Alex Beatson

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Experience

- **Redesign Science**
  Director of Machine Learning *Oct 2022 - Current*
  - Leading Redesign's ML team to build and deploy tools for ML-accelerated drug discovery. Closely working with drug discovery teams to ensure our tools maximize their productivity. Initiated and maintain team- and company-level sprint planning process.
  - Built platform which pretrains transformers to generate molecular structures from SMILES strings and fine-tunes them to optimize rewards defined by molecular dynamics simulations and chemist-prompt-specified constraints. Scaled NN-based active learning from training on 100K and ranking 10M molecules to training on 100M and ranking 10B molecules. Developed autoencoder and diffusion models to accelerate molecular dynamics simulation.
  - Modernized developer experience, CI/CD, and data/workflow infrastructure: migrated from individual research repos & projects to a monorepo with code review and unified CI/CD; from 20min+ Docker builds to launch a job after each code change to 1-2min with git+pip, and from scripts orchestrating individual Kubernetes jobs to workflow orchestration using Prefect, Ray, and a datagrok.ai frontend.

- **Genesis Therapeutics**
  Principal Research Scientist *July 2021 - Oct 2022*
  - Tech lead for Genesis' language-model-based molecule generation platform and graph neural net-based active learning platform, managing two engineers. Also worked on benchmarking and workflow orchestration.
  - Led virtual screening and molecule generation for a drug program for solid tumor cancer inhibition, leading to several orders-of-magnitude improvement in experimentally-validated potency.

- **Google**
  Intern *Summer 2016&2017*
  - **Google Brain (2017)**: Optimized GAN architectures and losses using Neural Architecture Search.
  - **Speech Team (2016)**: Used transfer learning to improve low-resource language speech recognition with LSTMs.

Education

- **Princeton University** Princeton, NJ
  PhD in Computer Science (Machine Learning). Advisor: Ryan P. Adams. *2015-2021*
  Awarded the Gordon Wu Fellowship in Engineering. Topics: deep learning, generative models, meta-learning/meta-optimization, and ML methods for engineering simulation and design.

- **University of Canterbury** Christchurch, New Zealand
  Bachelor of Engineering with Honors in Mechatronics Engineering; First Class Honors. *2010-2014*

Recent papers

- **Meta-PDE: Learning to solve PDEs quickly without a mesh**: Tian Qin, Alex Beatson, Deniz Oktay, Nick McGreivy, Ryan P. Adams. arXiv, 2022.
- **Randomized automatic differentiation**: Deniz Oktay, Nick McGreivy, Joshua Aduol, Alex Beatson, Ryan P. Adams. ICLR, 2021. Oral presentation (top 2% of papers).
- **Learning composable energy surrogates for PDE order reduction**: Alex Beatson, Jordan T. Ash, Geoffrey Roeder, Tianju Xue, Ryan P. Adams. NeurIPS, 2021. Oral presentation (top 1% of papers).
- **A data-driven computational scheme for the nonlinear mechanical properties of cellular mechanical metamaterials under large deformation**: Tianju Xue, Alex Beatson, Maurizio Chiaramonte, Geoffrey Roeder, Jordan T. Ash, Yigit Menguc, Sigrid Adriaenssens, Ryan P. Adams, Sheng Mao. Soft Matter, 2020.
- **Amortized finite element analysis for fast PDE-constrained optimization**: Tianju Xue, Alex Beatson, Sigrid Adri aenssens, Ryan P. Adams. ICML, 2020.
- **SUMO: Unbiased estimation of log marginal probability for latent variable models**: Yucen Luo, Alex Beatson, Mohammad Norouzi, Jun Zhu, David Duvenaud, Ryan P. Adams, Ricky T. Q. Chen. ICLR, 2020.
- **Efficient optimization of loops and limits with randomized telescoping sums**: Alex Beatson, Ryan P. Adams. ICML, 2019.
- **Amortized Bayesian meta-learning**: Sachin Ravi, Alex Beatson. ICLR, 2019.
- **Continual learning in generative adversarial nets**: Ari Seff, Alex Beatson, Daniel Suo, Han Liu. arXiv 2017.
- **Blind attacks on machine learners**: Alex Beatson, Zhaoran Wang, Han Liu. NeurIPS, 2016.