Conformal prediction and Venn-ABERS prediction using CPSign

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OpenRiskNet

RISK ASSESSMENT E-INFRASTRUCTURE

Outline

1. Conformal prediction
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   - Mondrian
2. Hands-on
   - What you might want to know
   - Let's get hands-on!
3. Venn-ABERS prediction
   - The consensus modelling
   - Non-Mondrian

Predict with confidence

Know how sure you are about each individual prediction

Current case in QSAR

Commonly in QSAR we estimate the performance of a model using a test set (or cross validation).

But when we make a prediction there is always the suspicion that the molecule that we are making a prediction for might be too different from the test set and then the question arise: Can we trust this particular prediction?

(One approach to this is based on the applicability domain concept)

Predict with confidence

Know how sure you are about each individual prediction

Conformal prediction

(*We will look only at classification today*)
With conformal prediction we are instead predicting one rank score (p-values) for each class indicating whether the molecule is of that class.

Mondrian method

The classes are treated separately

Mondrian method

We are modelling each class separately and get two independent predictions — one for each class (They don't sum up to 1)

Pros

- We get a confidence score for each prediction
- We are not sensitive to unbalanced data sets

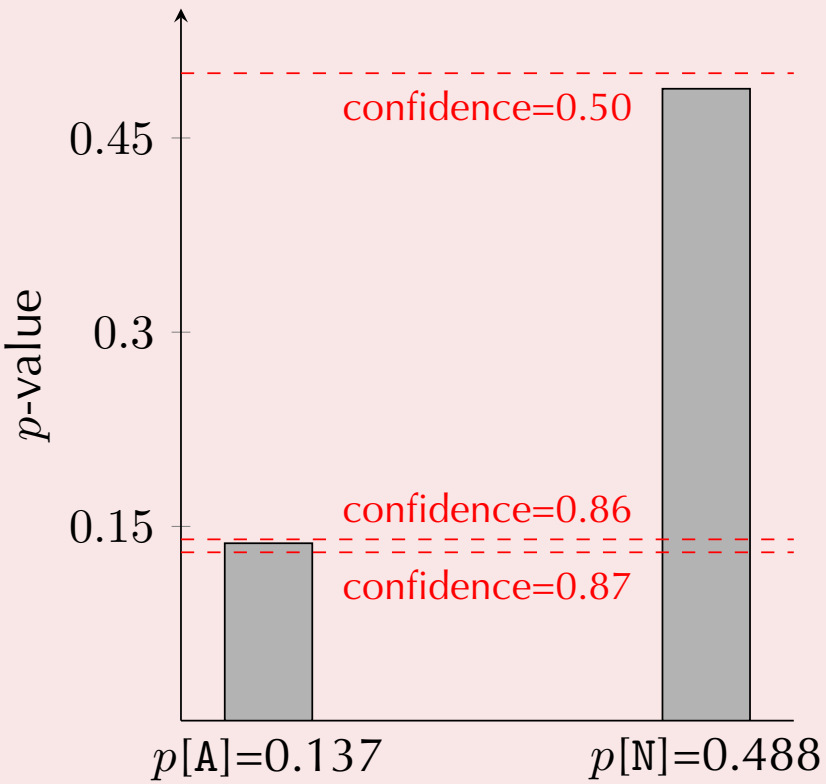
Cons

- We can't calculate common performance measures like, *e.g.*, area under ROC curve (AUROC).
- People are not used to this

Mondrian method

Let's look at an example

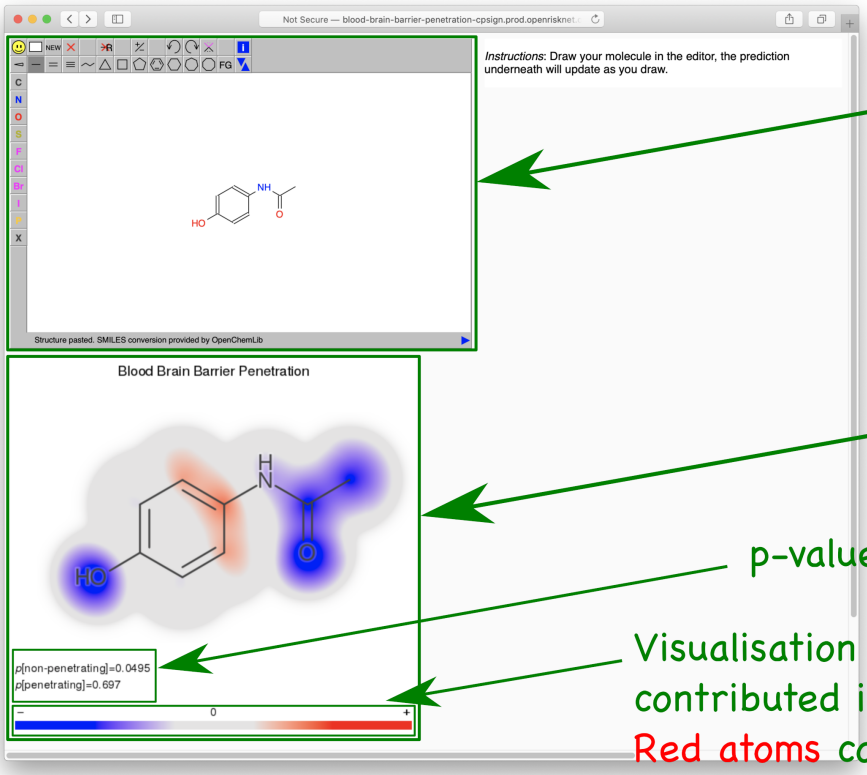
An example, classification (A or N?)



Confidence	p-value	Prediction
0.5	0.5	{Ø}
0.86	0.14	{N}
0.87	0.13	{A,N}

What you might want to know

Some info regarding our predictions



Draw a molecule

Get prediction

p-values for the different classes

Visualisation of which part of the molecule contributed in what way to the prediction

Red atoms contributed to the class with largest p-value

Blue atoms contributed to the class with lowest p-value

Let's get hands-on!

A chance to try it out a bit!

`http://blood-brain-barrier-penetration-cpsign.prod.openrisknet.org/draw/`

The consensus modelling

Consensus modelling

We have seen a number of prediction models now and it was suggested that we would use them together in a consensus approach.

The consensus modelling

Trouble

Trouble

Conformal prediction is Mondrian

$\Rightarrow$

The p-values does not sum up to 1

The consensus approach could not handle the p-values from our conformal prediction approach.

Non-Mondrian

Venn-ABERS produces probabilities

Non-Mondrian method

Venn-ABERS prediction is a more "classic" approach, *i.e.*, non-Mondrian.

Pros

- We get a predicted probability for each class
- We can calculate common performance measures like, *e.g.*, AUROC.

Cons

- We are sensitive to unbalanced data sets.


Thank you