Designing Transformers with Kernel Methods

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What I am interested in

Kernel methods and deep learning

- G. Mialon*, D. Chen*, M. Selosse*, J. Mairal. Structural Graph Transformers (to appear on arXiv).
- 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).

Causal inference

What I want to talk about today

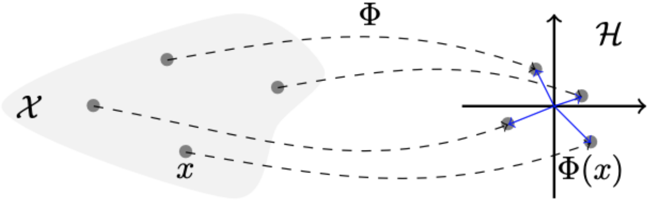
Kernel methods and transformers

- G. Mialon*, D. Chen*, M. Selosse*, J. Mairal. Structural Graph Transformers (to appear on arXiv).
- G. Mialon*, D. Chen*, A. d'Aspremont, J. Mairal. A Trainable Optimal Transport Embedding for Feature Aggregation and its Relationship to Attention (ICLR, 2021).

Why kernel methods?

- Reconciling deep learning with small data regimes.
- Understanding architectures with a kernel lens.

Kernel methods



Learning with Kernel methods

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

Transformers, self-attention, and kernel smoothing

Transformers (encoder).

- A sequence of layers processing an input set of d_{in} features 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 and "element-wise" feed-forward.

Transformers, self-attention, and kernel smoothing

Self-attention as a kernel smoothing.

- We can rewrite self-attention:

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

$$= \sum_{j=1}^{n} \frac{k(Q_i, K_j)}{\sum_{j'=1}^{n} k(Q_i, K_j)} V_j \in \mathbb{R}^{d_{\mathrm{out}}},$$

with k a non-negative kernel function, which can be seen as a kernel smoothing.

Kernel construction.

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

Self-attention for large (biological) sequences

Dealing with small datasets of large sequences.

- Sequence: a set of features with 1-D positional information.
- Important applications, *e.g*, protein sequences in bioinformatics.
- Long-range and potentially complex dependencies between elements.
- Varying size of the sequences.

Biological sequences bring two more problems.

- Long sequences (1000+ base pairs).
- Few labeled data (e.g, 20 samples per class for SCOP1.75).

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LDKVEAEVQIDRLITG
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Figure 1: Short part of mRNA sequence for the SARS-Cov-2 spike protein (each symbol represents an amino-acid).

Self-attention for large (biological) sequences

Transformers are delicate to use in this setting.

- Attractive inductive bias.
- Small amount of data.
- Memory issues for large sequences (although recently alleviated by the *efficient transformers* line of work, see [Tay et al., 2020]).

We propose a self-attention like embedding for sequences [Mialon et al., 2021a].

- Our embedding will provide a natural notion of pooling.
- The attention weights will be the output of a matching operation.
- We choose optimal transport, as it benefits from a rich theory and efficient solvers.

Optimal Transport

Distributing mass with minimal cost.

- Let a in Δ^n (probability simplex) and b in $\Delta^{n'}$ be weights of the discrete measures $\sum_i \mathrm{a}_i \delta_{\mathrm{x}_i}$ and $\sum_j \mathrm{b}_j \delta_{\mathrm{x}'_j}$ with respective locations x and x', where δ_{x} is the Dirac at position x.
- Let C in $\mathbb{R}^{n \times n'}$ be a pairwise cost matrix.
- The entropic regularized Kantorovich relaxation of OT from x to x' is

$$\min_{\mathrm{P} \in U(\mathrm{a},\mathrm{b})} \sum_{ij} \mathrm{C}_{ij}\mathrm{P}_{ij} - \varepsilon H(\mathrm{P}), \tag{2}$$

with $H(\mathrm{P}) = -\sum_{ij} \mathrm{P}_{ij}(\log(\mathrm{P}_{ij}) - 1)$ is the entropic regularization with parameter ε (controls sparsity of P), and U is the space of admissible couplings between a and b:

$$U(\mathrm{a},\mathrm{b}) = \{\mathrm{P} \in \mathbb{R}_+^{n \times n'} : \mathrm{P}1_n = \mathrm{a} \text{ and } \mathrm{P}^\top 1_{n'} = \mathrm{b}\}.$$

- Typically solved using Sinkhorn's algorithm [Sinkhorn and Knopp, 1967, Cuturi, 2013].
- In practice, a and b will be uniform measures.

Constructing a self-attention embedding

Optimal Transport Embedding and Kernel. Let $X \in \mathbb{R}^{n \times d}$, a sequence of features. κ a p.d. kernel with associated embedding φ.

- We define our embedding $\Phi_Z \in \mathbb{R}^{p \times d}$ as

$$\Phi_Z(X) = \sqrt{p} \times \mathrm{P}_\kappa(X, Z)^\top \varphi(X).$$

- $\mathrm{P}_\kappa(X, Z)$ the OT plan between X with cost $-\kappa$ and a learned reference $Z \in \mathbb{R}^{p \times d}$ item $\varphi(X) := [\varphi(\mathrm{X}_1), \dots, \varphi(X_n)]^\top$, with $\varphi : \mathbb{R}^d \to \mathcal{H}$
- Its associated p.d. kernel is

$$K_Z(X, X') = \sum_{i,j} \mathrm{P}_{\kappa,Z}(X, X')_{ij} \kappa(X_i, X'_j),$$

with $\mathrm{P}_{\kappa,Z}(X, X') := p \times \mathrm{P}_\kappa(X, Z)\mathrm{P}_\kappa(X', Z)^\top$.

Constructing a self-attention embedding

Kernel interpretation of our embedding.

- $\mathsf{P}_{\kappa,Z}(X, X')$: valid transport plan [Peyré and Cuturi, 2019], rough approximation of $\mathsf{P}_{\kappa}(X, X')$.
- K_Z is a p.d. surrogate for $K_{\mathrm{OT}}(X, X') = \sum_{i,j} \mathsf{P}_{\kappa}(X, X')_{ij} \kappa(X_i, X'_j)$.
- K_{OT} induces the 2-wasserstein distance and is not p.d. [Rubner et al., 2000].

Getting back to the kernel smoothing formula.

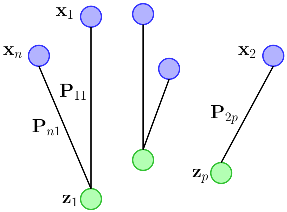
- We replaced $\frac{k(Q_i, K_j)}{\sum_{j'=1}^{n} k(Q_i, K_{j'})}$ by $\mathsf{P}_{\kappa}(X, Z)_{ij}$.

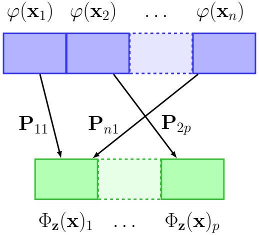
Result: a pooled self-attention embedding

- We introduced

$$\Phi_Z(X) = \sqrt{p} \times \mathrm{P}_\kappa(X, Z)^\top \varphi(X),$$

  which simultaneously embeds and pools elements of an input sequence.
- Non-linear embedding via φ.
- Pooling via P_κ, similar elements are pooled together.
- Natural notion of pooling by choosing $p < n$.





Result: a pooled self-attention embedding

Learning our embedding.

- Without supervision: simple k-means for Z and a tractable approximation of φ [Mairal, 2016].
- With supervision: back-propagating through a few steps of Sinkhorn iterations for Z. Classical back-propagation for a tractable approximation of φ [Mairal, 2016].

Extensions.

- Relative position encoding.
- Multi-head.

Experiments

SCOP1.75: Protein fold classification. $\sim$ 20000 samples, $\sim$ 1000 labels, many sequences longer than 1000 base pairs.

Table 1: Classification accuracy (top 1/5/10) on test set for SCOP 1.75 for different unsupervised and supervised baselines, averaged from 10 different runs. (q references $\times$ p supports).

Method	Unsupervised	Supervised
DeepSF [Hou et al., 2019]	Not available.	73.0/90.3/94.5
CKN [Chen et al., 2019a]	81.8±0.8/92.8±0.2/95.0±0.2	84.1±0.1/94.3±0.2/96.4±0.1
RKN [Chen et al., 2019b]	Not available.	85.3±0.3/95.0±0.2/96.5±0.1
Set Transformer [Lee et al., 2019]	Not available.	79.2±4.6/91.5±1.4/94.3±0.6
Approximate Rep the Set [Skianis et al., 2020]	Not available.	84.5±0.6/94.0±0.4/95.7±0.4
Ours (dot-product instead of OT)	78.2±1.9/93.1±0.7/96.0±0.4	87.5±0.3/95.5±0.2/96.9±0.1
Ours (Unsup.: 1 × 100 / Sup.: 5 × 10)	**85.8±0.2/95.3±0.1/96.8±0.1**	**88.7±0.3/95.9±0.2/97.3±0.1**

Discussion

Connection to transformers

- Relationship to efficient transformers [Kitaev et al., 2020].
- Kernel methods vs. few-shot learning with pre-trained models for biological sequences [Rives et al., 2019].

Code

- Freely available at `https://github.com/claying/OTK`.

Learning on graph data

Graph data are very valuable.

- Proteins in computational biology [Senior et al., 2020].
- Molecules in chemoinformatics [Duvenaud et al., 2015].
- Shapes in computer vision and computer graphics [Verma et al., 2018], etc.

Graph Neural Networks (GNNs).

- Originally introduced as an extension of convolutions for graph-structured data [Scarselli et al., 2008].
- Message passing paradigm in which vectors (messages) are exchanged (passed) between neighboring nodes whose representations are updated using neural networks.
- Many strategies to aggregate features of neighboring nodes [Bronstein et al., 2017, Duvenaud et al., 2015].
- De facto architecture for graph structured data.

Challenging GNNs with Structural Graph Transformers

GNNs and transformers are tightly connected, but...

- GNNs are the standard architecture for learning on graphs. Inductive bias: message passing between neighbors.
- Transformers: all input elements are allowed to communicate.
- Self-attention layer is permutation invariant, hence the need for structure encoding.

How to provide the transformer with graph structural information?

- Structural Graph Transformers [Mialon et al., 2021b]

Two mechanisms for providing transformers with graph structural information

Relative node position encoding.

- Position encoding: adding positional only information to the feature vector of an input node or to the attentions scores.
- As opposed to sequences or images, encoding positions of the elements in a graph is not trivial.
- [Dwivedi and Bresson, 2021] proposed absolute position encoding strategy based on the eigenvectors of the Laplacian. Blind spot with respect to transferability between graphs.

Leveraging substructures.

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

First mechanism: Relative position encoding with kernels on graphs

Spectral graph analysis.

- The Laplacian of a graph with n nodes defined as $L = D - A$. D is a $n \times n$ diagonal matrix of node degrees and A the adjacency matrix.
- Eigenvalue decomposition $L = \sum_i \lambda_i u_i u_i^\top$.
- The eigenvalue $\lambda_i = u_i^\top L u_i$ characterizes the amount of oscillation of the corresponding eigenvector u_i (a function on the nodes).
- For this reason, this decomposition is viewed as the discrete equivalent to the sine/cosine Fourier basis in $\mathbb{R}^n$ and associated frequencies.

Remark. Very often, the normalized Laplacian $I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$ is used instead of L, which does not change the above interpretation.

First mechanism: Relative position encoding with kernels on graphs

Kernels on graphs.

- It is possible to define a family of p.d. kernels on the graph [Smola and Kondor, 2003] by applying a regularization function r to the spectrum of L.
- We get a rich class of kernels

$$K_r = \sum_{i=1}^{m} r(\lambda_i) u_i u_i^\top, \tag{3}$$

  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.

First mechanism: Relative position encoding with kernels on graphs

Diffusion Kernel [Kondor and Vert, 2004].

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

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

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

First mechanism: Relative position encoding with kernels on graphs

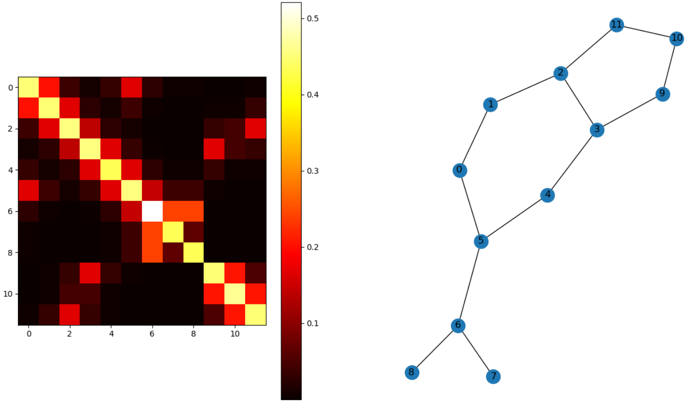


Figure 3: Diffusion kernel between the nodes of a MUTAG sample graph ($\beta = 1$).

First mechanism: Relative position encoding with kernels on graphs

Modulating the attention scores.

- Self-attention layer becomes

$$\text{PosAttention}(Q, V, K_r) = \text{normalize}\left(\exp\left(\frac{QQ^\top}{\sqrt{d_{\text{out}}}}\right) \odot K_r\right) V \in \mathbb{R}^{n \times d_{\text{out}}}, \tag{4}$$

  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:

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

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

Remark. As opposed to absolute position encoding, the model does not rely on the transferability of eigenvectors between different Laplacians.

First mechanism: Relative position encoding with kernels on graphs

Back to the kernel smoothing formula.

- We replaced $k(Q_i, K_j)$ by $k(Q_i, K_j) \times K_r(X_i, X_j)$.
- As observed in [Tsai et al., 2019] for sequences, this is an approach related to relative positional encoding [Shaw et al., 2018].

Second mechanism: Leveraging substructures via kernel embedding of paths

Graph convolutionnal kernel networks (GCKN) [Chen et al., 2020].

- Let us consider a graph G with n nodes, $\mathcal{P}_k(u)$ the set of paths shorter than or equal to k that start with node u, and p in $\mathcal{P}_k(u)$ will denote the concatenation of all node features encountered along the path.
- A layer of GCKN defines a feature map X in $\mathbb{R}^{n \times d}$ such that

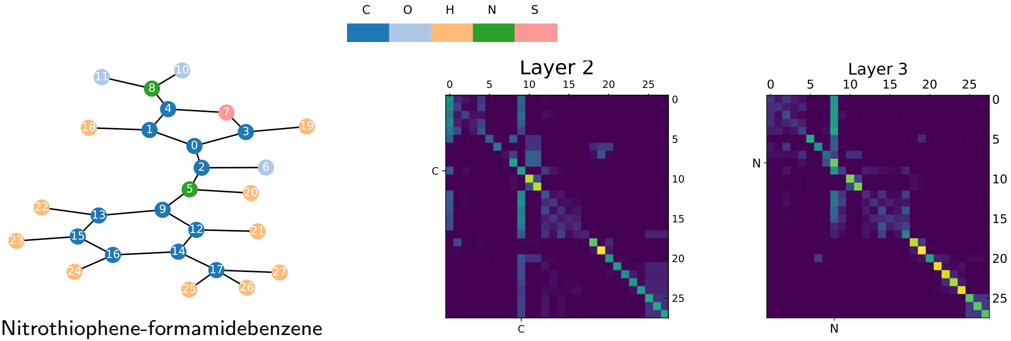
  $$X(u) = \sum_{p \in \mathcal{P}_k(u)} \psi(p),$$

  with $X(u)$ the column of X corresponding to node u and ψ is a d-dimensional embedding of the path features p.
- We encode a node as the sum of its features and those produced by one GCKN layer.

SGT is able to outperform popular GNNs

Method / Dataset	MUTAG	PROTEINS	PTC	NCI1	ZINC (no edge feat.)
Size	188	1113	344	4110	12k
Max. number of nodes	28	620	109	111	37
GCN [Kipf and Welling, 2017]	78.9±10.1	75.8±5.5	54.0±6.3	75.9±1.6	0.367±0.011
GAT [Veličković et al., 2018]	80.3±8.5	74.8±4.1	55.0±6.0	76.8±2.1	0.384±0.007
GIN [Xu et al., 2019]	82.6±6.2	73.1±4.6	55.0±8.7	**81.7±1.7**	0.387±0.015
[Dwivedi and Bresson, 2021]	83.9±6.5	70.1±3.2	57.7±3.1	80.0±1.9	0.323±0.013
Transformers (T)	82.2±6.3	75.6±4.9	58.1±10.5	70.0±4.5	0.696±0.007
T + LapPE	85.8±5.9	74.6±2.7	55.6±5.0	74.6±1.9	0.507±0.003
T + Adj PE	87.2±9.8	72.4±4.9	59.9±5.9	79.7±2.0	0.243±0.005
T + 2-step RW kernel	85.3±6.9	72.8±4.5	**62.0±9.4**	78.0±1.5	0.243±0.010
T + 3-step RW kernel	83.3±6.3	**76.2±4.4**	61.0±6.2	77.6±3.6	0.244±0.011
T + Diffusion kernel	82.7±7.6	74.6±4.2	59.1±7.4	78.9±1.6	0.255±0.010
T + GCKN	84.4±7.8	69.5±3.8	61.5±5.8	78.1±5.1	0.274±0.011
T + GCKN + 2-step RW kernel	90.4±5.8	72.5±4.6	58.4±7.6	81.0±1.8	0.213±0.016
T + GCKN + Adj PE	**90.5±7.0**	71.1±6.9	57.9±4.2	81.4±2.2	**0.211±0.010**

Patterns captured in the attention scores of SGT



Nitrothiophene-formamidebenzene

Figure 4: A molecule from the Mutagenicity data set [Kersting et al., 2016]. The attention scores are averaged by heads. *Left*: node 9 (C of aromatic cycle) is salient. *Right*: nodes 8 (N of NO_2) and 17 (C of CH_3) are salient. NO_2 is known for its mutagenetic properties.

Conclusions

Kernel methods

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

Optimal Transport Embedding

- Dealing with long sequences with few data.
- Connection to the recent line of work efficient transformers.
- Challenged by few-shot learning with pre-trained models.

Structural Graph Transformers

- Inductive bias of transformers is valid with graph.
- Attention provides promising intepretation tools.

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