Designing Transformers with Kernel Methods

Grégoire Mialon

DeepMind

About me

- 2016: Research intern at MIT, Nuclear Engineering.
- 2017: Graduated from École polytechnique (Theoretical physics, Statistics, Computer Science).
- 2017-2018: NLP data scientist at eXplain, Paris.
- 2018: Graduated from machine learning (M.S. MVA), ENS Paris-Saclay.
- 2018-today: PhD candidate, advised by Julien Mairal and Alexandre d'Aspremont.

An Offshore Floating Nuclear Plant.

What I have been doing in the past 3.5 years

Kernel methods and deep learning in constrained data regimes (100 to 10k samples).

- G. Mialon*, D. Chen*, M. Selosse*, J. Mairal. GraphiT: Encoding Graph Structure in Transformers (under review).
- G. Mialon*, D. Chen*, A. d'Aspremont, J. Mairal. A Trainable Optimal Transport Embedding for Feature Aggregation and its Relationship to Attention (ICLR, 2021).
- A. Bietti*, G. Mialon*, D. Chen, J. Mairal. A Kernel Perspective for Regularizing Deep Neural Networks (ICML, 2019).

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Convex optimization.

- G. Mialon, A. d'Aspremont, J. Mairal. Screening Data Points in Empirical Risk Minimization via Ellipsoidal Regions and Safe Loss Functions (AISTATS, 2020).

What I want to talk about today

Kernel methods and transformers in constrained data regime (100 to 10k samples). Application to scientific data.

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Motivation: designing strong models even when data is scarce

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- A path towards better models?
- Or, simply because there is too few available data:
  - Rare events: less than 30k people per rare disease in France (2021).
  - Expensive or complex data collection for fundamental science/econometrics.

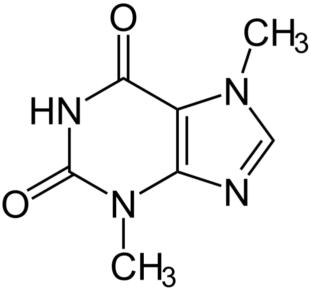
How to design strong models in constrained data regimes?

Encode inductive bias within trainable architectures with kernel methods.

Outline: Encoding inductive bias within trainable architectures with kernel methods

1. **Encoding Graph Structure in Transformers with Kernels on Graphs**
2. Embedding Sets of Features with Optimal Transport Kernels
3. Conclusion and perspectives

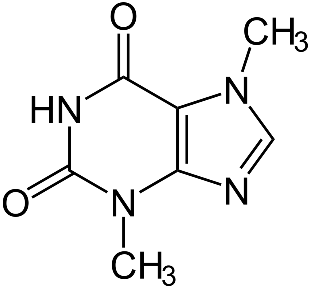
Graph data are an important research topic



A molecule of theobromin, or why chocolate makes us feel good.

Graph data are very valuable...

Graph data are an important research topic



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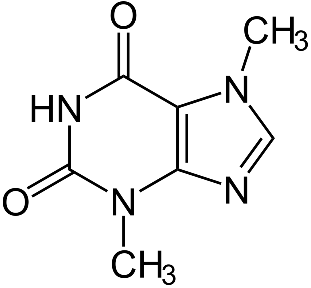

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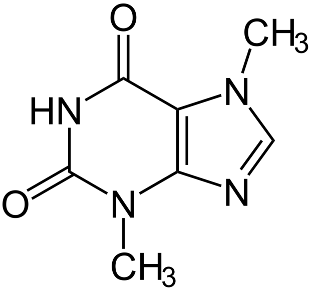

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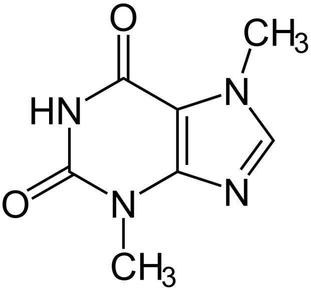

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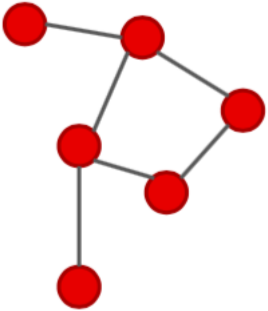
...but delicate to exploit.

- Non-euclidean structure.

Learning with Graph Neural Networks

Graph Neural Networks (GNNs).

- Introduced as an extension of neural networks for graph-structured data [Gori et al., 2005, Scarselli et al., 2008].
- Based on message passing.



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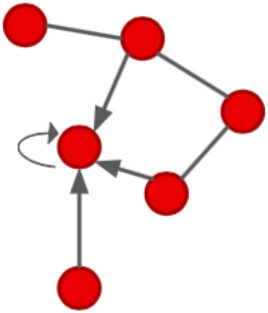

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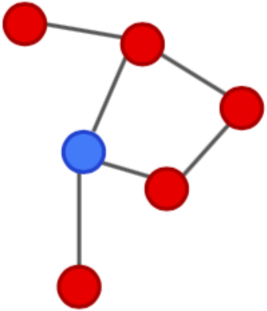

GNN, layer k+1 (for one node)

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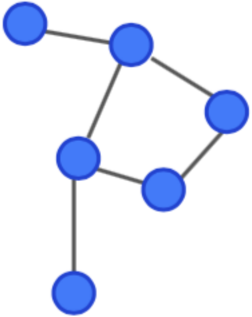

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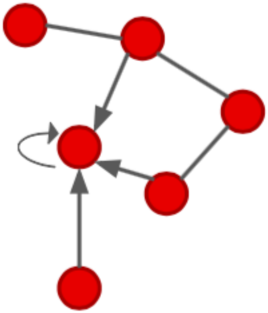
- Many strategies to aggregate features of neighboring nodes [Duvenaud et al., 2015, Bronstein et al., 2017, Veličković et al., 2018].
- Applications to molecules [Duvenaud et al., 2015], physical systems [Battaglia et al., 2016], materials [Xie et al., 2021], etc.

GNNs may struggle with long-range interactions



Only neighboring nodes communicate.

In GNNs, messages flow between neighbors only.

- Exploits the structure of the graph.

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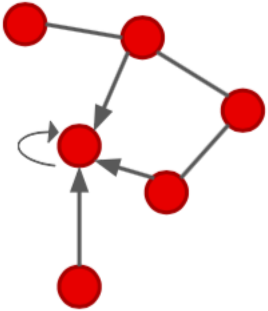

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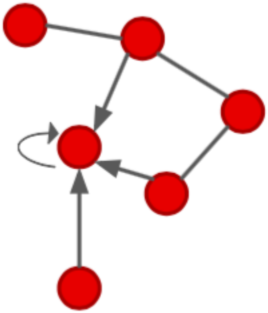

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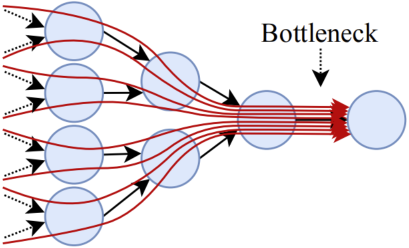

An illustration of oversquashing
(From Alon and Yahav).

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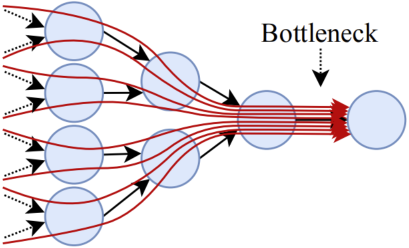

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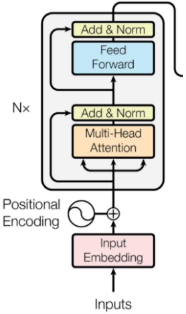
- Attempts at solving this issue [Godwin et al., 2021].

Transformers



Transformer encoder (from Vaswani et al.)

Transformers perform global aggregation!

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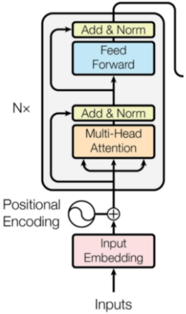

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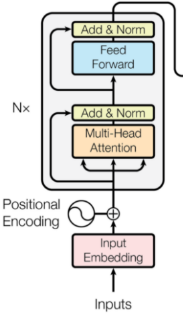

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- Question the paradigm "one data modality, one preferred architecture".

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Transformer encoder.

- Input: set of n elements X in $\mathbb{R}^{n \times d_{\text{in}}}$. Output: another set in $\mathbb{R}^{n \times d_{\text{out}}}$.

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with $Q^\top = W_Q X^\top$ and $K^\top = W_K X^\top$ resp. query and key matrices, $V^\top = W_V X^\top$ the value matrix, and W_Q, W_K, W_V in $\mathbb{R}^{d_{\text{out}} \times d_{\text{in}}}$ learned projection matrices.

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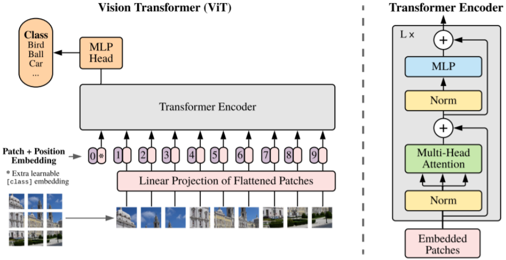
- Repeat.

Transformers for graphs require position encoding



Vision transformer (from [Dosovitskiy et al., 2021])

A nice inductive bias for graphs?

- All input elements communicate...

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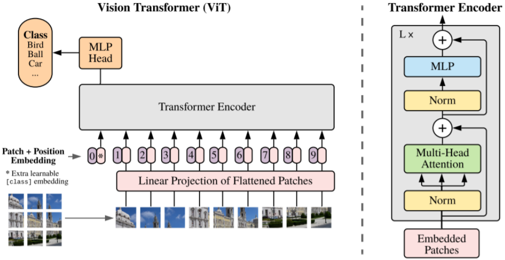

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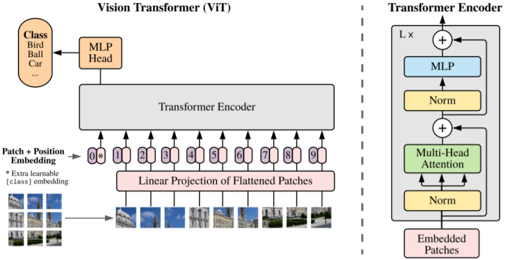

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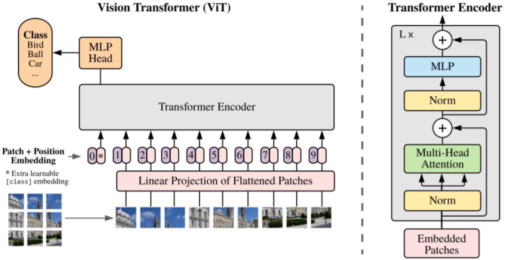

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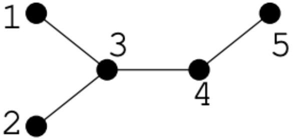
- ... but encoder output is permutation invariant.
- Hence, position encoding often required.
- Not trivial for graphs!

Previous attempts at using transformers with graphs



$$L = D - A = \begin{pmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

(From Vert, 2021)

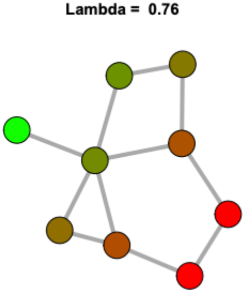
Dwivedi & Bresson, 2021: absolute PE using Laplacian eigenvectors.

- $A_{ij} = 1$ if two nodes are connected.
- Diagonal coefficients of D are node degrees.

Previous attempts at using transformers with graphs

Spectral graph analysis.

- Eigenvalue decomposition $L = \sum_i \lambda_i u_i u_i^\top$.
- $\lambda_i = u_i^\top L u_i = \sum_{j \sim k} (u_i(x_j) - u_i(x_k))^2$ characterizes amount of oscillation of u_i.



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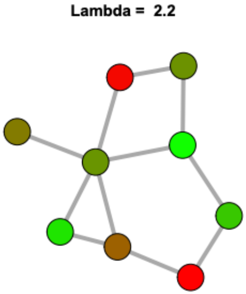

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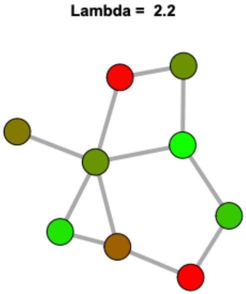

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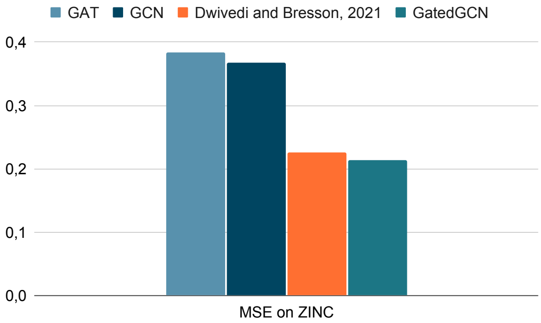
“Discrete equivalent” to sine/cosine Fourier basis in $\mathbb{R}^n$.

Promising results but...

ZINC: 12k graphs (regression).



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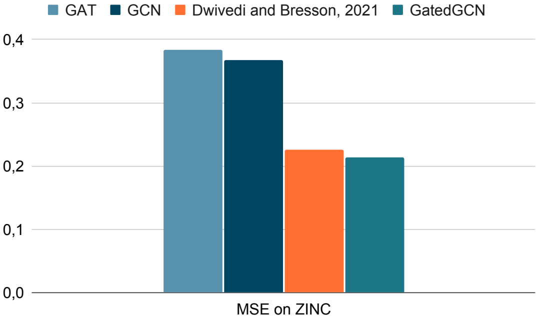

Problems with Laplacian absolute PE.

- Flipping sign at training.

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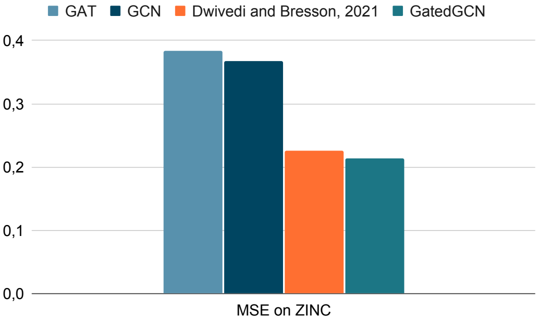

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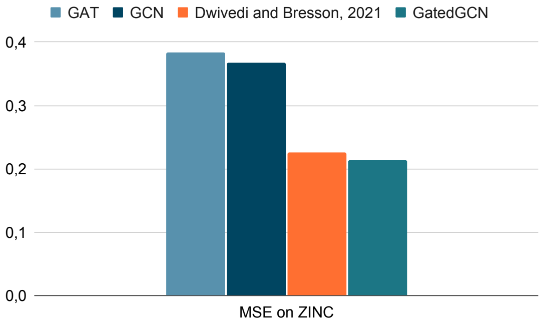

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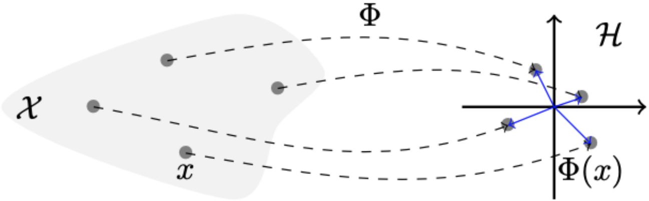
Can we improve graph structure encoding in transformers?

Our contribution: GraphiT, or two mechanisms for encoding graph structure in transformers

GraphiT: Encoding Graph Structure in Transformers
G. Mialon, D. Chen, M. Selosse, J. Mairal, 2021
Under review.
`https://github.com/inria-thoth/GraphiT`

Reminder: Kernel methods



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Learning with Kernel methods.

- Positive definite kernel K: defines a measure of similarity (prior?) between x and x'.

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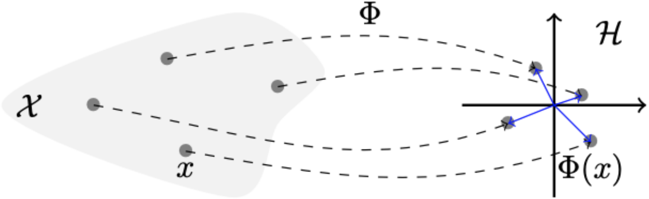

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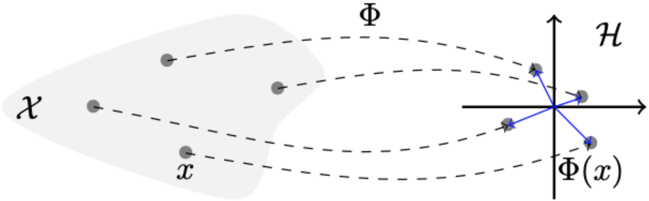

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- Associated to rich embedding Φ via $K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$.
- A surrogate for Φ can be learned with or without supervision [Williams and Seeger, 2001].

Kernels on graphs

Laplacian based kernels [Smola and Kondor, 2003].

- Rich family of p.d. kernels on the graph by applying regularization function r to the spectrum of L

$$K_r = \sum_{i=1}^{m} r(\lambda_i) u_i u_i^\top . \tag{2}$$

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$$K_r = \sum_{i=1}^{m} r(\lambda_i) u_i u_i^\top . \tag{2}$$

- Associated with the norm $\|f\|_r^2 = \sum_{i=1}^m (f_i^\top u_i)^2 / r(\lambda_i)$ from a reproducing kernel Hilbert space (RKHS), where $r : \mathbb{R} \mapsto \mathbb{R}_*^+$ is a non-increasing function such that smoother functions on the graph would have smaller norms in the RKHS.

A famous kernel on graphs: the diffusion kernel

Diffusion Kernel [Kondor and Vert, 2004].

- When $r(\lambda_i) = e^{-\beta\lambda_i}$,

$$K_D = \sum_{i=1}^{m} e^{-\beta\lambda_i} u_i u_i^\top = e^{-\beta L} = \lim_{p\to+\infty} \left(I - \frac{\beta}{p} L\right)^p .$$

A famous kernel on graphs: the diffusion kernel

Diffusion Kernel [Kondor and Vert, 2004].

- When $r(\lambda_i) = e^{-\beta \lambda_i}$,

$$K_D = \sum_{i=1}^{m} e^{-\beta \lambda_i} u_i u_i^\top = e^{-\beta L} = \lim_{p \to +\infty} \left(I - \frac{\beta}{p} L \right)^p .$$

- Physical interpretation: diffusion of a substance in the graph, controlled by β.

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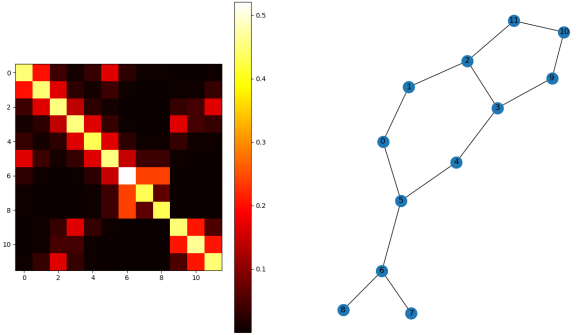
- Discrete equivalent of the Gaussian kernel, a solution to the heat equation in the continuous setting.

Kernels on graphs reflect structural similarity between nodes



Diffusion kernel between the nodes of a MUTAG sample graph ($\beta = 1$).

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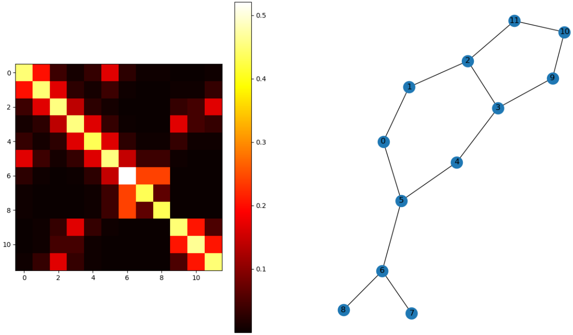

Diffusion kernel between the nodes of a MUTAG sample graph ($\beta = 1$).

Use kernel matrix to modulate self-attention!

Mechanism 1: node position encoding with kernels on graphs

Regular attention.

- Self-attention:

$$\text{Attention}(Q, V) = \text{normalize}\left(\exp\left(\frac{QQ^\top}{\sqrt{d_{\text{out}}}}\right)\right) V \in \mathbb{R}^{n \times d_{\text{out}}}. \tag{3}$$

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Remark. Same matrices for Q and K [Tsai et al., 2019].

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- Feature map X gets:

$$X = X + D^{-\frac{1}{2}} \text{PosAttention}(Q, V, K_r), \tag{6}$$

  with D the matrix of node degrees.

Mechanism 2: leveraging substructures via path embedding

- Substructures: local positional information *and* content, *e.g* paths [Borgwardt et al., 2020].

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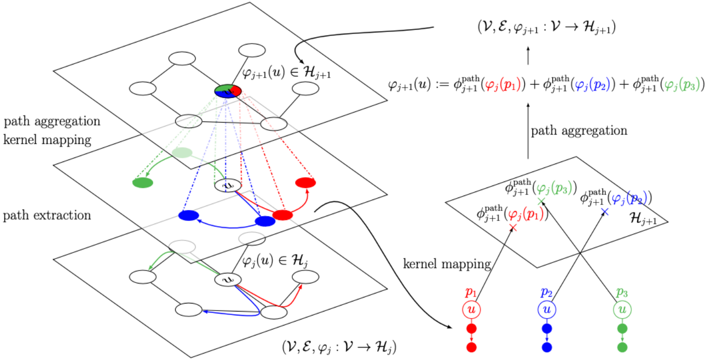
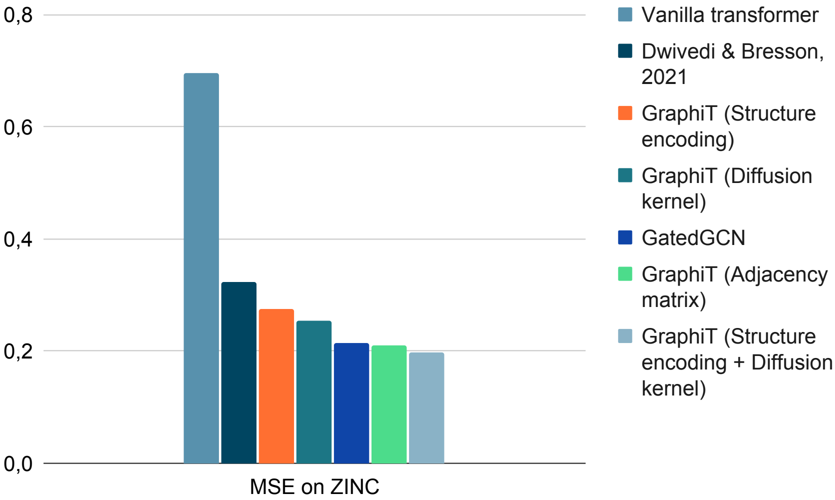
- Augmenting node features u using kernel neighborhood encoding [Chen et al., 2020].
- Kernel encoding learned with or without supervision.



$(\mathcal{V}, \mathcal{E}, \varphi_{j+1} : \mathcal{V} \to \mathcal{H}_{j+1})$
$\varphi_{j+1}(u) \in \mathcal{H}_{j+1}$
$\varphi_{j+1}(u) := \phi^{\text{path}}_{j+1}(\varphi_j(p_1)) + \phi^{\text{path}}_{j+1}(\varphi_j(p_2)) + \phi^{\text{path}}_{j+1}(\varphi_j(p_3))$
path aggregation
kernel mapping
path aggregation
$\phi^{\text{path}}_{j+1}(\varphi_j(p_3))$
$\phi^{\text{path}}_{j+1}(\varphi_j(p_2))$
$\phi^{\text{path}}_{j+1}(\varphi_j(p_1))$
$\mathcal{H}_{j+1}$
path extraction
u
kernel mapping
$\varphi_j(u) \in \mathcal{H}_j$
u
p_1
p_2
p_3
u
u
u
$(\mathcal{V}, \mathcal{E}, \varphi_j : \mathcal{V} \to \mathcal{H}_j)$

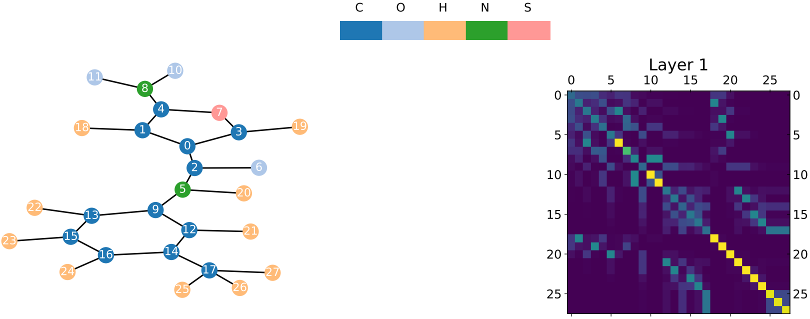
GraphiT is able to outperform popular GNNs

ZINC: 12k graphs (regression).



GraphiT captures meaningful interactions

Mutagenicity: 4k graphs (binary classification).



Nitrothiopheneamide-methylbenzene

Figure 1: *Left*: A molecule from the Mutagenicity data set [Kersting et al., 2016]. *Right*: approximate diffusion kernel for the molecular graph.

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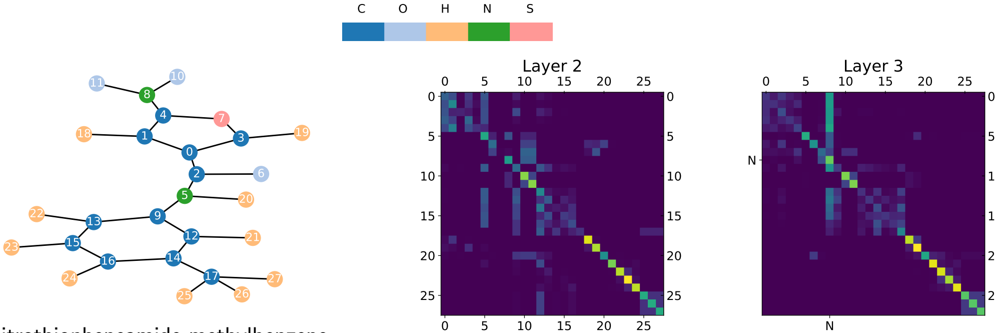
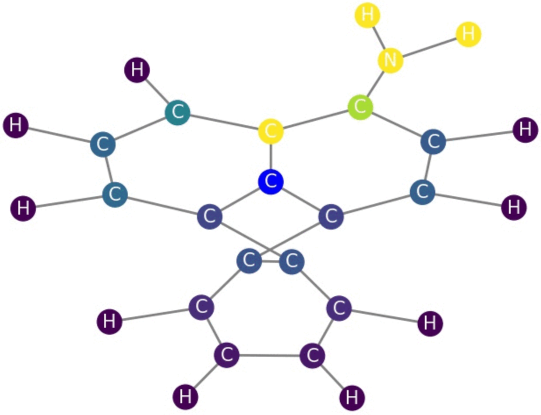


Nitrothiopheneamide-methylbenzene

Left: A molecule from the Mutagenicity data set [Kersting et al., 2016]. *Right*: nodes 8 (N of NO_2) is salient. NO_2 group is known for its mutagenetic properties. The attention scores are averaged by heads.

Attention from C atom



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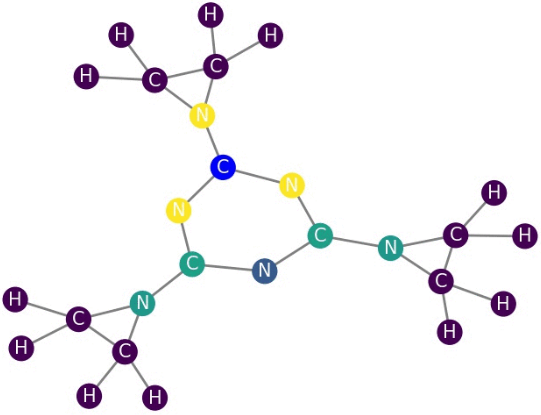

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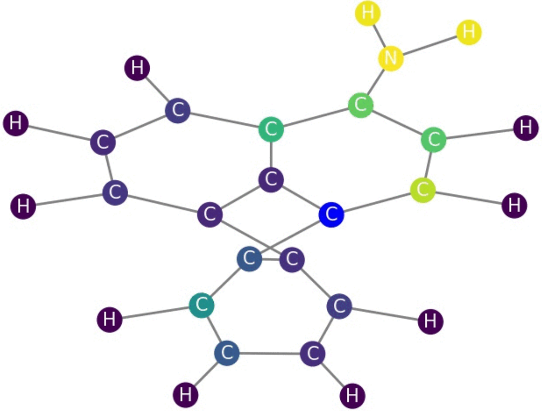
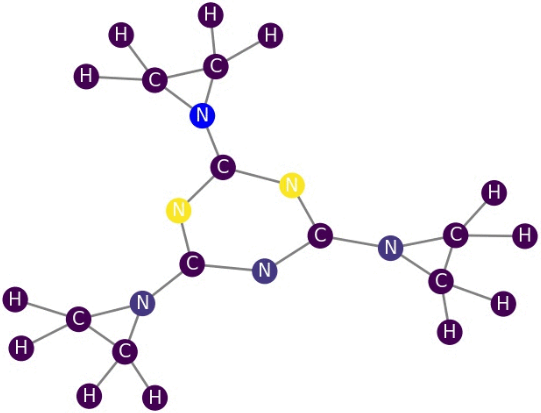


Attention from N atom



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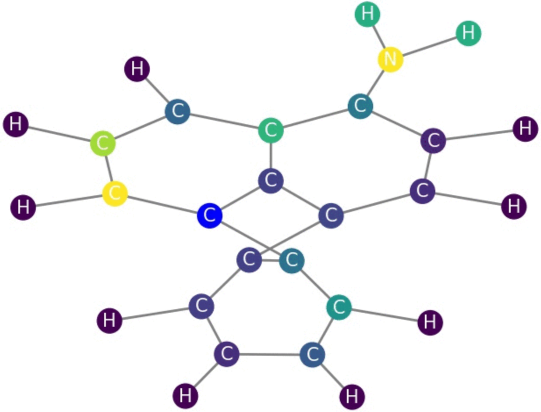

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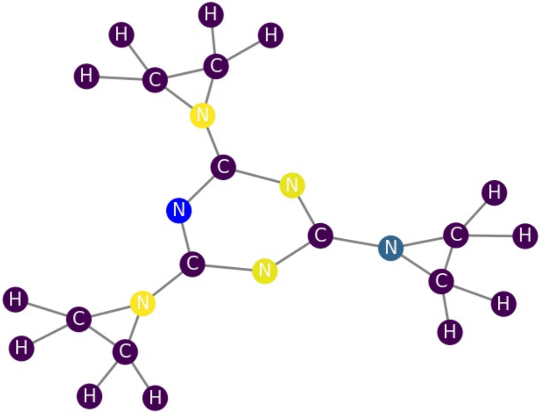

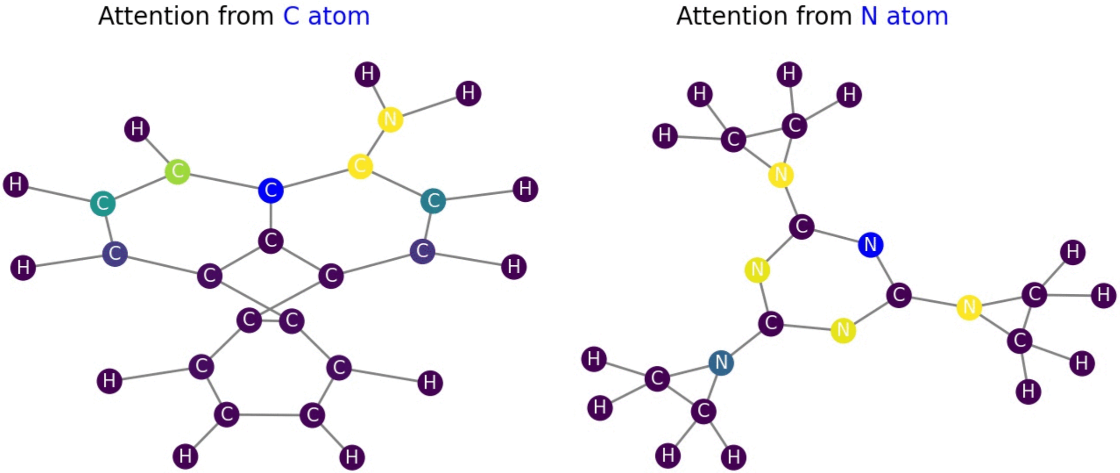

Attention from C atom

Attention from N atom

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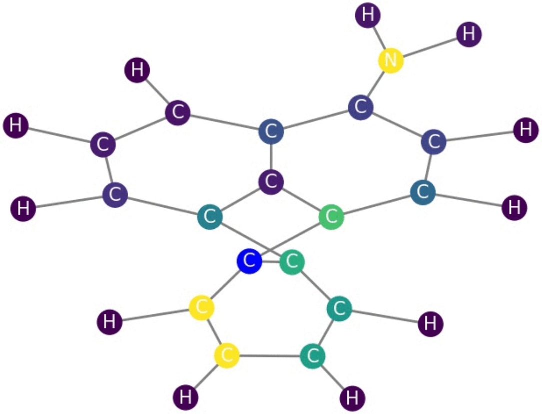

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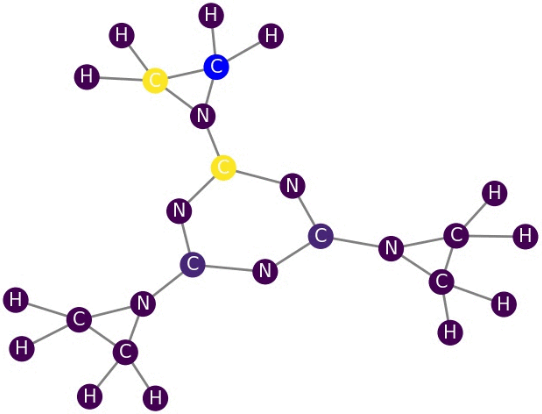

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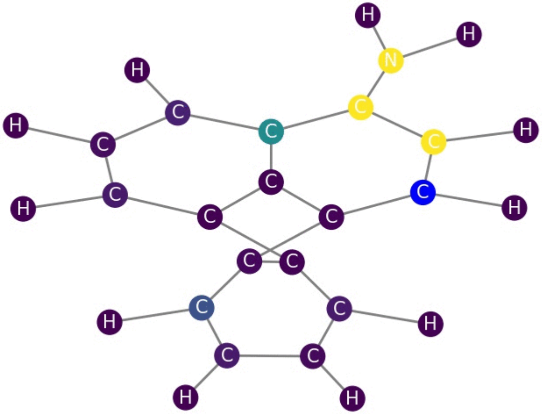

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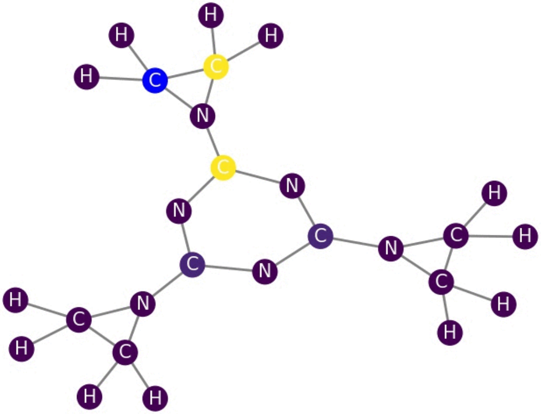

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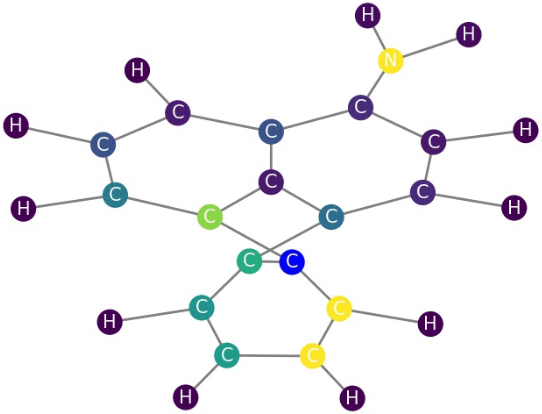

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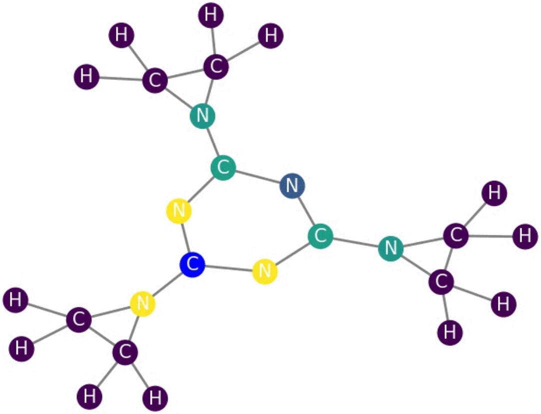

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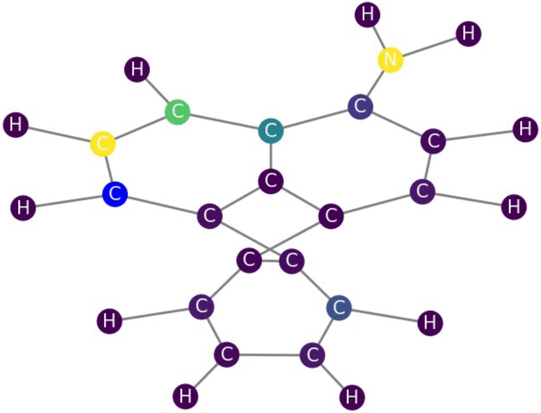

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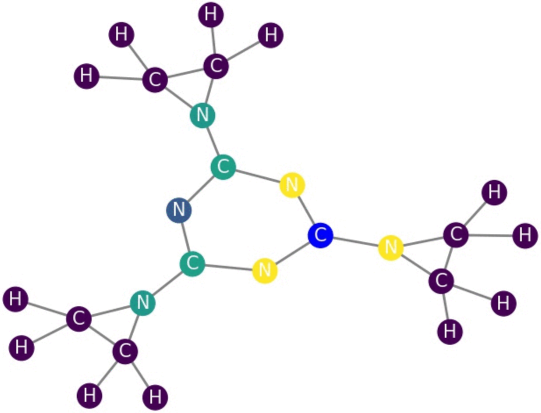

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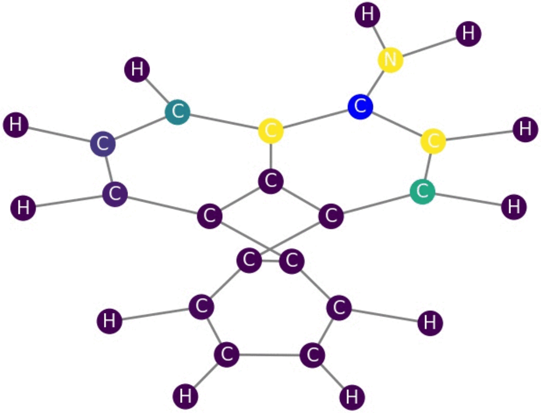

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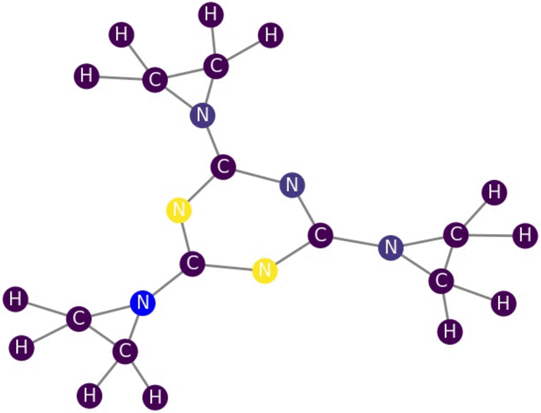

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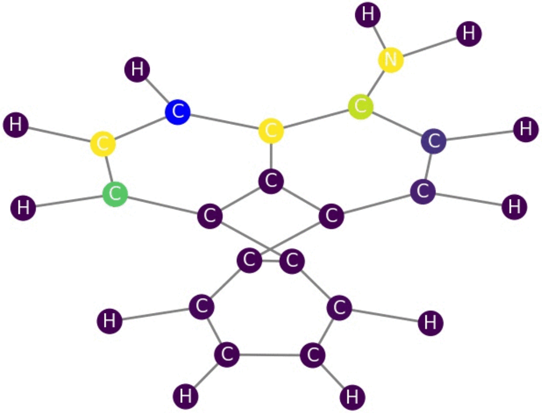

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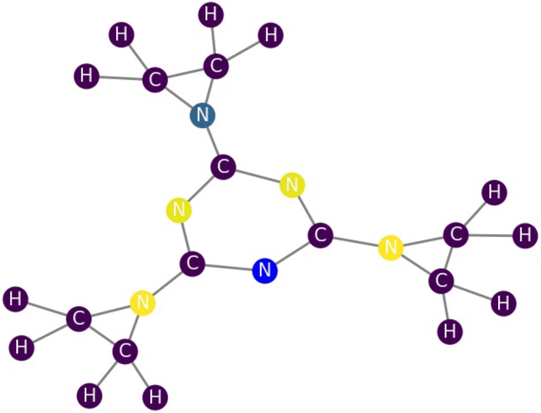

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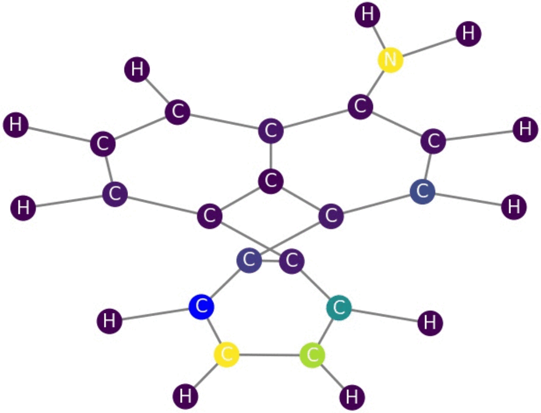

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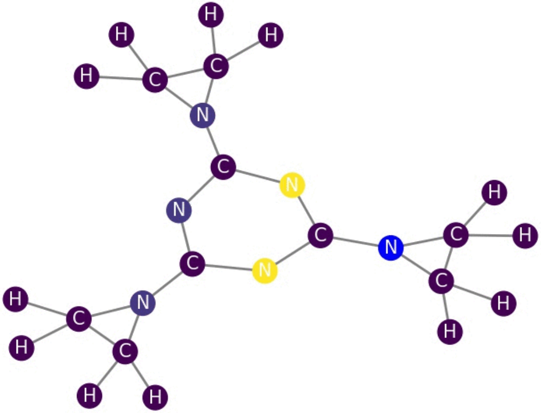

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- Evaluation on large scale datasets:
  OGB [Hu et al., 2020]?

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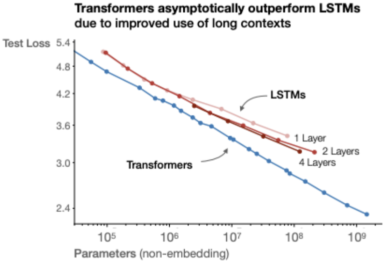
- Visualization for real-life applications?
- Pre-trained models? Self-supervised learning for graphs? [Thakoor et al., 2021]



(From [Kaplan et al., 2020]).

Kernel smoothing interpretation

Self-attention as a kernel smoothing [Tsai et al., 2019].

- We can rewrite self-attention:

$$\text{Attention}(Q, K, V)_i = \sum_{j=1}^{n} \frac{exp\left(\frac{Q_i K_j^\top}{\sqrt{d_{out}}}\right)}{\sum_{j'=1}^{n} exp\left(\frac{Q_i K_{j'}^\top}{\sqrt{d_{out}}}\right)} V_j \in \mathbb{R}^{d_{\text{out}}}$$

$$= \sum_{j=1}^{n} \frac{k(X_i, X_j)}{\sum_{j'=1}^{n} k(X_i, X_j)} v(X_j) \in \mathbb{R}^{d_{\text{out}}},$$

with $Q_i = W_Q X_i$, $K_j = W_K X_j$, $v(X_j) = W_V X_j$, k a non-negative kernel function: we get a kernel smoothing.

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Different choices for k suggest different transformers architectures.

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What if we pick a different similarity measure k?

Outline

1. Encoding Graph Structure in Transformers with Kernels on Graphs
2. **Embedding Sets of Features with Optimal Transport Kernels**
3. Conclusion and perspectives

Sets are another important data structure

Notre-Dame de Paris, LIDAR view (Andrew Tallon)

Sets can be found in various domains.

- 3D shape recognition (point clouds).

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Common characteristics with graphs.

- Size may vary.
- Potential interactions between elements.

Let’s focus on biological sequences

CUU	GAC	AAA	GUU	GAG	GCU	GAA	GUG	CAA	AUU	GAU	AGG	UUG	AUC	ACA	GGC
L	D	K	V	E	A	E	V	Q	I	D	R	L	I	T	G

Short part of mRNA sequence for the SARS-Cov-2 spike protein. Each triplet codes for an amino acid, represented below.

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- Sequences may be long.
- Potentially few labelled sample per class.

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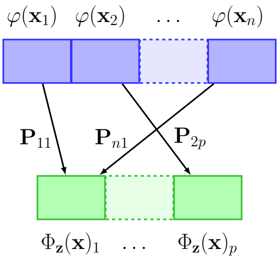
How to represent sets with low data and memory requirements?

Our contribution: OTKE, a data-efficient embedding for sets

A Trainable Optimal Transport Embedding for Feature Aggregation and its Relationship to Attention
G. Mialon, D. Chen, A. d'Aspremont, J. Mairal
ICLR 2021.
`https://github.com/claying/OTK`

OTKE: a data-efficient embedding for sets



Global, similarity-based pooling.

- Input: set or sequence $\mathsf{X} \in \mathbb{R}^{n \times d_{\text{in}}}$.

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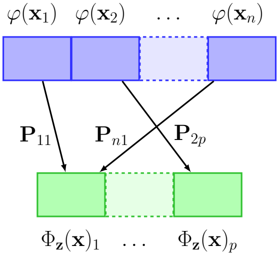

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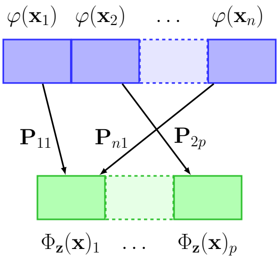

Global, similarity-based pooling.

- Input: set or sequence $\mathsf{X} \in \mathbb{R}^{n \times d_{\text{in}}}$.
- Element-wise, non-linear embedding φ.
- Pool elements $\varphi(\mathsf{x}_i)$ in p bins via weighted sums.

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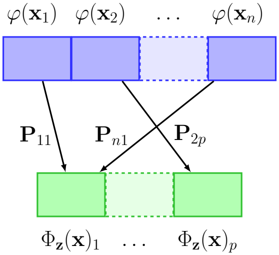
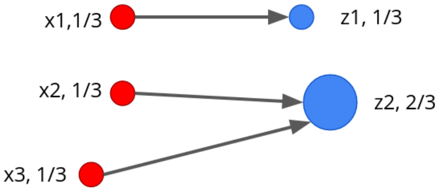


Global, similarity-based pooling.

- Input: set or sequence $\mathrm{X} \in \mathbb{R}^{n \times d_{\text{in}}}$.
- Element-wise, non-linear embedding φ.
- Pool elements $\varphi(\mathrm{x}_i)$ in p bins via weighted sums.
- To each bin corresponds a prototype (parameter) $z_j \in \mathbb{R}^{d_{\text{out}}}$, $j = 1 \ldots p$.

Pooling weight P_{ij} reflects similarity between x_i and z_j.

Our notion of similarity: optimal transport



$$P=\begin{pmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 1/3 \end{pmatrix}$$

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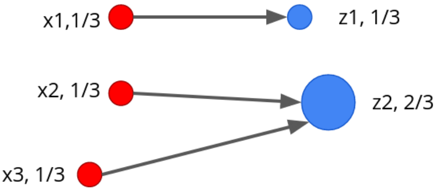

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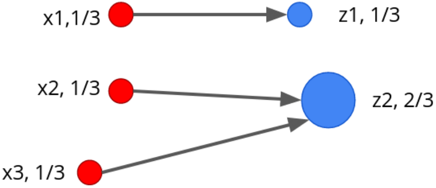

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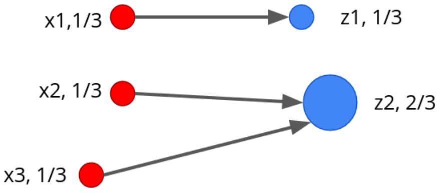

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What is optimal transport?

- "Most efficient way of transporting a mass distribution to another" [Peyré and Cuturi, 2019].
- Finding the transport plan minimizing a transportation cost.
- GPU-friendly solvers [Sinkhorn and Knopp, 1967, Cuturi and Doucet, 2013].

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- Embeds the sets in a space where ℓ_2 distance approximates the 2-Wasserstein distance [Wang et al., 2013].

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- Embeds the sets in a space where ℓ_2 distance approximates the 2-Wasserstein distance [Wang et al., 2013].
- Surrogate for a well-studied kernel [Rubner et al., 2000].

Reasonable memory/data requirements

Data efficient.

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- Kernel smoothing: we replaced $\frac{k(Q_i, K_j)}{\sum_{j'=1}^{n} k(Q_i, K_{j'})}$ by $\mathrm{P}(X, Z)_{ij}$.

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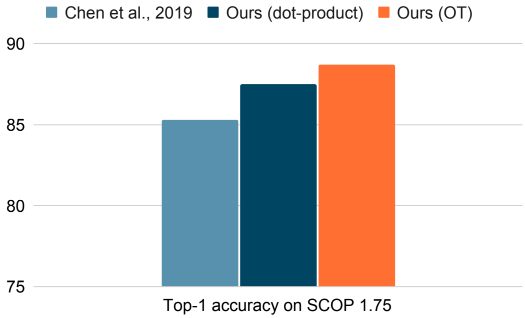
- Linear in the number of input elements.
- Similar ideas in efficient transformers [Wang et al., 2020, Choromanski et al., 2021], etc.

OTKE: (temporarily) sota for our bioinformatics tasks

SCOP 1.75: 20k samples (classification).

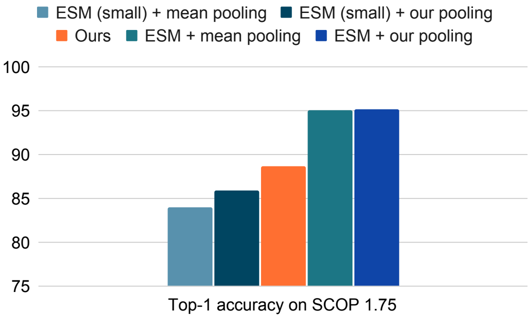
- Classify protein folding from amino-acid sequence: 1k labels!
- Sequence length from 10s to 1000s.



What about pre-trained models?

During ICLR rebuttal...

- ESM [Rives et al., 2019], a transformer protein language model trained on 250M protein sequences.
- Train a linear layer on top of ESM features.



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As an embedding.

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- Improved pooling for graph representation [Kolouri et al., 2021] or protein representation (ICLR rebuttal).
- Interesting improvement of OTKE by [Anonymous, 2022].

Outline

1. A new inductive bias for graphs
2. Embedding sets with low data requirements
3. **Conclusion and perspectives**

Take-home messages

GraphiT

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- Promising interpretation for graphs.

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Kernel methods

- Reconcile deep learning with smaller data regimes!
- Understanding architectures via a different lens.

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In constrained data regime, inductive biases such as kernel methods are still useful!

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- OTKE beaten by ESM [Rives et al., 2019].
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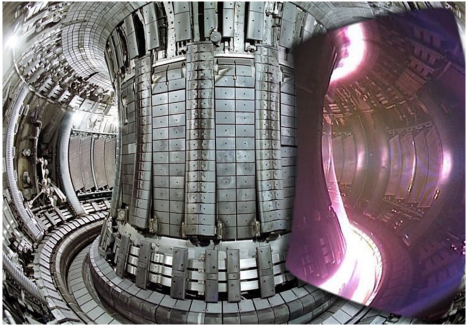
But in real life?

- AlphaFold2: physically motivated inductive biases.

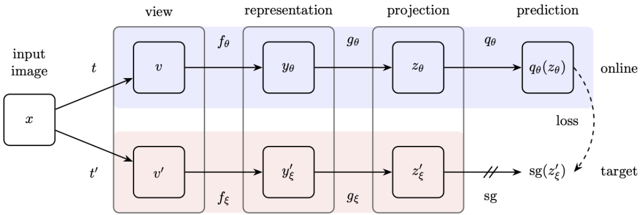
But in real life?



Seek progress elsewhere?

Inductive biases can be found in learning paradigms...

- Invariant Risk Minimization [Arjovsky et al., 2020].
- Data augmentation and loss in Self-supervised learning [He et al., 2020, Caron et al., 2020, Grill et al., 2020, Zbontar et al., 2021].



BYOL (from Grill et al.).

Thank you!

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