Charles C. Margossian

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Research interest

Bayesian modeling; Bayesian workflow; Hierarchical models; ODE-based models; Markov chain Monte Carlo; Variational Inference; Integrated Laplace approximations; Automatic differentiation; Pharmacometrics; Epidemiology; Statistical Physics; Probabilistic programming (Stan, Torsten, TensorFlow Probability)

Education

2017– 2022 **Ph.D. Statistics**, *Columbia University*, New York, NY.
- Thesis: *Modernizing Markov chains Monte Carlo for scientific and Bayesian modeling*
- Advisor: Andrew Gelman
- Dissertation Committee: Aki Vehtari, Matthew Hoffman, Sumit Mukherjee, David Blei

2011–2015 **B.Sci. Physics**, *Yale University*, New Haven, CT.

2009–2011 **Baccalauréat Scientifique**, *Ecole Jeannine Manuel (High school)*, Paris, France.

Appointments

2022–present **Research Fellow**, *Flatiron Institute, Center for Computational Mathematics*, Simons Foundation, New York, NY.

Summer 2021 **Research Intern**, *Google Research*, Bayesflow team, New York, NY.

Summer 2019 **Visiting Doctoral Student**, *Aalto University, Department of Computer Science*, Probabilistic Machine Learning group, Espoo, Finland.

2015–2017 **Visiting Scientist**, *Metrum Research Group LLC*, Pharmacometrics, Tariffville, CT and Cambridge, MA.

2013–2015 **Research Assistant**, *Yale University, Department of Astronomy*, New Haven, CT.

Summer 2014 **Patent Law, Technical Specialist**, *Leinweber & Zimmermann*, Munich, Germany.

Academic services

2023 - present **Stan Governing Body**.

2016 - present **Stan-Math core developer**, *Stan development team.*

2019 - present **Reviewer**, *Computational Statistics (2022), Nature (2021), AISTATS (2021), Methods in ecology (2021), Journal of data science (2021), NeurIPS (2020), Journal of pharmacokinetics and pharmacodynamics (2019).*

Skills

Progamming: R, Python, C++, Stan, TensorFlow Probability, LaTeX, GitHub
Languages: English, French, German

Google Scholar https://scholar.google.com/citations?user=nPtLsvIAAAAJ&hl=en

Preprints

[1] **Charles C Margossian**. General adjoint-differentiated Laplace approximation. *arXiv:2306.14976*, 2023.

[2] **Charles C Margossian**, Matthew D Hoffman, Pavel Sountsov, Lionel Riou-Durand, Aki Vehtari, and Andrew Gelman. Nested $\widehat{R}$: Assessing the convergence of Markov chain Monte Carlo when running many short chains. *arXiv:2110.13017*, 2022.

[3] **Charles C Margossian** and Michael Betancourt. Efficient Automatic Differentiation of Implicit Functions. *arXiv:2112.14217*, 2022.

[4] **Charles C Margossian** and Sumit Mukherjee. Simulating Ising and Potts models at critical and cold temperatures using auxiliary Gaussian variables. *arXiv:2110.10801*, 2021.

[5] Andrew Gelman, Aki Vehtari, Daniel Simpson, **Charles C Margossian**, Bob Carpenter, Yuling Yao, Lauren Kennedy, Jonah Gabry, Paul-Christian Bürkner, and Martin Modrák. Bayesian Workflow. *arXiv:2011.01808*, 2020.

[6] Michael Betancourt, **Charles C Margossian**, and Vianey Leos-Barajas. The Discrete Adjoint Method: Efficient Derivatives for Functions of Discrete Sequences. *arXiv:2002.00326*, 2020.

Published papers

*: Supervised student

[1] **Charles C Margossian** and Lawrence K Saul. The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference. *Selected for Oral Presentation, Uncertainty in Artificial Intelligence*, 2023.

[2] Lionel Riou-Durand, Pavel Sountsov, Jure Vogrinc, **Charles C Margossian**, and Sam Power. Adaptive Tuning for Metropolis Adjusted Langevin Trajectories. *Artificial Intelligence and Statistics*, 2023.

[3] **Charles C Margossian**, Yi Zhang, and William R Gillespie. Flexible and efficient Bayesian pharmacometrics modeling using Stan and Torsten, Part I. *CPT: Pharmacometrics & Systems Pharmacology*, 11:1151 – 1169, 2022.

[4] Philip Greengard, Jeremy Hoskins, **Charles C Margossian**, Jonah Gabry, Andrew Gelman, and Aki Vehtari. Fast methods for posterior inference of two-group normal-normal models. *Bayesian Analysis*, 2022.

[5] Léo Grinsztajn*, Elizaveta Semenova, **Charles C Margossian**, and Julien Riou. Bayesian workflow for disease transmission modeling in Stan. *Statistics in Medicine*, 40:6209 – 6234, 2021.

[6] **Charles C Margossian**, Aki Vehtari, Daniel Simpson, and Raj Agrawal. Hamiltonian Monte Carlo using an adjoint-differentiated Laplace approximation: Bayesian inference for latent Gaussian models and beyond. *Neural Information Processing Systems*, 2020.

[7] Anthony Hauser, Michel J Counotte, **Charles C Margossian**, Garyfallos Konstantinoudis, Nicola Low, Christian L Althaus, and Julien Riou. Estimation of SARS-CoV-2 mortality during the early stages of an epidemic: a modeling study in Hubei, China and six regions in Europe. *PLOS Medicine*, 17, 2020.

[8] **Charles C Margossian**. A Review of automatic differentiation and its efficient implementation. *Awarded "Top WIRES articles in 2022", WIRES: Data Mining and Knowledge Discovery*, 9, 2019.

[9] Joseph R Schmitt, Eric Agol, Katherine M Deck, Leslie A Rogers, J Zachary Gazak, Debra A Fischer, Ji Wang, Matthew J Holman, Kian J Jek, **Charles Margossian**, Mark R Omohundor, Troy Winarski, John M Brewer, Matthew J Giguere, Chris Lintott, Stuart Lynn, Michael Parrish, Kevin Schawinski, Megan E Schwamb, Robert Simpson, and Arfon M Smith. Planet Hunters. VII. Discovery of a new low-mass, low-density planet (PH3 C) orbiting KEPLER-289 with mass measurements of two additional Planets (PH3 B and D). *Astrophysical Journal*, 795(2), 2014.

Conference notebooks and posters

*: Supervised student

[1] **Charles C Margossian**, Matthew D Hoffman, Pavel Sountsov, Lionel Riou-Durand, Aki Vehtari, and Andrew Gelman. Assessing the convergence of Markov chains Monte Carlo when running many chains. *BayesComp*, 2023.

[2] Stanislas du Ché* and **Charles C Margossian**. Parallelization for Markov chains Monte Carlo with heterogeneous runtimes. *BayesComp*, 2023.

[3] **Charles C Margossian**, Lu Zhang, Sebastian Weber, and Andrew Gelman. Solving ODEs in a Bayesian context: challenges and opportunities. *Population Approach Group in Europe*, 2021.

[4] Aurélien Marc, Marion Kerioui, **Charles Margossian**, Julie Bertrand, Pauline Maisonnasse, Yoan Aldon, Rogier W Sanders, Marit Van Gils, Roger Le Grand, and Jérémie Guedj. Developping a model of SARS-CoV-2 viral dynamics under monoclonal antibody treatment. *Population Approach Group in Europe*, 2021.

[5] Johann D Gaebler* and **Charles C Margossian**. Propagating Derivatives through Implicit Functions in Reverse Mode Autodiff. *Stanford Institute for Computational & Mathematical Engineering*, 2021.

[6] **Charles C Margossian**, Aki Vehtari, Daniel Simpson, and Raj Agrawal. Approximate Bayesian inference for latent Gaussian models in Stan. *StanCon*, 2020.

[7] **Charles C Margossian** and Andrew Gelman. Bayesian model of planetary motion: exploring ideas for a modeling workflow when dealing with ordinary differential equations and multimodality. In *Stan Case Studies*, volume 7, 2020.

[8] **Charles C Margossian**. Computing Steady States with Stan's Nonlinear Algebraic Solver. *StanCon*, 2018.

[9] **Charles C Margossian** and William R Gillespie. Gaining Efficiency by Combining Analytical and Numerical Methods to Solve ODEs: Implementation in Stan and Application to Bayesian PK/PD. *American Conference on Pharmacometrics*, 2017.

[10] **Charles C Margossian** and William R Gillespie. Differential Equation Based Models in Stan. *StanCon*, 2017.

[11] **Charles C Margossian** and William R Gillespie. Stan Functions for Pharmacometrics Modeling. *American Conference on Pharmacometrics*, 2016.

Software

Core developer, *Stan: a probabilistic programming language*, mc-stan.org.

Co-creator, *Torsten: an extension of Stan for Bayesian pharmacometrics modeling*, GitHub link.

Contributor, *mrgSolve: Simulation from ODE-Based Population PK/PD and System Pharmacology Models*, GitHub link.

Awards and recognitions

2023 **UAI Oral presentation**, For *The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference*, top ∼15% articles accepted at the conference on Uncertainty in Artificial Intelligence.

2022 **WIRES Top Article**, For *A Review of Automatic Differentiation and its Efficient Implementation*, which was amongst the top 10 most cited articles in the 2021 Journal Citation Report for *WIRES, Data Mining and Knowledge Discovery*.

2022 **Minghui Yu Teaching Assistant Award**, *Department of Statistics, Columbia University*, Awarded by the Director of Graduated Studies based on student feedback.

2022 **AISTATS Top Reviewer**, The top reviewers were selected based on the feedback received from the Area Chairs and comprise the top-10% of AISTATS reviewers.

2017 **Dean's Fellowship**, *Department of Statistics, Columbia University*, 5 years funding for PhD degree.

2010 **Yale Book Award**, For "character and intellectual promise".

Supervised research projects

- Stanislas Du Ché (master student), Spring 2022
  Project: *Parallelization for Markov chain Monte Carlo with heterogeneous runtimes*

- Johann Gaebler (PhD student), Fall 2020
  Project: *Propagating Derivatives through implicit functions in reverse mode automatic differentiation*

- Léo Grinsztajn (master student), Summer 2020
  Project: *Bayesian Workflow for disease transmission models*

- Hyunjee Moon (undergraduate student), Summer 2020
  Project: *Simulation-based Calibration for the embedded Laplace approximation*

Teaching experience (selected)

2019 – 2023 **Lecturer**, *"Probability and Bayes", PHC 506: Biometry in Pharmaceutics*, University of Buffalo, School of Pharmacy, Buffalo, NY.

2019 – 2023 **Instructor**, *Building, fitting, and criticizing Bayesian PK/PD models*, one-day workshop, University of Buffalo, School of Pharmacy, Buffalo, NY.

2019, 2020 **Instructor**, *Stan for the people: two days introductory workshop on Bayesian modeling*, two-day workshop, McGill University, Montreal, Canada.

August 2019 **Co-instructor**, *Population and ODE-based models using Stan and Torsten*, two-day workshop, StanCon, Cambridge, UK.

January 2018 **Instructor**, *How to Develop for the Stan C++ Core Language*, StanCon, Pacific Grove, CA.

April 2017 **Invited Lecturer**, *"Introduction to Bayesian Data Analysis with Stan", STAT 220: Bayesian Statistics*, Harvard University, Cambridge, MA.

2021, 2022 **Teacher Assistant**, *Applied Statistics II, STAT 6102 (PhD level)*, Columbia University, New York, NY.

2019, 2020 **Teacher Assistant**, *Foundation of Graphical Models, STAT 6701 (PhD level)*, Columbia University, New York, NY.

Spring 2019 **Teacher Assistant**, *Statistical inference, STAT 5204 (Master level)*, Columbia University, New York, NY.

Fall 2018 **Teacher Assistant**, *Statistical Computing and Introduction to Data Science (Undergrad level)*, STAT 4206, Columbia University, New York, NY.

September 2017 **Teacher Assistant**, *Stan for Physics*, 5-day workshop, Massachusetts Institute of Technology, Cambridge, MA.

June 2017 **Teacher Assistant**, *Getting Started with Bayesian PKPD Modeling using Stan and Torsten*, Population Approach Group in Europe, Budapest, Hungary.

October 2016 **Teacher Assistant**, *Getting Started with Bayesian PKPD Modeling using Stan*, one-day workshop, American Conference on Pharmacometrics, Bellevue, WA.

October 2015 **Teacher Assistant**, *Getting Started with Bayesian PKPD Modeling using Stan*, one-day workshop, American Conference on Pharmacometrics, Arlington, VA.

2013–2015 **Peer Tutor**, *Science, Technology, and Research Scholars (STARS) program*, Yale University, New Haven, CT.

Presentations (selected)

June 2023 **Making Bayesian Pharmacometrics modeling simpler (but not too simple) with Torsten**, Stan for Pharmacometrics Day, INSERM, Paris, France.

June 2023 **Amortized Variational Inference: when and why?**, Flatiron-wide Meeting on Machine Learning, Flatiron Institute, New York, NY.

May 2023 **From high-performance algorithms to high-performance modeling**, Structural and Molecular Biophysics (SMBp) group meeting, Flatiron Institute, New York, NY.

October 2022 **Solving ODEs in a Bayesian model**, Flatiron-Wide Algorithms and Mathematics ($F_\omega(\alpha + m)!$), Flatiron Institute, New York, NY.

July 2022 **Nested $\hat{R}$: Assessing convergence for Markov chains Monte Carlo when running many short chains**, Center for Research in Economics and Statistics (CREST), École Polytechnique, Paris, France.

March 2021 **Bayesian inference for latent Gaussian models: MCMC, approximate methods, and hybrids**, Minghui Yu memorial conference, Columbia University, New York, NY.

November 2020 **Developing a Bayesian modeling workflow for population PBPK**, American Conference on Pharmacomertrics.

August 2020 **Approximate Bayesian inference for latent Gaussian models in Stan**, StanCon.

June 2020 **Developing a Bayesian workflow to model the Covid-19 outbreak**, 12^{th} Covid-19 symposium, Columbia University, New York, NY.

April 2020 **Laplace approximation for speeding up the computation of multilevel models**, MRP conference, Columbia University, New York, NY.

March 2020 **Building a probabilistic programming language to diagnose our inference**, University of Buffalo, School of Pharmacy, Buffalo, NY.

July 2018 **Understanding automatic differentiation to improve performance**, Stan for Pharmacometrics Day, Université Paris Diderot, School of Medicine, Paris, France.

January 2018 **Computing steady states with Stan's nonlinear algebraic solver**, StanCon, Pacific Grove, CA.

June 2017 **L'Avenir de Stan en pharmacométrie**, Université Paris Diderot, School of Medicine, Paris, France.

January 2017 **Differential equations based models in Stan**, *StanCon*, Columbia University, New York, NY.

November 2016 **Differential equations based models in Stan**, *Stan Meetup in Boston*, Harvard University, Cambridge, MA.

February 2016 **Practice (and malpractices!) of Bayesian analysis**, *Metrum Journal Minute*, Tariffville, CT.

March 2015 **How stars and planets Interact: testing the effects of close-in giant planets on stellar magnetic activity**, *Davenport Mellon Forum*, Yale University, New Haven, CT.

Modified June 2023