David Pfau

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Professional Experience

Google DeepMind, London, UK

Staff Research Scientist 2021 -

Senior Research Scientist 2019 - 2021

Research Scientist 2015 - 2019

Advancing research at the forefront of artificial intelligence, with a focus on AI for science. Did foundational work on the use of differential geometry in unsupervised learning. Pioneered the use of deep neural networks for solving problems in quantum chemistry from first principles, including first-author work in *Science*. Launched a collaboration with EPFL on reinforcement learning for nuclear fusion which led to a publication in *Nature* and significant press.

Imperial College London, London, UK

Visiting Professor, Department of Physics 2021 -

Co-advising students in the group of W. M. C. Foulkes on the use of deep neural networks for *ab-initio* computational quantum physics. Work published in *Physical Review Letters*, *Nature Communications* and *Physical Review X*.

Qadium, San Francisco, CA 2014 - 2015

Senior Research Scientist

Consulted on Data Microscopes, an open-source library of fast, modular nonparametric Bayesian models.

Education

Columbia University, New York, NY 2008 - 2014

Ph.D., Neurobiology and Behavior. July 2014.

- Advisor: Liam Paninski
- Thesis: *Learning Structure in Time Series for Neuroscience and Beyond*

M.Phil., Neurobiology and Behavior. November 2011.

Stanford University, Stanford, CA 2003 - 2007

B.S., Physics, Minor in Mathematics. GPA: 3.76, 3.88 in major.

Journal Publications

D. Pfau, S. Axelrod, H. Sutterud, I. von Glehn, J. S. Spencer (2024). *Accurate Computation of Quantum Excited States with Neural Networks*. Science 385, 6711.

W. T. Lou, H. Sutterud, G. Cassella, W. M. C. Foulkes, J. Knolle, **D. Pfau**, J. S. Spencer (2024). *Neural Wave Functions for Superfluids*. Physical Review X 14, 021030.

G. Cassella, W. M. C. Foulkes, **D. Pfau**, J. S. Spencer (2024). *Neural Network Variational Monte Carlo for Positronic Chemistry*. Nature Communications 15(1), 5124.

J. Citrin, P. Trochim, T. Goerler, **D. Pfau**, K. van de Plassche, F. Jenko (2023). *Fast Transport Simulations with Higher-Fidelity Surrogate Models of ITER*. Physics of Plasmas 30(6):062501.

G. Cassella, H. Sutterud, S. Azadi, N. D. Drummond, **D. Pfau**, J. S. Spencer, W. M. C. Foulkes (2023). *Discovering Quantum Phase Transitions with Fermionic Neural Networks*. Physical Review Letters 130(3):036401. **Editors' Suggestion**

J. Degrave,* F. Felici,* J. Buchli,* M. Neunert,* B. Tracey,* F. Carpanese,* T. Ewalds,* R. Hafner,* A. Abdolmaleki, D. de las Casas, C. Donner, L. Fritz, C. Galperti, A. Huber, J. Keeling, M. Tsimpoukelli, J. Kay, A. Merle, J.-M. Moret, S. Noury, F. Pesamosca, **D. Pfau**, O. Sauter, C.

Sommariva, S. Coda, B. Duval, A. Fasoli, P. Kohli, K. Kavukcuoglu, D. Hassabis, M. Riedmiller* (2022). *Magnetic Control of Tokamak Plasmas Through Deep Reinforcement Learning.* Nature 602:414-419.

J. Kirkpatrick,* B. McMorrow,* D. H. P. Turban,* A. L. Gaunt,* J. S. Spencer, A. G. de G. Matthews, A. Obika, L. Thiry, M. Fortunato, **D. Pfau**, L. Roman Castellanos, S. Petersen, A. W. R. Nelson, P. Kohli, P. Mori-Snchez, D. Hassabis, A. J. Cohen (2021). *Pushing the Frontiers of Density Functionals by Solving the Fractional Electron Problem.* Science 374(6573):1385-1389.

R. Evans, M. Bonjak, L. Buesing, K. Ellis, **D. Pfau**, P. Kohli, M. Sergot (2021). *Making Sense of Raw Input.* Artificial Intelligence 299:103521.

D. Pfau,* J. S. Spencer,* A. G. de G. Matthews, W. M. C. Foulkes (2020). *Ab-initio Solution of the Many-Electron Schrödinger Equation with Deep Neural Networks.* Physical Review Research 2(3):033429.

E. A. Pnevmatikakis, D. Soudry, Y. Gao, T. A. Machado, J. Merel, **D. Pfau**, T. Reardon, Y. Mu, C. Lacefield, W. Yang, M. Ahrens, R. Bruno, T. M. Jessell, D. S. Peterka, R. Yuste, L. Paninski (2016). *Simultaneous Denoising, Deconvolution, and Demixing of Calcium Imaging Data.* Neuron 89(2):285-299.

F. Doshi-Velez, **D. Pfau**, F. Wood, N. Roy (2015). *Bayesian Nonparametric Methods for Partially-Observable Reinforcement Learning.* IEEE Transactions on Pattern Analysis and Machine Intelligence 37(2):394-407.

J. Zylberberg, **D. Pfau**, M. DeWeese (2012). *Dead Leaves and the Dirty Ground: Low-level Image Statistics in Transmissive and Occlusive Imaging Environments.* Physical Review E 86, 066112. `http://arxiv.org/abs/1209.3277`

Conference Publications

I. von Glehn, J. S. Spencer, **D. Pfau** (2023). *A Self-Attention Ansatz for Ab-initio Quantum Chemistry.* 11th International Conference on Learning Representations, Kigali, Rwanda.

D. Pfau, I. Higgins, A. Botev, S. Racanire (2020). *Disentangling by Subspace Diffusion.* Advances in Neural Information Processing Systems 34, Vancouver, BC.

D. Pfau, S. Petersen, A. Agarwal, D. Barrett, K. L. Stachenfeld (2019). *Spectral Inference Networks: Unifying Deep and Spectral Learning.* 7th International Conference on Learning Representations, New Orleans, Louisiana.

L. Metz, B. Poole, **D. Pfau**, J. Sohl-Dickstein (2017). *Unrolled Generative Adversarial Networks.* 5th International Conference on Learning Representations, Toulon, France.

M. Andrychowicz, M. Denil, S. Gomez, M. W. Hoffman, **D. Pfau**, T. Schaul, N. de Freitas (2016). *Learning to Learn by Gradient Descent by Gradient Descent.* Advances in Neural Information Processing Systems 30, Barcelona, Spain.

C. Fernando, D. Banarse, M. Reynolds, F. Besse, **D. Pfau**, M. Jaderberg, M. Lanctot, D. Wierstra (2016). *Convolution by Evolution: Differentiable Pattern Producing Networks.* The Genetic and Evolutionary Computing Conference, Denver, CO.

D. Pfau, E. Pnevmatikakis, L. Paninski (2013). *Robust Learning of Low-Dimensional Dynamics from Large Neural Ensembles.* Advances in Neural Information Processing Systems 26, Lake Tahoe, NV.

Y. Wong, D. Putrino, M. Vigeral, **D. Pfau**, J. Merel, L. Paninski, B. Pesaran (2012). *Decoding Arm and Hand Movements Across Layers of the Macaque Frontal Cortices.* Proceedings of the 34th Conference of the IEEE Engineering in Medicine and Biology Society, San Diego, CA.

D. Pfau, N. Bartlett, F. Wood (2010). *Probabilistic Deterministic Infinite Automata.* Advances in Neural Information Processing Systems 23, Vancouver, Canada. **Poster Spotlight Presentation**.

N. Bartlett, **D. Pfau**, F. Wood (2010). *Forgetting Counts: Constant Memory Inference for a Dependent Hierarchical Pitman-Yor Process.* Proceedings of the Twenty-Seventh International Conference on Machine Learning, Haifa, Israel.

Review Articles

J. Hermann, J. S. Spencer, K. Choo, A. Mezzacapo, W. M. C. Foulkes, **D. Pfau**, G. Carleo, F. No (2023). *Ab-initio Quantum Chemistry with Neural-Network Wavefunctions.* Nature Reviews Chemistry 7(8).

Workshop Papers and Preprints

J. Citrin, I. Goodfellow, A. Raju, J. Chen, J. Degrave, C. Donner, F. Felici, P. Hamel, A. Huber, D. Nikulin, **D. Pfau**, B. Tracey, M. Riedmiller, P. Kohli (2024). *TORAX: A Fast and Differentiable Tokamak Transport Simulator in JAX.* arXiv:2406.06718.

D. Pfau, D. Rezende (2020). *Integrable Nonparametric Flows.* NeurIPS Workshop on Machine Learning and Physical Sciences, Vancouver, BC.

J. S. Spencer,* **D. Pfau**,* A. Botev, W. M. C. Foulkes (2020). *Better, Faster Fermionic Neural Networks.* NeurIPS Workshop on Machine Learning and Physical Sciences, Vancouver, BC.

I. Higgins,* D. Amos,* **D. Pfau**, S. Racaniere, L. Matthey, D. Rezende, A. Lerchner (2018). *Towards a Definition of Disentangled Representations.* arXiv:1812.02230.

D. Pfau, C. P. Burgess (2018). *Minimally Redundant Laplacian Eigenmaps.* 6th International Conference on Learning Representations, Workshop Track, Vancouver, Canada.

D. Pfau, O. Vinyals (2016). *Connecting Generative Adversarial Networks and Actor-Critic Methods.* NIPS Workshop on Adversarial Training, Barcelona, Spain. **Spotlight Presentation**.

Conference Abstracts and Poster Presentations

D. Pfau, J. Freeman, M. Ahrens, L. Paninski (2013). *Scalable Region of Interest Detection for Calcium Imaging.* NIPS Workshop: Acquiring and Analyzing the Activity of Large Neural Ensembles.

D. Pfau, E. Pnevmatikakis, L. Paninski (2013). *Robust Learning of Dynamics for Large Neural Ensembles.* Computational and Systems Neuroscience, Salt Lake City, UT.

K. Emmett, J. Rosenstein, **D. Pfau**, A. Bamberger, K. Shepard, C. Wiggins (2013). *Statistical Inference of DNA Translocation using Parallel Expectation Maximization.* Bulletin of the American Physical Society 58(1), Baltimore, MD.

D. Pfau, N. Bartlett, F. Wood (2010). *Bayesian Infinite Automata.* New York Machine Learning Symposium, New York, NY.

D. Pfau, X. Pitkow, L. Paninski (2009). *A Bayesian Method to Predict the Optimal Diffusion Coefficient in Random Fixational Eye Movements.* Computational and Systems Neuroscience, Salt Lake City, UT. doi:10.3389/conf.neuro.06.2009.03.049

Invited Academic Talks	ML in Physics Seminar, Princeton University, Princeton, NJ.	April 2024
	AMLab Seminar, University of Amsterdam, Amsterdam, Netherlands.	February 2024
	International Symposium on ML in QC, Uppsala University, Uppsala, Sweden.	December 2023
	ML@FI Seminar, Flatiron Institute, New York, NY.	October 2023
	Many-Body Quantum Physics with ML, ECT*, Trento, Italy.	September 2023
	Sensory Prediction, Engineering and Evolved, Santa Fe Institute, Santa Fe, NM.	July 2023
	Deep Learning Meets VMC, University of Vienna, Vienna, Austria.	July 2023
	Condensed Matter Theory Group Seminar, Imperial College, London, UK.	January 2023
	ML and Physical Sciences Workshop, NeurIPS, New Orleans, LA.	December 2022
	Imperial Computing Conference, Imperial College, London, UK.	December 2022
	ML for Materials Hard and Soft, Erwin Schrödinger Institute, Vienna, Austria.	July 2022
	The University of Toronto and The Vector Institute, Toronto, Canada.	March 2022
	ML and Informatics for Chemistry and Materials, TSRC, Telluride, CO.	September 2021
	Physics ∩ ML, Virtual.	June 2021
	University of Tübingen, Tübingen, Germany.	March 2021
	Baruch College, New York, NY.	February 2021
	Princeton Plasma Physics Laboratory, Princeton, NJ.	February 2021
	Quantum Comp. Material Science Roundtable, Osaka University, Osaka, Japan.	January 2021
	Monte Carlo and Quasi Monte Carlo Methods (MCQMC), Oxford, UK.	August 2020
	Baylor College of Medicine and Rice University, Houston, TX.	July 2020
	Deep Learning Seminar, Imperial College, London, UK.	February 2019
	Physics in Machine Learning Workshop, University of California, Berkeley, CA.	May 2019
	Machine Learning Summer School (MLSS), Buenos Aires, Argentina.	June 2018
	IML Machine Learning Workshop, CERN, Geneva, Switzerland.	April 2018
	International Conference on Computer Vision (ICCV), Venice, Italy.	October 2017
	Data, Learning and Inference (DALI), Tenerife, Spain.	April 2017
	York Plasma Institute, University of York, UK.	March 2017
	Redwood Center for Theoretical Neuroscience, Berkeley, CA.	April 2014
	CoSyNe Workshop: Discovering Structure in Neural Data, Snowbird, UT.	March 2014
Public Outreach	*The Gradient* Podcast	July 2024
	ARPA-E Advanced Technology Forum, Houston, TX.	June 2023
	British Film Institute, London, UK.	April 2019
	Creative AI Meetup, London, UK.	April 2018
	Somerset House, London, UK.	January 2018
	Jugular Dialogue, London, UK.	October 2016
	Gray Area Foundation for the Arts, San Francisco, CA.	February 2016
Teaching Experience	**Columbia University**, New York, NY	
	Guest Lecturer, W3995 Neuroscience and the Law	Fall 2013

Teaching Assistant, G8325 Statistical Analysis of Neural Data	Fall 2012
Teaching Assistant, G4360 Theoretical Neuroscience	Spring 2011

Professional Service

PhD Student Supervision

Jointly with W. M. C. Foulkes and James Spencer:

Gino Cassella, Imperial College London	2021 - present
Halvard Sutterud, Imperial College London	2021 - present

Thesis Committees

Janith Petangoda, Imperial College London	2022
Georgios Arvanitidis, TU Denmark	2019

Area Chairing

International Conference on Learning Representations	2022-2025
Artificial Intelligence and Statistics	2024-2025
International Conference on Machine Learning	2024
Neural Information Processing Systems	2021-2022

Reviewing and Program Committees

Nature Communications	2023
International Conference on Learning Representations	2017-2021
Nature Computational Science	2021
Neural Information Processing Systems	2011, 2013, 2015-2020
International Joint Conference on Artificial Intelligence	2019
International Conference of Machine Learning	2018
Nature	2017
Computational and Systems Neuroscience	2017
IEEE Transactions on Pattern Analysis and Machine Intelligence	2012
Journal of Machine Learning Research	2011
Artificial Intelligence and Statistics	2011

Workshop Organizing

Learning Disentangled Representations: from Perception to Control, NeurIPS	2017

Other

Reviewer Mentoring, International Conference on Learning Representations	2022
Volunteer, Neural Information Processing Systems	2010