

# Charles C. Margossian

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## 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– **Postdoctoral Research Fellow**, *Flatiron Institute*, Center for Computational Mathematics, New York, NY.
- Sum. 2021 **Research Intern**, *Google Research*, Bayesflow team, New York, NY.
- Sum. 2019 **Visiting Doctoral Student**, *Aalto University*, Department of Computer Science, Espoo, Finland.
- 2015–2017 **Visiting Scientist**, *Metrum Research Group*, Tariffville, CT and Cambridge, MA.
- 2013–2015 **Research Assistant**, *Yale University*, Department of Astronomy, New Haven, CT.
- Sum. 2014 **Patent Law Intern**, *Leinweber & Zimmermann*, Munich, Germany.

## Academic service

- Reviewer**, *PeerJ*, *Journal of Machine Learning Research* (2023 (2)), *Journal of Pharmacokinetics and Pharmacodynamics* (2023, 2019), *Computational Statistics* (2022), *Nature Geoscience* (2021), *Artificial Intelligence and Statistics* (2023, **Top Reviewer** 2021), *Methods in ecology* (2021), *Journal of data science* (2021), *Neural Information Processing Systems* (2020).
- 2016– **Core developer**, *Stan: a probabilistic programming language*, [mc-stan.org](https://mc-stan.org).
- 2022– **Elected Member**, *Stan Governing Body*, 2 year term.

## Skills

**Programming:** Python, R, C++, Stan, L<sup>A</sup>T<sub>E</sub>X, GitHub

**Languages:** English, French, German

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## Preprints

- [1] **Charles C Margossian**, Loucas Pillaud-Vivien, and Lawrence K Saul. An Ordering of Divergences for Variational Inference with Factorized Gaussian Approximations. *arXiv:2403.13748*, 2024.
- [2] **Charles C Margossian**, Matthew D Hoffman, Pavel Sountsov, Lionel Riou-Durand, Aki Vehtari, and Andrew Gelman. Nested  $\hat{R}$ : Assessing the convergence of Markov chain Monte Carlo when running many short chains. *arXiv:2110.13017*, 2024.
- [3] **Charles C Margossian** and David M Blei. Amortized Variational Inference: When and Why? *arXiv:2307.11018*, 2024.
- [4] David Heurtel-Depeiges, **Charles C Margossian**, Ruben Ohana, and Bruno Régaldo-Saint Blancard. Listening to the noise: Blind Denoising with Gibbs Diffusion. *arXiv:2402.19455*, 2024.
- [5] Diana Cai, Chirag Modi, Loucas Pillaud-Vivien, **Charles C Margossian**, Robert M Gower, David M Blei, and Lawrence K Saul. Batch and match: black-box variational inference with a score-based divergence. *arXiv:2402.14758*, 2024.
- [6] **Charles C Margossian**. General adjoint-differentiated Laplace approximation. *arXiv:2306.14976*, 2023.
- [7] **Charles C Margossian** and Michael Betancourt. Efficient Automatic Differentiation of Implicit Functions. *arXiv:2112.14217*, 2022.
- [8] **Charles C Margossian** and Sumit Mukherjee. Simulating Ising and Potts models at critical and cold temperatures using auxiliary Gaussian variables. *arXiv:2110.10801*, 2021.
- [9] 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.
- [10] Michael Betancourt, **Charles C Margossian**, and Vianey Leos-Barajas. The Discrete Adjoint Method: Efficient Derivatives for Functions of Discrete Sequences. *arXiv:2002.00326*, 2020.

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## Publications

\*: Supervised student

- [1] **Charles C Margossian** and Andrew 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.
- [2] **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, Proceedings of Machine Learning Research: Uncertainty in Artificial Intelligence*, 2023.
- [3] Lionel Riou-Durand, Pavel Sountsov, Jure Vogrinc, **Charles C Margossian**, and Sam Power. Adaptive Tuning for Metropolis Adjusted Langevin Trajectories. *Proceedings of Machine Learning Research: Artificial Intelligence and Statistics*, 2023.
- [4] Chirag Modi, **Charles C Margossian**, Yuling Yao, Robert Gower, David Blei, and Lawrence Saul. Variational Inference with Gaussian Score Matching. *Advances in Neural Information Processing Systems*, 2023.
- [5] **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.
- [6] 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.
- [7] 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.
- [8] **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. *Advances in Neural Information Processing Systems*, 2020.
- [9] 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.
- [10] **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.

- [11] 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.

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## 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.

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## 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](#).

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## 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”.

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## Supervised students

- 2023 **Manny Mokel (undergraduate student)**, *Nested  $\hat{R}$ : pooled sampling and variance approximation*, Flatiron Institute, New York, NY.
- 2022 **Stanislas Du Ché (master student)**, *Parallelization for Markov chain Monte Carlo with heterogeneous runtimes*, Columbia University, New York, NY.
- 2020 **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 **Hyunjee Moon (undergraduate student)**, *Simulation-based Calibration for the embedded Laplace approximation*, Columbia University, New York, NY.

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## Teaching

- 2023 **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.
- 2019–2023 **Instructor**, *Building, fitting, and criticizing Bayesian PK/PD models*, One day workshop, University of Buffalo, Buffalo, NY.
- 2019–2023 **Guest lecturer**, *Probability and Bayes*, Lecture for PHC 506: Biometry in Pharmaceutics, University of Buffalo, Buffalo, NY.
- 2019, 2020 **Instructor**, *Stan for the people: an introductory workshop to Bayesian modeling*, Two day workshop, McGill University, Montreal, Canada.
- 2019 **Instructor**, *Population and ODE-based models using Stan and Torsten*, Two day workshop, StanCon 2019, Cambridge University, Cambridge, UK.
- 2017 **Guest Lecturer**, *Introduction to Bayesian Data Analysis with Stan*, Lecture for STAT 2020: Bayesian Statistics, Harvard University, Cambridge, MA.
- 2017–2022 **Teaching Assistant**, *Recipient of the Minghui Yu Teaching Assistant Award*, Courses at all levels (undergrad, masters and PhD), Columbia University, New York, NY.
- 2013–2015 **Peer Tutor**, *Science, Technology, and Research Scholars (STARS) program*, Yale University, New Haven, CT.

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## Presentations (selected)

- 2023 **The Wisdom of Automatic Differentiation**, *Applied and Computational Math Group Meeting*, Courant Institute, New York University, New York, NY.
- 2023 **The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference**, *Conference on Uncertainty in Artificial Intelligence*, Pittsburgh, PA.
- 2023 **Amortized Variational Inference: when and why?**, *Flatiron-wide Meeting on Machine Learning*, Flatiron Institute, New York, NY.
- 2022 **Solving ODEs in a Bayesian model**, *Flatiron-Wide Algorithms and Mathematics ( $F_\omega(\alpha + m)!$ )*, Flatiron Institute, New York, NY.
- 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.*

- 2021 **Bayesian inference for latent Gaussian models: MCMC, approximate methods, and hybrids**, Minghui Yu memorial conference, Columbia University, New York, NY.
- 2020 **Developing a Bayesian modeling workflow for population PBPK**, American Conference on Pharmacometrics.
- 2020 **Approximate Bayesian inference for latent Gaussian models in Stan**, StanCon.
- 2020 **Developing a Bayesian workflow to model the Covid-19 outbreak**, 12<sup>th</sup> Covid-19 symposium, Columbia University, New York, NY.
- 2018 **Computing steady states with Stan's nonlinear algebraic solver**, *StanCon*, Pacific Grove, CA.
- 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.
- 2016 **Practice (and malpractices!) of Bayesian analysis**, *Metrum Journal Minute*, Tariffville, CT.
- 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 April 2024*