Wout Bittremieux

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Professional skills

Technical achievements:

- Developed an encoder-decoder deep learning model to assign peptide sequences to proteomics mass spectra, achieving an identification performance on par with or exceeding current state-of-the-art mass spectral search engines.
- Applied approximate nearest neighbor indexing techniques to perform similarity search of large bioinformatics data sets, resulting in tenfold speed-ups while identifying up to 50 % more unknown mass spectra during spectral library open modification searching.
- Developed an unsupervised outlier detection workflow to accurately discriminate between low-quality and high-quality mass spectrometry experiments. By replacing time-consuming manual analyses with automated decision-making this workflow boosts confidence in the experimental results and increases throughput. Special focus on interpretability for (non-technical) domain users.
- Established novel paradigms for mass spectrometry quality control by inspecting secondary metrics such as low-level instrument parameters and environmental variables. Implemented this functionality in robust tools for end users and APIs for developers.

Communication skills:

- Initiated and participated in local, national, and international multidisciplinary collaborations with academic and industry partners.
- Gave multiple oral presentations, poster presentations, and software demonstrations at leading local, national, and international scientific symposia and conferences.
- Received the 'outstanding oral presentation award' at the Benelux Bioinformatics Conference 2015.
- Successfully acquired multiple personal grants for international mobility, including a trimester research visit to Stellenbosch University in Cape Town, South Africa in the autumn of 2016.
- Authored five peer-reviewed publications, and co-authored an additional seven peer-reviewed publications.
- Assisted in teaching multiple courses on machine learning and bioinformatics.
- Supervised several master thesis students.

Organization and management skills:

- Acquired business insights by developing a valorization plan for a potential spin-off.
- Secretary for the Human Proteome Organization – Proteomics Standards Initiative (PSI) Quality Control working group. The PSI is a leading international body defining standards for mass spectrometry data, with the Quality Control working group the first newly formed working group in over ten years.
- Member of the local organizing committee for the Belgian Proteomics Association Symposium 2014 and the Benelux Bioinformatics Conference 2015.

Programming skills:

- Highly experienced in Python (NumPy, SciPy, scikit-learn, pandas, matplotlib, Keras) and Java.
- Experienced in R, C/C++, and SQL.

Selected software:

- ANN SoLo: Speeding up spectral library searching through approximate nearest neighbor indexing.
- iMonDB: User-friendly tool suite to automatically extract, store, manage, and visualize mass spectrometry quality control metrics.
- jqcML: Highly performant Java API for the qcML standard file format for mass spectrometry quality control data.
- QC analysis: Machine learning workflow to detect low-quality mass spectrometry experiments for automated decision-making.

Language skills

Dutch: Native language

English: Full professional proficiency

French: Limited working proficiency

German: Elementary proficiency

Work experience

University of Antwerp, Antwerp, Belgium

Postdoctoral researcher *2017–current*

Applied and developed various machine learning techniques to solve bioinformatics challenges, with a special focus on mass spectrometry proteomics.

Stellenbosch University, Cape Town, South Africa

Visiting researcher *2016*

Developed computational quality control techniques for mass spectrometry proteomics.

Testronic, Diepenbeek, Belgium

Software developer internship *2012*

Created a basic software framework for automated testing of TV set-top boxes.

Education

University of Antwerp, Antwerp, Belgium

PhD in Computer Science *2013–2017*

PhD thesis: 'Computational solutions for quality control of mass spectrometry-based proteomics.'

Hasselt University, Diepenbeek, Belgium

Master in Computer Science, completed with great honor *2010–2012*

Master thesis: 'Time series similarity search.'

Bachelor in Computer Science, completed with honor *2007–2010*

Interests

Certified referee at the Royal Belgian Football Association for over 13 years.

Publications

Bittremieux, **Wout**, Mathias Walzer, Stefan Tenzer, Weimin Zhu, et al.: *The HUPO-PSI Quality Control Working Group: Making Quality Control More Accessible for Biological Mass Spectrometry.* In: *Analytical Chemistry* (In press 2017). DOI: 10.1021/acs.analchem.6b04310.

De Neuter, Nicolas, **Wout Bittremieux**, Charlie Beirnaert, Bart Cuypers, et al.: *On the Feasibility of Mining CD8+ T-Cell Receptor Patterns Underlying Immunogenic Peptide Recognition.* In: *bioRxiv* (Mar. 20, 2017), p. 118539. DOI: 10.1101/118539.

Bittremieux, **Wout**, Dirk Valkenborg, Lennart Martens, and Kris Laukens: *Computational Quality Control Tools for Mass Spectrometry Proteomics.* In: *PROTEOMICS* 17 (3-4 Feb. 2017), p. 1600159. DOI: 10.1002/pmic.201600159.

Meysman, Pieter, Yvan Saeys, Ehsan Sabaghian, **Wout Bittremieux**, et al.: *Mining the Enriched Subgraphs for Specific Vertices in a Biological Graph.* In: *IEEE/ACM Transactions on Computational Biology and Bioinformatics* Early access (June 7, 2016), p. 1. DOI: 10.1109/TCBB.2016.2576440.

Maes, Evelyne, Pieter Kelchtermans, **Wout Bittremieux**, Kurt De Grave, et al.: *Designing Biomedical Proteomics Experiments: State-of-the-Art and Future Perspectives.* In: *Expert Review of Proteomics* 13.5 (Apr. 25, 2016), pp. 495–511. DOI: 10.1586/14789450.2016.1172967.

Bittremieux, **Wout**, Pieter Meysman, Lennart Martens, Dirk Valkenborg, et al.: *Unsupervised Quality Assessment of Mass Spectrometry Proteomics Experiments by Multivariate Quality Control Metrics.* In: *Journal of Proteome Research* 15.4 (Apr. 1, 2016), pp. 1300–1307. DOI: 10.1021/acs.jproteome.6b00028.

Meysman, Pieter, Yvan Saeys, Ehsan Sabaghian, **Wout Bittremieux**, et al.: "Discovery of Significantly Enriched Subgraphs Associated with Selected Vertices in a Single Graph". In: *Proceedings of the 14th International Workshop on Data Mining in Bioinformatics - BIOKDD '15.* Sydney, Australia, Aug. 10, 2015, p. 8.

Bittremieux, **Wout**, Hanny Willems, Pieter Kelchtermans, Lennart Martens, et al.: *iMonDB: Mass Spectrometry Quality Control through Instrument Monitoring.* In: *Journal of Proteome Research* 14.5 (May 1, 2015), pp. 2360–2366. DOI: 10.1021/acs.jproteome.5b00127.

Naulaerts, Stefan, Pieter Meysman, **Wout Bittremieux**, Trung Nghia Vu, et al.: *A Primer to Frequent Itemset Mining for Bioinformatics.* In: *Briefings in Bioinformatics* 16.2 (Mar. 2015), pp. 216–231. DOI: 10.1093/bib/bbt074.

Vu, Trung Nghia, **Wout Bittremieux**, Dirk Valkenborg, Bart Goethals, et al.: *Efficient Reduction of Candidate Matches in Peptide Spectrum Library Searching Using the Top k Most Intense Peaks.* In: *Journal of Proteome Research* 13.9 (Sept. 5, 2014), pp. 4175–4183. DOI: 10.1021/pr401269z.

Walzer, Mathias, Lucia Espona Pernas, Sara Nasso, **Wout Bittremieux**, et al.: *qcML: An Exchange Format for Quality Control Metrics from Mass Spectrometry Experiments.* In: *Molecular & Cellular Proteomics* 13.8 (Aug. 1, 2014), pp. 1905–1913. DOI: 10.1074/mcp.M113.035907.

Bittremieux, **Wout**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, et al.: *jqcML: An Open-Source Java API for Mass Spectrometry Quality Control Data in the qcML Format.* In: *Journal of Proteome Research* 13.7 (July 3, 2014), pp. 3484–3487. DOI: 10.1021/pr401274z.

Kelchtermans, Pieter, **Wout Bittremieux**, Kurt De Grave, Sven Degroeve, et al.: *Machine Learning Applications in Proteomics Research: How the Past Can Boost the Future.* In: *PROTEOMICS* 14 (4-5 Mar. 2014), pp. 353–366. DOI: 10.1002/pmic.201300289.

Presentations

Oral presentations

Bittremieux, **Wout**: *Shedding Light on Complex Mass Spectrometry Proteomics Processes through Advanced Data Mining.* In: *Faculty of Science Research Day* Antwerp, Belgium (Jan. 13, 2017). DOI: 10.5281/zenodo.242392.

Bittremieux, **Wout**: *Git: How Version Control Can Power Your Research.* In: *Biomina Lunch Talks* Antwerp, Belgium (June 24, 2016). DOI: 10.5281/zenodo.56352.

Bittremieux, **Wout**, Dirk Valkenborg, and Kris Laukens: *Optimized Open Modification Spectral Library Searching Using Approximate Nearest Neighbor Techniques.* In: *ASMS annual conference* San Antonio, TX, USA (June 9, 2016). DOI: 10.5281/zenodo.55999.

Bittremieux, **Wout**, Pieter Meysman, Lennart Martens, Bart Goethals, et al.: *Approaches for Mass Spectrometry Quality Control.* In: *Biomina Research Day* Antwerp, Belgium (Dec. 9, 2015). DOI: 10.5281/zenodo.56004.

Bittremieux, **Wout**, Pieter Meysman, Lennart Martens, Bart Goethals, et al.: *Analysis of Mass Spectrometry Quality Control Metrics.* In: *Benelux Bioinformatics Conference* Antwerp, Belgium (Dec. 7, 2015). DOI: 10.5281/zenodo.56001.

Bittremieux, **Wout** and Kris Laukens: *Precursor-Free and Fast Spectral Library Search Using Approximate Nearest Neighbor Techniques.* In: *Benelux Bioinformatics Conference Student Council Symposium* Antwerp, Belgium (Dec. 6, 2015). DOI: 10.5281/zenodo.56002.

Bittremieux, **Wout**, Emmanuel Müller, Dirk Valkenborg, Lennart Martens, et al.: *Pattern Mining of Mass Spectrometry Quality Control Data.* In: *Benelux Bioinformatics Conference* Luxembourg, Luxembourg (Dec. 9, 2014). DOI: 10.5281/zenodo.56000.

Bittremieux, **Wout**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, et al.: *Collecting and Mining Mass Spectrometry Quality Control Data.* In: *Biomina Research Day* Antwerp, Belgium (Feb. 20, 2014). DOI: 10.5281/zenodo.56003.

Poster presentations

Bittremieux, **Wout**, Pieter Meysman, Lennart Martens, Dirk Valkenborg, et al.: *Automatic Quality Assessment of Mass Spectrometry Experiments by Multivariate Quality Control Metrics.* In: *ASMS annual conference* San Antonio, TX, USA (June 9, 2016). DOI: 10.5281/zenodo.55998.

Bittremieux, **Wout**, Hanny Willems, Lennart Martens, Dirk Valkenborg, et al.: *Mass Spectrometry Quality Control: Instrument Monitoring and Pattern Mining Insights.* In: *ASMS annual conference* St. Louis, MO, USA (June 2, 2015). DOI: 10.5281/zenodo.55992.

Bittremieux, **Wout**, Hanny Willems, Lennart Martens, Bart Goethals, et al.: *A Comprehensive Approach to Mass Spectrometry Quality Control.* In: *Two-day symposium of the Belgian Proteomics Association* Brussels, Belgium (Dec. 18, 2014). DOI: 10.5281/zenodo.55990.

Bittremieux, **Wout**, Dirk Valkenborg, Aida Mrzic, Hanny Willems, et al.: *Pattern Mining of Mass Spectrometry Quality Control Data.* In: *European Conference on Computational Biology* Strasbourg, France (Sept. 7, 2014). DOI: 10.5281/zenodo.55989.

Bittremieux, **Wout**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, et al.: *Mining Mass Spectrometry Quality Control Data.* In: *ASMS annual conference* Baltimore, MD, USA (June 16, 2014). DOI: 10.5281/zenodo.55988.

Bittremieux, **Wout**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, et al.: *jqcML: An Open-Source Java API for Mass Spectrometry Quality Control Data in the qcML Format.* In: *Benelux Bioinformatics Conference* Brussels, Belgium (Dec. 9, 2013). DOI: 10.5281/zenodo.55986.

Software demonstrations

Bittremieux, **Wout** and Dirk Valkenborg: *iMonDB: Mass Spectrometry Instrument Monitoring for Quality Control.* In: *Methods and tools for intra- and inter-experiment LC MS performance tracking workshop, ASMS annual conference* St. Louis, MO, USA (June 1, 2015).