Samuel Stanton

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Research Interests

I am interested in foundational machine learning research with applications that promote human flourishing, particularly the life sciences. I wish to understand and design self-directed intelligent systems that automatically collect and incorporate the necessary information to make difficult decisions in consequential online settings. Applications of my work include control algorithms for robotic systems, efficient data collection strategies for public health surveillance, and lab-in-the-loop experimental design for antibody engineering.

PROFESSIONAL BACKGROUND

Prescient Design, Genentech Research and Early Development	New York City, NY
Principal Machine Learning Scientist	June 2022 - Present
Amazon Web Services	Remote
• Applied Science Intern	June 2020 - Aug. 2021
• Secondmind	Cambridge, U.K.
• Machine Learning Research Intern	June 2019 - Sept. 2019
• U.S. National Security Agency	San Antonio, TX
• Data Science Intern	May 2017 - Aug. 2017
Academic Background	
New York University	New York City, NY
Ph.D., Data Science, Thesis: Probabilistic Machine Learning for Online Decision-Making.	Aug 2019 - Sept 2022
• Cornell University	Ithaca, NY
• M.S., Operations Research	Aug 2017 - May 2019
• University of Colorado Denver	Denver, CO
• B.S. summa cum laude, Applied Mathematics	Aug 2013 - May 2017

Refereed Publications

- Chen, A.*, Stanton, S.*, Ding, F., Alberstein, R., ..., & Frey, N. (2025, July). Generalists vs. Specialists: Evaluating LLMs on Highly-Constrained Biophysical Sequence Optimization Tasks. In *Proceedings of the 42nd International Conference on Machine Learning*, tbd. PMLR.
- Prinster, D.*, Stanton, S.*, Liu, A., & Saria, S. (2024, July). Conformal Validity Guarantees Exist for Any Data Distribution. In *Proceedings of the 41st International Conference on Machine Learning*, 235:41086-41118. PMLR.
- Gruver, N.*, Stanton, S.*, Frey, N. C., Rudner, T. G., Hotzel, I., Lafrance-Vanasse, J., ... & Wilson, A. G. (2023, December). Protein Design with Guided Discrete Diffusion. Advances in Neural Information Processing Systems (spotlight), 36.
- Stanton, S., Maddox, W., & Wilson, A. G. (2023, April). Bayesian Optimization with Conformal Prediction Sets. In International Conference on Artificial Intelligence and Statistics (pp. 959-986). PMLR.
- Stanton, S., Maddox, W., Gruver, N., Maffettone, P., Delaney, E., Greenside, P., & Wilson, A. G. (2022, July). Accelerating Bayesian Optimization for Biological Sequence Design with Denoising Autoencoders. In *International Conference on Machine Learning* (spotlight) (pp. 20459-20478). PMLR.
- 6. Gruver, N., Finzi, M., **Stanton, S.**, & Wilson, A. G. (2022, April). Deconstructing the Inductive Biases of Hamiltonian Neural Networks. In *International Conference on Learning Representations* (spotlight).
- Stanton, S., Izmailov, P., Kirichenko, P., Alemi, A. A., & Wilson, A. G. (2021, December). Does Knowledge Distillation Really Work? Advances in Neural Information Processing Systems, 34, 6906-6919.
- Maddox, W. J., Stanton, S., & Wilson, A. G. (2021, December). Conditioning Sparse Variational Gaussian Processes for Online Decision-Making. Advances in Neural Information Processing Systems, 34, 6365-6379.
- 9. Amos, B., Stanton, S., Yarats, D., & Wilson, A. G. (2021, June). On the Model-Based Stochastic Value Gradient for Continuous Reinforcement Learning. In *Learning for Dynamics and Control* (pp. 6-20). PMLR.
- 10. Stanton, S., Maddox, W., Delbridge, I., & Wilson, A. G. (2021, April). Kernel Interpolation for Scalable Online Gaussian Processes. In International Conference on Artificial Intelligence and Statistics (pp. 3133-3141). PMLR.

 Finzi, M., Stanton, S., Izmailov, P., & Wilson, A. G. (2020, July). Generalizing Convolutional Neural Networks for Equivariance to Lie Groups on Arbitrary Continuous Data. In *International Conference on Machine Learning* (oral) (pp. 3165-3176). PMLR.

Refereed Workshop Papers

- Wang, A., Sang, Z., Stanton, S., ..., & Seeger, F. (2025, April). A Guided Design Framework for the Optimization of Therapeutic-Like Antibodies. 13th ICLR Workshop on Generative and Experimental Perspectives for Biomolecular Design.
- Stanton, S., Alberstein, R., Frey, N., Watkins, A., & Cho, K. (2024, July). Closed-Form Test Functions for Biophysical Sequence Optimization Algorithms. 1st ICML Workshop on Machine Learning for Life and Material Science.
- Adebayo, J., Stanton, S., Kelow, S., Maser, M., Bonneau, R., Gligorijevic, V., Cho, K., Ra, S., & Frey, N. (2023, December). Identifying Regularization Schemes That Make Feature Attributions Faithful. *NeurIPS Workshop on New Frontiers of AI for Drug Discovery and Development.*
- 4. Park, J. W., Stanton, S., Saremi, S., Watkins, A., Dwyer, H., Gligorijevic, V., ... & Cho, K. (2022, December). PropertyDAG: Multi-Objective Bayesian Optimization of Partially-Ordered, Mixed-Variable Properties for Biological Sequence Design. *NeurIPS Workshop on AI for Science*.
- 5. Stanton, S., Fakoor, R., Mueller, J., Wilson, A. G., & Smola, A. (2021, December). Robust Reinforcement Learning for Shifting Dynamics During Deployment. *NeurIPS Workshop on Safe and Robust Control of Uncertain Systems*.
- 6. Stanton, S., Wang, K. A., & Wilson, A. G. (2019, July). Model-based Policy Gradients with Entropy Exploration through Sampling. *ICML Generative Modeling and Model-Based Reasoning for Robotics and AI Workshop*.

Preprints

1. Frey, N.*, Hotzel, I.*, **Stanton, S.***, Kelly, R.*, Alberstein, R.*, ..., & Gligorijevic, V. (2025, March). Lab-in-the-loop therapeutic antibody design with deep learning. *Submitted to Nature Biotech, minor revisions requested*.

AWARDS

• NeurIPS Outstanding Reviewer	2021 - 2023
• ICML Outstanding Reviewer	2021 - 2024
• National Defense Science and Engineering Graduate (NDSEG) Fellowship	2018 - 2021

References

- Dr. Kyunghyun Cho, Senior Director of Frontier Research, Genentech Research and Early Development
- Dr. Andrew Gordon Wilson (Ph.D. advisor), Professor, Courant Institute of Mathematical Sciences, NYU
- Dr. Mark van der Wilk, Associate Professor, Department of Computer Science, University of Oxford