

## List of publications

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### Refereed journal publications

- [1] François Cornet, Bardi Benediktsson, Bjarke Hastrup, Mikkel N. Schmidt, and Arghya Bhowmik. “OM-Diff: inverse-design of organometallic catalysts with guided equivariant denoising diffusion”. In: *Digital Discovery* (2024). DOI: 10.1039/D4DD00099D.
- [2] Philip J. H. Jørgensen, Søren F. Nielsen, Jesper L. Hinrich, Mikkel N. Schmidt, Kristoffer H. Madsen, and Morten Mørup. “Probabilistic PARAFAC2”. In: *Entropy* (2024). DOI: 10.3390/e26080697.
- [3] Bo Li, Yasin Esfandiari, Mikkel N. Schmidt, Tommy S. Alstrøm, and Sebastian U. Stich. “Synthetic data shuffling accelerates the convergence of federated learning under data heterogeneity”. In: *Transactions on Machine Learning Research (TMLR)* (2024).
- [4] Jonas Busk, Mikkel N. Schmidt, Ole Winther, Tejs Vegge, and Peter Bjørn Jørgensen. “Graph neural network interatomic potential ensembles with calibrated aleatoric and epistemic uncertainty on energy and forces”. In: *Physical Chemistry Chemical Physics* (2023). DOI: 10.1039/D3CP02143B.
- [5] David Frich Hansen, Tommy Sonne Alstrøm, and Mikkel N. Schmidt. “Probabilistic signal estimation for vibrational spectroscopy with a flexible non-stationary Gaussian process baseline model”. In: *Chemometrics and Intelligent Laboratory Systems* (2023). DOI: 10.1016/j.chemolab.2023.104974.
- [6] Bo li, Giulia Zappalá, Elodie Dumont, Anja Boisen, Tomas Rindzevicius, Mikkel N. Schmidt, and Tommy S. Alstrøm. “Nitroaromatic explosives detection and quantification using attention-based transformer on surface-enhanced Raman spectroscopy maps”. In: *Analyst* (2023). DOI: 10.1039/D3AN00446E.
- [7] Muralikrishnan Srinivasan, Jinxiang Song, Alexander Grabowski, Krzysztof Szczerba, Holger K. Iversen, Mikkel N. Schmidt, Darko Zibar, Jochen Schröder, Anders Larsson, Christian Häger, and Henk Wymeersch. “End-to-End Learning for VCSEL-based Optical Interconnects: State-of-the-Art, Challenges, and Opportunities”. In: *Journal of Lightwave Technology* 41 (11 2023). DOI: 10.1109/JLT.2023.3251660. URL: <http://arxiv.org/abs/2211.14481>.
- [8] Kristoffer Jon Albers, Matthew G. Liptrot, Karen Sandø Ambrosen, Rasmus Røge, Tue Herlau, Kasper Winther Andersen, Hartwig R. Siebner, Lars Kai Hansen, Tim B. Dyrby, Kristoffer H. Madsen, Mikkel N. Schmidt, and Morten Mørup. “Uncovering Cortical Units of Processing from Multi-Layered Connectomes”. In: *Frontiers in Neuroscience* (2022). DOI: 10.3389/fnins.2022.836259.
- [9] Bo li, Mikkel N. Schmidt, and Tommy S. Alstrøm. “Raman Spectrum Matching with Contrastive Representation Learning”. In: *Analyst* (2022). DOI: 10.1039/D2AN00403H.
- [10] Kristoffer Jon Albers, Karen S. Ambrosen, Matthew G. Liptrot, Tim B. Dyrby, Mikkel N. Schmidt, and Morten Mørup. “Using connectomics for predictive assessment of brain parcellations”. In: *NeuroImage* 238 (Sept. 2021). DOI: 10.1016/j.neuroimage.2021.118170.
- [11] Rasmus Bonnevie and Mikkel N. Schmidt. “Matrix product states for inference in discrete probabilistic models”. In: *Journal of machine learning research* 22 (2021). URL: <http://jmlr.org/papers/v22/18-431.html>.
- [12] Jonas Busk, Peter Bjørn Jørgensen, Arghya Bhowmik, Mikkel N. Schmidt, Ole Winther, and Tejs Vegge. “Calibrated uncertainty for molecular property prediction using ensembles of message passing neural networks”. In: *Machine Learning: Science and Technology* 3.1 (2021). DOI: 10.1088/2632-2153/ac3eb3.
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- [16] Karen S. Ambrosen, Simon F. Eskildsen, Max Hinne, Kristine Krug, Henrik Lundell, Mikkel N. Schmidt, Marcel A. J. van Gerven, Morten Mørup, and Tim B. Dyrby. “Validation of structural brain connectivity networks: The impact of scanning parameters”. In: *NeuroImage* 204 (2019). DOI: 10.1016/j.neuroimage.2019.116207.
- [17] Kunal Ghosh, Annika Stuke, Milica Todorović, Peter Bjørn Jørgensen, Mikkel N. Schmidt, Aki Vehtari, and Patrick Rinke. “Deep Learning Spectroscopy: Neural Networks for Molecular Excitation Spectra”. In: *Advanced Science* 6 (9 May 2019). DOI: 10.1002/advs.201801367.
- [18] Peter Bjørn Jørgensen, Estefanía Garijo del Río, Mikkel N. Schmidt, and Karsten Wedel Jacobsen. “Materials property prediction using symmetry-labeled graphs as atomic-position independent descriptors”. In: *Physical Review B* 100.104114 (10 2019). DOI: 10.1103/PhysRevB.100.104114.
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- [20] Peter Bjørn Jørgensen, Murat Mesta, Suranjan Shil, Juan Maria García Lastra, Karsten Wedel Jacobsen, Kristian Sommer Thygesen, and Mikkel N. Schmidt. “Machine learning-based screening of complex molecules for polymer solar cells”. In: *The Journal of Chemical Physics* 148.241735 (2018). DOI: 10.1063/1.5023563.
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- [30] Darko Zibar, Ole Winther, Niccolo Franceschi, Robert Borkowski, Antonio Caballero, Valeria Arlunno, Mikkel N. Schmidt, Neil Guerrero Gonzales, Bangning Mao, Yabin Ye, Knud J. Larsen, and Idelfonso Tafur Monroy. “Nonlinear impairment compensation using expectation maximization for dispersion managed and unmanaged PDM 16-QAM transmission”. In: *Optics Express* 20.26 (2013), B181–B196. DOI: 10.1364/OE.20.00B181.
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- [34] Bo Li, Xiaowen Jiang, Mikkel N. Schmidt, Tommy S. Alstrøm, and Sebastian U. Stich. “An improved analysis of per-sample and per-update clipping in federated learning”. In: *Learning Representations, International Conference on (ICLR)*. 2024. URL: <https://iclr.cc/virtual/2024/poster/19208>.
- [35] Thea Brüsich, Mikkel N. Schmidt, and Tommy S. Alstrøm. “Multi-view self-supervised learning for multivariate variable-channel time series”. In: *Machine Learning for Signal Processing, IEEE International Workshop on, (MLSP)*. 2023. DOI: 10.1109/MLSP55844.2023.10285993.
- [36] François R. J. Cornet, Bardi Benediktsson, Bjarke Hastrup, Arghya Bhowmik, and Mikkel N. Schmidt. “Inverse-design of organometallic catalysts with guided equivariant diffusion”. In: *ELLIS Advancing Molecular Machine Learning Workshop (ML4Molecules) and AI for Accelerated Materials Design, NeurIPS Workshop (AI4MAT)*. 2023.
- [37] David Frich Hansen, Tommy S. Alstrøm, and Mikkel N. Schmidt. “Amortized variational peak fitting for spectroscopic data”. In: *Machine Learning for Signal Processing, IEEE International Workshop on, (MLSP)*. 2023. DOI: 10.1109/MLSP55844.2023.10285981.
- [38] Peter Bjørn Jørgensen, Jonas Busk, Ole Winther, and Mikkel N. Schmidt. “Coherent Energy and Force Uncertainty in Deep Learning Force Fields”. In: *ELLIS Advancing Molecular Machine Learning Workshop (ML4Molecules)*. 2023.

- [39] Bo Li, Mikkel N. Schmidt, Tommy S. Alstrøm, and Sebastian U. Stich. “On the Effectiveness of Partial Variance Reduction in Federated Learning With Heterogeneous Data”. In: *Computer Vision and Pattern Recognition Conference, The IEEE/CVF (CVPR)*. 2023, pp. 3964–3973. URL: [https://openaccess.thecvf.com/content/CVPR2023/html/Li\\_On\\_the\\_Effectiveness\\_of\\_Partial\\_Variance\\_Reduction\\_in\\_Federated\\_Learning\\_CVPR\\_2023\\_paper.html](https://openaccess.thecvf.com/content/CVPR2023/html/Li_On_the_Effectiveness_of_Partial_Variance_Reduction_in_Federated_Learning_CVPR_2023_paper.html).
- [40] Anders S. Olsen, Emil Ortvald, Kristoffer H. Madsen, Mikkel N. Schmidt, and Morten Mørup. “Angular central Gaussian and Watson mixture models for assessing dynamic functional brain connectivity during a motor task”. In: *Unraveling the Brain, Data Science and Learning Workshop (DSLW), ICASSP Satellite*. 2023. DOI: 10.1109/ICASSPW59220.2023.10193021.
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- [43] Mikkel N. Schmidt, Tommy S. Alstrøm, Marcus Svendstorp, and Jan Larsen. “Peak detection and baseline correction using a convolutional neural network”. In: *Acoustics, speech and signal processing, IEEE international conference on (ICASSP)*. 2019. DOI: 10.1109/ICASSP.2019.8682311.
- [44] Maximillian F. Vording, Peter O. Okeyo, Juan J. R. Guillamon, Peter E. Larsen, Mikkel N. Schmidt, and Tommy S. Alstrøm. “A Bayesian generative model with Gaussian process priors for termomechanical analysis of micro-resonators”. In: *Machine Learning for Signal Processing, IEEE International Workshop on, (MLSP)*. 2019. DOI: 10.1109/MLSP.2019.8918876.
- [45] Kristoffer Jon Albers, Mikkel N. Schmidt, Morten Mørup, Marisciel Litong-Palima, Rasmus Bonnevie, and Fumiko Kano Glückstad. “Understanding Mindsets Across Markets, Internationally: A Public-Private Innovation Project for Developing a Tourist Data Analytic Platform”. In: *Computer Software and Applications Conference (COMPSAC)*. July 2018, pp. 159–164. DOI: 10.1109/COMPSAC.2018.10221.
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- [47] Søren F. V. Nielsen, Diego Vidaurre, Mikkel N. Schmidt, Kristoffer H. Madsen, and Morten Mørup. “Testing group differences in state transition structure of dynamic functional connectivity models”. In: *Pattern Recognition in NeuroImaging (PRNI)*. 2018. DOI: 10.1109/PRNI.2018.8423966.
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- [52] Rasmus Røge, Karen Sandø Ambrosen, Kristoffer Jon Albers, Casper Tabassum Eriksen, Matthew George Lip-trot, Mikkel N. Schmidt, Kristoffer Hougaard Madsen, and Morten Mørup. “Whole brain functional connectivity predicted by indirect structural connections”. In: *Pattern Recognition in NeuroImaging (PRNI)*. 2017. DOI: 10.1109/PRNI.2017.7981496.
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- [55] Philip H. Jørgensen, Morten Mørup, Mikkel N. Schmidt, and Tue Herlau. “Bayesian latent feature modeling for modeling bipartite networks with overlapping groups”. In: *Machine Learning for Signal Processing, IEEE International Workshop on, (MLSP)*. 2016. DOI: 10.1109/MLSP.2016.7738845.
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#### Refereed abstracts and workshop contributions

- [87] Philip H. Jørgensen, Søren F. V. Nielsen, Jesper L. Hinrich, Mikkel N. Schmidt, Kristoffer H. Madsen, and Morten Mørup. “Analysis of Chromatographic Data using the Probabilistic PARAFAC2”. In: *Machine Learning and the Physical Sciences, NeurIPS Workshop on*. 2019.
- [88] Fumiko K. Glückstad, Mikkel N. Schmidt, and Morten Mørup. “Testing a model of destination image formation: Application of nonparametric Bayesian relational modeling to destination image analysis”. In: *Global Marketing Conference at Tokyo*. July 2018, pp. 63–64. DOI: 10.15444/GMC2018.01.07.02.
- [89] Kasper B. Frøhling, Tommy S. Alstrøm, Michael Bache, Michael S. Schmidt, Mikkel N. Schmidt, Jan larsen, Mogens H. Jakobsen, and Anja Boisen. “Statistical analysis of large areas of Raman mapped DNA functionalized gold coated silicon nanopillar SERS substrates”. In: *Advanced Vibrational Spectroscopy, International Conference on (ICAVS)*. 2015.
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- [92] Tue Herlau, Morten Mørup, and Mikkel N. Schmidt. “Temporally Evolving Hierarchies in Networks”. In: *NetSci*. 2013.
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- [94] Sune Lehmann, Morten Mørup, and Mikkel N. Schmidt. “A Bayesian Generative Model for Pervasive Overlap”. In: *NetSci*. 2012.
- [95] Morten Mørup and Mikkel N. Schmidt. “Efficient inference in the infinite multiple membership relational model”. In: *NIPS workshop on Bayesian nonparametric: Hope or hype*. 2011.
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