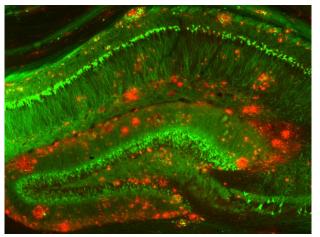
AmyloGram 2.0: MBO in the prediction of amyloid proteins

Dominik Rafacz

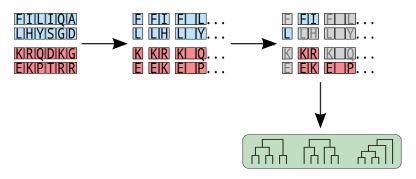
Warsaw University of Technology

Amyloidogenic proteins



Amyloid aggregates (red) around neurons (green). Strittmatter Laboratory, Yale University.

AmyloGram - n-grams analysis



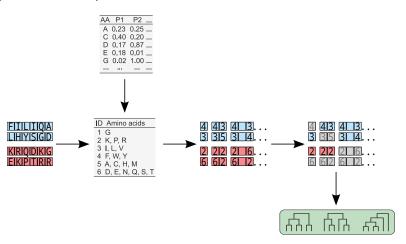
Example 1-grams: A, L, G

Example 2-grams: AL, MM, MY

Example 2-grams (with a gap): A-L, M-M, M-Y

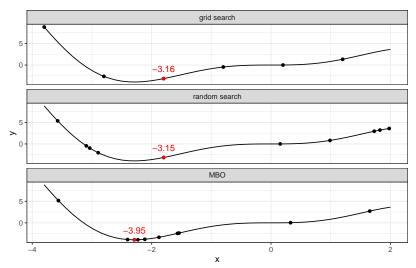
Burdukiewicz, M., Sobczyk, P., Rödiger, S., Duda-Madej, A., Mackiewicz, P., and Kotulska, M. (2017). Amyloidogenic motifs revealed by n-gram analysis. Scientific Reports 7, 12961

AmyloGram - alphabet reduction



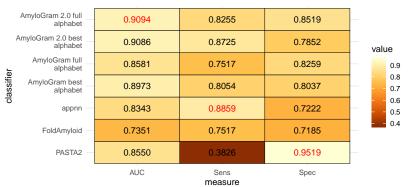
Burdukiewicz, M., Sobczyk, P., Rödiger, S., Duda-Madej, A., Mackiewicz, P., and Kotulska, M. (2017). Amyloidogenic motifs revealed by n-gram analysis. Scientific Reports 7, 12961

MBO



Results

Scores of classifiers



Features used in the model in original model: 262
Features used in the model with full alphabet: 33620
Features used in the model with best alphabet: 1014

Results

MBO shows an improvement compared to the grid optimization, but feature engineering (development of new alphabets and n-grams) requires further adjustment of the tuning method.

Acknowledgements & references

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Burdukiewicz, M., Sobczyk, P., Rödiger, S., Duda-Madej, A., Mackiewicz, P., and Kotulska, M. (2017). Amyloidogenic motifs revealed by n-gram analysis. Scientific Reports 7, 12961 Bischl, B., Richter, J., Bossek, J., Horn, D., Thomas, J. and Lang, M. (2017). mlrMBO: A Modular Framework for Model-Based Optimization of Expensive Black-Box Functions.