

# David Kristjanson Duvenaud

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PROFESSIONAL EXPERIENCE	<b>Vector Institute</b> <i>Founding Member</i>	September 2017 – present
	<b>University of Toronto</b> <i>Assistant Professor</i> , Computer Science and Statistical Sciences Canada Research Chair in Generative Models	July 2016 – present
	<b>Harvard School of Engineering and Applied Sciences</b> <i>Postdoctoral Fellow</i> , Intelligent Probabilistic Systems group Worked with Prof. Ryan P. Adams on Bayesian optimization, deep learning, molecular modeling, and variational inference.	Sept 2014 – June 2016
	<b>Max Planck Institute for Intelligent Systems</b> <i>Visiting Researcher</i> , Schölkopf group Worked with Phillip Hennig on stochastic quasi-Newton optimization, model-based ordinary differential equation solvers, and nonparametric inference methods.	Summer 2012
	<b>Google Research</b> <i>Software Engineering Intern</i> , Video Content Analysis team Used machine vision to solve YouTube video classification problems at scale. Contributed to DistBelief, a close-to-the-metal distributed deep learning framework, and precursor to TensorFlow.	Summers 2010 and 2011
	<b>Invenia</b> <i>Cofounder</i> Recruited, trained and supervised five research assistants, plus consultants. Wrote, presented and was awarded several research grants. Led two research contracts applying machine learning methods to energy forecasts. These projects led to the deployment of automated forecasting systems for several major utilities. Invenia currently has a full-time staff of 35.	2006 – present
EDUCATION	<b>University of Cambridge, Machine Learning Group</b> Ph.D., Engineering Advisors: Carl Rasmussen and Zoubin Ghahramani Thesis: Automatic model construction with Gaussian processes	2010 – 2014
	<b>University of British Columbia, Laboratory for Computational Intelligence</b> M. Sc., Computer Science Advisor: Kevin P. Murphy Thesis: Multiscale conditional random fields for machine vision	2008 – 2010
	<b>University of Manitoba</b> B. Sc. Hons., Computer Science. First class honours.	2001 – 2006
GRANTS AND AWARDS	Google faculty award: \$45,000 NIPS Best paper award Samsung research gift: \$67,250 NVIDIA Compute the Cure research grant: \$250,000 Tier II Canada Research Chair: \$500,000 NSERC Discovery Grant: \$140,000	2019 2018 2018 2017 2017 2017

PREPRINTS

**Invertible Residual Networks** Behrmann, J., Grathwohl, W., Chen, R. T. Q., Duvenaud, D., Jacobsen, J. *arXiv:1802.09419*, 2019

**Stochastic Hyperparameter Optimization through Hypernetworks.** Lorraine, J., Duvenaud, D., *arXiv:1802.09419*, 2018

REFEREED  
PUBLICATIONS

**FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models.** Grathwohl, W., Chen, T. Q., Bettencourt, J., Sutskever, I., Duvenaud, D., *International Conference on Learning Representations*, 2019. Oral presentation.

**Self-Tuning Networks: Bilevel Optimization of Hyperparameters using Structured Best-Response Functions.** MacKay, M., Vicol, P., Lorraine, J., Duvenaud, D., Grosse, R. *International Conference on Learning Representations*, 2019.

**Explaining Image Classifiers by Counterfactual Generation.** Chang, C., Creager, E., Gold-  
enberg, A., Duvenaud, D., *International Conference on Learning Representations*, 2019.

**Latent-space Dynamics for Reduced Deformable Simulation.** Fulton, L., Modi, V., Duve-  
naud, D., Levin, D. I. W., Jacobson, A. *Eurographics*, 2019.

**Neural Ordinary Differential Equations.** Chen, T. Q., Rubanova, Y., Bettencourt, J., Duve-  
naud, D., *Neural Information Processing Systems*, 2018. Best paper award.

Chen, T., Li, X., Grosse, R., Duvenaud, D.. **Isolating Sources of Disentanglement in Varia-  
tional Autoencoders.** *Neural Information Processing Systems*, 2018. Oral presentation.

Cremer, C., Li, X., Duvenaud, D.. **Inference Suboptimality in Variational Autoencoders.**  
*International Conference on Machine Learning*, 2018.

G Zhang, S Sun, Duvenaud, D., Grosse, R., **Noisy Natural Gradient as Variational Inference.**  
*International Conference on Machine Learning*, 2018.

Grathwohl, G., Choi, D., Wu, Y., Roeder, G., Duvenaud, D., **Backpropagation through the  
Void: Optimizing control variates for black-box gradient estimation.** *International Con-  
ference on Learning Representations, 2018*

Gómez-Bombarelli, R., Wei, N., Duvenaud, D., Hernández-Lobato, J.M., Sánchez-Lengeling, B.,  
Sheberla, D., Aguilera-Iparraguirre, J., Hirzel, T., Adams, R.P., and Aspuru-Guzik, A. **Automatic  
chemical design using a data-driven continuous representation of molecules.** *ACS Central  
Science*, 2018

Schulz, E., Tenenbaum, J., Duvenaud, D., Speekenbrink, M., Gershman, S. **Compositional In-  
ductive Biases in Function Learning.** *Cognitive Psychology*, 2017.

Roeder, G., Wu, Y., Duvenaud, D., **Sticking the Landing: Simple, Lower-variance Gradient  
Estimators for Variational Inference.** *Neural Information Processing Systems*, 2017.

Wei, J.N., Duvenaud, D., Aspuru-Guzik, A. **Neural Networks for the Prediction of Organic  
Chemistry Reactions.** *American Chemical Society Central Science*, 2016.

Johnson, M.J., Duvenaud, D., Wiltschko, A.B., Datta, S.R., Adams, R.P. **Composing Graphical  
Models with Neural Networks for Structured Representations and Fast Inference.** *Neu-  
ral Information Processing Systems*, 2016.

Schulz, E., Tenenbaum, J., Duvenaud, D., Speekenbrink, M., Gershman, S. **Probing the Compo-  
sitionality of Intuitive Functions.** *Neural Information Processing Systems*, 2016.

Gómez-Bombarelli, R., Aguilera-Iparraguirre, R., Hirzel T., Duvenaud, D., Maclaurin, M., Blood-  
Forsythe, M., Chae H., Einzinger, M., Ha, D., Wu, T., Markopoulos, G., Jeon, S., Kang, H., Sekine,  
W., Miyazaki, H., Numata, M., Kim, S., Huang, W., Hong, S., Buchwald, S., Baldo, M., Adams,  
R. P. Aspuru-Guzik, A. **Design of Efficient Molecular Organic Light-emitting Diodes by a  
High-throughput Virtual Screening and Experimental Approach.** *Nature Materials*, 2016.

- Duvenaud, D.\*, Maclaurin, D.\*, Adams, R.P. **Early Stopping as Nonparametric Variational Inference.** *Artificial Intelligence and Statistics*, 2016. Oral Presentation (Top 6.5% of submissions)
- Huang, A., Duvenaud, D., Gajos, K. **ChordRipple: Recommending Chords to Help Novice Composers Go Beyond the Ordinary.** *Intelligent User Interfaces*, 2016.
- Duvenaud, D.\*, Maclaurin, D.\*, Aguilera-Iparraguirre, J., Gómez-Bombarelli, R., Hirzel, T., Aspuru-Guzik, A., Adams, R.P. **Convolutional Networks on Graphs for Learning Molecular Fingerprints.** *Neural Information Processing Systems*, 2015.
- Maclaurin, D.\*, Duvenaud, D.\*, Adams, R.P. **Gradient-based Hyperparameter Optimization through Reversible Learning.** *International Conference on Machine Learning*, 2015.
- Schober, M., Duvenaud, D., Hennig, P. **Probabilistic ODE Solvers with Runge-Kutta Means.** *Neural Information Processing Systems*, 2014. Oral Presentation (Top 1.2% of submissions)
- Lloyd, J.R., Duvenaud, D., Grosse, R., Tenenbaum, J. B., Ghahramani, Z. **Automatic Construction and Natural-Language Description of Nonparametric Regression Models.** *Association for the Advancement of Artificial Intelligence*, 2014.
- Duvenaud, D., Rippel, O., Adams, R.P., Ghahramani, Z. **Avoiding Pathologies in Very Deep Networks.** *Artificial Intelligence and Statistics*, 2014.
- Huang, A., Duvenaud, D., Arnold, K., Partridge, B., Oberholtzer, J., Gajos, K. **Active Learning of Intuitive Control Knobs for Synthesizers Using Gaussian Processes.** *Intelligent User Interfaces*, 2014.
- Iwata, T., Duvenaud, D., Ghahramani, Z. **Warped Mixtures for Nonparametric Cluster Shapes.** *Uncertainty in Artificial Intelligence*, 2013.
- Duvenaud, D.\*, Lloyd, J.R.\*, Grosse, R., Tenenbaum, J. B., Ghahramani, Z. **Structure Discovery in Nonparametric Regression through Compositional Kernel Search.** *International Conference on Machine Learning*, 2013.
- Osborne, M., Duvenaud, D., Garnett, R., Rasmussen, C. E., Roberts, S., Ghahramani, Z. **Active Learning of Model Evidence using Bayesian Quadrature.** *Neural Information Processing Systems*, 2012.
- Huszár, F. Duvenaud, D. **Optimally-Weighted Herding is Bayesian Quadrature.** *Uncertainty in Artificial Intelligence*, 2012. Oral Presentation (Top 8% of submissions)
- Duvenaud, D., Nickisch, H., Rasmussen, C. E. **Additive Gaussian Processes.** *Neural Information Processing Systems*, 2011.
- Duvenaud, D., Marlin, B., Murphy, K. **Multiscale Conditional Random Fields for Semi-supervised Labeling and Classification.** *Conference on Computer and Robot Vision*, 2011.
- Roeder, G., Killoran, N., Grathwohl, W., Duvenaud, D. **Design Motifs for Probabilistic Generative Design** *ICLR workshop track*, 2018
- Nado, Z., Snoek, J., Grosse, R., Duvenaud, D., Xu, B., Martens, J. **Stochastic Gradient Langevin Dynamics that Exploit Neural Network Structure** *ICLR workshop track*, 2018
- Killoran, N., Lee, L., DeLong, A., Duvenaud, D., Frey, B., **Generating and designing DNA with deep generative models** *NIPS workshop on Machine Learning in Computational Biology*, 2017.
- Cremer, C., Q Morris, Q., and Duvenaud, D.. **Reinterpreting Importance-Weighted Autoencoders.** *ICLR workshop track*, 2017
- Duvenaud, D., and Adams, R.P. **Black-box Stochastic Variational Inference in Five Lines of Python.** *NIPS workshop on Black-box inference methods*, 2015
- Altieri, N. and Duvenaud, D. **Variational Inference with Gradient Flows.** *NIPS workshop on*

*Advances in Approximate Bayesian Inference*, 2015

Maclaurin, D., Duvenaud, D., and Adams, R.P. **Autograd: Reverse-mode Differentiation of Native Python.** *ICML workshop on Automatic Machine Learning*, 2015

Grosse, R., and Duvenaud, D.. **Testing Markov-chain Monte Carlo code.** *NIPS Workshop on Software Engineering for Machine Learning*, 2014

Swersky, K., Duvenaud, D., Snoek, J., Hutter, F., and Osborne, M.A. **Raiders of the Lost Architecture: Kernels for Bayesian Optimization in Conditional Parameter Spaces.** *NIPS workshop on Bayesian Optimization*, 2013.

Duvenaud, D., Eaton, D., Murphy, K., and Schmidt, M. **Causal learning without DAGs.** *Journal of Machine Learning Research, Workshop & Conference Proceedings*, 2010.

PATENTS Aspuru-Guzik, A., Gomez-Bombarelli, R., Hirzel, T.D., Aguilera-Iparraguirre, J., Adams, R.P., Maclaurin, D., and Duvenaud, D. **Organic light-emitting diode materials.** WO2015175678

INVITED TALKS	NVIDIA Research	December 2018
	Symposium on Advances in Approximate Bayesian Inference	December 2018
	Toronto Machine Learning Summit	November 2018
	CIFAR Deep Learning Summer School	July 2018
	University of Oxford, Robotics Research Group	July 2018
	Microsoft Research Cambridge	July 2018
	Google Deepmind	July 2018
	ICML Workshop on Credit Assignment in Reinforcement Learning	July 2018
	Google Brain, San Francisco	June 2018
	UC Berkeley, Center for Human-Compatible AI	June 2018
	NIPS Workshop on Machine Learning for Molecules and Materials	December 2017
	Toronto Machine Learning Summit	November 2017
	Montréal Deep Learning Summit	October 2017
	Simons Institute, Workshop on Machine Learning	May 2017
	Data Learning and Inference Meeting (DALI)	April 2017
	Google Brain, Mountain View	February 2017
	University of Waterloo, Computational Mathematics Colloquium	January 2017
	NIPS Workshop on Automatic Differentiation	December 2016
	NIPS Workshop on Optimizing the Optimizers	December 2016
	American Chemical Society National Meeting, Machine Learning Workshop	August 2016
	OpenAI	April 2016
	University of Toronto, Department of Computer Science	March 2016
	University of British Columbia, Department of Computer Science	March 2016
	New York University, Computer Science Department	February 2016
	Princeton University, Department of Computer Science	February 2016
	Université de Montréal, Institute for Learning Algorithms	February 2016
	Cambridge University, Computational and Biological Learning Lab	February 2016
	Twitter Cortex	February 2016
	NIPS Workshop on Probabilistic Integration	December 2015
	MIT Media Lab, Laboratory for Social Machines	November 2015
	UMass Amherst, Machine Learning and Friends Lunch	November 2015
	Broad Institute, Stat Math Reading Club	November 2015
	Brown University, Scientific Computing Group	November 2015
	University of Toronto, Machine Learning Group	October 2015
	Microsoft Research Cambridge	July 2015
	University of Oxford, Robotics Research Group	July 2015
	University of Oxford, Future of Humanity Institute	July 2015

	Google DeepMind	July 2015
	Cambridge University, Computational and Biological Learning Lab	July 2015
	ICML Workshop on Automatic Machine Learning	July 2015
	Conference on Bayesian Nonparametrics	June 2015
	Boston Machine Learning Meetup	February 2015
	Harvard Society for Mind, Brain and Behavior	December 2014
	Sheffield University, Deep Probabilistic Models Workshop	October 2014
	MIT CSAIL, Clinical Decision Making Group	October 2014
	London Machine Learning Meetup	June 2014
	University of Oxford, Future of Humanity Institute	January 2014
	University of Toronto, Machine Learning Group	January 2014
	University of Oxford, Robotics Research Group	April 2013
	Microsoft Research Cambridge	March 2013
	Sheffield University, Institute for Translational Neuroscience	February 2013
	NIPS Workshop on Confluence between Kernel Methods and Graphical Models	December 2012
	NIPS Workshop on Probabilistic Numerics	December 2012
	ICML Workshop on RKHS and Kernel-based methods	July 2012
	University of Washington, Statistics Department	January 2011
	DeepMind Technologies	November 2011
SERVICE	Area Chair, International Conference on Machine Learning (ICML)	2017, 2018, 2019
	Area Chair, International Conference on Learning Representations (ICLR)	2017, 2018, 2019
	Area Chair, Neural Information Processing Systems (NIPS)	2017, 2018
	Area Chair, Artificial Intelligence and Statistics (AISTATS)	2017, 2018
	Co-organizer, NIPS Workshop on Aligned Artificial Intelligence	2017
	Area Chair, Association for the Advancement of Artificial Intelligence (AAAI)	2017
	Co-organizer, NIPS Workshop on Reliable Machine learning	2016
REVIEWING	European Physical Journal C	2019
	Workshop on Language for Inference (LAFI)	2019
	Journal of Machine Learning Research (JMLR)	2012, 2013, 2015, 2018
	Journal of Chemical Information and Modeling	2018
	Science	2018
	Computer Graphics and Interactive Techniques (SIGGRAPH)	2018
	American Chemical Society Central Science (ACS)	2017, 2108
	Nature	2017
	IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)	2012, 2017
	International Joint Conferences on Artificial Intelligence (IJCAI)	2016
	International Conference on Learning Representations (ICLR)	2016
	Neural Information Processing Systems (NIPS)	2013, 2014, 2015, 2016
	International Conference on Machine Learning (ICML)	2013, 2014, 2015, 2016
	Artificial Intelligence and Statistics (AISTATS)	2014, 2015
	Statistics and Computing	2013, 2014, 2015
PRESS COVERAGE	New AI Method Wins Coveted NeurIPS Award. <i>Psychology Today</i>	January 14, 2019
	A radical new neural network design. <i>MIT Technology Review</i>	December 12, 2018
	Interview: <i>Talking Machines podcast</i>	Sept 8, 2018
	Should Artificial Intelligence Copy the Human Brain? <i>Wall Street Journal</i>	August 4, 2018
	Interview: New frontiers in deep learning research. <i>In Context Podcast</i>	March 29, 2018
	Interview: <i>This week in machine learning &amp; AI podcast</i>	January 15, 2018
	Is AI riding a one-trick pony? <i>MIT Tech. Rev.</i>	September 29, 2017
	Finally, a way to halt Canada's 'brain drain'. <i>Globe and Mail.</i>	July 10, 2017
	Software dreams up new molecules in quest for wonder drugs. <i>MIT Tech. Rev.</i>	November 3, 2016

‘Artificial brain’ aces undergrad organic chemistry test. <i>Chemistry World</i>	October 17, 2016
The hunt for tomorrow’s diodes is tangled up in blue. <i>Wall Street Journal</i>	August 19, 2016
‘Molecular Tinder’ may change the game for OLED screens. <i>Techcrunch</i>	August 8, 2016
The growing influence of statisticians. <i>Phys-org</i>	June 4, 2015
The Automatic Statistician and electrified meat. <i>Talking Machines podcast</i>	March 26, 2015
Automating the data scientists. <i>MIT Technology Review</i>	February 13, 2015
How machines learned to think statistically. <i>Significance magazine</i>	February 3, 2015
Google is funding an artificial intelligence for data science. <i>Yahoo! News</i>	December 2, 2014