Unsupervised Dependency Graph Network

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Abstract

Recent work has identified properties of pretrained self-attention models that mirror those of dependency parse structures. In particular, some self-attention heads correspond well to individual dependency types. Inspired by these developments, we propose a new competitive mechanism that encourages these attention heads to model different dependency relations. We introduce a new model, the Unsupervised Dependency Graph Network (UDGN), that can induce dependency structures from raw corpora and the masked language modeling task. Experiment results show that UDGN achieves very strong unsupervised dependency parsing performance without gold POS tags and any other external information. The competitive gated heads show a strong correlation with human-annotated dependency types. Furthermore, the UDGN can also achieve competitive performance on masked language modeling and sentence textual similarity tasks [1].

1 Introduction

The goal of unsupervised dependency parsing is to induce dependency grammar from corpora that don't have annotated parse trees (Marecek, 2016). Although the task is difficult, one advantage of unsupervised methods is that they can leverage vast amount of unannotated raw corpus (Han et al., 2020). Thus, adapting the task into a pretraining framework is increasingly tempting. The induced dependency trees can also help solve other NLP problems such as unsupervised discourse parsing (Nishida and Nakayama, 2020), aspect-based sentiment analysis (Dai et al., 2021) and intent discovery (Liu et al., 2021). Furthermore, the task can also be used as a probe to verify cognitive theories for human language acquistition (Yang et al., 2020; Pate and Goldwater, 2013; Katzir, 2014; Solan et al., 2002).

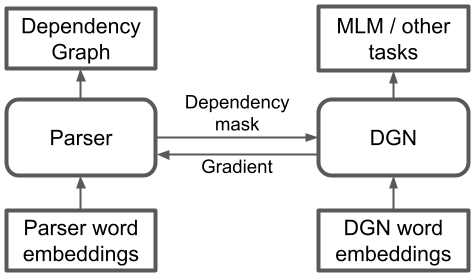

Figure 1: The architecture of Unsupervised Dependency Graph Network (UDGN). Given an input sentence, the parser can predict the dependency relation between tokens and generate a soft mask to approximate the undirected dependency graph. Conditioning on the mask, the DGN computes contextual word embeddings for the training task. Since the mask is soft, the gradient can be backpropagated from the DGN into the parser. Thus UDGN can induce grammar while training on masked language modeling or other downstream tasks.

Pretrained Language Models (PLMs) have become the foundation of modern natural language processing in the last few years (Bommasani et al., 2021). They dominate the most if not all NLP tasks. But Recent works show that, beyond pretraining big models on large-scale corpora, deep learning methods can improve performance by increasing models' awareness of syntactic information (Kuncoro et al., 2020). These methods either include known structural information as input to the model (Sundararaman et al., 2019; Bai et al., 2021), or incorporate structural prediction tasks into the training process (Wang et al., 2019a). However, these attempts require access to large datasets with supervised parses, which may be complicated and expensive.

Recent work also identified properties of pretrained self-attention models that mirror those of dependency parse structures (Htut et al., 2019; Hewitt

[1]Our code is publicly available at https://github.com/yikangshen/UDGN.

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and Manning, 2019; Jawahar et al., 2019). StructFormer (Shen et al., 2020) shows that a transformer-based model can induce a good dependency structure. The belief that linguistic structure may be embedded in these models is of interest to the community. Furthermore, Dai et al. (2021) shows that the induced trees from finetuned RoBERTa outperform parser-provided trees on aspect-based sentiment analysis tasks. This result brings interest to study task-specific structures. From this perspective, the unsupervised acquisition of dependency structure from raw data or downstream tasks appears important and feasible.

Traditionally, dependency grammars consider the dependency types (a.k.a. syntactic functions) as primitive and then derive the dependency graph (Debusmann, 2000). Every head-dependent dependency bears a syntactic function (Mel'cuk et al., 1988). Htut et al. (2019) shows that some attention heads in BERT (Devlin et al., 2018) and RoBERTa (Liu et al., 2019) track individual dependency types. In other words, these heads model different syntactic functions. Inspired by this observation and syntactic functions, we introduce *competitive gated heads* to model different syntactic parts and the process of selecting the proper syntactic function for each edge. These heads include two key components:

- A set of gated heads that model different information propagation processes between tokens;
- A competitive controller that selects the most suitable gated head for each pair of tokens.

Building on these components, we propose a novel architecture, the Unsupervised Dependency Graph Network (UDGN). As shown in Figure 1, the UDGN is composed of two networks: a *parser* that computes the dependency head distribution p_i for each word w_i in the input sentence and then converts it to a matrix of edge probability m_{ij} that approximates an undirected dependency graph; a *Dependency Graph Network* (DGN) that uses the edge probabilities $\{m_{ij}\}$ and competitive gated heads to propagate information between words to compute a contextualized embedding h_i for each word w_i. While training with the masked language modeling or other objectives, the gradient can flow through the DGN to the parser network through its dependence on m_{ij}. As a result, UDGN can induce a dependency grammar while solely relying on the masked language modeling objective.

In the experiment section, we first train the UDGN with masked language modeling, then evaluate it on unsupervised dependency parsing. Our experimental results show that UDGN can: 1) achieve very strong unsupervised parsing results among models that don't have access to extra annotations (including POS tags); 2) learn attention heads that are strongly correlated to human-annotated dependency types; 3) achieve competitive performance on language modeling tasks. We also finetune the pretrained UDGN on Semantic Textual Similarity (STS) tasks. Our experiments show that UDGN outperforms a Transformer baseline trained on the same corpus.

2 Related Work

Unsupervised dependency parsing Unsupervised dependency parsing is a long-standing task for computational linguistics. Dependency Model with Valence (DMV; Klein and Manning 2004) is the basis of several unsupervised dependency parsing methods (Daumé III, 2009; Gillenwater et al., 2010). Jiang et al. (2016) updates the method using neural networks to predict grammar rule probabilities. While previous methods mostly require additional Part-of-Speech (POS) information, Spitkovsky et al. (2011) tackled the issue by performing clustering based on word context information and then assigning the cluster ID to each word as their tag. He et al. (2018) incorporate an invertible neural network into DMV model to jointly model dependency grammar and word embeddings. Recently, NL-PCFG (Zhu et al., 2020) and NBL-PCFG (Yang et al., 2021) combined neural network and L-PCFG to achieve good performance in a joint unsupervised dependency and constituency parsing setting. StructFormer (Shen et al., 2020) proposes a joint constituency and dependency parser and uses the dependency distribution to regularize the self-attention heads in the transformer model. This joint parser-language model framework can induce grammar from masked language modeling tasks.

The UDGN's architecture is similar to StructFormer, both models include a parser and masked language model. Our model, however, has three major differences: 1) it uses competitive gated heads to improve models performance on grammar induction; 2) it uses a neural head selective parser that can produce both projective and non-projective dependency trees, whereas the distance parser in StructFormer can only produce projective

trees; 3) it uses a simplified method to generate an undirected dependency mask.

Transformers, Graph Neural Networks and Dependency Graphs In many Transformer-based models, attention masks are often used to limit the input tokens that a particular timestep can attend over. In Yang et al. (2019), for example, a mask derived from the permutation of inputs is used to induce a factorization over the tokens so that the resulting model is a valid probabilistic model. This attention mask can be viewed as an adjacency matrix over a graph whose nodes are the input tokens. From this perspective, Transformers are a form of Graph Neural Network (Scarselli et al., 2008) — specifically, a Graph Attention Network (GAT; Veličković et al. 2017), as it attends over the features of its neighbors. Several works have made this connection, and integrated dependency structures into transformers (Ahmad et al., 2021; Wang et al., 2019b; Tang et al., 2020). Results from Omote et al. (2019) and Deguchi et al. (2019) suggest that embedding these structures can improve translation models.

However, these dependency parses may not always be present to be used as input to the model. Strubell et al. (2018) trains the self-attention to attend the syntactic governor (head) of a particular token, resulting in a model that does not require dependency structure as input during inference time. We take a further step in our work and attempt to learn these structures in an unsupervised fashion from the MLM objective.

Differentiable Structured Prediction While the head selection is a good approximation of a tree structure, there are methods to obtain a relaxed adjacency matrix as the output of the parser. Previous work have used such methods for predicting structure. Koo et al. (2007) proposed using the Kirchoff matrix tree theorem for dependency parsing. They explain how the marginals of the edge potentials are computed, and these marginals have properties similar to a tree adjacency matrix (sum over the marginals are equal to $N-1$ for example, where N is the length of the sentence). Eisner (2016) describes how backpropagation can be used to compute marginals of some structured prediction algorithm. We also tried using the Kirchhoff method to normalize our dependency distributions in Appendix A.3. Corro and Titov (2018) uses similar notions but relaxes projective trees using Gumbel-softmax. Kim et al. (2017) proposed a structured form of attention and show that they are useful for certain sequence-to-sequence tasks. Mensch and Blondel (2018) gives a general theoretical treatment for these types of relaxations, while Paulus et al. (2020) gives a practical treatment of possible applications for these methods.

3 Model Architecture

As shown in Figure 2, the parser computes a dependency head distribution for each token and then converts it to a soft dependency mask m_{ij}. The DGN takes m_{ij} and the sentence as input and uses a competitive mechanism to propagate information between tokens.

3.1 Head Selective Parser

We use a simplified version of the Dependency Neural Selection parser (DENSE; Zhang et al. 2016) that only predicts unlabelled dependency relations. The parser takes the sentence $\mathbf{s} = w_1 w_2 ... w_T$ as input, and, for each token w_i, it produces a distribution p_i over all tokens in the sentence, resulting in a $T \times T$ weight matrix.

The parser first maps the sequence of tokens $w_1 w_2 ... w_T$ into a sequence of embeddings $[\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_T]$. Then the word embeddings are fed into a stack of a bidirectional LSTM (BiLSTM):

$$\mathbf{h}_i = \text{BiLSTM}(\mathbf{x}_i) \tag{1}$$

where $\mathbf{h}_i$ is the output of the BiLSTM at i-th timestep. Linear transforms are applied to the output of the BiLSTM to extract head and dependent information.

$$\mathbf{h}_i^{\text{H}} = \mathbf{W}_{\text{H}} \mathbf{h}_i + \mathbf{b}_{\text{H}} \tag{2}$$

$$\mathbf{h}_i^{\text{D}} = \mathbf{W}_{\text{D}} \mathbf{h}_i + \mathbf{b}_{\text{D}} \tag{3}$$

To map the head and dependents, we use bilinear attention:

$$e_{ij} = \frac{\mathbf{h}_i^{\text{D}} \mathbf{h}_j^{\text{H}}}{\sqrt{D}} \tag{4}$$

$$p_{ij} = \frac{\exp(e_{ij})}{\sum_k \exp(e_{ik})} \tag{5}$$

where p_{ij} is the probability that w_i depends on w_j, D is the dimension of hidden states. During the inference for parsing, the Chu-Liu/Edmonds' algorithm (Chu and Liu, 1965b) is used to extract the most likely directed dependency graph from the matrix p.

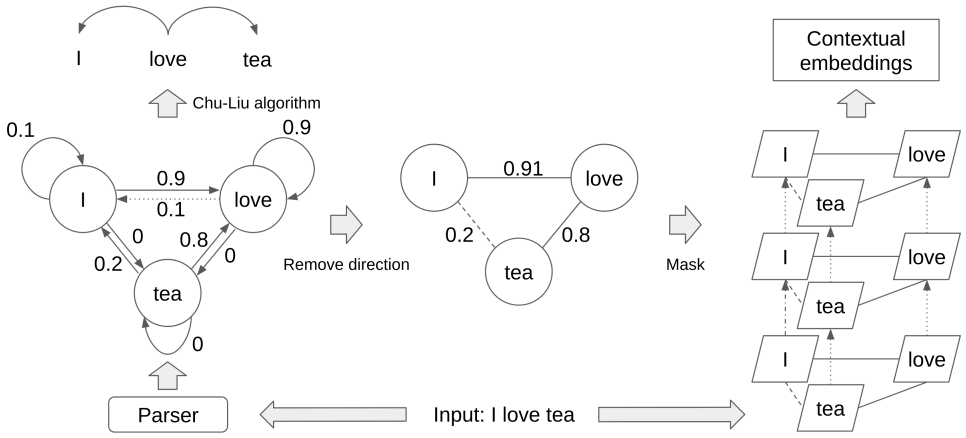

Figure 2: Details of the UDGN. Given the input sentence, the parser (left) produces a dependency head distribution for each token. These distributions form a distribution matrix p_{ij}. To do unsupervised parsing, the Chu-Liu algorithm (Chu and Liu, 1965a) generates the most likely dependency graph given p_{ij}. While training, however, we remove the direction of dependency in p_{ij} and obtain an undirected dependency mask m_{ij} (middle). m_{ij} is symmetric and with zeroes along the diagonal. The DGN (right) takes m_{ij} and the sentence as input and uses competitive gated heads to propagate information between tokens. m_{ij} controls the amount of information being propagated between nodes. If m_{ij} is small then less information will be communicated between x_i and x_j, and vice versa.

3.2 Dependency Mask

Given the dependency probabilities, StructFormer (Shen et al., 2020) uses a weighted sum of matrix p and $p^\top$ to produce a mask for self-attention layers in the transformer. We found that simply using the adjacency matrix of the undirected dependency graph provides better parsing results and perplexities. However, simply using the sum of the matrix and its transpose to create a symmetric weight matrix does not ensure that the attention mask has values < 1. When $p_{ij} = 1$ and $p_{ji} = 1$, for instance, the mask violates the constraints of a dependency mask. Thus, we treat p_{ij} and p_{ji} as parameters for independent Bernoulli variables, and we compute the probability that either w_i depends on w_j **or** w_j depends on w_i.

$$\begin{aligned} m_{ij} &= p(i \to j \quad \textbf{or} \quad j \to i) \\ &= p_{ij} + p_{ji} - p_{ij} \times p_{ji} \end{aligned} \tag{6}$$

3.3 Dependency Graph Network

To better induce and model the dependency relations, we propose a new Dependency Graph Network (DGN). One DGN layer includes several gated heads and a competitive controller. A gated head can process and propagate information from one node to another. Different heads can learn to process and propagate different types of information. The competitive controller is designed to select the correct head to propagate information between a specific pair of nodes.

We take inspiration from the linguistic theory that dependencies are associated with different syntactic functions. These functions can appear as labels, e.g. ATTR (attribute), COMP-P (complement of preposition), and COMP-TO (complement of to). However, DGN learns these functions from training tasks, which in our experiments is the masked language model objective. Since these objectives tend to be statistical in nature, these functions may not be correlated with ground truth labels given by human experts.

Inside each layer, the input vector h_i^{l-1} is first projected into N groups of vectors, where N is the number of heads. Each group contains four different vectors, namely, query $\mathbf{q}$, key $\mathbf{k}$, value $\mathbf{v}$ and gate $\mathbf{g}$:

$$\begin{bmatrix} \mathbf{q}_{ik} \\ \mathbf{k}_{ik} \\ \mathbf{v}_{ik} \\ \mathbf{g}_{ik} \end{bmatrix} = \mathbf{W}_{\text{head}_k} \mathbf{h}_i^{l-1} + \mathbf{b}_{\text{head}_k} \tag{7}$$

Gated Head To model the information propagation from node j to node i, we proposed a gated head:

$$\mathbf{c}_{ijk} = \sigma(\mathbf{v}_{jk}) \odot \text{sigmoid}(\mathbf{g}_{ik}) \tag{8}$$

where σ is a non-linear activation function, and gates $\text{sigmoid}(\mathbf{g})$ allows the i-th token to filter the extracted information. We also found that the gate effectively improves the model's ability to induce

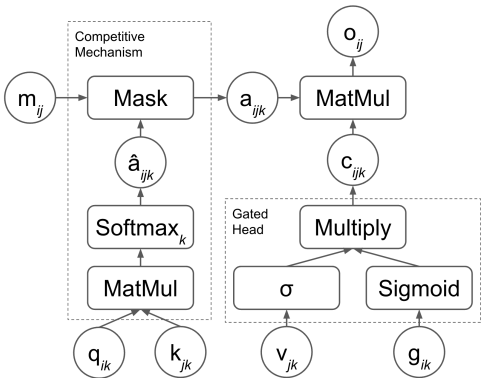

Figure 3: Competitive Gated Heads. Suppose that the information should be propagated from node j to node i, the competitive controller takes $\mathbf{q}_{i\cdot}, \mathbf{k}_{j\cdot}$ as input, output a probability distribution $\hat{a}_{ij}$ across different heads. This allows the model to select a head for the information propagation. Then the probability $\hat{a}_{ijk}$ is multiplied by dependency mask m_{ij} to get a_{ijk}. The mask m_{ij} functions as a macro gate to control the amount of information propagate between the node pair. For the k-th head, the node j send representation $\mathbf{v}_{jk}$, the node i uses a gate $\mathbf{g}_{ik}$ to filter the incoming representation.

latent dependency structures that are coherent to human-annotated trees. The activation function can be chosen from a wide variety of functions, including the identity function, tanh, ReLU, and ELU, etc. In our experiment, we found that tanh function provides the best overall performance. This is probably due to two reasons: a) tanh function provides a bounded output (between -1 and 1), and b) gates and head weights are more effective while controlling a bounded value.

Competitive Controller Lamb et al. (2021) proposed the idea of using a competition method to encourage heads to specialize over training iterations to learn different functions. This idea is coherent with our intuition different heads should model different dependency relations. In UDGN, a competitive controller is designed to select a head for each pair of nodes (i, j). However discrete assignment is hard to optimize, we replace it with a soft relaxation:

$$e_{ijk} = \frac{\mathbf{q}_{ik}\mathbf{k}_{jk}}{\sqrt{D}} \tag{9}$$

$$\hat{a}_{ijk} = \mathrm{softmax}_k(e_{ijk}) \tag{10}$$

where $\hat{a}_{ijk}$ is the probability that the k-th head is assigned to propagate information from the j-th token to the i-th token. To obtain the actual head weights, we multiply the probability of edge existence with the probability of choosing a specific attention head:

$$a_{ijk} = \hat{a}_{ijk} \times m_{ij} \tag{11}$$

where a_{ijk} is the weight from the node j to the node i for k-th attention head.

Relative Position Bias Transformer models use positional encoding to represent the absolute position for each token. In DGN, we only model whether the token is before or after the current token. The motivating intuition is the association of different heads with different directions. In equation 10, we can introduce a relative position bias:

$$\hat{a}_{ijk} = \mathrm{softmax}_k(e_{ijk} + b^{lr}_k) \tag{12}$$

$$b^{lr}_k = \begin{cases} b^l_k, & i > j \\ b^r_k, & i < j \end{cases} \tag{13}$$

where b^l_k and b^r_k are trainable parameters. The relative position bias allows the attention head k to prioritize forward or backward directions. A mere forward and backward differentiation may seem weak compared to other parameterizations of positional encoding (Vaswani et al., 2017; Shaw et al., 2018), but in conjunction with the dependency constraints, this method is a more effective way to model the relative position in a tree structure. As shown in Table 4, the relative position bias achieves stronger masked language modeling and parsing performance than positional encoding.

At the end, a matrix multiplication is used to aggregate information from different positions.

$$\mathbf{o}_{ik} = \sum_j a_{ijk}\mathbf{c}_{ijk} \tag{14}$$

Then, the output $\mathbf{o}$ from different heads are concatenated, and then projected back to the hidden state space with a linear layer.

$$\mathbf{h}^l_i = \mathbf{h}^{l-1}_i + \mathbf{W}_o \begin{bmatrix} \mathbf{o}_{i1} \\ \vdots \\ \mathbf{o}_{in} \end{bmatrix} + \mathbf{b}_o \tag{15}$$

where $\mathbf{h}^l_i$ is the output of the l-th gated self attention layers. The shared hidden state space can be seen as the shared global workspace (Goyal et al., 2021) for different independent mechanisms (heads).

Model	PTB	BLLIP -SM	BLLIP -MD	BLLIP -XL
Transformer	68.9	44.6	22.8	17.0
StructFormer	64.8	43.1	23.4	16.8
UDGN	59.3	40.2	24.2	19.7

Table 1: Masked Language Model perplexities on different datasets.

Methods	DDA	UDA
DMV (Klein and Manning, 2004)	35.8	
E-DMV (Headden III et al., 2009)	38.2	
UR-A E-DMV (Tu and Honavar, 2012)	46.1	
Neural E-DMV (Jiang et al., 2016)	42.7	
Gaussian DMV (He et al., 2018)	43.1	
INP (He et al., 2018)	47.9	
NL-PCFGs (Zhu et al., 2020)	40.5	55.9
NBL-PCFGs (Yang et al., 2021)	39.1	56.1
StructFormer (Shen et al., 2020)	46.2	61.6
UDGN	**49.9**	**61.8**

Table 2: Dependency Parsing Results on WSJ test set without gold POS tags. DMV-based baseline results are from He et al. (2018). DDA stands for Directed Dependency Accuracy. UDA stands for Undirected Dependency Accuracy. Unsupervised dependency parsing results with the knowledge of gold POS tags or other external knowledge are excluded from this table.

4 Experiments

4.1 Masked Language Modeling

Language Modeling tasks evaluate the model's general ability to model different semantic and syntactic phenomena (e.g., words co-occurrence, verb-subject agreement, etc.). The performance of MLM is evaluated by measuring perplexity on masked words. We perform experiments on two corpora: the Penn TreeBank (PTB) and Brown Laboratory for Linguistic Information Processing (BLLIP). In this experiment, we randomly replace each token with a mask token <mask>, such that the model is required to predict the original token. But we never replace <unk> token.

PTB The Penn Treebank (Marcus et al., 1993) is a standard dataset for language modeling (Mikolov et al., 2012) and unsupervised constituency parsing (Shen et al., 2018; Kim et al., 2019). It contains 1M words (2499 stories) from Wall Street Journal. Following the setting proposed in Shen et al. (2020), we preprocess the Penn Treebank dataset by removing all punctuations, lower case all letters, and replaces low frequency tokens (< 5) with <unk>. The preprocessing results in a vocabulary size of 10798 (including <unk>, <pad> and <mask>).

BLLIP The Brown Laboratory for Linguistic Information Processing dataset is a large corpus, parsed in the same style as the PTB dataset. It contains 24 million sentences from Wall Street Journal. We perform experiments on four subsets of BLLIP: BLLIP-XS (40k sentences, 1M tokens), BLLIP-SM (200K sentences, 5M tokens), BLLIP-MD (600K sentences, 14M tokens), and BLLIP-LG (2M sentences, 42M tokens). Following the same setting proposed in Hu et al. (2020) for sentence selection, each subset is a superset of smaller subsets. Models trained on different subsets are tested on a shared held-out test set (20k sentences, 500k tokens). We use a shared vocabulary for all splits to make the mask language modeling and parsing results comparable. Like the PTB dataset, we preprocess the BLLIP dataset by removing all punctuations and lower case letters. The shared vocabulary is obtained by counting word frequencies on the BLLIP-LG dataset and selecting the words that appear more than 27 times. The resulting vocabulary size is 30232 (including <unk>, <pad> and <mask>), and covers more than 98% tokens in BLLIP-LG split.

The mask rate is 30% when training on both corpora. In Section A.4, we further explore the relationship between mask rate and parsing results. Other hyperparameters are tuned separately for each model and dataset. Details are further described in Section A.1. Table 1 shows The masked language model results. UDGN outperforms the baselines on smaller datasets (PTB, BLLIP-SM), but underperforms against baselines trained on large datasets (BLLIP-MD, BLLIP-LG). However, in Section 4.5, we find that the UDGN pretrained on BLLIP-LG dataset can achieve stronger performance when finetuned on a downstream task. This result may suggest that our model learns more generic contextual embeddings.

4.2 Unsupervised Dependency Parsing

Following previous research (Shen et al., 2020), we use the model trained on the PTB training set (section 0-20, no punctuations) and test its parsing accuracy on section 23 of the PTB corpus. Punctuations are ignored during the evaluation. We convert the human-annotated constituency trees in the PTB test set (Marcus et al., 1993) to dependency trees with Stanford CoreNLP (Manning et al., 2014) and use the Directed Dependency Accuracy (DDA) as our metric. To derive valid trees from the attention

Models	prep	pobj	det	compound	nsubj	amod	dobj	aux
UDGN	0.65(0.12)	0.60(0.11)	0.68(0.15)	0.42(0.04)	0.50(0.06)	0.39(0.07)	0.39(0.07)	0.62(0.10)
StructFormer	0.39(0.05)	0.38(0.07)	0.57(0.03)	0.33(0.01)	0.25(0.06)	0.26(0.01)	0.22(0.05)	0.23(0.04)
Transformer	0.43(0.00)	0.46(0.03)	0.46(0.12)	0.30(0.01)	0.39(0.15)	0.26(0.02)	0.28(0.01)	0.30(0.10)

Table 3: The *pearson correlation coefficients* between most frequent dependency types and their most correlated head. All results are average across four random seeds, standard derivation are in parentheses. Types are arranged from the highest frequency to lowest frequency. PCC heat maps between all types and all heads are in Appendix A.2.

mask, we use the Chu-Liu (Chu and Liu, 1965b) (or Edmonds' (Edmonds, 1967)) algorithm to obtain the maximum directed spanning tree.

Table 2 shows that our model outperforms baseline models. This result suggests that, given our minimum inductive bias (a token must attach to another, but the graph is not necessarily a tree), predicting missing tokens implicitly learns a good graph that correlates well with human-annotated dependency trees. In other words, some of the dependency relations proposed by linguists may correspond with efficient ways of propagating information through the sentence. Parsing examples of our model can be found in Appendix A.5.

4.3 Correlation Between Heads and Dependency Types

In this section, we test the correlation between heads and dependency types. We consider each dependency edge $i \rightarrow j$ (i depends on j) in the ground truth structure as a data point. Given all the edges, we can obtain three sets of quantities: head probabilities $A^k = \{\hat{a}^k_{ji}\}$ and type values $Y^l = \{y^l_{ij}\}$. $\hat{a}^k_{ij}$ is a real value between 0 and 1, represents the probability that heads k is used to model the information propagation from the child i to the parent j. Details about this value can be found at Equation 12. y^l_{ij} is a binary value, represents whether the label l is assigned to edge $i \rightarrow j$. We can then compute Pearson Correlation Coefficient (PCC) for every pair of A^k and Y^l across all ground truth edges $\{i \rightarrow j\}$:

$$\rho_{A^k,Y^l} = \frac{\text{cov}(A^k, Y^l)}{\sigma_{A^k}\sigma_{Y^l}} \tag{16}$$

where $\text{cov}(\cdot)$ is the covariance function, $\sigma_\cdot$ is the standard deviation of the respective variable. Hence, ρ_{A^k,Y^l} measures the correlation between head k and dependency type l. $\rho_{A^k,Y^l} > 0$ means that the model tends to use head k for propagating information from child to parent for dependency edges of the type l. Here, we only consider the information propagation from child to parent even though information can propagate in both directions in masked language models. In Appendix A.2, we also computed the PCC for the parent to child direction.

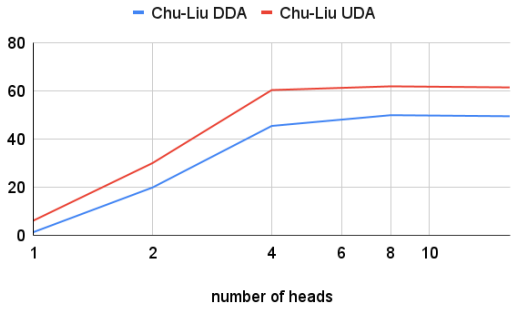

Figure 4: Relationship between the parsing performance and the number of heads in each layer. The hidden state size of heads are adjusted to maintain the same number of total parameters.

Table 3 shows the PCC between the most frequent dependency types and their most correlated heads. We can observe that all three models have heads that are positively correlated to human-annotated dependency types. This result is coherent with the observation of Htut et al. (2019). Meanwhile, the UDGN achieves a significantly better correlation than the StructFormer and the Transformer. This confirms our intuition that competitive gated heads can better induce dependency types.

4.4 Ablation Experiments

Figure 4 shows the relation between the number of heads in each UDGN layer and the model's unsupervised parsing performance. Table 4 shows the model's performance when individual components are removed. We can observe that the number of heads has the most significant influence on unsupervised parsing performance. While this is only one head, the model fails to learn any meaningful structure. Then the parsing performance increase as the number of heads increase. And we observe

Model	MLM	Argmax		Chu-Liu	
	PPL	DDA	UDA	DDA	UDA
UDGN	59.3(0.5)	52.7(0.9)	58.3(0.7)	49.9(1.6)	61.8(0.9)
- Gates	69.5(1.9)	31.5(2.2)	40.7(0.3)	26.1(2.1)	48.9(0.5)
- Competition	73.6(3.1)	44.7(1.9)	54.4(1.9)	40.4(1.6)	56.6(2.1)
- relative pos bias	62.1(1.0)	51.6(1.6)	59.8(0.8)	47.4(2.6)	62.1(1.1)

Table 4: The performance of UDGN after removing different components. "- Gates" means removing the gate g in gated heads. "- Competition" means using a non-competitive sigmoid function to replace the softmax in the competitive controller. "- relative pos bias" means removing the relative positional bias. "Chu-Liu" means that we use the Chu-Liu algorithm to extract the maximum directed spanning tree. "Argmax" means that we take the word at the maximum p value as the dependency head. This could result in non-tree structures, but we believe that this metric gives a better indication of how often the parser predicts the right head of each word.

Model	STS12	STS13	STS14	STS15	STS16	STS-B	SICK-R	Avg.
Transformer	76.17	61.48	73.97	74.35	53.72	64.26	80.00	69.14
UDGN (Freeze parser)	77.71	71.17	78.71	82.30	66.04	70.13	82.17	75.46
UDGN	80.51	75.02	80.54	82.16	64.73	72.49	81.94	76.77

Table 5: Sentence embedding performance on STS tasks. All models are pretrained on BLLIP-LG, and finetuned on STS. Freeze parser means that the parameters for the parser are not updated during finetuning.

marginal improvement after the number of heads reaching 8. The second most significant parsing performance decrease is caused by removing the gating mechanism. This change forces each head to always extract the same information from a given key node h_j, regardless of the query node h_i. This has a similar effect as the previous change, reducing the diversity of different functions that can be modeled by heads. These two observations may suggest that the diversity of information propagation function (multiple heads) is essential to induce a meaningful structure.

The competitive controller also has an important influence on parsing performance. Its non-competitive version is the sigmoid controller used in StructFormer. If we replace it with the non-competitive controller, the DDA decreases to 44.7 which is similar to the result of StructFormer (46.2). Another interesting observation is that removing relative position bias has the least influence on parsing and language modeling. This may suggest that the dependency structure already encoded certain positional information. More ablation experiment results can be found in Appendix A.3.

4.5 Fine-tuning

In this experiment, the goal was to determine if a better representation of semantics can be encoded if the model was constrained for structure. We pretrain a UDGN model on the BLLIP-XL dataset, and then finetune it on the STS-B (Cer et al., 2017) dataset. For a controlled experiment, we compare the results we attain with the previously mentioned Transformer model. We then evaluate the resulting classifier on the STS 2012-2016 (Agirre et al., 2012, 2013, 2014, 2015, 2016), the SICK-Relatedness (Marelli et al., 2014) dataset, and STS-B (Cer et al., 2017). We then report the Spearman correlation score for each dataset (the 'all' setting in Gao et al. 2021).

We find that the UDGN model performs better overall than the transformer model. While these are not state-of-the-art results for these tasks, our comparison aimed to examine the benefit of the UDGN model over the Transformer architecture. It's also interesting to notice that if parameters in the parser are frozen during the finetuning, the model will get worse performance. This result suggests that finetuning on STS forces pretrained language models to learn more task-oriented trees. Dai et al. (2021) observed similar results with finetuned RoBERTa on Aspect-Based Sentiment Analysis tasks.

5 Conclusion

In this paper, we proposed the Unsupervised Dependency Graph Network (UDGN), a novel architecture to induce and accommodate dependency graphs in a transformer-like framework. The model is inspired by linguistic theories. Experiment results show that UDGN achieves state-of-the-art dependency grammar induction performance. The competitive gated heads show a strong correlation

to human-annotated dependency types. We hope these interesting observations will build new connections between classic linguistic theories and modern neural network models. Another interesting future research direction is exploring how the newly proposed components can help large-scale pretrained languages models.

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A Appendix

A.1 Hyperparameters

Model	Hidden Size	head/Head Size	Dropout	DropAtt	lr	#tags	Feedforward Size
UDGN (PTB)	512	128	0.2	0.1	0.001	6	–
UDGN (BLLIP-XS,SM)	512	128	0.2	0.1	0.001	6	–
UDGN (BLLIP-MD,LG)	512	128	0.2	0.1	0.001	6	–
Transformer	512	64	0.1	0.1	0.0003	–	2048
StructFormer	512	64	0.1	0.1	0.0003	–	2048

Table 6: Hyperparameters used in Masked Language Modeling experiments. All model has 8 layers and 8 heads or attention heads. For UDGN, we apply dropout in front of all linear layers; dropatt randomly drops heads; the parser is a 3-layer biLSTM model, which has 6 tag embeddings, 1 of them is a zero vector, 5 of them are trainable. For transformer and structformer, the dropout is applied to the output of each sublayers; dropatt randomly drops attention weights; the size of their feedforward sublayers is 2048.

A.2 Correlation between Heads and Dependency Types

Models	prep	pobj	det	compound	nsubj	amod	dobj	aux
UDGN	0.45(0.15)	0.84(0.05)	0.59(0.08)	0.38(0.03)	0.47(0.08)	0.43(0.08)	0.32(0.04)	0.45(0.08)
StructFormer	0.28(0.04)	0.43(0.13)	0.38(0.06)	0.34(0.02)	0.30(0.03)	0.27(0.01)	0.19(0.02)	0.22(0.02)
Transformer	0.44(0.03)	0.31(0.05)	0.37(0.03)	0.32(0.00)	0.16(0.01)	0.28(0.01)	0.20(0.01)	0.26(0.03)

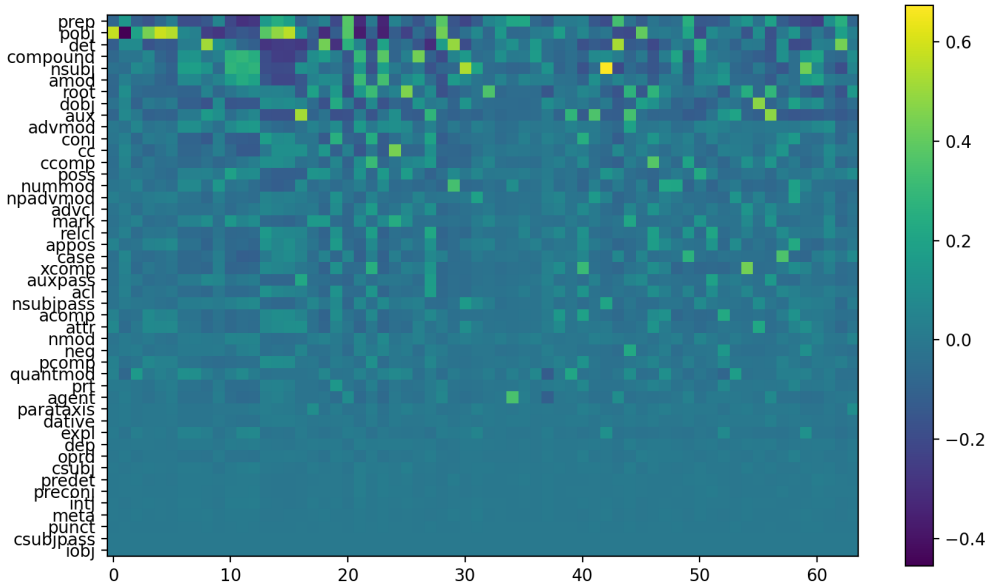
Table 7: The pearson correlation coefficients between most frequent dependency types (*the child to parent direction*) and their most correlated head. Types are arrange from the highest frequency to lower frequency.

A.3 More Ablation Experiments

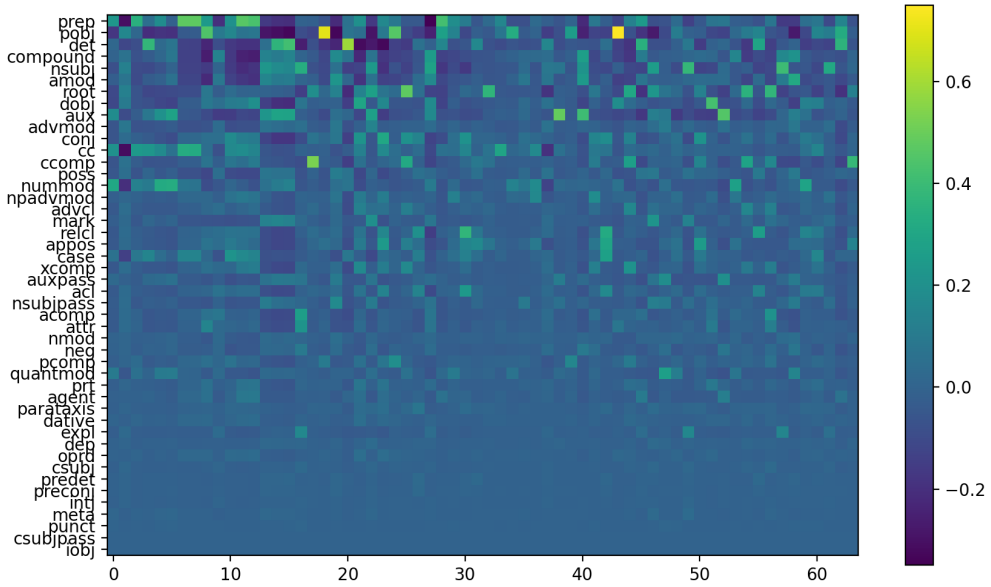
In this section, we evaluate UDGN's performance after removing the nonlinear function in gated heads, replacing relative positional bias with a standard positional encoding, and using Kirchhoff matrix tree theorem (Koo et al., 2007) to normalize the dependency probabilities. It's interesting to notice that, although Kirchhoff method can produce a valid marginal distribution for dependency probabilities, adding the normalization can't improve the unsupervised parsing performance. We believe it's due to the extra optimization complexity introduced by the matrix inversion in Kirchhoff method. Another observation is that relative position bias helps the model to achieve better perplexity and parsing performance in comparison with positional encoding. This may suggest that the combination of dependency graphs and relative positions is more informative than absolute positions.

Model	MLM	Argmax		Chu-Liu	
	PPL	DDA	UDA	DDA	UDA
UDGN	60.4(0.8)	52.5(0.7)	58.8(0.9)	50.2(1.5)	61.2(0.4)
- Nonlinear	61.2(1.0)	49.5(1.1)	56.8(1.4)	45.6(2.0)	60.8(1.4)
- relative pos bias + pos encoding	65.2(3.4)	47.1(7.3)	55.4(4.1)	44.8(7.2)	58.2(5.2)
+ Kirchhoff	59.7(0.5)	50.2(2.2)	58.4(1.2)	46.5(2.1)	60.7(1.2)

Table 8: The performance of UDGN after removing different components. "- Nonlinear" means remove the tanh activation function in gated heads. "- relative pos bias + pos enc" means using a trainable positional encoding to replace the relative position bias. "+ Kirchhoff" means using Kirchhoff matrix tree theorem (Koo et al., 2007) to compute the marginal probabilities of each edge, and these marginals have properties similar to a tree adjacency matrix (sum over the marginals are equal to N-1 for example, where N is the length of the sentence).



(a) PCC heat map for heads and child to parent dependency relations.



(b) PCC heat map for heads and parent to child dependency relations.

Figure 5: Pearson Correlation Coefficients heat maps. Dependency types are arranged from highest frequency to lowest. We can observe that high frequent types have more strongly correlated heads. Strongly correlated heads also evenly distributed across layers.

Dataset	#tokens	MLM PPL	Argmax DDA	Argmax UDA	Chu-Liu DDA	Chu-Liu UDA
BLLIP-XS	1M	133.7(3.1)	51.4(2.0)	57.6(1.6)	47.9(2.7)	61.2(1.6)
BLLIP-SM	5M	40.2(0.8)	53.7(2.5)	60.7(0.6)	50.9(5.3)	65.1(1.6)
BLLIP-MD	14M	24.2(0.5)	50.5(6.1)	59.8(2.9)	47.7(8.1)	63.0(4.2)
BLLIP-LG	42M	19.7(0.3)	45.6(2.9)	61.7(1.8)	41.6(4.2)	62.5(1.6)

Table 9: The performance of UDGN after trained on different BLLIP splits. Since all BLLIP splits share the same vocabulary and test set, results are comparable. While DDA have a high variance, UDA remain stable across different corpus sizes. This may due to the reason that DGN only use an undirected dependency mask, the choice of dependency direction could be arbitrary. This result may suggest that syntax can be acquired with a relatively small amount of data. It is possible then, that where extra data helps is in terms of semantic knowledge, like common sense.

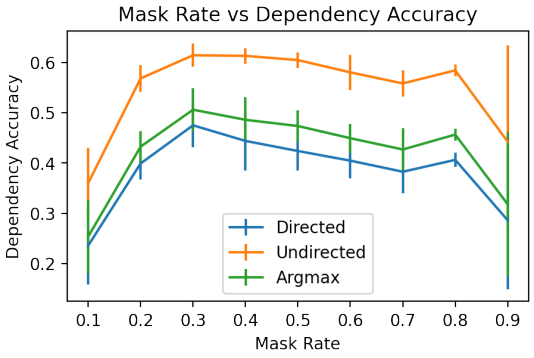


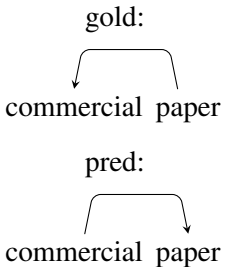
Figure 6: Relationship between the parsing performance and the mask rate for MLM.

A.4 Mask rate

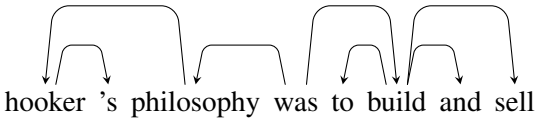
One of the more surprising findings in our experiments with this architecture was the relationship between the word mask rate in the MLM task and how much the resulting parse trees corresponded to the ground-truth parse trees. We trained 5 models for different word masking rates from 0.1 to 0.9, in 0.1 increments, and computed the argmax, DDA, and undirected DDA (UDA) scores for each of these models. Figure 6 shows the plot for these results.

Firstly, we observe that the acceptable range of masking rate for achieving a decent UDA score was fairly large: the optimal was at about 0.3, but values of 0.2 up to 0.8 worked to induce tree structures that resulted in fairly good undirected trees. Secondly, as we move away from the optimum of 0.3-0.4, the variance of our results increases, with the highest variance when we mask at a rate of 0.9. Finally, our model supplies the attention mask as a symmetric matrix— the directionality of the mask is decimated when we perform Equation 6. Consequently, we find that the variance of the DDA is higher than UDA as the connectivity of the nodes in the tree is more important than the direction of the connection in our architecture.

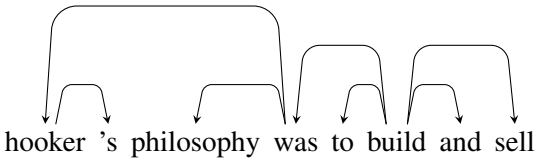
A.5 Dependency Graph Examples



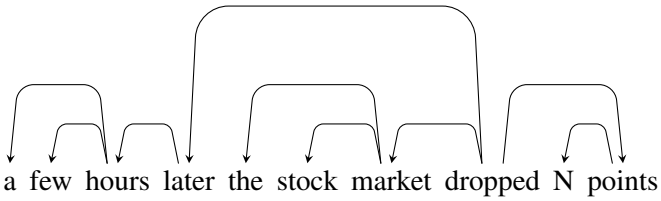
Gold tree:



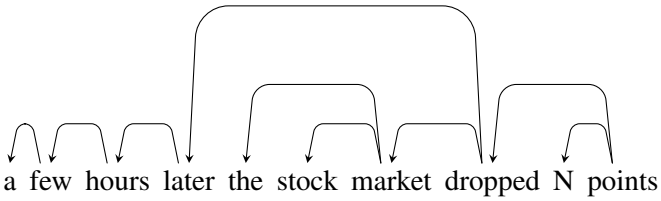
Induced tree:



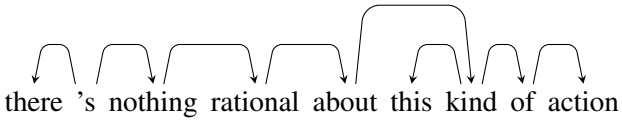
gold:



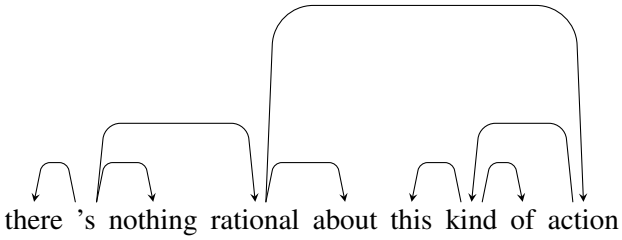
pred:



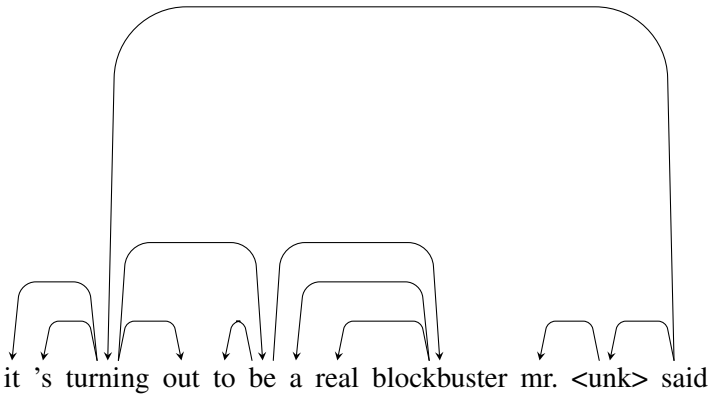
gold:



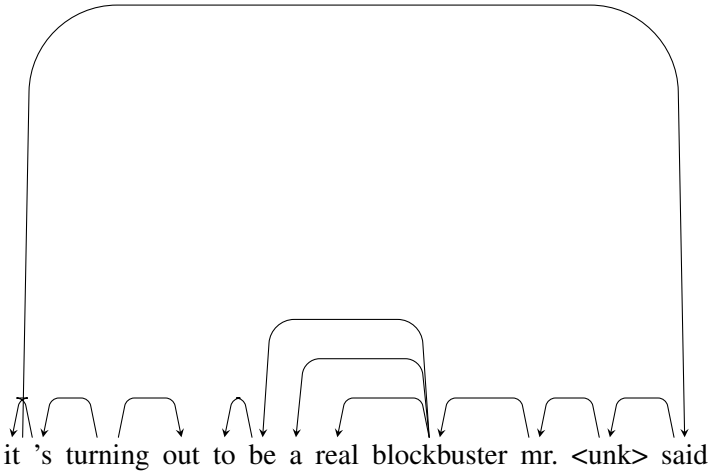
pred:



gold:



pred:



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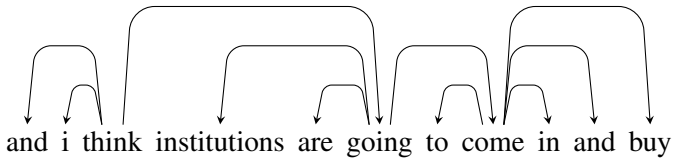

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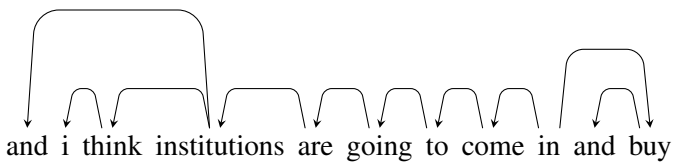

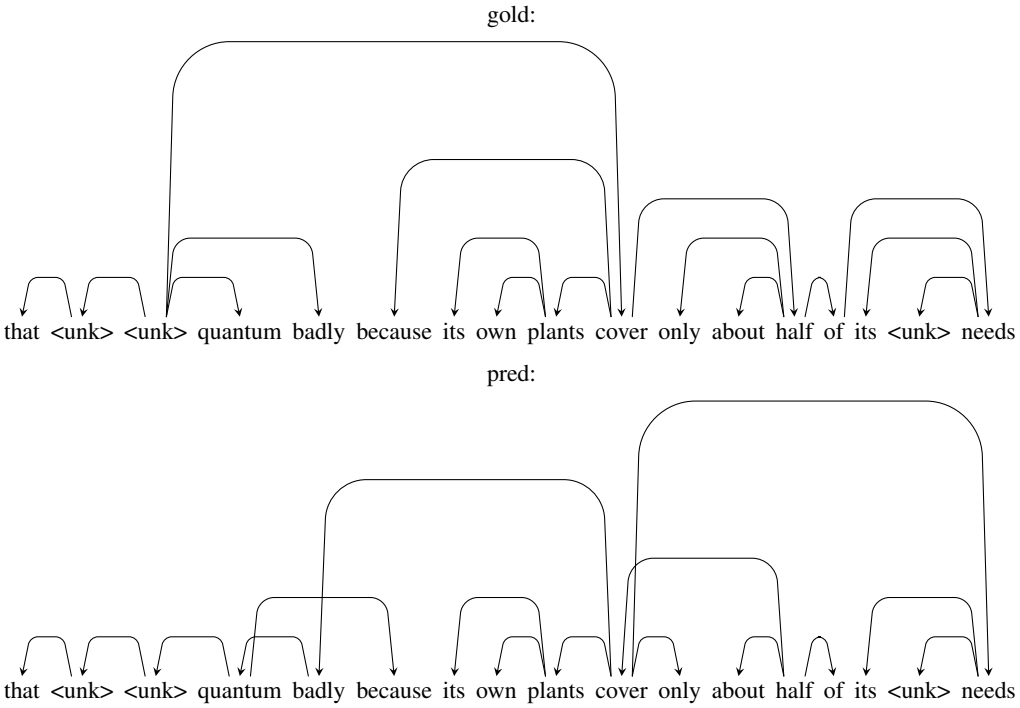
gold:
that <unk> <unk> quantum badly because its own plants cover only about half of its <unk> needs
pred:
that <unk> <unk> quantum badly because its own plants cover only about half of its <unk> needs