Imre Risi Kondor

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Legal Name	**Imre Miklós Kondor**
Name used in publications	**Risi Kondor**

Research interests

1. Machine learning for science (molecular modeling, drug discovery, etc.)
2. Equivariant deep learning architectures for learning graphs and other combinatorial objects
3. Multiresolution and multiscale matrix factorizations
4. Permutation problems and Fourier analysis on the symmetric group
5. High performance large scale machine learning systems

Employment

Department of Computer Science, Department of Statistics, Computational and Applied Mathematics Initiative — **The University of Chicago**
Associate professor — Jul 2018 –
Assistant professor — Jul 2011 – Jun 2018

Center for Computational Mathematics, — **Flatiron Insitute, New York**
Senior research scientist and leader of the machine learning group
(on leave from the University of Chicago) — Jul 2019 – Sep 2021

Center for the Mathematics of Information, — **California Institute of Technology**
Postdoctoral fellow — Sep 2009 – Jun 2011

Gatsby Computational Neuroscience Unit, — **University College London**
Senior post-doctoral research associate — Sep 2007 – Aug 2009

Education

Columbia University — 2002 – 2007
Ph.D. in computer science (thesis defended 08/13/07, degree awarded 10/08).
Thesis: "Group theoretical methods in machine learning"
Advisor: Tony Jebara.

Carnegie Mellon University — 2000 – 2002
M.Sc. in knowledge discovery and data mining (machine learning).
Advisor: John Lafferty.

Von Karman Institute for Fluid Dynamics (Brussels, Belgium) — 1999 – 2000
Diploma in computational fluid dynamics. Advisor: Herman Deconinck.

Eötvös University (Budapest, Hungary) — 1997 – 1999
Diploma in physics, specializing in particle physics, statistical physics and environmental fluid dynamics (without final exam). Advisor: Tamás Tél.

University of Cambridge — 1992 – 1995
B.A. in mathematics

Industry experience

Amazon Web Services — July – Dec 2017
Palo Alto, CA (Alex Smola's Deep Learning Group)

Awards

DARPA Young Faculty Award for "Multiresolution Machine Learning for Molecular Modeling" 2016

Notable student paper award at AISTATS 2016 for **Multiresolution Matrix Compression** (N. Teneva, P.K. Mudrakarta and R. Kondor) 2016

Test of time award at ICML 2012 (most influential paper from 10 years ago) for Diffusion Kernels on Graphs and Other Discrete Input Spaces (R. Kondor and J. Lafferty) 2012

Best student paper award at ICML 2003 for
A kernel between sets of vectors (R. Kondor and T. Jebara). 2003

Postdoctoral researchers advised

Wenda Zhou (Ph.D. Statistics, Columbia University)
OpenAI Jul 2020 –

Erik Thiede (Ph.D. Chemistry, University of Chicago)
Assistant Professor in Chemistry at Cornell Jul 2019 –

Brandon Anderson (Ph.D. Physics, University of Maryland)
One of the founders of Atomic AI Nov 2017 – Sep 2019

Ph.D students graduated

Horace Pan (UChicago CS)
Thesis: Leveraging symmetry and structure in machine learning
Currently Machine Learning Engineer at Gauntlet Oct 2015 – Jun 2022

Truong Son Hy (UChicago CS)
Thesis: Graph representation learning, deep generative models on graphs, group equivariant molecular neural networks and multiresolution machine learning
Currently Assistant Professor at Indiana State University Oct 2016 – Jun 2022

Jonathan Eskreis–Winkler (UChicago Stat)
Thesis: Multiresolution analysis on discrete spaces
Currently Senior Applied Scientist at Etsy Oct 2015 – Dec 2019

Pramod K Mudrakarta (UChicago CS)
Thesis: Challenges in modern machine learning: multiresolution structure, model understanding and transfer learning
Currently Software Developer at Google Oct 2014 – Aug 2019

Nedelina Teneva (UChicago CS)
Thesis: Multiresolution Matrix Factorization
Currently Research Scientist at Megagon Jan 2013 – Jul 2017

Maia Fraser (UChicago CS)
Thesis: Group Actions in Topological Data Analysis and Hierarchical Learning
(Maia started her Ph.D. with Partha Niyogi)
Currently Associate Professor at the University of Ottawa Apr 2012 – Jul 2013

Ph.D students currently advised

Andrew Hands (UChicago CS)
Specializing in higher order equivariant graph neural networks Jul 2022 –

Han Zheng (UChicago CS)
Specializing in machine learning for quantum computing Jul 2022 –

Soumyabrata Kundu (UChicago Stats)
Specializing in steerable neural networks Jul 2022 –

Ryan Wong (UChicago Physics)
Specializing in rotation equivariant neural networks for Physics Sep 2022 –

Ryan Keane (UChicago CS)
Specializing in high performance systems for AIxScience Sep 2023 –

Richard Xu (UChicago CS)
Specializing in graph neural networks Sep 2023 –

	Su Hyeong Lee (UChicago CAM) Specializing in generative graph models	Sep 2023 –
	Anastasya Bershanska (UChicago CS) Specializing in quantum computing	
PhD students co-advised	**Samira Sheikhi** (UChicago CS) Research advisor: Nathan Srebro (TTI-C)	Oct 2014 – June 2017
	Stephen Basart (Uchicago CS) Research advior: Greg Shakhnarovich	Oct 2015 –
	Zewei Chu (UChicago CS) Research advisor: Kevin Gimpel (TTI-C)	Nov 2016 –
Ph.D students co-mentored	**Shubhendu Trivedi** (TTI-C) Advisor: Greg Shakhnarovich	Jan 2016 – Aug 2018
	Deepti Pachauri (UW Madison) advisor: Vikas Singh Thesis defended Apr 2015: Group theoretic algorithms for matching problems with applications to computer vision	Jan 2012 – Apr 2015
	Walter Dempsey (UChicago Stat) advisor: Peter McCullagh Thesis defended May 2015: Statistical Methods in joint modeling of longitudinal and survival data	Jan 2012 – Mar 2013
	Vikas Garg (formerly at TTI-C, MIT) Advisor: Tommi Jaakkola	Jan 2013 – Jun 2014
M.S. students advised	**Qinqi Zhang** (UChicago CAM)	May 2023 –
	Tianyi Sun (UChicago CAM)	Jun 2022 – Aug 2023
	Han Zheng (UChicago CAM)	Oct 2021 – Jun 2022
	Yifeng Shi (UChicago Stat)	April 2017 – Jun 2018
	Nick Chase (UChicago Stat) Thesis: An Application of RNNs and LSTM to Financial Markets	Sep 2016 – Feb 2017
	Chang Cheng (UChicago Stat) Thesis: Graph partitioning for large real world dataset	Oct 2015 – May 2016
	Cheng Gao (UChicago Stat) Thesis: Generalized semi-supervised learning on undirected graphs with multiscale spectral graph wavelet transformation	Oct 2012 – Mar 2013
Undergraduate students mentored	**Nancy Cheng** (UChicago Mathematics and Statistics)	Jun 2018 – Jun 2019
	Matthew Joseph (UChicago Mathematics)	
	Dan Mané (UChicago CS)	
Ph.D. committees	**Stephen Fitz** (UChicago CS)	Jun 2021 – Oct 2023
	Taco Cohen (University of Amsterdam)	Nov 2020 – Jun 2021
	Tri Huyn (UChicago CS) advisor: Michael Maire	Feb 2020 –
	Hanxin Zhang (UChicago GGSB) advisor Andrey Rzhetsky	Feb 2017 –
	Liwen Zhang (UChicago CS) advisor: Lek-Heng Lim	Oct 2017 –
	Yunlong Jiao (Mines ParisTech) advisor: Jean-Philipp Vert	June 2017 – August 2017
	Gustav Larsson (UChicago CS) advisor: Yali Amit and Greg Shaknarovich	Oct 2016 – June 2017
	Qinqing Zheng (UChicago CS) advisor: John Lafferty	Feb 2015 – July 2017
	Eric Sibony (Telecom ParisTech) advisor: Stephan Clémençon	Dec 2015 – Jun 2016
	Marc Goessling (Stat) advisor: Yali Amit	Feb 2014 – Jul 2016
	Lian Huan Ng (Stat) advisor: Yali Amit	Feb 2012 – Jul 2015
	Deepti Pachauri (UW Madison) advisor: Vikas Singh	Jun 2013 – Apr 2015
	Ankan Saha (UChicago CS) advisor: John Lafferty	Jan 2012 – Jul 2013

M.S. committees

Owen Melia (UChicago CS)	Mar 2023
Stephen Fitz (UChicago CS)	Mar 2017
Samira Sheikhi (UChicago CS)	Nov 2016
Kai Li (UChicago CS)	April 2016
Jialei Wang (UChicago CS)	May 2015
Jiajun Shen (UChicago CS)	Apr 2015
Liwen Zhang (UChicago CS)	Mar 2015
Alex Kolchinski (UChicago CS)	Jun 2014

Courses taught

CMSC 35430 Machine learning on graphs, groups and manifolds
Spring 2022, Winter 2023, Winter 2024

CMSC 35401 Topics in machine learning: Machine learning for molecular modeling
Spring 2022, Winter 2023, Winter 2024

STAT 37796 Topics in machine leaning: Symmetries and harmonic analysis
Autumn 2021

STAT 37790 Topics in Machine Learning: High performance machine learning system design Spring 2019

CMSC 35246 Deep Learning (graduate level) with Shubhendu Trivedi
Spring 2017

STAT 37710/CMSC 35400 Machine Learning (graduate level)
Autumn 2012, Spring 2014, Spring 2015, Spring 2016, Spring 2017, Spring 2018, Spring 2019, Spring 2024

CMSC 25400/STAT 27725 Machine Learning (undergraduate level)
Winter 2014, Winter 2015, Autumn 2015, Winter 2017, Autumn 2018, Winter 2019

CMSC 35900 Topics in Artificial Intelligence
Spring 2012, Spring 2014, Winter 2015, Spring 2018

STAT 37730 Topics in Computational Harmonic Analysis and Representation Theory
Spring 2012.

CMSC 25010 Introduction to Artificial Intelligence
Winter 2012, Spring 2013.

CMSC 15300 Foundations of Software
Autumn 2011.

Machine Learning II (with Yee-Whye Teh and Maneesh Sahani at the Gatsby Unit)
Spring 2008, Spring 2009

University service roles

Data Science Institute Search Committee	Oct 2022–
Data Science Insititute AI+Science Initiative leadership team	March 2022–
James Franck Institute Emerging Frontiers program leadership on Stat. Mach. driven Machine Learning	Oct 2021–
CS graduate committee	Nov 2018 – Jun 2020
CS hiring committee	Oct 2017 – Jun 2018
CCAM (Computational and Applied Math) admissions committee	Jan 2017 –

Programs organized

IMSI program on Data Driven Materials Informatics
(with Claudia Draxl, Marina Meila, Danny Perez, Gabriel Stoltz and Francois Williaime)
Institute for Mathematical and Statistical Innovation at the University of Chicago Spring 2024

The University of Chicago and Caltech Conference on AI+Science (with Rebecca Willett, Aaron Dinner, David Miller, Juan de Pablo, David Uminsky, Anima Anandkumar and Pietro Perona)

The University of Chicago March 28-30, 2023

Conference on the Interplay between AI and mathematical modelling in the post-structural genomics era (with Jessica Andreani, Arne Elofsson, Krzysztof Fidelis, Serge Grudinin and Elodie Laine)
Centre International de Recontres Mathematiques, Marseille, France March 20-24, 2023

Summer schools organized

Data Science Institute AI+Science Summer School (with Y. Chen, A. Dinner, I. Foster, E. Jonas, Y. Khoo, D. Miller, B. Nord, S. Vaikuntanathan and R. Willett) August 2022

IMA Summer Graduate Program on Modern Applications of Representation Theory (with Jason Morton and Lek-Heng Lim) Jul 20 – Aug 6, 2014

AMS Mathematical Research Community on Algebraic and Geometric Methods in Applied Discrete Mathematics (senior assistant in Michael Orrison's group on Representation Theory in Data Analysis) Jun 15 – 21, 2104

Workshops organized

Flatiron-wide algorithms and mathematics
Internal workshop at the Flatiron Insitute Oct 2020

Minding the gap: between fairness and ethics (NeurIPS 2019)
Co-organized with Igor Rubinov, Jack Poulson, Manfred K. Warmuth, Emanuel Moss and Alexa Hagerty Dec 2019

Workshop on Multiresolution Methods for Large Scale Learning (NIPS 2015)
Co-organized with Inderjit Dhillon, Rob Nowak, Michael O'Neil and Nedelina Teneva Dec 2015

Workshop on Learning with Orderings (NIPS 2009)
with Tiberio Caetano, Carlos Guestrin, Jonathan Huang, Guy Lebanon, Marina Meila Dec 2009

Symposium and workshop on Algebraic methods in machine learning at NIPS 2008 (with Guy Lebanon and Jason Morton) Dec 2008

Tutorials taught

Equivariant neural networks (NeurIPS 2020)
with Taco Cohen Dec 2020

Fourier space neural networks (IPAM) Nov 2019

Representation theory, Fourier analysis and invariants (IPAM)
Part of the "Understanding many-particle systems with machine learning" program Sep 2016

Machine learning for engineers Aug 2013
Mini-course in Michelle Khine's lab at the Dept. of Biomedical Engineering, UC Irvine

Representation theoretical methods in machine learning Oct 2008
Eight lecture mini-course at the Gatsby Unit

Group theory and machine learning Oct 2007
Machine learning tutorial at the University of Cambridge

Group theoretical methods in machine learning Jun 2007
Tutorial at the International Conference of Machine Learning, Corvallis, OR

Non-commutative harmonic analysis Jun 2007
Tutorial at the Complex Systems Summer School, Santa Fe

Participant in Research Programs

Geometry and learning from data in 3D and beyond
Semester long program at IPAM Mar – Jun 2019

NSF innovation lab: Learning the power of data in chemistry Dec 17–21, 2018

Understanding many-particle systems with machine learning
Semester long program at IPAM Sep – Dec 2016

NSF ideas lab: Interdisciplinary approaches to biomedical data science Jul 2015

Algorithmic Spectral Graph Theory
Semester long program at the Simons Institute, Berkeley — Sep – Dec 2014

Reviewer

Journals
IEEE Transactions on Pattern Matching and Artificial Intelligence
IEEE Signal Processing Letters
Journal of Machine Learning Research (action editor)
Journal of Selected Topics in Signal Processing
Machine Learning Journal
Conferences
Artificial Intelligence and Statistics (AISTATS)
International Conference on Machine Learning (area chair) (ICML) (yearly)
Neural Information Processing Systems (area chair) (NeurIPS) (most years)
International Conference on Learning Representations (ICLR) (most years)

Grants

University of Chicago and Vienna Faculty award on **Algebraic aspects of graph neural networks** with Balázs Szendröi and Lek-Heng Lim: $11,500 — Jan 2023 – Dec 2023

DARPA HR00111890038 Distruption engineering program on the Physics of AI: **"Multiscale, group covariant neural networks for learning Physics"** $887,718 — Sept 2018 – March 2020

UChicago FACCTS (France and Chicago Collaborating in the Sciences) grant on **Multiscale Matrix Decompositions for ML** with Rémi Gribonval (INRIA): $12,000 — Jan 2017 – Jan 2019

DARPA D16AP00112 Young Faculty Award: **Multiresolution Machine Learning for Molecular Modeling**: $500,000 (also see under "Awards") — Sep 2016 – Sep 2018

NSF CCF 1405959: **RIVER: A Research Infrastructure to explore Volatility, Energy-efficiency, and Resilience.** PI: Andrew Chien. Co-PIs: Ian Foster, Haryadi Gunawi, Ridgway Scott, John Goldsmith, Varun Gupta, Risi Kondor. Total amount (anticipated): $997,432 Aug 2014 – Aug 2017

NSF CCF III (small) 1320344: **Solving matching problems in machine learning with non-commutative harmonic analysis.** PIs: Risi Kondor and Vikas Singh (University of Wisconsin, Madison). Total award: 424,205. UChicago part: $221,993. — Aug 2013 – Jul 2017

NSF DMS 1417916: **IMA Summer school on modern applications of representation theory (supplementary grant).** PIs: Risi Kondor, Jason Morton and Lek-Heng Lim. Total amount: $39,920 — June, 2014

Preprints

Note: * denotes students or postdocs advised or co-mentored by me at the time of writing. Unless noted otherwise, preprints can be found on `arXiv`.

P-tensors: a general formalism for constructing higher order message passing networks
Tianyi Sun*, Andrew Hands*, Risi Kondor — Jun 2023

Modeling polypharmacy and predicting drug-drug Interactions using deep generative models on multimodal graphs
Nhat Khang Ngo, Truong Son Hy* and Risi Kondor — Feb 2023

Group-equivariant neural networks with fusion diagrams
Zimu Li, Han Zheng*, Erik Thiede*, Junyu Liu and Risi Kondor — Nov 2022

Predicting drug-drug interactions using deep generative models on graphs
Nhat Khang Ngo, Truong Son Hy*, R. Kondor — Sep 2022

On the Super-exponential Quantum Speedup of Equivariant Quantum Machine Learning Algorithms with SU(d) Symmetry
Han Zheng*, Zimu Li, Junyu Liu, Sergii Strelchuk and Risi Kondor — Jul 2022

Symmetry group equivariant architectures for physics
Alexander Bogatskiy et al. — Mar 2022

Speeding up Learning Quantum States through Group Equivariant Convolutional Quantum Ansätze
Han Zheng*, Zimu Li, Junyu Liu, Sergii Strelchuk and Risi Kondor — Dec 2021

Learning Multiresolution Matrix Factorization and its Wavelet Networks on Graphs
Truong Son Hy* and R. Kondor — Nov 2021

Multiresolution Graph Variational Autoencoder
Truong Son Hy* and Risi Kondor — 2021

The general theory of permutation equivarant neural networks and higher order graph variational encoders
Erik H. Thiede*, Truong Son Hy* and Risi Kondor — 2020

Asymmetric multiresolution matrix factorization
Pramod K. Mudrakarta*, Shubhendu Trivedi* and R. Kondor — 2019

A generic multiresolution preconditioner for sparse symmetric systems
Pramod K. Mudrakarta* and R. Kondor

Parallel MMF: a multiresolution approach to matrix computation
Risi Kondor, Nedelina Teneva* and Pramod K. Mudrakarta* — 2015

The skew spectrum of functions on finite groups and their homogeneous spaces
Risi Kondor — 2007

A novel set of rotationally and translationally invariant features for images based on the non-commutative bispectrum
Risi Kondor — 2007

Multi-facet learning in Hilbert spaces
Risi Kondor, Gábor Csányi, Sebastian E. Ahnert and Tony Jebara
Columbia University, CUCS-054-05 — 2005

Refereed workshop publications

Note: * denotes students or postdocs advised or co-mentored by me at the time of writing.

Transformers are efficient hierarchical chemical graph learners
Zihan Pengmei*, Zimu Li, Chih-chan Tien, Risi Kondor, Aaron R. Dinner
AI4Science workshop at NeurIPS 2023 — Dec 2023

Fast Temporal Wavelet Graph Neural Networks
Duc Thien Nguyen, Manh Duc Tuan Nguyen, Truong Son Hy* and Risi Kondor
Temporal graph learning workshop at NeurIPS 2023 — Dec 2023

Multiresolution matrix factorization and its wavelet networks on graphs
Truong Son Hy* and Risi Kondor
Topological, Algebraic, and Geometric Learning Workshops, 2022 — Dec 2022

Molecular fingerprints are a simple yet effective solution to the drug-drug interaction problem Yanan Long, Horace Pan, Chao Zhang, Hy Truong Song, Risi Kondor, Andrey Rzhetsky
ICML workshop on computational biology — Jul 2022

Temporal multiresolution graph neural networks for epidemic prediction Truong Son Hy, Viet Bach Nguyen, Long Tran-Thanh, Risi Kondor
ICML Workshop on healthcare and AI — Jul 2022

Refereed publications in journals and major conferences

Note: * denotes students or postdocs advised or co-mentored by me at the time of writing.

NIPS, NeurIPS: Neural Information Processing Systems conference (acceptance rate: 22%)
ICML: International Conference on Machine Learning conference (acceptance rate: 25%)
AISTATS: Artificial Intelligence and Statistics conference (acceptance rate: 31%)
COLT: Conference on Learning Theory (acceptance rate: $\sim 35\%$)
SODA: ACM–SIAM Symposium on Discrete Algorithms (acceptance rate: $\sim 30\%$)
CVPR: Conference on Computer Vision and Pattern Recognition (acceptance rate: $\sim 30\%$)

JMLR: Journal of Machine Learning Research

Multiresolution graph transformers and wavelet positional encoding for learning hierarchical structures
Nhat Khang Ngo, Truong Son Hy and Risi Kondor The Journal of Chemical Physics, July 2023

Multiresolution equivariant graph variational autoencoder
Truong Son Hy* and Risi Kondor Machine Learning: Science and Technology, March 2023

Speeding up Learning Quantum States through Group Equivariant Convolutional Quantum Ansätze
Han Zheng*, Zimu Li, Junyu Liu, Sergii Strelchuk and R. Kondor PRX Quantum, May 2023

Permutation equivariant layers for higher order interactions
Horace Pan* and Risi Kondor AISTATS 2022

Autobahn: automorphism based graph neural nets
Erik H. Thiede*, Wenda Zhou* and Risi Kondor NeurIPS 2021 (poster)

ATOM3D: tasks on molecules in three dimensions
Raphael J. L. Townshend, Martin Vögele, Patricia Suriana, Alexander Derry, Alexander Powers, Yianni Laloudakis, Sidhika Balachandar, Brandon Anderson*, Stephan Eismann, Risi Kondor, Russ B. Altman, Ron O. Dror NeurIPS 2021 (datasets track, joint winner of best datasets paper)

A community-powered search of machine learning strategy space to find NMR property prediction models
Lars A. Bratholm et al. PLOS ONE, July 2021

Fourier bases for solving permutation puzzles
Horace Pan* and Risi Kondor AISTATS 2021

Lorentz group equivariant neural network for particle physics
A. Bogatskiy, B. Anderson*, J. Offermann, M. Roussi, D. Miller, R. Kondor ICML 2020

Deep learning for automated classification and characterization of amorphous materials
K. Swanson, S. Trivedi*, J. Lequieu, K. Swanson and R. Kondor Soft Matter, 2020

Cormorant: covariant molecular neural networks
Brandon Anderson*, Truong Son Hy*, Risi Kondor NeurIPS 2019

Clebsch-Gordan nets: a fully Fourier space spherical convolutional neural network
Risi Kondor, Zhen Lin* and Shubhendu Trivedi* NIPS 2018

Predicting molecular properties with covariant compositional networks
Truong Son Hy*, Shubhendu Trivedi, Horace Pan, Brandon Anderson and Risi Kondor
The Journal of Chemical Physics, Jun 2018

On the generalization of equivariance and convolution in neural networks to the action of compact groups
Risi Kondor and Shubhendu Trivedi* ICML 2018 (oral)

Multiresolution kernel approximation for Gaussian process regression
Y. Ding*, J. Eskreis–Winkler* and R. Kondor NIPS 2017 (oral)

Data mining when each data point is a matrix
K. Rajendran, A. A. Kattis, A. Holiday, R. Kondor, Y. Kevrekidis Patterns in Dynamics, 2017

The incremental multiresolution matrix factorization algorithm
V. Ithapu*, R. Kondor and V. Singh CVPR 2017

The multiscale Laplacian graph kernel
Risi Kondor and Horace Pan* NIPS 2016 (oral)

Multiresolution matrix compression N. Teneva*, P. K. Mudrakarta* and R. Kondor
Oral presentation (6.5% rate) and winner of Notable Student Paper Award. AISTATS 2016

$\mathbb{S}_n$FFT: A Julia toolkit for for harmonic analysis on the symmetric group
G. Plumb, D. Pachauri*, R. Kondor and V. Singh JMLR, 2016.

Permutation diffusion maps with application to the image association problem in computer vision
D. Pachauri*, R. Kondor, G. Sargur and V. Singh — NIPS 2014

Multiresolution matrix factorization
R. Kondor, N. Teneva* and V. Garg* — ICML 2014

Solving the multi-way matching problem by permutation synchronziation
D. Pachauri*, R. Kondor and V. Singh — NIPS 2013

On representing chemical environments
Albert P. Bartók, Risi Kondor and Gábor Csányi — Physical Review B 87, 2013

Multiresolution analysis on the symmetric group
Risi Kondor and Walter Dempsey* — NIPS 2012

Incorporating domain knowledge in matching problems via harmonic analysis
D. Pachauri*, M. Collins, R. Kondor, V. Singh — ICML 2012

Ranking with kernels in Fourier space
Risi Kondor and Marconi Barbosa* — COLT 2010

Graph kernels
S. V. N. Vishwanathan, Karsten M. Borgardt, Risi Kondor, Nicol n. Schraudolf — JMLR, 2010

Gaussian approximation potentials: the accuracy of quantum mechanics, without the electrons
Albert P. Bartók, Michael C. Payne, Risi Kondor, Gábor Csányi — Physical Review Letters **104**, 2010

A Fourier space algorithm for solving quadratic assignment problems
Risi Kondor — SODA 2010

The graphlet spectrum
Risi Kondor, Nino Shervashidze and Karsten M. Borgwardt — ICML 2009

The skew spectrum of graphs
Risi Kondor and Karsten M. Borgwardt — ICML 2008

Multi-object tracking with representations of the symmetric group
Risi Kondor, Andrew Howard and Tony Jebara — AISTATS 2007

Gaussian and Wishart hyperkernels
Risi Kondor and Tony Jebara — NIPS 2006

Probability product kernels
Tony Jebara, Risi Kondor and Andrew Howard) — JMLR 2004

Kernels and regularization on graphs
Alex Smola and Risi Kondor — COLT 2003

Bhattacharyya and expected likelihood kernels
Tony Jebara and Risi Kondor — COLT 2003

A kernel between sets of vectors
R. Kondor and T. Jebara (best student paper award) — ICML 2003

Diffusion kernels on graphs and other discrete input spaces
Risi Kondor and John Lafferty) (Winner of "Test of Time" award) — ICML 2002

Book chapters

Non-commutative harmonic analysis in multi-object tracking (R. Kondor) in "Inference and Estimation in Probabilistic Time-series models" ed. David Barber, A. Taylan Cemgil, Silvia Chiappa, Cambridge University Press, 2011 (in press).

Diffusion kernels (R. Kondor and J.-P. Vert) in "Kernel Methods in Computational Biology" ed. B. Schölkopf, K. Tsuda and J.-P. Vert, The MIT Press, 2004.

Software

cnine. Lightweight C++/CUDA tensor library (2021–)

`https://github.com/risi-kondor/cnine`

Snob2. Symmetric group FFT library with Python interface (2021–)
`https://github.com/risi-kondor/Snob2`

GElib. C++/CUDA SO(3) equivariant neural network library (2021–)
`https://github.com/risi-kondor/GElib`

ptens permutation equivariant message passing library (2022–)
`https://github.com/risi-kondor/ptens`

Mondrian. Parallel blocked matrix library (2016)
`http://people.cs.uchicago.edu/~risi/Mondrian/index.html`

pMMF. A high peformance parallel MMF library in C++
(with N. Teneva and P. K. Mudrakarta, 2015)
`http://people.cs.uchicago.edu/~risi/MMF/index.html`

$\mathbb{S}_n$**–FFT.** A Julia toolkit for for harmonic analysis on the symmetric group
(with G. Plumb, D. Pachauri and V. Singh, 2016)
`https://github.com/GDPlumb/SnFFT.jl`

$\mathbb{S}_n$**ob.** C++ symmetric group FFT library (2006 –)
`http://people.cs.uchicago.edu/~risi/SnOB/index.html`

Patents

A Fully Fourier Space Spherical Convolutional Neural Network based on Clebsch-Gordan Transforms
Risi Kondor, Shubhendu Trivedi and Zhen Lin — US patent application PCT/US2019/38236

Covariant neural network architecture for determining atomic potentials
R. Kondor — US patent application 16/975962

Method and system for estimating properties of atoms and molecules
G. Csányi, A P. Bartók, R. Kondor — US Patent 8,843,509 B2

International Patent Application PCT/GB2009/001414 filed 5/6/09 by Cambridge Enterprise Limited, publication WO2009/147408 A2 (G. Csányi, A P. Bartók, R. Kondor) on Gaussian Approximation Potential invention.