

Charles C. Margossian

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

Education

- Ph.D. Statistics**, Columbia University, New York, NY. 2017– 2022
- Thesis: *Modernizing Markov chains Monte Carlo for scientific and Bayesian modeling*
 - Advisor: Andrew Gelman
 - 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, NY. 2022–
- Independent research in computational mathematics, 3 years funding
 - 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...)
- Research Intern**, Google Research, New York, NY. Sum. 2021
- 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, Finland. Sum. 2019
- 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*
 - 2015–2016: Pharmacometrics bootcamp
 - Supervisor: Bill Gillespie
- Research Assist.**, Yale University, Department of Astronomy, New Haven, CT. 2013–2015
- Senior Thesis: *Testing the Effects of Close-in Giant Planets on Stellar Magnetic Activity*
 - Exoplanet group
 - Advisors: Debra Fischer and Ji Wang
- Patent Law Intern**, Leinweber & Zimmermann, Munich, Germany. Sum. 2014

Skills

Programming: R, Python, C++, Stan, \LaTeX , GitHub
Languages: English, French, German

Papers

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

- [1] C. C. Margossian and L. K. Saul. **Variational Inference in Location-Scale Families: Exact Recovery of the Mean and Correlation Matrix.** *arXiv:2410.11067 (submitted)*, 2024.
- [2] C. C. Margossian, 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 \hat{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] C. C. Margossian 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. Régaldou-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] C. C. Margossian, 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, C. C. Margossian, 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, C. C. Margossian, 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, C. C. Margossian, 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, C. Margossian, 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. Mokol* 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] C. C. Margossian. **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] C. C. Margossian, 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] C. C. Margossian 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] C. C. Margossian and W. R. Gillespie. **Differential Equation Based Models in Stan**. *StanCon*, 2017.
- [13] C. C. Margossian and W. 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 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

NeurIPS spotlight, For *EigenVI: score-based variational inference with orthogonal function expansions*, submitted to the conference on Neural Information Processing Systems . 2024

ISBA best poster award, For *Monitoring Nonstationary Variance to Assess Convergence of MCMC*, presented at the International Society of Bayesian Analysis (ISBA): World Meeting. 2024

ICML spotlight, For *Batch and Match: black box variational inference with a score-based divergence*, top ~13% articles accepted at the International Conference on Machine Learning. 2024

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. 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). 2020–

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 Convergence of MCMC*, Flatiron Institute, New York, NY. 2023

Stanislas Du Ché (master student), *Parallelization for Markov chain Monte Carlo with heterogeneous runtimes*, Columbia University, New York, NY. 2022

Johann Gaebker (PhD student), *Propagating Derivatives through implicit functions in reverse mode automatic differentiation*, Columbia University, New York, NY. 2020

Léo Grinsztajn (master student), *Bayesian Workflow for disease transmission models*, Columbia University, New York, NY. 2020

Hyunji (Angie) Moon (undergraduate student), *Simulation-based Calibration for the embedded Laplace approximation*, Columbia University, New York, NY. 2020

Teaching

Instructor, *Monte Carlo Methods*, Half-a-day course, Nordic Summer School on Probabilistic AI, Copenhagen, Denmark. 2024

Instructor, *Bayesian Workflow for hierarchical and ODE-based models*, Three day workshop, Summer School on Advanced Bayesian Methods, Leuven, Belgium. 2023

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

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

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

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, 2019
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 2017–2022
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, *Monte Carlo methods using modern hardware*, International Society of 2024
Bayesian Analysis (ISBA): World Meeting, Venice, Italy.

Invited talk, *Variational Inference for Uncertainty Quantification: An Analysis of Trade-offs*, 2024
International Society of Bayesian Analysis (ISBA): World Meeting, Venice, Italy.

Invited talk, *The Wisdom of Automatic Differentiation*, Applied and Computational Math 2023
Group Meeting, Courant Institute, New York University, New York, NY.

Oral Presentation, *The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian 2023*
Approximations for Variational Inference, Conference on Uncertainty in Artificial Intelligence,
Pittsburgh, PA.

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

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

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

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

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

Invited talk, *Developing a Bayesian modeling workflow for population PBPK*, American 2020
Conference on Pharmacometrics, Online.

Invited talk, *Developing a Bayesian workflow to model the Covid-19 outbreak*, 12th Covid-19 2020
symposium, Columbia University, New York, NY.

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

- Proposed talk**, *Differential equations based models in Stan*, StanCon, Columbia University, New York, NY. 2017
- Invited talk**, *Differential equations based models in Stan*, Stan Meetup in Boston, Harvard University, Cambridge, MA. 2016
- Lecture**, *Practice (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 2024