

# Imre Risi Kondor

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Legal Name	<b>Imre Miklós Kondor</b>
Name used in publications	<b>Risi Kondor</b>
Research interests	<b>Statistical machine learning and computational harmonic analysis:</b> <ol style="list-style-type: none"><li>1. Machine learning for science (molecular modeling, drug discovery, etc.)</li><li>2. Covariant deep learning architectures for learning graphs and other combinatorial objects</li><li>3. Multiresolution and multiscale matrix factorizations</li><li>4. Permutation problems and Fourier analysis on the symmetric group</li><li>5. High performance large scale machine learning systems</li></ol>
Employment	<p><b>Department of Computer Science, Department of Statistics, Computational and Applied Mathematics Initiative</b> <b>The University of Chicago</b> Associate professor Jul 2018 – Assistant professor Jul 2011 – Jun 2018</p> <p><b>Center for Computational Mathematics,</b> <b>Flatiron Institute, New York</b> Senior research scientist and group leader of the machine learning group (on leave from the University of Chicago) Jul 2019 – Sep 2021</p> <p><b>Center for the Mathematics of Information,</b> <b>California Institute of Technology</b> Postdoctoral fellow Sep 2009 – Jun 2011</p> <p><b>Gatsby Computational Neuroscience Unit,</b> <b>University College London</b> Senior post-doctoral research associate Sep 2007 – Aug 2009</p>
Education	<p><b>Columbia University</b> 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.</p> <p><b>Carnegie Mellon University</b> 2000 – 2002 M.Sc. in knowledge discovery and data mining (machine learning). Advisor: John Lafferty.</p> <p><b>Von Karman Institute for Fluid Dynamics</b> (Brussels, Belgium) 1999 – 2000 Diploma in computational fluid dynamics. Advisor: Herman Deconinck.</p> <p><b>Eötvös University</b> (Budapest, Hungary) 1997 – 1999 Diploma in physics, specializing in particle physics, statistical physics and environmental fluid dynamics (without final exam). Advisor: Tamás Tél.</p> <p><b>University of Cambridge</b> 1992 – 1995 B.A. in mathematics</p>
Industry experience	<b>Amazon Web Services</b> July – Dec 2017 Palo Alto, CA (Alex Smola’s Deep Learning Group)

Awards	<b>DARPA Young Faculty Award</b> for “Multiresolution Machine Learning for Molecular Modeling” 2016	
	<b>Notable student paper award</b> at AISTATS 2016 for <b>Multiresolution Matrix Compression</b> (N. Teneva, P.K. Mudrakarta and R. Kondor)	2016
	<b>Test of time award</b> at ICML 2012 (most influential paper from 10 years ago) for <b>Diffusion Kernels on Graphs and Other Discrete Input Spaces</b> (R. Kondor and J. Lafferty)	2012
	<b>Best student paper award</b> at ICML 2003 for <b>A kernel between sets of vectors</b> (R. Kondor and T. Jebara).	2003
Postdoctoral researchers advised	<b>Erik Thiede</b> (Ph.D. Chemistry, University of Chicago) Flatiron Insititute	Jul 2019 – Jun 2021
	<b>Brandon Anderson</b> (Ph.D. Physics, University of Maryland) Currently Senior Machine Learning Engineer at Atomwise	Nov 2017 – Sep 2019
Ph.D students graduated	<b>Jonathan Eskreis–Winkler</b> (UChicago Stat) Thesis: Multiresolution analysis on discrete spaces Currently at Etsy	Oct 2015 – Dec 2019
	<b>Pramod K Mudrakarta</b> (UChicago CS) Thesis: <b>Challenges in modern machine learning: multiresolution structure, model understanding and transfer learning</b> Currently at Google Research	Oct 2014 – Aug 2019
	<b>Nedelina Teneva</b> (UChicago CS) Thesis: <b>Multiresolution Matrix Factorization</b> Currently at Amazon	Jan 2013 – Jul 2017
	<b>Maia Fraser</b> (UChicago CS) Thesis: Group Actions in Topological Data Analysis and Hierarchical Learning (Maia started her Ph.D. with Partha Niyogi) Currently assistant professor at the University of Ottawa	Apr 2012 – Jul 2013
Ph.D students currently advised	<b>Horace Pan</b> (UChicago CS) Specializing in multiscale graph kernels	Oct 2015 –
	<b>Truong Son Hy</b> (UChicago CS) Specializing in graph kernels for applications in Chemistry and Physics	Oct 2016 –
PhD students co-advised	<b>Samira Sheikhi</b> (UChicago CS) Research advisor: Nathan Srebro (TTI-C)	Oct 2014 – June 2017
	<b>Stephen Basart</b> (UChicago CS) Research advior: Greg Shakhnarovich	Oct 2015 –
	<b>Zewei Chu</b> (UChicago CS) Research advisor: Kevin Gimpel (TTI-C)	Nov 2016 –
Ph.D students co-mentored	<b>Shubhendu Trivedi</b> (TTI-C) Advisor: Greg Shakhnarovich	Jan 2016 – Aug 2018
	<b>Deepti Pachauri</b> (UW Madison) advisor: Vikas Singh Thesis defended Apr 2015: Group theoretic algorithms for matching problems with applications to computer vision	Jan 2012 – Apr 2015
	<b>Walter Dempsey</b> (UChicago Stat) advisor: Peter McCullagh Thesis defended May 2015: Statistical Methods in joint modeling of longitudinal and survival data	Jan 2012 – Mar 2013
	<b>Vikas Garg</b> (formerly at TTI-C, MIT) Advisor: Tommi Jaakkola	Jan 2013 – Jun 2014

M.S. students advised	<b>Yifeng Shi</b> (UChicago Stat)	April 2017–
	<b>Nick Chase</b> (UChicago Stat) Thesis: An Application of RNNs and LSTM to Financial Markets	Sep 2016 – Feb 2017
	<b>Chang Cheng</b> (UChicago Stat) Thesis: Graph partitioning for large real world dataset	Oct 2015 – May 2016
	<b>Cheng Gao</b> (UChicago Stat) Thesis: Generalized semi-supervised learning on undirected graphs with multiscale spectral graph wavelet transformation	Oct 2012 – Mar 2013
Undergraduate students mentored	<b>Nancy Cheng</b> (UChicago Mathematics and Statistics)	Jun 2018 – Jun 2019
	<b>Matthew Joseph</b> (UChicago Mathematics) Currently at Google	2014
	<b>Dan Mané</b> (UChicago CS) Currently at Google	summer 2012
Ph.D. committees	<b>Taco Cohen</b> (University of Amsterdam)	Nov 2020 –
	<b>Tri Huyn</b> (UChicago CS) advisor: Michael Maire	Feb 2020 –
	<b>Hanxin Zhang</b> (UChicago GGSB) advisor: Andrey Rzhetsky	Feb 2017 –
	<b>Liwen Zhang</b> (UChicago CS) advisor: Lek-Heng Lim	Oct 2017 –
	<b>Yunlong Jiao</b> (Mines ParisTech) advisor: Jean-Philipp Vert	June 2017 – August 2017
	<b>Gustav Larsson</b> (UChicago CS) advisor: Yali Amit and Greg Shakhnarovich	Oct 2016 – June 2017
	<b>Qinqing Zheng</b> (UChicago CS) advisor: John Lafferty	Feb 2015 – July 2017
	<b>Eric Sibony</b> (Telecom ParisTech) advisor: Stephan Cléménçon	Dec 2015 – Jun 2016
	<b>Marc Goessling</b> (Stat) advisor: Yali Amit	Feb 2014 – Jul 2016
	<b>Lian Huan Ng</b> (Stat) advisor: Yali Amit	Feb 2012 – Jul 2015
<b>Deepti Pachauri</b> (UW Madison) advisor: Vikas Singh	Jun 2013 – Apr 2015	
<b>Ankan Saha</b> (UChicago CS) advisor: John Lafferty	Jan 2012 – Jul 2013	
M.S. committees	<b>Stephen Fitz</b> (UChicago CS)	Mar 2017
	<b>Samira Sheikhi</b> (UChicago CS)	Nov 2016
	<b>Kai Li</b> (UChicago CS)	April 2016
	<b>Jialei Wang</b> (UChicago CS)	May 2015
	<b>Jiajun Shen</b> (UChicago CS)	Apr 2015
	<b>Liwen Zhang</b> (UChicago CS)	Mar 2015
	<b>Alex Kolchinski</b> (UChicago CS)	Jun 2014
Courses taught	<b>STAT 37796 Topics in Machine Learning: Symmetries and harmonic analysis</b> Autumn 2021	
	<b>STAT 37790 Topics in Machine Learning: High performance machine learning system design</b> Spring 2019	
	<b>CMSC 35246 Deep Learning (graduate level) with Shubhendu Trivedi</b> Spring 2017	
	<b>STAT 37710/CMSC 35400 Machine Learning (graduate level)</b> Autumn 2012, Spring 2014, Spring 2015, Spring 2016, Spring 2017, Spring 2018, Spring 2019	
	<b>CMSC 25400/STAT 27725 Machine Learning (undergraduate level)</b> Winter 2014, Winter 2015, Autumn 2015, Winter 2017, Autumn 2018, Winter 2019	
	<b>CMSC 35900 Topics in Artificial Intelligence</b> Spring 2012, Spring 2014, Winter 2015, Spring 2018	
	<b>STAT 37730 Topics in Computational Harmonic Analysis and Representation Theory</b> Spring 2012.	
	<b>CMSC 25010 Introduction to Artificial Intelligence</b> Winter 2012, Spring 2013.	
<b>CMSC 15300 Foundations of Software</b>		

Autumn 2011.

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

Departmental Service	<b>CS graduate committee</b>	Nov 2018 –
	<b>CS hiring committee</b>	Oct 2017 – Jun 2018
	<b>CCAM (Computational and Applied Math) admissions committee</b>	Jan 2017 –
Summer schools organized	<b>IMA Summer Graduate Program on Modern Applications of Representation Theory</b> (with Jason Morton and Lek-Heng Lim)	Jul 20 – Aug 6, 2014
	<b>AMS Mathematical Research Community on Algebraic and Geometric Methods in Applied Discrete Mathematics</b> (senior assistant in Michael Orrison’s group on Representation Theory in Data Analysis)	Jun 15 – 21, 2104
Workshops organized	<b>Flatiron-wide algorithms and mathematics</b> Internal workshop at the Flatiron Insitute	Oct 2020
	<b>Minding the gap: between fairness and ethics</b> (NeurIPS 2019) Co-organized with Igor Rubinov, Jack Poulson, Manfred K. Warmuth, Emanuel Moss and Alexa Hagerty	Dec 2019
	<b>Workshop on Multiresolution Methods for Large Scale Learning</b> (NIPS 2015) Co-organized with Inderjit Dhillon, Rob Nowak, Michael O’Neil and Nedelina Teneva	Dec 2015
	<b>Workshop on Learning with Orderings</b> (NIPS 2009) with Tiberio Caetano, Carlos Guestrin, Jonathan Huang, Guy Lebanon, Marina Meila	Dec 2009
	<b>Symposium and workshop on Algebraic methods in machine learning at NIPS 2008</b> (with Guy Lebanon and Jason Morton)	Dec 2008
Tutorials taught	<b>Equivariant neural networks</b> (NeurIPS 2020) with Taco Cohen	Dec 2020
	<b>Fourier space neural networks</b> (IPAM)	Nov 2019
	<b>Representation theory, Fourier analysis and invariants</b> (IPAM) Part of the “Understanding many-particle systems with machine learning” program	Sep 2016
	<b>Machine learning for engineers</b> Mini-course in Michelle Khine’s lab at the Dept. of Biomedical Engineering, UC Irvine	Aug 2013
	<b>Representation theoretical methods in machine learning</b> Eight lecture mini-course at the Gatsby Unit	Oct 2008
	<b>Group theory and machine learning</b> Machine learning tutorial at the University of Cambridge	Oct 2007
	<b>Group theoretical methods in machine learning</b> Tutorial at the International Conference of Machine Learning, Corvallis, OR	Jun 2007
	<b>Non-commutative harmonic analysis</b> Tutorial at the Complex Systems Summer School, Santa Fe	Jun 2007
Participant in Research Programs	<b>Geometry and learning from data in 3D and beyond</b> Semester long program at IPAM	Mar – Jun 2019
	<b>NSF innovation lab: Learning the power of data in chemistry</b>	Dec 17–21, 2018
	<b>Understanding many-particle systems with machine learning</b> Semester long program at IPAM	Sep – Dec 2016
	<b>NSF ideas lab: Interdisciplinary approaches to biomedical data science</b>	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) (yearly)

### Grants

DARPA HR00111890038 Disruption 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, Ridgeway 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.

#### [Multiresolution Graph Variational Autoencoder](#)

(Truong Son Hy\* and Risi Kondor)

arXiv 2021

#### [The general theory of permutation equivariant neural networks and higher order graph variational encoders](#)

Erik H. Thiede\*, Truong Son Hy\* and Risi Kondor

arXiv 2020

#### [Asymmetric multiresolution matrix factorization](#)

Pramod K. Mudrakarta\*, Shubhendu Trivedi\* and R. Kondor

arXiv 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\*

arXiv 2015

#### [The skew spectrum of functions on finite groups and their homogeneous spaces](#)

Risi Kondor

arXiv 2007

#### [A novel set of rotationally and translationally invariant features for images based on the non-commutative bispectrum](#)

Risi Kondor

arXiv 2007

#### [Multi-facet learning in Hilbert spaces](#)

(R. Kondor, G. Csanyi, S. E. Ahnert and T. Jebara)

Columbia University, CUCS-054-05. 2005

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

**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)

**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 synchroniziation** (D. Pachauri\*, R. Kondor and V. Singh) NIPS 2013
- On representing chemical environments** (A. P. Bartók, R. Kondor and G. Csányi) Physical Review B 87, 2013
- Multiresolution analysis on the symmetric group** (R. Kondor and W. 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** (R. Kondor and M. Barbosa\*) COLT 2010
- Graph kernels** (S. V. N. Vishwanathan, K. M. Borgardt, R. Kondor, N. Schraudolf) Journal of Machine Learning Research **11**, 2010
- Gaussian approximation potentials: the accuracy of quantum mechanics, without the electrons** (A. P. Bartók, M. C. Payne, R. Kondor, G. Csányi) Physical Review Letters **104**, 2010
- A Fourier space algorithm for solving quadratic assignment problems** (R. Kondor) SODA 2010
- The graphlet spectrum** (R. Kondor, N. Shervashidze and K. M. Borgwardt) ICML 2009
- The skew spectrum of graphs** (R. Kondor and K. M. Borgwardt) ICML 2008
- Multi-object tracking with representations of the symmetric group** (R. Kondor, A. Howard and T. Jebara) AISTATS 2007
- Gaussian and Wishart hyperkernels** (R. Kondor and T. Jebara) NIPS 2006
- Probability product kernels** (T. Jebara, R. Kondor and A. Howard) of Machine Learning Research **5**:819-844, 2004
- Kernels and regularization on graphs** (A. Smola and R. Kondor) COLT 2003
- Bhattacharyya and expected likelihood kernels** (T. Jebara and R. 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** (R. Kondor and J. 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.

#### 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.

## 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 library for  $SO(3)$  operations (2021–)

<https://github.com/risi-kondor/GELib>

**Mondrian.** Parallel blocked matrix library (2016)

<http://people.cs.uchicago.edu/~risi/Mondrian/index.html>

**pMMF.** A high performance parallel MMF library in C++

(with N. Teneva and P. K. Mudrakarta, 2015) <http://people.cs.uchicago.edu/~risi/MMF/index.html>

**$S_n$ -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>

**$S_n$ ob.** A C++ library for computing fast Fourier transforms on the symmetric group (2006–)

<http://people.cs.uchicago.edu/~risi/SnOB/index.html>