Ji Won Park

Research Scientist

San Francisco Bay Area

✉ jiwoncpark@gmail.com | ⌂ jiwoncpark.github.io | 🔗 ji-won-park | 🐦 @jiwoncpark

Research Areas

- **Decision-making under uncertainty**
    - Designing acquisition functions for multi-objective Bayesian optimization tailored for molecular property spaces
    - Productionalizing machine-guided design of antibodies, small molecules, and molecular glues with specific project desiderata
- **Inference in high dimensions**
    - Non/semi-parametric Bayes, adaptation, targeted learning
    - Post-hoc calibration methods including conformal prediction
    - Causality-inspired domain generalization methods for out-of-distribution robustness
- **Sampling in high dimensions**
    - Sampling algorithms for non-log-concave distributions
    - Hybridizing MCMC with variational methods to balance accuracy and speed

Education

Stanford University   *Stanford, CA*

Ph.D. Physics   *Sept 2017 – March 2022*
- Co-advised by Philip J. Marshall, Aaron Roodman

Duke University   *Durham, NC*

B.S. Physics, B.S. Math   *Aug 2013 – May 2017*
- Honors thesis advisor: Christopher Walter
- Graduation with High Distinction

Professional Experience

Genentech   *South San Francisco, CA*

Principal Machine Learning Scientist   *Nov 2023 - Present*

Senior Machine Learning Scientist II   *Nov 2021 - Nov 2023*
- Developing algorithms to improve uncertainty quantification in active, machine-guided molecular design
- Advising experimental and applied machine learning scientists on active data acquisition and probabilistic modeling
- Worked with Kyunghyun Cho, Saeed Saremi, Nataša Tagasovska.

Stanford University / SLAC National Accelerator Laboratory   *Stanford, CA*

Graduate Research Assistant   *April 2018 - Present*

My thesis developed approximate inference methods under a hierarchical Bayesian framework. I applied this approach to multi-modal astronomical datasets to infer the Hubble constant, a key cosmological parameter governing the Universe's accelerated expansion. Dissertation: "All the Lenses: Hierarchical Inference of the Hubble Constant from Strong Gravitational Time Delays with Bayesian Deep Learning"

Simons Foundation Flatiron Institute, Center for Computational Astrophysics (CCA)   *New York City, NY*

Visiting Researcher (Supervisor: Shirley Ho)   *April-July 2021*

Extended latent stochastic differential equations to reconstruct the multivariate time series of active galactic nuclei (AGNs) and infer their black hole properties. Among the Universe's most extreme objects, AGNs are luminous galactic centers hosting black holes, whose physical attributes trace the Universe's evolutionary history.

NASA Ames Research Center   *Mountain View, CA*
Summer Ph.D. Intern   *June-Oct 2019 (part-time)*
Developed a Pix2Pix video-to-image model to predict solar flux emergence from time-series magnetograms. Forecasting solar flux emergence is critical for astronaut safety below low-Earth orbit.

Publications

* indicates equal contribution.

Published

[20] **Park, J.W.**, Tibshirani, R., Cho, K. Semiparametric conformal prediction. AISTATS (2025). [arXiv]

[19] Bazgir, O., Wang, Z., **Park, J. W.**, Hafner, M., Lu, J. Integration of Graph Neural Network and Neural-ODEs for Tumor Dynamic Prediction. ICLR (2024) MLGenX Workshop. [arXiv]

[18] Griffiths, R. and 24 others including **Park, J.W.**. GAUCHE: a library for Gaussian processes in chemistry. NeurIPS (2024). [arXiv]

[17] Fagin, J., **Park, J. W.**, Best, H., Chan, J. H., Ford, K. S., Graham, M. J., ..., O'Dowd, M. Latent Stochastic Differential Equations for Modeling Quasar Variability and Inferring Black Hole Properties. *The Astrophysical Journal* (2024), 965(2): 104. [arXiv] [ADS]

[16] Saremi, S., **Park, J. W.**, Bach, F. Chain of Log-Concave Markov Chains. ICLR (2024). [arXiv]

[15] **Park, J.W.***, Tagasovska, N.*, Maser, M., Ra, S., Cho, K. BOtied: Multi-objective Bayesian optimization with tied multivariate ranks. ICML (2024). [arXiv]

[14] Ng, N., **Park, J.W.**, Lee, J.H., Kelly, R., Cho, K. Blind Sequence Denoising with Self-Supervised Set Learning. TMLR (2023).

[13] **Park, J.W.**, Birrer, S., Ueland, M., Cranmer, M., Wagner-Carena, S., Marshall, P.J., Roodman, A. 2021. Hierarchical Inference of Weak Lensing Convergence from Photometric Catalogs with Bayesian Graph Neural Networks. *The Astrophysical Journal* (2023), 953(2): 178. [arXiv] [ADS] [ApJ]

[12] Maser, M., **Park, J.W.**, Lin, J.Y.Y., Lee, J.H., Frey, N., Watkins, A. SupSiam: Non-contrastive Auxiliary Loss for Learning from Molecular Conformers. ICLR (2023) Machine Learning for Drug Discovery Workshop. [arXiv]

[11] Fagin, J.* **Park, J.W.***, Best, H., Ford, S., Graham, M., Villar, A., Ho, S., Chan, J., O'Dowd, M. Latent Stochastic Differential Equations for Modeling Quasar Variability and Inferring Black Hole Properties. ICLR (2023) *Physics for Machine Learning* Workshop. Spotlight. [arXiv]

[10] **Park, J.W.**, Stanton, S., Saremi, S., Watkins, A., Dwyer, H., Gligorijevic, V., Bonneau, R., Ra, S., Cho, K. PropertyDAG: Multi-objective Bayesian Optimization of Partially Ordered, Mixed-Variable Properties for Biological Sequence Design. NeurIPS (2022) AI for Science Workshop. [arXiv]

[9] Berenberg, D., Lee, J.H., Kelow, S., **Park, J.W.**, Watkins, A., Gligorijevic, V. Bonneau, R., Ra, S., Cho, K. Multi-Segment Preserving Sampling for Deep Manifold Sampler. ICLR (2022) Machine Learning for Drug Discovery Workshop. Spotlight. [arXiv]

[8] Morgan, R., Nord, B., Bechtol, K., Gonzalez, J., Buckley-Geer, E., Moller, A., **Park, J.W.** followed by 38 others. Deepzipper: A Novel Deep-Learning Architecture for Lensed Supernovae Identification. *The Astrophysical Journal* (2022), 927(1): 109-9. [ADS]

[7] **Park, J.W.**, Villar, A., Li, Y., Jiang, Y.F., Ho, S., Lin, J.Y.Y., Marshall, P.J., Roodman, A. Inferring Black Hole Properties from Astronomical Multivariate Time Series with Bayesian Attentive Neural Processes. ICML (2021) Uncertainty and Robustness

in Deep Learning and Time Series Workshops. [arXiv] [ADS]

[6] **Park, J.W.**, Wagner-Carena, S., Birrer, S., Marshall, P.J., Lin, J.Y.Y., Roodman, A. (LSST Dark Energy Science Collaboration). Large-scale Gravitational Lens Modeling with Bayesian Neural Networks for Accurate and Precise Inference of the Hubble Constant. *The Astrophysical Journal* (2021), 910(1): 39. [arXiv] [ADS]

[5] Wagner-Carena, S., **Park, J.W.**, Birrer, S., Marshall, P.J., Roodman, A., Wechsler, R.H. (LSST Dark Energy Science Collaboration). Hierarchical Inference with Bayesian Neural Networks: An Application to Strong Gravitational Lensing. *The Astrophysical Journal* (2021), 909(2): 187. [arXiv] [ADS]

[4] LSST Dark Energy Science Collaboration including **Park, J.W.** The LSST DESC DC2 Simulated Sky Survey. *The Astrophysical Journal Supplement Series* (2021), 253(1): 31-34. [arXiv] [ADS]

[3] Ding, X., Treu, T., and 26 others including **Park, J.W.** Time Delay Lens Modeling Challenge. *Monthly Notices of the Royal Astronomical Society* (2021), 503(1): 1096-1123. [arXiv] [ADS]

[2] Birrer S., Shajib, A.J., Gilman, D., Galan, A., and 16 others including **Park, J.W.** Lenstronomy II: A Gravitational Lensing Software Ecosystem. *The Journal Open Science Software* (2021), 03283. [arXiv] [ADS]

[1] Birrer S., Shajib, A.J., Galan, A., Millon, M., Treu, T. and 22 others including **Park, J.W.** TDCOSMO IV: Hierarchical Time-Delay Cosmography — Joint Inference of the Hubble Constant and Galaxy Density Profiles. *Astronomy and Astrophysics* (2020), 643(A165): 40. [arXiv] [ADS]

In Prep

[25] Fannjiang, C., **Park, J.W.** Reliable algorithm selection for machine learning-guided design. In prep.

[24] Lahiri, P., **Park, J.W.**., Vasilaki, S., Dreyer, F., Stanton, S., Seeger, F., Kelly, R. (Author list and ordering TBD.) High-throughput affinity characterization with AffiMapper. In prep.

[23] Kim, K., **Park, J.W.**. Bayesian optimization with control functionals. In prep.

[22] Nerli, S.*, **Park, J.W.***, Lu, C., Davidson, D., Kelow, S., Bonneau, R., Cho, K., Watkins, A. P-flex: Modeling peptide conformational flexibility in pHLA-I molecules with machine-learned structural descriptors. In prep.

[21] Tagasovska, N.*, **Park, J.W.***, Kirchmeyer, M., Frey, N., Ismail, A., Jamasb, A., Lee, E., Bryson, T., Ra, S., Cho, K. 2023. Antibody DomainBed: Out-of-Distribution Generalization in Therapeutic Protein Design. In prep. [arXiv]

Patents

Provisional applications

Six patent applications under review (details withheld for confidentiality)

Published patents

[1] Berenberg, D., Lee, J.H., Kelow, S., **Park, J.W.**, Watkins, A., Gligorijevic, V. Bonneau, R., Ra, S., Cho, K. 2022. "Multi-Segment Preserving Sampling for Deep Manifold Sampler." [068893-506P01US] [GNE Ref. P37421-US]

Presentations

External presentations

November 2024. Poster presentation, "Semiparametric conformal prediction for molecular property prediction ." Cambridge, MA.

October 2024. Invited panelist at the CMG AI Summit, "How to win in the age of AI." South San Francisco, CA.

June 2024. *Finding Signal in the Noise for Lab-in-the-Loop Molecular Design*. Invited talk: Stanford University Bio-X (Interdisciplinary Biosciences Institute).

June 2024. *Multi-objective optimization for molecular design using multivariate ranks and quantiles*. Invited talk: Cradle.ai. Zurich, Switzerland.

March 2024. *BOtied: Multi-objective Bayesian optimization with tied multivariate ranks*. Invited talk: Neural Concept and EPFL. Lausanne, Switzerland.

February 2024. *BOtied: Multi-objective Bayesian optimization with tied multivariate ranks*. Invited talk: 2024 SIAM Conference on Uncertainty Quantification. Trieste, Italy.

January 2024. *Multi-Objective Bayesian Optimization for Molecular Design*. Invited talk: KASBP-SF Annual Symposium. South San Francisco, CA.

January 2024. Invited plenary panelist at the American Physical Society 2024 Conference for Undergraduate Women in Physics (APS CUWiP) at Stanford University. The goal of CUWiP is to encourage undergraduate women and gender minorities to continue in physics.

November 2023. *Multi-Objective Bayesian Optimization for Molecular Design*. Industry Research Workshop: Machine Learning for Health Care and Life Sciences. ETH Zurich, Zurich, Switzerland.

June 2023. *A Tail of Many Tails: Multi-Objective Bayesian Optimization for Molecular Design.* Invited talk: Seoul National University, Seoul, South Korea.

June 2023. *A Tail of Many Tails: Multi-Objective Bayesian Optimization for Molecular Design.* Invited talk: Korea Advanced Institute of Science & Technology, Daejeon, South Korea.

May 2022. *Inferring the Hubble Constant from Strong Lensing Time Delays with Bayesian Deep Learning*. Departmental tea talk: Kavli Institute of Particle Astrophysics and Cosmology, Stanford, CA.

May 2021. *Inferring the Hubble Constant from Strong Lensing Time Delays with Bayesian Deep Learning*. Departmental tea talk: Kavli Institute of Particle Astrophysics and Cosmology, Stanford, CA.

April 2021. *Large-Scale Gravitational Lens Modeling with Bayesian Neural Networks for Accurate and Precise Inference of the Hubble Constant.* Oral presentation, competitive. Time-Domain Cosmology with Strong Gravitational Lensing Workshop, virtual.

July 2021. *Inferring Black Hole Properties from Astronomical Multivariate Time Series with Bayesian Attentive Neural Processes*. Poster presentation, competitive. International Conference on Machine Learning (ICML) Uncertainty and Robustness in Deep Learning and Time Series Workshops, virtual.

July 2021. *Joint Light Curve Reconstruction and Parameter Inference from LSST-like Active Galactic Nuclei (AGN) Light Curves with Bayesian Neural Networks*. Oral presentation, competitive. Supermassive Black Hole Studies with the Legacy Survey of Space and Time – The 2021 Summer Meeting of the LSST AGN Science Collaboration, virtual.

February 2020. *Validation of AGN Variability in DC2 (the Second Data Challenge)*. Oral presentation: Winter 2020 DESC Collaboration Meeting, Tucson, AZ.

November 2019. *Inference of the Hubble Constant Using Bayesian Neural Networks*. Oral presentation: Bay Area Likelihood-Free Inference Workshop, Berkeley, CA.

July 2019. *Hierarchical Inference of the Hubble Constant: Simulation Design*. Oral presentation: Summer 2019 DESC Collaboration Meeting, Paris, France.

July 2019. *Catalog-Level Detection of Strong Lenses with Probabilistic Machine Learning*. Oral presentation: Summer 2019 DESC Collaboration Meeting, Paris, France.

February 2019. Emulating LSST Catalogs with Deep Learning. Invited keynote. Plenary session at the Winter 2019 DESC Collaboration Meeting, Berkeley, CA.

July 2018. *Catalog-Level Lens Finding with Variational Recurrent Autoencoders*. Oral presentation: Summer 2018 DESC Collaboration Meeting, Pittsburgh, PA.

Research Mentoring

2024-2025	**Kyurae Kim** Graduate Student	*University of Pennsylvania*
2023	**Taro Makino** Graduate Student	*New York University*
2022	**Nathan Ng** Graduate Student	*University of Toronto*
2022-2023	**Joshua Fagin** Graduate Student	*City University of New York*
2021-2020	**Madison Ueland** Undergraduate Summer Research Student	*Stanford University*
2019	**Alex Feghhi** Undergraduate Intern	*NASA Ames Research Center*

Outreach

February 2024	**US Particle Physics** Featured in periodical *Particle Physics Builds STEM Leaders*	*Online*
January 2024	**APS Conferences for Undergraduate Women in Physics (CUWiP)** Invited Plenary Panelist	*Stanford, CA*
2019–2021	**Stanford Physics Peer Mentoring Program** Graduate Peer Mentor	*Stanford, CA*

Professional Development

2024–Present	**Korean American Society in Biotech and Pharmaceuticals (KASBP)** Organizing Committee, San Francisco Chapter	*San Francisco Bay Area*
2021–Present	**Prescient Design Machine Learning Journal Club** Organizer	*South San Francisco, CA*
2019–2021	**Breakfast Club (journal club on probabilistic ML for high energy physics)** Organizer	*Stanford, CA*
2020	**Summer 2020 DESC Collaboration Meeting** Scientific Organizing Committee	*Virtual*
2016–2017	**Korean-American Scientists and Engineers Association (KSEA)** Co-President, Duke Chapter	*Durham, NC*
2013–2017	**CHANCE (volunteer tutoring organization)** Tutor, Vice President of Treasury	*Durham, NC*