Rory Donovan-Maiye

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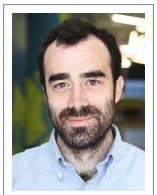

Employment

2017– **Scientist**, *Allen Institute for Cell Science*.
Modeling Team – Integrative methods for cell modeling, primarily focused on deep learning techniques

2016–2017 **Postdoctoral Fellow**, *Institute for System Biology*.
Price Lab – personalized medicine & wellness, mouse and human genomics

Education

2011–2016 **Ph.D.**, *Carnegie Mellon–University of Pittsburgh Program in Computational Biology*.
Systems Biology & Machine Learning

2004–2005 **M.S.**, *University of Washington*.
Physics

2000–2004 **B.A**, *Reed College*.
Physics

Research

Integrated Cell Modeling.
I've been working in collaboration with Greg Johnson to build integrated models of single cells. We use conditional generative adversarial networks (GANs) to fuse data from multiple fluorescence microscopy experiments into a coherent model of sub-cellular structure localization in single cells.

Sparse Time-Series Models.
This project aims to integrate data across time-points to build sparse regression models for time-series data, such that the sparse regressors at neighboring time points vary smoothly. This would be useful for e.g. RNA-seq experiments with multiple time-points, if you wanted to predict the set genes driving a phenotype, and see how that set changes over time.

Integrated Workflow for Transcription Factor Binding Site Prediction.
In an effort to find the best candidate transcriptions factors to input to the Price Lab's transcriptional regulatory network inference tools, I constructed a machine learning pipeline to integrate an array of genome-scale data and predictive tools to output a single high confidence prediction of transcriptional activity at arbitrary sites across the genome.

Graphical Models for Free Energy Estimation.
Computationally estimating how strongly two biomolecules bind together is often either overly time consuming (e.g. molecular dynamics) or overly empirical (e.g. docking). Alternatively, using graphical models of proteins to compute the Bethe free energy of binding can be both fast and accurate.

Weighted Ensemble Systems Biology.
By applying weighted ensemble sampling to stochastic models of biological processes, we achieved orders of magnitude speed-ups in simulating events of interest in these complex systems. Our first paper dealt with non-spatial models, and our second paper addresses models of spatially resolved cellular processes.

Quantitative Evolution and the ATP Synthase.
Using simple state-based models of proton transport and free energy transduction, we probe the optimality of the curiously engineered rotary mechanism of the ATP synthase, using models that are entirely agnostic to structure and are optimized over all unknown parameters that are thermodynamically permissible.

Stochastic Models of Cellular Heterogeneity.
Simple stochastic models can recapitulate the population-level heterogeneity of protein abundance found in, for example, colonies of E. coli. This work employs a non-spatial model of gene expression, stochastically simulated with a modified Gillespie algorithm that takes into account cell division.

Computational Skills

Languages, *Python, Julia, R, Matlab, Mathematica, Fortran, C, C++, Bash, HTML & CSS, LaTeX.*
Scientific programming with a focus on simulation algorithms, data analysis, computational efficiency, machine learning, and GPU-dirven deep learning. Strong abilities and interests in:

- Expertise in Python, Matlab, R, and Julia, with additional proficiency in lower-level compiled languages.
- Machine learning and the automated extraction of knowledge from data.
- Web design and the visual display of quantitative information.

Training Experience

2012–2015 **Research Assistant**, *Carnegie Mellon–University of Pittsburgh Program in Computational Biology*.
Working with Prof. Daniel Zuckerman, applying the weighted ensemble formalism to systems biology models.

2012–2015 **Teaching Assistant**, *Carnegie Mellon–University of Pittsburgh Program in Computational Biology*.
Graduate-level computational structural biology.

2004–2006 **Research Assistant**, *University of Washington*.
Worked with Prof. John Rehr, developing *ab initio* methods for computing Compton scattering profiles.

2005–2006 **Teaching Assistant**, *University of Washington*.
Introductory and advanced undergraduate physics curriculum.

Publications

Rory M Donovan-Maiye, Christopher J Langmead, and Daniel Zuckerman. Systematic testing of belief-propagation estimates for absolute free energies in atomistic peptides and proteins. *Journal of chemical theory and computation*, 2017.

Gregory R Johnson, Rory M Donovan-Maiye, and Mary M Maleckar. Generative modeling with conditional autoencoders: Building an integrated cell. *arXiv preprint arXiv:1705.00092*, 2017.

Ramu Anandakrishnan, Zining Zhang, Rory Donovan-Maiye, and Daniel M Zuckerman. Biophysical comparison of atp synthesis mechanisms shows a kinetic advantage for the rotary process. *Proceedings of the National Academy of Sciences*, 113(40):11220–11225, 2016.

Rory M. Donovan, Jose-Juan Tapia, Devin P. Sullivan, James R. Faeder, Robert F. Murphy, Markus Dittrich, and Daniel M. Zuckerman. Unbiased rare event sampling in spatial stochastic systems biology models using a weighted ensemble of trajectories. *PLoS Computational Biology*, 2016.

Andrew J. Sedgewick, Ivy Shi, Rory M. Donovan, and Panatiotis V. Benos. Learning mixed graphical models with separate sparsity parameters and stability-based model selection. *BMC Genomics*, 2014.

Rory M. Donovan, Andrew J. Sedgewick, James R. Faeder, and Daniel M. Zuckerman. Efficient stochastic simulation of chemical kinetics networks using a weighted ensemble of trajectories. *The Journal of Chemical Physics*, 139(11):115105, 2013.

Rory M. Donovan. *Quantization of constrained systems*. Bachelor's thesis, Reed College, 2004.

Posters

2015 **q-bio**, *Rare Event Sampling in Spatial Stochastic Systems Biology Models Using A Weighted Ensemble Of Trajectories*.

2015 **Biophysical Society**, *Rare Event Sampling in Stochastic Systems Biology Models Using A Weighted Ensemble Of Trajectories*.

2014 **RECOMB**, *Accelerating systems biology computation: Rapid estimation of equilibrium and kinetic quantities via weighted ensemble sampling*.

2013 **q-bio**, *Rare Event Sampling of Chemical Kinetics Networks Using A Weighted Ensemble Of Trajectories*.

Awards

2015 **Best Poster**, *ARC 2015*, $500 travel award.

2015 **Outstanding Student Research Accomplishment**, *CMU–Pitt. Program in Computational Biology*.

2013 **Best Poster**, *CMU–Pitt. Program in Computational Biology*, Program Retreat.

2012–2014 **NRSA Institutional Training Grant predoctoral fellowship**, *CMU–Pitt. Program in Computational Biology*.

2004–2005 **Graduate Fellow**, *University of Washington*.

Miscellaneous

2013-2015 **Student Senator**, *CMU–Pitt. Program in Computational Biology*.
Formed and elected to the student government. Served with faculty on the admissions committee for the Ph.D. program.

2013 **Scholarship**, *q-bio Summer School*.
Highly selective two-week graduate level summer school / workshop. Worked on decoding stochastic gene regulatory networks from data.