

David Li-Bland

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Employment History

- 2024–2025 **Staff Machine Learning Research Scientist, Genesis Molecular AI**
Goal: Drug Discovery
Selected Contributions:
- Reinforcement Learning & inference time alignment strategies for diffusion based all-atom structure prediction model
- Analytical optimization of training and inference schedules for diffusion models that directly target RMSD of samples, while reducing the number of hyperparameters
- Improved statistical analysis of benchmark metrics
- Active learning system for drug discovery
- 2019–2024 **Machine Learning Research Scientist, Unlearn.ai**
Goal: Model disease progression in individuals
Selected Contributions:
- Novel generative machine learning architectures
- Modeling of multiple diseases
- Statistical methods with variance reduction guarantees
- Novel model selection and hyperparameter optimization schemes
- 2017–2019 **Research Engineer, Machine Learning, Human Diagnosis Project**
Goal: Collective medical intelligence system
Selected Contributions:
- ML systems to model symptoms and diagnoses
- Search service
- Clustering algorithm for diagnoses
- 2016–2017 **Research Scientist, Verseon**
Goal: Drug discovery platform
Primary Contribution: Preliminary development of high-dimensional optimization procedure (via compressed sensing)
- 2014–2016 **Visiting Assistant Professor, U.C. Berkeley, Department of Mathematics**
2012–2016 **NSF Postdoctoral Researcher, U.C. Berkeley, Department of Mathematics**

Education

- 2007–2012 **Ph. D., Mathematics, University of Toronto**
2006–2007 **M. Sc., Mathematics, University of Chicago**
2001–2005 **Hons. B. Sc., Mathematics, University of Toronto, High Distinction**

Research Interests

Generative Modeling & Molecular Biology, Generative Models, Reinforcement Learning & Alignment, Stochastic Processes, Control Theory, Probabilistic Inference, Optimization, Information Geometry, Geometry, Topology

Expertise

Machine Learning Diffusion Models, Alignment of Diffusion Models, Generative Models, Deep Neural Networks, MCMC Sampling, Variational Inference, Model Selection, Hyperparameter Optimization, Graphical Models, Bayesian Inference

Statistical modeling Stochastic processes, Stochastic differential equations, Bayesian Inference

Programming Languages Python, Javascript, C++/C

Communication Invited speaker for international conferences and minicourses, Instructor for 6+ university courses, Delivered 30+ invited talks/lectures.

Leadership/Teamwork Project lead at Genesis Molecular AI, Project lead at Unlearn.ai, Team lead at HumanDx, Supervised 4 graduate students, Administered large university courses with multiple instructors, Multiple interdisciplinary research collaborations

Selected Honours and Awards

2025 **GenBio Workshop, Panelist**, (*ICML*)

2014 **André Lichnerowicz prize in Poisson geometry**, (*International Conference on Poisson Geometry in Mathematics and Physics*)

2012–2016 **NSF Mathematical Sciences Postdoctoral Research Fellowship**, Award No.: DMS-1204779

Research and Publications

Patents

- [1] Maruan Al-Shedivat, Leidal Kenneth Knute, Arthur Deng, and David Li-Bland. Training generative machine learning models for 3d molecular structure prediction using alignment objective, U.S. Patent, 2025/179253, US2025016976, 2025.
- [2] Maruan Al-Shedivat and David Li-Bland. Systems and methods for optimizing generative models for predicting 3d structures of molecular systems, U.S. Patent App, 63/715, 289, 2024.
- [3] David Li-Bland, Aaron Smith, and Anton Loukianov. Systems and methods for model selection, U.S. Patent App. 17/658, 228, 2022.

Manuscripts

- [4] Genesis Research Team, Alejandro Dobles, Nina Jovic, Kenneth Leidal, Pranav Murugan, David C. Williams, Drausin Wulsin, Nate Gruver, Christina X. Ji, Korrawat Pruegsanusak, Gianluca Scarpellini, Ansh Sharma, Wojciech Swiderski, Andrea Bootsma, Richard Strong Bowen, Charlotte Chen, Jamin Chen, Marc André Dämgen, Benjamin DiFrancesco, J. D. Fishman, Alla Ivanova, Zach Kagin, David Li-Bland, Zuli Liu, Igor Morozov, Jeffrey Ouyang-Zhang, Frank C. Pickard IV, Kushal S. Shah, Ben Shor, Gabriel Monteiro da Silva, Roy Tal, Maxx Tessmer, Carl Tilbury, Cyr Vetcher, Daniel Zeng, Maruan Al-Shedivat, Aleksandra Faust, Evan N. Feinberg, Michael V. LeVine, and Matteus Pan. Pearl: A foundation model for placing every atom in the right location. *arXiv preprint arXiv:2510.24670*, 2025.
- [5] Daniele Bertolini, Anton D Loukianov, Aaron M Smith, David Li-Bland, Yannick

- Pouliot, Jonathan R Walsh, and Charles K Fisher. Modeling disease progression in mild cognitive impairment and alzheimer’s disease with digital twins. 2020.
URL <https://arxiv.org/abs/2012.13455>
- [6] Jonathan R Walsh, Aaron M Smith, Yannick Pouliot, David Li-Bland, Anton Loukianov, and Charles K Fisher. Generating digital twins with multiple sclerosis using probabilistic neural networks. 2020.
URL <https://arxiv.org/abs/2002.02779>
 - [7] David Li-Bland. Saddle Points and Stochastic Gradient Descent. <https://davidlibland.github.io/posts/2018-11-10-saddle-points-and-sdg.html>, 2018.
 - [8] David Li-Bland. The stack of higher internal categories and stacks of iterated spans. 2015. 38 pages.
URL <http://arxiv.org/abs/1506.08870>
 - [9] Theodore Johnson-Freyd, David Li-Bland, and Alan Weinstein. Quantization of the linear symplectic category: a field theoretic approach.
[Published](#)
 - [10] David Li-Bland and Eckhard Meinrenken. On the integration of manin pairs. *Differential Geometry and its Applications*, 99:page 102246, 2025.
 - [11] David Li-Bland. Designing faster and more efficient multiple sclerosis clinical trials by incorporating machine learning predictions. In *Multiple Sclerosis Journal*, volume 28, pages 64–64. SAGE Publications Ltd 1 Olivers Yard, 55 City Road, London EC1Y 1SP, England, 2022.
 - [12] Daniele Bertolini, Anton D Loukianov, Aaron Smith, David Li-Bland, Yannick Pouliot, Jonathan R Walsh, and Charles K Fisher. Forecasting progression of mild cognitive impairment (mci) and alzheimer’s disease (ad) with digital twins. *Alzheimer’s & Dementia*, 17:page e054414, 2021.
 - [13] Jonathan Walsh, Aaron Smith, Yannick Pouliot, David Li-Bland, Anton Loukianov, and Charles Fisher. Modeling subject-level disease progression for multiple sclerosis clinical trials with machine learning (2232). *Neurology*, 94(15, supplement), 2020.
URL https://www.neurology.org/doi/10.1212/WNL.94.15_supplement.2232
 - [14] David Li-Bland and Pavol Ševera. Coherent Quantization using Coloured Surfaces. *Mathematical Research Letters*, 26(3):pages 805–850, 2019. 35 pages.
URL <http://arxiv.org/abs/1510.05615>
 - [15] David Li-Bland and Pavol Ševera. Moduli spaces for quilted surfaces and Poisson structures. *Documenta Mathematica*, 20:pages 1071–1135, 2015.
URL <http://arxiv.org/abs/1212.2097>
 - [16] David Li-Bland and Pavol Ševera. On deformation quantization of poisson lie groups and moduli spaces of flat connections. *International Mathematics Research Notices*, 2015(15):pages 6734–6751, 2015.
URL <http://arxiv.org/abs/1307.2047>
 - [17] David Li-Bland and Pavol Ševera. Symplectic and poisson geometry of the moduli spaces of flat connections over quilted surfaces. In Damien Calaque and Thomas Strobl,

editors, *Mathematical Aspects of Quantum Field Theories*, Mathematical Physics Studies, pages 343–411. Springer International Publishing, 2015. ISBN 978-3-319-09948-4.

URL <http://arxiv.org/abs/1304.0737>

- [18] David Li-Bland. Pseudo-dirac structures. *Indagationes Mathematicae*, 25(5):pages 1054–1101, 2014. Poisson 2012: Poisson Geometry in Mathematics and Physics.
URL <http://arxiv.org/abs/1408.5365>
- [19] David Li-Bland and Eckhard Meinrenken. Dirac Lie groups. *Asian Journal of Mathematics*, 18(5):pages 779–815, 2014.
URL <http://arxiv.org/abs/1110.1525>
- [20] David Li-Bland and Eckhard Meinrenken. On the Van Est homomorphism for Lie groupoids. *L'Enseignement Mathématique*, 61(1-2), 2014.
URL <http://arxiv.org/abs/1403.1191>
- [21] David Li-Bland and Alan Weinstein. Selective Categories and Linear Canonical Relations. *SIGMA Symmetry Integrability and Geometry: Methods and Applications*, 10(100):pages 1–31, 2014.
URL <http://arxiv.org/abs/1401.7302>
- [22] David Li-Bland and Pavol Ševera. Integration of Exact Courant Algebroids. *Electronic Research Announcements in Mathematical Sciences*, 19:pages 58–76, 2012.
URL <http://arxiv.org/abs/1101.3996>
- [23] David Li-Bland. AV-Courant Algebroids and Generalized CR Structures. *Canadian Journal of Mathematics*, 63(4):pages 938–960, 2011.
URL <http://arxiv.org/abs/0811.4470>
- [24] David Li-Bland and Pavol Ševera. Quasi-Hamiltonian groupoids and multiplicative Manin pairs. *International Mathematics Research Notices*, (10):pages 2295–2350, 2011.
URL <http://arxiv.org/abs/0911.2179>
- [25] David Li-Bland and Eckhard Meinrenken. Courant algebroids and Poisson geometry. *International Mathematics Research Notices*, (11):pages 2106–2145, 2009.
URL <http://arxiv.org/abs/0811.4554>

Ph. D. Thesis

- [26] David Li-Bland. *LA-Courant algebroids, and applications*. Ph.D. thesis, University of Toronto, 2012.
URL <http://arxiv.org/abs/1204.2796>

Volunteer Experiences

- 2013, 2025 **African Institute for Mathematical Sciences**, *Research Project Supervisor*, Ghana
- 2016 **International Mathematical Union’s Commission for Developing Countries**, *Volunteer Lecturer*, University of Dar Es Salaam
- 2014 **African Institute for Mathematical Sciences**, *Volunteer Lecturer*, Ghana