Learning with invariants

Master's Thesis

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Introduction

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- But the data may have useful statistical information...
- Enter the Learning Using Statistical Invariants (LUSI) paradigm!
- Goal: Exploit statistical information of the training data in order to find better approximations of the goal function.

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4. Extend the learning paradigm to multiclass classification problems.

Learning using statistical invariants

Strong and weak modes of convergence (I)

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2. The inner product between functions

$$R(f_1, f_2) = \langle f_1(x), f_2(x) \rangle$$

   which has to satisfy the corresponding requirements.

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$$\lim_{l \to \infty} \langle P_l(y = 1|x) - P(y = 1|x), \psi(x) \rangle = 0 \quad \forall \psi(x) \in L_2$$

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- These important properties are called invariants.

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The main goal of this paradigm is to find an approximation of the conditional probability function that preserves the specified invariants. Mathematically, this can be expressed as:

$$\frac{1}{l}\sum_{i=1}^{l}\psi_s(x_i)P_l(y=1|x_i) \approx \frac{1}{l}\sum_{i=1}^{l}y_i\psi_s(x_i), \quad s=1,\ldots,m$$

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Invariant selection

The authors propose a method to select new invariants. Given a predicate ψ_{m+1}, we first evaluate the following expression:

$$\mathcal{T} = \frac{\left|\sum_{i=1}^{l} \psi_{m+1}(x_i) P_l^m(y=1|x_i) - \sum_{i=1}^{l} y_i \psi_{m+1}(x_i)\right|}{\sum_{i=1}^{l} y_i \psi_{m+1}(x_i)}$$

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If $\mathcal{T} \geq \delta$ for some small threshold δ, then the new invariant defined by predicate ψ_{m+1} is selected. Otherwise, it is disregarded.

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  - First order invariant (mean or centroid of positive class elements):

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$$f(x) = \underbrace{\overbrace{A^T}^{\text{vector of coefficients}} \mathcal{K}(x)}_{\mathcal{K}(x):\ \text{vector of kernel functions evaluated on training data}} + \overbrace{c}^{\text{bias}}$$

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Note

In the most simple case, the $V-$matrix can be replaced with the identity matrix.

Solving the learning problem (III)

We can formulate and solve a minimization problem subject to the invariants equality constraints that has a closed-form solution.

The coefficients vector A can be computed as

$$A = (A_V - cA_c) - \left(\sum_{s=1}^{m} \mu_s A_s \right)$$

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$$A = (A_V - cA_c) - \left(\sum_{s=1}^{m} \mu_s A_s \right)$$

where

$$A_V = (VK + \gamma I)^{-1} VY$$
$$A_c = (VK + \gamma I)^{-1} V 1_l$$
$$A_s = (VK + \gamma I)^{-1} \Phi_s, \quad s = 1, \ldots, n$$

Solving the learning problem (IV)

The values of c and the m coefficients μ_s can be obtained solving the following system of equations:

$$c[1_l^T VKA_c - 1_l^T V1_l] + \sum_{s=1}^{m} \mu_s [1_l^T VKA_s - 1_l^T \Phi_s] = [1_l^T VKA_V - 1_l^T VY]$$

$$c[A_c^T K\Phi_k - 1_l^T \Phi_k] + \sum_{s=1}^{m} \mu_s A_s^T K\Phi_k = [A_V^T K\Phi_k - Y^T \Phi_k], \quad k = 1, \dots, m$$

Overview of the LUSI algorithm

Step 1: Construct an estimate of the conditional probability function without considering the predicates.

Step 2: Find the maximal disagreement value $\mathcal{T}_s$ for vectors

$$\Phi_k = (\psi_k(x_1), \ldots, \psi_k(x_l))^T, \quad k = 1, \ldots, m$$

Step 3: If $\mathcal{T}_s > \delta$, add the invariant associated to the predicate ψ_s; otherwise stop.

Step 4: Find a new approximation of the conditional probability function and go back to **Step 2**; otherwise stop.

Main results and limitations

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Limitations

- Invariants are problem specific.
- Invariant selection can sometimes be a "black-art".
- Invariants only consider statistical information of the positive class, hence it cannot be directly applied to multiclass classification problems.

Proposals

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- Two new general use invariants based on random processes: random projections and random hyperplanes.
- An extension of the original algorithm to consider the negative class and all classes in multiclass classification problems using Error Correcting Output Codes (ECOC).

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$p \sim \mathcal{N}(\mu, \Sigma)$, projection vector

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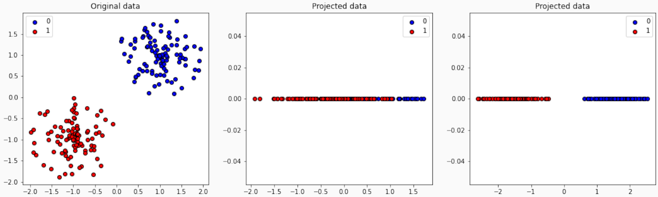

Figure 1: Examples of the random projection invariant.

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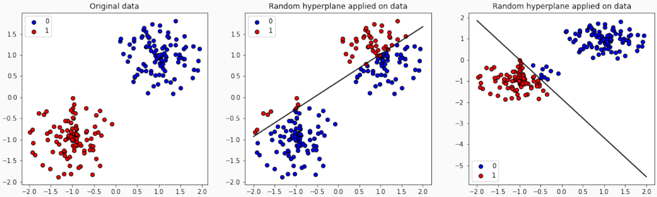

Figure 2: Examples of the random hyperplane invariant.

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1. Generate new invariants at each iteration.
2. Allow the algorithm to try new invariants when no invariant is selected.
3. Limit the number of tries so that the algorithm does not end up in an infinite loop.

Extending LUSI with ECOC (I)

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- For each one of the N_c classes we create a codeword of length n. These codewords are organized as the rows of a matrix $M \in \{0, 1\}^{N_c \times n}$ called the coding matrix.

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- Each column of the matrix is treated as an individual classification problem and a binary classifier is fit with the transformed data.

Extending LUSI with ECOC (II)

	h_1	h_2	h_3	h_4	h_5
C1	1	0	0	0	0
C2	0	1	0	0	0
C3	0	0	1	0	0
C4	0	0	0	1	0
C5	0	0	0	0	1

	h_1	h_2	h_3	h_4	h_5
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C2	0	1	1	0	1
C3	1	0	0	1	0
C4	0	1	0	1	0
C5	0	0	1	0	1

Table 1: Two examples of coding matrices. The left one represents a special coding called one-against-all.

Extending LUSI with ECOC (III)

Let $f(x) = (f_1(x), \dots, f_n(x))$ be the vector containing the predictions for each one of the problems. In order to obtain the final output class, we have to decode this vector, which can be done using the following expression:

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In our proposal we use a vector of predicted probabilities and the Euclidean distance.

Experimentation and results

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Experimentation with two types of datasets with different goals in mind:

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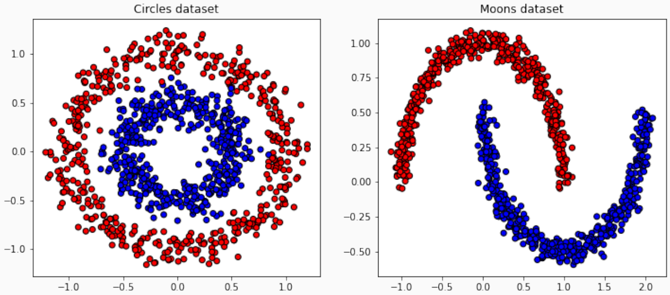
- Toy datasets
    - Compare the different invariants.
    - Compare the original algorithm with the ECOC version.
    - Find interesting properties of the invariants.
- Real datasets
    - Assess the quality of the proposed invariants.

Experimentation with toy datasets

Compare Vapnik's invariants (zeroth and first order) with random projections and random hyperplanes on the Circles and Moons datasets.



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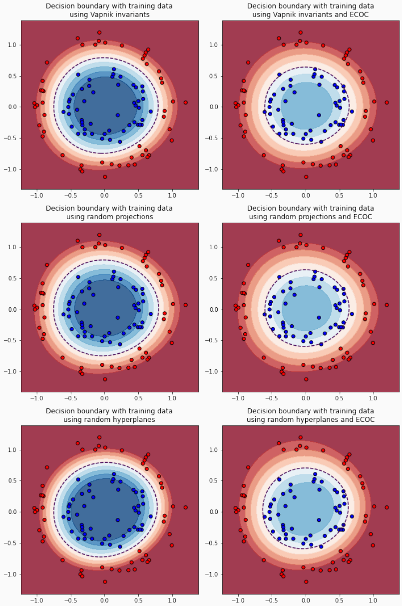
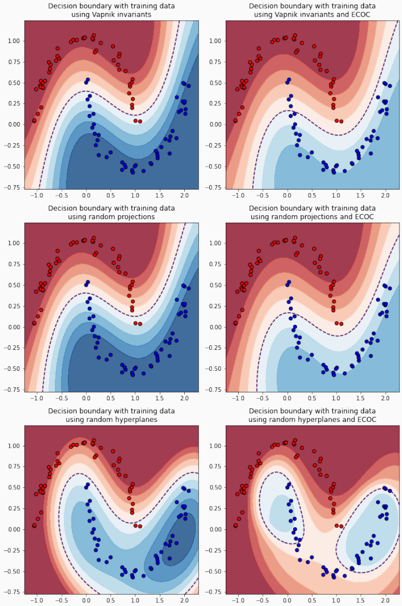
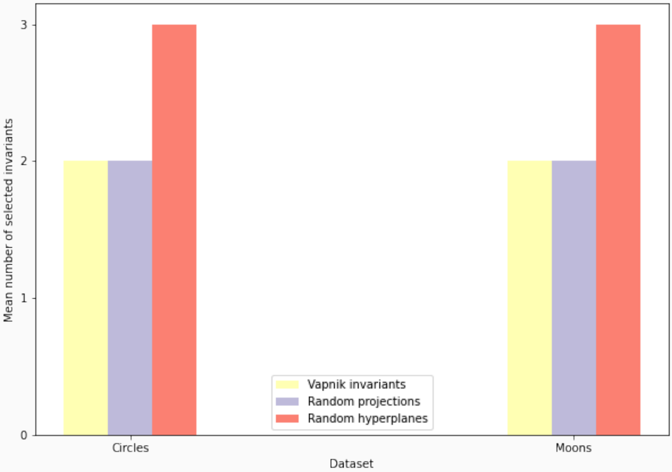


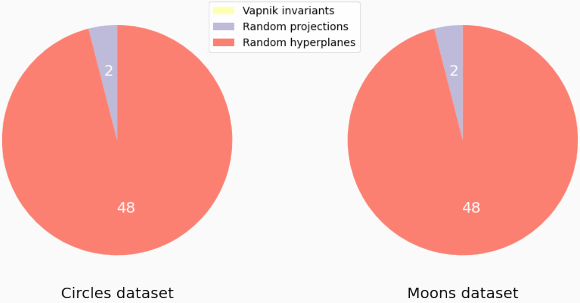
Comparing LUSI with the ECOC version (II)



Comparing the number of selected invariants



Exploring the bias towards certain types of invariants



Experimentation with real datasets

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- Evaluate the models using different subsamples of the training data: 100%, 50% and 10% of the training partition.

Selected datasets

Problem	Num. examples	Attributes	Classes
Balance Scale	625	4	3
Ecoli	336	8	8
Glass	214	9	6
Iris	150	4	3
Yeast	1484	8	10

Results

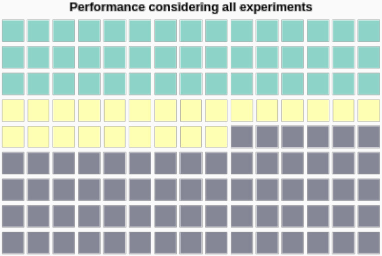
Dataset	Baseline model	Vapnik invariants	Random projections	Random hyperplanes
Balance Scale	$91.47 \pm 0.38\%$	$91.47 \pm 0.38\%$	$\mathbf{91.73 \pm 0.38}\%$	$90.13 \pm 1.51\%$
Ecoli	$85.29 \pm 2.08\%$	$\mathbf{85.29 \pm 1.20}\%$	$84.15 \pm 2.05\%$	$75.98 \pm 6.28\%$
Glass	$\mathbf{72.87 \pm 7.91}\%$	$\mathbf{72.87 \pm 7.91}\%$	$72.09 \pm 7.44\%$	$71.06 \pm 7.60\%$
Iris	$\mathbf{96.67 \pm 0.00}\%$	$95.56 \pm 1.57\%$	$95.19 \pm 1.66\%$	$88.52 \pm 11.56\%$
Yeast	$53.76 \pm 1.04\%$	$\mathbf{53.87 \pm 1.20}\%$	$52.53 \pm 5.44\%$	$50.39 \pm 5.33\%$

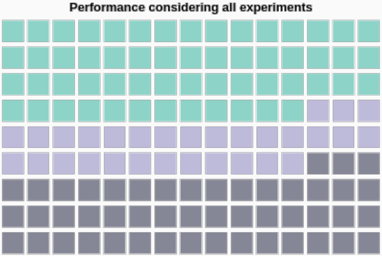
Table 2: Results using 100% of the training data.

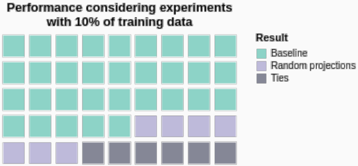
Dataset	Baseline model	Vapnik invariants	Random projections	Random hyperplanes
Balance Scale	$\mathbf{88.80 \pm 1.73}\%$	$87.73 \pm 2.10\%$	$83.73 \pm 7.17\%$	$76.00 \pm 12.77\%$
Ecoli	$71.57 \pm 1.39\%$	$\mathbf{72.55 \pm 4.22}\%$	$67.32 \pm 4.03\%$	$63.89 \pm 9.61\%$
Glass	$\mathbf{56.59 \pm 4.78}\%$	$45.74 \pm 6.67\%$	$52.45 \pm 7.03\%$	$45.48 \pm 9.50\%$
Iris	$\mathbf{93.33 \pm 2.72}\%$	$90.00 \pm 4.71\%$	$77.78 \pm 22.93\%$	$84.81 \pm 9.04\%$
Yeast	$\mathbf{47.92 \pm 2.08}\%$	$47.92 \pm 2.14\%$	$45.68 \pm 4.60\%$	$37.82 \pm 7.92\%$

Table 3: Results using a subsample of 10% of the training data.

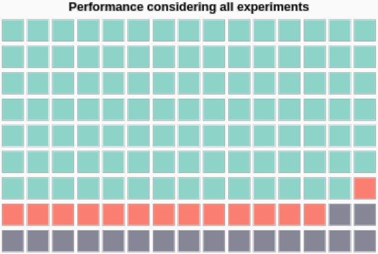
Comparing the invariants on individual problems (I)

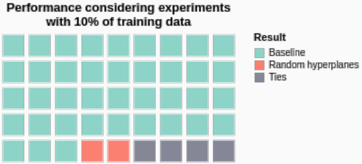


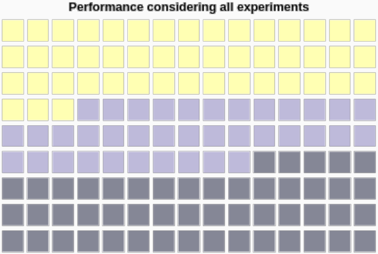




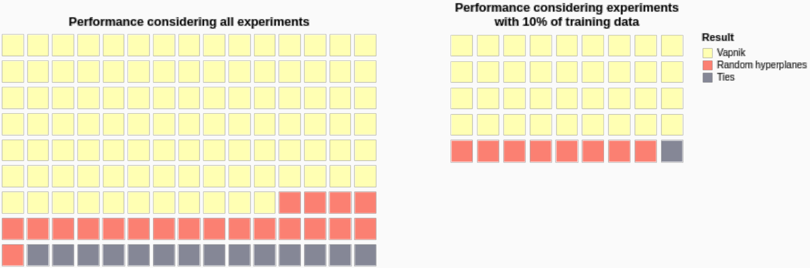
Comparing the invariants on individual problems (II)

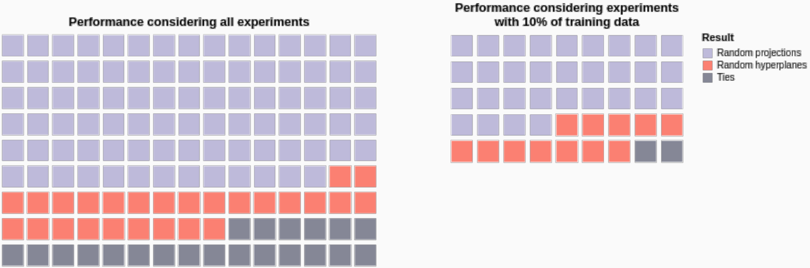






Comparing the invariants on individual problems (III)





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- ✗ Automatized the selection process of the most suitable invariants for a given problem.
- ✓ Extend the learning paradigm to multiclass classification problems.
  - Created a small software module containing the different invariants and both the original and ECOC version of LUSI.

Future work

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- Improve random projections by constructing an orthogonal space from random vectors.

Thank you for your attention!

Questions?