

Adaptive Distances on Sets of Vectors

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Motivation

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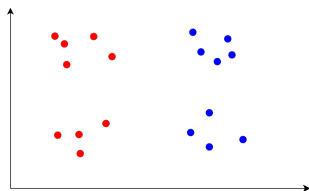
Distance learning for kNN:

- ▶ Learn distance to better separates classes
- ▶ Works well in practice
- ▶ Efficient implementations
- ▶ **Mostly for vectorial data**
 - ▶ Focus on Mahalanobis distance (=linear transformation)

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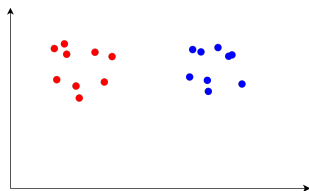
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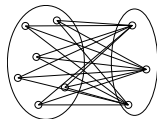
Other structures (sets, graphs)?

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- ▶ Possible to kernelize existing methods

$$K(X_i, X_j) = \sum_{(x_i, x_j) \in X_i \times X_j} k(x_i, x_j)$$

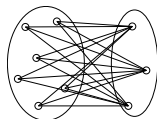


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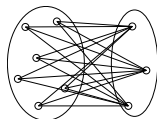
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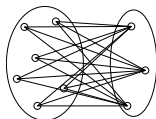
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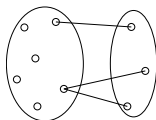
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Our solution:

Learn matching based set distances



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- Artificial Data

- Real world Data

Conclusions and Future Research

Matching Based Set Distances

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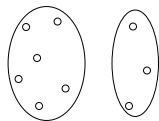
$$D(X_i, X_j) = \mathcal{A}\{d(F) \mid F \in \mathcal{F}\}$$

- ▶ \mathcal{F} : mapping family
- ▶ $F \subseteq X_i \times X_j$
- ▶ $d(F)$: set of pairwise distances d
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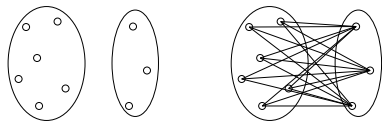
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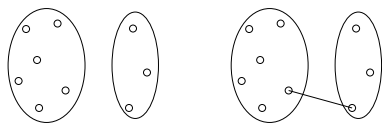


Average Linkage

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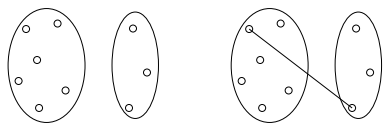


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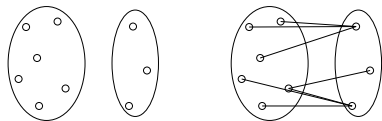


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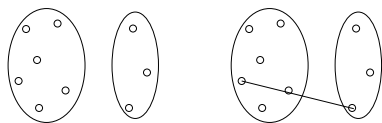


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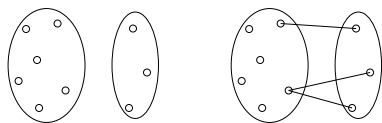


Hausdorff

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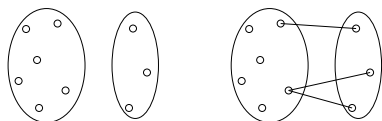


RIBL

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RIBL

- ▶ Other options possible

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Details and empirical results in the paper

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- ▶ We focus on learning \mathbf{A}
 - ▶ Equivalent to learning representation of sets' elements

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- ▶ NCA : **N**eighborhood **C**omponent **A**nalysis

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- ▶ 1 to 10 vectors per set; in \mathbb{R}^{100}
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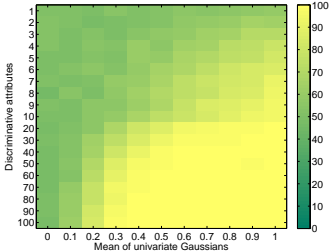
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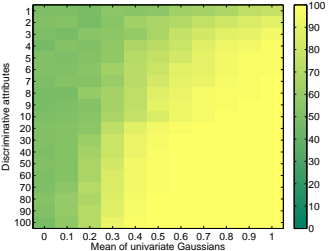
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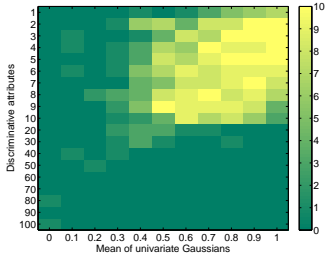
Results



(a) standard set distances



(b) adaptive set distances



(c) significance tests

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Datasets:

Datasets	n	m	p	c
musk1	92	5.17	167	2
musk2	102	64.69	167	2
muta	188	27.89	101	2
fm	349	25.62	51	2
mm	336	25.40	51	2
tiger	200	6.1	230	2
fox	200	6.95	230	2
elephant	200	6.6	230	2

Adaptive distances vs. standard distances

		musk1	musk2	muta	fm	mm	tiger	fox	eleph.
D ^{AL}	D	76.4	71.0	57.6	58.6	63.0	72.0	52.0	76.0
	D_A^f	75.9	71.5	58.2	50.1-	53.5-	74.0	56.5	79.5
	D_A^d	78.0	76.5	68.4+	40.4-	48.1-	78.5+	59.5+	77.0
D ^{SL}	D	81.1	77.2	42.2	41.6	39.3	76.0	56.5	71.5
	D_A^f	78.4	69.5	41.6	41.6	39.3	73.5	57.5	72.5
	D_A^d	82.4	68.5-	42.8	41.6	39.3	79.0	61.5+	72.5
D ^{CL}	D	67.5	71.5	39.4	43.2	40.9	67.5	54.5	64.5
	D_A^f	71.7	65.5	56.3+	47.3	46.6+	68.5	47.0	55.5
	D_A^d	77.3+	79.5+	58.2+	52.1+	58.1+	72.5	51.5	74.0+
D ^H	D	81.3	78.0	75.5	46.8	48.3	74.0	51.5	74.5
	D_A^f	83.5	73.3	77.5	57.5+	57.2+	74.0	55.5	65.5
	D_A^d	78.8	77.2	80.6+	57.2+	53.8+	76.5	65.5+	75.5
D ^{SMD}	D	83.3	75.2	79.4	56.6	58.2	77.5	60.0	79.5
	D_A^f	77.1	73.3	81.4+	58.5	58.3	76.0	59.0	77.5
	D_A^d	81.3	73.3	80.5	56.6	58.7	85.0+	62.0	85.5+

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- Usually there exists a mapping better than cross product

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D ^H	D	81.3	78.0	75.5	46.8	48.3	74.0	51.5	74.5
	D_A^f	83.5	73.3	77.5	57.5+	57.2+	74.0	55.5	65.5
	D_A^d	78.8	77.2	80.6+	57.2+	53.8+	76.5	65.5+	75.5
D ^{SMD}	D	83.3	75.2	79.4	56.6	58.2	77.5	60.0	79.5
	D_A^f	77.1	73.3	81.4+	58.5	58.3	76.0	59.0	77.5
	D_A^d	81.3	73.3	80.5	56.6	58.7	85.0+	62.0	85.5+

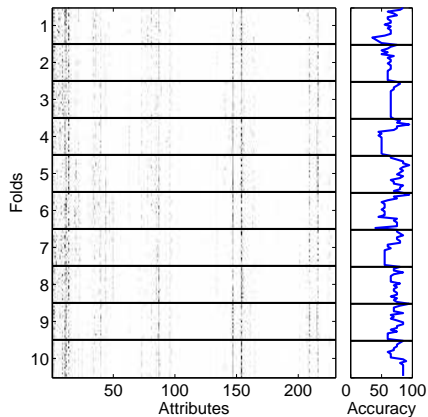
- ▶ Usually there exists a mapping better than cross product
- ▶ D_A^d usually better than D

Adaptive distances vs. standard distances

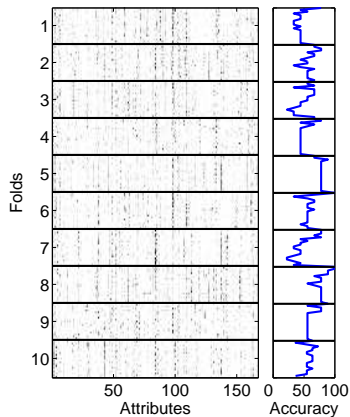
		musk1	musk2	muta	fm	mm	tiger	fox	eleph.
D ^{AL}	D	76.4	71.0	57.6	58.6	63.0	72.0	52.0	76.0
	D_A^f	75.9	71.5	58.2	50.1-	53.5-	74.0	56.5	79.5
	D_A^d	78.0	76.5	68.4+	40.4-	48.1-	78.5+	59.5+	77.0
D ^{SL}	D	81.1	77.2	42.2	41.6	39.3	76.0	56.5	71.5
	D_A^f	78.4	69.5	41.6	41.6	39.3	73.5	57.5	72.5
	D_A^d	82.4	68.5-	42.8	41.6	39.3	79.0	61.5+	72.5
D ^{CL}	D	67.5	71.5	39.4	43.2	40.9	67.5	54.5	64.5
	D_A^f	71.7	65.5	56.3+	47.3	46.6+	68.5	47.0	55.5
	D_A^d	77.3+	79.5+	58.2+	52.1+	58.1+	72.5	51.5	74.0+
D ^H	D	81.3	78.0	75.5	46.8	48.3	74.0	51.5	74.5
	D_A^f	83.5	73.3	77.5	57.5+	57.2+	74.0	55.5	65.5
	D_A^d	78.8	77.2	80.6+	57.2+	53.8+	76.5	65.5+	75.5
D ^{SMD}	D	83.3	75.2	79.4	56.6	58.2	77.5	60.0	79.5
	D_A^f	77.1	73.3	81.4+	58.5	58.3	76.0	59.0	77.5
	D_A^d	81.3	73.3	80.5	56.6	58.7	85.0+	62.0	85.5+

- ▶ Usually there exists a mapping better than cross product
- ▶ D_A^d usually better than D
- ▶ D_A^f are not as good

Non-convexity of NCA

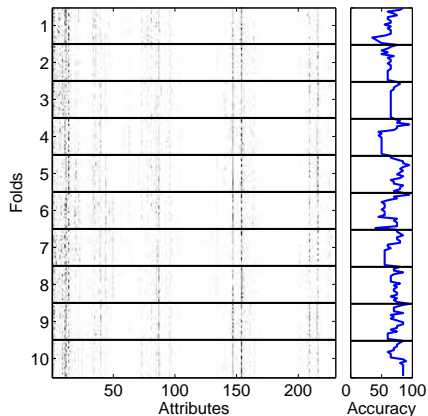


(e) tiger, D^H

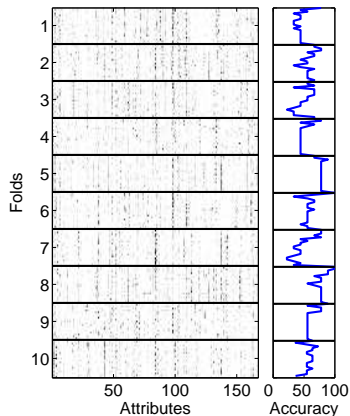


(g) musk1, D^H

Non-convexity of NCA



(i) tiger, D^H



(k) musk1, D^H

- ▶ Local optimas are present

Outline

Set Distances

Learning Set Distances

Experiments

- Artificial Data

- Real world Data

Conclusions and Future Research

Conclusions and Open Problems

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Pros:

- ▶ Practical problem with many applications
- ▶ General framework

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Future research:

- ▶ Directly learn \mathcal{F} and \mathcal{A} in

$$D(X_i, X_j) = \mathcal{A}\{d(F) \mid F \in \mathcal{F}\}$$

Thank you!