Generative Supervised Explainable artificial intelligence for the untargeted analysis of LCMS data

Andrea Jr Carnoli, Melissa Broeren, Ane Arrizabalaga Larrañaga, Bas H.M. van der Velden, Marco H. Blokland

Wageningen Food Safety Research, Wageningen, Netherlands

Introduction

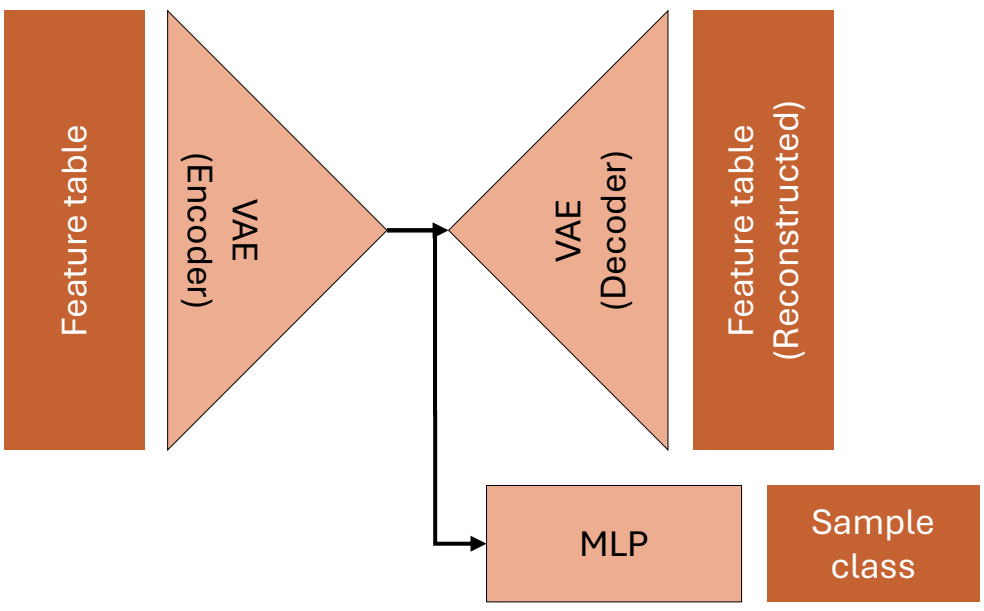
Feature tables obtained from untargeted Liquid Chromatography – High Resolution Mass Spectrometry studies are very common in food safety studies. Artificial Intelligence can be very useful, but its application is constrained by the limited amount of data. In this work we studied how transfer learning can be helpful, even when the tables are derived from completely different experiments

Conclusion

- - Transfer Learning is helpful for the development and application of Artificial Intelligence models
- - Transfer Learning can be applied even if the experiments are different

Artificial Intelligence

Beta – Branched Variational Autoencoder



$$Loss_{\beta-BVAE} = \alpha Loss_{rec} + \beta Loss_{KLD} + \gamma Loss_{class}$$

Pretraining

Open-Access steroids data

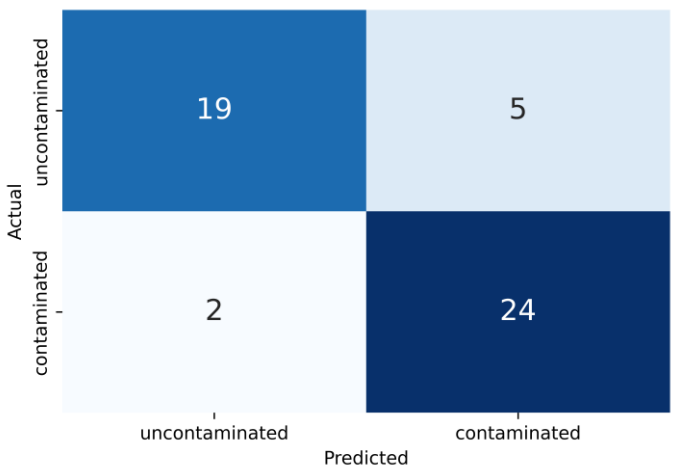
1241 bovine urine
- 5% spiked
- Recorded across 3 years

Finetuning

Chicken muscles data

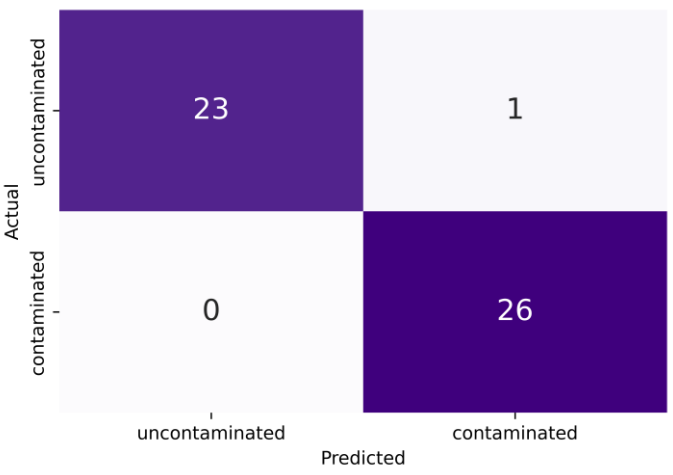
156 chicken muscles:
- 50% spiked
- Recorded across 2 days

Without transfer learning



-Misleading results (Acc:0.86)
-Shortcut learning (day)

With transfer learning



-Performance improved (Acc:0.98)
-No shortcuts

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101059813