Support Fuzzy-Set Machines

From Kernels on Fuzzy Sets to Machine Learning Applications
Tutorial IEEE-FUZZ 2019

Jorge Guevara Díaz[1] Roberto Hirata Jr.[2] Stéphane Canu[3]

[1]IBM Research

[2]Institute of Mathematics and Statistics
University of Sao Paulo-Brazil

[3]Institut National de Sciences Appliquees
University of Normandy-France

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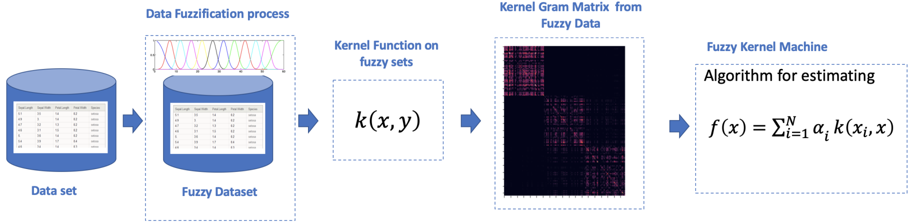
Outline

Outline

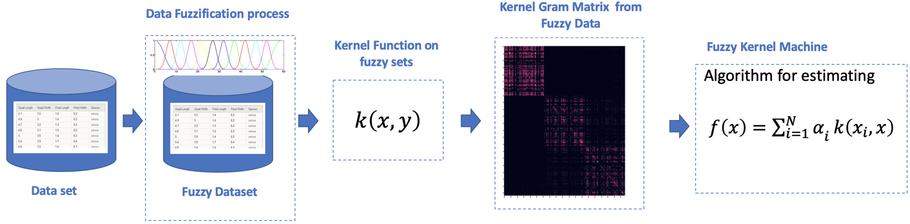
Overall picture

- how to use the kernel trick for constructing a fuzzy kernel machines



Overall picture

- In this tutorial we are going to construct a support fuzzy-set machine



Overall picture

- This novel approach differs from other *fuzzy support machines*, because we are not modifying the machine learning algorithm but using kernels on fuzzy sets.

All the following approaches modify the SVM algorithm in some sense, but not the kernel:

- Lin, Chun-Fu, and Sheng-De Wang. "Fuzzy support vector machines." IEEE transactions on neural networks 13.2 (2002): 464-471.
- Inoue, Takuya, and Shigeo Abe. "Fuzzy support vector machines for pattern classification." IJCNN'01. International Joint Conference on Neural Networks. Proceedings (Cat. No. 01CH37222). Vol. 2. IEEE, 2001.
- Wang, Yongqiao, Shouyang Wang, and Kin Keung Lai. "A new fuzzy support vector machine to evaluate credit risk." IEEE Transactions on Fuzzy Systems 13.6 (2005): 820-831.
- Abe, Shigeo, and Takuya Inoue. "Fuzzy support vector machines for multiclass problems." ESANN. 2002.
- etc.

Overall picture

- Our approach differs from other *"fuzzy support machines"*, because we do not modify the machine learning algorithm, instead we construct kernels on fuzzy sets.

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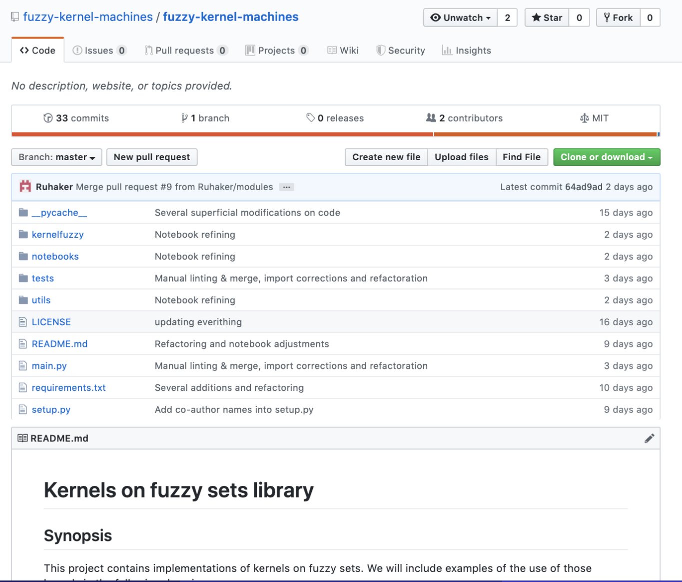
- The kernel trick given by kernels on fuzzy sets can be used for any kernel method (support vector regression, kernel PCA, Gaussian process, etc)

Overall picture

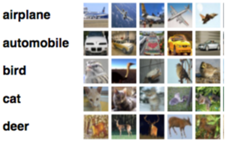
- Our approach differs from other *"fuzzy support machines"*, because we do not modify the machine learning algorithm, instead we construct kernels on fuzzy sets.
- The kernel trick given by kernels on fuzzy sets can be used for any kernel method (support vector regression, kernel PCA, Gaussian process, etc)
- for instance, a support fuzzy-set machine is a SVM with kernel on fuzzy sets. We call it "**support fuzzy-set machine**" because the solution (decision function) will depend only by a subset of the training examples (fuzzy sets).

Overall picture

Kernel on fuzzy set library (collaboration with Lucas Yau from University of Sao Paulo)



Data



Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
5.1	3.5	1.4	0.2	setosa
4.9	3.	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
5.	3.6	1.4	0.2	setosa
5.4	3.9	1.7	0.4	setosa
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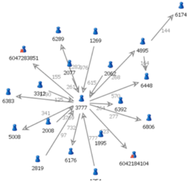
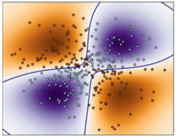
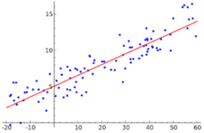


Tasks

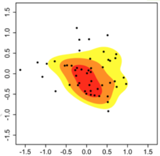
Classification



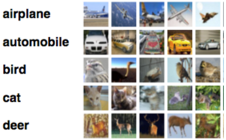
Regression



Density estimation



Data



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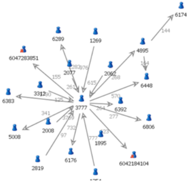

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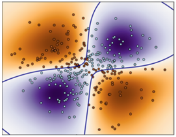
Classification



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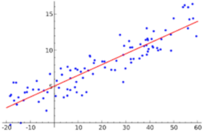
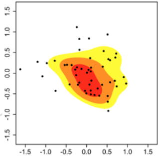


Density estimation



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Learn

y= $f(x)$

Tasks

Classification

Regression

Density estimation

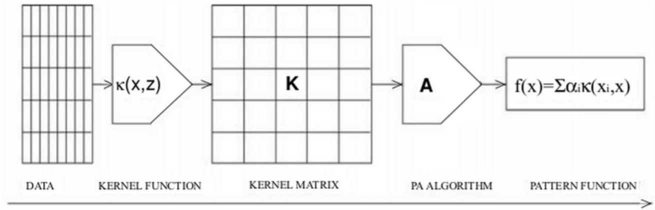
Introduction

- Data representation
  - Images
    - Vectors
    - Conditional random fields
  - Structured data
    - logical predicates
    - Graphs
    - Distributions
  - Uncertain data
    - Probability measures
    - Fuzzy sets
  - Granular data
    - Fuzzy sets
    - Granular representations

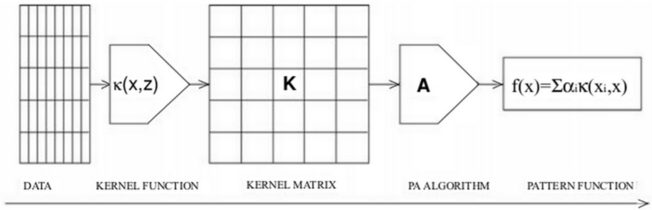
- Similarity measures
  - A real valued function that quantifies the similarity between two objects
  - Many of them:
    - Inner products (Kernels)
    - Cosine similarity
    - Fuzzy similarity measures
    - etc
- Property
  - Inverse of distance metrics (in some sense)

Outline

Kernel methods



Kernel methods

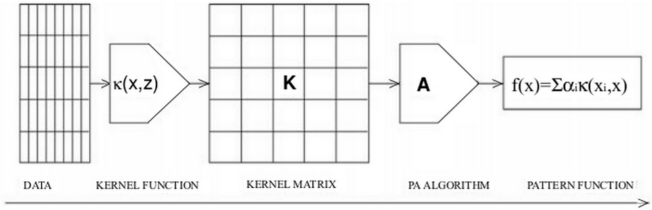


Support Vector Machines

$$\begin{aligned}
\min_{\boldsymbol{\alpha}\in\mathbb{R}^N} \quad & \frac{1}{2}\boldsymbol{\alpha}^\top K\boldsymbol{\alpha} - \mathbf{1}^\top\boldsymbol{\alpha} \\
\text{subject to} \quad & \boldsymbol{\alpha}^\top \mathbf{y} = 0. \\
& 0 \le \alpha_i \le \lambda,\ \ i = 1,\dots,N.
\end{aligned}$$

Cortes, Corinna, and Vladimir Vapnik. "Support-vector networks." Machine learning 20.3 (1995): 273-297
Figure from Shawe-Taylor, John, and Nello Cristianini. Kernel methods for pattern analysis. Cambridge university press, 2004.

Kernel methods



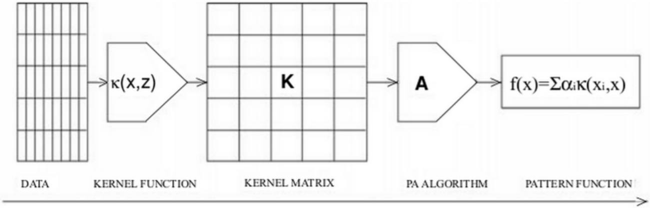
Kernel PCA

$$\begin{array}{ll} \text{Solve} & M\lambda\boldsymbol{\alpha} = K\boldsymbol{\alpha} \\ \text{subject to} & \boldsymbol{\alpha}^\top K\boldsymbol{\alpha} = 1. \end{array}$$

where the eigen functions are given by $V(.) = \sum_i \alpha_i k(x_i, .)$

Schölkopf, Bernhard, Alexander Smola, and Klaus-Robert Müller. "Nonlinear component analysis as a kernel eigenvalue problem." Neural computation 10.5 (1998): 1299-1319.

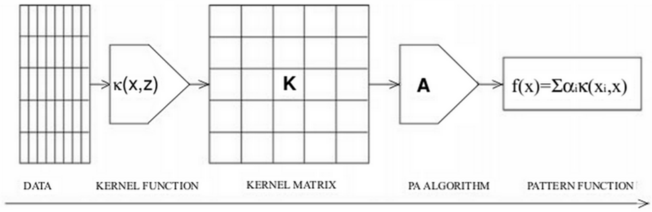
Kernel methods



Gaussian process regression

- $f \sim \mathcal{GP}\left(\mathbb{E}[f(X)], k(x,x)\right) = \mathcal{GP}\left(m(x), k(x,x)\right)$
- Predictive distribution $y_i \mid x_*, x, \mathbf{y} \sim \mathcal{N}\left(k(x_*,x)k(x,x)^{-\mathbf{1}}\mathbf{y}, k(x_*,x_*) - k(x_*,x)k(x,x)^{-\mathbf{1}}k(x,x_*)\right)$
- thus, $y = \hat{f}(x_*) \equiv k(x_*,x)k(x,x)^{-\mathbf{1}}\mathbf{y} = \sum_i \alpha_i k(x_i,x_*)$, , where $\boldsymbol{\alpha} = K^{-\mathbf{1}}\mathbf{y}$

Rasmussen, Carl Edward. "Gaussian processes in machine learning." Advanced lectures on machine learning. Springer, Berlin, Heidelberg, 2004. 63-71.

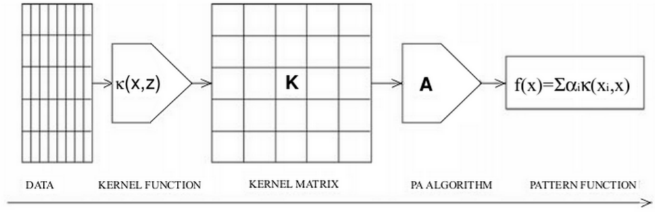


Support Vector Data Description

$$\begin{aligned}
\min_{\boldsymbol{\alpha} \in \mathbb{R}^N} \quad & \boldsymbol{\alpha}^\top K \boldsymbol{\alpha} - \boldsymbol{\alpha}^\top diag(K) \\
\text{subject to} \quad & \boldsymbol{\alpha}^\top \mathbf{1} = 0. \\
& 0 \leq \alpha_i \leq \lambda, \ i = 1, \ldots, N,
\end{aligned}$$

Tax, David MJ, and Robert PW Duin. "Support vector data description." Machine learning 54.1 (2004): 45-66.

Kernel methods

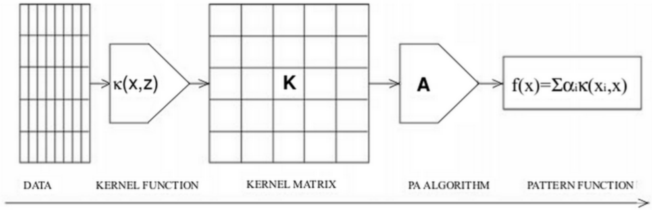


Radial basis function neural network

$$f(x) = \sum_{l=1}^{L} w_l \exp(-\gamma \|x - \mu_k\|^2)$$

Broomhead, David S., and David Lowe. Radial basis functions, multi-variable functional interpolation and adaptive networks. No. RSRE-MEMO-4148. Royal Signals and Radar Establishment Malvern (United Kingdom), 1988.

Kernel methods



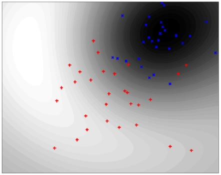
- SVM
- kernel PCA
- Gaussian process
- SVDD
- MKL
- SMDD
- Kernel regression
- Kernel two-sample test
- kernel spectral clustering

Representer Theorem

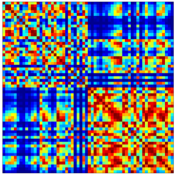
$$f^* = \underset{f \in \mathcal{H}}{\text{argmin}}\ Cost\left((x_1, y_1, f(x_1)), \ldots, (x_N, y_N, f(x_N))\right) + \Omega(\|f\|) \quad (1)$$

$$f^*(.) = \sum_{i=1}^{N} \alpha_i k(., x_i) \quad (2)$$

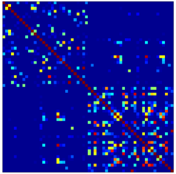
A kernel matrix is a similarity matrix



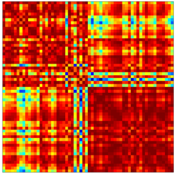
raw data



Gram matrix for $b = 2$



$b = .5$



$b = 10$

RKHS, where the magic happens

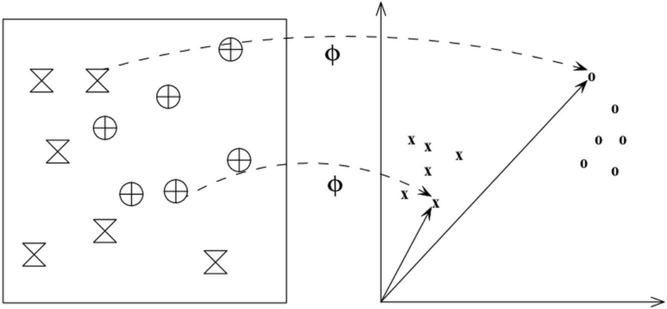


Figure: Kernel mapping[a]

Figure from Shawe-Taylor et al. "Kernel Methods for Pattern Analysis". Cambridge University Press.

Main ingredient

- A real-valued symmetric positive definite kernel k.
  $\sum_{i=1,j=1}^{N} c_i c_j k(x_i, x_j) \geq 0$

$$\boxed{\begin{aligned} \mathcal{X} &\to \mathcal{H} \\ x &\mapsto k(.,x) \end{aligned}}$$

$$k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$

$$\begin{array}{ll} \forall x \in \mathcal{X},\ k(.,x) \in \mathcal{H} & \\ \forall x \in \mathcal{X},\ \forall f \in \mathcal{H} & \langle f, k(.,x) \rangle = f(x) \\ \forall x, x' \in \mathcal{X} & k(x,x') = \langle k(.,x), k(.,x') \rangle \end{array}$$

Reproducing Kernel Hilbert Spaces

Definition (Reproducing kernel)

A function

$$\begin{aligned} k : \mathcal{X} \times \mathcal{X} &\rightarrow \mathbb{R} \\ (x, y) &\mapsto k(x, t) \end{aligned} \tag{3}$$

is called a reproducing kernel of the Hilbert space $\mathcal{H}$ *if and only if:*

1. $\forall x \in \mathcal{X},\ k(.,x) \in \mathcal{H}$
2. $\forall x \in \mathcal{X},\ \forall f \in \mathcal{H}\ \ \langle f, k(.,x)\rangle_{\mathcal{H}} = f(x)$

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Reproducing property

$$\forall (x, y) \in \mathcal{X} \times \mathcal{X},\ k(x, y) = \langle k(., x), k(., y)\rangle_{\mathcal{H}} \qquad (4)$$

Reproducing Kernel Hilbert Spaces

Definition (Real RKHS)

A Hilbert Space of real valued functions on $\mathcal{X}$, denoted by $\mathcal{H}$, with reproducing kernel is called a real Reproducing Kernel Hilbert Space or real RKHS.

Reproducing Kernel Hilbert Spaces

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Characterization

All the evaluation functionals are continuous on $\mathcal{H}$. :

$$
\begin{aligned}
e_x : \mathcal{H} &\rightarrow \mathbb{R} && (5)\\
f &\mapsto e_x(f) = f(x) && (6)
\end{aligned}
$$

Berlinet, Alain, and Christine Thomas-Agnan. Reproducing kernel Hilbert spaces in probability and statistics. Springer Science Business Media, 2011.

Positive Definite Kernel

Lemma

Any reproducing kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ *is a symmetric positive definite function, that is, it satisfies:*

$$\sum_{i=1}^{N} \sum_{j=1}^{N} c_i c_j k(x_i, x_j) \geq 0 \tag{7}$$

$\forall N \in \mathbb{N}$, $\forall c_i, c_j \in \mathbb{R}$ *and* $k(x, y) = k(y, x)$, $\forall x, y \in \mathcal{X}$. *The converse is true.*

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Consequently

Kernels k are reproducing kernels of some RKHS. The space spanned by $k(x, .)$ generates a RKHS or a Hilbert space with reproducing kernel k.

Positive Definite Kernel

If k is a reproducing kernel, then

$$
\begin{aligned}
\sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j k(x_i, x_j) &= \sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j \langle k(., x_i), k(., x_j)\rangle_{\mathcal{H}} \\
&= \langle \sum_{i=1}^{N} c_i k(., x_i), \sum_{j=1}^{N} c_j k(., x_j)\rangle_{\mathcal{H}} \\
&= \| \sum_{i=1}^{N} c_i k(., x_i)\|_{\mathcal{H}}^2 \\
&\geq 0
\end{aligned}
$$

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&= \| \sum_{i=1}^{N} c_i k(., x_i)\|_{\mathcal{H}}^2 \\
&\geq 0
\end{aligned}$$

That is

Elements of the RKHS are real-valued functions on $\mathcal{X}$ of the form $f(.) = \sum_{i=1}^{N} c_i k(., x_i)$.

Polynomial kernel $k(\mathbf{x}, \mathbf{x}') = (a + b\mathbf{x}^\top \mathbf{x}')^\gamma$

Examples of reproducing kernels or positive definite kernels

$$
\begin{aligned}
k(\mathbf{x},\mathbf{x}') &= (1+\mathbf{x}^\top\mathbf{x}')^2 \\
&= (1+x_1x_1'+x_2x_2')^2 \\
&= (1+x_1^2x_1'^2+x_2^2x_2'^2+2x_1x_1'+2x_2x_2'+2x_1x_1'x_2x_2') \\
&= \left\langle (1,x_1^2,x_2^2,\sqrt{2}x_1,\sqrt{2}x_2\ ,\ \sqrt{2}x_1x_2),(1,x_1'^2,x_2'^2,\sqrt{2}x_1',\sqrt{2}x_2',\sqrt{2}x_1'x_2') \right\rangle
\end{aligned}
$$

Polynomial kernel $k(\mathbf{x},\mathbf{x}') = (a+b\mathbf{x}^\top\mathbf{x}')^\gamma$

Positive Definite Kernel

Examples of reproducing kernels or positive definite kernels

$$
\begin{aligned}
k(x, x') &= \exp\big(-(x - x')^2\big) \\
&= \exp(-x^2)\exp(-x'^2)\sum_{i=0}^{\infty}\frac{2^i x^i x'^i}{i!}
\end{aligned}
$$

infinite dimensional

Positive Definite Kernel

Examples of reproducing kernels or positive definite kernels

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infinite dimensional
RBF kernel $k(\mathbf{x}, \mathbf{x}') = \exp(-0.5 * \gamma\|\mathbf{x} - \mathbf{x}'\|^2)$

Positive Definite Kernel

Examples of reproducing kernels or positive definite kernels
The real-valued kernel on $\mathcal{P} \times \mathcal{P}$, defined by

$$\begin{aligned}\tilde{k}(\mathbb{P}, \mathbb{Q}) =& \langle \mathbb{E}_{\mathbb{P}}[k(X, .)], \mathbb{E}_{\mathbb{Q}}[k(X', .)] \rangle_{\mathcal{H}} \\ =& \int_{\mathbf{x} \in \mathbb{R}^D} \int_{\mathbf{x}' \in \mathbb{R}^D} k(\mathbf{x}, \mathbf{x}') d\mathbb{P}(\mathbf{x}) d\mathbb{Q}(\mathbf{x}')\end{aligned} \tag{8}$$

is positive definite.

Positive Definite Kernel

Examples of reproducing kernels or positive definite kernels

- Mean maps with stationary kernels do not have constant norm
  $\|\mu_{\mathbb{P}}\|_{\mathcal{H}} = \|\mathbb{E}_{\mathbb{P}}[k_I(X.,)]\|_{\mathcal{H}} \ \leq \ \mathbb{E}_{\mathbb{P}}[\|k_I(X.,)\|_{\mathcal{H}}] = \sqrt{|\epsilon|}$
- normalize mean maps to lie on a surface of some hypersphere

$$\tilde{\tilde{k}}(\mathbb{P}_i, \mathbb{P}_j) = \frac{\langle \mu_{\mathbb{P}}, \mu_{\mathbb{Q}} \rangle_{\mathcal{H}}}{\sqrt{\langle \mu_{\mathbb{P}}, \mu_{\mathbb{P}} \rangle_{\mathcal{H}} \langle \mu_{\mathbb{Q}}, \mu_{\mathbb{Q}} \rangle_{\mathcal{H}}}}, \tag{9}$$

- the injectivity of $\mu : \mathcal{P} \to \mathcal{H}$ is preserved.

Muandet et al "One-class support measure machines for group anomaly detection."

Positive Definite Kernel

$$k_{\nu=p+1/2}(r) \;=\; \exp\left(-\frac{\sqrt{2\nu}r}{\ell}\right)\frac{\Gamma(p+1)}{\Gamma(2p+1)}\sum_{i=0}^{p}\frac{(p+i)!}{i!(p-i)!}\left(\frac{\sqrt{8\nu}r}{\ell}\right)^{p-i}.$$

$$k_{\nu=p+1/2}(r) = \exp\left(-\frac{\sqrt{2\nu}r}{\ell}\right)\frac{\Gamma(p+1)}{\Gamma(2p+1)}\sum_{i=0}^{p}\frac{(p+i)!}{i!(p-i)!}\left(\frac{\sqrt{8\nu}r}{\ell}\right)^{p-i}.$$

The Matern kernel, widely used in kriging procedures by geostatisticians

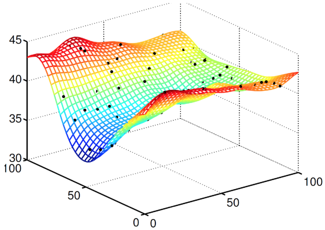

Figure from: https://www.ethz.ch/content/specialinterest/baug/institute-ibk/risk-safety-and-uncertainty/en/research/past-projects/polynomial-chaos-kriging.html

Positive Definite Kernel

Examples of reproducing kernels or positive definite kernels

- Linear kernel $k(x, y) = \langle x, y \rangle \; x, y \in \mathbb{R}^D$

Positive Definite Kernel

Examples of reproducing kernels or positive definite kernels

- Linear kernel $k(x, y) = \langle x, y \rangle \; x, y \in \mathbb{R}^D$
- Polynomial kernel $k(x, y) = (\langle x, y \rangle + 1)^D \; x, y \in \mathbb{R}^D$

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- Probability product kernel $\tilde{k}(\mathbb{P}, \mathbb{Q}) = \int_{\mathcal{X}} \mathbb{P}(x)^\rho \mathbb{Q}(x)^\rho dx$
- Kernel on probability measures for $X \sim \mathbb{P}, X' \sim \mathbb{Q}$,
  $\tilde{k}(\mathbb{P}, \mathbb{Q}) = \langle \mathbb{E}_{\mathbb{P}}[k(X.,)], \mathbb{E}_{\mathbb{Q}}[k(X'.,)] \rangle_{\mathcal{H}}$

Positive Definite Kernel

Making new kernels from old If k_1 and k_2 are PD kernels, by closure properties of PD kernels, also are PD kernels:

1. $k_1(x, y) + k_2(x, y)$;
2. $\alpha k_1(x, y), \quad \alpha \in \mathbb{R}^+$;
3. $k_1(x, y)k_2(x, y)$;
4. $k(f(x), f(y))$
5. $\exp(k_1(x, y))$;
6. $p(k_1(x, y)), \quad p$ is a polynomial with positive coefficients.

Kernels

Positive definite kernels are

- coovariance functions, i.e., $k(x, x') = \mathbb{E}\big[f(x)f(x')\big]$,

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- the main ingredient to define RKHS
- very useful in practice in machine learning, i.e., they define gram matrices $K_{i,j} = k(x_i, x_j)$ used in ML algorithms
- defined on non empty sets: That enables its use on non-vectorial spaces. (sets, graphs, strings, etc)

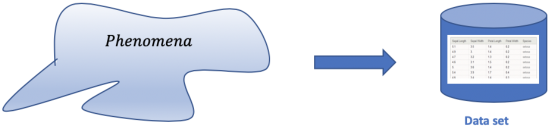
Outline

Kernels on Fuzzy sets

Material

- https://github.com/fuzzy-kernel-machines/fuzzy-kernel-machines
- Guevara, Jorge, et.al. **"Learning with Kernels on Fuzzy Sets"** (Arxiv) In-preparation
- Guevara, Jorge, et.al. **"Kernels on Fuzzy Sets: an Overview"**, Learning on Distributions, Functions, Graphs and Groups @ NIPS-2017
- Guevara, Jorge, et.al. **"Cross product kernels for fuzzy set similarity."** Fuzzy Systems (FUZZ-IEEE), 2017.
- Guevara, Jorge, et.al. **"Fuzzy Set Similarity using a Distance-Based Kernel on Fuzzy Sets"**, 2016, Book Chapter, Handbook of Fuzzy Sets Comparison - Theory, Algorithms and Applications,pages 103-120.
- Guevara, Jorge, et.al. **"Positive Definite Kernel Functions on Fuzzy Sets."** Fuzzy Systems (FUZZ-IEEE), 2014.
- Guevara, Jorge, et.al.**"Kernel Functions in Takagi-Sugeno-Kang Fuzzy System with Nonsingleton Fuzzy Input."** Fuzzy Systems (FUZZ-IEEE), 2013.

Motivation



- study, analysis and understanding of the nature of a research object.
- testing (causal) hypotheses
- discovering hidden patterns and correlations
- postulate theories,
- give explanations
- make predictions on unobserved cases

Kernels on Fuzzy sets

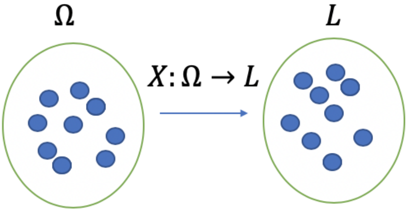
Set-valued information

- Ontic (conjuctive sets)
  - set of pixels denoting a region within a image
  - cluster of galaxies
- Epistemic (disjuntive sets)
  - a set containing the unknown age of a person
  - an interval containing a non-precise measurement

Couso, Inés, and Didier Dubois. "Statistical reasoning with set-valued information: Ontic vs. epistemic views." International Journal of Approximate Reasoning 55.7 (2014): 1502-1518.

Kernels on Fuzzy sets

Fuzzy Sets



We can have both views ontic and epistemic

Kernels on Fuzzy sets

Fuzzy data

Var 1	Var 2	Var 3	Var 4	Var 5	Var 6	MD
234	345	34	654	345	56	0.5
56	45	546	345	345	45	1
345	345	767	564	435	456	0.3

Kernels on Fuzzy sets

Fuzzy data

Var 1	Var 2	Var 3	Var 4
234	345	34	654
56	45	546	345
345	345	767	564

MD 1	MD 2	MD 3	MD 4
0.3	0.5	1	0.4
0.6	0.7	0.4	1
0	0.3	0.1	0.9

Kernels on Fuzzy sets

Fuzzy data

Var 1	Var 2	Var 3	Var 4	Var 5
X_1^1	X_2^1	X_3^1	X_4^1	X_5^1
X_1^2	X_2^2	X_3^2	X_4^2	X_5^2
X_1^3	X_2^3	X_3^3	X_4^3	X_5^3
X_1^4	X_2^4	X_3^4	X_4^4	X_5^4

$$
\begin{aligned}
X : \Omega \quad &\rightarrow \quad [0, 1] \\
x \quad &\mapsto \quad X(x).
\end{aligned}
$$

Kernels on Fuzzy sets

Motivation

- similarity measure between fuzzy sets given by kernels

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- similarity measure between fuzzy sets given by kernels
- geometric interpretation of similarity between fuzzy set in RKHS
- embedding of fuzzy sets into RKHS
- using fuzzy data "as is" in kernel methods
- covariance matrix for fuzzy samples

Fuzzy Set

- Fuzzy sets on Ω are denoted by X, Y, Z.

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Definition (Support of a fuzzy set)

The support of a fuzzy set is the set

$$\mathrm{supp}(X) = \{x \in \Omega | X(x) > 0\}.$$

Cross product kernel on fuzzy sets

Definition (Cross product kernel on fuzzy sets)

The cross product kernel on fuzzy sets is a function $k_\times : \mathcal{F}(\Omega) \times \mathcal{F}(\Omega) \to \mathbb{R}$ *given by:*

$$k_\times(X, Y) = \sum_{\substack{x \in \mathrm{supp}(X),\\ y \in \mathrm{supp}(Y)}} k_1 \otimes k_2\big((x, X(x)), (y, Y(y))\big), \tag{10}$$

where: $k_1 : \Omega \times \Omega \to \mathbb{R}$, $k_2 : [0,1] \times [0,1] \to \mathbb{R}$,

$$k_1 \otimes k_2\big(x, X(x), y, Y(y)\big) = k_1(x, y)\, k_2(X(x), Y(y)). \tag{11}$$

Guevara, Jorge, et.al. **"Cross product kernels for fuzzy set similarity."** Fuzzy Systems (FUZZ-IEEE), 2017.

Cross product kernel on fuzzy sets

Lemma

If k_1 and k_2 are real-valued pd kernels, then the cross product kernel on fuzzy sets is pd.

Cross product kernel on fuzzy sets

Lemma

If k_1 and k_2 are real-valued pd kernels, then the cross product kernel on fuzzy sets is pd.

Corollary

Kernel $k_\times$ defines a similarity measure for two fuzzy sets $X, Y \in \mathcal{F}(\Omega)$ as follows:

$$k_\times(X, Y) = \langle \phi_X, \phi_Y \rangle_{\mathcal{H}}, \tag{12}$$

Guevara, Jorge, et.al. **"Cross product kernels for fuzzy set similarity."** Fuzzy Systems (FUZZ-IEEE), 2017.

Cross product kernel on fuzzy sets

$k_1(x,y)$	$k_\times(X,Y)$
linear	$\sum_{\substack{x\in \mathrm{supp}(X),\\ y\in \mathrm{supp}(Y)}} xyX(x)Y(y)$
polynomial	$\sum_{\substack{x\in \mathrm{supp}(X),\\ y\in \mathrm{supp}(Y)}} (\gamma\langle x,y\rangle + b)^\beta X(x)Y(y)$
exponential	$\sum_{\substack{x\in \mathrm{supp}(X),\\ y\in \mathrm{supp}(Y)}} \exp(\gamma\langle x,y\rangle)X(x)Y(y)$
Gaussian	$\sum_{\substack{x\in \mathrm{supp}(X),\\ y\in \mathrm{supp}(Y)}} \exp(-\gamma\|x-y\|^2)X(x)Y(y)$

Table: Examples of cross product kernels on fuzzy sets.

Guevara, Jorge, et.al. **"Cross product kernels for fuzzy set similarity."** Fuzzy Systems (FUZZ-IEEE), 2017.

Cross product kernel on fuzzy sets

Example

Let $(\Omega, \mathcal{A}, \mu)$ *be a finite measure space. Let* $k_{\mathbf{1}}, k_{\mathbf{2}}$ *be continuous functions with finite integral. The kernel*

$$k_{\times}(X, Y) = \iint_{\substack{x \in \mathrm{supp}(X), \\ y \in \mathrm{supp}(Y)}} k_{\mathbf{1}} \otimes k_{\mathbf{2}}((x, X(x)), (y, Y(y)))\, d\mu(x) d\mu(y), \tag{13}$$

is a cross product kernel on fuzzy sets.

Example

Replacing the measure μ *of the previous example with a probability measure* $\mathbb{P}$ *results in the following cross product kernel on fuzzy sets:*

$$k_{\times}(X, Y) = \iint_{\substack{x \in \mathrm{supp}(X), \\ y \in \mathrm{supp}(Y)}} k_{\mathbf{1}} \otimes k_{\mathbf{2}}((x, X(x)), (y, Y(y)))\, d\mathbb{P}(x) d\mathbb{P}(y), \tag{14}$$

Guevara, Jorge, et.al. **"Cross product kernels for fuzzy set similarity."** Fuzzy Systems (FUZZ-IEEE), 2017.

Cross product kernel on fuzzy sets

A generalization of $k_\times$ to deal with a D-tuple of fuzzy sets, i.e., $(X_1, \ldots, X_D) \in \mathcal{F}(\Omega_1) \times \cdots \times \mathcal{F}(\Omega_D)$ is implemented by the following kernel:

$$k_\times^\pi((X_1, \ldots, X_D), (Y_1, \ldots, Y_D)) = \prod_{d=1}^{D} k_\times^d(X_d, Y_d). \tag{15}$$

If all the kernels $k_\times^d$ are positive definite then $k_\times^\pi$ is positive definite by closure properties of kernels. Another generalization based on addition of positive definite kernels is also possible:

$$k_\times^\Sigma((X_1, \ldots, X_D), (Y_1, \ldots, Y_D)) = \sum_{d=1}^{D} \alpha_i k_\times^d(X_d, Y_d). \tag{16}$$

Kernel $k_\times^\Sigma$ is positive definite if only if $\alpha_i \in \mathbb{R}^+$ and all the $k_\times^D$ kernels are positive definite.

Cross product kernel on fuzzy sets

Properties

- $k_\times$ is a convolution kernel, i.e., it can be derived from $k_{conv}(e, e') = \sum_{\vec{e} \in R^{-1}(e), \vec{e}' \in R^{-1}(e')} \prod_{l=1}^{L} k_l(e_l, e'_l)$,

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- $k_\times$ generalize the cross product kernel on sets, i.e., $k(A, A')$
- $k_\times$ embeds probability distributions into a RKHS.
- fuzzines and radomness modeling (see example when $\mu = \mathbb{P}$)
- noise resistant under supervised classification experiments on attribute noisy datasets (see Paper below)

Guevara, Jorge, et.al. **"Cross product kernels for fuzzy set similarity."** Fuzzy Systems (FUZZ-IEEE), 2017.

Cross product kernel on fuzzy sets

Example of this kernel using the **fuzzy-kernel-machines** library (see notebook 2)

```
from kernelfuzzy.fuzzyset import FuzzySet
from kernelfuzzy.memberships import gaussmf

elements = np.random.uniform(0, 100, 2)
X = FuzzySet(elements=elements, mf=gaussmf, params=[np.mean(elements), np.std(elements)])

elements = np.random.uniform(0, 100, 2)
Y = FuzzySet(elements= elements, mf=gaussmf, params=[np.mean(elements), np.std(elements)])

print("Fuzzy set: ", X.get_pair())
print("Fuzzy set: ", Y.get_pair())
```

```
Fuzzy set:  [(3.5582410565239586, 0.36787944117144233), (42.5806658890677, 0.36787944117144245)]
Fuzzy set:  [(70.57530755417343, 0.3678794411714424), (20.89244684919256, 0.36787944117144217)]
```

Cross-Product kernels: linear kernel with RBF kernel

This example calculates the Cross-Product of different kernels: the RBF with a linear kernel

```
#cross product kernel with RBF kernel and linear kernels
from sklearn.metrics.pairwise import rbf_kernel

print(kernels.cross_product_kernel(X, Y, rbf_kernel, 0.05, kernels.linear_kernel, ''))
print(kernels.cross_product_kernel(X, Y, rbf_kernel, 0.5, kernels.linear_kernel, ''))
print(kernels.cross_product_kernel(X, Y, rbf_kernel, 5.0, kernels.linear_kernel, ''))
```

```
4.043661711650557e-08
7.658805252340087e-67
0.0
```

Cross product kernel on fuzzy sets

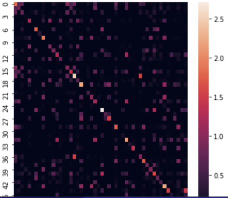
Kernel gram matrix example using the **fuzzy-kernel-machines** library (see notebook 3)

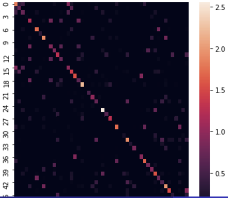
Kernel Gram Matrix: RBF kernel and linear kernel

The Gram Matrix kernels are created from a fuzzy dataset. Each Gram Matrix is estimated via the cross-product kernel on the fuzzy sets, with a RBF kernel for the elements and a linear kernel for the membership degrees

In [6]:

```
from sklearn.metrics.pairwise import rbf_kernel
import matplotlib.pyplot as plt

# fuzzy dataset
fuzzy_dataset = FuzzyData.create_toy_fuzzy_dataset(num_rows=50, num_cols=2
)

kernel_bandwidth=[0.05, 0.5, 5, 50]

# plotting
fig, axn = plt.subplots(2, 2, figsize=(10,10))
for i, ax in enumerate(axn.flat):
    K = gram_matrix_cross_product_kernel(fuzzy_dataset, fuzzy_dataset, rbf
_kernel, kernel_bandwidth[i], linear_kernel, '')
    sns.heatmap(K, ax=ax)

fig.tight_layout()
```





The intersection kernel on fuzzy sets

A triangular norm or **T-norm** is the function $T : [0,1]^2 \to [0,1]$, such that, for all $x, y, z \in [0,1]$ satisfies:

- T1 commutativity: $T(x,y) = T(y,x)$;
- T2 associativity: $T(x, T(y,z)) = T(T(x,y),z)$;
- T3 monotonicity: $y \leq z \Rightarrow T(x,y) \leq T(x,z)$;
- T4 boundary condition $T(x,1) = x$.

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a multiple-valued extension

Using $n \in \mathbb{N}, n \ge 2$ and associativity, a multiple-valued extension $T_n : [0,1]^n \to [0,1]$ of a T-norm T is given by $T_2 = T$ and

$$T_n(x_1, x_2, \ldots, x_n) = T(x_1, T_{n-1}(x_2, x_3, \ldots, x_n)). \tag{17}$$

We will use T to denote T or T_n.

The intersection kernel on fuzzy sets

A **semi-ring of sets**, $\mathcal{S}$ on Ω, is a subset of the power set $\mathcal{P}(\Omega)$, that is, a set of sets satisfying:

1. $\phi \in \mathcal{S}$, ϕ denotes the empty set;
2. $A, B \in \mathcal{S}, \implies A \cap B \in \mathcal{S}$;
3. for all $A, A_1 \in \mathcal{S}$ and $A_1 \subseteq A$, there exists a sequence of pairwise disjoint sets $A_2, A_3, \ldots A_N \subseteq \mathcal{S}$, such

$$A = \bigcup_{i=1}^{N} A_i.$$

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Finite decomposition

Condition 3 is called *finite decomposition of A*.

The intersection kernel on fuzzy sets

Definition (Measure)

Let $\mathcal{S}$ be a semi-ring and let $\rho : \mathcal{S} \to [0, \infty]$ be a pre-measure, i.e., ρ satisfy:

1. $\rho(\phi) = 0$;
2. *for a finite decomposition of $A \in \mathcal{S}$, $\rho(A) = \sum_{i=1}^{N} \rho(A_i)$;*

by Carathéodory's extension theorem, ρ is a measure on $\sigma(\mathcal{S})$, where $\sigma(S)$ is the smallest σ-algebra containing S.

Gartner et.al., shows that a kernel $k : \mathcal{S} \times \mathcal{S} \to \mathbb{R}$ defined by $k(A, A') = \rho(A \cap A')$ is positive definite, where $\rho : \mathcal{S} \to [0, \infty]$ is a measure.

Gartner, Thomas. Kernels for structured data. Vol. 72. World Scientific, 2008.

The intersection kernel on fuzzy sets

Remark

Notation $\mathcal{F}_{\mathcal{S}}(\Omega)$ stands for the set of all fuzzy sets over Ω whose support belongs to $\mathcal{S}$, i.e.,

$$\mathcal{F}_{\mathcal{S}}(\Omega) = \{X \subset \Omega | \, \text{supp}(X) \in \mathcal{S}\}.$$

where $\mathcal{S}$ is a semi-ring of sets on Ω

The intersection kernel on fuzzy sets

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where $\mathcal{S}$ is a semi-ring of sets on Ω

Example

If $X \cap Y \in \mathcal{F}_{\mathcal{S}}(\Omega)$ then satisfy (finite decomposition):

$$\text{supp}(X \cap Y) = \bigcup_{i \in I} A_i, \; A_i \in \mathcal{S},$$

where $\{A_1, A_2, \ldots, A_N\}$. are pairwise disjoint sets

Intersection Kernel on Fuzzy Sets

Example cont.

We can measure $\mathrm{supp}(X \cap Y) = \bigcup_{i \in I} A_i,\ A_i \in \mathcal{S}$ using the measure $\rho : \mathcal{S} \to [0, \infty]$ as follows:

$$\rho\big(\,\mathrm{supp}(X \cap Y)\big) = \rho\Big(\bigcup_{i \in I} A_i\Big) = \sum_{i \in I} \rho(A_i),$$

Intersection Kernel on Fuzzy Sets

Example cont.

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Adding fuzziness

The idea to include fuzziness is to weight each $\rho(A_i)$ by a value given by the contribution of the membership function on all the elements of the set A_i.

Intersection Kernel on Fuzzy Sets

Definition

The intersection kernel on fuzzy sets is a function:
$k_\cap : \mathcal{F}_\mathcal{S}(\Omega) \times \mathcal{F}_\mathcal{S}(\Omega) \to \mathbb{R}$, *defined by:*

$$k_\cap(X, Y) = \sum_{i \in I} \big(X \cap Y\big)(A_i)\rho(A_i), \tag{18}$$

where $\big(X \cap Y\big)(A) \equiv \sum_{x \in A} \big(X \cap Y\big)\,(x)$

Guevara, Jorge, et.al. **"Positive Definite Kernel Functions on Fuzzy Sets."** Fuzzy Systems (FUZZ-IEEE), 2014.

Intersection Kernel on Fuzzy Sets

Kernel $k_\cap$ can be implemented via T-norm operators:

$$
\begin{aligned}
k_\cap(\mathrm{X,Y}) &= \sum_{i \in I} \big(X \cap Y\big)(A_i)\rho(A_i) \\
&= \sum_{i \in I} \sum_{x \in A_i} \big(X \cap Y\big)(x)\rho(A_i) \\
&= \sum_{i \in I} \sum_{x \in A_i} T(X(x), Y(x))\rho(A_i)
\end{aligned}
$$

Intersection Kernel on Fuzzy Sets

Examples

Some kernel examples for different T-norm operators

Kernel $k_\cap$	T-norm
$k_{\cap\_\min}(X,Y) = \sum_{i\in I}\sum_{x\in A_i} \min(X(x),Y(x))\rho(A)$	minimum
$k_{\cap\_\mathrm{pro}}(X,Y) = \sum_{i\in I}\sum_{x\in A_i} X(x)Y(x)\rho(A)$	product
$k_{\cap\_\text{Łuk}}(X,Y) = \sum_{i\in I}\sum_{x\in A_i} \max(X(x)+Y(x)-1,0)\rho(A)$	Łukasiewicz
$k_{\cap\_\mathrm{Dra}}(X,Y) = \sum_{i\in I}\sum_{x\in A_i} f(X(x),Y(x))\rho(A)$	Drastic

where f is defined as

$$f(X(x),Y(x)) = \begin{cases} X(x), \text{ if } Y(x) = 1 \\ Y(x), \text{ if } X(x) = 1 \\ 0, \ \textit{otherwise} \end{cases}$$

Intersection Kernel on Fuzzy Sets

Lemma

$k_{\min}(X, Y) = \sum_{i \in I} \sum_{x \in A_i} \min(\mu_X(x), \mu_Y(x))\rho(A_i)$
is positive definite

Lemma

$k_P(X, Y) = \sum_{i \in I} \sum_{x \in A_i} \mu_X(x)\mu_Y(x)\rho(A_i)$
is positive definite.

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```
%membershipFunction(type, points)
K(X,Y)=sum(min(X(data(i,:)),Y(data(i,:))))
```

The non-singleton kernel on fuzzy sets

Definition

This kernel is a function $k_{nsk} : \mathcal{F}(\Omega) \times \mathcal{F}(\Omega) \to [0,1]$ *defined by:*

$$\begin{aligned} k_{nsk}(X, Y) &= \sup_{x \in \Omega} \Big(X \cap Y\Big)(x) \\ &= \sup_{x \in \Omega} \Big(T\big(X(x), Y(x)\big) \Big), \end{aligned}$$

where sup *is the supremum.*

Derived from non-singleton fuzzy systems.

Guevara, Jorge, et.al.**"Kernel Functions in Takagi-Sugeno-Kang Fuzzy System with Nonsingleton Fuzzy Input."**

The non-singleton kernel on fuzzy sets

Examples Given $X = (X_1, \ldots, X_d, \ldots, X_D)$ and $Y = (Y_1, \ldots, X_d, \ldots, Y_D)$, such that: $X_d(.) = \exp\left(-\frac{1}{2}\frac{(.-m_d)^2}{\sigma_d^2}\right)$, where, $m_d \in \mathbb{R}$ amd $\sigma_d \in \mathbb{R}^+$, then, the following kernel

$$k_{nsk}(X, Y) = \prod_{d=1}^{D} \exp\left(-\frac{1}{2}\frac{(m_d - m'_d)^2}{\sigma_d^2 + (\sigma'_d)^2}\right), \tag{19}$$

is a positive definite kernel.

Guevara, Jorge, et.al.**"Kernel Functions in Takagi-Sugeno-Kang Fuzzy System with Nonsingleton Fuzzy Input."**

Examples Given $X = (X_1, \dots, X_d, \dots, X_D)$ and $Y = (Y_1, \dots, X_d, \dots, Y_D)$, such that: $X_d(.) = \exp\left(-\frac{1}{2}\frac{(. - m_d)^2}{\sigma_d^2}\right)$, where, $m_d \in \mathbb{R}$ amd $\sigma_d \in \mathbb{R}^+$, then, the following kernel

$$k_{nsk}^{\gamma}(X, Y) = \prod_{d=1}^{D} \exp\left(-\frac{1}{2}\frac{(m_d - m'_d)^2}{\sigma_d^2 + (\sigma'_d)^2 + \gamma}\right), \qquad (20)$$

is a positive definite kernel.

Guevara, Jorge, et.al."**Kernel Functions in Takagi-Sugeno-Kang Fuzzy System with Nonsingleton Fuzzy Input.**"

Distance-based kernels on fuzzy sets

Based on the concept of *distance substitution kernels*. **Examples** Kernel $K_D(X, X') = \exp(-\lambda D(X, X')^2)$,is PD when we use the following metric on fuzzy sets: $D(X, X') = \dfrac{\sum_{x\in\Omega} |X(x) - X'(x)|}{\sum_{x\in\Omega} |X(x) + X'(x)|}$.

Guevara, Jorge, et.al. **"Fuzzy Set Similarity using a Distance-Based Kernel on Fuzzy Sets"**, 2016, Book Chapter, Handbook of Fuzzy Sets Comparison - Theory, Algorithms and Applications,pages 103-120

Outline

Fuzzy kernel machines

Definition (Support fuzzy-set machines)

Kernels machines with kernel gram matrix constructed by kernels on fuzzy sets.

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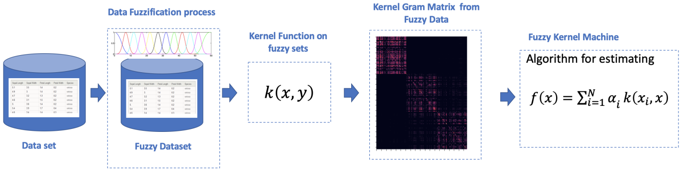
Support fuzzy-set machines learn $f = \sum_i \alpha_i k(X,)$ using the SVM algorithm

Definition (Support fuzzy-sets)

Is the set given by all the fuzzy sets used in a kernel machine such the correspondent $\alpha_i > 0$.

Support fuzzy-set machine example using the **fuzzy-kernel-machines** library (see notebook 4 and 5)



Practical example on supervised classification on noisy data:

Table: Summary of the PIMA dataset

Dataset	%Noise
pima-5an-nn	5%
pima-10an-nn	10%
pima-15an-nn	15%
pima-20an-nn	20%
pima-5an-nc	5%
pima-10an-nc	10%
pima-15an-nc	15%
pima-20an-nc	20%

Pima, 768 observations, 35/65 class rate

Support fuzzy-set machines

Algorithm 1 First fuzzification approach

Input: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$
Output: $\mathcal{MF} = \Big\{\big(x_i, X_1(x_i^1), \ldots, X_D(x_i^D), y_i\big)\Big\}_{i=1}^N$
  for each class y_i **do**
    for $d = 1$ to D **do**
      $q_1, q_2, q_3 = quantile(x^d_{1 \le i \le N}, (0.25, 0.5, 0.75))$
      $\mu_d = q_2$
      $\sigma_d = |q_3 - q_1| / (2 * \sqrt{2 * \log 2})$
      $X_d(.) = \exp(-0.5(. - \mu_d)^2 / \sigma_d^2)$
    end for
  end for

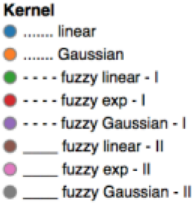
Support fuzzy-set machines

Algorithm 2 Second fuzzification approach

Input: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}$
Output: $\mathcal{MF} = \left\{\left(x_i, X_1(x_i^1), \ldots, X_D(x_i^D), y_i\right)\right\}_{i=1}^{N}$

```
for each class y_i do
    for d = 1 to D do
        h = histogram(x^d_{1≤i≤N})
        h = h/ max(h)
        X_d(.) = linearInterpolation(h)
    end for
end for
```

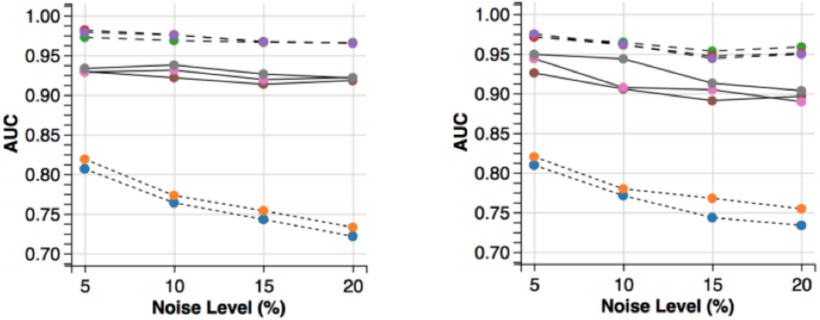
Kernels used on the experiment



$k_1(x, y)$	$k_\times(X, Y)$
Fuzzy linear	$\sum_{\substack{x \in \mathrm{supp}(X), \\ y \in \mathrm{supp}(Y)}} xyX(x)Y(y)$
Fuzzy exp	$\sum_{\substack{x \in \mathrm{supp}(X), \\ y \in \mathrm{supp}(Y)}} \exp(\gamma \langle x, y \rangle) X(x)Y(y)$
Fuzzy Gaussian	$\sum_{\substack{x \in \mathrm{supp}(X), \\ y \in \mathrm{supp}(Y)}} \exp(-\gamma \lVert x - y \rVert^{2}) X(x)Y(y)$

Table

Support fuzzy-set machines



(a) (b)

Conclusions and next steps

- similarity measure between fuzzy sets given by kernels

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- embedding of fuzzy sets into RKHS
- using fuzzy data "as is" in kernel methods
- covariance matrix for fuzzy samples