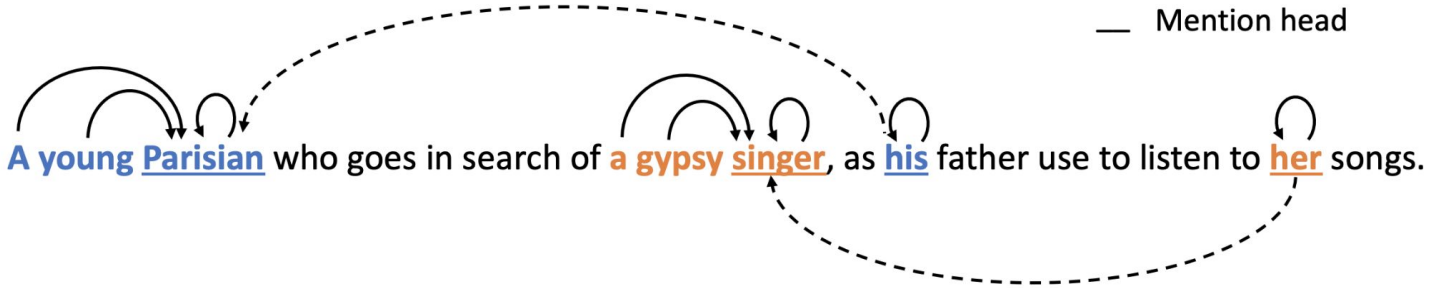
Transformers as Graph-to-Graph Models

Andrei Catalin Coman

Graphs in Transformers



- Transformers are essentially latent graph processing models, with sequences just being a special case.
- Attention weights are functionally equivalent to graph edges, since they determine how information propagates.
- Attention weights are computed from a set of vectors.
- Graphs are encoded in Transformers' set-of-vector embeddings.

James Henderson, Alireza Mohammadshahi, Andrei Coman, and Lesly Miculicich. 2023. Transformers as Graph-to-Graph Models. In Proceedings of the Big Picture Workshop, pages 93–107, Singapore, Singapore. Association for Computational Linguistics.

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"Transformers are latent graph models"

Graph2Graph Transformers (G2GT)

- Our G2GT makes this graph processing ability explicit.
- Observed graphs are input to the attention weight computations as relation embeddings.
- Predicted graphs are output with attention-like functions.
- Latent graphs are computed by pretrained Transformer weights.

	A	young	Parisian	...	a	gypsy	singer	,	as	his	use	her	songs
A	0	0	0	0	0	0	0	0	0	0	0	0	0
young	0	0	0	0	0	0	0	0	0	0	0	0	0
Parisian	1	0	0	0	0	0	0	0	0	0	0	0	0
...	0	0	0	0	0	0	0	0	0	0	0	0	0
a	0	0	0	0	0	0	0	0	0	0	0	0	0
gypsy	0	0	0	0	0	0	0	0	0	0	0	0	0
singer	0	0	0	0	1	0	0	0	0	0	0	0	0
,	0	0	0	0	0	0	0	0	0	0	0	0	0
as	0	0	0	0	0	0	0	0	0	0	0	0	0
his	0	0	2	0	0	0	0	0	0	1	0	0	0
use	0	0	0	0	0	0	0	0	0	0	0	0	0
to	0	0	0	0	0	0	0	0	0	0	0	0	0
her	0	0	0	0	0	0	2	0	0	0	0	1	0
songs	0	0	0	0	0	0	0	0	0	0	0	0	0

query-key | query-relation | relation-key

$$e_{ij} = \frac{1}{\sqrt{d}}\left[x_i \boldsymbol{W^Q}(x_j \boldsymbol{W^K})^T + x_i \boldsymbol{W^Q}(r_{ij} \boldsymbol{W_1^R})^T + r_{ij} \boldsymbol{W_2^R}(x_j \boldsymbol{W^K})^T\right]$$

$$z_i = \sum_j \alpha_{ij}\underbrace{(x_j \boldsymbol{W^V} + r_{ij} \boldsymbol{W_3^R})}_{\text{value-relation}}$$

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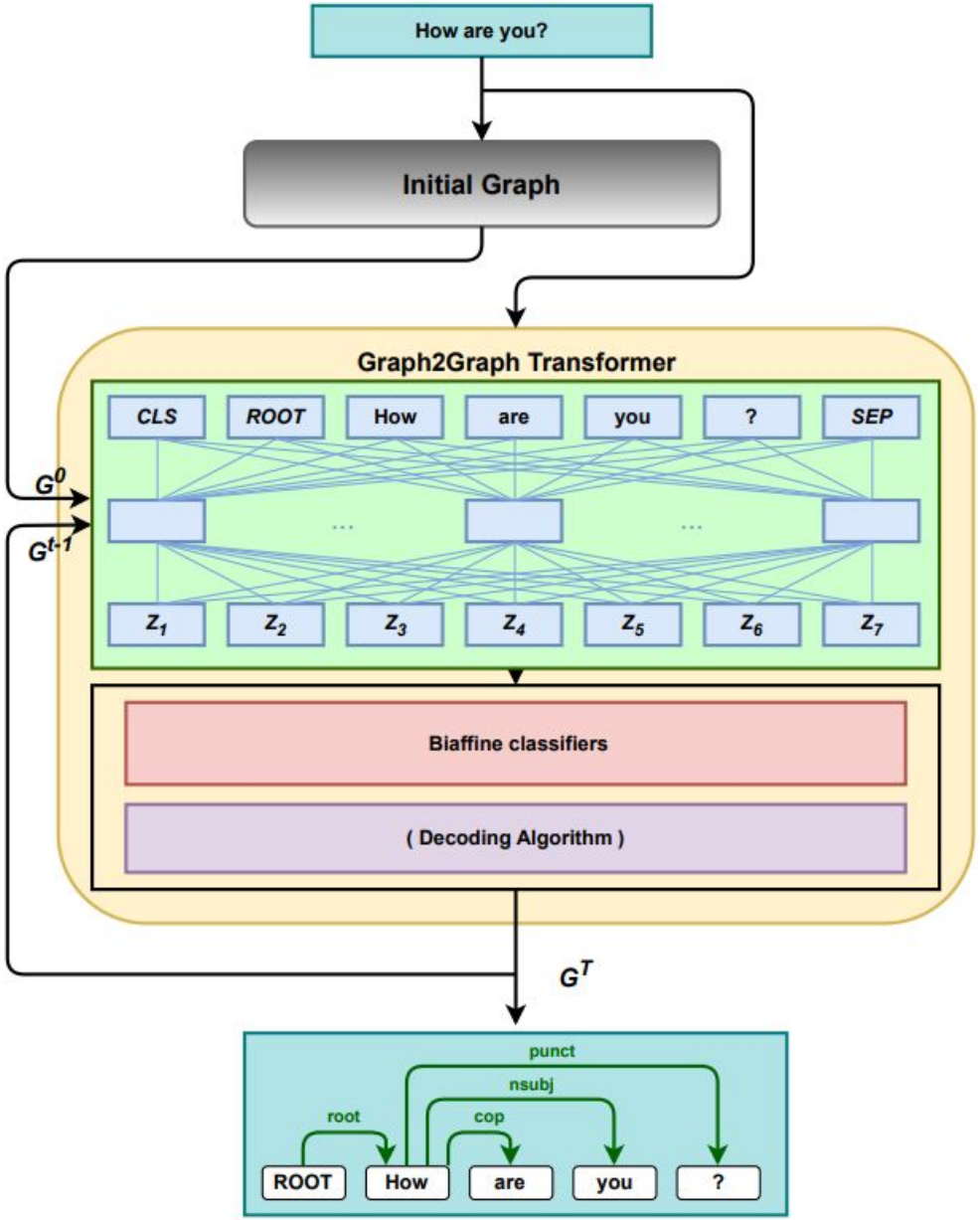
Efficient Global Graph Prediction

- G2GT encodes the observed graph, predicted graph, and latent graph in a single joint Transformer embedding.
- G2GT enables iterative refinement of the predicted graph to capture global patterns over the graph and text, without any bespoke pipeline or decoding strategy.



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