

# Nicholas T Franklin, Ph.D.

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## Summary

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Research scientist with 10+ years developing novel methods in generative models, reinforcement learning and Bayesian inference. I build general methods and apply them to problems in molecular modeling. Published at NeurIPS, Psychological Review, eLife, and other leading venues.

## Experience

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### Flagship Pioneering

*Senior Scientist, Machine Learning*

Cambridge, MA

*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 application in biomolecular modeling. My work is published at leading ML venues.

*Technical Leadership:* Set technical research direction, supervise and recruit junior scientists and interns, and lead cross-team research collaborations.

*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  $2\text{--}3\times$  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).

### Hyperscience

*Applied Scientist*

New York, NY

*Feb 2021–Jul 2022*

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

### Harvard University

*Postdoctoral Fellow, Lab of Samuel J. Gershman*

Cambridge, MA

*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

*Graduate Researcher, Lab of Michael J. Frank*

Providence, RI

*Sep 2011–Aug 2017*

Developed novel nonparametric Bayesian reinforcement learning models and biological neural networks.

Published theoretical and empirical work in leading computational neuroscience journals (PLOS Computational Biology, eLife).

## Education

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**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

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

**Engineering:** Python, PyTorch, Git, Lightning

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

## Selected Publications

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1. Ko J, Rontogiannis A, Ban YEA, Elaldi A, **Franklin NT**<sup>†</sup> (2025): Relaxed Sequence Sampling for Diverse Protein Design. *Machine Learning for Structural Biology Workshop* (<sup>†</sup>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* (\*Equal Contribution)
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*