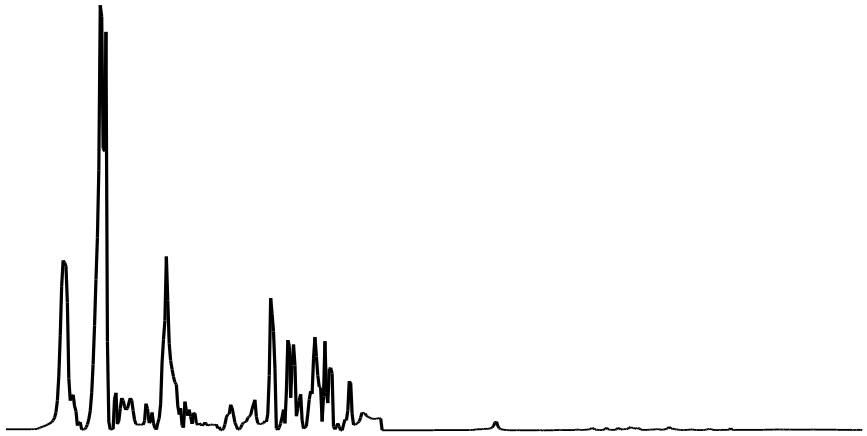
BASES GIVING DISTANCES

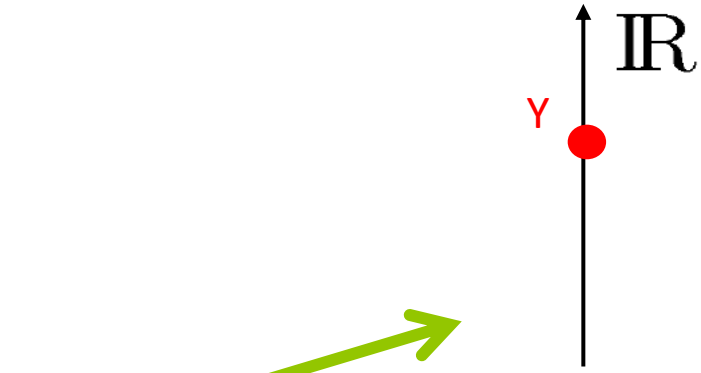
Advantages of the BAGIDIS methodology for comparing spectra in metabonomics

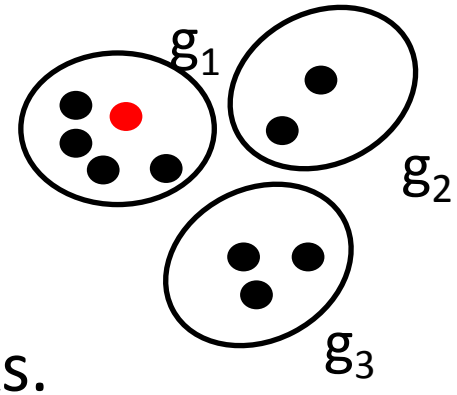
Catherine Timmermans and co-authors

The goal

- Predicting a scalar value or a group membership from a curve with sharp patterns.





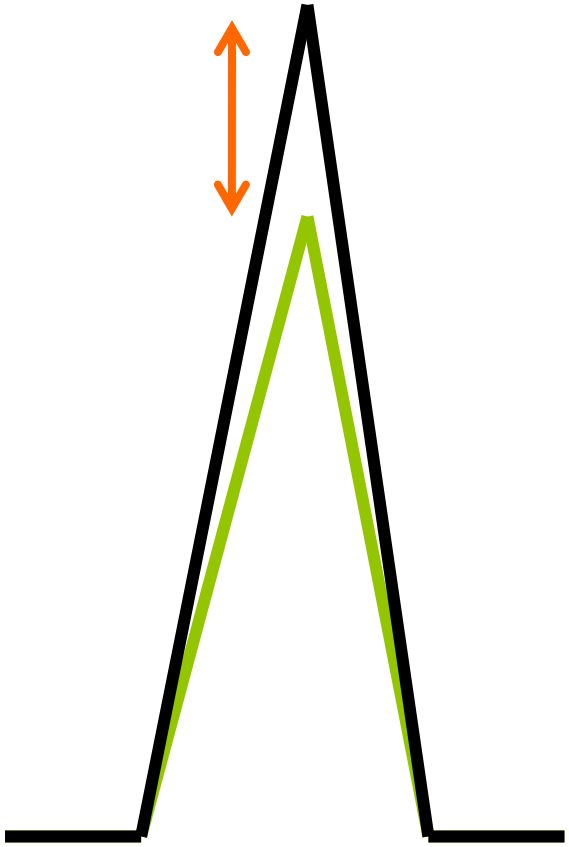


- Identifying significantly discriminative peaks.

The challenge

Defining an efficient measure of dissimilarity between spectra.

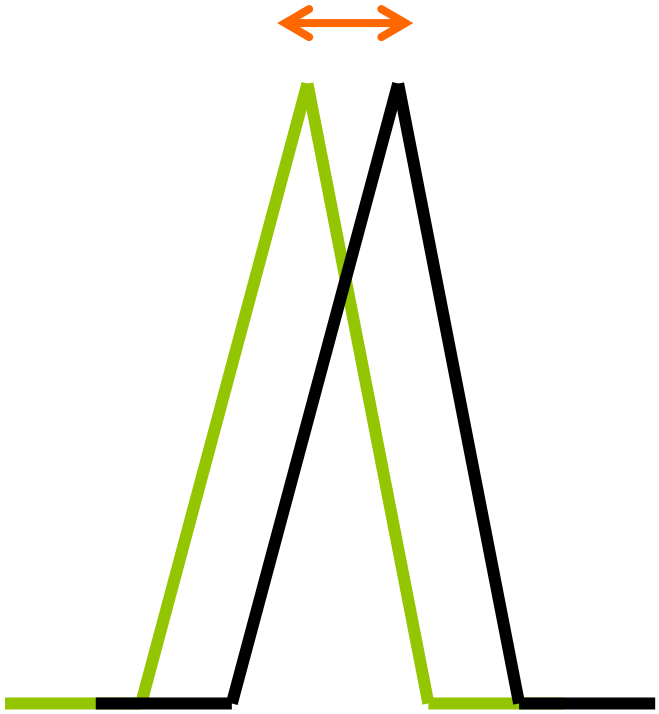
The challenge



A peak can be affected by

a vertical amplification

The challenge

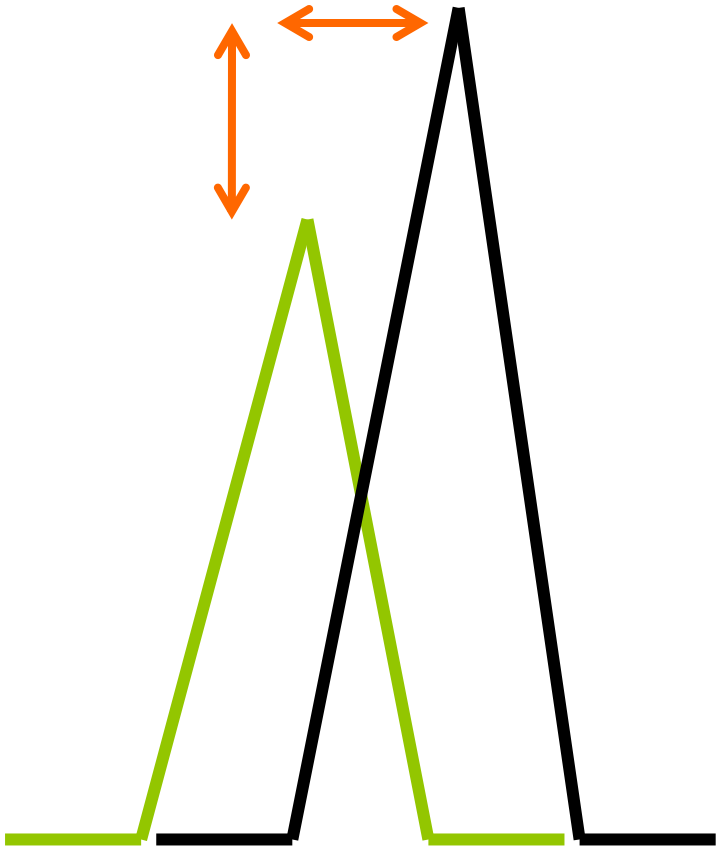


A peak can be affected by

a vertical amplification,

an horizontal shift

The challenge



A peak can be affected by

a vertical amplification,

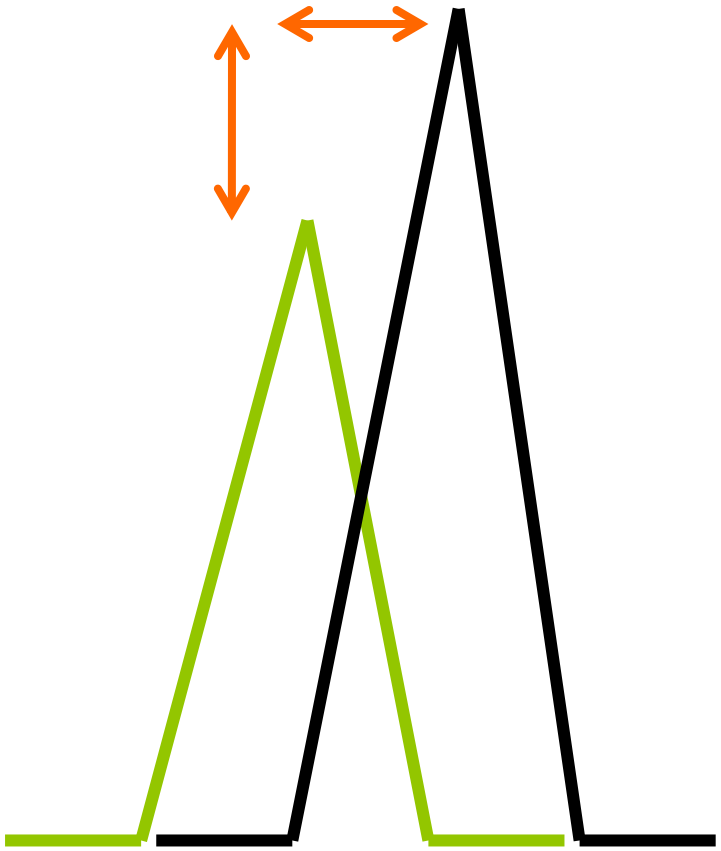
an horizontal shift,

… or both.

The challenge

Commonly used distance measures fail as soon as there is an horizontal shift from one spectra to another.

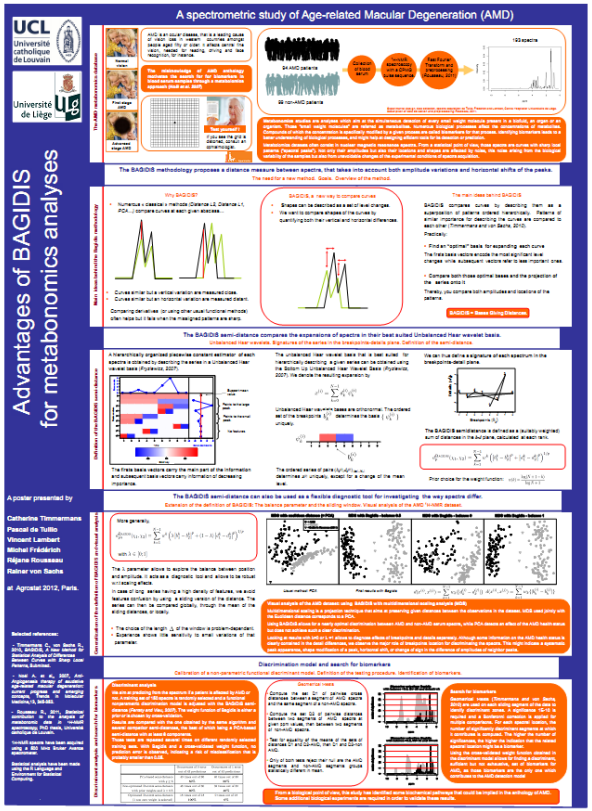
Our solution



The BAGIDIS semi-distance has the ability to capture the variations of patterns that are affected simultaneously by horizontal shifts and vertical amplifications.

Timmermans & von Sachs

Our solution



Talk with me or

have a look at the poster

for more details and an

application in

pharmaceutical sciences .

Catherine Timmermans