# Designing Transformers with Kernel Methods

Grégoire Mialon

FAIR

# 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 Msc MVA, ENS Paris-Saclay
- Since 2018: PhD student at Inria and ENS, Paris, advised by Julien Mairal and Alexandre d'Aspremont.

# What I have been doing in the past 3.5 years

**Kernel methods and deep learning in the small/medium data regime.**

- 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).

**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 the small/medium data regime.**

- 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).

# Motivation: designing strong models even when labelled data is scarce

**Learning with few data is one of the biggest problems in machine learning.**

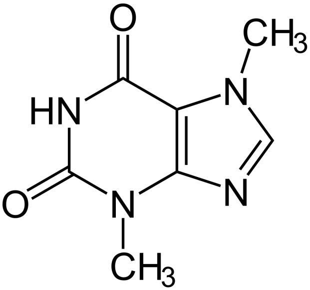
- A path towards better models.
- Or, simply because there is too few available data.

# How to design strong models in the small data regime?

# Outline: Encoding inductive bias within trainable architecture with kernel methods

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

# Graph data are an important research topic




A molecule of theobromin, or why chocolate is so good.

**Graph data are very valuable...**

- Proteins in computational biology.
- Molecules in chemoinformatics.
- Shapes in computer vision and computer graphics, etc.

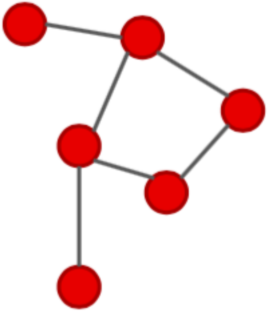
**... but delicate to handle.**

- 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.



GNN, layer k

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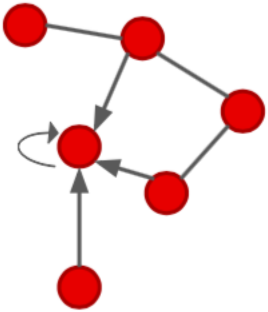

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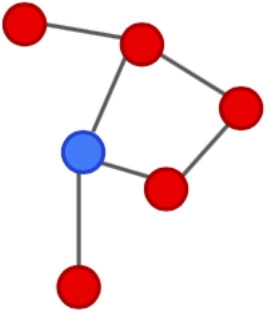
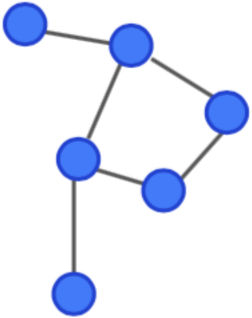


GNN, layer k+1 (for one node)

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

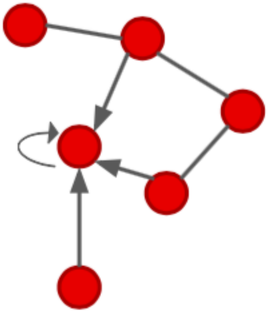


GNN, layer k+1

# Current limitations of GNNs

**In GNNs, messages flow between neighbors only.**

- Exploits the structure of the graph.
- But $n$ layers for $n$-hop neighbors to interact.
- Oversmoothing [Hamilton, 2020].



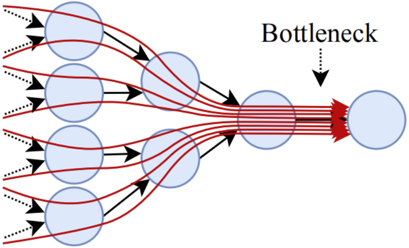
Only neighboring nodes communicate.

# Current limitations of GNNs

**In GNNs, messages flow between neighbors only.**

- Exploits the structure of the graph.
- But $n$ layers for $n$-hop neighbors to interact.
- Oversmoothing [Hamilton, 2020].
- Long-range interactions?
  Oversquashing [Alon and Yahav, 2021].

**Transformers perform global aggregation!**

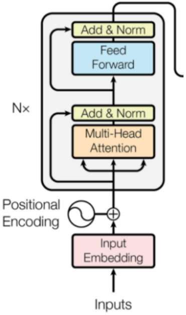



An illustration of oversquashing
(From Alon and Yahav, 2020).

# Transformers

**Why transformers?**

- Initially introduced in natural language processing [Vaswani et al., 2017, Devlin et al., 2019].
- Bioinformatics [Rives et al., 2019].
- Computer vision [Dosovitskiy et al., 2021].
- Transformers put into question the paradigm "one data modality, one preferred architecture".




Transformer encoder
(from Vaswani et al., 2017)

# Transformers

**Transformer encoder.**

- A sequence of layers processing an input set of $n$ elements $X$ in $\mathbb{R}^{n \times d_{\text{in}}}$, and compute another set in $\mathbb{R}^{n \times d_{\text{out}}}$.
- Self-attention mechanism:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_{out}}}\right) V \in \mathbb{R}^{n \times d_{\text{out}}}, \tag{1}$$

  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.
- During forward pass, feature map $X$ updated via:

$$X = X + \text{Attention}(Q, K, V).$$

- LayerNorm then "element-wise" feed-forward.
- Repeat.

# Kernel smoothing interpretation

**Self-attention as a kernel smoothing.**

- We can rewrite self-attention:

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

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

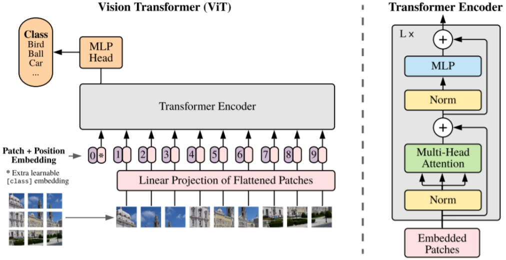
with $Q_i = W_Q X_i$, $K_j = W_K X_j$, $v(X_j) = W_V X_j$, $k$ a non-negative kernel function: we get a kernel smoothing.

**Different choices for $k$ suggest different transformers architectures [Tsai et al., 2019].**

# Transformers for graphs require position encoding

**Inductive bias of transformers for graphs?**

- All input elements are allowed to communicate.
- Self-attention layer is permutation equivariant.
- Hence, position encoding often required.
- Not trivial for graphs!

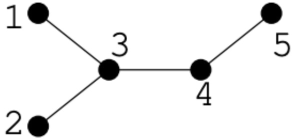



Vision transformer (from [Dosovitskiy et al., 2021])

# Previous attempts at using transformers with graphs

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

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



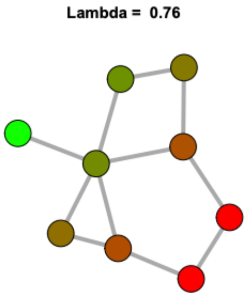

$$L = D - A = \begin{pmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ -1 & -1 & 3 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

(From Vert, 2021)

# 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 $u_i$.
- "Discrete equivalent" to sine/cosine Fourier basis in $\mathbb{R}^n$ and associated frequencies.

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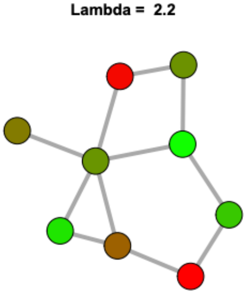


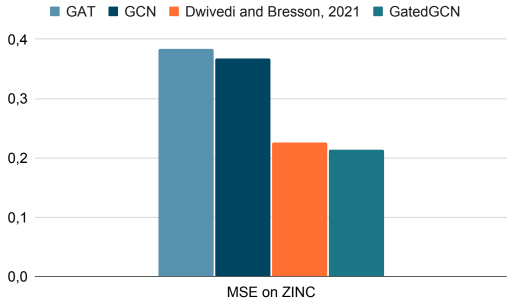

(From Vert, 2021)

# Promising results but...

**Problems with Laplacian absolute PE.**

- Flipping sign at training.
- Bounded by size of smallest graph.
- Do these vectors transfer between different graphs?

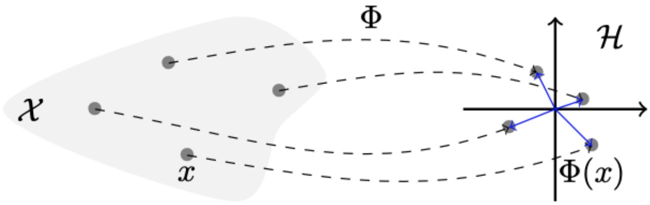
**Can we improve graph structure encoding in transformers?**



# 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




(From Bietti, 2019)

**Learning with Kernel methods**

- Map data $x$ to high-dimensional space, $\Phi(x) \in \mathcal{H}$ (RKHS).
- $\Phi$ associated to a positive definite kernel $K$: $K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$.
- Convex optimization for learning linear decision function in the RKHS (non-linear in the original space, kernel trick).

# Kernels on graphs

**Laplacian based kernels [Smola and Kondor, 2003].**

- Define a rich family of p.d. kernels on the graph by applying a regularization function $r$ to the spectrum of $L$

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

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

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

- Interpretation in terms of diffusion of a substance in the graph, controlled by $\beta$.
- Discrete equivalent of the Gaussian kernel, a solution to the heat equation in the continuous setting, hence its name.

# Kernels on graphs reflect structural similarity between nodes

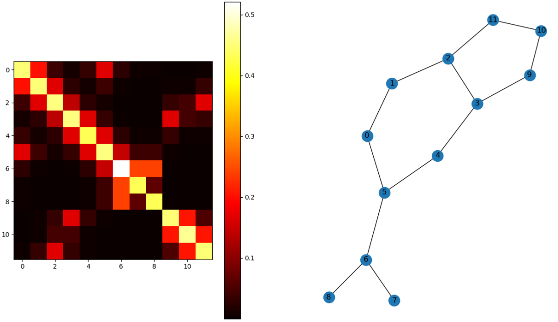



Figure 1: Diffusion kernel between the nodes of a MUTAG sample graph ($\beta = 1$).

**Use kernel matrix to modulate self-attention!**

# Mechanism 1: node position encoding with kernels on graphs

**Regular attention.**

- Self-attention layer

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

- During forward pass, feature map $X$ is updated as follows:

$$X = X + \text{Attention}(Q, V). \quad (4)$$

**Remark.** As in [Tsai et al., 2019], we use the same matrices for $Q$ and $K$.

# Mechanism 1: node position encoding with kernels on graphs

**Modulated attention.**

- Self-attention layer becomes

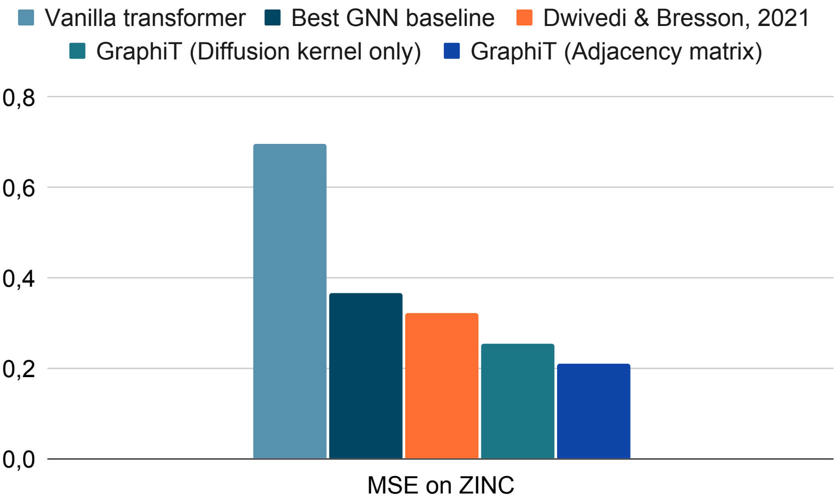
$$\text{PosAttention}(Q, V, K_r) = \text{normalize}\left(\exp\left(\frac{QQ^\top}{\sqrt{d_{\text{out}}}}\right) \odot K_r\right) V \in \mathbb{R}^{n \times d_{\text{out}}}, \tag{5}$$

  with the same $Q$ and $V$ matrices, and $K_r$ a kernel on the graph.
- During forward pass, feature map $X$ is updated as follows:

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

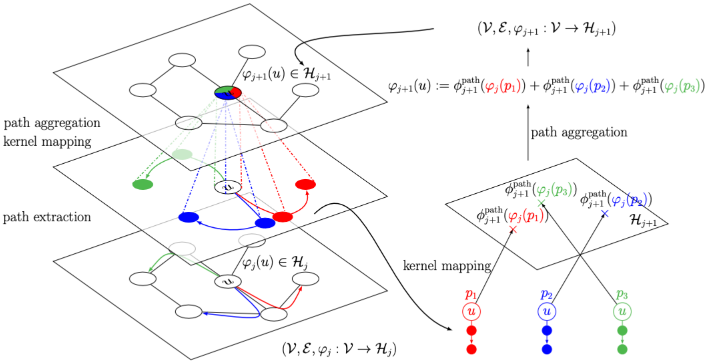
  with $D$ the matrix of node degrees and $K_r$ a kernel on the graph.

# Graph kernels allow effective position encoding



# Mechanism 2: leveraging substructures via path embedding

- Substructures: carry local positional information and content, *e.g* walks, subtrees, graphlets.
- Heavily used within graph kernels [Borgwardt et al., 2020].



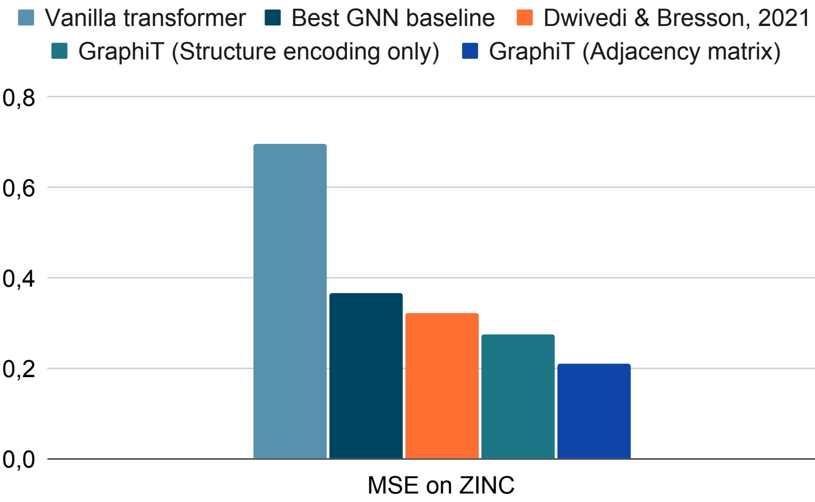

(from Chen et al., 2020)

# Leveraging substructures via path embedding

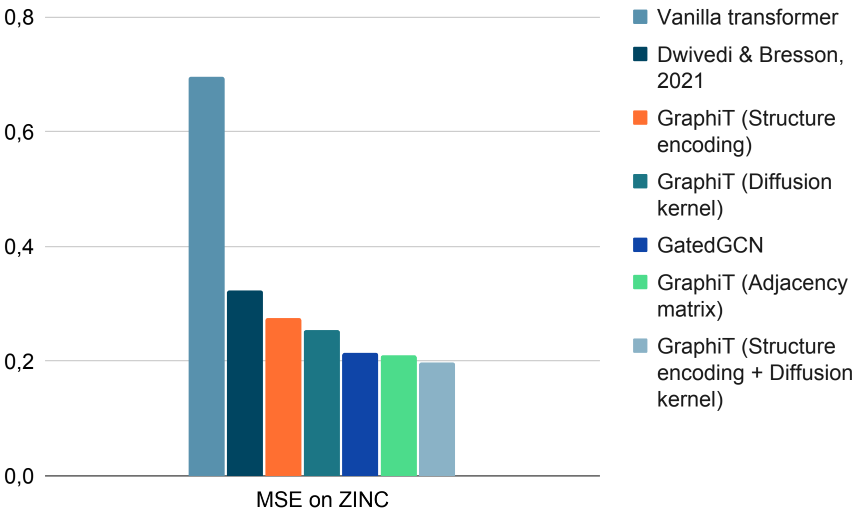
**In practice.**

- Encoding local substructure around node $u$ using method from [Chen et al., 2020].
- Add the resulting vector to the feature vector of $u$ at the transformer input.
- Somehow similar approach in [Dosovitskiy et al., 2021].

# Substructures are an effective inductive bias



# GraphiT is able to outperform popular GNNs



# GraphiT captures meaningful interactions

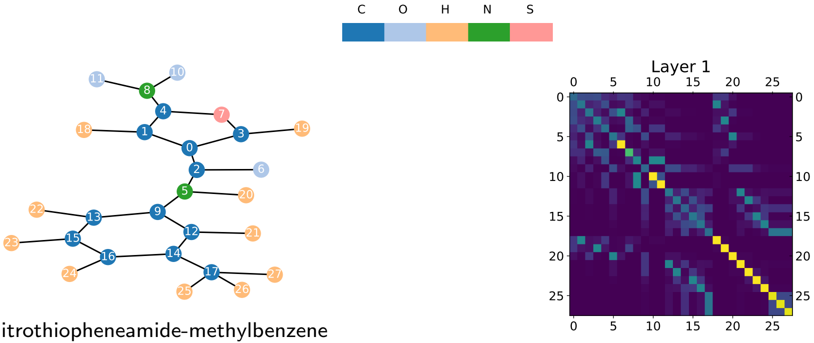



Figure 2: *Left*: A molecule from the Mutagenicity data set [Kersting et al., 2016]. *Right*: approximate diffusion kernel for the molecular graph.

# GraphiT captures meaningful interactions

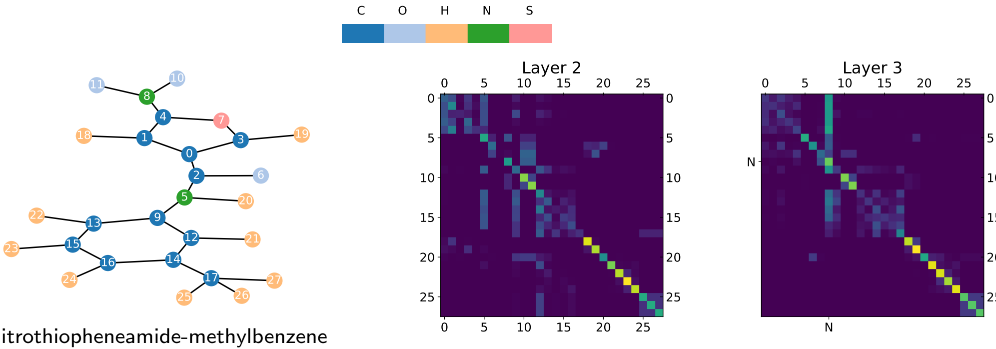
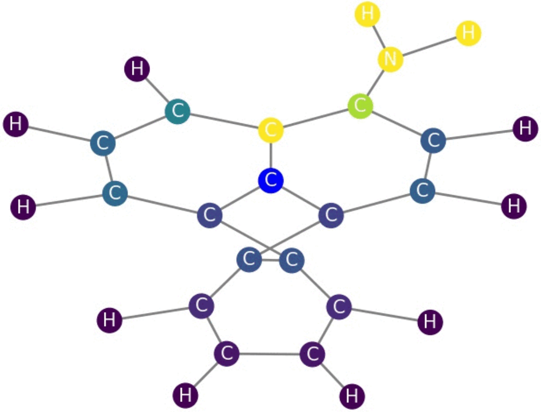



Figure 3: *Left*: A molecule from the Mutagenicity data set [Kersting et al., 2016]. *Right*: nodes 8 (N of $NO_2$) is salient. $NO_2$ group is known for its mutagenetic properties. The attention scores are averaged by heads.

Attention from C atom



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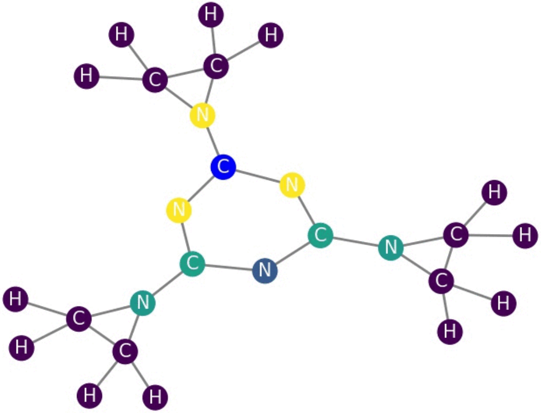

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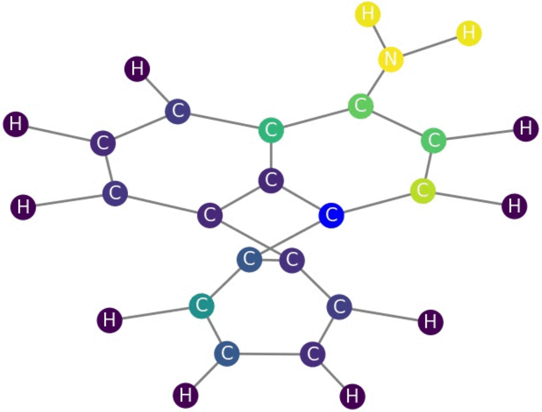
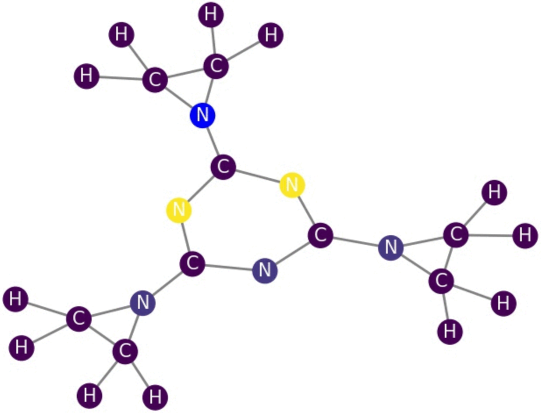


Attention from N atom



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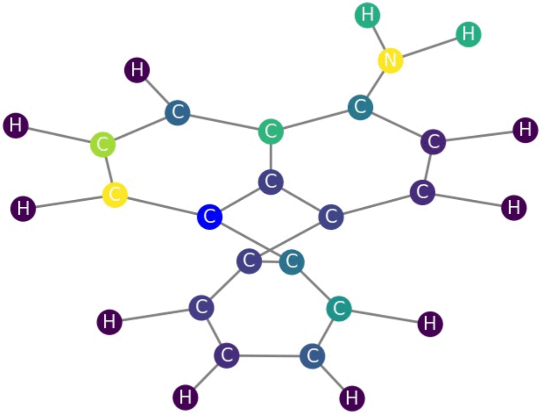

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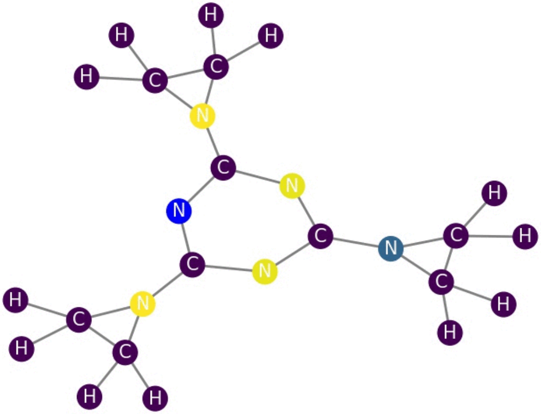

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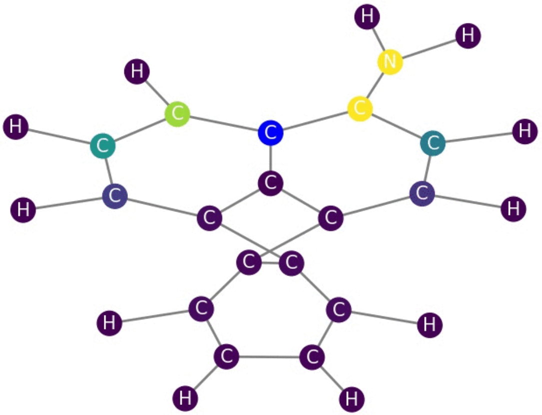

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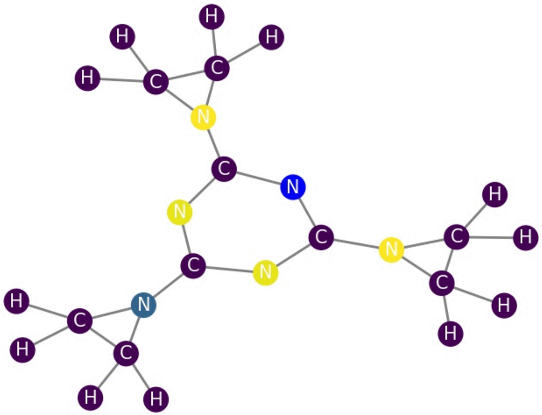

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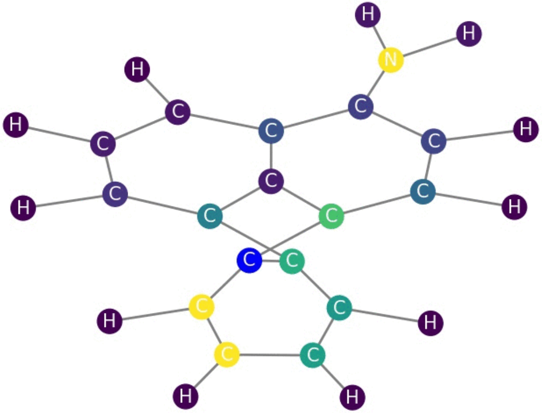

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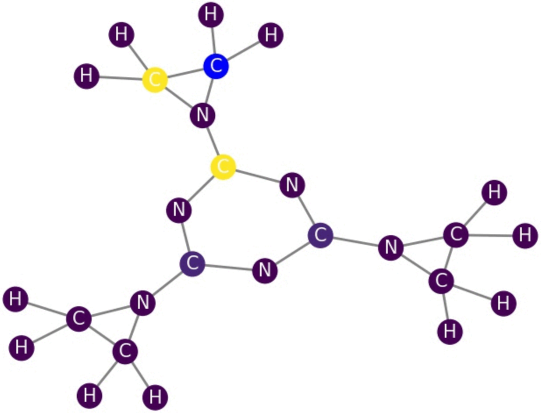

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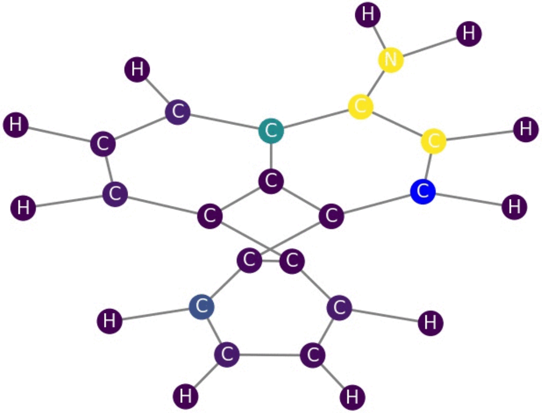

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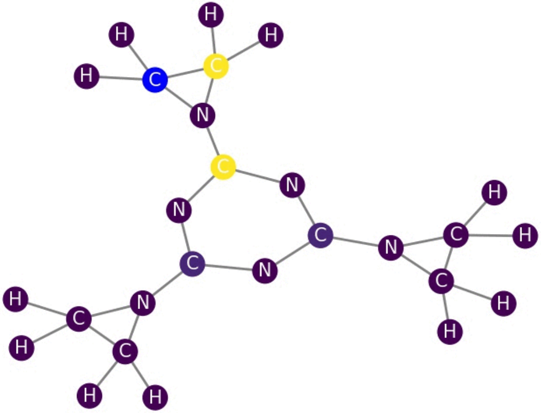

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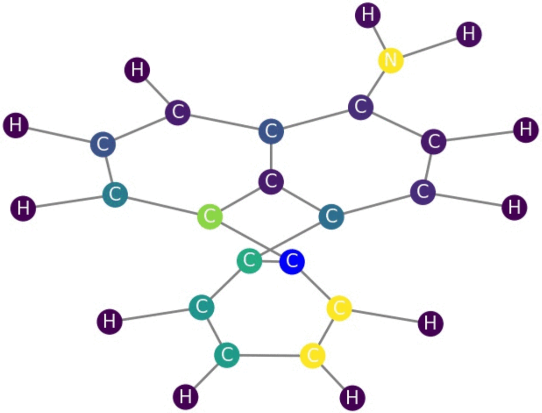

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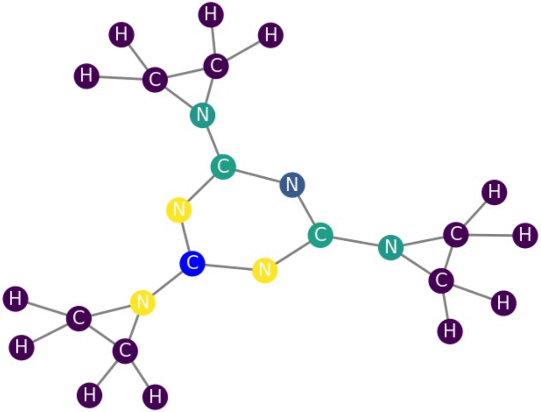

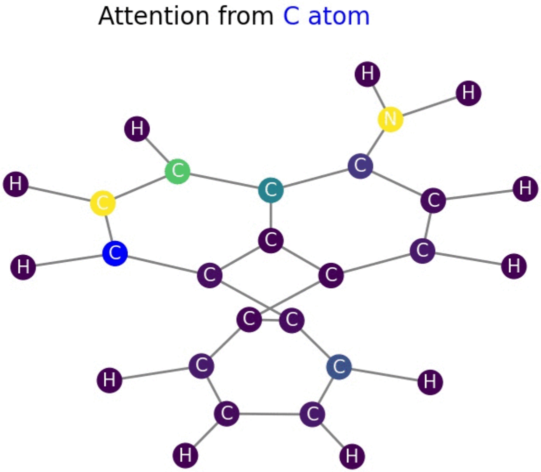
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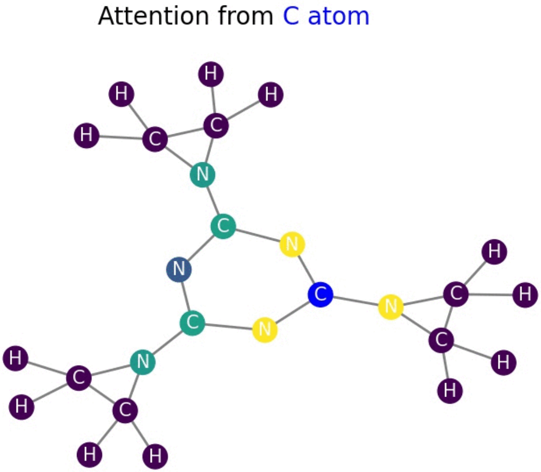
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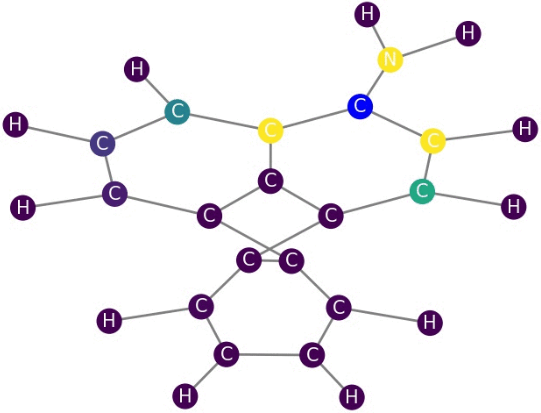
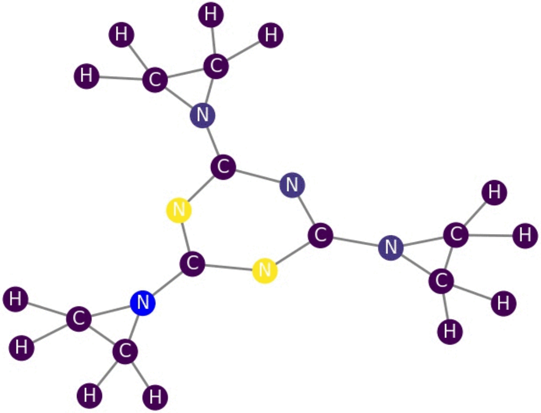


Attention from N atom



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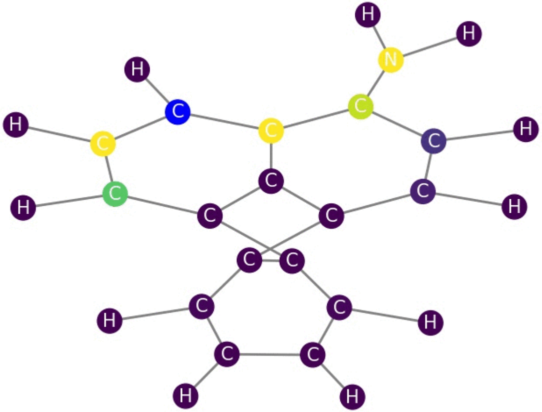

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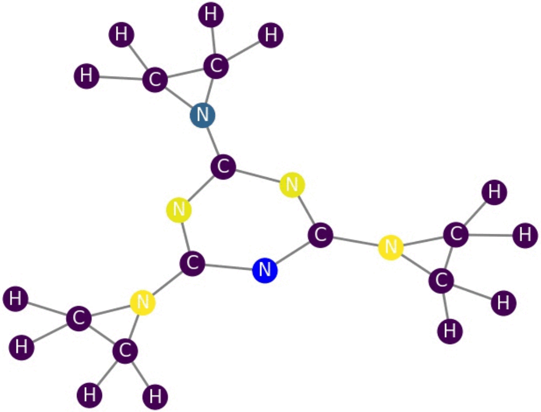
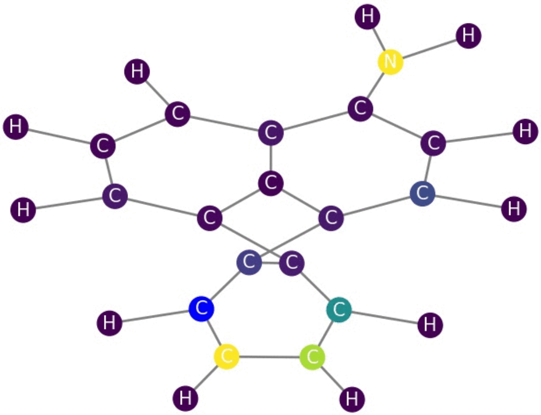
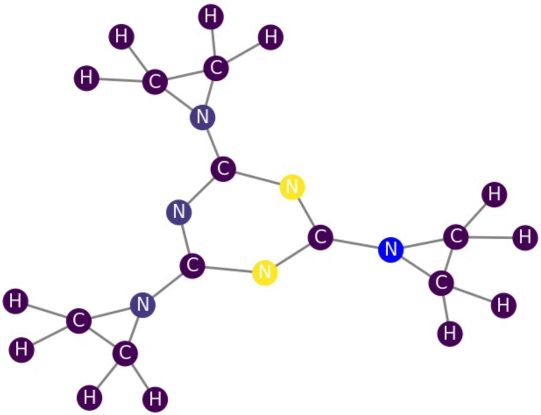


Attention from C atom




Attention from N atom



# Inductive bias of GraphiT is competitive, but has its limitations

**Small scale datasets.**

- Varying results with graph kernel and parameter.

**Larger scale datasets: OGB [Hu et al., 2020].**

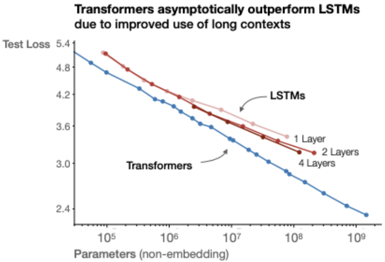
**Quadratic cost of self-attention.**

- What about large graphs?
- Recent line of work on efficient tranformers [Tay et al., 2020].

# Perspectives of GraphiT

**GraphiT opens exciting questions.**

- Scaling laws of graph transformers?
- Interactions with self-supervised learning for graphs? [Zhu et al., 2020, Thakoor et al., 2021]
- Leverage visualization for real-life applications?
- Graph transformers are currently an active domain of research [Ying et al., 2021, Kreuzer et al., 2021, Choromanski et al., 2021a].




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

# Back to the smoothing formula

**Self-attention as a kernel smoothing.**

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

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.

- We replaced $k(X_i, X_j)$ by $k(X_i, X_j) \times K_r(i, j)$. $k$ based on node content, $K_r$ based on node structural similarity.
- Related to relative positional encoding [Shaw et al., 2018].

**What if we pick another similarity measure?**

# Outline

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

# Sets are also an important data modality

**Sets can be found in various domains.**

- 3D shape recognition (point clouds).
- Protein sequences (set of features where order matters) in computational biology.
- Sentences in NLP.

**Common characteristics with graphs.**

- Size may vary.
- Potential interactions between elements.

# Let's focus on biological sequences

**Biological sequences may pose more problems: SCOP 1.75 [Murzin et al., 1995].**

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

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 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.

# Our sequences require specific embedding

**Existing methods do not yield satisfactory results for our data.**

- Kernel methods for sets [Lyu, 2004]: not expressive enough.
- Transformers, deep architectures for sets [Lee et al., 2019, Skianis et al., 2020]: empirically mixed results.

**How to represent sets with low data and memory requirements?**

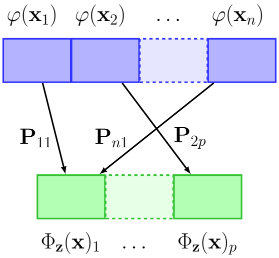
# Our contribution: OTK, a data-efficient embedding for sets

**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`

# OTK: a data-efficient embedding for sets

**Global, similarity-based pooling.**

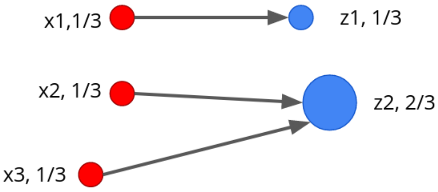
- Input set or sequence X.
- Element-wise, non-linear embedding $\varphi$.
- Pool elements $\varphi(x_i)$ in bins via weighted sums.
- To each p bin corresponds a prototype (parameter) $z_j, j = 1 \ldots p$.
- Pooling weights P reflect similarity between x and z.



# Our notion of similarity: optimal transport

**What is optimal transport?**

- Pooling weights P: optimal transport plan between X and Z.
- Most efficient way of transporting a mass distribution to another.
- Finding the transport plan minimizing a transportation cost.
- GPU-friendly solvers [Sinkhorn and Knopp, 1967, Cuturi and Doucet, 2013].




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

# Our notion of similarity: optimal transport

**Two interpretations**

- Empirically: better than dot-product.
- Embeds the set in a space where $\ell_2$ 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.**

- Z can be learned with or without supervision.

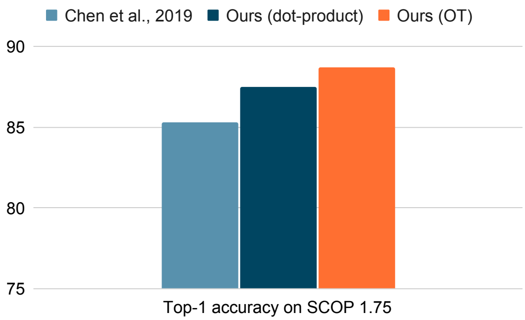
**A linearized variant of attention.**

- Kernel smoothing: we replaced $\frac{k(Q_i, K_j)}{\sum_{j'=1}^{n} k(Q_i, K_{j'})}$ by $\mathrm{P}_{\kappa}(X, Z)_{ij}$.
- Linear in the number of input elements.
- Similar ideas in efficient transformers [Wang et al., 2020, Choromanski et al., 2021b].

# OTKE: (temporarily) sota for two bioinformatics tasks

**SCOP 1.75**

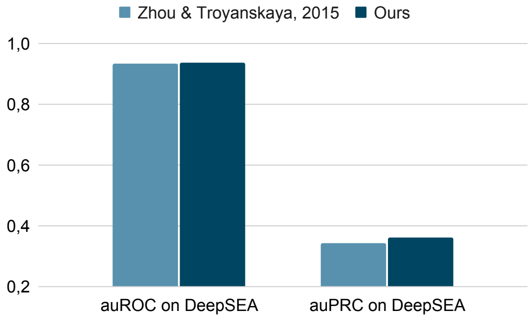
- Classify protein folding from amino-acid sequence.



# OTKE: (temporarily) sota for two bioinformatics tasks

**DeepSEA**

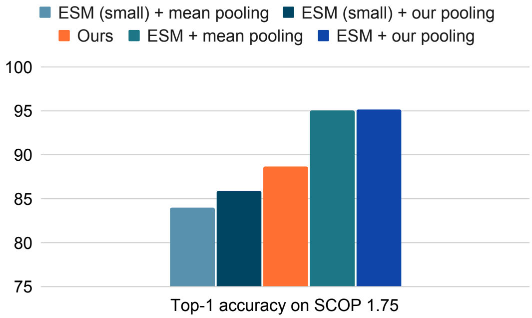
- Predicting chromatin profile from raw genomic sequence.



# What about pre-training?

**During ICLR rebuttal...**

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



# Limitations and further work

**As an embedding.**

- Multi-layer version not trivial.
- Outperformed by available pre-trained model.

**As an adaptive pooling mechanism for deep architectures?**

- Improved pooling for graph representation [Kolouri et al., 2021] or protein representation (ICLR rebuttal).
- Dot-product instead of computationally more intensive OT?

# Outline

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

# How to design strong models in smaller data regimes?

**GraphiT**

- Inductive bias of transformers is valid with graph with small/medium scale datasets.
- Attention provides promising intepretation tools for graphs.

**OTK Embedding**

- Dealing with long sequences with few data.
- Interesting pooling mechanism connected to the recent line of work efficient transformers.
- Challenged by transfer learning from pre-trained models.

**Kernel methods**

- Reconciles deep learning with smaller data regimes!
- Understanding architectures via a new lens.

# Are inductive biases still useful?

**In the small data regime, inductive biases such as kernel methods are still useful!**

- Pre-training is not always possible.
- Not all domains have large data.
- Even when large unlabelled data is available, self-supervised learning frameworks may be not mature enough.

# Are inductive biases still useful?

**But in the large data regime?**

- OTK beaten by ESM [Rives et al., 2019].
- ResMLP [Touvron et al., 2021], DeiT [Touvron et al., 2020], BiT [Kolesnikov et al., 2020].
- In the large data regime, the bitter lesson of machine learning seems more true than ever.

# What about learning paradigms?

**Inductive biases are elsewhere.**

- 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].

Thank you!

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