The World of Graph Neural Networks: From the Mystery of Generalization to Foundational Limitations

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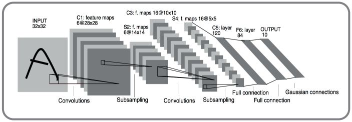
(Ludwig-Maximilians-Universität München and University of Tromsø)

Mathematics for Deep Learning Opening Workshop
University of Bath, April 21 – 22, 2022

The Dawn of Deep Learning in Public Life

Self-Driving Cars

Telecommunication/
Speech Recognition



Legal Issues

Health Care

Impact on Mathematical Problem Settings

Some Examples:

- Inverse Probleme/Imaging Science *(2012–)*
  - $\rightsquigarrow$ *Denoising*
  - $\rightsquigarrow$ *Edge Detection*
  - $\rightsquigarrow$ *Inpainting*
  - $\rightsquigarrow$ *Classification*
  - $\rightsquigarrow$ *Superresolution*
  - $\rightsquigarrow$ *Limited-Angle Computed Tomography*
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- Numerical Analysis of Partial Differential Equations *(2017–)*
  $\rightsquigarrow$ *Black-Scholes PDE*
  $\rightsquigarrow$ *Allen-Cahn PDE*
  $\rightsquigarrow$ *Parametric PDEs*
  $\rightsquigarrow$ ...

Problem with Trustworthiness

By *Linda Geddes* 5th December 2018

Computers can be made to see a sea turtle as a gun or hear a concerto as someone's voice, which is raising concerns about using artificial intelligence in the real world.

MACHINE MINDS | ARTIFICIAL INTELLIGENCE BBC

Role of Mathematics

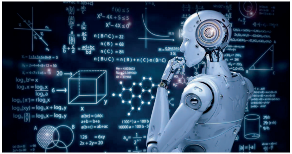
Two Key Challenges for Mathematics:

Mathematics for Deep Learning!

- Can we derive a deep mathematical understanding of deep learning?
- How can we make deep learning more robust?
- ...

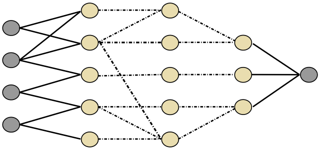
Deep Learning for Mathematics!

- How can we use deep learning to improve imaging science?
- Can we develop superior PDE solvers via deep learning?
- ...



Delving Deeper into Deep Neural Networks...

Definition of a Deep Neural Network



Definition:

Assume the following notions:

- $d \in \mathbb{N}$: Dimension of input layer.
- L: Number of layers.
- $\rho : \mathbb{R} \to \mathbb{R}$: (Non-linear) function called *activation function*.
- $T_\ell : \mathbb{R}^{N_{\ell-1}} \to \mathbb{R}^{N_\ell}$, $\ell = 1, \ldots, L$, where $T_\ell x = W^{(\ell)} x + b^{(\ell)}$

Then $\Phi : \mathbb{R}^d \to \mathbb{R}^{N_L}$ given by

$$\Phi(x) = T_L \rho(T_{L-1} \rho(\ldots \rho(T_1(x)))), \quad x \in \mathbb{R}^d,$$

is called *(deep) neural network (DNN)*.

Second Appearance of Neural Networks

Key Observations by Y. LeCun et al. (around 2000):

- Drastic improvement of computing power.
  $\rightsquigarrow$ *Networks with hundreds of layers can be trained.*
  $\rightsquigarrow$ *Deep Neural Networks!*
- Age of Data starts.
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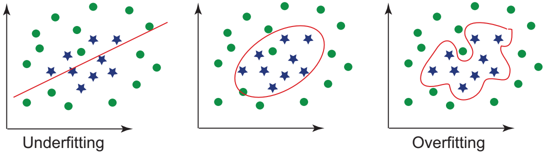
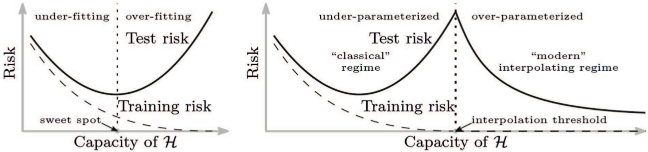
Surprising Phenomenon:





(Source: Belkin, Hsu, Ma, Mandal; 2019)

- **Expressivity:**
  - Which *aspects of a neural network architecture* affect the performance of deep learning?

$\rightsquigarrow$ *Applied Harmonic Analysis, Approximation Theory, ...*

Mathematics for Deep Learning

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  - Why do large neural networks *not overfit*?

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- **Explainability:**
  - Why did a trained deep neural network *reach a certain decision*?
  - Which *features of data* are learned by deep architectures?

  $\rightsquigarrow$ *Information Theory, Uncertainty Quantification, ...*

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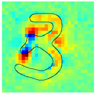
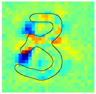
Explainability

Main Goal: We aim to *understand* decisions of "black-box" predictors!

map for digit 3



map for digit 8



Selected Questions:

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- What about a theory for *optimal relevance maps*?

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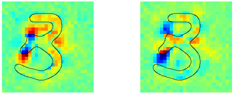

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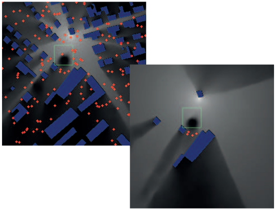
Rate-Distortion Explanation & CartoonX *(Kolek, Nguyen, Levie, Bruna, K; 2021):*



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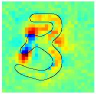

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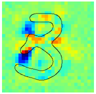

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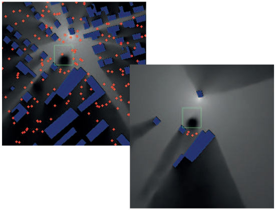

Vision for the Future:

Human-like answer to any question about a decision!

Deep Learning for Mathematical Problem Settings

- **Inverse Problems:**
  - How do we *optimally combine* deep learning with model-based approaches?

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- **Partial Differential Equations:**
  - Why do neural networks perform well in *very high-dimensional environments*?
  - Are neural networks capable of *replacing highly specialized numerical algorithms* in natural sciences?

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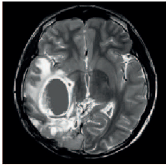
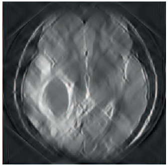
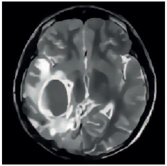
Deep Microlocal Reconstruction *(Andrade-Loarca, K, Öktem, Petersen; 2022):*



Original



Sparse Regularization/Shearlets

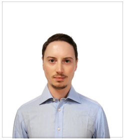


Deep Microlocal Reconstruction

Let's now consider Graph Neural Networks

Collaborators:

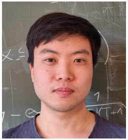
Michael Bronstein
(Imperial College London)



Lorenzo Bucci
(U. della Svizzera italiana)

Wei Huang
(U. della Svizzera italiana)

Ron Levie
(LMU Munich/Technion)

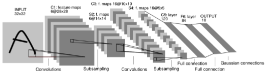


Yunseok Lee
(LMU Munich)

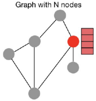
Sohir Maskey
(LMU Munich)

Some Facts about Graph Convolutional Neural Networks

Graph convolutional neural networks generalize classical CNNs to signals over graph domains. [Sperduti, Starita; 1997], [Gori, Monfardini, Scarselli; 2005], [Bruna, Zaremba, Szlam, LeCun; 2013], [Masci, Boscaini, Bronstein, Vandergheynst; 2015], ...



LeCun et al. 1989



Graph signal: s : graph nodes $\to \mathbb{R}^c$

Graph CNN: graph signal $\to$ convolution $\to$ activation $\to$ pooling $\to \ldots$

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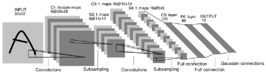

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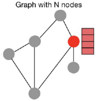

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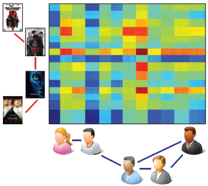
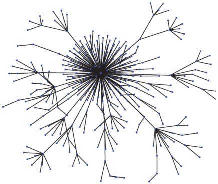
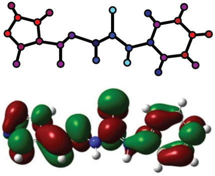
Some Applications:



Recommender system

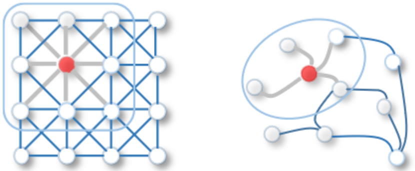


Fake news detection



Chemistry

Two Approaches to Convolution on Graphs



Spatial Approaches:

- Sliding window
- Aggregating feature information from the neighbors of each node

Spectral Approaches:

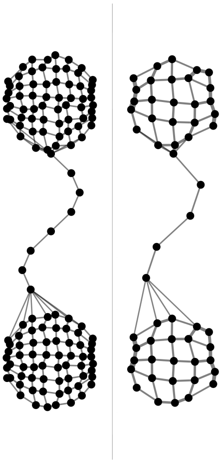
- Convolution theorem
- Defined in frequency domain
- Filter = multiplication in the frequency domain

Transferability of Spectral-based GCNNs

A Special Form of Generalization Capability

Desirable Feature:

Graph convolutional neural networks should *generalize* to graphs and signals unseen in the training set.



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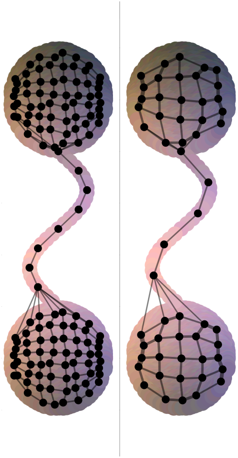
The Concept of Transferability:

If two graphs *model the same phenomenon*, a fixed filter/Graph CNN should have approximately the same repercussion on both graphs.



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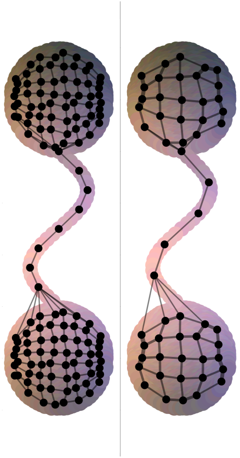

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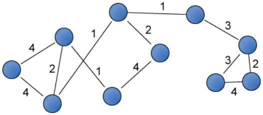
We prove transferability for spectral graph filters/Graph CNNs!

Graph Theory

Notation:

We will in the following consider *undirected weighted graphs* $G = \{V, E, W\}$, where



- $V = \{1, \ldots, N\}$ are the *vertices*,
- $E \subset V^2$ are the *edges*,
- W is the *adjacency matrix*, i.e.,

$$w_{i,j} = 0, \quad \text{if} \quad (i,j) \notin E,$$
$$w_{i,j} > 0, \quad \text{if} \quad (i,j) \in E,$$

- the *degree matrix* is given by

$$D = \mathrm{diag}\left\{\sum_{j \neq i} w_{i,j}\right\}_{i=1}^{N}.$$

Graph Laplacian: Oscillations on Graphs

Definition: Let D be the degree matrix and W the adjacency matrix. Then the *unnormalized Graph Laplacian* is defined by

$$\Delta_u = D - W$$

and the *normalized Graph Laplacian* is given by

$$\Delta_n = D^{-1/2} \Delta_u D^{-1/2}.$$

As a generic notation, we will in the following use Δ.

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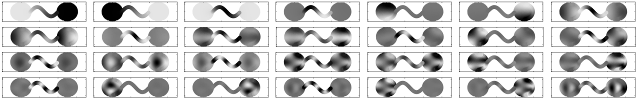
Remark: The Graph Laplacian Δ is self-adjoint. We will denote its

- eigenvalues by $\{\lambda_j\}_j \rightsquigarrow$ *Frequencies*,
- eigenvectors by $\{u_j\}_j \rightsquigarrow$ *Fourier modes*.

The graph Laplacian Δ encapsulates the geometry of the graph!

Graph Laplacian Eigenvectors



Spectral Graph Convolution

Definition:

Letting $\{u_j\}_j$ denote the eigenvectors of the graph Laplacian, we define the *spectral graph convolution operator* by

$$Cf = \sum_j c_j \langle f, u_j \rangle u_j.$$

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Problem with the Implementation:

- Computationally demanding
  - Eigendecomposition is slow.
  - No general FFT for graphs.
- Not transferable
  - The eigendecomposition is not stable to graph perturbations.
  - A fixed filter has different repercussions on similar graphs.

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Solution: Implement convolution using functional calculus!

Functional Calculus

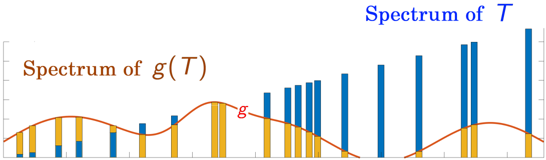
Definition:

Let T be a self-adjoint operator with discrete spectrum

$$Tv = \sum_j \lambda_j \langle v, u_j \rangle u_j.$$

A function $g : \mathbb{R} \to \mathbb{C}$ of T is then defined via

$$g(T)v = \sum_j g(\lambda_j) \langle v, u_j \rangle u_j.$$



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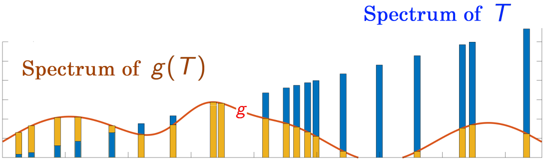
Remark:

If $g(\lambda) = \frac{\sum_{l=0}^{L} c_l \lambda^l}{\sum_{l=0}^{L} d_l \lambda^l}$, then $g(T) = \left(\sum_{l=0}^{L} c_l T^l\right) \left(\sum_{l=0}^{L} d_l T^l\right)^{-1}$.



Spectral Filtering using Functional Calculus

Functional Calculus Filters:

The functional calculus for $g : \mathbb{R} \to \mathbb{C}$ applied to the graph Laplacian yields

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Recall:

The previous implementation used

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Advantages of Functional Calculus Viewpoint:

This approach...

- *...solves the instability problem* (Levie, Isufi, K; 2019).
- *...solves the computational problem*, if g is a rational function.

Towards Transferability

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Three Approaches to Transferability

Stability under Perturbation [Levie, Isufi, K; 2019], [Kenlay, Thanou, Dong; 2021]**:**

- Two graphs which are small perturbations of each other.

Topological Space Sampling [Levie, Huang, Bucci, Bronstein, K; 2019],[Keriven, Bietti, Vaiter; 2020]**:**

- Two graphs which sample the same underlying continuous space.

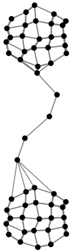
Graphon Approach [Ruiz, Chamon, Ribeiro; 2020], [Maskey, Levie, K; 2021]**:**

- Two graphs that come from the same sequence that converges to a graphon in a homomorphism density sense.

Topological Space Sampling

Interpretation:

- Weighted graphs:
  $\rightsquigarrow$ *Points and strength of correspondence between pairs of points.*



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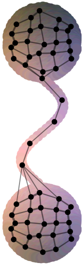
  $\rightsquigarrow$ *Points and distances.*

Our Viewpoint:

Think of graphs as discretizations of metric spaces

$$\text{distance} \nearrow \iff \text{edge weight} \searrow$$



Graphs that represent the same phenomenon are discretizations of the same metric space!

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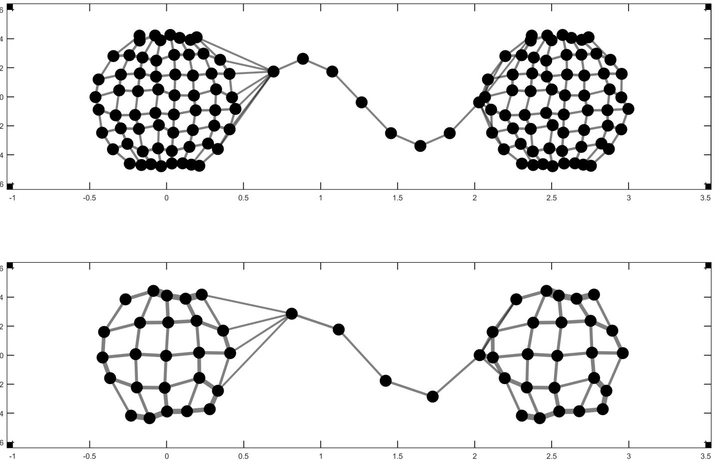
Comparing the Repercussion of a Filter on Two Graphs



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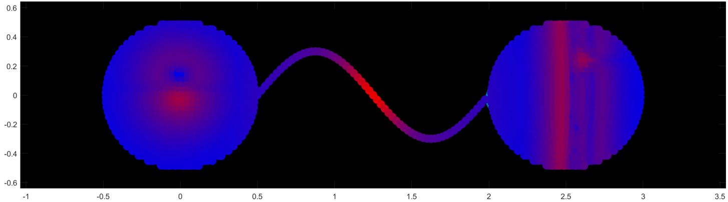
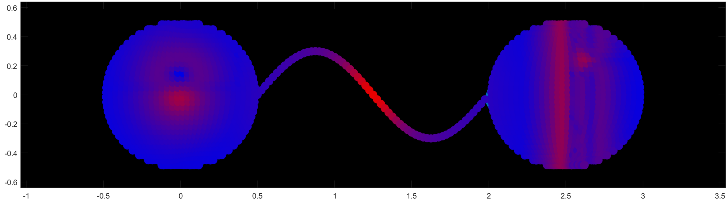


Take a generic signal $f : \mathcal{M} \to \mathbb{C}$



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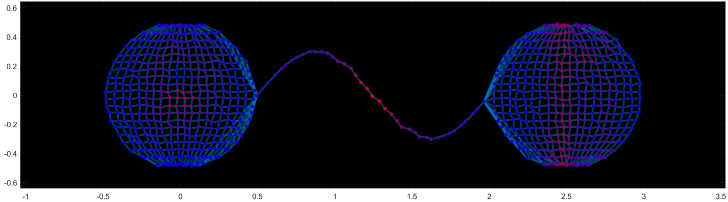
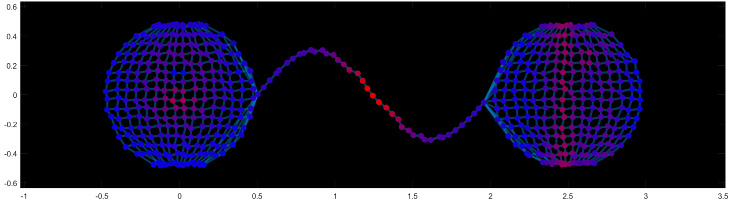


Sample to both graphs $\quad S_1 f : G_1 \to \mathbb{C}, \quad S_2 f : G_2 \to \mathbb{C}$



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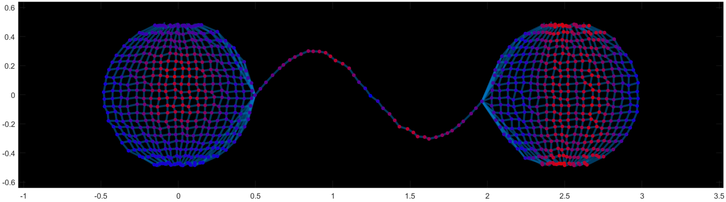
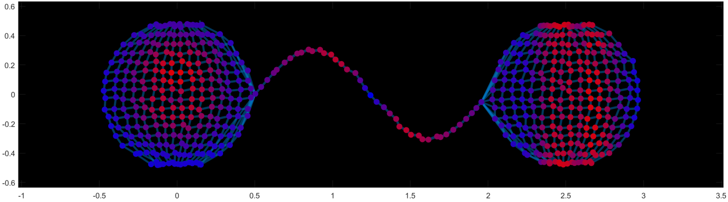


Apply both graph filters $g(\mathbf{\Delta}_1)S_1 f, \quad g(\mathbf{\Delta}_2)S_2 f$



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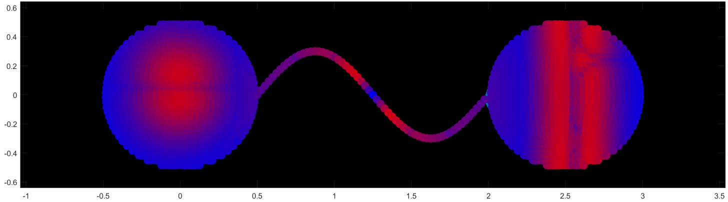
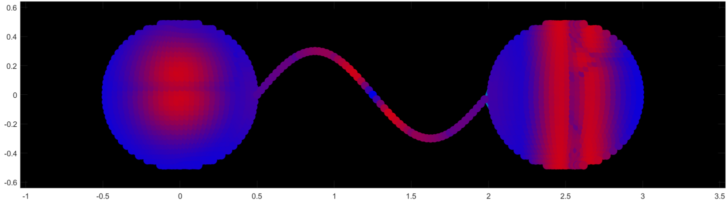


Interpolate back to $L^2(\mathcal{M})$ to get $\|R_1 g(\boldsymbol{\Delta}_1) S_1 f - R_2 g(\boldsymbol{\Delta}_2) S_2 f\| \approx 0$

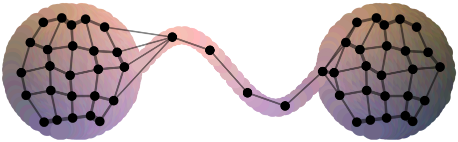


DSP Framework akin to the Nyquist–Shannon Approach

Our New Setting:

- *Analogue domain*: Borel space $\mathcal{M}$, with Laplacian $\mathcal{L}$.
- *Digital domains*: Graphs G with graph Laplacians Δ.
- *Paley Wiener spaces*: Band-limited spaces corresponding to $\mathcal{L}$.
- *Sampling operators*: $S^\lambda : PW(\lambda) \to L^2(G)$.
- *Interpolation operator*:

$$R^\lambda := (S^\lambda P(\lambda))^* := (S^\lambda P_{PW(\lambda)})^* : L^2(G) \to PW(\lambda).$$



What is Transferability precisely?

Definition:
The *transferability error of the filter f* on the signal $s \in L^2(\mathcal{M})$, is now defined by

$$\|f(\mathcal{L})s - R^\lambda f(\Delta) S^\lambda s\|,$$

the *transferability error of the Laplacian* is defined by

$$\|\mathcal{L}s - R^l \Delta S^\lambda s\|,$$

and the *consistency error* is defined by

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(Informal Version) Theorem (Levie, Huang, Bucci, Bronstein, K; 2020):

Transferability of Filter

$\leq$ *Transferability of Laplacian* $+$ *Consistency Error*

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Transferability of Functional Calculus GCNNs

Theorem (Levie, Huang, Bucci, Bronstein, K; 2020):
Consider two graphs G_j, $j = 1, 2$ and two graph Laplacians Δ_j, $j = 1, 2$, approximating the same Laplacian $\mathcal{L}$ in $\mathcal{M}$, and consider a ReLU graph CNN with Lipschitz filters. Further, let $G_{j,l}$ be the graph in layer l with graph Laplacians $\Delta_{j,l}$. Also, assume that, for all layers l, bands λ_l, and $j = 1, 2$,

$$\|S_{j,l}^{\lambda_l} \mathcal{L} P(\lambda_l) - \Delta_{j,l} S_{j,l}^{\lambda_l} P(\lambda_l)\| \leq \delta$$

and

$$\|P(\lambda_L) - R_{j,L}^{\lambda_L} S_{j,L}^{\lambda_L} P(\lambda_L)\| \leq \delta$$

for some $0 < \delta < 1$. Then, for all output-channels k and mappings $\Phi_{j,L}^k$ given by the graph CNN,

$$\begin{aligned} &\|R_{1,L}^{\lambda_L} \Phi_{1,L}^k S_{1,1}^{\lambda_0} P(\lambda_0) - R_{2,L}^{\lambda_L} \Phi_{2,L}^k S_{2,1}^{\lambda_0} P(\lambda_0)\| \\ &\qquad \leq 2\Big(LD\sqrt{\dim(PW(\lambda))} + L + 1\Big)\delta. \end{aligned}$$

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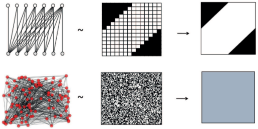
Further Results on Generalization Ability of GNNs

Graph Convolutional Neural Networks:

- *Similar results on transferability* for the *graphon* setting (Maskey, Levie, K; 2021).
- This builds on (Ruiz, Wang, Ribeiro; 2021).



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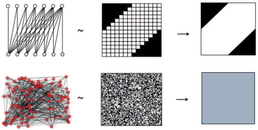
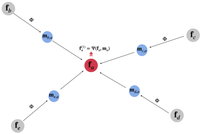


Message Passing Graph Neural Networks:



- *Non-asymptotic generalization bounds*, only depending on the regularity of the network and space (Maskey, Levie, Lee, K; 2021).
- Builds on (Garg, Jegelka, Jaakkola; 2020), (Verma, Zhang; 2019), (Yehudai, Fetaya, Meirom, Chechik, Maron; 2022).

A Word of Caution: Computability Aspects

Collaborators:

Holger Boche
(TU Munich)

Adalbert Fono
(LMU Munich)

Problem with Computability

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Computability on Digital Machines (informal):

A *computable problem (function)* is one for which the input-output relation can be computed on a digital machine for any given accuracy.

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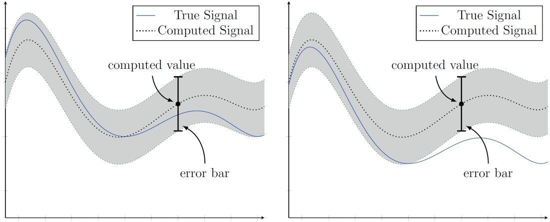
A *computable problem (function)* is one for which the input-output relation can be computed on a digital machine for any given accuracy.

Theorem (Boche, Fono, K; 2022):

The solution of a finite-dimensional inverse problem is *not (Banach-Mazur/Turing-)computable* (by a deep neural network).

Illustration of the Problem:



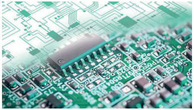
Some Thoughts on the Result

Remarks:

- *No algorithm exists*, which on digital hardware derives neural networks approximating the solution for any given accuracy.
- The output of trained neural networks *not reliable (no guarantees)*.
- This result could point towards why *instabilities* and *non-robustness* occurs for deep neural networks.

General Barrier:

- Limits of **computability** on today's hardware



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Other Models of Computations:

- New emerging hardware
  - *Neuromorphic computing*: Elements of computer modeled after systems in the human brain and nervous system.
  - *Biocomputing*: Living cells as the substrate for performing human-defined computations
- Different models of computation required

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Key Future Question:

Does the non-computability result also hold for different computation models such as analog computers as well?

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Key Future Question:

Does the non-computability result also hold for different computation models such as analog computers as well?

Theorem (Boche, Fono, K; 2022):
The solution of a finite-dim. inverse problem is *computable* (by a deep neural network) *on an analog machine!*

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Conclusions

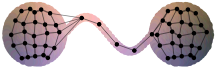
What to take Home...?

Deep Learning:

- *Stability* is a major concern!
- The amazing *generalization capability* is still a mystery!

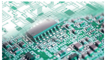
Transferability of Graph Convolutional Neural Networks:

- *Transferability* is a special type of generalization.
- We consider graphs as *discretizations of metric spaces*.
- We show *spectral GCNNs* (based on *functional calculus*) are transferable.
- Similar results: Graphs as *arising from a graphon*.



Generalization of Message Passing Graph Neural Networks:

- We consider graphs as *sampled from (continuous) models*.
- We derive *non-asymptotic* generalization bounds, *only depending on the regularity* of the network and space.



Caution: Problems with computability on digital hardware!

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THANK YOU!

References available at:

`www.ai.math.lmu.de/kutyniok`

Survey Paper (arXiv:2105.04026):

Berner, Grohs, K, Petersen, *The Modern Mathematics of Deep Learning*.

Check related information on Twitter at:

`@GittaKutyniok`

Upcoming Book:

- Grohs and K, eds.
  Mathematical Aspects of Deep Learning
  Cambridge University Press, to appear.

Convergence of Δ to Metric-Measure Laplacians

Transferability of Filter
$\leq$ *Transferability of Laplacian* $+$ *Consistency Error*

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Is it reasonable to assume that the transferability error of the Laplacian is small?

Informal Statement (Levie, Huang, Bucci, Bronstein, K; 2020)**:**
If graphs are constructed by sampling random points from $\mathcal{M}$, then graph Laplacians Δ approximate the continuous Laplacian $\mathcal{L}$ with high probability $\Rightarrow$ *Transferability in high probability!*

Towards Transferability:

Graphon Approach

Graphons

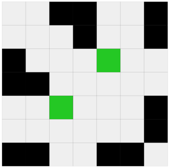
Definition:

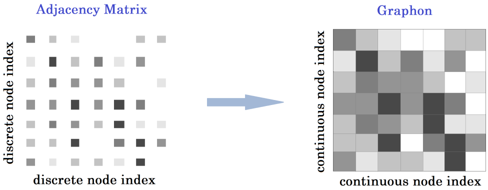
A *graphon* is a symmetric measurable function $W : [0,1]^2 \to [0,1]$.

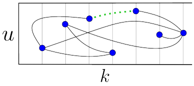
Intuition:

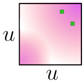
A graphon is understood as defining an exchangeable random graph model:

- Each vertex j of the graph is assigned an independent random value $x_j \sim U[0,1]$.
- Edge (i,j) is independently included in the graph with probability $W(x_i, x_j)$.



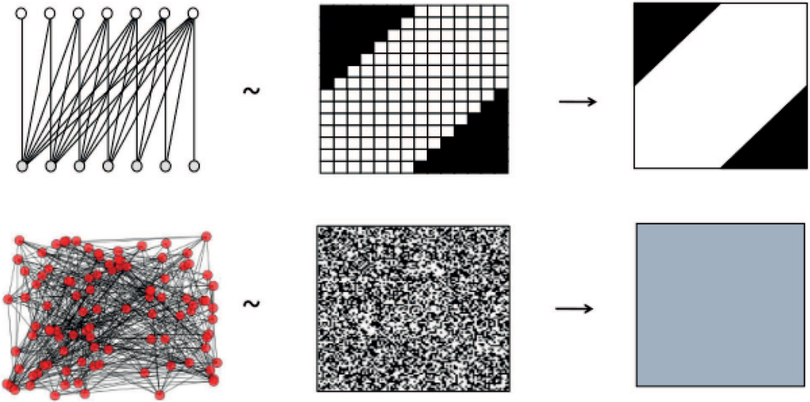






Examples of Graphons

Graphs, Empirical Graphons, and Limits:



Local Convergence: Homomorphism Density

Definition:
For F, G simple graphs, let $t(F, G)$ the probability that a random map $V(F) \to V(G)$ is a homomorphism. Then a sequence G_n is *convergent to a graphon W*, if

$$t(F, G_n) \to t(F, W) := \int_{[0,1]^{v(F)}} \prod_{i,j \in E} W(x_i, x_j) \prod_{i \in V} dx_i$$

for all simple graphs F. For a graph G, the *induced kernel W_G* is defined by

$$W_G(u, v) := \sum_{i,j \leq n} \Delta(i, j) \chi_{I_i}(u) \chi_{I_j}(v)$$

and the *Hilbert-Schmidt operator T_W* associated to a kernel W is given by

$$T_W \psi(v) := \int_0^1 W(u, v) \psi(u) du, \quad \psi \in L^2(0, 1).$$

$\rightsquigarrow$ *We can use functional calculus (filters)!*

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Transferability of Continuous Filters

Theorem (Maskey, Levie, K; 2021):
Let $(G_n)_n$ be a sequence of graphs with uniformly bounded Laplacians. Suppose that there exists a graphon W such that

$$G_n \to W$$

in homomorphism density. Let h be a continuous function. Then, there exists a sequence of permutations $(\pi_n)_n$ such that

$$h(T_{W_{\pi_n(G_n)}}) \to h(T_W)$$

in operator norm.

Numerical Results

Rethinking Transferability

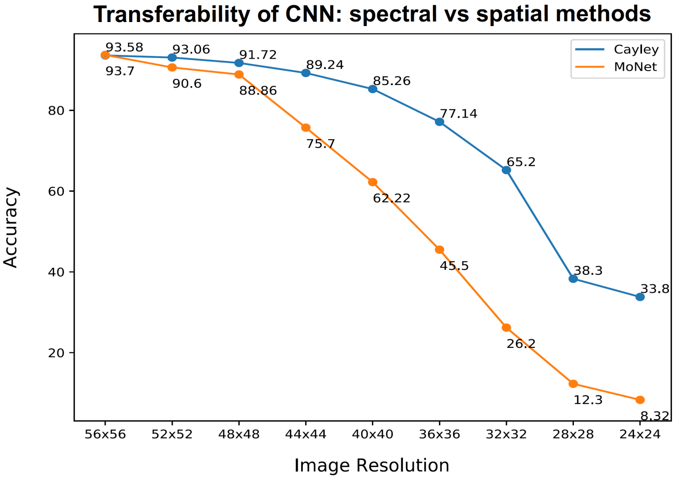
Graph CNNs can manage transferability in different ways!

- **Concept-Based Transferability:**
  - *Multi-graph training set*
  - The network learns "concepts" that promote transferability.
- **Principle Transferability:**
  - *Single or multi-graph training set*
  - A built-in capability of graph CNNs, independent of their specific filters, which requires no training.

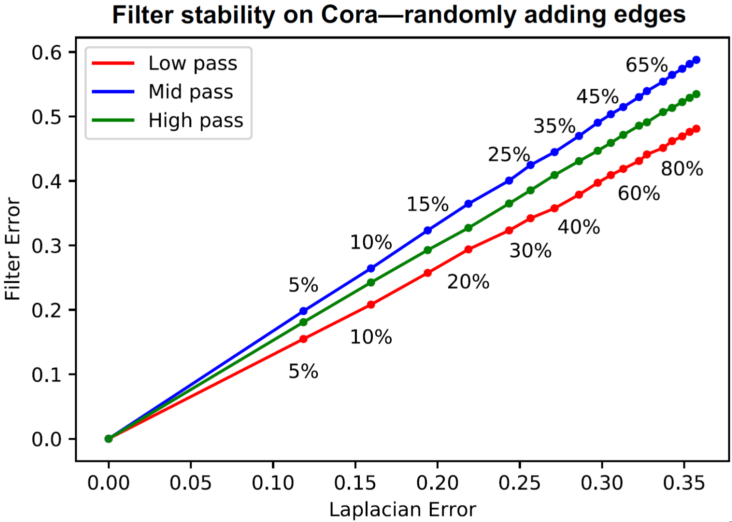
The success of spectral graph CNNs in multi-graph settings relies on both types of transferability!

Some Examples

Isolate principle transferability from concept-based transferability:
Train the network on one single graph and test on other graphs.



Transferability under Graph Perturbation



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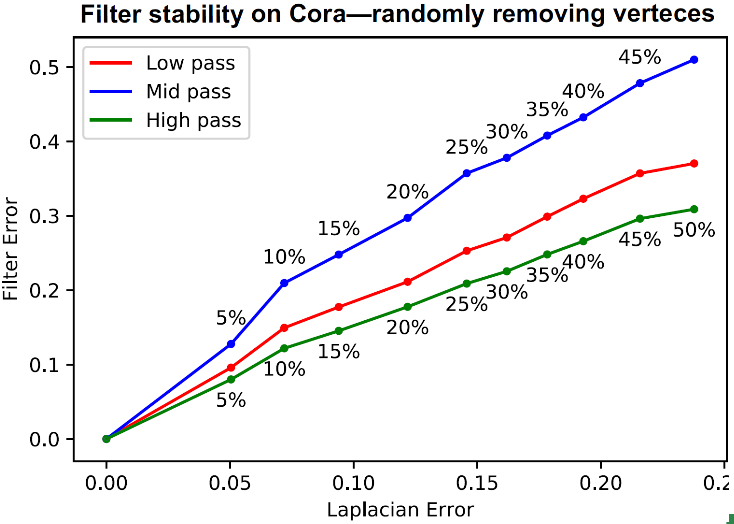

An Experimental Study of Transferability

Spectral method were tested only in single-graph settings.

Benchmark ChebNet (Defferrard et al. 2016) in multi-graph settings:

- *Graph benchmarks*:

  Hu et al. Open Graph Benchmark: *Datasets for Machine Learning on Graphs.* 2020.

  Dwivedi et at. *Benchmarking Graph Neural Networks.* 2020.
- *Tasks*: graph regression, graph classification, node classification.
- *Rules*: different for each benchmark, e.g., budget of parameters, fixed number of layers, fixed hyperparameters, no specialized data augmentation techniques.

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$\rightarrow$ *ChebNet reaches state-of-the-art results (Nilsson, Bresson; 2020)*