How to define a rejection class based on model learning?

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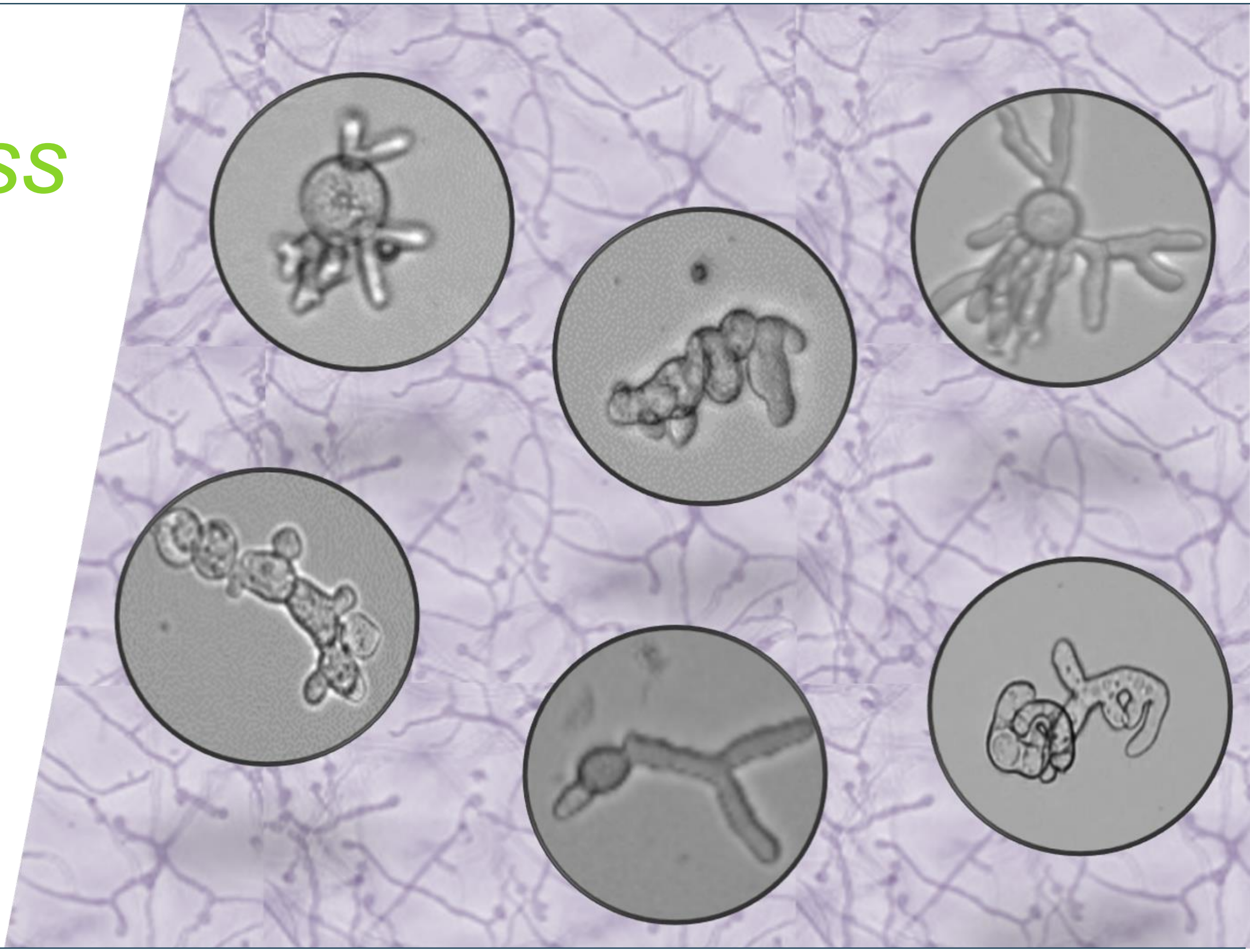


Outline

1

Introduction: Short review on rejection class

2

Proposed strategy

- Model learning
  - Fuzzy membership function (FMF)
    - Here, FMF = Probability Density Function (PDF)
  - Thresholds on the PDFs

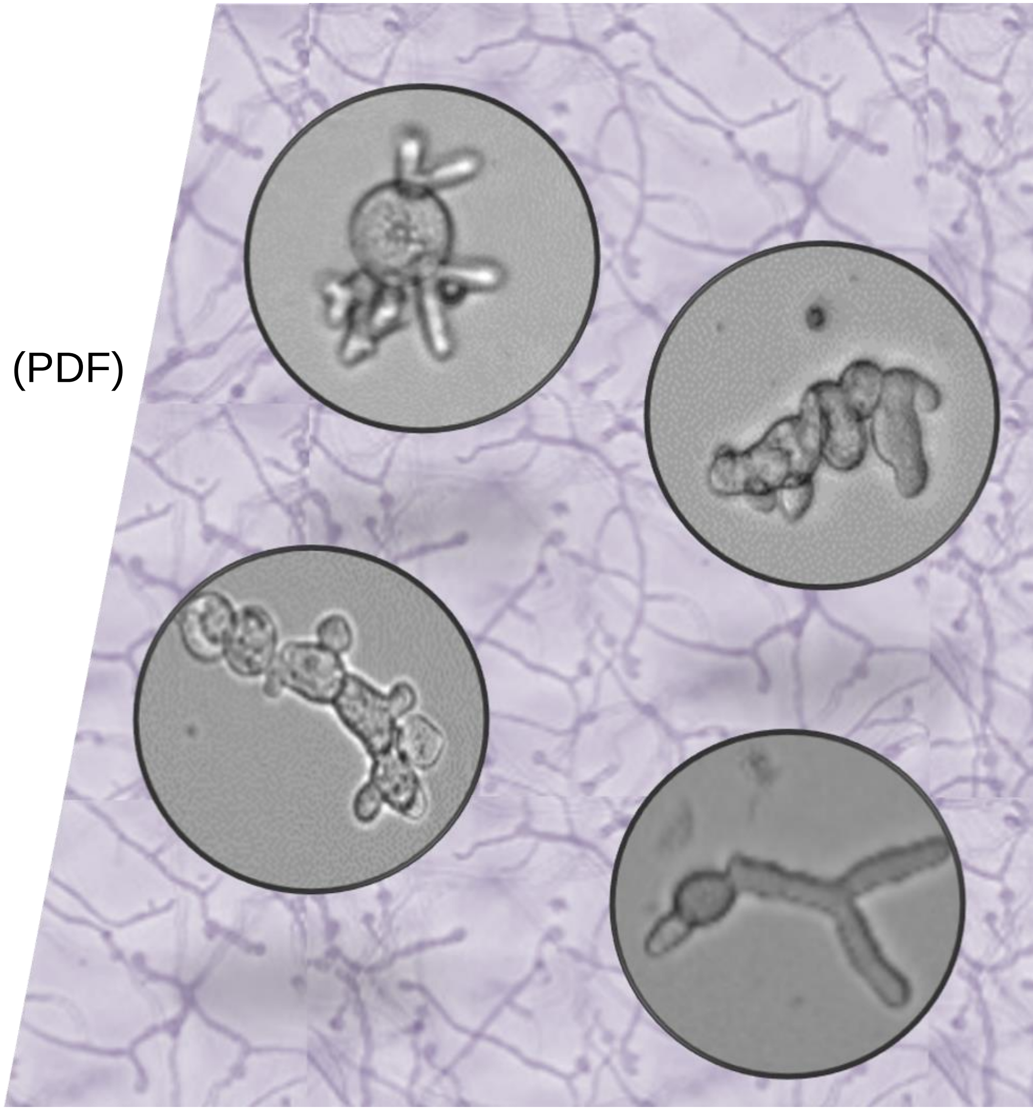
3

Experimental results

- Biological context
- Learning set and feature vectors for model estimation
  - Deep Neural Network (DNN)
    - Bottlenecks
    - Outputs layer
- Learning and Test Procedure
- Results and analysis

4

Conclusion



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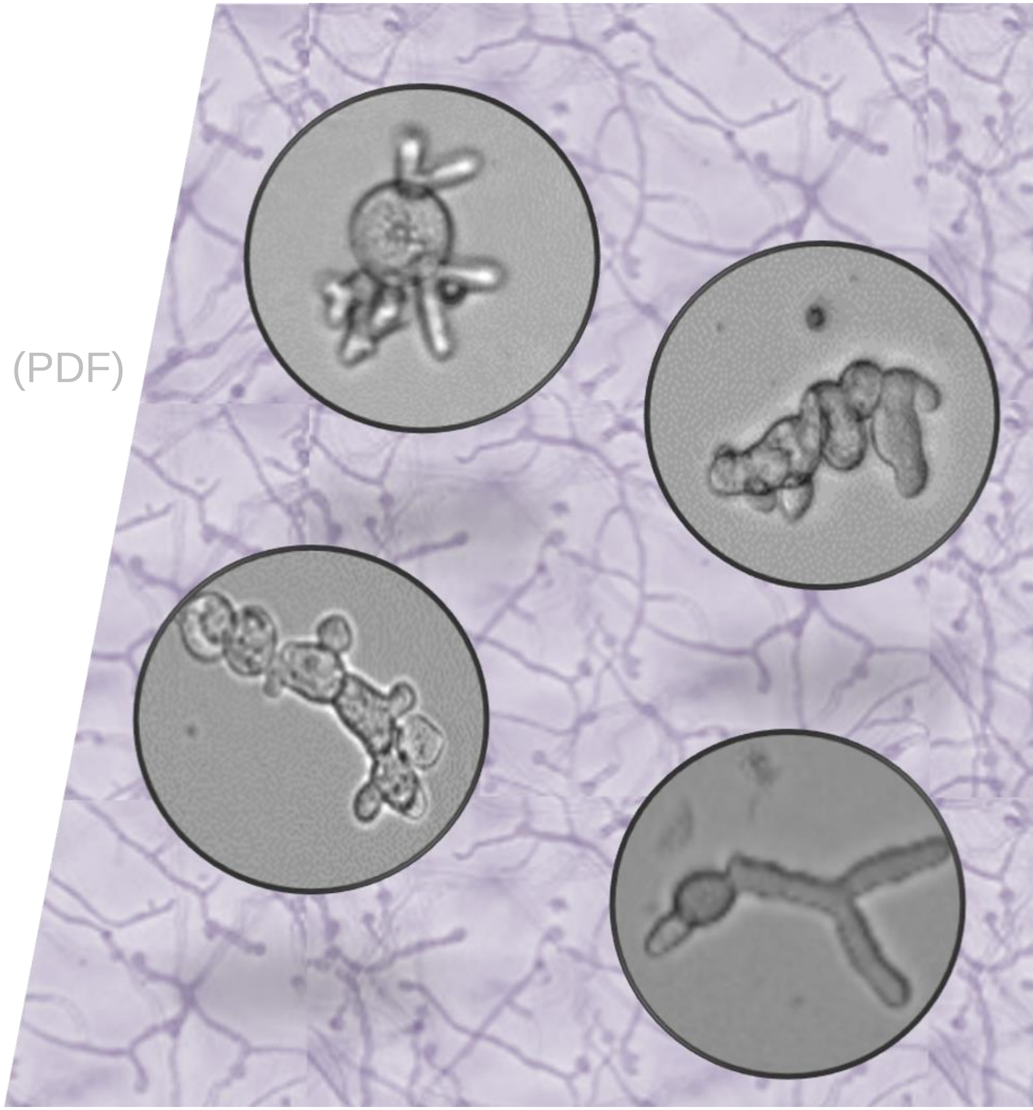

Introduction

State of the Art : How to classify images with rejection class ?

Supervised classification: optimize the accuracy of classifying data into the classes that appear in the learning set

- Classifier = feature space splitter which focuses on optimizing the frontiers between classes

Rejection option added to a classifier

- Examples in literature:
  - k-Nearest neighbor classifier: threshold on the distance to the neighbors (1)
  - SVM: threshold on the distance to the maximum-margin hyperplane (2)
  - Deep Neural Network: threshold on the output = confidence score of the prediction (3)

System where the prediction model **and** the selection mechanism are optimized simultaneously

- Examples in literature:
  - Deep Neural Network (4)(5)

Better approach:

- Take into account the possibility of rejecting a sample in the classifier design
- Pay attention to the space in-between known classes or away from them

(1) Mukherjee, Sayan, et al. *Support vector machine classification of microarray data*. AI Memo 1677, Massachusetts Institute of Technology, 1999.
(2) Hellman, Martin E. "The nearest neighbor classification rule with a reject option." *IEEE Transactions on Systems Science and Cybernetics* 6.3 (1970): 179-185.
(3) Chow, C. "On optimum recognition error and reject tradeoff." *IEEE Transactions on information theory* 16.1 (1970): 41-46.
(4) Geifman, Yonatan, and Ran El-Yaniv. "Selective classification for deep neural networks." *Advances in neural information processing systems* 30 (2017): 4878-4887.
(5) Geifman, Yonatan, and Ran El-Yaniv. "Selectivenet: A deep neural network with an integrated reject option." *arXiv preprint arXiv:1901.09192* (2019).

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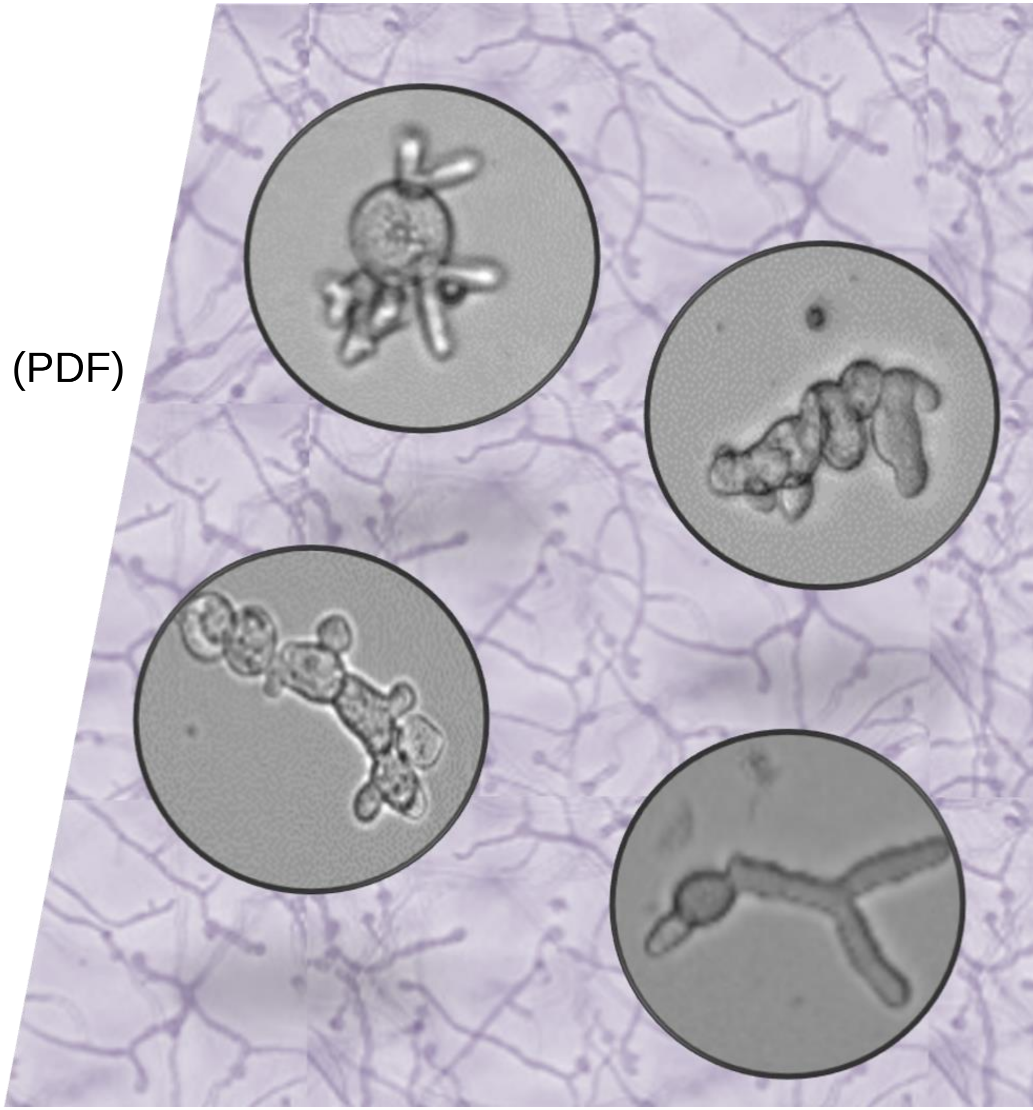
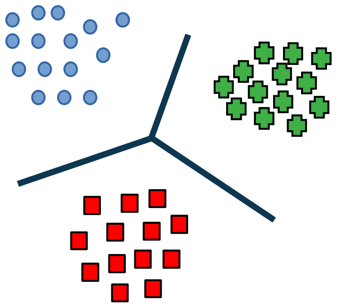
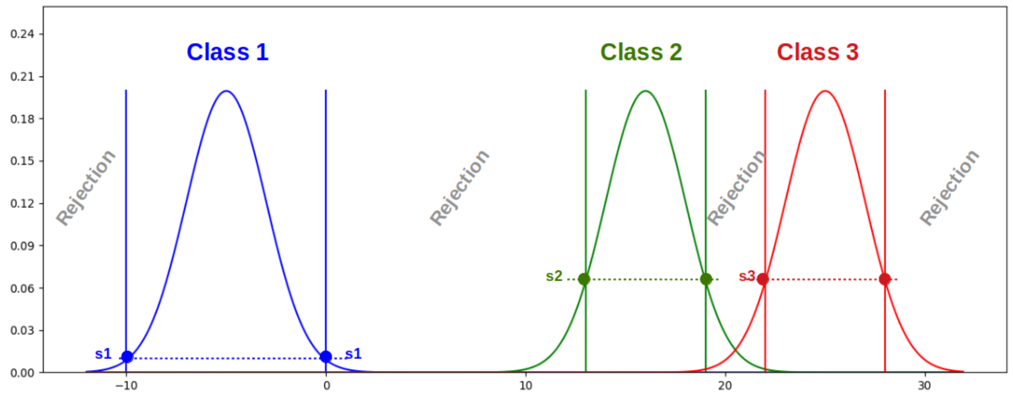


Proposed strategy

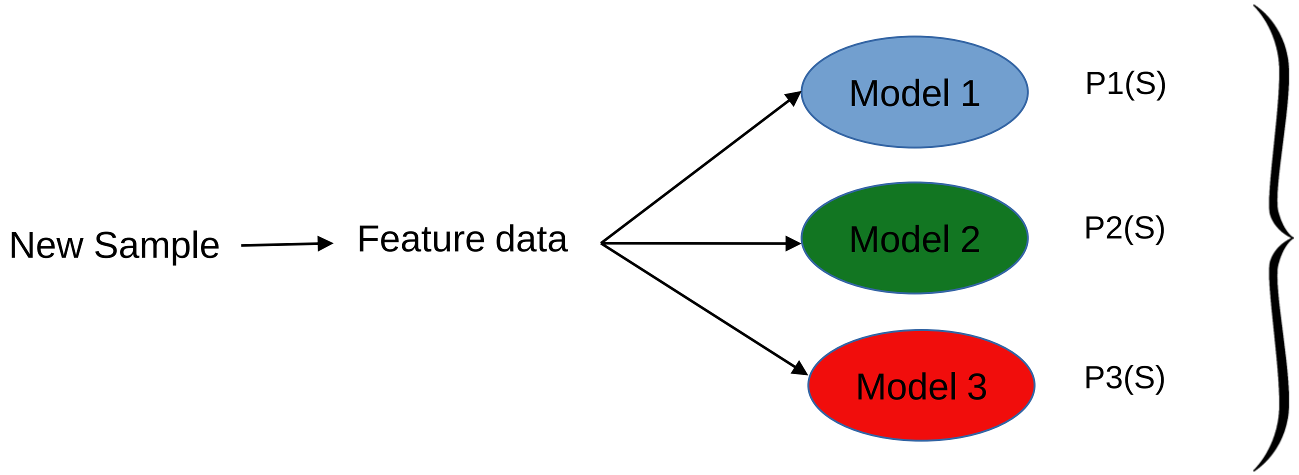
Model and Model Threshold Learning



- Learning
  - One model per class, independently
  - One threshold per model, accounting for classes overlapping



- Prediction
  - Each model accepts or rejects a new sample based on threshold



- One model accepts => associate class
- Several models accept => associate class of <u>hightest</u> model acceptance value
- All models reject => rejection class

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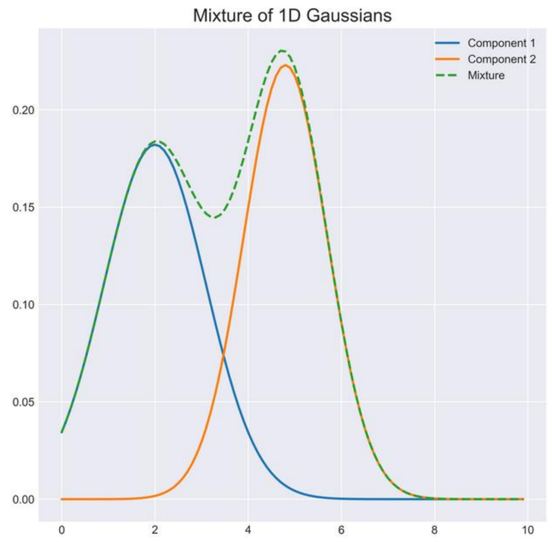
Proposed strategy

Model and Model Threshold Learning



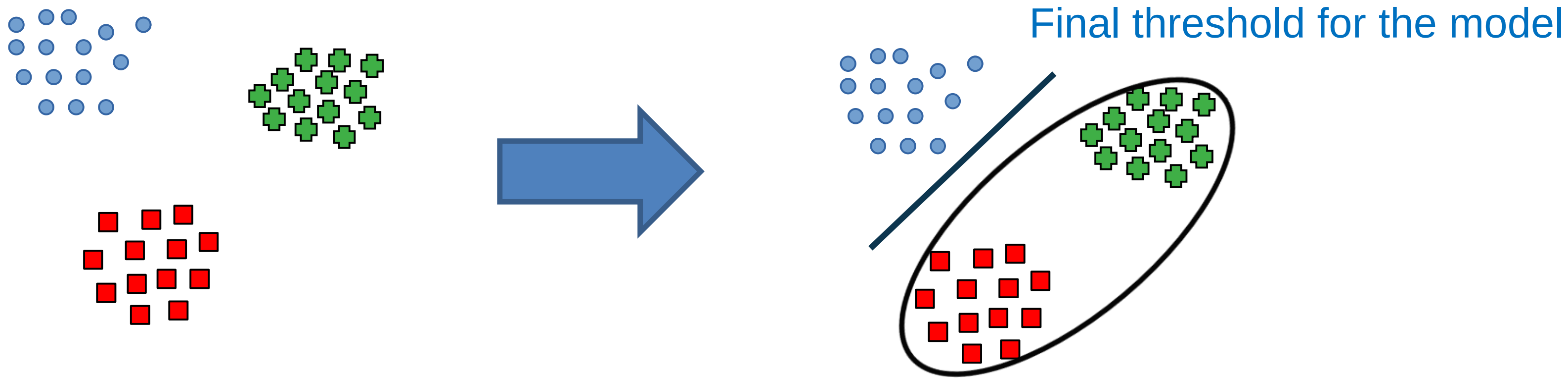
- Model type : Gaussian mixture

  → Probability distributions represented as combination of simpler “component” distributions

  → Estimation using EM algorithm

- PDF threshold learning: Two options

  - **1-vs.-all** : Meta-class 0: sample from current class (blue) / Meta-class 1: samples from all other classes



1 vs. all

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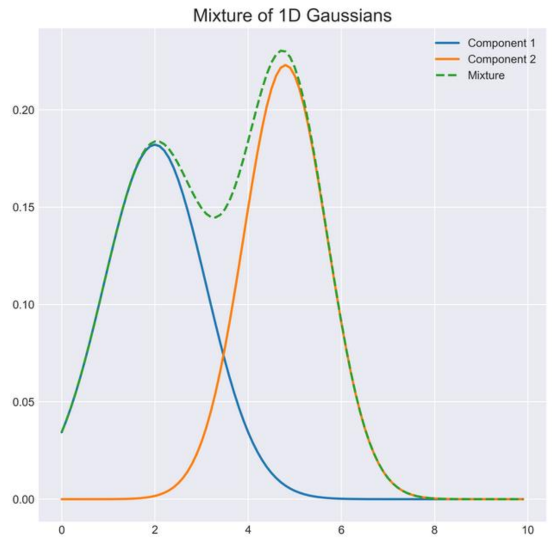
Proposed strategy

Model and Model Threshold Learning



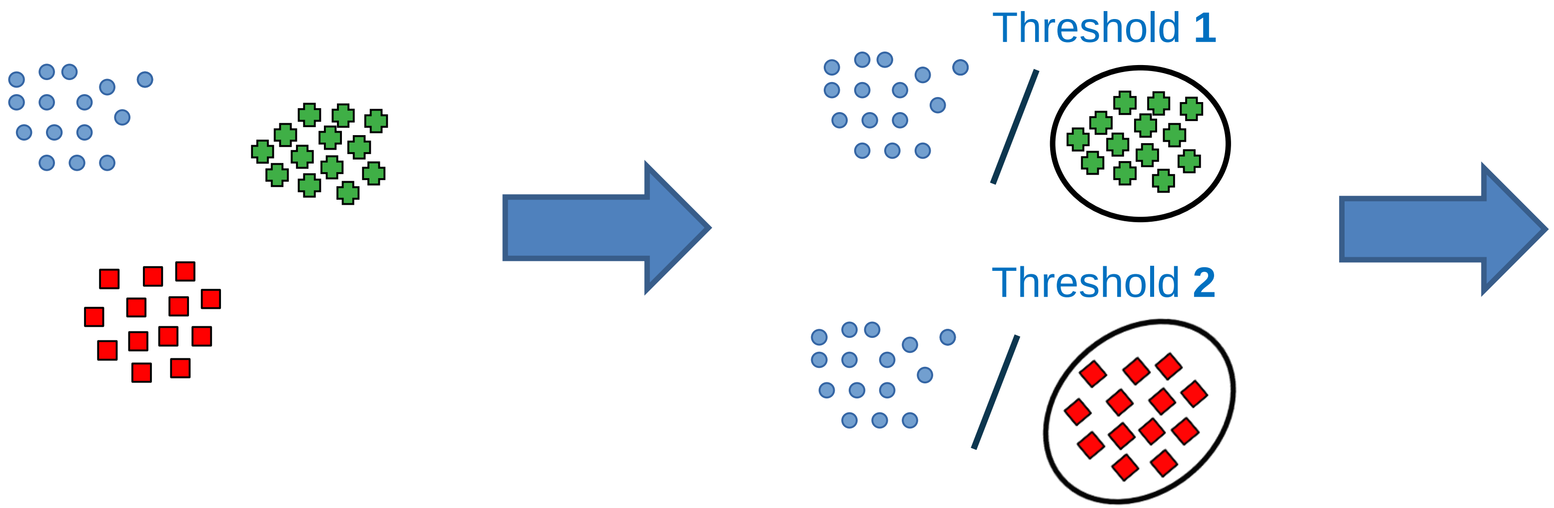
- Model type : Gaussian mixture

  → Probability distributions represented as combination of simpler “component” distributions

  → Estimation using EM algorithm

- PDF threshold learning: Two options

  - **1-vs.-1** : Meta-class 0: sample from current class (blue) / Meta-class 1: sample from each of other classes in turn



Final threshold for the model = maximum between them

1 vs. 1

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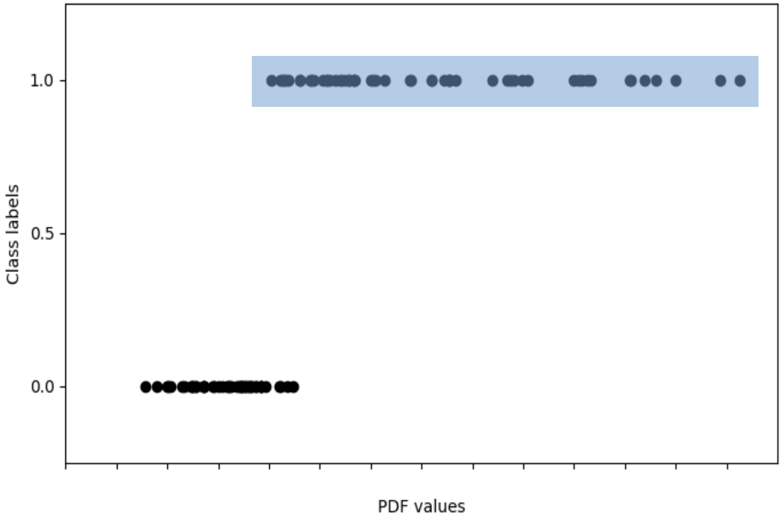
Proposed strategy

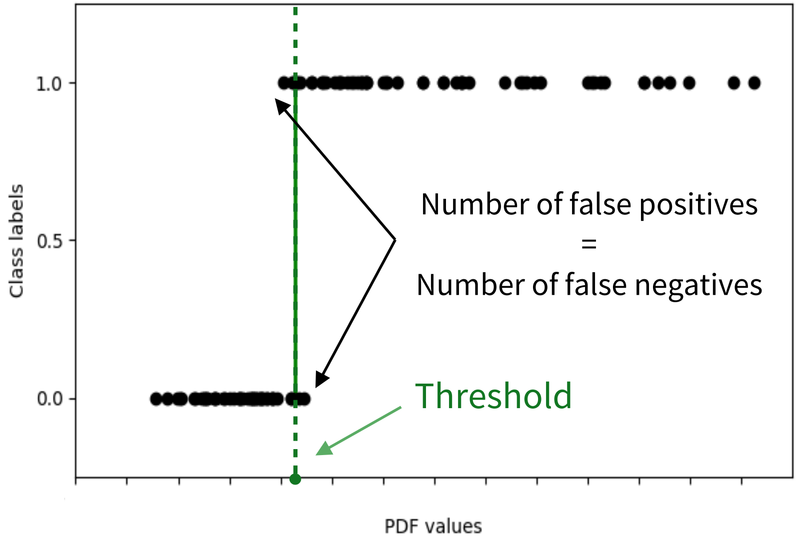
Model and Model Threshold Learning

- PDF threshold learning:

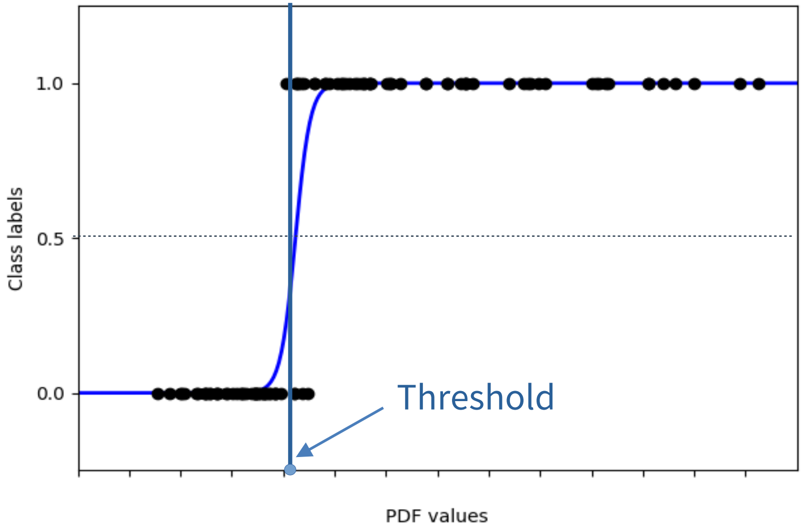
- Two options (1 vs. All or 1 vs. 1)
- Two methods:



Misclassification-based



Regression-based



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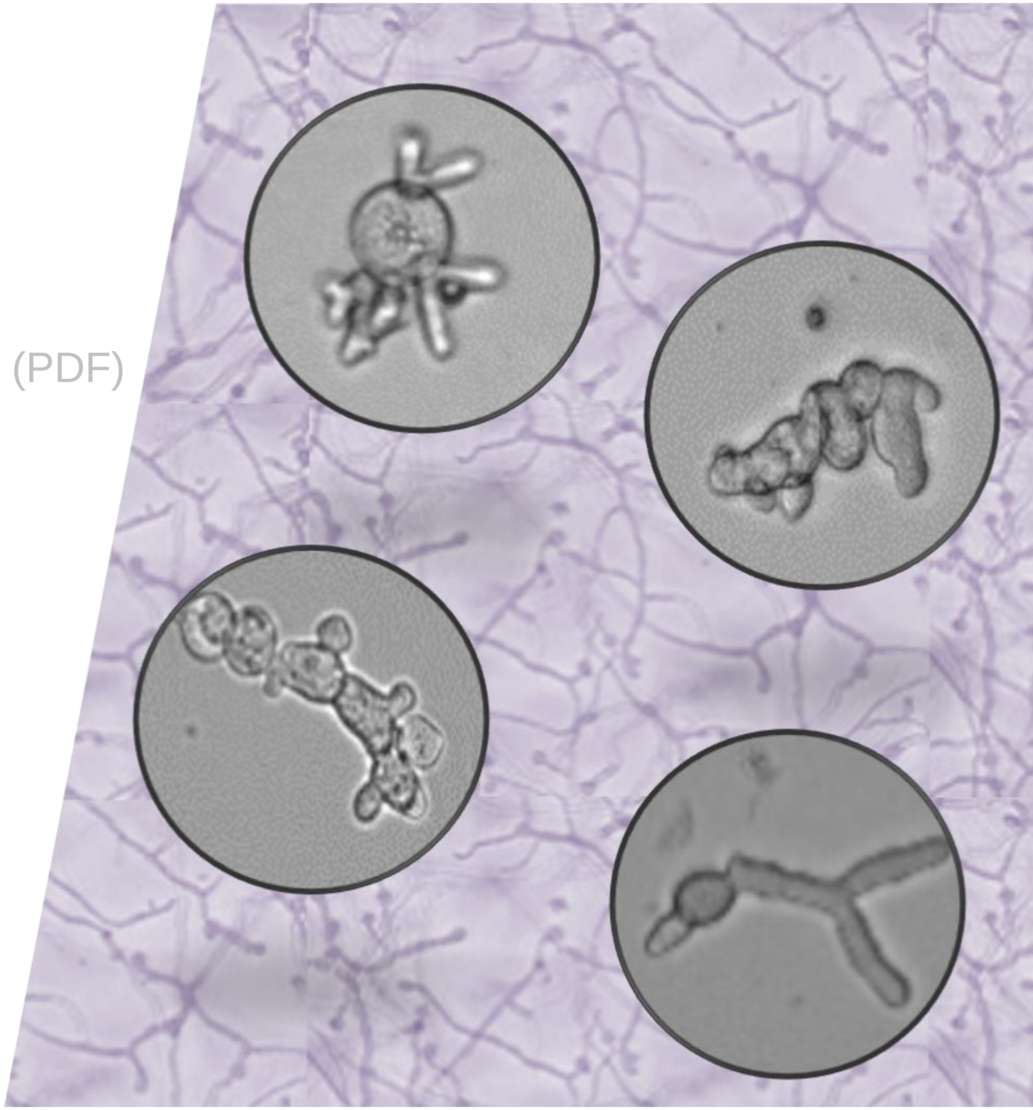

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Experimental results

Biological context: the power of fungi phenotyping to classify molecules based on their Mode of Action

<u>Bayer Disease Control Research</u>
Center focusing on Disease Control

Fungal Pathogens

Fungicides

- Fungicides are classified based on their Mode of Action
- Fungicides with different Mode of Action can show remarkable phenotype *in vitro* liquid culture conditions
- Model of interest : the gray mold *Botrytis cinerea*

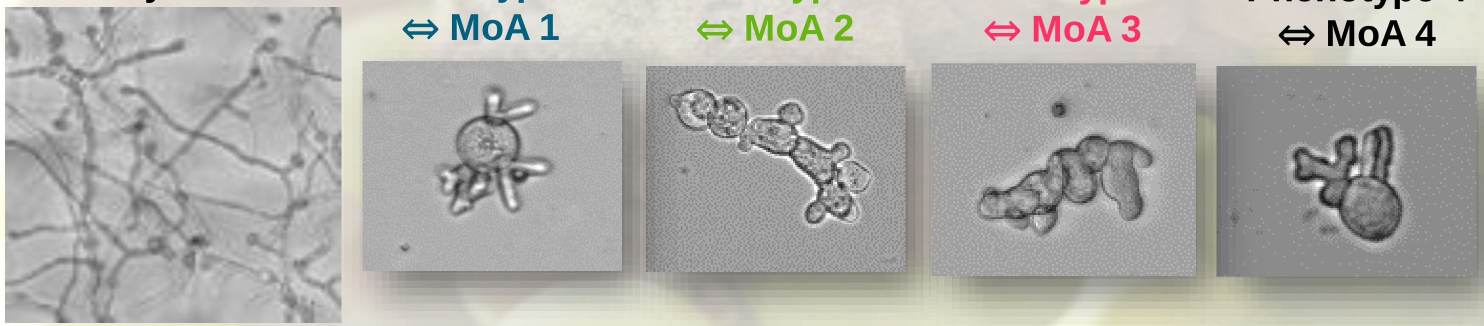
Untreated ⇔ Mycelium

Phenotype 1 ⇔ MoA 1

Phenotype 2 ⇔ MoA 2

Phenotype 3 ⇔ MoA 3

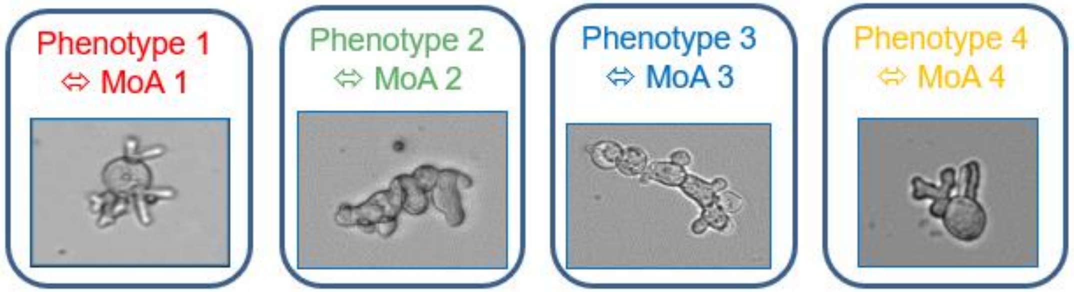
Phenotype 4 ⇔ MoA 4



- Fungicides can be clustered according to morphological induced defects

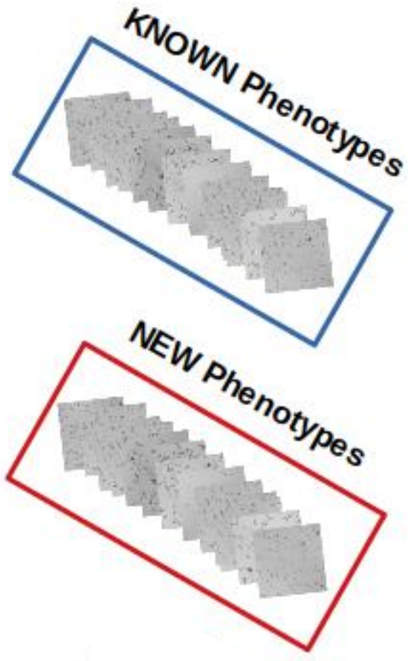
Experimental results

Learning set and feature vectors for model estimation



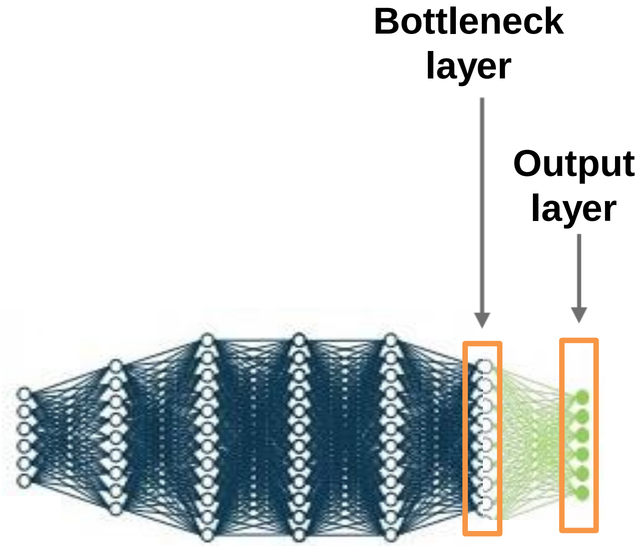
- 4 known classes = 4 fungi phenotypes
- 1 rejection class = future new phenotypes

- 2 feature choices
  - Bottleneck (layer)
  - Output (layer)



Class	Sub_Images Number
0	4752
1	3600
2	3728
3	2760
4	4607
5	6928
6	3998
NEW PH	10352

*Images pre-processing:
1 Image (2160*2160) → 16 sub-images
(500*500) → 16 resized sub-images (240*240)



MobileNet Network fine tuning
*Trained on ImageNet database

Experimental results

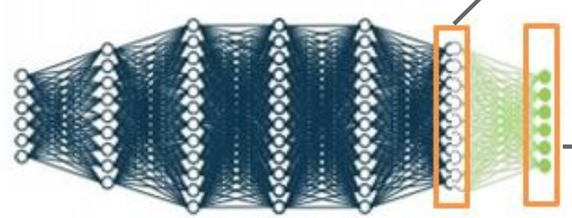
Learning set and feature vectors for model estimation

Feature preprocessing

Bottlenecks

- Dimension = 1001

⇒ Dimension reduction: Variable importance or PCA



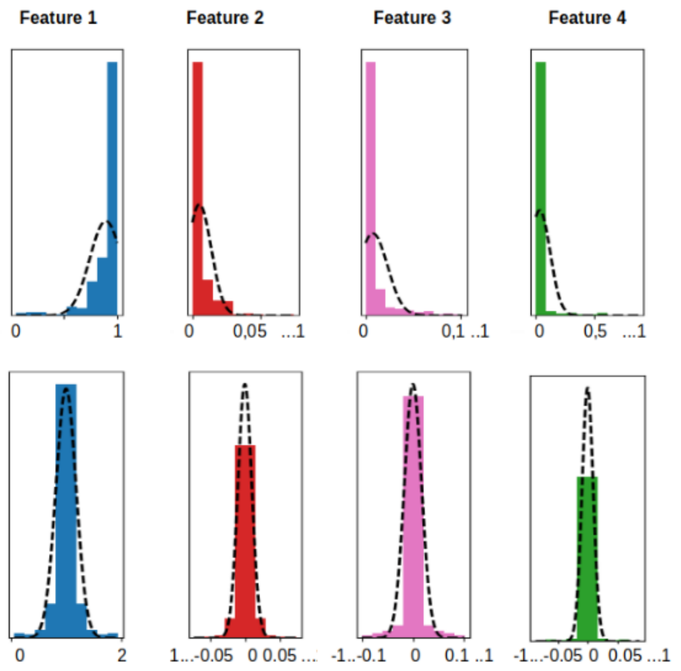
MobileNet Network fine tuning
*Trained on ImageNet database

Output

- Dimension = number of class

Components in [0,1]
with high density close to 0 or close to one

⇒ Not adapted to Gaussian mixture modeling
⇒ Data symmetrization (2^d more samples)



Original and symmetrized data output class 1

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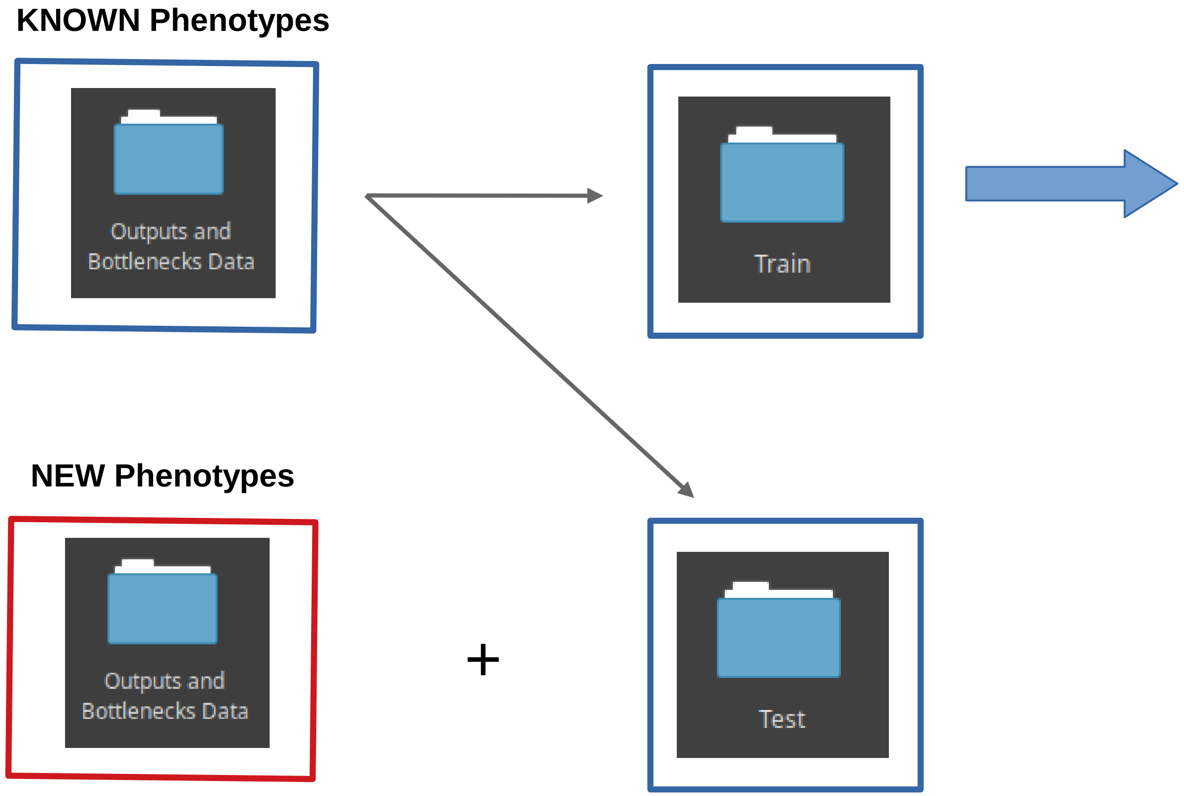
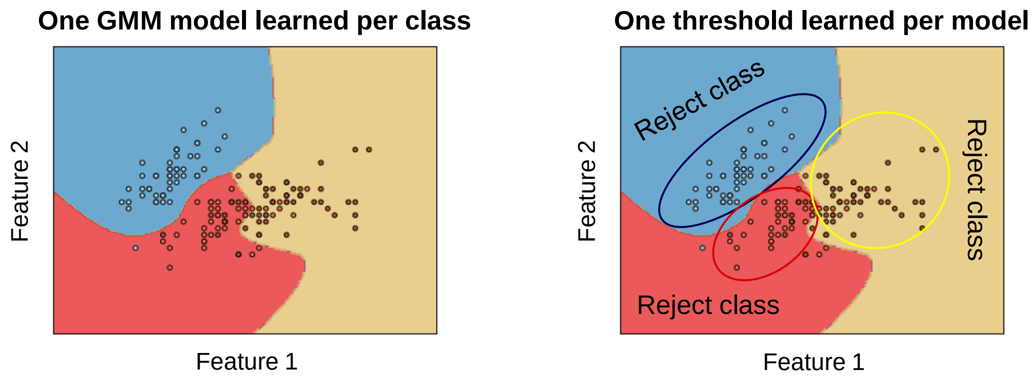
Experimental results

Learning and Test Procedure





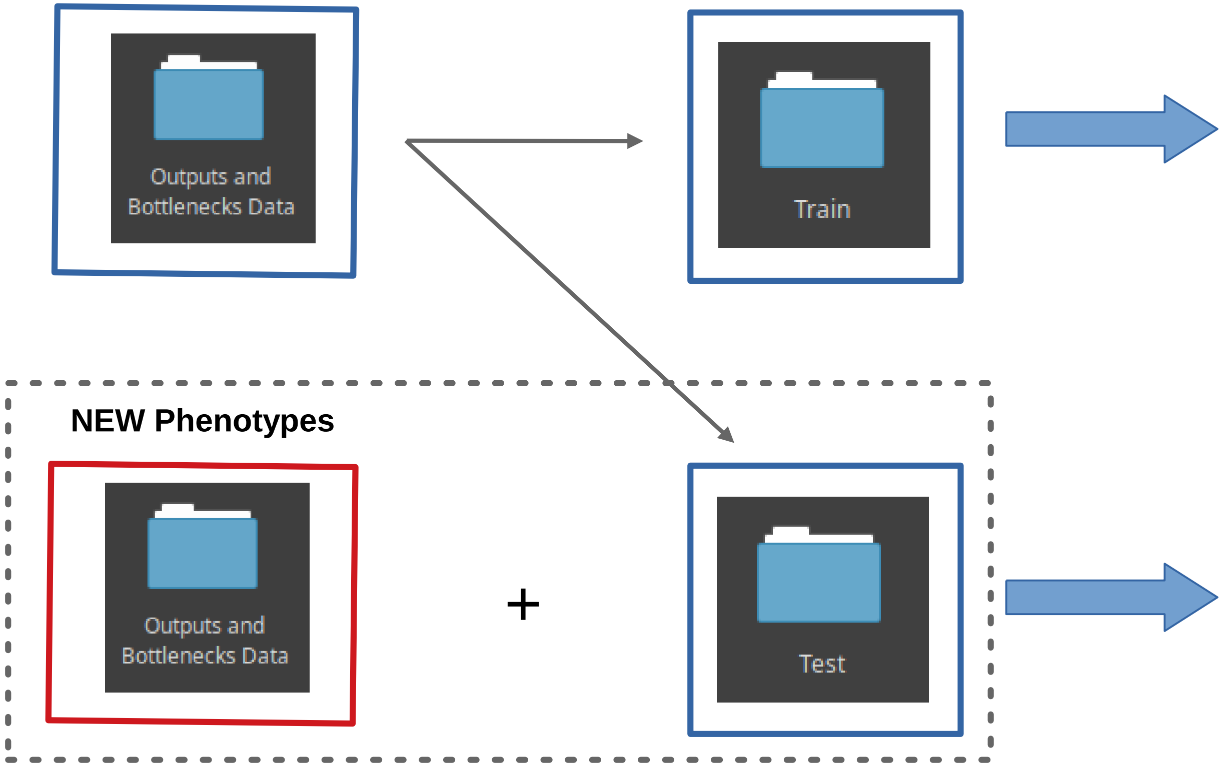
<u>Parameter tuning:</u>

- **Features**
  - Dimension reduction
  - Symmetrization
- **GMM parameters**
  - Number of components (nc)
  - Type of covariance matrix
- **Threshold learning**
  - 1 vs. 1 or 1 vs. All
  - LR/Misclassification

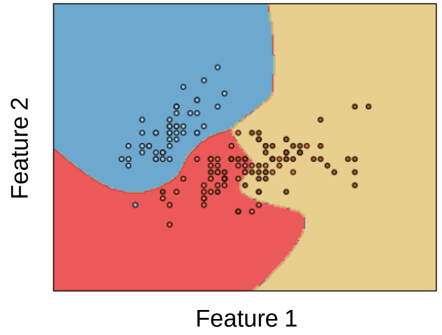
Experimental results

Learning and Test Procedure

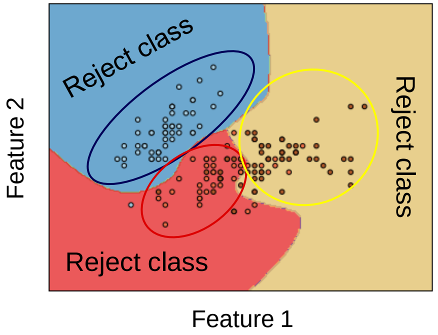
KNOWN Phenotypes



One GMM model learned per class



One threshold learned per model



Prediction results on KNOWN and NEW phenotypes

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Experimental results

Results and analysis

Methods	Features		Results	Threshold learning			
				Regression		*Misclassif.*	
				`1-vs-all`	`1-vs-1`	`1-vs-all`	`1-vs-1`
Proposed	Bottleneck (Spheric GMM)	Var. importance	Known	94	88	**91**	86
			Rejection	77	87	**98**	91
			Dimension	90	90	90	90
			Nb components	10	6	10	6
		PCA	Known	93	92	88	90
			Rejection	82	85	90	89
			Dimension	30	30	30	30
			Nb components	10	11	11	10
	Output (Diagonal GMM)	Original	Known	97	97	78	95
			Rejection	72	73	75	71
			Dimension	7			
			Nb components	6	11	11	10
		Symmetrized	Known	97	**96**	52	73
			Rejection	71	**76**	91	79
			Dimension	7			
			Nb components	7	10	9	8

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Experimental results

Results and analysis

De Stefano, Claudio & Sansone, Carlo & Vento, Mario. (2000). *To reject or not to reject: That is the question* - An answer in case of neural classifiers. Systems, Man, and Cybernetics, Part C: Applications and Reviews, IEEE Transactions on. 30. 84 - 94. 10.1109/5326.827457.

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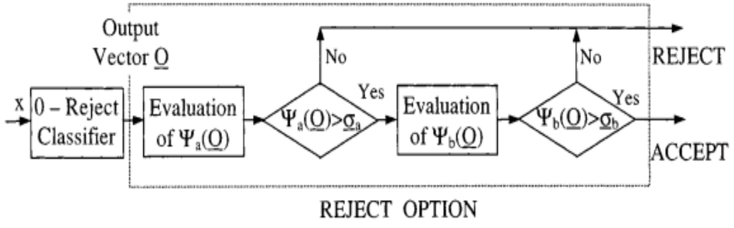
CNNro			Known	65			
			Rejection	100			



⇒ Better result with our proposed method (94,5 % against 82,5 % of accuracy)

⇒ In their method they prefer to reject than to predict badly

Successful detection on known & new phenotypes
→ Better results with our method than with Stefano *et al.*

Conclusion

How to define a rejection class based on model learning?

Innovative method of supervised classification with rejection class
=> which accounts for the neighboring relationships between the known classes

- Model = Gaussian mixture
- Threshold learning = Misclassification-based / Regression-based (LR)
- Options=«1 vs. All» / «1 vs.1»

Method validated on real data:

- Data = Transmitted light microscopy images
- Classes = Phenotypes / Molecule's MoA = 4 identified phenotypes + a pool of new phenotypes
- Features = Output / Bottlenecks (with or without preprocessing)

  Best results with :
  - Features = **Bottlenecks**,
  - Feature reduction dimension: **Variable importance**
  - Threshlod learning = **1 vs. All, Misclassification**

  Classification accuracy =~ **94 %**

⇒ With **91 %** on known phenotypes and **98 %** on rejection class

Comparison with existing method:

- Deep Neural Network: threshold on the output = confidence score of the prediction
- **Best result with our proposed method**: 94.5 % against 82.5 % of accuracy

⇒ **65%** on known classes and **100%** on rejection class

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Thank you!

Sarah Laroui

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