David Kristjanson Duvenaud

Professional Experience

Vector Institute — September 2017 – present
Founding Member

University of Toronto — July 2016 – present
Assistant Professor, Computer Science and Statistical Sciences
Canada Research Chair in Generative Models

Harvard School of Engineering and Applied Sciences — Sept 2014 – June 2016
Postdoctoral Fellow, Intelligent Probabilistic Systems group
Worked with Prof. Ryan P. Adams on Bayesian optimization, deep learning, molecular modeling, and variational inference.

Max Planck Institute for Intelligent Systems — Summer 2012
Visiting Researcher, Schölkopf group
Worked with Phillip Hennig on stochastic quasi-Newton optimization, model-based ordinary differential equation solvers, and nonparametric inference methods.

Google Research — Summers 2010 and 2011
Software Engineering Intern, 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.

Invenia — 2006 – present
Cofounder
Co-founded a machine learning research consulting company. 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.

Education

University of Cambridge, Machine Learning Group — 2010 – 2014
Ph.D., Engineering
Advisors: Carl Rasmussen and Zoubin Ghahramani
Thesis: Automatic model construction with Gaussian processes

University of British Columbia, Laboratory for Computational Intelligence — 2008 – 2010
M. Sc., Computer Science
Advisor: Kevin P. Murphy
Thesis: Multiscale conditional random fields for machine vision

University of Manitoba — 2001 – 2006
B. Sc. Hons., Computer Science. First class honours.

Grants and Awards (CAD)

CIFAR AI Chair: $750,000	2021
Google faculty award: $45,000	2019
NeurIPS Best paper award	2018
Samsung research gift: $67,250	2018
NVIDIA Compute the Cure research grant: $250,000	2017
Tier II Canada Research Chair: $500,000	2017
NSERC Discovery Grant: $140,000	2017

Refereed Publications

[47] Raghu, A., Raghu, M., Kornblith, S., Duvenaud, D., & Hinton, G. (2021). Teaching with commentaries. In *International conference on learning representations.*

[46] Grathowhl, W., Kelly, J., Hashemi, M., Norouzi, M., Swersky, K., & Duvenaud, D. (2021). No MCMC for me: Amortized sampling for fast and stable training of energy-based models. In *International conference on learning representations.*

[45] Tonekaboni, S., Joshi, S., Campbell, K., Duvenaud, D., & Goldenberg, A. (2020). What went wrong and when? instance-wise feature importance for time-series models. In *Neural information processing systems.*

[44] Kelly, J., Bettencourt, J., Johnson, M. J., & Duvenaud, D. (2020). Learning differential equations that are easy to solve. In *Neural information processing systems.*

[43] Grathwohl, W., Wang, K.-C., Jacobsen, J.-H., Duvenaud, D., & Zemel., R. (2020). Learning the Stein discrepancy for training and evaluating energy-based models without sampling. In *International conference on machine learning.*

[42] Li, X., Chen, R. T. Q., Wong, T.-K. L., & Duvenaud, D. (2020). Scalable gradients for stochastic differential equations. In *Artificial intelligence and statistics.*

[41] Lorraine, J., Vicol, P., & Duvenaud, D. (2020). Optimizing millions of hyperparameters by implicit differentiation. In *Artificial intelligence and statistics.*

[40] Grathwohl, W., Wang, K.-C., Jacobsen, J.-H., Duvenaud, D., Norouzi, M., & Swersky, K. (2020). Your classifier is secretly an energy based model and you should treat it like one. In *International conference on learning representations.*

[39] Luo, Y., Beatson, A., Norouzi, M., Zhu, J., Duvenaud, D., Adams, R. P., & Chen, R. T. (2020). SUMO: Unbiased estimation of log marginal probability for latent variable models. In *International conference on learning representations.*

[38] Chen, R. T. Q., & Duvenaud, D. (2019). Neural networks with cheap differential operators. In *Neural information processing systems.*

[37] Chen, R. T. Q., Rubanova, Y., & Duvenaud, D. (2019). Latent ODEs for irregularly-sampled time series. In *Neural information processing systems.*

[36] Liao, R., Li, Y., Song, Y., Wang, S., Hamilton, W., Duvenaud, D., ... Zemel, R. (2019). Efficient graph generation with graph recurrent attention networks. In *Neural information processing systems.*

[35] Chen, R. T., mann, J., Duvenaud, D., & Jacobsen, J.-H. (2019). Residual flows for invertible generative modeling. In *Neural information processing systems.*

[34] Ethayarajh, K., Duvenaud, D., & Hirst, G. (2019a). Towards understanding linear word analogies. In *Association for computational linguistics.*

[33] Ethayarajh, K., Duvenaud, D., & Hirst, G. (2019b). Understanding undesirable word embedding associations. In *Association for computational linguistics.*

[32] Chen, R. T., mann, J., Duvenaud, D., & Jacobsen, J.-H. (2019). Residual flows for invertible generative modeling. In *Neural information processing systems.*

[31] Behrmann, J., Grathwohl, W., Chen, R. T. Q., Duvenaud, D., & Jacobsen, J.-H. (2019). Invertible residual networks. In *International conference on machine learning.* Oral presentation.

[30] Grathwohl, W., Chen, R. T. Q., Bettencourt, J., Sutskever, I., & Duvenaud, D. (2019). Ffjord: Free-form continuous dynamics for scalable reversible generative models. *International Conference on Learning Representations*. Oral presentation.

[29] MacKay, M., Vicol, P., Lorraine, J., Duvenaud, D., & Grosse, R. (2019). Self-tuning networks: Bilevel optimization of hyperparameters using structured best-response functions. In *International conference on learning representations.*

[28] Chang, C.-H., Creager, E., Goldenberg, A., & Duvenaud, D. (2019). Explaining image classifiers by adaptive dropout and generative in-filling. In *International conference on learning representations.*

[27] Fulton, L., Modi, V., Duvenaud, D., Levin, D. I., & Jacobson, A. (2019). Latent-space dynamics for reduced deformable simulation. In *Computer graphics forum* (Vol. 38, pp. 379–391).

[26] Chen, R. T. Q., Rubanova, Y., Bettencourt, J., & Duvenaud, D. (2018). Neural ordinary differential equations. *Neural Information Processing Systems*. Best paper award.

[25] Chen, R. T. Q., Li, X., Grosse, R., & Duvenaud, D. (2018). Isolating sources of disentanglement in variational autoencoders. *Neural Information Processing Systems*. Oral Presentation.

[24] Cremer, C., Li, X., & Duvenaud, D. (2018). Inference suboptimality in variational autoencoders. *International Conference on Machine Learning*.

[23] Zhang, G., Sun, S., Duvenaud, D., & Grosse, R. (2018). Noisy natural gradient as variational inference. *International Conference on Machine Learning*.

[22] Grathwohl, W., Choi, D., Wu, Y., Roeder, G., & Duvenaud, D. (2018). Backpropagation through the void: Optimizing control variates for black-box gradient estimation. In *International conference on learning representations.*

[21] Gomez-Bombarelli, R., Wei, J. N., Duvenaud, D., Hernandez-Lobato, J. M., Sanchez-Lengeling, B., Sheberla, D., . . . Aspuru-Guzik, A. (2018). Automatic chemical design using a data-driven continuous representation of molecules. *American Chemical Society Central Science*.

[20] Schulz, E., Tenenbaum, J. B., Duvenaud, D., Speekenbrink, M., & Gershman, S. J. (2017). Compositional inductive biases in function learning. *Cognitive psychology*, *99*, 44–79.

[19] Roeder, G., Wu, Y., & Duvenaud, D. (2017). Sticking the landing: Simple, lower-variance gradient estimators for variational inference. In *Neural information processing systems.*

[18] Wei, J. N., Duvenaud, D., & Aspuru-Guzik, A. (2016). Neural networks for the prediction of organic chemistry reactions. *ACS Central Science*, *2*(10), 725-732.

[17] Johnson, M. J., Duvenaud, D., Wiltschko, A., Datta, S., & Adams, R. P. (2016). Composing graphical models with neural networks for structured representations and fast inference. In *Neural information processing systems.*

[16] Shulz, E., Tenenbaum, J. B., Duvenaud, D., Speekenbrink, M., & Gershman, S. J. (2016). Probing the compositionality of intuitive functions. In *Neural information processing systems.*

[15] Gómez-Bombarelli, R., Aguilera-Iparraguirre, J., Hirzel, T. D., Duvenaud, D., Maclaurin, D., Blood-Forsythe, M. A., ... Aspuru-Guzik, A. (2016). Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. *Nature materials*, *15*(10), 1120.

[14] Duvenaud, D., Maclaurin, D., & Adams, R. (2016). Early stopping as nonparametric variational inference. In *Artificial intelligence and statistics* (pp. 1070–1077).

[13] Huang, C.-Z. A., Duvenaud, D., & Gajos, K. Z. (2016). Chordripple: Recommending chords to help novice composers go beyond the ordinary. In *Intelligent user interfaces* (pp. 241–250).

[12] Duvenaud, D., Maclaurin, D., Aguilera-Iparraguirre, J., Gómez-Bombarelli, R., Hirzel, T., Aspuru-Guzik, A., & Adams, R. P. (2015). Convolutional networks on graphs for learning molecular fingerprints. In *Neural information processing systems.*

[11] Maclaurin, D., Duvenaud, D., & Adams, R. P. (2015, July). Gradient-based hyperparameter optimization through reversible learning. In *International conference on machine learning.*

[10] Schober, M., Duvenaud, D., & Hennig, P. (2014). Probabilistic ODE solvers with Runge-Kutta means. In *Neural information processing systems.* Oral presentation.

[9] Lloyd, J. R., Duvenaud, D., Grosse, R., Tenenbaum, J. B., & Ghahramani, Z. (2014). Automatic construction and natural-language description of nonparametric regression models. In *Association for the advancement of artificial intelligence (aaai).*

[8] Duvenaud, D., Rippel, O., Adams, R. P., & Ghahramani, Z. (2014). Avoiding pathologies in very deep networks. In *Artificial intelligence and statistics.*

[7] Anna Huang, C.-Z., Duvenaud, D., Arnold, K., Partridge, B., W. Oberholtzer, J., & Z. Gajos, K. (2014, 02). Active learning of intuitive control knobs for synthesizers using Gaussian processes. In (p. 115-124).

[6] Tomoharu Iwata, Z. G., David Duvenaud. (2013). Warped mixtures for nonparametric cluster shapes. In *Uncertainty in artificial intelligence* (p. 311-319).

[5] Duvenaud, D., Lloyd, J. R., Grosse, R., Tenenbaum, J. B., & Ghahramani, Z. (2013). Structure discovery in nonparametric regression through compositional kernel search. In *International conference on machine learning* (pp. 1166–1174).

[4] Osborne, M. A., Duvenaud, D., Garnett, R., Rasmussen, C. E., Roberts, S. J., & Ghahramani, Z. (2012). Active learning of model evidence using Bayesian quadrature. In *Neural information processing systems.*

[3] Huszár, F., & Duvenaud, D. (2012). Optimally-weighted herding is Bayesian quadrature. In *Uncertainty in artificial intelligence* (pp. 377–385). Oral presentation.

[2] Duvenaud, D., Nickisch, H., & Rasmussen, C. E. (2011). Additive Gaussian processes. In *Neural information processing systems* (pp. 226–234).

[1] Duvenaud, D., Marlin, B., & Murphy, K. (2011). Multiscale conditional random fields for semi-supervised labeling and classification. In *Proceedings of the 8th Canadian conference on computer and robot vision* (pp. 371–378). IEEE Computer Society.

Workshop Publications

[9] Nado, Z., Snoek, J., Grosse, R., Duvenaud, D., Xu, B., & Martens, J. (2018). Stochastic gradient langevin dynamics that exploit neural network structure. In *International conference on learning representations workshop track.*

[8] Killoran, N., Lee, L. J., Delong, A., Duvenaud, D., & Frey, B. J. (2017). Generating and designing DNA with deep generative models. In *NIPS workshop on machine learning in computational biology.*

[7] Cremer, C., Morris, Q., & Duvenaud, D. (2017). Reinterpreting importance-weighted autoencoders. *International Conference on Learning Represenations Workshop Track*.

[6] Duvenaud, D., & Adams, R. P. (2015). Black-box stochastic variational inference in five lines of python. *NIPS Workshop on Black-box Learning and Inference*.

[5] Altieri, N., & Duvenaud, D. (2015). Variational inference with gradient flows. In *NIPS workshop on advances in approximate bayesian inference.*

[4] Maclaurin, D., Duvenaud, D., Johnson, M. J., & Adams, R. P. (2015). Autograd: Reverse-mode differentiation of native python. *ICML workshop on Automatic Machine Learning*.

[3] Grosse, R., & Duvenaud, D. (2014). Testing markov-chain monte carlo code. In *NIPS workshop on software engineering for machine learning.*

[2] Swersky, K., Duvenaud, D., Snoek, J., Hutter, F., & Osborne, M. (2013). Raiders of the lost architecture: Kernels for Bayesian optimization in conditional parameter spaces. In *NIPS workshop on bayesian optimization.*

[1] Duvenaud, D., Eaton, D., Murphy, K., & Schmidt, M. (2010). Causal learning without DAGs. In *Journal of machine learning research workshop and conference proceedings* (Vol. 6, pp. 177–190).

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

University College London, DeepMind/ELLIS CSML Seminar Series (remote)	February 2021
NeurIPS Europe meetup on Bayesian Deep Learning (remote)	December 2020
NeurIPS Workshop: Beyond Backpropagation (remote)	December 2020
NeurIPS Tutorial: Deep Implicit Layers (remote)	December 2020
Toronto Machine Learning Summit (remote)	November 2020
University of Amsterdam Machine Learning Seminar (remote)	November 2020
Toronto Machine Learning Summit (remote)	November 2020
University of Washington, Applied Math seminar series (remote)	October 2020
ODSC West Virtual Conference (remote)	October 2020
University of Toronto, Computer Science Student Union Seminar (remote)	October 2020
University of Pennsylvania, Applied Math Colliquium Series (remote)	October 2020
Tenth International Workshop on Climate Informatics (remote)	September 2020
Symposium on Sparse Recovery and Machine Learning, SIAM Annual Meeting (remote)	July 2020
World AI Conference, Beijing (remote)	July 2020
Institute for Advanced Study, Princeton University (remote)	April 2020
Guest Lecture, Yale University (remote)	March 2020
Deep Structures Workshop, Aalto University, Finland	December 2019
NeurIPS Retrospectives Workshop	December 2019
NeurIPS Workshop on Learning Meaningful Representations of Life	December 2019
NeurIPS Communications Practicum	December 2019

University of British Columbia	December 2019
Toronto Machine Learning Summit	November 2019
Fields Institute, Conference on Data Science	November 2019
MIT CSAIL Machine Learning Seminar	October 2019
Google Brain, Cambridge, Massachusetts	October 2019
Harvard University, Data to Actionable Knowledge Group	October 2019
Broad Institute, Models, Inference & Algorithms Initiative	October 2019
Gatsby Computational Neuroscience Unit, University College London	May 2019
Oxford Undergraduate Maths Society	May 2019
NVIDIA Research Toronto	December 2018
Symposium on Advances in Approximate Bayesian Inference, Montréal	December 2018
Canada-UK Colloquium on AI	November 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
NeurIPS 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
NeurIPS Workshop on Automatic Differentiation	December 2016
NeurIPS 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 Algorthms	February 2016
Cambridge University, Computational and Biological Learning Lab	February 2016
Twitter Cortex	February 2016
NeurIPS 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
	NeurIPS Workshop on Confluence between Kernel Methods and Graphical Models	December 2012
	NeurIPS 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	Senior Area Chair, Neural Information Processing Systems (NeurIPS)	2020, 2021
	Area Chair, Intl. Conference on Learning Representations (ICLR)	2017, 2018, 2019, 2020, 2021
	Area Chair, International Conference on Machine Learning (ICML)	2017, 2018, 2019, 2021
	Sponsorships Chair, Uncertainty in Artificial Intelligence (UAI)	2020
	Area Chair, Neural Information Processing Systems (NeurIPS)	2017, 2018, 2019
	Area Chair, Artificial Intelligence and Statistics (AISTATS)	2017, 2018
	Co-organizer, NeurIPS Workshop on Aligned Artificial Intelligence	2017
	Area Chair, Association for the Advancement of Artificial Intelligence (AAAI)	2017
	Co-organizer, NeurIPS Workshop on Reliable Machine learning	2016
Reviewing	Nature Communications	2020
	Journal of Machine Learning Research (JMLR)	2012, 2013, 2015, 2018, 2019, 2020
	Neural Computation	2020
	ICML Workshop on Invertible Neural Networks and Normalizing Flows	2020
	Proceedings of the National Academy of Sciences of the United States of America (PNAS)	2020
	NeurIPS Workshop Proposals	2019
	European Physical Journal C	2019
	Workshop on Language for Inference (LAFI)	2019
	Journal of Chemical Information and Modeling	2018
	Science	2018
	Computer Graphics and Interactive Techniques (SIGGRAPH)	2018
	Nature	2017
	American Chemical Society Central Science (ACS)	2017, 2108
	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 (NeurIPS)	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	AI makes predictions about random events like market trades. *VentureBeat*	May 7, 2020
	Profile: The Chosen Few. *Report on Business Magazine*	February 25, 2019
	New AI Method Wins Coveted NeurIPS Award. *Psychology Today*	January 14, 2019
	NeurIPS 2018 Best Paper Team: “Math Is Forever” *Synced Newsletter*	December 21, 2018
	A radical new neural network design. *MIT Technology Review*	December 12, 2018
	Interview: *Talking Machines podcast*	Sept 8, 2018
	Should Artificial Intelligence Copy the Human Brain? *Wall Street Journal*	August 4, 2018
	Interview: New frontiers in deep learning research. *In Context Podcast*	March 29, 2018
	Interview: *This week in machine learning & AI podcast*	January 15, 2018

Is AI riding a one-trick pony? *MIT Tech. Rev.*	September 29, 2017
Finally, a way to halt Canada's 'brain drain'. *Globe and Mail.*	July 10, 2017
Software dreams up new molecules in quest for wonder drugs. *MIT Tech. Rev.*	November 3, 2016
'Artificial brain' aces undergrad organic chemistry test. *Chemistry World*	October 17, 2016
The hunt for tomorrow's diodes is tangled up in blue. *Wall Street Journal*	August 19, 2016
'Molecular Tinder' may change the game for OLED screens. *Techcrunch*	August 8, 2016
The growing influence of statisticians. *Phys-org*	June 4, 2015
The Automatic Statistician and electrified meat. *Talking Machines podcast*	March 26, 2015
Automating the data scientists. *MIT Technology Review*	February 13, 2015
How machines learned to think statistically. *Significance magazine*	February 3, 2015
Google is funding an artificial intelligence for data science. *Yahoo! News*	December 2, 2014