

# Charles C. Margossian

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## Research interest

- **Bayesian modeling:** Bayesian workflow, Hierarchical models, ODE models
- **Computation:** Markov chain Monte Carlo, Variational inference, Integrated Laplace approximation, Automatic differentiation
- **Application:** Pharmacometrics; Epidemiology, Statistical physics, Astronomy

## 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– **Research Fellow**, *Flatiron Institute, Center for Computational Mathematics*.  
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*, 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 service

- Reviewer**, *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).
- 2022– **Elected Member**, *Stan Governing Body*, 1 year term.
- 2016– **Core developer**, *Stan: a probabilistic programming language*, [mc-stan.org](https://mc-stan.org).

## Skills

**Programming:** R, Python, C++, Stan, TensorFlow Probability, PyTorch, L<sup>A</sup>T<sub>E</sub>X, GitHub  
**Languages:** English, French, German

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## Preprints

- [1] **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*, 2023.
- [2] **Charles C Margossian** and Andrew Gelman. For how many iterations should we run Markov chain Monte Carlo? *arXiv:2311.02726*, 2023.
- [3] **Charles C Margossian** and David M Blei. Amortized Variational Inference: When and Why? *arXiv:2307.11018*, 2023.
- [4] **Charles C Margossian**. General adjoint-differentiated Laplace approximation. *arXiv:2306.14976*, 2023.
- [5] **Charles C Margossian** and Michael Betancourt. Efficient Automatic Differentiation of Implicit Functions. *arXiv:2112.14217*, 2022.
- [6] **Charles C Margossian** and Sumit Mukherjee. Simulating Ising and Potts models at critical and cold temperatures using auxiliary Gaussian variables. *arXiv:2110.10801*, 2021.
- [7] 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.
- [8] 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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## 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] Chirag Modi, **Charles C Margossian**, Yuling Yao, Robert Gower, David Blei, and Lawrence Saul. Variational Inference with Gaussian Score Matching. *Neural Information Processing Systems*, 2023.
- [4] **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.

- [5] 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.
- [6] 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.
- [7] **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.
- [8] Anthony Hauser, Michel J Cournotte, **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.
- [9] **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.
- [10] 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. Developing 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.

## Open-source Software

- **Stan**: a probabilistic programming language, **Core developer**, [mc-stan.org](https://mc-stan.org)
- **Torsten**: an extension of **Stan** for pharmacometrics modeling, **Co-creator**, [GitHub](#)
- **mrgSolve**: Simulation from ODE-Based Population PK/PD and System Pharmacology Models, **Contributor**, [GitHub](#)
- **bayesplot**: Plotting for Bayesian Models in R, **Contributor**, [Cran](#)

## 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

- Manny Mokel (undergraduate student), Summer 2023  
Project: *Nested  $\hat{R}$ : pooled sampling and variance approximation*
- 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

### Instructor:

- *Bayesian Workflow for hierarchical and ODE-based models*, three day workshop, Summer School on Advanced Bayesian Methods, Leuven, Belgium (2023)
- *Stan for the people: an introductory workshop to Bayesian modeling*, two day workshop, McGill University, Montreal, Canada (2019, 2020)
- *Introduction to Bayesian Data Analysis with Stan*, lecture, STAT 220: Bayesian Statistics, Harvard University, Cambridge, MA, April 2017.
- University of Buffalo, School of Pharmacy, Buffalo, NY (2019 – 2023)
  - *Probability and Bayes*, lecture, PHC 506: Biometry in Pharmaceutics
  - *Building, fitting, and criticizing Bayesian PK/PD models*, one day workshop
- StanCon
  - *Fundamentals of Stan*, half-day workshop, StanCon 2023, University of Washington, Saint-Louis, MO
  - *Population and ODE-based models using Stan and Torsten*, two day workshop, StanCon 2019, Cambridge, UK
  - *How to Develop for the Stan C++ Core Language*, lecture, StanCon 2018, Pacific Grove, CA

### Teaching Assistant (selected):

- Columbia University, New York, NY  
**Recipient of the Minghui Yu Teaching Assistant Award**
  - *Applied Statistics II* (PhD level, 2021 – 2022)
  - *Foundations of Graphical Modeling* (PhD level, 2019 – 2020)
  - *Statistical Inference* (Masters level, 2019)
  - *Statistical Computing and Introduction to Data Science* (Undergrad level, 2018)
  - *Bayesian Statistics* (Masters level, 2018)
  - *Linear Regression Models* (Undergrad level, 2017)
- Metrum Research Group:
  - Getting Started with Bayesian PKPD Modeling using Stan and Torsten*, one day workshop
  - Population Approach Group in Europe, Budapest, Hungary (2017)
  - American Conference on Pharmacometrics, Bellevue, WA (2016)
  - American Conference on Pharmacometrics, Arlington, VA (2015)

- Other:
  - *Stan for Physics*, five day workshop, Massachusetts Institute of Technology, Cambridge, MA (2017)

**Peer Tutor:**

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

## Presentations (selected)

- November 2023 **The Wisdom of Automatic Differentiation**, *Applied and Computational Math Group Meeting*, Courant Institute, New York University, New York, NY.
- July 2023 **The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference**, Conference on Uncertainty in Artificial Intelligence, Pittsburgh, PA.
- 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 Pharmacometrics.
- 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<sup>th</sup> 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 November 2023*