

David Kristjanson Duvenaud

PROFESSIONAL EXPERIENCE	University of Toronto July 2016 – present <i>Assistant Professor</i> , Computer Science and Statistics
	Harvard School of Engineering and Applied Sciences Sept 2014 – June 2016 <i>Postdoctoral Fellow</i> , 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 <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.
	Google Research Summers 2010 and 2011 <i>Software Engineering Intern</i> , Video Content Analysis team Used machine vision to solve YouTube video classification problems at scale. Contributed to Dist-Belief, a close-to-the-metal distributed deep learning framework, precursor to TensorFlow.
	Invenia 2006 – present 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 20.
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 honors
HONORS AND AWARDS	NSERC Postdoctoral Fellowship: \$80,000 (declined) 2014 Cambridge Commonwealth Trust Scholarship: £36,000 2010 NSERC Postgraduate Scholarship: \$42,000 2010 Vanier Canada Graduate Scholarship: \$100,000 (declined) 2010 Best Prediction Score, DREAM Protein Signaling Network Challenge 2009 Alexander Graham Bell Canada Graduate Scholarship: \$35,000 2008 First Place, International Student Unmanned Aerial Vehicle Competition 2006

PREPRINTS

Gómez-Bombarelli, R.*, Duvenaud, D.*, Hernández-Lobato, J.M.*, Aguilera-Iparraguirre, J., Hirzel, T., Adams, R.P., and Aspuru-Guzik, A. **Automatic chemical design using a data-driven continuous representation of molecules.** *ArXiv:1610.02415*, 2016.

REFEREED
PUBLICATIONS

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

Johnson, M.J., Duvenaud, D., Wiltchko, A.B., Datta, S.R., Adams, R.P. **Composing Graphical Models with Neural Networks for Structured Representations and Fast Inference** To appear in *Neural Information Processing Systems*, 2016.

Schulz, E., Tenenbaum, J., Duvenaud, D., Speekenbrink, M., Gershman, S. **Probing the Compositionality of Intuitive Functions** To appear in *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. and 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.*, and Adams, R.P. **Early Stopping as Nonparametric Variational Inference.** To appear in *Artificial Intelligence and Statistics*, 2016. **Oral Presentation** (Top 6.5% of submissions)

Huang, A., Duvenaud, D., and 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., and Adams, R.P. **Convolutional Networks on Graphs for Learning Molecular Fingerprints.** *Neural Information Processing Systems*, 2015.

Maclaurin, D.*, Duvenaud, D.*, and Adams, R.P. **Gradient-based Hyperparameter Optimization through Reversible Learning.** *International Conference on Machine Learning*, 2015.

Schober, M., Duvenaud, D., and 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., and 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., and Ghahramani, Z. **Avoiding Pathologies in Very Deep Networks.** *Artificial Intelligence and Statistics*, 2014.

Huang, A., Duvenaud, D., Arnold, K., Partridge, B., Oberholtzer, J., and Gajos, K. **Active Learning of Intuitive Control Knobs for Synthesizers Using Gaussian Processes.** *Intelligent User Interfaces*, 2014.

Iwata, T., Duvenaud, D., and Ghahramani, Z. **Warped Mixtures for Nonparametric Cluster Shapes.** *Uncertainty in Artificial Intelligence*, 2013.

Duvenaud, D.*, Lloyd, J.R.*, Grosse, R., Tenenbaum, J. B., and 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., and Ghahramani, Z. **Active Learning of Model Evidence using Bayesian Quadrature.** *Neural Information Processing Systems*, 2012.

Huszár, F. and Duvenaud, D. **Optimally-Weighted Herding is Bayesian Quadrature.** *Uncer-*

tainty in Artificial Intelligence, 2012. **Oral Presentation** (Top 8% of submissions)

Duvenaud, D., Nickisch, H., and Rasmussen, C. E. **Additive Gaussian Processes**. *Neural Information Processing Systems*, 2011.

Duvenaud, D., Marlin, B., and Murphy, K. **Multiscale Conditional Random Fields for Semi-supervised Labeling and Classification**. *Conference on Computer and Robot Vision*, 2011.

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

WORKSHOP
PUBLICATIONS

Duvenaud, D. and Adams, R.P. **Black-box Stochastic Variational Inference in Five Lines of Python**. *NIPS workshop on Black-box inference methods*, 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.

PATENTS

Adams, R.P., Aguilera-Iparraguirre, J., Aspuru-Guzik, A., Duvenaud, D., Gomez-Bombarelli, R., Hirzel, T.D., and Maclaurin, D. **Combinatorial assembly of donor-bridge-acceptor fragments for organic light emitting diodes**. US patent pending, filed 2014

INVITED TALKS

(upcoming) Simons Institute workshop on Machine Learning	May 2017
(upcoming) Data Learning and Inference Meeting	May 2017
Google Brain	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, Association for the Advancement of Artificial Intelligence (AAAI) (upcoming)	2017
	Area Chair, Neural Information Processing Systems (NIPS)	2017
	Area Chair, International Conference on Machine Learning (ICML)	2017
	Area Chair, International Conference on Learning Representations (ICLR)	2017
	Area Chair, Artificial Intelligence and Statistics (AISTATS)	2017
	Co-organizer, NIPS Workshop on Reliable Machine learning	2016
REVIEWING	American Chemical Society Central Science (ACS)	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 (SC)	2013, 2014, 2015
	Journal of Machine Learning Research (JMLR)	2012, 2013, 2015
	IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)	2012
PRESS COVERAGE	Software dreams up new molecules in quest for wonder drugs. <i>MIT Tech. Rev.</i>	November 3rd, 2016
	‘Artificial brain’ aces undergrad organic chemistry test. <i>Chemistry World</i>	October 17th, 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