

# 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, 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,  $\text{\LaTeX}$ , GitHub

**Languages:** English, French, German

## Publications

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

- [1] 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.
- [2] 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, (upcoming) 2nd edition, 2024.
- [3] C. C. Margossian and D. M. Blei. **Amortized Variational Inference: When and Why?** *Uncertainty in Artificial Intelligence*, PMLR (accepted), 2024.
- [4] 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.
- [5] 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.
- [6] 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.
- [7] 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.
- [8] 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.
- [9] 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.
- [10] 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.

- [11] 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.
- [12] 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.
- [13] 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.
- [14] 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.
- [15] 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.

## Preprints

- [1] 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.
- [2] 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.** *(in preparation, submitted)*, 2024.
- [3] 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.

## 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](https://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

<b>ISBA best poster award</b> , For <i>Monitoring Nonstationary Variance to Assess Convergence of MCMC</i> , presented at the International Society of Bayesian Analysis (ISBA): World Meeting.	2024
<b>ICML spotlight</b> , 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
<b>UAI oral presentation</b> , 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
<b>WIRES top article</b> , For <i>A Review of Automatic Differentiation and its Efficient Implementation</i> , which was amongst the top 10 most cited articles in the <a href="#">2021 Journal Citation Report</a> for <i>WIRES: Data Mining and Knowledge Discovery</i> .	2022
<b>Minghui Yu teaching assistant award</b> , Department of Statistics, Columbia University, Awarded by the Director of Graduated Studies based on student feedback.	2022
<b>AISTATS top reviewer</b> , The top reviewers were selected based on the feedback received from the Area Chairs and comprise the top-10% of AISTATS reviewers.	2022
<b>Dean's fellowship</b> , Department of Statistics, Columbia University, 5 years funding for PhD degree.	2017
<b>Yale book award</b> , For "character and intellectual promise".	2010

## Academic services

**Reviewer**, 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/ID 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*, Two day workshop, McGill University, Montreal, Canada. 2019, 2020

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

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

**Teaching Assistant**, **Recipient of the Minghui Yu Teaching Assistant Award**, Courses at all levels (undergrad, masters and PhD), Columbia University, New York, NY. 2017–2022

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

## Invited talks (selected)

**Chaired session**, *Monte Carlo methods using modern hardware*, 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 ( $F_w(\alpha + m)!$ ), 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 Pharmacometrics, Online. 2020

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

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

**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 September 2024*