DAVID H. BROOKES

(240) 499-4647 ⋄ david.brookes@berkeley.edu ⋄ Berkeley, CA
github.com/dhbrookes

EDUCATION

Ph.D., Biophysics Graduate Group August 2016 - May 2021
Berkeley AI Research Lab
University of California, Berkeley

B.S., Bioengineering August 2011 - May 2015
Concentration in Computational Biology
University of California, Berkeley

Relevant coursework: Theoretical Statistics, Graduate Statistical Mechanics I & II, Graduate Quantum Mechanics I, Introduction to Machine Learning, Efficient Algorithms and Intractable Problems, Numerical Analysis, Introduction to Artificial Intelligence.

PROFESSIONAL EXPERIENCE

AI Resident, *Google X* May 2019 - August 2019

· Combined machine learning expertise with software engineering skills to bolster an early-stage confidential project, as well as shape the project's future direction.
· Effectively communicated advanced modeling ideas to a team of people with vastly different expertise.

RESEARCH EXPERIENCE

Graduate Student Researcher, *Berkeley AI Research Lab* February 2018 - Present
Supervisor: Prof. Jennifer Listgarten

· Developed probabilistic modeling approaches for biological sequence design. Specifically, a rigorous probabilistic framework for sampling sequences that satisfy desired properties using joint supervised and generative modeling approaches ([2] and [3], below).
· Used insights from the above practical work to derive a novel connection between Estimation of Distribution algorithms and Expectation Maximization ([1], below).
· In upcoming work, we will apply our design methods in conjunction with novel modeling strategies to design a library of viral capsid sequences to be used in a downstream Directed Evolution experiment run by collaborators.

Student Researcher, *UC Berkeley College of Chemistry* October 2014 - February 2018
Supervisor: Prof. Teresa Head-Gordon

· Developed advanced simulation methods for studying the structure and dynamics of biological macromolecules.
· Designed custom Gaussian Process Regression kernels for enforcing rotational symmetry in atomistic force prediction, yielding closed-form data augmentation.
· Developed a Bayesian inference procedure for determining the ensemble of intrinsically disordered protein structures that are most likely given a set of experimental data ([4]).
· Lead developer of software suite to solve for electrostatic interactions on the surface of biological macromolecules. ([2] and [3], with code below available at `github.com/dhbrookes/pbsolvers`)
· Solved a linear model of basis functions to find the distribution of possible structures of liquid water that satisfy a set of experimental data ([5]).

RESEARCH

Papers

[1] **D. H. Brookes**, A. Busia, C. Fannjiang, K. Murphy, and J. Listgarten. A view of Estimation of Distribution Algorithms through the lens of Expectation Maximization. Accepted at *The Genetic and Evolutionary Computation Conference*, 2020.

[2] **D. H. Brookes**, H. Park, and J. Listgarten. Conditioning by adaptive sampling for robust design. *Proceedings of ICML*, 2019. **Selected for a 20 minute oral presentation (< 5% of submissions)**.

[3] **D. H. Brookes** and J. Listgarten. Design by adaptive sampling. *NeurIPS Workshop on Machine Learning for Molecules and Materials*, 2018.

[4] E. Jurrus, D. Engel, K. Star, K. Monson, J. Brandi, L. E. Felberg, **D. H. Brookes**, L. Wilson, J. Chen, K. Liles, M. Chun, P. Li, T. Dolinsky, R. Konecny, D. Koes, J. E. Nielsen, T. Head-Gordon, W. Geng, R. Krasny, M. Gunner, G.-W. Wei, M. J. Holst, J. A. McCammon, N. A. Baker. Improvements to the APBS biomolecular solvation software suite. *Protein Sci.* 27 (1), pp. 112-128, 2018.

[5] L. E. Felberg, **D. H. Brookes**, E. Jurrus, N. Baker, and T. Head-Gordon. PB-AM: An open-source, fully analytical linear Poisson-Boltzmann solver. *J. Comp. Chem.* 38 (15), pp. 1275-1282, 2017.

[6] **D. H. Brookes** and T. Head-Gordon. Experimental inferential structure determination of ensembles for intrinsically disordered proteins *J. Am. Chem. Soc.* 138 (13), pp. 4530-4538, 2016.

[7] **D. H. Brookes** and T. Head-Gordon. The family of oxygen-oxygen radial distribution functions for water. *J. Phys. Chem. Lett.* 6 (15), pp. 2938-2943, 2015

[8] L. E. Felberg, **D. H. Brookes**, J. E. Rice, T. Head-Gordon, and W. Swope. Role of hydrophilicity and length of diblock arms for determining star polymer physical properties. *J. Phys. Chem. B.* 119 (3), pp. 944-957, 2015.

Invited talks and posters

1. A view of Estimation of Distribution Algorithms through the lens of Expectation Maximization *The Genetic and Evolutionary Computation Conference*, Jul. 2020.
2. Conditioning by adaptive sampling for robust design. *ICML*, Jun. 2019.
3. Design by Adaptive Sampling. *Google AI, Mountain View*, Jan. 2019.
4. Design by Adaptive Sampling. *NeurIPS Workshop on Machine Learning for Molecules and Materials*, Dec. 2018.
5. Sequence Design by Adaptive Sampling. *Berkeley Center for Computational Biology Retreat*, Nov. 2018.