

GRAPH REPRESENTATION LEARNING AND BEYOND (GRL+)

ICML 2020 Workshop

ORGANISERS



Petar Veličković
DeepMind



Michael Bronstein
Twitter / Imperial
/ USI Lugano



Andreea Deac
Mila / UdeM



Will Hamilton
Mila / McGill



Jess Hamrick
DeepMind



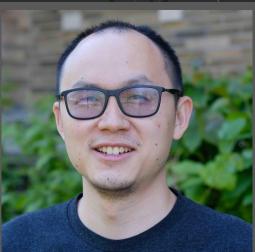
Milad Hashemi
Google



Stefanie Jegelka
MIT



Jure Leskovec
Stanford / Pinterest



Renjie Liao
University of Toronto



Federico Monti
Twitter / USI Lugano



Yizhou Sun
UCLA



Kevin Swersky
Google Brain

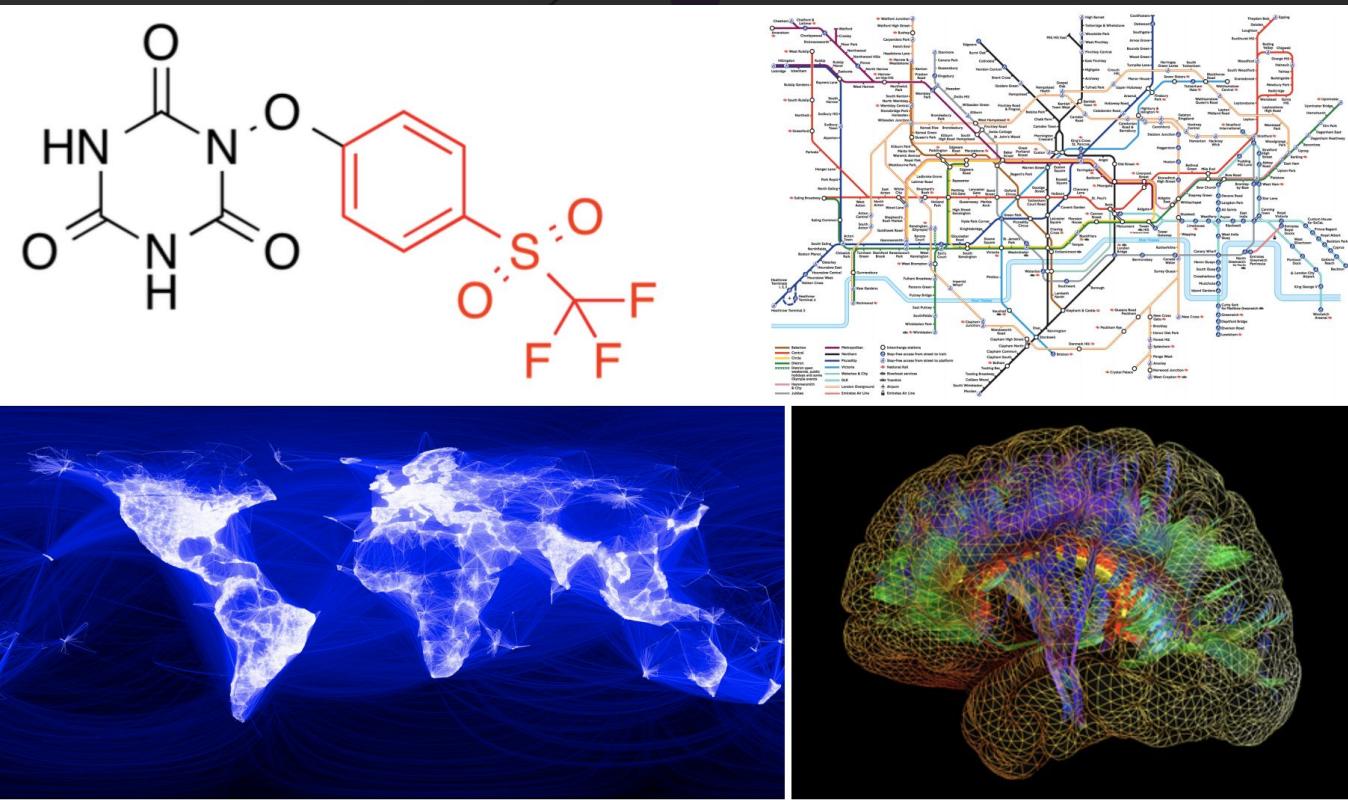


Rex Ying
Stanford

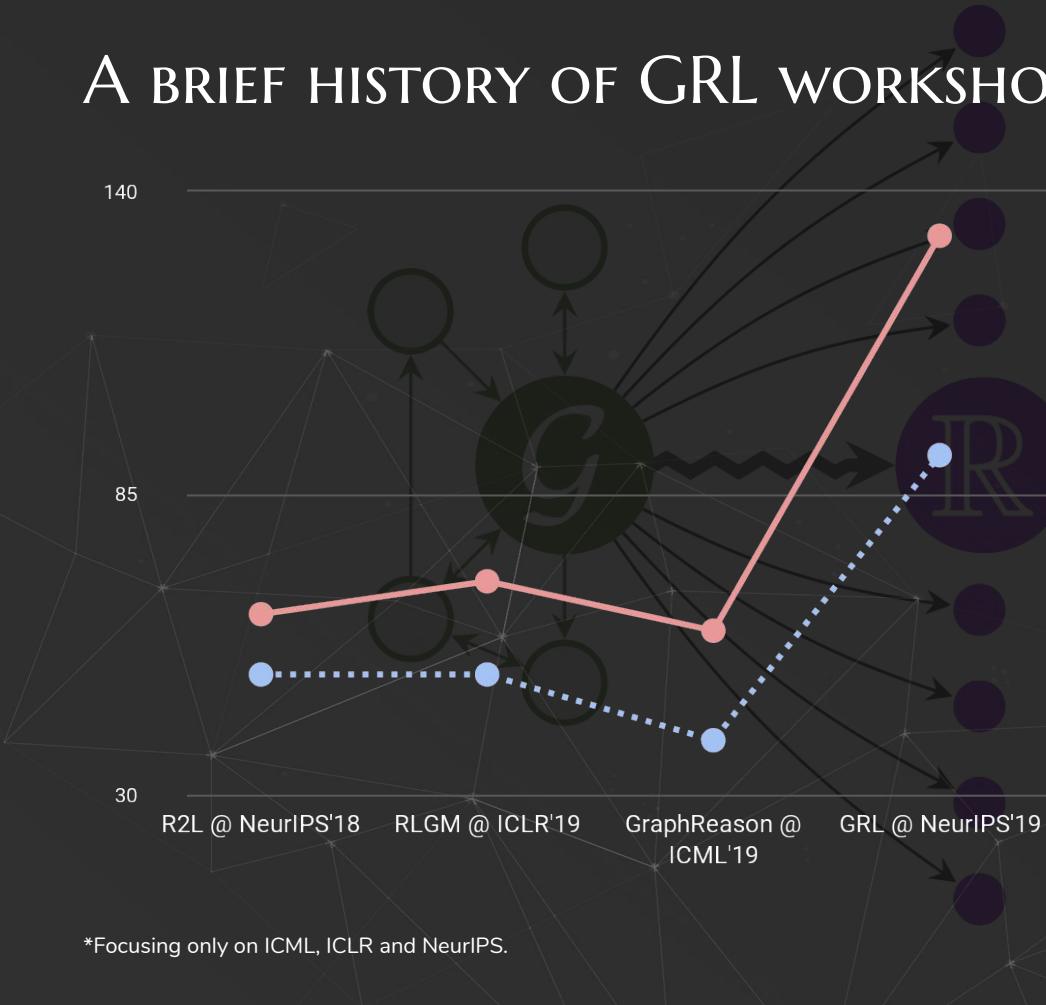


Marinka Žitnik
Harvard

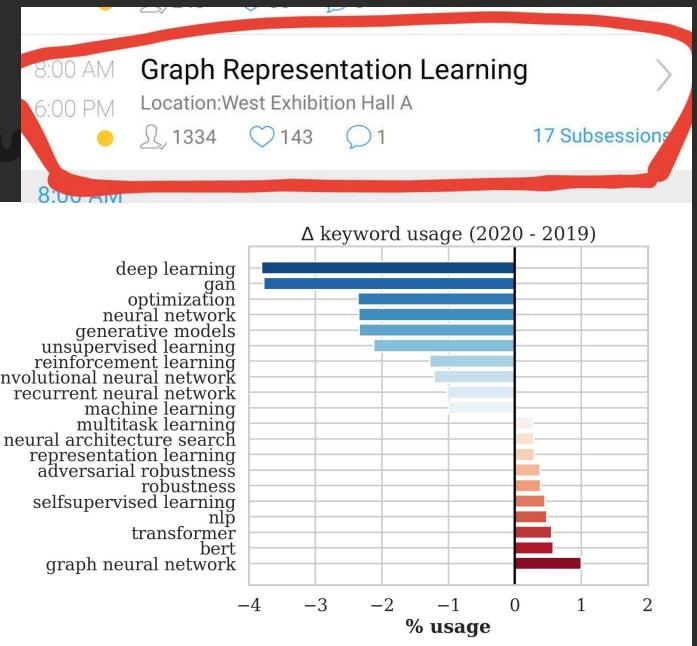
GRAPHS ARE EVERYWHERE!



A BRIEF HISTORY OF GRL WORKSHOPS*



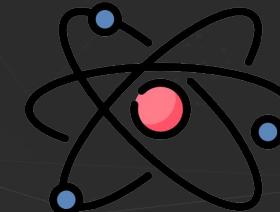
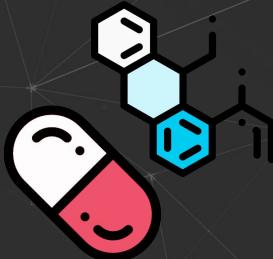
- Submissions
- Accepted



*Focusing only on ICML, ICLR and NeurIPS.

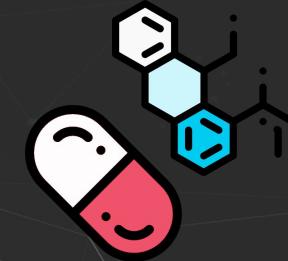
GRL BROKE INTO THE REAL WORLD!

- GNNs discover **novel antibiotics** (Stokes et al., Cell'20)
- GNNs power **web-scale recommender systems** (Ying et al., KDD'18; Pal et al., KDD'20)
- GNNs assist **particle physicists** (Martinez et al., Eur. Phys. J. Plus'19)



EMERGING APPLICATIONS OF GRL

- GNNs enhance **fake news detection** (Monti et al., 2019)
- GNNs applied for **autonomous vehicle perception** (Gao et al., CVPR'20)
- GNNs offer **repurposing candidates for COVID-19** (Gysi et al., 2020)



GRL+ ACCEPTANCE STATS

- **95** papers submitted
 - Out of which **41** tagged as a **Novel Application**
 - Out of which **9** tagged as a **COVID-19 Application**
- **73** papers accepted (Acceptance rate: ~**77%**)
 - One of the **largest** ICML 2020 workshops!
- **9** papers selected for contributed talks
 - Three each in **Original Research**, **Novel Applications**, and **COVID-19 Applications**
 - **Best paper awards** announced during **Closing Remarks!**

PROGRAM COMMITTEE (~110 REVIEWERS!)



Aaron Zweig, New York University, Agnieszka Słowiak, University of Cambridge, Aleksandar Bojchevski, TU Munich, Aleksandar Stanić, IDSIA, Alvaro Sanchez-Gonzalez, DeepMind, Andreea Deac, Mila, Andrei Nicolicioiu, Bitdefender, Andrew Wang, Stanford University, Arantxa Casanova, Mila, Arian Jamasb, University of Cambridge, Bahare Fatemi, University of British Columbia, Beliz Gunel, Stanford University, Ben Day, University of Cambridge, Benoît Corsini, Element AI, Boris Knyazev, University of Guelph, Bowen Liu, Stanford University, Bruno Ribeiro, Purdue University, Bryan Perozzi, Google Research, Cătălina Cangea, University of Cambridge, Chaitanya Joshi, Nanyang Technological University, Charles Blundell, DeepMind, Charlie Nash, DeepMind, Chi Thang Duong, EPFL, Christopher Morris, Polytechnique Montréal, Cinjon Resnick, New York University, Cristian Bodnar, University of Cambridge, Daniel Daza, Vrije Universiteit Amsterdam, Daniele Grattarola, Università della Svizzera Italiana, Davide Bacci, University of Pisa, Davide Belli, University of Amsterdam, Dominique Beaini, InVivo AI, Dongkwan Kim, KAIST, Duo Wang, University of Cambridge, Dylan Bourgeois, EPFL, Edward Smith, McGill University, Emanuele Rossi, Twitter, Emma Rocheteau, University of Cambridge, Fabrizio Frasca, Twitter, Felix Opolka, University of Cambridge, Gabriele Corso, University of Cambridge, Guangtao Wang, JD.com, Guillem Cucurull, Blue Prism, Guy Wolf, Université de Montréal, Haggai Maron, NVIDIA Research, Hanjun Dai, Georgia Institute of Technology, Helena Andrés-Terre, University of Cambridge, Ines Chami, Stanford University, Iulia Duță, Bitdefender, Jakub Tomczak, Vrije Universiteit Amsterdam, Jan Svoboda, NNAISENSE, Jessica Hamrick, DeepMind, Jiaxuan You, Stanford University, Jiezhong Qiu, Tsinghua University, Jin Dong, McGill University, Jingling Li, University of Maryland, Joey Bose, McGill University, Johannes Klicpera, TU Munich, Jordan Hoffmann, Harvard University, Jun Gao, University of Toronto, NVIDIA, Kevin Swersky, Google Brain, Komal Teru, McGill University, Koustuv Sinha, McGill University, Louis Tiao, University of Sydney, Louis-Pascal Xhonneux, Mila/Université de Montréal, Lu Liu, University of Technology Sydney, Luca Cavalleri, University of Cambridge, Lukas Galke, Kiel University / ZBW, Marc Brockschmidt, Microsoft Research Cambridge, Mariana Vargas Vieyra, INRIA Lille Nord Europe, Marinka Žitnik, Harvard University, Matthias Fey, TU Dortmund, Michal Valko, DeepMind, Milad Hashemi, Google, Min Jae Song, New York University, Momchil Peychev, ETH Zürich, Nick Choma, New York University, Niklas Stoehr, ETH Zürich, Otilia Stretcu, Carnegie Mellon University, Patrick Fernandes, Unbabel, Pau Riba, Computer Vision Center, Paul Scherer, University of Cambridge, Rafael Gómez-Bombarelli, Massachusetts Institute of Technology, Razvan Pascanu, DeepMind, Rex Ying, Stanford University, Ron Levie, TU Berlin, Ryoma Sato, Kyoto University, Sergey Ivanov, Criteo, Sergio Casas Romero, Uber ATG / University of Toronto, Shagun Sodhani, Facebook AI, Shengchao Liu, Mila, Sitao Luan, Mila, Sofia Ira Ktena, Twitter, Sri Charan Ragireddy, IIT Kharagpur, Thomas Kipf, Google Brain, Tiago Azevedo, University of Cambridge, Ting Chen, Google Brain, Vijay Prakash Dwivedi, Nanyang Technological University, Vikas Verma, Aalto University, Vikash Singh, Heal, Weihua Hu, Stanford University, Wengong Jin, Massachusetts Institute of Technology, Wenyuan Zeng, Uber ATG / University of Toronto, Will Hamilton, McGill University, Xiang Ren, University of Southern California, Xiaohui Zeng, University of Toronto, Xiaowen Dong, University of Oxford, Yizhou Sun, University of California, Los Angeles, Yujia Li, DeepMind, Yujun Yan, University of Michigan, Yunsheng Bai, University of California, Los Angeles, Yuwen Xiong, Uber ATG / University of Toronto, Zichao Yan, McGill University

OUTSTANDING REVIEWERS



Guy Wolf
Université de Montréal



Iulia Dută
Bitdefender



Niklas Stoehr
ETH Zürich

EMERGING TRENDS

KEYNOTE SPEAKERS



Benchmarking Graph Neural Networks

Xavier Bresson
Nanyang Technological University

KEYNOTE SPEAKERS



Relational Structure
Discovery

R

L

Thomas Kipf
Google Brain

KEYNOTE SPEAKERS



Insights from Physics on
Graphs and Relational
Inductive Bias



Kyle Cranmer
New York University

KEYNOTE SPEAKERS



GCNs:
From Summarization to
Heterophily

Danai Koutra
University of Michigan, Ann Arbor

KEYNOTE SPEAKERS



**Geometric and Topological
Graph Analysis for Machine
Learning Applications**



Tina Eliassi-Rad
Northeastern University

KEYNOTE SPEAKERS



Graph Neural Networks for Self-Driving

R



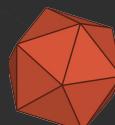
Raquel Urtasun

University of Toronto / Uber ATG

UPDATE TALKS



Matthias Fey
TU Dortmund University



**PyTorch
geometric**



Zheng Zhang
NYU Shanghai / AWS



Jure Leskovec
Stanford / Pinterest

DGL

OGB

GRL+ SCHEDULE (VIENNA TIME)

8:40--9:00AM: **Opening Remarks**

9:00--10:00AM: **Invited Talks** (Xavier Bresson, Thomas Kipf)

10:00--10:30AM: **Q&A / Discussion / Coffee 1**

10:30--11:30AM: **Virtual Poster Session #1**

11:30AM--12:00PM: **Contributed Talks (Novel Applications)**

12:00--12:30PM: **Updates** (PyTorch Geometric, Deep Graph Library, Open Graph Benchmark)

12:30--1:30PM: **Lunch Break**

1:30--2:15PM: **Contributed Talks (Original Research)**

2:15--3:15PM: **Invited Talks** (Kyle Cranmer, Danai Koutra)

3:15--3:45PM: **Q&A / Discussion / Coffee 2**

3:45--4:15PM: **Contributed Talks (COVID-19 Applications)**

4:15--5:15PM: **Invited Talks** (Tina Eliassi-Rad, Raquel Urtasun)

5:15--5:45PM: **Q&A / Discussion / Coffee 3**

5:45--6:45PM: **Virtual Poster Session #2**

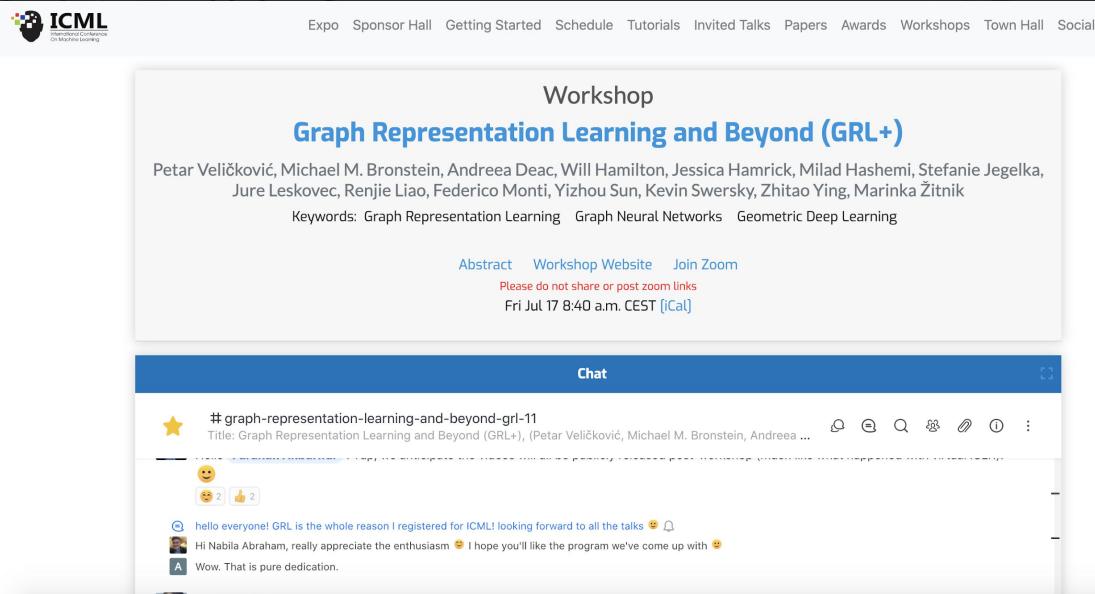
6:45--7:00PM: **Closing Remarks**

<https://grlplus.github.io/schedule/>

INTERACTING WITH THE WORKSHOP: VIRTUAL WEBSITE

Virtual workshop website at:

<https://icml.cc/virtual/2020/workshop/5715>



The screenshot shows the ICML virtual workshop website for the "Graph Representation Learning and Beyond (GRL+)" workshop. The top navigation bar includes links for Expo, Sponsor Hall, Getting Started, Schedule, Tutorials, Invited Talks, Papers, Awards, Workshops, Town Hall, and Socials. The main content area features the workshop title "Workshop Graph Representation Learning and Beyond (GRL+)" and the names of the organizers: Petar Veličković, Michael M. Bronstein, Andreea Deac, Will Hamilton, Jessica Hamrick, Milad Hashemi, Stefanie Jegelka, Jure Leskovec, Renjie Liao, Federico Monti, Yizhou Sun, Kevin Swersky, Zhitao Ying, Marinka Žitnik. Below the title are keywords: Graph Representation Learning, Graph Neural Networks, Geometric Deep Learning. A "Chat" section at the bottom shows a message from a user named Nabila Abraham expressing enthusiasm about the program.

Expo Sponsor Hall Getting Started Schedule Tutorials Invited Talks Papers Awards Workshops Town Hall Socials

Workshop
Graph Representation Learning and Beyond (GRL+)

Petar Veličković, Michael M. Bronstein, Andreea Deac, Will Hamilton, Jessica Hamrick, Milad Hashemi, Stefanie Jegelka, Jure Leskovec, Renjie Liao, Federico Monti, Yizhou Sun, Kevin Swersky, Zhitao Ying, Marinka Žitnik

Keywords: Graph Representation Learning Graph Neural Networks Geometric Deep Learning

Abstract Workshop Website Join Zoom
Please do not share or post zoom links
Fri Jul 17 8:40 a.m. CEST [iCal]

Chat

#graph-representation-learning-and-beyond-grl-11
Title: Graph Representation Learning and Beyond (GRL+), (Petar Veličković, Michael M. Bronstein, Andreea ...

Hi Nabila Abraham, really appreciate the enthusiasm 😊 I hope you'll like the program we've come up with 😊

Wow. That is pure dedication.

INTERACTING WITH THE WORKSHOP: ROCKETCHAT

We will use **RocketChat** throughout the workshop for async communication

The screenshot shows a screenshot of the RocketChat interface. At the top, there's a blue header bar with the word "Chat". Below it is a list of messages in a white background area. The first message is a pinned post by a user with a yellow star icon, titled "# graph-representation-learning-and-beyond-grl-11" and "Title: Graph Representation Learning and Beyond (GRL+), (Petar Veličković, Michael M. Bronstein, Andreea ...)". This message has several reaction icons (handshake, question mark, magnifying glass, etc.) and a three-dot menu. Below this is a message from Cuong Nguyen (@cuong-nguyen23538) at 6:58 PM, saying "Hi Everyone! Very excited to participate in this workshop 😊". This message has a reply count of 5. Next is a message from Nabila Abraham (@nabila-abraham) at 8:35 PM, saying "hello everyone! GRL is the whole reason I registered for ICML! looking forward to all the talks 😊". This message has 2 replies and 1 like. A timestamp indicates the screenshot was taken on July 16, 2020 at 9:57 PM. At the bottom, there's a message input field with a smiley face icon, the word "Message", and a plus sign button.

graph-representation-learning-and-beyond-grl-11
Title: Graph Representation Learning and Beyond (GRL+), (Petar Veličković, Michael M. Bronstein, Andreea ...)

Cuong Nguyen @cuong-nguyen23538 6:58 PM
Hi Everyone! Very excited to participate in this workshop 😊

Nabila Abraham @nabila-abraham 8:35 PM
hello everyone! GRL is the whole reason I registered for ICML! looking forward to all the talks 😊

2 replies July 16, 2020 9:57 PM

anyone else in Canada waking up for 3am?

Message +

INTERACTING WITH THE WORKSHOP: LIVESTREAM

Follow keynote, update and contributed talks live via the [livestream](#)

Abstract Workshop Website Join Zoom
Please do not share or post zoom links
Fri Jul 17 8:40 a.m. CEST [\[iCal\]](#)

S Livestream will start soon!

ICML
International Conference
On Machine Learning

**Graph Representation Learning
and Beyond (GRL+)**

INTERACTING WITH THE WORKSHOP: ZOOM

Opening / Closing Remarks, and Q&A / Discussions in the main **Zoom**

Workshop

Graph Representation Learning and Beyond (GRL+)

Petar Veličković, Michael M. Bronstein, Andreea Deac, Will Hamilton, Jessica Hamrick, Milad Hashemi, Stefanie Jegelka, Jure Leskovec, Renjie Liao, Federico Monti, Yizhou Sun, Kevin Swersky, Zhitao Ying, Marinka Žitnik

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[Abstract](#)

[Workshop Website](#)

[Join Zoom](#)

Please do not share or post zoom links

Fri Jul 17 8:40 a.m. CEST [\[iCal\]](#)

INTERACTING WITH THE WORKSHOP: SLIDO

For asking / upvoting questions for our keynote speakers, please use **slido**:



A screenshot of the Slido web interface. At the top, there's a purple circle containing a large white letter "R". To its right is a gear icon. Below this, a box contains the text "Ask the speaker". Underneath is a placeholder text area with "Placeholder question for Xavier". To the right of the text area is the number "129". At the bottom left is a user icon with the placeholder text "Your name (optional)". On the far right is a green button labeled "SEND".

129

SEND

INTERACTING WITH THE WORKSHOP: POSTERS

For each accepted paper:

- Camera-Ready version & Session ID: <https://grlplus.github.io/papers/>
- Poster Teaser / Link to join Zoom Room: Virtual Website

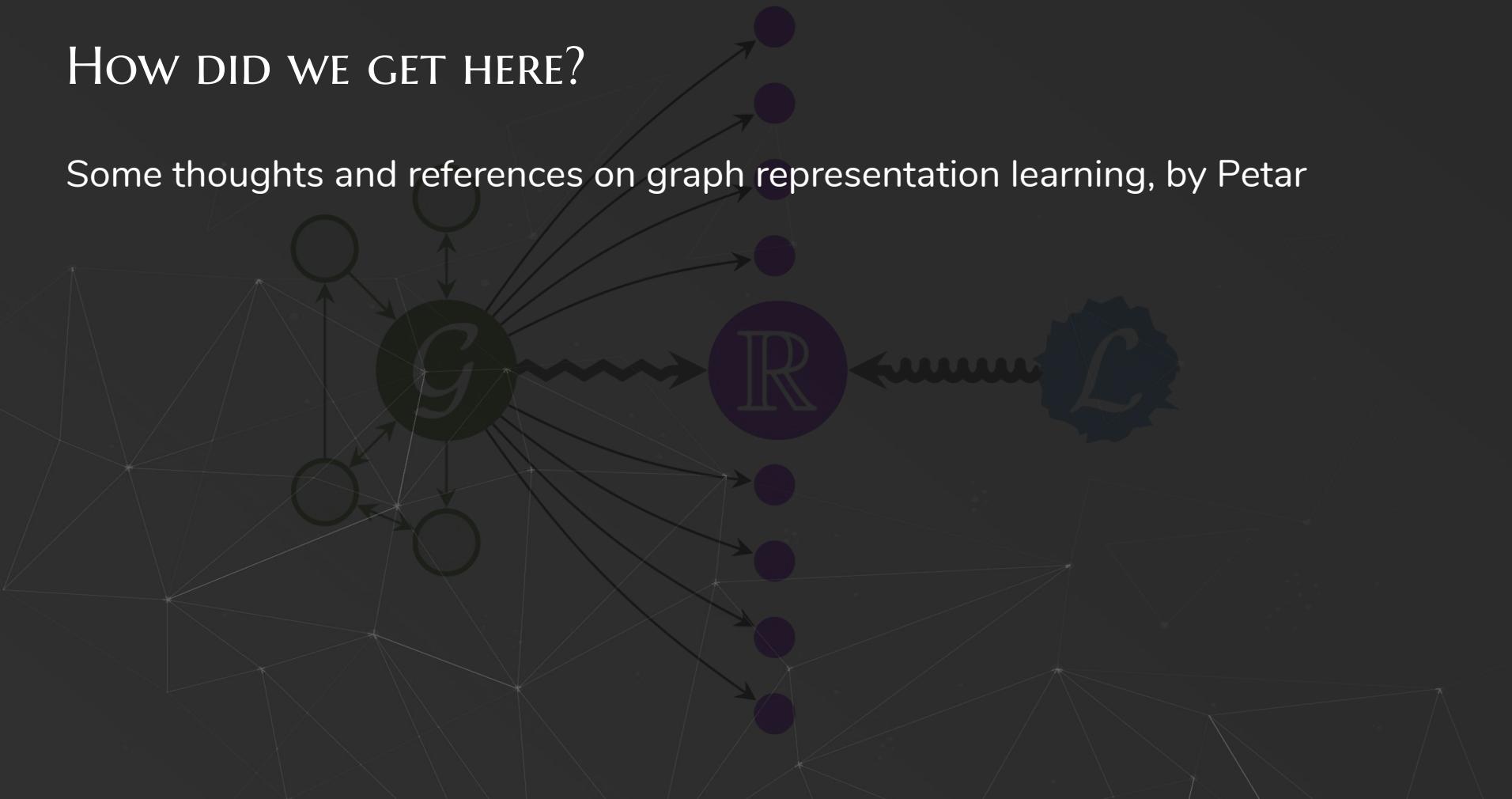
(#82 / Sess. 2) Scattering GCN: Overcoming Oversmoothness in Graph
Convolutional Networks (Poster Teaser) » *Frederik Wenkel*

Graph convolutional networks (GCNs) are widely used for semi-supervised node classification on graphs today. The graph structure is however only accounted for by considering the similarity of activations between adjacent nodes, in turn degrading the results. In this work, we augment GCN models by incorporating richer notions of regularity by leveraging cascades of band-pass filters, known as geometric scatterings. We introduce a new hybrid architecture for the task and demonstrate its potential on multiple graph datasets, where it outperforms leading GCN models.

[Teaser video](#) | [Zoom join link](#)

HOW DID WE GET HERE?

Some thoughts and references on graph representation learning, by Petar



HOW DID WE GET HERE?

Embedding techniques on graphs



Bordes et al., NeurIPS'13 Perozzi et al., KDD'14 Tang et al., WWW'15 Grover & Leskovec, KDD'16

HOW DID WE GET HERE?

Embedding techniques on graphs



Spectral generalisation of image convolutions

Graph Fourier Transform

Bruna et al., ICLR'14

Chebyshev Nets

Defferrard et al., NeurIPS'16

GCNs

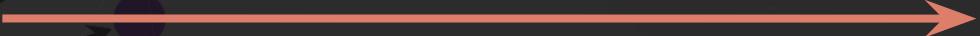
Kipf & Welling, ICLR'17

GWNNs

Xu et al., ICLR'19

HOW DID WE GET HERE?

Embedding techniques on graphs



Spectral generalisation of image convolutions



Message-passing in the spatial domain

GGNNs

Li et al., ICLR'16 Monti et al., CVPR'17

MoNet



Molecular Fingerprints

Duvenaud et al., NeurIPS'15

MPNNs

Gilmer et al., ICML'17

GATs

Veličković et al., ICLR'18

Graph Nets

Battaglia et al., 2018

Patchy-SAN

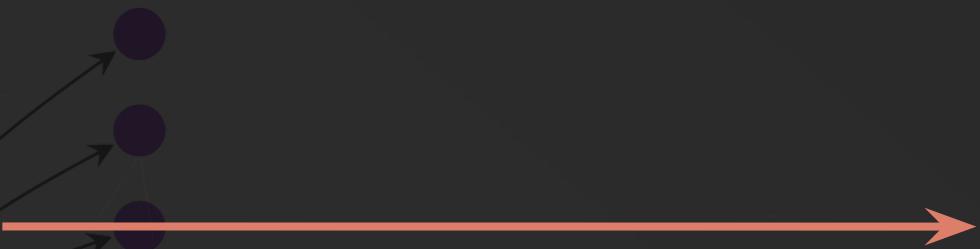
Niepert et al., ICML'16

GraphSAGE

Hamilton et al., NeurIPS'17

HOW DID WE GET HERE?

Embedding techniques on graphs



Spectral generalisation of image convolutions



Message-passing in the spatial domain



Probabilistic Graphical Model concepts



structure2vec

Dai et al., ICML'16

GMNNs

Qu et al., ICML'19

ExpressGNN

Zhang et al., ICLR'20

HOW DID WE GET HERE?

Embedding techniques on graphs



Spectral generalisation of image convolutions



Message-passing in the spatial domain



Probabilistic Graphical Model concepts



Graph Isomorphism algorithms



k-GNNs

Morris et al., AAAI'19

GINs

Xu et al., ICLR'19

RP-GIN

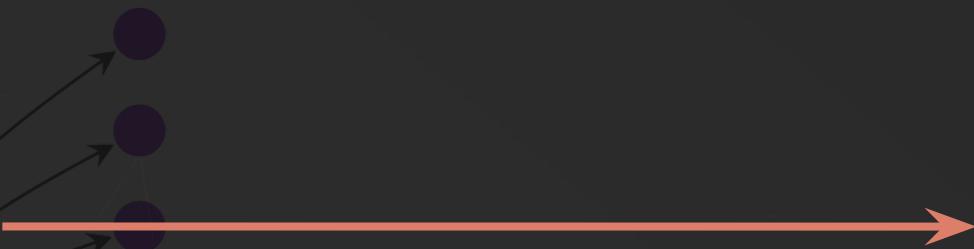
Murphy et al., ICML'19

Provably powerful GNNs

Maron et al., NeurIPS'19

HOW DID WE GET HERE?

Embedding techniques on graphs



Spectral generalisation of image convolutions

Message-passing in the spatial domain

Probabilistic Graphical Model concepts

Graph Isomorphism algorithms

Historical GRL papers



GNNs

Gori et al., IJCNN'05;
Scarselli et al., TNN'07

Recursive NNs

Sperduti & Starita, TNN'97; Frasconi et al., TNN'98

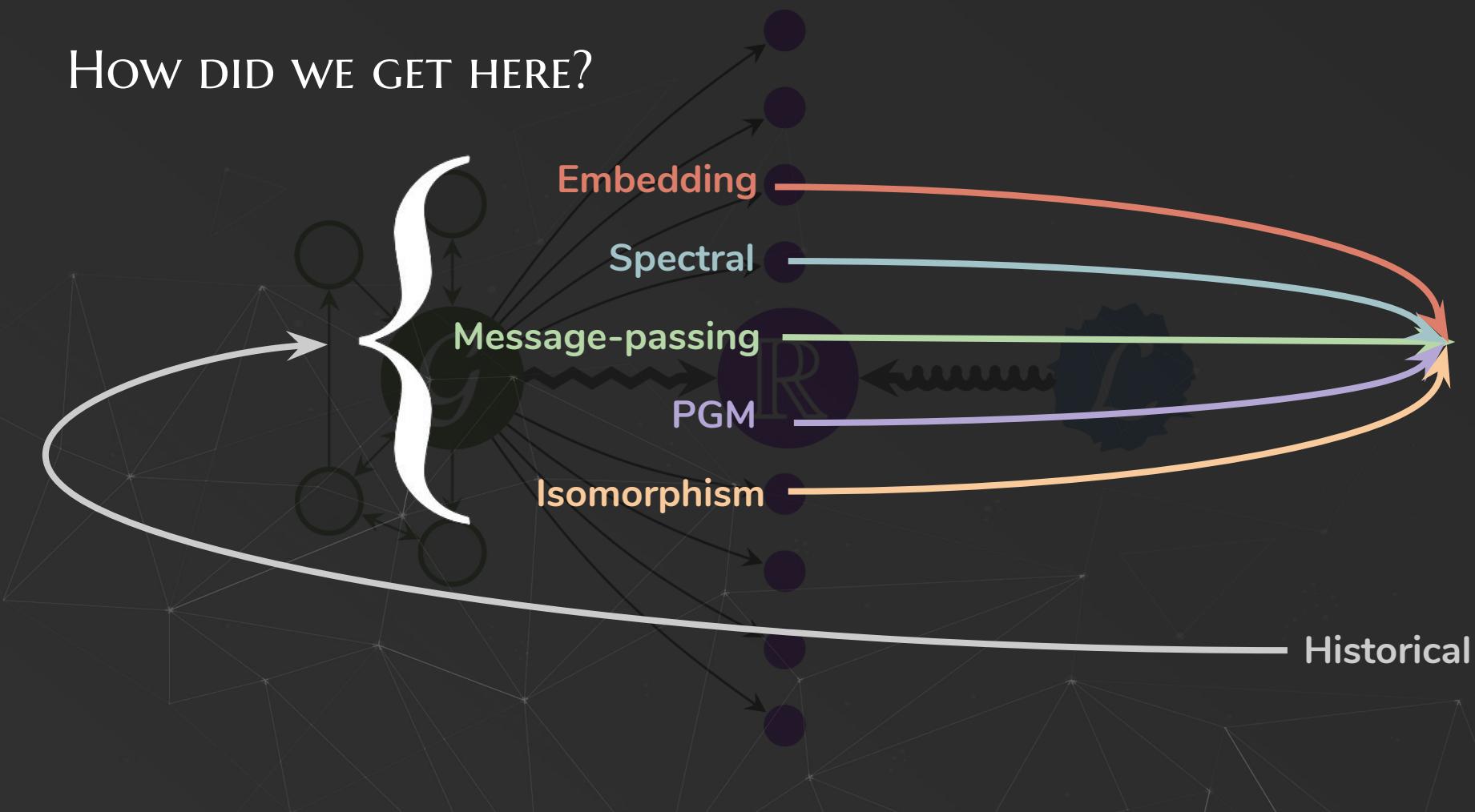
Backprop through structure

Goller & Küchler, ICNN'96

Labeling RAAM

Sperduti, NeurIPS'93

HOW DID WE GET HERE?





THANK YOU!

Enjoy the workshop!