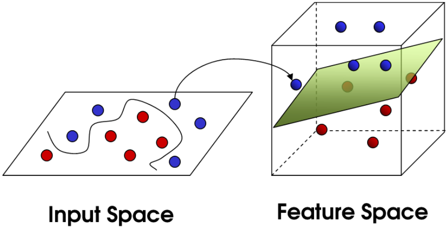
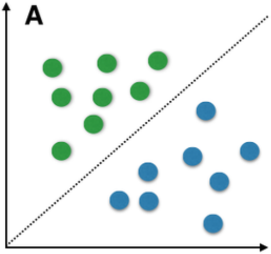




Example-1: continued – linear separability

Idealized situation



Decision surface:

$$\{\mathbf{x} : \langle \mathbf{w}, \mathbf{x} \rangle = 0\}$$

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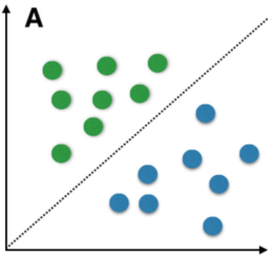

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classes:

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Example-1: continued – non-linear separability

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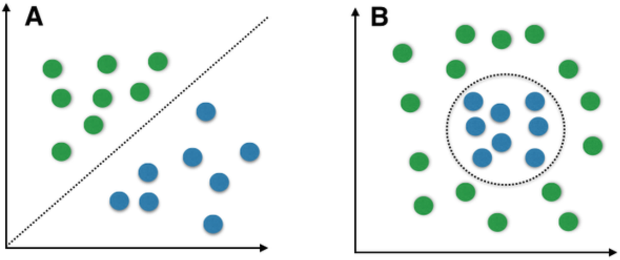
Real world



Decision surface (left):

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Example-1: non-linear separability – continued

On the ellipse

$$\left\{ \mathbf{x} : \frac{(x_1 - c_1)^2}{a^2} + \frac{(x_2 - c_2)^2}{b^2} = 1 \right\}$$

Example-1: non-linear separability – continued

On the ellipse, outside

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With polynomial feature: $\boxed{\varphi(\mathbf{x}) = (x_1^2, x_1, 1, x_2^2, x_2)}$:

- Decision surface: $\{\mathbf{x} : \langle \mathbf{w}, \varphi(\mathbf{x}) \rangle = 0\}$.

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Example-1: quadratic & polynomial features

Still in $\mathbb{R}^2$:

$$\varphi(\mathbf{x}) = \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right),$$

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$\langle \mathbf{x}, \mathbf{x}' \rangle^d = \langle \varphi(\mathbf{x}), \varphi(\mathbf{x}') \rangle$: $\varphi(\mathbf{x}) =$ d-order polynomial. $\Rightarrow$

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$\langle\mathbf{x}, \mathbf{x}'\rangle^d = \langle\varphi(\mathbf{x}), \varphi(\mathbf{x}')\rangle$: $\varphi(\mathbf{x}) =$ d-order polynomial. $\Rightarrow$ Explicit computation would be heavy!

Example-2: characterizing distributions / independence

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- Goal: to measure the dependence of X and Y.
- Desiderata for a $Q(\mathbb{P}_{XY})$ independence measure [Rényi, 1959]:

  1. $Q(\mathbb{P}_{XY})$ is well-defined,
  2. $Q(\mathbb{P}_{XY}) \in [0, 1]$,
  3. $Q(\mathbb{P}_{XY}) = 0$ iff. $X \perp Y$.
  4. $Q(\mathbb{P}_{XY}) = 1$ iff. $Y = f(X)$ or $X = g(Y)$.

Example-2: continued

- He showed:

$$Q(\mathbb{P}_{XY}) = \sup_{f,g:\ \text{measurable}} \operatorname{corr}(f(X), g(Y)),$$

  satisfies 1-4.
- Too ambitious:
  - computationally intractable.
  - many measurable functions.

Example-2: continued; measurable $\rightarrow$ continuous

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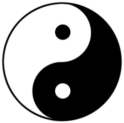
Key: balance

denseness $\rightarrow$ universality, computation $\rightarrow$ RKHS.



Motivation: kernels = generalized inner product

1. Various data types.
2. RKHS: flexible ($\overset{1:1}{\longleftrightarrow}$ probability measures).
3. Still computationally tractable: enough $k(x_i, x_j) \in \mathbb{R}$.
4. RKHS: Hilbert $\Rightarrow$ statistical analysis.
5. v-RKHS $[k(x, x') \in \mathcal{L}(Y)]$: dependency among output coordinates.

Kernel, RKHS: definition, kernel factory

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- Def-2 (reproducing kernel):

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Kernel, RKHS: generalized inner product, -linear methods

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- All these definitions are equivalent, $k \overset{1:1}{\leftrightarrow} \mathcal{H}_k$.
- Examples on $\mathbb{R}^d$ ($\gamma > 0$, $p \in \mathbb{Z}^+$): $k_p(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + \gamma)^p$, $k_G(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2^2}$, $k_e(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2}$.

Some kernel-enriched domains: $(\mathcal{X}, k)$

- Strings [Watkins, 1999, Lodhi et al., 2002, Leslie et al., 2002, Kuang et al., 2004, Leslie and Kuang, 2004, Saigo et al., 2004, Cuturi and Vert, 2005],
- time series [Rüping, 2001, Cuturi et al., 2007, Cuturi, 2011, Király and Oberhauser, 2019],
- trees [Collins and Duffy, 2001, Kashima and Koyanagi, 2002],
- groups and specifically rankings [Cuturi et al., 2005, Jiao and Vert, 2016],
- sets [Haussler, 1999, Gärtner et al., 2002, Balanca and Herbin, 2012, Fellmann et al., 2023], probability distributions [Berlinet and Thomas-Agnan, 2004, Hein and Bousquet, 2005, Smola et al., 2007, Sriperumbudur et al., 2010a],
- various generative models [Jaakkola and Haussler, 1999, Tsuda et al., 2002, Seeger, 2002, Jebara et al., 2004],
- fuzzy domains [Guevara et al., 2017], or
- graphs [Kondor and Lafferty, 2002, Gärtner et al., 2003, Kashima et al., 2003, Borgwardt and Kriegel, 2005, Shervashidze et al., 2009, Vishwanathan et al., 2010, Kondor and Pan, 2016, Bai et al., 2020, Borgwardt et al., 2020, Schulz et al., 2022, Nikolentzos and Vazirgiannis, 2023].

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  2. Cone. If $k_m : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ kernel, $\alpha_m \geq 0$ ($m = 1,\ldots,M$), then

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Example: $\oplus_{m=1}^{M} \mathbb{R} = \mathbb{R}^M$.

Kernel factory – continued

4. Product. If $(k_m)_{m=1}^{M}$ are kernels on $\mathcal{X}_m$, then

$$\left(\otimes_{m=1}^{M} k_m\right)\left(\left(x_1,\ldots,x_M\right),\left(x_1',\ldots,x_M'\right)\right) = \prod_{m=1}^{M} k_m\left(x_m, x_m'\right).$$

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- Thus, $(k_m)_{m=1}^M : \mathcal{X}\times\mathcal{X}\to\mathbb{R}$ kernels $\Rightarrow \prod_{m=1}^M k_m(x,x')$: kernel on $\mathcal{X}$.
- Consequence ($\gamma \geq 0$, $p\in\mathbb{Z}^+$):

$$k(\mathbf{x},\mathbf{y}) = \left(\langle\mathbf{x},\mathbf{y}\rangle_2 + \gamma\right)^p$$

is a kernel.

Kernel factory: product indeed

Let $M = 2$ and assume that $\varphi_m(x) \in \mathbb{R}^{d_m}$:

$$(k_1 \otimes k_2)\left((x, y), (x', y')\right) = k_1(x, x')k_2(y, y')$$

Kernel factory: product indeed

Let $M = 2$ and assume that $\varphi_m(x) \in \mathbb{R}^{d_m}$:

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&= \varphi_1(x)^\top \varphi_1(x') \varphi_2\left(y'\right)^\top \varphi_2(y)
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&= \operatorname{tr}\left(\varphi_2(y)\varphi_1(x)^\top \varphi_1(x')\varphi_2(y')^\top\right) \\
&= \left\langle \underbrace{\varphi_1(x)\varphi_2(y)^\top}_{\in \mathbb{R}^{d_1 \times d_2}}, \underbrace{\varphi_1(x')\varphi_2(y')^\top}_{\in \mathbb{R}^{d_1 \times d_2}} \right\rangle_{\mathsf{F}},
\end{aligned}
$$

where $\langle \mathbf{A}, \mathbf{B}\rangle_{\mathsf{F}} = \operatorname{tr}\left(\mathbf{A}^\top \mathbf{B}\right) = \sqrt{\sum_{ij} A_{ij}B_{ij}}$ is the Frobenius inner product.

Kernel factory

6. Limit. If $(k_n)_{n\in\mathbb{N}}$ are kernels on $\mathcal{X}$, then

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$$k(\mathbf{x},\mathbf{y}) = e^{\gamma\langle \mathbf{x},\mathbf{y}\rangle_2} = \sum_{n\in\mathbb{N}} \frac{\left(\gamma\left\langle \mathbf{x},\mathbf{y}\right\rangle_2\right)^n}{n!}$$

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Reason: polynomial kernel & limit rule.

7. Pre-post multiplication. k kernel on $\mathcal{X}$, $f : \mathcal{X} \to \mathbb{R}$, then

$$\tilde{k}(x, y) = f(x)k(x, y)f(y)$$

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Example (Gaussian kernel, $\gamma > 0$): previous example & new rule

$$k(\mathbf{x},\mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|_2^2}$$

by using $\|\mathbf{x}-\mathbf{y}\|_2^2 = \|\mathbf{x}\|_2^2 + \|\mathbf{y}\|_2^2 - 2\langle\mathbf{x},\mathbf{y}\rangle$.

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$$k(\mathbf{x},\mathbf{y}) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|_2^2} = e^{-\gamma\|\mathbf{x}\|_2^2} e^{2\gamma\langle \mathbf{x},\mathbf{y}\rangle_2} e^{-\gamma\|\mathbf{y}\|_2^2}$$

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Properties of $\mathcal{H}_k$, computational tractability

Properties of k control that of $\mathcal{H}_k$

[Steinwart and Christmann, 2008, Chapter 4]:

- k: bounded $[\sup_{x,y\in\mathcal{X}} k(x,y) \le C] \Rightarrow \forall f \in \mathcal{H}_k$ is bounded

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- k: analytic $\Rightarrow \forall f \in \mathcal{H}_k$ is analytic.

Representer theorem [Schölkopf et al., 2001, Yu et al., 2013]

- Given: $\{(x_i, y_i)\}_{i=1}^n$, say classification/regression.
- Goal:

$$J(f) = V(x_1, y_1, f(x_1), \ldots, x_n, y_n, f(x_n)) + r\left(\|f\|^2_{\mathcal{H}_k}\right) \to \min_{f \in \mathcal{H}_k},$$

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- Example:

$$V(\ldots) = \frac{1}{n}\sum_{i=1}^{n} \max(1 - y_i f(x_i), 0) \quad \text{(soft classification)},$$

$$V(\ldots) = \frac{1}{n}\sum_{i=1}^{n} [f(x_i) - y_i]^2 \quad \text{(regression)}.$$

Representer theorem – continued

...then

- $\boxed{\exists \text{ solution}}$ in the form:

$$\boxed{f^* = \sum_{i=1}^{n} \alpha_i k(\cdot, x_i)}, \quad \alpha_i \in \mathbb{R}.$$

- r: strictly increasing $\Rightarrow$ $\forall$ solution is of this form.
- Example: $r(z) = \lambda z$, $\lambda > 0$.

Representer theorem – proof

Objective

$$J(f) = V(x_1, y_1, f(x_1), \dots, x_n, y_n, f(x_n)) + r\left(\|f\|_{\mathcal{H}_k}^2\right) \to \min_{f \in \mathcal{H}_k}.$$

Decompose & Pythagorean theorem:

$$\begin{aligned} S &= \operatorname{span}\left(k(\cdot, x_i) \,:\, i \in [n]\right), \\ f &= f_S + f_\perp, \\ \|f\|_{\mathcal{H}_k}^2 &= \|f_S\|_{\mathcal{H}_k}^2 + \underbrace{\|f_\perp\|_{\mathcal{H}_k}^2}_{\geq 0} \geq \|f_S\|_{\mathcal{H}_k}^2. \end{aligned}$$

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In J

- 1st term: depends on f_S only, $f(x_i) = \langle f, k(\cdot, x_i)\rangle_{\mathcal{H}_k}$.

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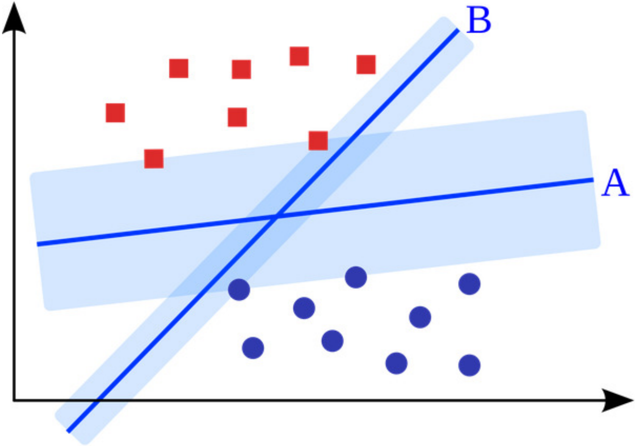
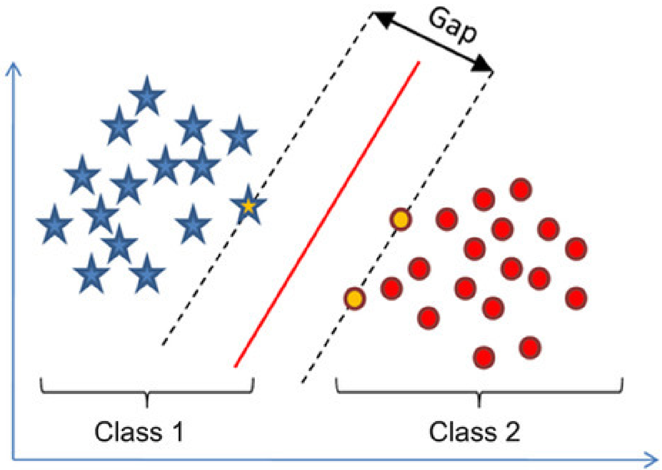
- 1st term: depends on f_S only, $f(x_i) = \langle f, k(\cdot, x_i)\rangle_{\mathcal{H}_k}$.
- 2nd term: can only decrease by neglecting $f_\perp$ ($r \nearrow$).

Classification: SVMC

Which separating line is the 'best'?



Answer / intuition: the one with the largest margin.



SVM formulation: hard classification

- Hyperplane: $f_{\mathbf{w},b}(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b$,
  - $\mathbf{w}$: normal vector, b: offset.

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- Shortly,

$$\min_{\mathbf{w},b} \|\mathbf{w}\|_2^2, \text{ s.t. } y_i \left(\langle \mathbf{w}, \mathbf{x}_i \rangle + b \right) \geq 1, \forall i.$$

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- Decision: $\hat{y}(\mathbf{x}) = \text{sign}\left(\langle \mathbf{w}, \mathbf{x} \rangle + b \right)$.

SVM formulation: soft classification

- Hard classification objective:

$$\min_{\mathbf{w},b} \|\mathbf{w}\|_2^2 \;\; \text{s.t.} \;\; y_i \left(\langle \mathbf{w}, \mathbf{x}_i \rangle + b \right) \geq 1, \forall i.$$

There might not be solution! (non-linearly separable case)

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  There might not be solution! (non-linearly separable case)

- Soft classification objective ($C > 0$):

$$\min_{\mathbf{w},b,\boldsymbol{\xi}} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^n \xi_i \;\text{ s.t. }\; y_i\left(\langle \mathbf{w}, \mathbf{x}_i\rangle + b\right) \geq 1 - \xi_i,\; \xi_i \geq 0,\; \forall i.$$

  Linear penalty on misclassification.

Note on the soft objective of SVMC

$$\min_{\mathbf{w},b,\xi} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n} \xi_i \text{ s.t. } y_i\left(\langle \mathbf{w}, \mathbf{x}_i\rangle + b\right) \geq 1 - \xi_i,\ \xi_i \geq 0,\ \forall i$$

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$$, \min_{\mathbf{w},b,\boldsymbol{\xi}} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n}\underbrace{\max\Big(1 - y_i(\underbrace{\langle \mathbf{w}, \mathbf{x}_i\rangle + b}_{=f(\mathbf{x}_i)}), 0\Big)}_{=:h(y_i f(\mathbf{x}_i))},$$

where $h(u) = \max(1-u, 0)$ is the hinge loss.

Note on the soft objective of SVMC – continued

The hinge loss is the **convex envelope of the zero-one loss**:

$$z(u) = \mathbb{I}_{\{u<0\}}, \qquad u = y_i f(x_i),$$
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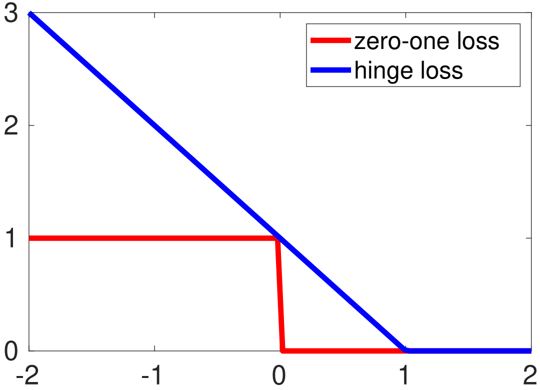

Soft classification objective:

$$\min_{\mathbf{w},b,\boldsymbol{\xi}} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n}\xi_i, \text{ s.t. } y_i\left(\langle \mathbf{w}, \mathbf{x}_i\rangle + b\right) \geq 1 - \xi_i,\ \xi_i \geq 0 \quad (\forall i).$$

Lagrangian function: with $\alpha_i \geq 0, \beta_i \geq 0$ $(\forall i)$

$L(\mathbf{w}, b, \boldsymbol{\xi}; \boldsymbol{\alpha}, \boldsymbol{\beta})$ = objective - Lagrangian multipliers $\times$ conditions

$$= \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i\left[y_i\left(\langle \mathbf{w}, \mathbf{x}_i\rangle + b\right) - 1 + \xi_i\right] - \sum_{i=1}^{n}\beta_i\xi_i.$$

Solving for $\frac{\partial L}{\partial \text{primal}} = 0$, we get ...

SVM formulation: soft classification

$$L(\mathbf{w}, b, \boldsymbol{\xi}; \boldsymbol{\alpha}, \boldsymbol{\beta}) =$$
$$= \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\alpha_i\left[y_i\left(\langle \mathbf{w}, \mathbf{x}_i\rangle + b\right) - 1 + \xi_i\right] - \sum_{i=1}^{n}\beta_i\xi_i.$$

Optimality equations:

$$\mathbf{0} = \frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i \quad (\mathbf{w} \leftrightarrow \boldsymbol{\alpha}),$$
$$0 = \frac{\partial L}{\partial b} = \sum_{i=1}^{n}\alpha_i y_i,$$
$$0 = \frac{\partial L}{\partial \xi_i} = C - \alpha_i - \beta_i.$$

Plugging these equations back to L, we have ...

SVM formulation: soft classification

Dual form:

$$\max_{\boldsymbol{\alpha}} \underbrace{\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle}_{\text{quadratic in } \boldsymbol{\alpha}}, \text{ s.t. } \underbrace{0 \leq \alpha_i \leq C, \sum_{i=1}^{n} \alpha_i y_i = 0}_{\text{linear in } \boldsymbol{\alpha}}.$$

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$$\max_{\boldsymbol{\alpha}} \underbrace{\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle}_{\text{quadratic in } \boldsymbol{\alpha}}, \text{ s.t. } \underbrace{0 \le \alpha_i \le C, \sum_{i=1}^{n} \alpha_i y_i = 0}_{\text{linear in } \boldsymbol{\alpha}}.$$

- $b \Leftarrow y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) = 1 \Leftarrow \alpha_i > 0$ [complementary slackness].

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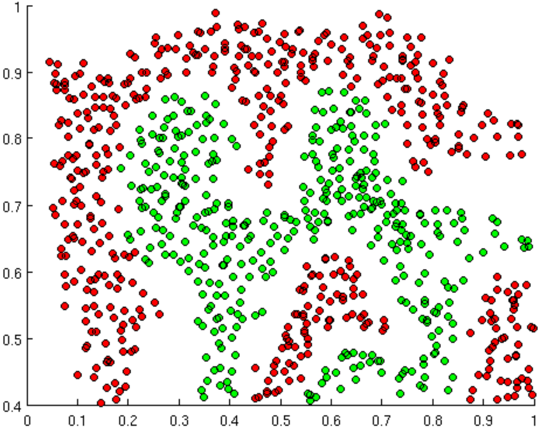
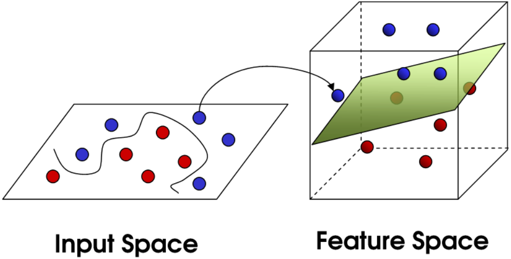
- Now:



If linear separability does not hold: kernel trick



Nonlinear SVM

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- Nonlinear SVM (primal):

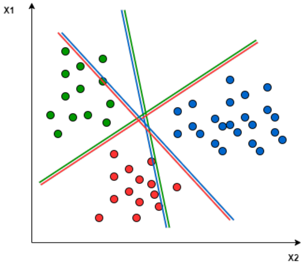
$$\min_{f \in \mathcal{H}_k, \boldsymbol{\xi}} \frac{1}{2} \|f\|_{\mathcal{H}_k}^2 + C \sum_{i=1}^{n} \xi_i, \text{ s.t. } y_i f(x_i) \ge 1 - \xi_i,\ \xi_i \ge 0,\ \forall i.$$

Multiclass (say M) classification with SVM

Idea

Break down the problem to multiple binary classification problems.

1. one-to-one approach:
   - $\frac{M(M-1)}{2}$ SVMC-s, i vs. j ($i \neq j$),
   - on new input x: the class with the most votes is predicted.



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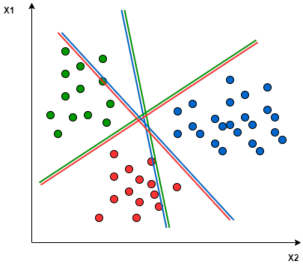
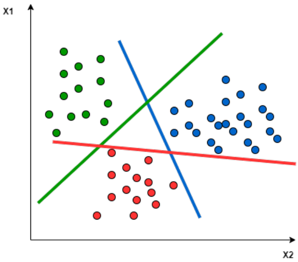
2. one-to-rest approach:
   - M SVMC-s, each predicts one class.
   - Classifiers give real-valued confidence scores: $f_m(x)$, $m \in [M]$.
   - Decision: $\hat{m} = \arg\max_{m \in [M]} f_m(x)$.





Parameter selection $\rightarrow$ cost: C, kernel parameter: σ

M-fold cross-validation $[\theta := (C, \sigma)]$:

1. Split data:
   - training set $(X_{\text{tr}}, Y_{\text{tr}})$: $X_{\text{val},m}$, $Y_{\text{val},m}$, $m \in [M]$.
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4. Report: performance of θ^* on X_{te}, Y_{te}.

Regression: kernel ridge regression

Kernel ridge regression (KRR)

- Given: $\{(x_i, y_i)\}_{i=1}^n$, $\mathcal{H} := \mathcal{H}_k$, $y_i \in \mathbb{R}$.
- Task ($\lambda > 0$):

$$J(f) = \frac{1}{n}\sum_{i=1}^n [y_i - f(x_i)]^2 + \lambda \|f\|_{\mathcal{H}}^2 \to \min_{f \in \mathcal{H}}.$$

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- Analytical solution:

$$f(x) = [k(x_1, x), \ldots, k(x_n, x)]\,(\mathbf{G} + \lambda n \mathbf{I}_n)^{-1}[y_1; \ldots; y_n],$$
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Question

How do we get this solution?

Kernel ridge regression

By the representer theorem

$$f = \sum_{i=1}^{n} a_i k(\cdot, x_i), \quad (a_i \in \mathbb{R}).$$

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Multiplying the objective by n, using the reproducing property:

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\tilde{J}(f) &= \sum_{j=1}^{n} [y_j - \langle f, k(\cdot, x_j) \rangle_{\mathcal{H}}]^2 + \lambda n \|f\|_{\mathcal{H}}^2 \\
&= \|\mathbf{y} - \mathbf{G}\mathbf{a}\|_2^2 + (\lambda n)\mathbf{a}^\top \mathbf{G}\mathbf{a} \\
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$$\frac{\partial \mathbf{a}^\top \mathbf{B}\mathbf{a}}{\partial \mathbf{a}} = \left(\mathbf{B} + \mathbf{B}^\top\right)\mathbf{a}, \quad \frac{\partial \mathbf{c}^\top \mathbf{a}}{\partial \mathbf{a}} = \mathbf{c}.$$

Kernel machines: a simple algorithm = SGD [Kivinen et al., 2004]

Empirical regularized risk:

$$\min_{f\in\mathcal{H}_k} J(f) = \frac{1}{n}\sum_{i=1}^{n}\ell(f(x_i), y_i) + \frac{\lambda}{2}\|f\|^2_{\mathcal{H}_k} \quad (\lambda > 0).$$

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Update (learning rate: $\eta_t > 0$):

$$f_{t+1} = f_t - \eta_t \underbrace{\left.\frac{\partial J_{\text{inst}}(f, (x_t, y_t))}{\partial f}\right|_{f = f_t}}_{\left.\frac{\partial \ell(z,y)}{\partial z}\right|_{z = f_t(x_t), y = y_t} k(\cdot, x_t) + \lambda f_t} .$$

Note: if ℓ is non-differentiable, subgradient is taken.

SGD implementation

1. Initialization: $f_1 = 0$.
2. By the representer theorem:

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4. $\Leftrightarrow$ Update (in terms of coefficients): For $i \in [t]$,

$$\alpha_i := \begin{cases} -\eta_t \ell'(f_t(x_t), y_t) & \text{if } i = t, \\ (1 - \eta_t \lambda) \alpha_i & \text{if } i < t. \end{cases}$$

Optimizers+

1. Recall the dual problem:

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2. For KRR:
   - scaling to billions of points [Meanti et al., 2020],
   - idea: Nyström method + pre-conditioned conjugate gradient solver + GPU.
3. For large-scale classification (+recent survey), see [Tanji et al., 2023]:
   - Nyström technique + accelerated stochastic subgradient descent.

Maximal correlation: KCCA

KCCA: definition

- Given: $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$.
- Associated:
  - feature maps $\varphi(x) = k(\cdot, x)$, $\psi(y) = \ell(\cdot, y)$,
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- KCCA measure of $(X, Y) \in \mathcal{X} \times \mathcal{Y}$

$$\rho_{\mathsf{KCCA}}(X, Y; \mathcal{H}_k, \mathcal{H}_\ell) = \sup_{f \in \mathcal{H}_k, g \in \mathcal{H}_\ell} \mathrm{corr}(f(X), g(Y)),$$

$$\mathrm{corr}(f(X), g(Y)) = \frac{\mathrm{cov}(f(X), g(Y))}{\sqrt{\mathrm{var}[f(X)]\, \mathrm{var}[g(Y)]}}.$$

KCCA: notes

- Optimization domain: $\mathcal{H}_k \times \mathcal{H}_\ell \ni (f, g)$.
- By reproducing property: we will get a finite-D task.
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Recall the reproducing property

$$f(x) = \langle f, k(\cdot, x)\rangle_{\mathcal{H}_k} \quad \forall f \in \mathcal{H}_k, x \in \mathcal{X}.$$

KCCA: empirical estimate

$$\widehat{\mathrm{cov}}(f(X), g(Y)) = \frac{1}{N}\sum_{n=1}^{N} \underbrace{\left[f(x_n) - \frac{1}{N}\sum_{i=1}^{N} f(x_i) \right]}_{\left\langle f, \varphi(x_n) - \frac{1}{N}\sum_{i=1}^{N}\varphi(x_i) \right\rangle_{\mathcal{H}_k}} \underbrace{\left[g(y_n) - \frac{1}{N}\sum_{i=1}^{N} g(y_i) \right]}_{\left\langle g, \psi(y_n) - \frac{1}{N}\sum_{i=1}^{N}\psi(y_i) \right\rangle_{\mathcal{H}_\ell}}$$

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Similarly:

$$\widehat{\mathrm{var}}[f(X)] = \frac{1}{N}\sum_{n=1}^{N} \left[f(x_n) - \frac{1}{N}\sum_{i=1}^{N} f(x_i) \right]^2$$

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- f: appears only as $\langle f, \tilde{\varphi}(x_n) \rangle_{\mathcal{H}_k}$ [similarly: g in $\langle g, \tilde{\psi}(y_n) \rangle_{\mathcal{H}_\ell}$]. $\Rightarrow$

KCCA: empirical estimate

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- $\forall$ component of f $\perp$

$$\mathrm{span}\left(\{\tilde{\varphi}(x_n)\}_{n=1}^N\right) = \left\{\sum_{n=1}^N c_n \tilde{\varphi}(x_n), \mathbf{c} = [c_n] \in \mathbb{R}^N\right\}$$

has no affect in the objective.

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has no affect in the objective.

Key idea

Enough to consider $f = \sum_{i=1}^N c_i \tilde{\varphi}(x_i)$, $g = \sum_{i=1}^N d_i \tilde{\psi}(y_i)$.

KCCA: empirical estimate

Using that $f = \sum_{i=1}^{N} c_i \tilde{\varphi}(x_i)$, $g = \sum_{i=1}^{N} d_i \tilde{\psi}(y_i)$:

$$\langle f, \tilde{\varphi}(x_n) \rangle_{\mathcal{H}_k} = \sum_{i=1}^{N} c_i \langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_n) \rangle_{\mathcal{H}_k}$$

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$$\langle g, \tilde{\psi}(y_n)\rangle_{\mathcal{H}_\ell} = (\mathbf{d}^\top \tilde{\mathbf{G}}_Y)_n,$$

with the centered kernels ($\tilde{k}$, $\tilde{\ell}$) and Gram matrices ($\tilde{\mathbf{G}}_X$, $\tilde{\mathbf{G}}_Y$).

Until now

All the objective terms can be expressed by $\mathbf{c}$, $\mathbf{d}$, $\tilde{\mathbf{G}}_X$, $\tilde{\mathbf{G}}_Y$.

KCCA: empirical estimate

$$\widehat{\mathrm{cov}}(f(X), g(Y)) = \frac{1}{N}\sum_{n=1}^{N} \langle f, \tilde{\varphi}(x_n)\rangle_{\mathcal{H}_k} \langle g, \tilde{\psi}(y_n)\rangle_{\mathcal{H}_\ell},$$

$$\widehat{\mathrm{var}}[f(X)] = \frac{1}{N}\sum_{n=1}^{N} \langle f, \tilde{\varphi}(x_n)\rangle^2_{\mathcal{H}_k}, \widehat{\mathrm{var}}[g(Y)] = \frac{1}{N}\sum_{n=1}^{N} \langle g, \tilde{\psi}(y_n)\rangle^2_{\mathcal{H}_\ell},$$

and we have

$$\langle f, \tilde{\varphi}(x_n)\rangle_{\mathcal{H}_k} = (\mathbf{c}^\top \tilde{\mathbf{G}}_X)_n, \qquad \langle g, \tilde{\psi}(y_n)\rangle_{\mathcal{H}_\ell} = (\mathbf{d}^\top \tilde{\mathbf{G}}_Y)_n.$$

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Thus,

$$\widehat{\mathrm{cov}}(f(X), g(Y)) = \frac{1}{N} \mathbf{c}^\top \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \mathbf{d},$$

$$\widehat{\mathrm{var}}[f(X)] = \frac{1}{N} \mathbf{c}^\top (\tilde{\mathbf{G}}_X)^2 \mathbf{c}, \quad \widehat{\mathrm{var}}[g(Y)] = \frac{1}{N} \mathbf{d}^\top (\tilde{\mathbf{G}}_Y)^2 \mathbf{d}.$$

KCCA: finite-D form

Empirical estimate of KCCA:

$$\widehat{\rho_{\text{KCCA}}}^{\text{temp}}(X, Y; \mathcal{H}_k, \mathcal{H}_\ell) = \sup_{\mathbf{c}\in\mathbb{R}^N, \mathbf{d}\in\mathbb{R}^N} \frac{\mathbf{c}^\top \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \mathbf{d}}{\sqrt{\mathbf{c}^\top (\tilde{\mathbf{G}}_X)^2 \mathbf{c}}\sqrt{\mathbf{d}^\top (\tilde{\mathbf{G}}_Y)^2 \mathbf{d}}}.$$

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In practice ($\kappa > 0$):

$$\begin{aligned}\widehat{\rho_{\mathrm{KCCA}}}(X, Y) &:= \widehat{\rho_{\mathrm{KCCA}}}(X, Y; \mathcal{H}_k, \mathcal{H}_\ell, \kappa) \\ &= \sup_{\mathbf{c}\in\mathbb{R}^N, \mathbf{d}\in\mathbb{R}^N} \frac{\mathbf{c}^\top \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \mathbf{d}}{\sqrt{\mathbf{c}^\top \left(\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N\right)^2 \mathbf{c}}\sqrt{\mathbf{d}^\top \left(\tilde{\mathbf{G}}_Y + \kappa \mathbf{I}_N\right)^2 \mathbf{d}}}.\end{aligned}$$

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Question

How do we solve it?

KCCA: solution

Stationary points of $\widehat{\rho_{\mathrm{KCCA}}}(X, Y)$:

$$\mathbf{0} = \frac{\partial \widehat{\rho_{\mathrm{KCCA}}}(X, Y)}{\partial \mathbf{c}}, \qquad \mathbf{0} = \frac{\partial \widehat{\rho_{\mathrm{KCCA}}}(X, Y)}{\partial \mathbf{d}},$$

which simplifies to

$$\tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \mathbf{d} = \frac{(\mathbf{c}^\top \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \mathbf{d})(\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N)^2 \mathbf{c}}{\mathbf{c}^\top (\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N)^2 \mathbf{c}}, \quad \tilde{\mathbf{G}}_Y \tilde{\mathbf{G}}_X \mathbf{c} = \frac{(\mathbf{d}^\top \tilde{\mathbf{G}}_Y \tilde{\mathbf{G}}_X \mathbf{c})(\tilde{\mathbf{G}}_Y + \kappa \mathbf{I}_N)^2 \mathbf{d}}{\mathbf{d}^\top (\tilde{\mathbf{G}}_Y + \kappa \mathbf{I}_N)^2 \mathbf{d}}$$

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Normalization:

- $(\mathbf{c}, \mathbf{d})$: solution $\Rightarrow$ $(a\mathbf{c}, b\mathbf{d})$: solution $a, b \in \mathbb{R} \backslash \{0\}$.
- denominators $:= 1$.

KCCA: final task

Find the maximal eigenvalue, $\lambda := \mathbf{c}^\top \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \mathbf{d}$, of the generalized eigenvalue problem:

$$\begin{bmatrix} \mathbf{0} & \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \\ \tilde{\mathbf{G}}_Y \tilde{\mathbf{G}}_X & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \mathbf{c}^\top \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \mathbf{d} \begin{bmatrix} (\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_Y + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

$$\mathbf{A}\mathbf{z} = \lambda \mathbf{B}\mathbf{z}.$$

Note: Python implementation in the ITE toolbox ($M \geq 2$, with acceleration).

Summary

- Kernel, RKHS: generalized inner product, - linear methods.
- Computational tractability: representer theorem.
- Classification: SVMC.
- Regression: kernel ridge regression.
- Maximal correlation: KCCA.

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- Classification: SVMC.
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Contents (KCCA: questions)

1. Is KCCA an independence measure? $(\Leftarrow$ universality$)$
2. Meaning/handling of the regularization (κ).
3. $M \geq 2$ components.
4. Computation of $\tilde{\mathbf{G}}_X$, $\tilde{\mathbf{G}}_Y$.

Q1 (independence measure) $\Leftarrow$ universal k, ℓ

If $X \perp Y$, then $\rho_{\text{KCCA}}(X, Y; \mathcal{H}_k, \mathcal{H}_\ell, \kappa) = 0$. Opposite direction:

- For 'rich' $\mathcal{H}_k$, $\mathcal{H}_\ell$
  [Bach and Jordan, 2002, Gretton et al., 2005].

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- Enough: universal kernel on a compact metric domain.
- Example ($\gamma > 0$):
  - Gaussian: $k(\mathbf{x}, \mathbf{x}') = e^{-\gamma \|\mathbf{x}-\mathbf{x}'\|_2^2}$.
  - Laplacian kernel: $k(\mathbf{x}, \mathbf{x}') = e^{-\gamma \|\mathbf{x}-\mathbf{x}'\|_2}$.

Q1: universal kernel, $C(\mathcal{X}) = \{f : \mathcal{X} \to \mathbb{R} \text{ continuous}\}$

Definition

Assume:

- $\mathcal{X}$: compact metric space.
- k: continuous kernel on $\mathcal{X}$.

k is called *(c)-universal* [Steinwart, 2001] if $\mathcal{H}_k$ is dense in $(C(\mathcal{X}), \|\cdot\|_\infty)$.

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Assumptions

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- k: continuous, bounded $\Rightarrow \mathcal{H}_k \subset C(\mathcal{X})$ [Steinwart and Christmann, 2008].
- Extensions of c-universality to non-compact spaces:
  - c_0-universality, cc-universality, ... [Carmeli et al., 2010, Sriperumbudur et al., 2010b, Simon-Gabriel and Schölkopf, 2018].

Q1: properties of universal kernels [Steinwart, 2001, Steinwart and Christmann, 2008]

If k is universal, then

- $k(x, x) > 0$ for all $x \in \mathcal{X}$.

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  is a metric.
- The normalized kernel (recall: corr)

  $$\tilde{k}(x,y) := \frac{k(x,y)}{\sqrt{k(x,x)k(y,y)}}$$

  is universal.

Q1: universal Taylor kernels [Steinwart, 2001, Steinwart and Christmann, 2008]

- For an $C^\infty \ni f : (-r, r) \to \mathbb{R}$

$$f(t) = \sum_{n=0}^{\infty} a_n t^n \quad t \in (-r, r), \; r \in (0, \infty].$$

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$$f(t) = \sum_{n=0}^{\infty} a_n t^n \quad t \in (-r, r),\ r \in (0, \infty].$$

- If $a_n > 0\ \forall n$, then

$$k(\mathbf{x}, \mathbf{y}) = f(\langle \mathbf{x}, \mathbf{y} \rangle)$$

is universal on $\mathcal{X} := \left\{ \mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\|_2 \leq \sqrt{r} \right\}$.

Q1: universal kernels on compact subsets of $\mathbb{R}^d$, $\alpha > 0$

- $k(\mathbf{x}, \mathbf{y}) = e^{\alpha \langle \mathbf{x}, \mathbf{y} \rangle}$: previous result with $f(t) = e^{\alpha t} \Rightarrow a_n = \frac{\alpha^n}{n!}$.

Q1: universal kernels on compact subsets of $\mathbb{R}^d$, $\alpha > 0$

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- $k(\mathbf{x}, \mathbf{y}) = e^{-\alpha \|\mathbf{x} - \mathbf{y}\|_2^2}$: exp. kernel & normalization.

Q1: universal kernels on compact subsets of $\mathbb{R}^d$, $\alpha > 0$

- $k(\mathbf{x}, \mathbf{y}) = (1 - \langle \mathbf{x}, \mathbf{y} \rangle)^{-\alpha}$ binomial kernel
    - on $\mathcal{X}$ compact $\subset \{\mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\|_2 < 1\}$.
    - $f(t) = (1 - t)^{-\alpha} = \sum_{n=0}^{\infty} \underbrace{\binom{-\alpha}{n} (-1)^n}_{>0} t^n \quad (|t| < 1)$,

where $\binom{b}{n} = \sum_{i=1}^{n} \frac{b-i+1}{i}$.

Contents

Q2 (κ)

In fact, we estimated

$$\rho_{\mathrm{KCCA}}(X, Y; \mathcal{H}_k, \mathcal{H}_\ell, \kappa) = \sup_{f \in \mathcal{H}_k, g \in \mathcal{H}_\ell} \mathrm{corr}(f(X), g(Y); \kappa),$$

$$\mathrm{corr}(f(X), g(Y); \kappa) = \frac{\mathrm{cov}(f(X), g(Y))}{\sqrt{\mathrm{var}[f(X)] + \kappa \|f\|^2_{\mathcal{H}_k}}\sqrt{\mathrm{var}[g(Y)] + \kappa \|g\|^2_{\mathcal{H}_\ell}}}.$$

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For consistent KCCA estimate:

- $\kappa_N \to 0$ [Leurgans et al., 1993](spline-RKHS), [Fukumizu et al., 2007] (general RKHS).
- analysis: covariance operators.

Contents

Q3 ($M \geq 2$): symmetry, other form

For

$$\begin{bmatrix} \mathbf{0} & \tilde{\mathbf{G}}_X\tilde{\mathbf{G}}_Y \\ \tilde{\mathbf{G}}_Y\tilde{\mathbf{G}}_X & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = \mathbf{c}^\top \tilde{\mathbf{G}}_X\tilde{\mathbf{G}}_Y \mathbf{d} \begin{bmatrix} (\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_Y + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

$([\mathbf{c}, \mathbf{d}], \lambda)$ solution $\Rightarrow$ $([-\mathbf{c}; \mathbf{d}], -\lambda)$: solution. Thus, eigenvalues:

$$\{\lambda_1, -\lambda_1, \ldots, \lambda_N, -\lambda_N\}.$$

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Adding the r.h.s. to both sides:

$$\begin{bmatrix} (\tilde{\mathbf{G}}_X + \kappa\mathbf{I}_N)^2 & \tilde{\mathbf{G}}_X\tilde{\mathbf{G}}_Y \\ \tilde{\mathbf{G}}_Y\tilde{\mathbf{G}}_X & (\tilde{\mathbf{G}}_\mathbf{Y} + \kappa\mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = (1+\lambda) \begin{bmatrix} (\tilde{\mathbf{G}}_X + \kappa\mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_X + \kappa\mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

with eigenvalues $\{1+\lambda_1, 1-\lambda_1, \ldots, 1+\lambda_N, 1-\lambda_N\}$.

Q3 $(M \geq 2)$

2-variables $[(X, Y)]$:

$$\begin{bmatrix} (\tilde{\mathbf{G}}_{\mathbf{X}} + \kappa \mathbf{I}_N)^2 & \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \\ \tilde{\mathbf{G}}_Y \tilde{\mathbf{G}}_X & (\tilde{\mathbf{G}}_{\mathbf{Y}} + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = (1 + \lambda) \begin{bmatrix} (\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

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$$\begin{bmatrix} (\tilde{\mathbf{G}}_{\mathbf{X}} + \kappa \mathbf{I}_N)^2 & \tilde{\mathbf{G}}_X \tilde{\mathbf{G}}_Y \\ \tilde{\mathbf{G}}_Y \tilde{\mathbf{G}}_X & (\tilde{\mathbf{G}}_{\mathbf{Y}} + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix} = (1+\lambda) \begin{bmatrix} (\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N)^2 & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_X + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \mathbf{d} \end{bmatrix}$$

For M-variables (pairwise dependence):

$$\begin{bmatrix} (\tilde{\mathbf{G}}_1 + \kappa \mathbf{I}_N)^2 & \tilde{\mathbf{G}}_1 \tilde{\mathbf{G}}_2 & \dots & \tilde{\mathbf{G}}_1 \tilde{\mathbf{G}}_M \\ \tilde{\mathbf{G}}_2 \tilde{\mathbf{G}}_1 & (\tilde{\mathbf{G}}_2 + \kappa \mathbf{I}_N)^2 & \dots & \tilde{\mathbf{G}}_2 \tilde{\mathbf{G}}_M \\ \vdots & \vdots & & \vdots \\ \tilde{\mathbf{G}}_M \tilde{\mathbf{G}}_1 & \tilde{\mathbf{G}}_M \tilde{\mathbf{G}}_2 & \dots & (\tilde{\mathbf{G}}_M + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \\ \vdots \\ \mathbf{c}_M \end{bmatrix} =$$

$$\gamma \begin{bmatrix} (\tilde{\mathbf{G}}_1 + \kappa \mathbf{I}_N)^2 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & (\tilde{\mathbf{G}}_2 + \kappa \mathbf{I}_N)^2 & \dots & \mathbf{0} \\ \vdots & \vdots & & \\ \mathbf{0} & \mathbf{0} & \dots & (\tilde{\mathbf{G}}_M + \kappa \mathbf{I}_N)^2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \\ \vdots \\ \mathbf{c}_M \end{bmatrix}.$$

Contents

Q4: Centered Gram matrix

In short

$\tilde{\mathbf{G}}_X = \mathbf{H}\mathbf{G}_X\mathbf{H}$ with $\mathbf{H} = \mathbf{I}_N - \frac{\mathbf{E}_N}{N}$; $\mathbf{H}; \mathbf{E}_N \in \mathbb{R}^{N \times N}$.

$$(\tilde{\mathbf{G}}_X)_{ij} = \tilde{k}(x_i, x_j) = \langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_j) \rangle_{\mathcal{H}_k}$$

Q4: Centered Gram matrix

In short

$\tilde{\mathbf{G}}_X = \mathbf{H}\mathbf{G}_X\mathbf{H}$ with $\mathbf{H} = \mathbf{I}_N - \frac{\mathbf{E}_N}{N}$; $\mathbf{H}; \mathbf{E}_N \in \mathbb{R}^{N \times N}$.

$$
\begin{aligned}
(\tilde{\mathbf{G}}_X)_{ij} &= \tilde{k}(x_i, x_j) = \langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_j) \rangle_{\mathcal{H}_k} \\
&= \langle \varphi(x_i) - \frac{1}{N} \sum_{n=1}^{N} \varphi(x_n), \varphi(x_j) - \frac{1}{N} \sum_{m=1}^{N} \varphi(x_m) \rangle_{\mathcal{H}_k}
\end{aligned}
$$

Q4: Centered Gram matrix

In short

$\tilde{\mathbf{G}}_X = \mathbf{H}\mathbf{G}_X\mathbf{H}$ with $\mathbf{H} = \mathbf{I}_N - \frac{\mathbf{E}_N}{N}$; $\mathbf{H}; \mathbf{E}_N \in \mathbb{R}^{N \times N}$.

$$
\begin{aligned}
(\tilde{\mathbf{G}}_X)_{ij} &= \tilde{k}(x_i, x_j) = \langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_j) \rangle_{\mathcal{H}_k} \\
&= \left\langle \varphi(x_i) - \frac{1}{N}\sum_{n=1}^{N} \varphi(x_n), \varphi(x_j) - \frac{1}{N}\sum_{m=1}^{N} \varphi(x_m) \right\rangle_{\mathcal{H}_k} \\
&= (\mathbf{G}_X)_{ij} - \frac{1}{N}\sum_{m=1}^{N}(\mathbf{G}_X)_{im} - \frac{1}{N}\sum_{n=1}^{N}(\mathbf{G}_X)_{nj} - \frac{1}{N^2}\sum_{n,m=1}^{N}(\mathbf{G}_X)_{nm}
\end{aligned}
$$

Q4: Centered Gram matrix

In short

$\tilde{\mathbf{G}}_X = \mathbf{H}\mathbf{G}_X\mathbf{H}$ with $\mathbf{H} = \mathbf{I}_N - \frac{\mathbf{E}_N}{N}$; $\mathbf{H}; \mathbf{E}_N \in \mathbb{R}^{N\times N}$.

$$
\begin{aligned}
(\tilde{\mathbf{G}}_X)_{ij} &= \tilde{k}(x_i, x_j) = \langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_j) \rangle_{\mathcal{H}_k} \\
&= \left\langle \varphi(x_i) - \frac{1}{N}\sum_{n=1}^{N} \varphi(x_n), \varphi(x_j) - \frac{1}{N}\sum_{m=1}^{N} \varphi(x_m) \right\rangle_{\mathcal{H}_k} \\
&= (\mathbf{G}_X)_{ij} - \frac{1}{N}\sum_{m=1}^{N}(\mathbf{G}_X)_{im} - \frac{1}{N}\sum_{n=1}^{N}(\mathbf{G}_X)_{nj} - \frac{1}{N^2}\sum_{n,m=1}^{N}(\mathbf{G}_X)_{nm} \\
&= \left(\mathbf{G}_X - \mathbf{G}_X\frac{\mathbf{E}_N}{N} - \frac{\mathbf{E}_N}{N}\mathbf{G}_X - \frac{\mathbf{E}_N}{N}\mathbf{G}_X\frac{\mathbf{E}_N}{N}\right)_{ij},
\end{aligned}
$$

Q4: Centered Gram matrix

In short

$\tilde{\mathbf{G}}_X = \mathbf{H}\mathbf{G}_X\mathbf{H}$ with $\mathbf{H} = \mathbf{I}_N - \frac{\mathbf{E}_N}{N}$; $\mathbf{H}; \mathbf{E}_N \in \mathbb{R}^{N\times N}$.

$$
\begin{aligned}
(\tilde{\mathbf{G}}_X)_{ij} &= \tilde{k}(x_i, x_j) = \langle \tilde{\varphi}(x_i), \tilde{\varphi}(x_j) \rangle_{\mathcal{H}_k} \\
&= \left\langle \varphi(x_i) - \frac{1}{N}\sum_{n=1}^{N} \varphi(x_n), \varphi(x_j) - \frac{1}{N}\sum_{m=1}^{N} \varphi(x_m) \right\rangle_{\mathcal{H}_k} \\
&= (\mathbf{G}_X)_{ij} - \frac{1}{N}\sum_{m=1}^{N} (\mathbf{G}_X)_{im} - \frac{1}{N}\sum_{n=1}^{N} (\mathbf{G}_X)_{nj} - \frac{1}{N^2}\sum_{n,m=1}^{N} (\mathbf{G}_X)_{nm} \\
&= \left(\mathbf{G}_X - \mathbf{G}_X \frac{\mathbf{E}_N}{N} - \frac{\mathbf{E}_N}{N}\mathbf{G}_X - \frac{\mathbf{E}_N}{N}\mathbf{G}_X\frac{\mathbf{E}_N}{N} \right)_{ij}, \\
&= (\mathbf{H}\mathbf{G}_X\mathbf{H})_{ij},
\end{aligned}
$$

$\mathbf{H}$: symmetric ($\mathbf{H} = \mathbf{H}^\top$), idempotent ($\mathbf{H}^2 = \mathbf{H}$). Contents

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