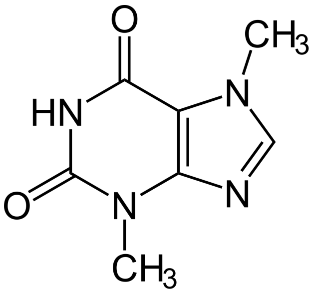
Transformers on graphs: challenge and perspectives

Grégoire Mialon

SGDMAL, Rennes. 21 juin 2022

Joint work with: Dexiong Chen (ETH Zürich), Margot Selosse, Julien Mairal (Inria).

Graph data are an important research topic



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- Molecules in chemoinformatics.

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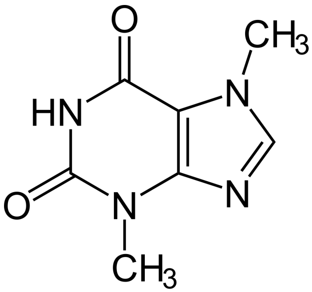

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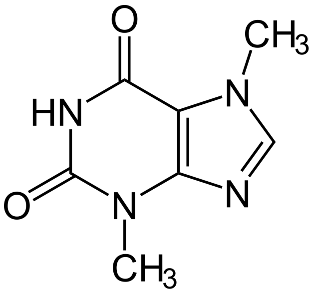

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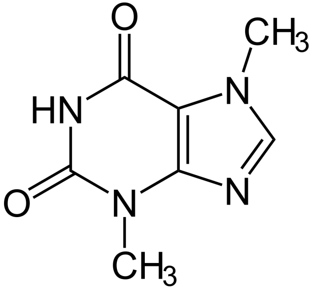

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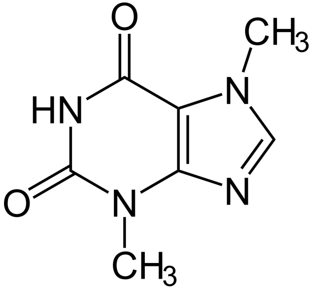
...but delicate to exploit.

- Non-Euclidean structure.

Success and current limits of neural networks for graphs



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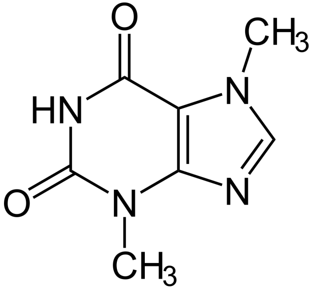

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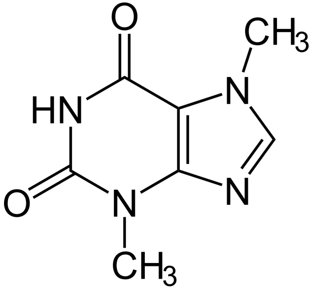

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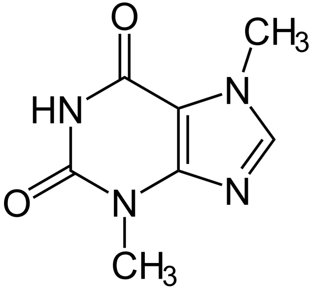

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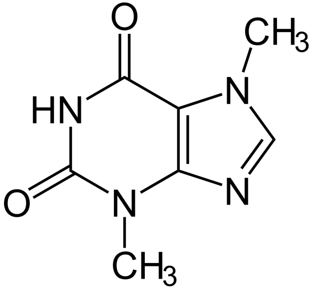

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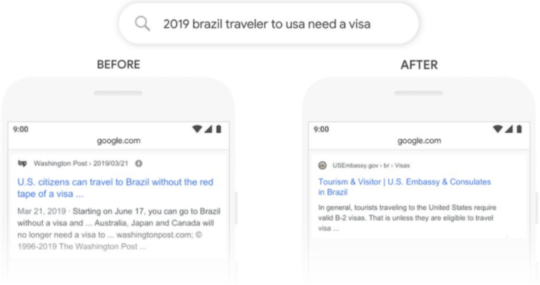
Let us connect all the nodes!

Transformers: a scalable, multi-purpose architecture



Improved web search engines.

"Vibrant portrait painting of Salvador Dalí with a robotic half face".

Transformers for graph are tempting but not straightforward

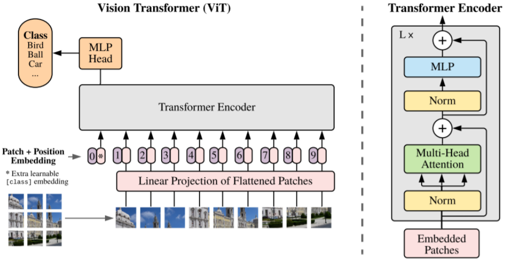


Image transformer (from [Dosovitskiy et al., 2021]).
Input: image seen as a set of patches.
Output: class label.

Success of transformers [Vaswani et al., 2017].

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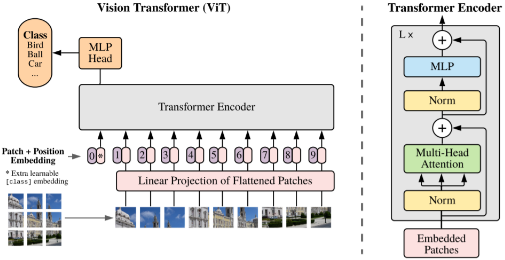

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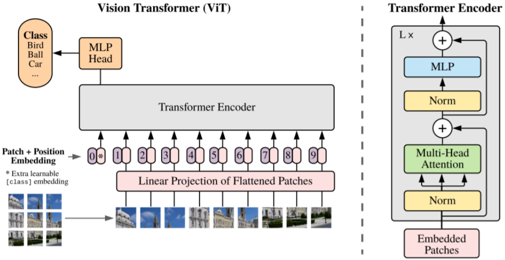

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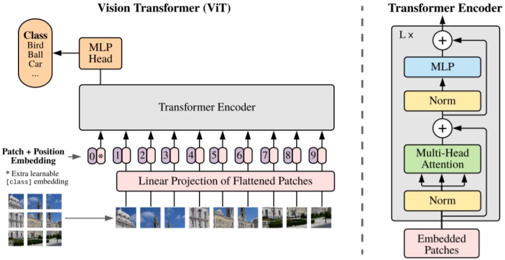

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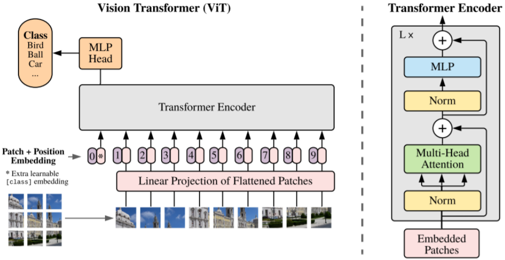

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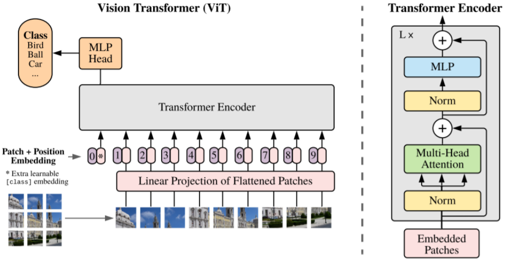

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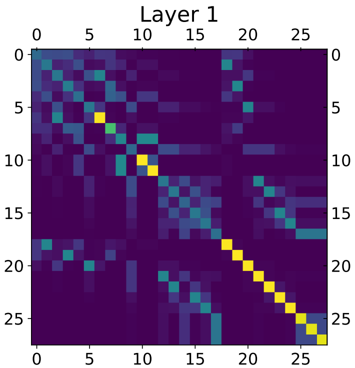
How to provide information on the structure of the graphs?

One example: GraphiT, encoding graph structure in transformers



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

[Mialon et al., 2021]

We propose two mechanisms:

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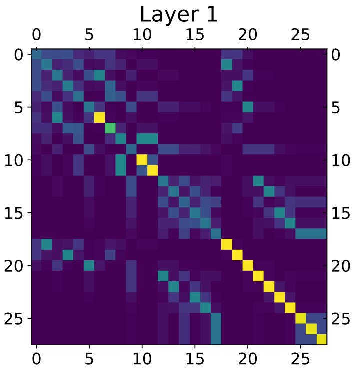

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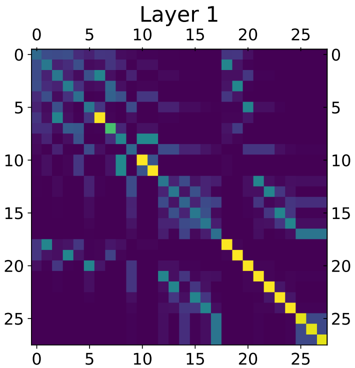

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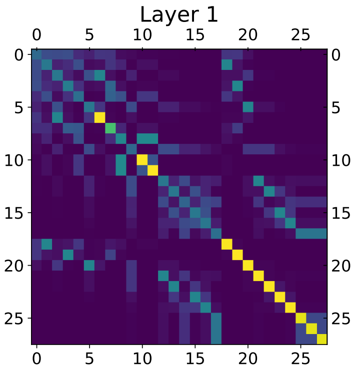

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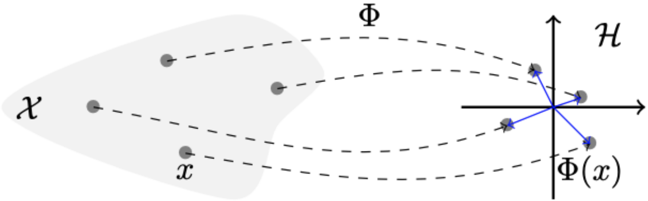
- Modulating attention with **kernels on the graph** [Tsai et al., 2019, Kondor and Vert, 2004].
- Encoding **local neighborhood** of each node [Chen et al., 2020].
- Possible to encode edge features in both mechanisms.

Reminder: Kernel methods



(From Bietti, 2019)

Learning with Kernel methods.

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

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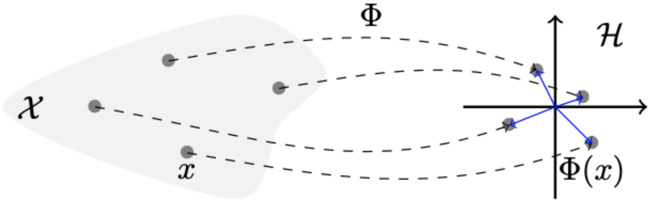

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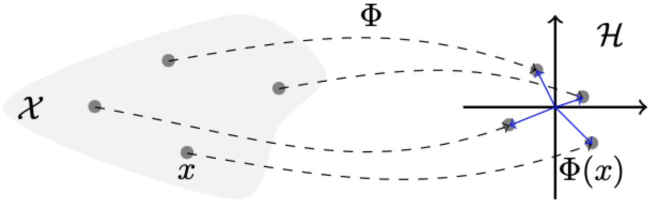

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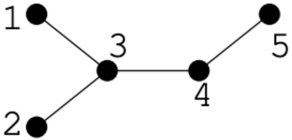
- A surrogate for Φ can be learned with or without supervision [Williams and Seeger, 2001].

Reminder: Graph Laplacians



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

(From Vert, 2021)

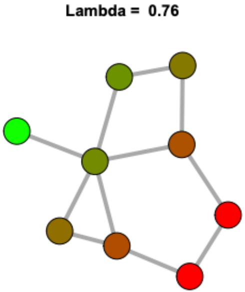
The Laplacian is a representation of the graph.

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

Reminder: Graph Laplacian

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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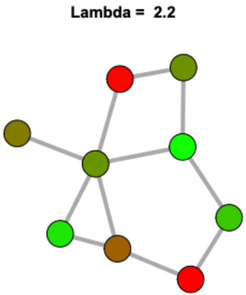

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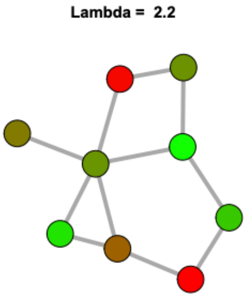

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"Discrete equivalent" to sine/cosine Fourier basis in $\mathbb{R}^n$.

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

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

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

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

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

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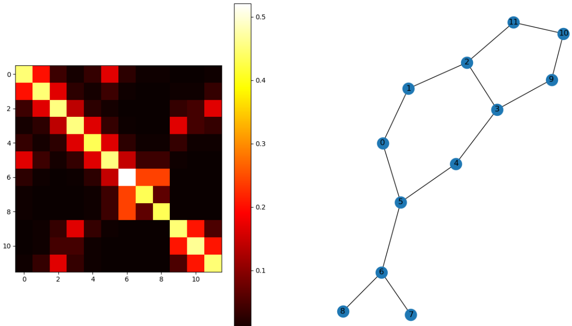
- Discrete equivalent of the Gaussian kernel, a solution to the heat equation in the continuous setting.

Kernels on graphs provide smooth structural similarity between nodes



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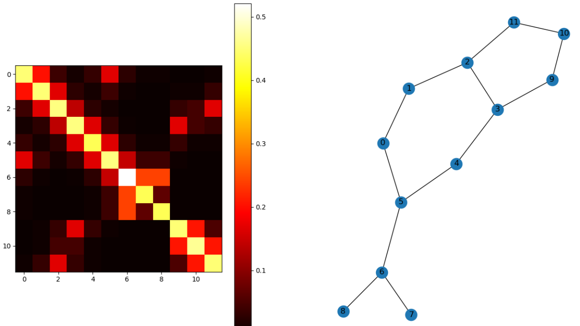

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Use kernel matrix to modulate self-attention!

Mechanism 1: node position encoding with kernels on graphs

Regular attention.

- Self-attention:

$$\text{Attention}(Q, V) = \text{normalize}\left(\exp\left(\frac{QQ^\top}{\sqrt{d_{\text{out}}}}\right)\right) V \in \mathbb{R}^{n \times d_{\text{out}}}. \tag{2}$$

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

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  with K_r a kernel on the graph.
- Feature map X gets:

$$X = X + D^{-\frac{1}{2}} \text{PosAttention}(Q, V, K_r), \quad (5)$$

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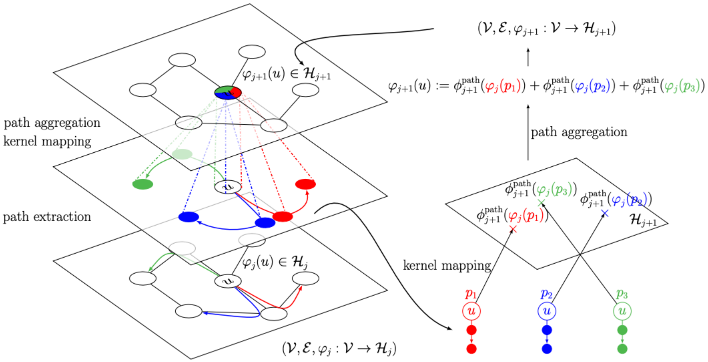
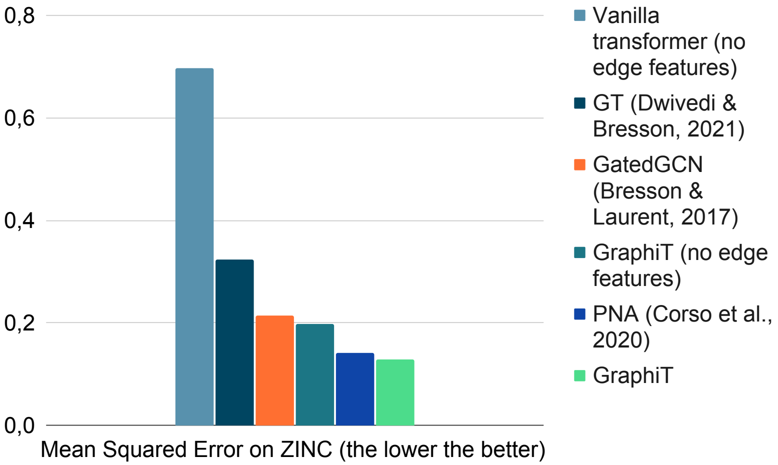
- Augmenting node features u using kernel neighborhood encoding [Chen et al., 2020].
- Kernel encoding learned with or without supervision.



(from Chen et al.)

GraphiT is able to outperform popular GNNs

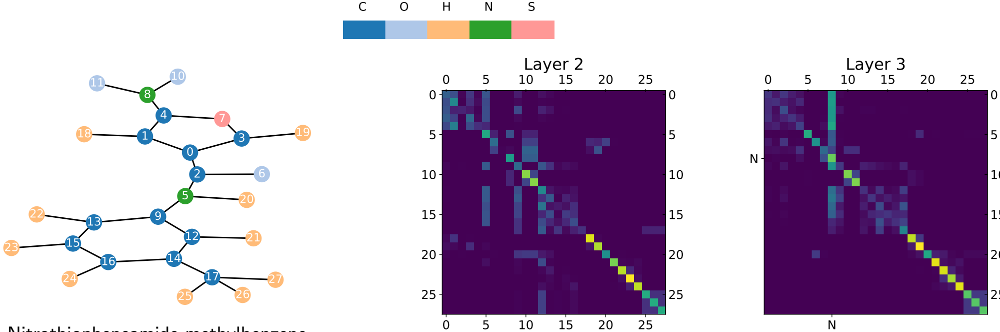
ZINC (12k graphs, regression): Predicting the constrained differential solubility of molecules.



[Mialon et al., 2021]

GraphiT captures meaningful interactions

Mutagenicity: 4k samples (binary classification).



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.

[Mialon et al., 2021]

Related work

There are many ways to incorporate graph structure into the transformer.

- Position encoding with eigenvectors of L [Dwivedi and Bresson, 2021].
- Fully learned position encoding [Ying et al., 2021].
- Message passing with position encoding [Dwivedi et al., 2021].
- And many others! [Kreuzer et al., 2021, Choromanski et al., 2021] . . .

Scaling to larger datasets

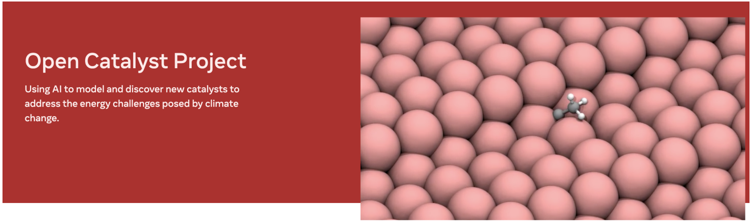
PCQM4M-LSC 2021 [Hu et al., 2020]:

- Goal: chemistry knowledge gain by pre-training.
- Task: predict an energy gap of molecules from DFT simulations.
- 3.8M graphs.
- Winner: (Ensemble of) Graphormer [Ying et al., 2021].
- 47M parameters per model.
- ? on NVIDIA V100 GPUs on Microsoft Azure Cloud.

Scaling to larger datasets

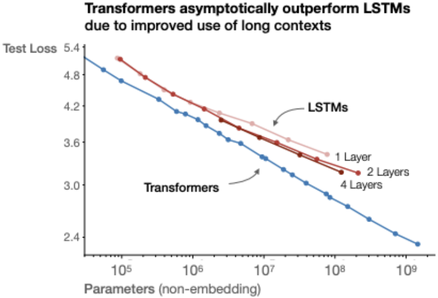
Open Catalyst 2020 [Zitnick et al., 2020]:

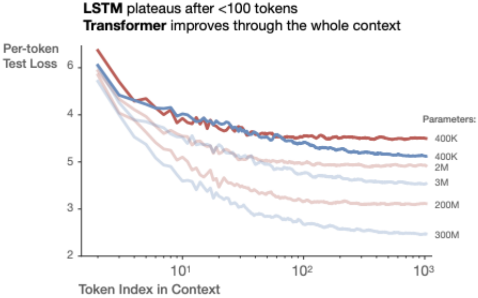
- Goal: accelerating catalyst discovery for systems such as renewable fertilizer, energy storage.
- Task: predicting an adsorbate-catalyst energy from simulations.
- 140M structure-energy estimation.
- Winner: Graphormer [Ying et al., 2021].
- 150M parameters?
- 1.5 days on 8 Nvidia A100.



Conclusion

- Inductive bias of transformers is valid for graphs.
- Promising interpretation capabilities.
- Scaling laws with respect to graphs?





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