

Shashank Singh

Curriculum Vitae
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CONTACT INFORMATION

Address: Neckarstraße 190
70190 Stuttgart
Germany
Website: <https://sss1.github.io>

Mobile Phone: +49 0176/58976800
Email: shashankssingh44@gmail.com
ORCID ID: [0000-0002-7305-673X](https://orcid.org/0000-0002-7305-673X)
[Google Scholar Profile](#)

EDUCATION

Ph.D.	Statistics & Machine Learning, Carnegie Mellon University	Aug 2019
	Thesis: Estimating Probability Distributions and Their Properties	
M.S.	Machine Learning, Carnegie Mellon University	Aug 2017
M.S.	Mathematical Sciences, Carnegie Mellon University	May 2014
	Thesis: Concentration Inequalities for Density Functionals	
B.S.	Mathematical Sciences, Carnegie Mellon University	May 2014
B.S.	Computer Science, Carnegie Mellon University	May 2014

EMPLOYMENT

2021-	Max Planck Institute for Intelligent Systems (Tübingen, Germany) Postdoctoral Researcher, hosted by Bernhard Schölkopf
2019-2020	Software Engineer at Google, Cloud AI Deployments Team (Pittsburgh, PA) <i>Designed, implemented, and evaluated machine learning systems for industrial and public sector applications (see, e.g., paper "Interpretable COVID-19 Forecasting").</i>
2018 Sep-Dec	Applied Scientist Intern at Amazon Web Services (New York, NY) <i>Developed new algorithms to compress deep neural networks used in computer vision (see paper "DARC: Differentiable ARchitecture Compression").</i>
2015 May-Aug	Software Engineering Intern at Google (Mountain View, CA) <i>Designed, implemented, and tested anomaly detection pipeline for detecting fraudulent activity amongst billions of daily user engagements with online products.</i>

RESEARCH INTERESTS

Theory: Statistical Machine Learning (especially nonparametric methods, fundamental limits of learning from data, generative modeling, out-of-distribution generalization, and causal inference), Sequential Optimization and Experimental Design, Information Theory

Applications: Applications of mathematical modeling, statistics, and machine learning, including Computational Biology (genomics, biological systems modeling), Cognitive Science (behavior modeling, cognitive development), and Epidemiological Forecasting

FELLOWSHIPS AND AWARDS

2019	NeurIPS 2019 Honorable Mention for Outstanding Paper (3/6743 submissions)
2017	Mellon Foundation Presidential Fellow in Life Sciences (1 year graduate funding)
2015	National Science Foundation Graduate Research Fellow (3 years graduate funding)
2012	Undergraduate Research Fellow in Computational Neuroscience, Center for the Neural Basis of Cognition, Carnegie Mellon University. (1 year research stipend)

PUBLICATIONS

Submitted Papers (Under Review)

Singh, S. [Nonparametric Indirect Active Learning](#).

Uppal, K., Kim, J., & **Singh, S.** [Decoding Attention from Gaze: A Benchmark Dataset and End-to-End Models](#).

Kim, J., **Singh, S.**, Vales, C., Keebler, E., Fisher, A.V., & Thiessen, E.D. [Staying and Returning Dynamics of Young Children's Attention](#).

Journal Articles

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| 2021 | Ledsam, J., Arik, S., Shor, J., Sinha, R., Yoon, J., Le, L., Dusenberry, M., Yoder, N., Popenndorf, K., Epshteyn, A., Euphrosine, J., Kanal, E., Jones, I., Li, C.-L., Luan, B., Mckenna, J., Menon, V., Singh, S. , Sun, M., Ravi, A.S., Zhang, L., Sava, D., Kayama, H., Tsai, T., Yoneoka, D., Nomura, S., Miyata, H., and Pfister, T. A prospective evaluation of AI-augmented epidemiology to forecast COVID-19 in the USA and Japan . In <i>Nature Digital Medicine</i> . |
| 2020 | Kim, J., Singh, S. , Thiessen, E. D., & Fisher, A. V. "A Hidden Markov Model for Analyzing Eye-Tracking of Moving Objects" . In <i>Behavior Research Methods</i> . |
| 2019 | Rashid, S., Long, Z., Singh, S. , Kohram, M., Vashistha, H., Navlakha, S., Salman, H., Oltvai, Z. N., Bar-Joseph, Z. "Adjustment in tumbling rates improves bacterial chemotaxis on obstacle-laden terrains" . In <i>Proceedings of the National Academy of Sciences (PNAS)</i> . |
| | Rashid, S., Singh, S. , Navlakha, S., & Bar-Joseph, Z. "A Bacterial based Distributed Gradient Descent Model for Mass Scale Evacuations" . In <i>Swarm and Evolutionary Computation</i> . |
| 2018 | Singh, S. , Yang, Y., Póczos, B., & Ma, J. "Predicting Enhancer-Promoter Interaction from Genomic Sequence with Deep Neural Networks" . <i>Quantitative Biology</i> , Special Issue on Applications of Deep Learning to Biology. |

Conference Papers

- 2022 **Singh, S.** & Khim, J. *Optimal Binary Classification Beyond Accuracy*. Accepted to Neural Information Processing Systems (NeurIPS). (25.6% accept rate)
- Eastwood, C., Robey, A., **Singh, S.**, von Kügelgen, J., Hassani, H., Pappas, G. J., & Schölkopf, B. *Probable Domain Generalization via Quantile Risk Minimization*. Accepted to Neural Information Processing Systems (NeurIPS). (25.6% accept rate)
- Kim, J., **Singh, S.**, Yurovsky, D., Fisher, A. V., & Thiessen, E. D. *A Hierarchical Model of Visual Attention over Time*. Full paper presented orally in Annual Meeting of the Cognitive Science Society (CogSci). (26.9% accept rate)
- 2021 **Singh, S.** *Continuum-Armed Bandits: A Function Space Perspective*. To be presented in International Conference on Artificial Intelligence and Statistics (AISTATS). (29.8% accept rate)
- 2020 Uppal, A., **Singh, S.** & Póczos, B. *Robust Density Estimation under Besov IPM Losses*. Neural Information Processing Systems (NeurIPS). (20.1% accept rate; Spotlight Presentation; 20.3% of accepted papers)
- Arik, S. O., Li, C.-L., Yoon, J., Sinha, R., Epshteyn, A., Le, L., Menon, V., **Singh, S.**, Zhang, L., Yoder, N., Nikoltchev, M., Sonthalia, Y., Nakhost, H., Kanal, E., & Pfister, T. *Interpretable Covid-19 Forecasting*. Neural Information Processing Systems (NeurIPS). (20.1% accept rate; Spotlight Presentation; 20.3% of accepted papers)
- Kim, J., **Singh, S.**, Thiessen, E. D., & Fisher, A. V. *Staying and Returning Dynamics of Sustained Attention in Young Children*. Poster presented at Annual Meeting of the Cognitive Science Society (CogSci). (63% accept rate)
- 2019 Uppal, A., **Singh, S.** & Póczos, B. *Nonparametric Density Estimation & Convergence of GANs under Besov IPM Losses*. Oral Presentation in Neural Information Processing Systems (NeurIPS). (21.0% accept rate; **Honorable Mention for Outstanding Paper Award**; 0.2% of accepted papers)
- 2018 **Singh, S.**, Uppal, A., Li, B., Li, C.-L., Zaheer, M., & Póczos, B. *Nonparametric Density Estimation under Adversarial Losses*. Poster Presentation in Neural Information Processing Systems (NeurIPS). (20.8% accept rate)
- Kim, J., **Singh, S.**, Vande Velde, A., Thiessen, E.D., & Fisher, A.V. *A Hidden Markov Model for Analyzing Eye-Tracking of Moving Objects*. Full paper presented orally in Annual Meeting of the Cognitive Science Society (CogSci). (22.5% accept rate)
- Singh, S.**, Póczos, B., & Ma, J. *Minimax Reconstruction Risk of Convolutional Sparse Dictionary Learning*. International Conference on Artificial Intelligence and Statistics (AISTATS). (33.2% accept rate)

- 2017 **Singh, S.** & Póczos, B. *Nonparanormal Information Estimation*. International Conference on Machine Learning (ICML). (25.5% accept rate)
- Yang, Y., Zhang, R., **Singh, S.**, & Ma, J. *Exploiting sequence-based features for predicting enhancer-promoter interactions*. Full Paper in Intelligent Systems for Molecular Biology (ISMB). (16.5% accept rate; **F1000Prime Recommended**)
- 2016 **Singh, S.**, Du, S., & Póczos, B. *Efficient Nonparametric Smoothness Estimation*. Neural Information Processing Systems (NIPS). (22.7% accept rate)
- Singh, S.** & Póczos, B. *Finite-Sample Analysis of Fixed-k Nearest Neighbor Density Functional Estimators*. Neural Information Processing Systems (NIPS). (22.7% accept rate)
- Singh, S.**, Rashid, S., Navlakha, S., & Bar-Joseph, Z. *Distributed Gradient Descent in Bacterial Food Search*. Full Paper in Research in Computational Molecular Biology (RECOMB). (20.6% accept rate)
- 2014 **Singh, S.** & Póczos, B. *Exponential Concentration of a Density Functional Estimator*. Neural Information Processing Systems (NIPS). (24.7% accept rate)
- Singh, S.** & Póczos, B. *Generalized Exponential Concentration Inequality for Rényi Divergence Estimation*. International Conference on Machine Learning (ICML). (Cycle 1; 14.7% accept rate; **1 of 18 papers nominated for JMLR fast-track**)

Workshop Papers

- 2022 **Singh, S.** *Indirect Active Learning*. ICML Workshop on Adaptive Experimental Design and Active Learning in the Real World (ReALML).
- 2020 Arik, S. O., Li, C.-L., Nikoltchev, M., Sinha, R., Epshteyn, A., Yoon, J., Le, L., Menon, V., **Singh, S.**, Sonthalia, Y., Nakhost, H., Zhang, L., Kanak, E., & Pfister, T. *Interpretable Covid-19 Forecasting*. ICML Workshop on Healthcare Systems, Population Health, and the role of Health-tech.
- Singh, S.**, Khetan, A., & Karnin, Z. *DARC: Differentiable ARchitecture Compression*. ICLR Workshop on Neural Architecture Search.
- 2017 **Singh, S.**, Póczos, B., & Ma, J. *Minimax Reconstruction Risk of Convolutional Sparse Dictionary Learning*. 55th Annual Allerton Conference on Communication, Control, and Computing.
- 2016 **Singh, S.**, Yang, Y., Póczos, B., and Ma, J. *Predicting Enhancer-Promoter Interaction from Genomic Sequence with Deep Learning*. NIPS Workshop on Machine Learning in Computational Biology.
- 2014 **Singh, S.**, Navlakha, S., and Bar-Joseph, Z. *Distributed and computationally efficient belief propagation based on swarms of foraging bacteria*.

Technical Reports

- 2018 | **Singh, S.** & Póczos, B. [Minimax Distribution Estimation in Wasserstein Distance](#).
- Singh, S.**, Sriperumbudur, B.K., & Póczos, B., [Nonparametric estimation of Fourier-weighted inner products](#).
- 2016 | **Singh, S.** & Póczos, B. *Analysis of k -Nearest Neighbor Distances with Application to Entropy Estimation*.

PRESENTATIONS

Invited Conference Talks

- 2019 | *Accelerating Convergence in Wasserstein Distribution in High Dimensions*. 2019 INFORMS Annual Meeting, Session on Recent Advances in Learning and Distributionally Robust Optimization. At the Washington State Convention Center, Seattle, WA, USA, October 20. (20 minutes)

Contributed Conference/Workshop Talks

- 2022 | [A Hierarchical Model of Internal Attentional State over Time](#). 44th Annual Meeting of the Cognitive Science Society (CogSci). At the Metro Toronto Convention Centre, Toronto, Canada, July 30. (15 minutes)
- 2019 | [Nonparametric Density Estimation & Convergence Rates for GANs under Besov IPM Losses](#). 33rd Conference on Neural Information Processing Systems (NeurIPS). At the Vancouver Convention Centre, Vancouver, British Columbia, Canada, December 12. (15 minutes)
- 2017 | *On the Reconstruction Risk of Convolutional Sparse Dictionary Learning*. 55th Annual Allerton Conference on Communication, Control, and Computing. At the Allerton Retreat Center, Monticello, IL, USA, October 4. (20 minutes)
- Nonparanormal Information Estimation: Realistic High-Dimensional Dependence Estimation*. 34th International Conference on Machine Learning (ICML). At the International Convention Center, Sydney, Australia, August 8. (20 minutes)
- 2014 | *Low-Communication Distributed Optimization via E. Coli Swarm Foraging*. 2nd Workshop on Biological Distributed Algorithms, Austin, TX, Oct 12. (20 minutes)
- [Generalized Exponential Concentration Inequality for Rényi Divergence Estimation](#). At 31st International Conference on Machine Learning (ICML), Beijing, China, June 22. (20 minutes)

Other Talks and Poster Presentations

- 2022 | *Indirect Active Learning*. Poster at Adaptive Experimental Design and Active Learning in the Real World (RealML) workshop at ICML 2022, July 22.

- Indirect Active Learning.*
- Probable Generalization via Quantile Risk Minimization.* "Cake Talk" (department seminar), Max Planck Institute for Intelligent Systems. Remote, June 1. (45 minutes).
- 2020 *Measuring Selective Sustained Attention in Children with TrackIt and Eyetracking.* Virtual poster at Annual Meeting of the Cognitive Science Society (CogSci), July 30.
- 2019 *Nonparametric Density Estimation under IPM Losses.* Poster at Joint Statistical Meetings (JSM), Denver, CO, USA, July 29.
- Measuring Selective Sustained Attention in Children with TrackIt and Eyetracking.* Poster at Annual Meeting of the Cognitive Science Society (CogSci), Montreal, Canada, July 27.
- 2018 *Nonparametric Density Estimation under Adversarial Losses.* Poster at Neural Information Processing Systems (NeurIPS), Montreal, Canada.
- Minimax Reconstruction Risk of Convolutional Sparse Dictionary Learning.* Poster at International Conference on Artificial Intelligence and Statistics (AISTATS), Lanzarote, Spain.
- 2017 *Nonparanormal Information Estimation.* Poster at International Conference on Machine Learning (ICML), Sydney, Australia.
- Predicting Enhancer-Promoter Interaction using only Genomic Sequence Features.* Poster at Cold Spring Harbor Laboratory Meeting on Systems Biology: Global Regulation of Gene Expression. Cold Spring Harbor, NY, USA, Feb. 28.
- 2016 *Predicting Enhancer-Promoter Interaction from Genomic Sequence with Deep Learning.* Poster at NIPS Workshop on Machine Learning in Computational Biology, Barcelona, Spain, Dec 10.
- Finite-Sample Analysis of Fixed- k Nearest Neighbor Density Functional Estimators.* Poster, Neural Information Processing Systems (NIPS), Barcelona, Spain, Dec 6.
- Efficient Nonparametric Smoothness Estimation.* Poster at Neural Information Processing Systems (NIPS), Barcelona, Spain, Dec 5.
- 2014 *Exponential Concentration of a Density Functional Estimator.* Poster at Neural Information Processing Systems (NIPS), in Montreal, Canada.
- Exponential Concentration Inequality for a Rényi- α Divergence Estimator.* Poster at International Conference on Machine Learning (ICML), Beijing, China.

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| 2012 | <i>Neuronal interaction and dynamics of uncertainty resolution in V2</i> . CNBC Undergraduate Program in Neural Computation, in Pittsburgh, PA, USA. |
| 2011 | <i>Temporal evolution of probabilistic population codes for stereo vision in V1</i> . Meeting of the Minds CMU Research Symposium, in Pittsburgh, PA, USA. |

OPEN-SOURCE SOFTWARE

Some free, open-source software that I have authored in connection to my scientific projects:

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| 2018 | <i>eyetracking</i> . Hidden Markov Model and pre-processing utilities for decoding visual object-tracking experiments, written to support a CogSci 2018 paper.
Python. https://github.com/sss1/eyetracking |
| 2017 | <i>convolutional-dictionary</i> . An implementation of convolutional sparse dictionary learning and related simulations, written to support an AISTATS 2018 paper.
MATLAB. https://github.com/sss1/convolutional-dictionary |
| 2017 | <i>nonparanormal-information</i> . Estimators for entropy and mutual information assuming a nonparanormal model, written to support an ICML 2017 paper.
MATLAB. https://github.com/sss1/nonparanormal-information |
| 2016 | <i>sobolev-estimation</i> . Nonparametric estimators for Sobolev norms, distances, and inner products of probability densities, written to support a NIPS 2016 paper.
MATLAB. https://github.com/sss1/sobolev-estimation |

OTHER PROFESSIONAL ACTIVITIES

Reviewer for the following journals:

Annals of Statistics
Journal of Machine Learning Research (JMLR)
Bernoulli
IEEE Transactions on Information Theory
Machine Learning Journal (MLJ)
PLOS ONE
Communications on Pure and Applied Analysis

Reviewer for the following conferences:

Neural Information Processing Systems (NeurIPS) Conference, 2016–2022
 International Conference on Machine Learning (ICML), 2018–2022
 – 2020 Top 33% Reviewer award – 2019 Top 5% Reviewer (awarded free registration)
 Artificial Intelligence and Statistics (AISTATS), 2017–2023
 Conference on Learning Theory (COLT), 2018
 IEEE International Symposium on Information Theory (ISIT), 2019
 International Joint Conference on Artificial Intelligence (IJCAI), 2016, 2021 (SPC)
 Biological Distributed Algorithms Workshop (BDA), 2016

Mentoring of PhD Students

Ananya Uppal	PhD in Mathematical Sciences Project: <i>Density Estimation under Besov IPM Losses</i>	03/18-05/21
Cian Eastwood	PhD in Mathematical Sciences Project: <i>Robust Multi-Environment Generalization</i>	08/21-Present

Mentoring of MS Students

Karan Uppal	MS in Mathematics & Computing Project: <i>Neural network models for attentional decoding</i> DAAD WISE Internship Host	05/22-07/22
Rui Peng	MS in Machine Learning Project: <i>Predicting Higher-order Chromatin Interaction from Human Gene Sequence with Deep Neural Networks</i> Member of Data Analysis Project Committee	08/16-12/17
Boyue Li	MS in Biotech. Innovation and Computation Project: <i>Estimating KL Divergence in Exponential Families</i>	08/17-08/18

Teaching Assistantships at Carnegie Mellon University

10-704	Information Processing and Learning <i>Professor Aarti Singh</i>	Fall 2016
36-462	Data Mining <i>Professor Max G'Sell</i>	Spring 2015
36-309	Experimental Design for Behavioral and Social Sciences <i>Professor Howard Seltman</i>	Fall 2014
21-373	Algebraic Structures <i>Professor Rick Statman</i>	Fall 2013
15-251	Great Theoretical Ideas in Computer Science <i>Professors Ryan O'Donnell & Danny Sleator</i>	Spring 2012
15-211	Fundamental Data Structures and Algorithms <i>Professors Jim Morris & Chris Langmead</i>	Fall 2011