Charles C. Margossian

cmargossian@flatironinstitute.org • charlesm93.github.io • New York, NY

Education

Ph.D. Statistics, Columbia University, New York, NY. 2017-2022 o Thesis: Modernizing Markov chains Monte Carlo for scientific and Bayesian modeling • Advisor: Andrew Gelman o Committee: Aki Vehtari, Matt Hoffman, Sumit Mukherjee and David Blei B.Sci. Physics, Yale University, New Haven, CT. 2011-2015 Baccalauréat Scientifique, Ecole Jeannine Manuel (High school), Paris, France. 2009-2011 Experience Research Fellow, Flatiron Institute, Center for Computational Mathematics, New York, 2022-NY. • Independent research in computational mathematics, 3 years funding o Computational Statistics and Machine Learning groups Core Developer, Stan Development Team, https://mc-stan.org/. 2016-• Open-source, Bayesian inference and automatic differentiation in C++ • Main contribution: support for implicit functions (ODEs, algebraic equations...) Sum. 2021 Research Intern, Google Research, New York, NY. • TensorFlow Probability team: inference on modern hardware (GPUs, TPUs) • Hosts: Matt Hoffman and Pavel Sountsov Visiting Doctoral Student, Aalto University, Department of Computer Science, Espoo, Sum. 2019 Finland. • Probabilistic machine learning group • Advisor: Aki Vehtari Visiting Scientist, Metrum Research Group, Tariffville, CT and Cambridge, MA. 2015-2017 • Co-creator of Torsten: an extension of Stan for pharmacometrics modeling o 2015–2016: Phamacometrics bootcamp • Supervisor: Bill Gillespie Research Assist., Yale University, Department of Astronomy, New Haven, CT. 2013-2015 o Senior Thesis: Testing the Effects of Close-in Giant Planets on Stellar Magnetic Activity • Exoplanet group • Advisors: Debra Fischer and Ji Wang

Skills

Progamming: R, Python, C++, Stan, ATEX, GitHub

Patent Law Intern, Leinweber & Zimmermann, Munich, Germany.

Languages: English, French, German

Sum. 2014

Papers

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

- [1] C. C. Margossian and L. K. Saul. Variational Inference in Location–Scale Families: Exact Recovery of the Mean and Correlation Matrix. Selected for oral presentation, Artificial Intelligence and Statistics, PMLR (accepted), 2025.
- [2] <u>C. C. Margossian</u>, L. Pillaud-Vivien, and L. K. Saul. **Variational Inference for Uncertainty Quantification:** an Analysis of Trade-Offs. *arXiv:2403.13748. (submitted)*, 2024.
- [3] C. C. Margossian, M. D. Hoffman, P. Sountsov, L. Riou-Durand, A. Vehtari, and A. Gelman. Nested \widehat{R} : Assessing the convergence of Markov chain Monte Carlo when running many short chains. *Bayesian Analysis*, Advance Publication:1–28, 2024.
- [4] C. C. Margossian and A. Gelman. For how many iterations should we run Markov chain Monte Carlo? In Handbook of Markov chain Monte Carlo. Chapman & Hall/CRC, (in press) 2nd edition, 2024.
- [5] <u>C. C. Margossian</u> and D. M. Blei. **Amortized Variational Inference: When** and Why? *Uncertainty in Artificial Intelligence*, PMLR 244:2434–2449, 2024.
- [6] F. Heurtel-Depeiges, C. C. Margossian, R. Ohana, and B. Régaldo-Saint Blancard. Listening to the noise: Blind Denoising with Gibbs Diffusion. International Conference on Machine Learning, PMLR 235:18284–18304, 2024.
- [7] D. Cai, C. Modi, C. C. Margossian, R. M. Gower, D. M. Blei, and L. K. Saul. EigenVI: score-based variational inference with orthogonal function expansions. *Selected for spotlight, Advances in Neural Information Processing Systems*, (in press), 2024.
- [8] D. Cai, C. Modi, L. Pillaud-Vivien, C. C. Margossian, R. M. Gower, D. M. Blei, and L. K. Saul. Batch and match: black-box variational inference with a score-based divergence. Selected for spotlight, International Conference on Machine Learning, PMLR 235:5258–5297, 2024.
- [9] C. C. Margossian and L. K. Saul. The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference. Selected for oral presentation, Uncertainty in Artificial Intelligence, PMLR 216:1358–1367, 2023.

- [10] L. Riou-Durand, P. Sountsov, J. Vogrinc, C. C. Margossian, and S. Power. Adaptive Tuning for Metropolis Adjusted Langevin Trajectories. Artificial Intelligence and Statistics, PMLR 206:8102–8116, 2023.
- [11] C. Modi, C. C. Margossian, Y. Yao, R. M. Gower, D. M. Blei, and L. K. Saul. Variational Inference with Gaussian Score Matching. *Advances in Neural Information Processing Systems*, 37, 2023.
- [12] <u>C. C. Margossian</u>, Y. Zhang, and W. R. Gillespie. Flexible and efficient Bayesian pharmacometrics modeling using Stan and Torsten, Part I. *CPT: Pharmacometrics & Systems Pharmacology*, 11(9):1151–1169, 2022.
- [13] P. Greengard, J. Hoskins, <u>C. C. Margossian</u>, J. Gabry, A. Gelman, and A. Vehtari. Fast methods for posterior inference of two-group normal-normal models. *Bayesian Analysis*, 18(3):889–907, 2022.
- [14] L. L. Grinsztajn (supervised student), E. Semenova, <u>C. C. Margossian</u>, and J. Riou. Bayesian workflow for disease transmission modeling in Stan. *Statistics in Medicine*, 40(27):6209–6234, 2021.
- [15] C. C. Margossian, A. Vehtari, D. Simpson, and R. Agrawal. Hamiltonian Monte Carlo using an adjoint-differentiated Laplace approximation: Bayesian inference for latent Gaussian models and beyond. Advances in Neural Information Processing Systems, 34, 2020.
- [16] A. Hauser, M. J. Counotte, C. C. Margossian, G. Konstantinoudis, N. Low, C. L. Althaus, and J. 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(7), 2020.
- [17] A. Gelman, A. Vehtari, D. Simpson, <u>C. C. Margossian</u>, B. Carpenter, Y. Yao, L. Kennedy, J. Gabry, P-C. Bürkner, and M. Modrák. **Bayesian Workflow**. *arXiv:2011.01808.* (full book in preparation), 2020.
- [18] C. C. Margossian. Review of automatic differentiation and its efficient implementation. Awarded "Top WIRES articles in 2022", WIRES: Data Mining and Knowledge Discovery, 9(4), 2019.
- [19] J. R. Schmitt, E. Agol, K. M. Deck, L. A. Rogers, Z. J. Gazak, D. A. Fischer, J. Wang, M. J. Holman, K. J. Jek, <u>C. Margossian</u>, M. R. Omohundor, T. Winarski, J. M. Brewer, M. J. Giguere, C. Lintott, S. Lynn, M. Parrish, K. Schawinski, M. E. Schwamb, R. Simpson, and A. 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.

Posters and technical reports (selected)

*supervised student

- [1] E. Mokel* and C. C. Margossian. Monitoring Nonstationary Variance to Assess Convergence of MCMC. Best poster award, International Society of Bayesian Analysis (ISBA) world meeting, 2024.
- [2] <u>C. C. Margossian</u>. **General adjoint-differentiated Laplace approximation**. *arXiv:2306.14976*., 2023.
- [3] S. du Ché* and C. C. Margossian. Parallelization for Markov chains Monte Carlo with heterogeneous runtimes. *BayesComp*, 2023.
- [4] C. C. Margossian and M. Betancourt. **Efficient Automatic Differentiation** of Implicit Functions. *arXiv:2112.14217.*, 2022.
- [5] <u>C. C. Margossian</u>, L. Zhang, S. Weber, and A. Gelman. **Solving ODEs in a Bayesian context: challenges and opportunities**. *Population Approach Group in Europe*, 2021.
- [6] A. Marc, M. Kerioui, C. Margossian, J. Bertrand, P. Maisonnasse, Y. Aldon, R. W. Sanders, M. Van Gils, R. Le Grand, and J. Guedj. Developing a model of SARS-CoV-2 viral dynamics under monoclonal antibody treatment. Population Approach Group in Europe, 2021.
- [7] J. D. Gaebler* and C. C. Margossian. Propagating Derivatives through Implicit Functions in Reverse Mode Autodiff. Stanford Institute for Computational & Mathematical Engineering, 2021.
- [8] <u>C. C. Margossian</u> and A. 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.
- [9] M. Betancourt, C. C. Margossian, and V. Leos-Barajas. The Discrete Adjoint Method: Efficient Derivatives for Functions of Discrete Sequences. arXiv:2002.00326., 2020.
- [10] C. C. Margossian. Computing Steady States with Stan's Nonlinear Algebraic Solver. StanCon, 2018.
- [11] C. C. Margossian and W. 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.

- [12] <u>C. C. Margossian</u> and W. R. Gillespie. **Differential Equation Based Models** in Stan. *StanCon*, 2017.
- [13] <u>C. C. Margossian</u> and W. R. Gillespie. **Stan Functions for Pharmacomet**rics 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 pharmacometrics modeling, GitHub.

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

Contributor, bayesplot: Plotting for Bayesian Models in R, Cran.

Awards and recognitions

3	
AISTATS oral presentation, For Variational Inference in Location–Scale Families: exact recovery of the mean and correlation matrix, top \sim 2% of submitted papers at the conference on Artificial Intelligence and Statistics.	2025
NeurIPS spotlight , For <i>EigenVI: score-based variational inference with orthogonal function expansions</i> , submitted to the conference on Neural Information Processing Systems .	2024
ISBA best poster award , For <i>Monitoring Nonstationary Variance to Assess Convergence of MCMC</i> , presented at the International Society of Bayesian Analysis (ISBA): World Meeting.	2024
ICML spotlight, For <i>Batch and Match: black box variational inference with a score-based divergence</i> , top ~13% articles accepted at the International Conference on Machine Learning.	2024
UAI oral presentation , For <i>The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference</i> , top ~15% articles accepted at the conference on Uncertainty in Artificial Intelligence.	2023
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.	2022
Dean's fellowship , Department of Statistics, Columbia University, 5 years funding for PhD degree.	2017
Yale book award, For "character and intellectual promise".	2010

Academic services

Reviewer, Transactions of Machine Learning (2024), Handbook of Markov chain Monte Carlo (2024 (2)), Transactions of Machine Learning (2024), Bayesian Analysis (2024), SIAM review (2024), Advances in Neural Information Processing Systems (2024, 2020), Statistics and Computing (2024), CPT: Pharmacometrics and Systems Pharmacology (2024), PeerJ (2023), Journal of Machine Learning Research (2023 (2)), PMLR: Artificial Intelligence and Statistics (2023, Top Reviewer Award 2021), Journal of Pharmacokinetics and Pharmacodynamics (2023, 2019), Computational Statistics (2022), Nature Geoscience (2021), Methods in ecology (2021), Journal of data science (2021).

Elected Member, Stan Governing Body, Two year term.	2022-
Organizer, StanCon 2024, Oxford, UK.	2024
Organizer, StanCon 2023, St Louis, MO.	2023
Student representative, PhD program in statistics at Columbia University.	2019 - 2020

Supervised students

Manny Mokel (undergraduate student), Monitoring Nonstationary Variance to Assess	2023
Convergence of MCMC, Flatiron Institute, New York, NY.	

Stanislas Du Ché (master student), Parallelization for Markov chain Monte Carlo with heterogeneous runtimes, Columbia University, New York, NY.

Johann Gaebker (PhD student), Propagating Derivatives through implicit functions in reverse mode automatic differentiation, Columbia University, New York, NY.

Léo Grinsztajn (master student), Bayesian Workflow for disease transmission models, Columbia University, New York, NY.

Hyunji (Angie) Moon (undergraduate student), Simulation-based Calibration for the embedded Laplace approximation, Columbia University, New York, NY.

Teaching

Instructor, *Monte Carlo Methods*, Half-a-day course, Nordic Summer School on Probabilistic AI, Copenhagen, Denmark.

Instructor, *Bayesian Workflow for hierarchical and ODE-based models*, Three day workshop, Summer School on Advanced Bayesian Methods, Leuven, Belgium.

Instructor, *Fundamentals of Stan*, Half-day workshop, StanCon 2023, Washington University in St Louis, St Louis, MO.

Instructor, *Building*, *fitting*, *and criticizing Bayesian PK/PD models*, One day workshop, University of Buffalo, Buffalo, NY.

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

Instructor, Stan for the people: an introductory workshop to Bayesian modeling, 2019, 2020 Two day workshop, McGill University, Montreal, Canada.

Instructor, *Population and ODE-based models using Stan and Torsten*, Two day workshop, StanCon 2019, Cambridge University, Cambridge, UK.

Guest Lecturer, *Introduction to Bayesian Data Analysis with Stan*, Lecture for STAT 2020: **2017** Bayesian Statistics, Harvard University, Cambridge, MA.

Teaching Assistant, Recipient of the Minghui Yu Teaching Assistant Award, Courses at all levels (undergrad, masters and PhD), Columbia University, New York, NY.

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

Invited talks (selected)

Chaired session , <i>Monte Carlo methods using modern hardware</i> , International Society of Bayesian Analysis (ISBA): World Meeting, Venice, Italy.	2024
Invited talk, Variational Inference for Uncertainty Quantification: An Analysis of Trade-offs, International Society of Bayesian Analysis (ISBA): World Meeting, Venice, Italy.	2024
Invited talk, The Wisdom of Automatic Differentiation, Applied and Computational Math Group Meeting, Courant Institute, New York University, New York, NY.	2023
Oral Presentation , The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference, Conference on Uncertainty in Artificial Intelligence, Pittsburgh, PA.	2023
Invited talk, Making Bayesian Pharmacometrics modeling simpler (but not too simple) with Torsten, Stan for Pharmacometrics Day, INSERM, Paris, France.	2023
Invited talk , Amortized Variational Inference: when and why?, Flatiron-wide Meeting on Machine Learning, Flatiron Institute, New York, NY.	2023
Lecture , Solving ODEs in a Bayesian model, Flatiron-Wide Algorithms and Mathematics $(F_{\omega}(\alpha + m)!)$, Flatiron Institute, New York, NY.	2022
Invited talk, 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.	2022
Talk , Bayesian inference for latent Gaussian models: MCMC, approximate methods, and hybrids, Minghui Yu memorial conference, Columbia University, New York, NY.	2021
Invited talk , Developing a Bayesian modeling workflow for population PBPK, American Conference on Pharmacomertrics, Online.	2020

Invited talk, Developing a Bayesian workflow to model the Covid-19 outbreak, 12th Covid-19

Proposed talk, Computing steady states with Stan's nonlinear algebraic solver, StanCon,

symposium, Columbia University, New York, NY.

Pacific Grove, CA.

2020

2018

Proposed talk , <i>Differential equations based models in Stan</i> , StanCon, Columbia University, New York, NY.	2017
Invited talk , <i>Differential equations based models in Stan</i> , Stan Meetup in Boston, Harvard University, Cambridge, MA.	2016
Lecture , <i>Practice</i> (and malpractices!) of Bayesian analysis, Metrum Journal Minute, Tariffville, CT.	2016
Talk , 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.	2015
Modified January	j 2024