Nicholas T Franklin, Ph.D.

nthompsonfranklin@gmail.com　•　nicktfranklin.github.io

Summary

Research scientist with 10+ years developing novel methods for learning and generalization over structured spaces, spanning deep generative models, reinforcement learning, and Bayesian inference. Published at NeurIPS, Psychological Review, eLife, and other leading venues. My current work applies these methods to biomolecular design, developing generative approaches for molecular modeling and *de novo* design.

Experience

Flagship Pioneering　　　　　　　　　　　　　　　　　　　　　　　Cambridge, MA
Senior Scientist, Machine Learning　　　　　　　　　　　　　　　　*Nov 2023–Present*

Research scientist in Pioneering Intelligence, Flagship's ML/AI research group. I develop novel methods in deep generative modeling and reinforcement learning, with a focus on developing new methods in molecular modeling. My work is published at leading ML venues.

Selected research:

- **Gradient-based sampling for inverting structure prediction models.** Supervised the development of Relaxed Sequence Sampling (RSS), an MCMC framework that inverts AlphaFold2 via gradient-based sampling with protein language model priors, producing $5\times$ more designable structures and 2–$3\times$ greater diversity than baselines (MLSB Workshop; senior author).
- **Autoregressive GFlowNets for diverse sequence generation.** Extended GFlowNet sampling methods with autoregressive language models for *de novo* design of discrete sequences.
- **Mechanistic interpretability in structure prediction models.** Investigated learned representations in co-folding architectures using sparse autoencoders, yielding interpretable features from pair representations (MLSB Workshop).
- **Efficient attention mechanisms.** Co-developed Flash Invariant Point Attention, an efficient reformulation of geometric attention that achieves linear scaling for structure prediction, enabling generation of proteins with thousands of residues (NeurIPS 2025, Spotlight).

Research leadership: Set technical research direction, supervise and recruit junior scientists and interns, and lead cross-team research collaborations.

Hyperscience　　　　　　　　　　　　　　　　　　　　　　　　　　New York, NY
Applied Scientist　　　　　　　　　　　　　　　　　　　　　　　*Feb 2021–Jul 2022*

Applied ML research on document understanding (computer vision and NLP) at a growth-stage start-up.

Harvard University　　　　　　　　　　　　　　　　　　　　　　　Cambridge, MA
Postdoctoral Fellow, Lab of Samuel J. Gershman　　　　　　　　　*Sep 2017–Jan 2021*

Developed Structured Event Memory (SEM), a first-authored neurosymbolic generative model combining LSTMs with Bayesian nonparametric inference over structured representations (Psychological Review). Published additional work on probabilistic Bayesian methods for learning and memory (Cognitive Psychology). Created open-source research software. Supervised student research in computational neuroscience and deep learning.

Brown University　　　　　　　　　　　　　　　　　　　　　　　Providence, RI
Graduate Researcher, Lab of Michael J. Frank　　　　　　　　　*Sep 2011–Aug 2017*

Developed novel models of reinforcement learning and biological neural networks using nonparametric Bayesian methods. Published theoretical and empirical work in leading journals (PLOS Computational Biology, eLife).

Education

Ph.D. in Cognitive Science, Brown University — August 2017
B.S. Biology, B.A. Spanish, The University of Texas at Austin — May 2009

Technical Skills

Research Methods: Deep generative models (diffusion, flow-matching, VAEs, autoregressive models), reinforcement learning (GFlowNets, PPO), Bayesian nonparametrics, probabilistic inference, mechanistic interpretability

Domains: Protein modeling and design, small molecule modeling, biomolecular simulation, computational neuroscience

Engineering: Python, PyTorch, transformers, NumPy, Git, AWS, Lightning

Languages: English (native), Spanish (professionally proficient), French (intermediate)

Selected Publications

1. Ko J, Rontogiannis A, Ban YEA, Elaldi A, **Franklin NT**[†] (2025): Relaxed Sequence Sampling for Diverse Protein Design. *Machine Learning for Structural Biology Workshop* ([†]senior author)

2. Migliorini G, Rontogiannis A, Guitchounts G, **Franklin NT**, Elaldi A, Viessmann O (2025): PairSAE: Mechanistic Interpretability from Pair Representations In Protein Co-Folding. *Machine Learning for Structural Biology Workshop*

3. Liu A, Elaldi A, **Franklin NT**, Russell N, Atwal GS, Ban YEA, Viessmann O (2025): Flash Invariant Point Attention. *NeurIPS 2025* (Spotlight)

4. Buekers AO, Collin Silvy HP, Kempner RP, **Franklin NT**, Gershman SJ, Norman KA (2024) Blocked training facilitates learning of multiple schemas. *Communications Psychology*

5. **Franklin NT** & Frank MJ (2020). Generalizing to generalize: humans flexibly switch between compositional and conjunctive structures during reinforcement learning. *PLOS Computational Biology*

6. **Franklin NT**, Norman KA, Ranganath C, Zacks JM, Gershman SJ (2020) Structured event memory: a neuro-symbolic model of event cognition. *Psychological Review*

7. Schulz E, **Franklin NT**, Gershman SJ (2020). Finding structure in multi-armed bandits. *Cognitive Psychology*

8. **Franklin NT**, Frank MJ (2018). Compositional clustering in task structure learning. *PLOS Computational Biology*

9. **Franklin NT** & Frank MJ (2015). A cholinergic feedback circuit to regulate striatal population uncertainty and optimize reinforcement learning. *eLife*