Transformer Query-Target Knowledge Discovery (TEND): Drug Discovery from CORD-19

Leo K. Tam  
NVIDIA  
2788 San Tomas Expy  
Santa Clara, CA. 95051

Xiaosong Wang  
NVIDIA  
2788 San Tomas Expy  
Santa Clara, CA. 95051

Daguang Xu  
NVIDIA  
2788 San Tomas Expy  
Santa Clara, CA. 95051

Abstract

Previous work established skip-gram word2vec models could be used to mine knowledge in the materials science literature for the discovery of thermoelectrics. Recent transformer architectures have shown great progress in language modeling and associated fine-tuned tasks, but they have yet to be adapted for drug discovery. We present a RoBERTa transformer-based method that extends the masked language token prediction using query-target conditioning to treat the specificity challenge. The transformer discovery method entails several benefits over the word2vec method including domain-specific (antiviral) analogy performance, negation handling, and flexible query analysis (specific) and is demonstrated on influenza drug discovery. To stimulate COVID-19 research, we release an influenza clinical trials and antiviral analogies dataset used in conjunction with the COVID-19 Open Research Dataset Challenge (CORD-19) literature dataset in the study. We examine k-shot fine-tuning to improve the downstream analogies performance as well as to mine analogies for model explainability. Further, the query-target analysis is verified in a forward chaining analysis against the influenza drug clinical trials dataset, before adapted for COVID-19 drugs (combinations and side-effects) and on-going clinical trials. In consideration of the present topic, we release the model, dataset, and code.1

1 Introduction

The COVID-19 literature has experienced exponential growth and analysis tools have arisen to digest the literature (Brainard, 2020). To mine the literature, word embedding methods (Huang et al., 2012; Mikolov et al., 2013) operate in a high-dimensional space where semantic relationships are exposed through interrogation with metrics such as cosine similarity. Advances in transformer attention-based architectures treat one possible weakness in word embedding learning approaches by conditioning on contextual information for a downstream task (Vaswani et al., 2017). The pretrain-finetune paradigm, whereby a language model is trained on a large corpus through a task such as masked cloze or autoregressive variants and then trained again (fine-tuned) for a specific application encountered success (Dai and Le, 2015; Collobert and Weston, 2008). While word2vec implementations focused on analogies evaluation as a downstream task indicative of semantic learning, transformer architectures surveyed a collection of downstream tasks such as sentiment, sentence similarity, natural language (NL) inference, question and answering, and reading comprehension, etc. present in the GLUE and super GLUE benchmark (Wang et al., 2019b,a). Word2vec discovery methods (Tshitoyan et al., 2019) constitute a return to analogy evaluation, though eschewing generic semantic analogies to highlight analogies in materials science. It is hypothesized that resolving analogies may form the basis for higher reasoning such as advancing the limits of domain-specific research (Kuniyoshi et al., 2020; Hansson et al., 2020) and measuring scholastic achievement (Khot et al., 2017). For the case of applications in the medical domain (Lee et al., 2020), transformer pretrain-finetune performance was dependent on the quality and in-domain nature of source and target datasets.

Similar to novel materials discovery, drug discovery is an intensive and arduous process requiring trial and error. Drug discovery is the problem of allocating resources to numerous promising candidates, and thus ranking promising candidates assists the discovery process in a top-down fashion. To date globally, only nine influenza drugs have received full approval for use (De Clercq and Li, 2020) and...
Where the Tshitoyan et al. (2019) method uses a rigid prediction method to mine associative analogies for undiscovered materials, the advances in tokenization (Sennrich et al., 2016) have relaxed exact vocabulary registration though complicating the method. The present work examines a query-target (QT) token conditioning method, which extends the masked language modeling (MLM) inference. The QT method is used to rank prediction association with clinical trials efficacy treating a specificity problem when moving from a fixed vocabulary to whole language tokenization. Moreover, the RoBERTa-large model trained on the CORD-19 literature dataset (29500 provided at the time of work and now updated to over 200000 articles) can be enhanced for drug analogies evaluation via a k-shot method (Raffel et al., 2019; Brown et al., 2020).

2 Related work

Previous work has examined drug and side-effect relationships in a bipartite graph focusing on literature in a four year range (Jeong et al., 2020). While Jeong et al. (2020) considered 169766 PubMed abstracts across drugs, Hansson et al. (2020) considered solely type II diabetes related drugs, clustering them around heuristic expert topics. Scoring was conducted via co-mention weighting and a five year look-back literature mention weighting. Both previous methods incorporate expert information in a semi-supervised method, the first through database registration for drug - side effect pairs and the second through semantic concept selection. The present method is an unsupervised method excepting for physician review for the auxiliary analogies task. Further, the method uses a majority of full texts in a narrow focus (Kohlmeier et al., 2020). Results from Alsntzer et al. (2019); Lee et al. (2020) revealed how the detail and relevance of the dataset influences the final result. We corroborate that domain-specific datasets improve domain-specific analogy performance.

3 Methods

The overview of our method is presented in Fig. 1, which depicts both training and inference modes. During training, the MLM task is held without modification from Liu et al. (2019), namely 13.5% of tokens are targeted for replacement with 90% replaced with <mask>, 10% corrupted with a random token. The MLM task is chosen as it closely replaces the function in Tshitoyan et al. (2019) for predicting a target word given the context around the word. The RoBERTa transformer method is a pure application of MLM, removing the next sentence prediction task while scaling to longer sequences with dynamic masking. A cross-entropy loss is used for prediction, the RoBERTa 50K byte-pair encoding tokenization is used, and hyper-parameters are left at default settings from Wolf et al. (2019). During training, the inputs are the CORD-19 dataset described in sec. 3.1 dynamically masked ten times. The MLM training from scratch runs across 16 NVIDIA V100 GPUs in a single-node (DGX-2) configuration for 100000 steps over approximately 36 hours. The MLM prediction is used for analogy evaluation via the structure “A is to B as C is to <mask>” as suggested by Raffel et al. (2019). The complete set of analogies is provided with the code. For the word2vec implementation, the procedure followed Tshitoyan et al. (2019), including vocabulary generation and evaluation. The QT inference mode is discussed in Sec. 3.2.

3.1 Datasets

Table 1: CORD-19 Dataset

| Sources  | Records | License  | Count |
|----------|---------|----------|-------|
| CZI      | 1236    | Custom   | 17102 |
| PMC      | 27337   | Noncomm. | 2353  |
| bioRxiv  | 566     | Commercial | 9118  |
| medRxiv  | 361     | Arxiv    | 927   |
| Total    | 29500   |          | 29500 |

The United States Food and Drug Administration (FDA) approved drugs and global clinical trials data are drawn from De Clercq and Li (2016) and USGov (2020) respectively. In Tab. 2, counts such as the number of trials and drugs trialed per year’s end is collected. Namely, we use influenza
Figure 1: A RoBERTa-large transformer query-target method for drug discovery reveals positive and negative associations.

Figure 2: The black line represents influenza drugs receiving FDA approval. To date, there are only eight antiviral drugs approved for influenza strains globally with a ninth drug, remdesivir receiving emergency approval subsequent to the analyses performed here.
as the condition, check the search term to filter by drug treatments, and focus on years prior to 2016, when the last antiviral drug was approved. De-duplication is performed on trade and scientific names using the chart from De Clercq and Li (2016). The number of candidate and approved drugs specifically for influenza per year is plotted on Fig. 2.

For analogy evaluation, the set of language (grammar) analogies and drug analogies are drawn from relationships in Tshitoyan et al. (2019) and De Clercq and Li (2016) respectively. A list of the analogy categories is presented in Tab. 3. For k-shot training, a random set of k=5 analogies from each category is used as additional pretraining for MLM (Brown et al., 2020).

### 3.2 Query-target inference

During inference, a query and target phrase are selected based on the relationships of interest. We examine the relationship with the RoBERTa training objective, adopting the formulation from Yang et al. (2019) for the objective as:

$$\max_\theta \log p_\theta(\bar{x}|\hat{x}) \approx \sum_t \delta_t \log \sum_{x'} \exp \left( H^\theta_l(\hat{x})^T e(x_t) \right)$$  \hspace{1cm} (1)

where $\delta_t$ is 1 if $t$ indicates a masked token and 0 otherwise, $x = [x_1, \cdots, x_S]$ is a text sequence, $\hat{x}$ represents a corrupted token, $\bar{x}$ represents a masked token, $e(x)$ is the embedding of the sequence, and $H^\theta_l$ is the RoBERTa-large architecture with parameters $\theta$ that maps a $S$ length text sequence into a sequence of hidden vectors. Optimizing the training objective results in accurate MLM inference. For MLM inference (Devlin et al., 2019), the $K$ masked tokens in the query $q = [q_1, \cdots, q_K]$ are targeted for token prediction, i.e.

$$P_k = \frac{\exp \left( H^\theta_l(q_k) \right)}{\sum_j \exp \left( H^\theta_l(q_j) \right)}.$$  \hspace{1cm} (2)

For QT prediction, we condition the masked token targets on the query targets $y = [y_1, \cdots, y_L]$:

$$R := P_k(q_k|q_k \in y) = \frac{\sum_j \exp \left( H^\theta_l(q_k) \right)}{\sum_j \exp \left( H^\theta_l(q_j) \right)}$$  \hspace{1cm} (3)

follows by independence assumption in Eqn. 1 and therefore is contained in the training objective (i.e. accurate QT prediction is implied). When $q = y$, we observe the QT conditioning decomposes to the MLM task prediction. The QT conditioning is more focused than reformulating a span prediction method such as in Devlin et al. (2019) due to rejection of extraneous tokens that would be admitted in a dot product formulation. Once QT prediction has been formed, the analogy MLM task may be permuted with the QT terms using “$Q$ is to $T$ as $Q$ is to $<mask>$” to analyze the top-$k$ related terms without conditioning. For rank prediction, tokens with positive and negative associations are not intentionally mixed as they are for visualization purposes.

### 3.3 Attention visualization

Typically transformer attention visualization examines the sequence to sequence attention (Vaswani et al., 2017; Huang et al., 2019), namely plotting the per-token attention:

$$A_t = \frac{\exp \left( H^\theta_l(x_t)^T e(x_t) \right)}{\sum_j \exp \left( H^\theta_l(x_t)^T e(x_j) \right)}.$$  \hspace{1cm} (4)

For QT visualization, the token attention per $l$-th query targets, namely:

$$R_l = \frac{\exp \left( H^\theta_l(q_k)^T e(q_k) \right)}{\sum_j \exp \left( H^\theta_l(q_k)^T e(q_j) \right)}.$$  \hspace{1cm} (5)
Table 3: Analogy Semantic Learning Evaluation

| Category                  | Number | Subcategory |
|---------------------------|--------|-------------|
| drug – inhibition         | 211    | antiviral   |
| drug – group              | 57     | antiviral   |
| drug – abbreviation       | 57     | antiviral   |
| drug – approved target    | 73     | antiviral   |
| opposites                 | 703    | grammar     |
| comparatives              | 651    | grammar     |
| superlatives              | 651    | grammar     |
| present participles       | 4031   | grammar     |
| past tense                | 4031   | grammar     |
| plural                    | 4169   | grammar     |
| plural verbs              | 993    | grammar     |

Figure 3: Self attention visualization (top) and query-target function (bottom left) show associated (light) and unassociated (dark) values. A passage from De Clercq and Li (2016) is highlighted on a per-sentence basis using the target term “efficacy”.

Favipiravir (also known as T-705), 6-Fluoro-3-hydroxy-3-pyrroline-2-carboxamide, has been primarily pursued for the treatment of influenza infections (539–543). Approved in Japan, favipiravir can be used in the treatment of influenza A, B, and C virus infections (Table 2). According to the mechanism of drug action postulated by Furuta et al. (332), favipiravir is converted intracellularly to its ribonucleoside monophosphate form by the phosphonate transferase, two phosphorylations subsequently convert the ribonucleoside monophosphate form to the triphosphate form, the active metabolite of favipiravir. Importantly, favipiravir triphosphate shows broad-spectrum inhibitory activities against the RNA polymerases of influenza A viruses (including the highly pathogenic H5N1 avian strain) (330), SARS (SARS-CoV-2), and many other positive-sense RNA and negative-sense RNA viruses (332). Recently, favipiravir has been proposed to treat patients infected with Covid-19 (334). Preliminary results suggest that favipiravir efficiently inhibits influenza infections in mice models (335, 336), but further investigations are still needed (337). In addition, favipiravir can inhibit the replication of human rhinovirus (332, 338) and human arenaviruses (Junin, Machupo, and Pichinde viruses) (338, 339), but these new applications require further evidence from clinical trials.
3.4 Forward chaining (FC) analysis

To preserve the casual nature of time series data, the rank calculation from Eqn. 3 is performed on the year-limited data in Tab. 3. The target query is set as “clinical trials efficacy” and the candidate drugs are drawn from the number specified in column 2 of Tab. 2. The candidate drugs are a subset of the total drugs tested as trials cover additional diseases (column 4, Tab. 2).

4 Results

After training for 100000 steps, the MLM task reached a perplexity of 2.4696 on the held-out test data. The attention relationship for self-sequence to sequence and QT is visualized in Fig. 3 as per eqns. 3 and 4. While the QT scoring may be adapted to sentence highlighting (Fig. 3), a comparison with the span extraction or abstractive summarization method in Devlin et al. (2019) is beyond the scope of the current work. While negation handling (Fig. 3) is an expected result Devlin et al. (2019); Wang et al. (2019a), it represents an advancement over the word2vec scoring method. Analogies evaluation is collected in Tab. 4. Although a comparison on simple grammar analogies can be conducted, a simple extension cannot be performed as the 600000+ word2vec vocabulary built from standard procedures does not adequately capture the phrases in the drug analogies. In the categories where RoBERTa-large can be compared to word2vec (opposites, comparatives, superlatives) significant improvement is observed (83.0% accuracy vs 50.4% accuracy). The few-shot and semi-supervised learning approaches are critical to performance, generating 23.8% and 18.8% improvement in top-1 accuracy for grammar and antiviral analogies respectively.

While synthetic analogies can be captured to some degree by the CORD-19 RoBERTa-large model, is the model relevant for forward predictions as in Tshitoyan et al. (2019)? Fig. 4 shows the FC analysis for the period where clinical trials data is reliably available. Below the FC figure, a ranking of drugs under current clinical trials is presented. Shortly after the analysis was issued ([anon URL]), the antiviral remdesivir entered emergency FDA approval, reflecting Fig. 4. As a possible failure mode, hydroxychloroquine was ranked as a distant third and was later shown to have no correlation with positive or negative outcomes (Geleris et al., 2020). In Fig. 4 (bottom), the permuted MLM task mines relationships that mirror the relationship of remdesivir with clinical trials efficacy. Inverting the analogy mining operation (not pictured) does not recover the QT function as predicted terms are too generic to focus on candidate drugs. While further experiments are collected on negative terms (side effects) and drug combinations in Fig. 5, a reliable method to test and verify these results has not been collected.

5 Conclusion and perspectives

A transformer QT conditioning specifies the discovery method on a narrow literature dataset to predict clinical trials approval as verified by FC, real-time prediction, and relationship mining. The conditioning operation is a straightforward calculation at inference time for the transformer language model permissible by the independence assumption during pretraining. For language models where independence is not assumed, such as the permutation language objective (Yang et al., 2019), conditioning would be performed via estimation of the posterior distribution, i.e. via a Metropolis-Hastings algorithm. The ranking task can be used to determine a per-sentence passage highlighting (Fig. 3) with a specific query. The scope of the QT method can be given since $q, y \in X$ is in the set of all statements in the corpus, and only finite sets could be generated (though by motivation this is unwieldy). For more validation, the field of online learning may offer independent verification through the marginal contribution to accuracy of each datum (Jia et al., 2019).

Besides the accessible resource of clinical drug trials, other quantitative methods of determining drug function are feasible given detailed dataset formulation. Such methods could focus on canonical measures such as the inhibitory constant ($K_i$), effective dose at 95% (ED95), or number needed to treat (NNT). Still further are works examining protein receptor binding, but the connection to literature machine learning methods is unclear as well requiring specialized dataset expertise. Due to the relatively limited number of successes for antiviral drugs, analysis suffers from sample bias. Further comparison on the materials dataset was not possible due to unavailability of the dataset after request. Despite limitations, the study suggests transformer language models are a flexible tool in mining literature.
Table 4: Analogies accuracy using language models trained on various corpora. *The word2vec cannot adequately adapt to the phrases used in drug analogies at 600000+ vocabulary with standard procedures.

| Model               | Top-5 Accuracy | Grammar | Antivirals |
|---------------------|----------------|---------|------------|
| RoBERTa-large       | 0.241          | 0.365   |
| k-shot (k=5) RoBERTa-large | 0.925   | 0.538   |
| CORD-19 RoBERTa-large | 0.727   | 0.525   |
| k-shot (k=5) CORD-19 RoBERTa-large | 0.705   | 0.579   |

| Model               | Top-1 Accuracy | Grammar | Antivirals |
|---------------------|----------------|---------|------------|
| RoBERTa-large       | 0.082          | 0.124   |
| k-shot (k=5) RoBERTa-large | 0.830   | 0.312   |
| CORD-19 RoBERTa-large | 0.428   | 0.190   |
| k-shot (k=5) CORD-19 RoBERTa-large | 0.572   | 0.396   |
| word2vec skip-gram  | 0.504          | *       |
| COVID word2vec skip-gram | 0.592   | *       |

Figure 4: (Left) A year-limited FC ranking analysis of influenza drugs under clinical trials for FDA approval. Only two drugs received approval in the period between 2005 and 2016. (Right) Ranking of current clinical trials for COVID-19 drugs. (Bottom) The permuted MLM task probes the relationship of remdesivir with clinical trials efficacy.
Figure 5: (Top) Examination of side effects using the transformer query-target method. (Bottom) Drug combinations are evaluated via concatenation.
References

Emily Alsentzer, John R. Murphy, Willie Boag, Wei-Hung Wang, Di Jin, Tristan Naumann, and Matthew B. A. McDermott. 2019. Publicly available clinical BERT embeddings. CoRR, abs/1904.03323.

Jeffrey Brainard. 2020. New tools aim to tame pandemic paper tsunami. Science, 368(6494):924–925.

Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel M. Ziegler, Jeffrey Wu, Clemens Winter, Christopher Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. 2020. Language models are few-shot learners. CoRR, abs/2005.14165.

Ronan Collobert and Jason Weston. 2008. A unified architecture for natural language processing: deep neural networks with multitask learning. In Machine Learning, Proceedings of the Twenty-Fifth International Conference (ICML 2008), Helsinki, Finland, June 5-9, 2008, volume 307 of ACM International Conference Proceeding Series, pages 160–167. ACM.

Andrew M. Dai and Quoc V. Le. 2015. Semi-supervised sequence learning. In Advances in Neural Information Processing Systems 28: Annual Conference on Neural Information Processing Systems 2015, December 7-12, 2015, Montreal, Quebec, Canada, pages 3079–3087.

Erik De Clercq and Guangdi Li. 2016. Approved antiviral drugs over the past 50 years. Clin Microbiol Rev, 29(3):695–747.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. 2019. BERT: pre-training of deep bidirectional transformers for language understanding. In Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT 2019, Minneapolis, MN, USA, June 2-7, 2019, Volume 1 (Long and Short Papers), pages 4171–4186. Association for Computational Linguistics.

Joshua Geleris, Yifei Sun, Jonathan Platt, Jason Zucker, Matthew Baldwin, George Hripecsak, Angelena Labella, Daniel K Manson, Christine Kubin, R Graham Barr, Magdalena E Sobieszczyk, and Neil W Schluger. 2020. Observational study of hydroxychloroquine in hospitalized patients with covid-19. N Engl J Med, 382(25):2411–2418.

Lena K Hansson, Rasmus Borup Hansen, Sune Pletscher-Frankild, Rudolf Berzins, Daniel Hvidberg Hansen, Dennis Madsen, Sten B Christensen, Malene Revsbech Christiansen, Ulrika Boulund, Xenia Asbaek Wolf, Sonny Kim Kjaerulf, Martijn van de Bunt, Soren Tulin, Thomas Skot Jensen, Rasmus Wernersson, and Jan Nygaard Jensen. 2020. Semantic text mining in early drug discovery for type 2 diabetes. PLoS One, 15(6):e0233956.

Eric H. Huang, Richard Socher, Christopher D. Manning, and Andrew Y. Ng. 2012. Improving word representations via global context and multiple word prototypes. In The 50th Annual Meeting of the Association for Computational Linguistics. Proceedings of the Conference, July 8-14, 2012, Jeju Island, Korea - Volume 1: Long Papers, pages 873–882. The Association for Computer Linguistics.

Kexin Huang, Jaan Altsasaar, and Rajesh Ranganath. 2019. Clinicalbert: Modeling clinical notes and predicting hospital readmission. CoRR, abs/1904.05342.

Yoo Kyung Jeong, Qing Xie, Erjia Yan, and Min Song. 2020. Examining drug and side effect relation using author-entity pair bipartite networks. Journal of Informetrics, 14(1):100999.

Ruoxi Jia, David Dao, Boxin Wang, Frances Ann Hubis, Nick Hynes, Nezhihe Merve Gürel, Bo Li, Ce Zhang, Dawn Song, and Costas J. Spanos. 2019. Towards efficient data valuation based on the shapley value. In The 22nd International Conference on Artificial Intelligence and Statistics, AISTATS 2019, 16-18 April 2019, Naha, Okinawa, Japan, volume 89 of Proceedings of Machine Learning Research, pages 1167–1176. PMLR.

Tushar Khot, Ashish Sabharwal, and Peter Clark. 2017. Answering complex questions using open information extraction. In Proceedings of the 55th Annual Meeting of the Association for Computational Linguistics, ACL 2017, Vancouver, Canada, July 30 - August 4, Volume 2: Short Papers, pages 311–316. Association for Computational Linguistics.

Sebastian Kohlmeier, Kyle Lo, Lucy Lu Wang, and JJ Yang. 2020. Covid-19 open research dataset (cord-19).

Fusataka Kuniyoshi, Kohei Makino, Jun Ozawa, and Makoto Miwa. 2020. Annotating and extracting synthesis process of all-solid-state batteries from scientific literature. In Proceedings of The 12th Language Resources and Evaluation Conference, LREC 2020, Marseille, France, May 11-16, 2020, pages 1941–1950. European Language Resources Association.

Jinhyuk Lee, Wonjin Yoon, Sungdong Kim, Donghyeon Kim, Sunkyu Kim, Chan Ho So, and Jaewoo Kang. 2020. Biobert: a pre-trained biomedical language representation model for biomedical text mining. Bioinform., 36(4):1234–1240.

Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis,
Luke Zettlemoyer, and Veselin Stoyanov. 2019. Roberta: A robustly optimized BERT pretraining approach. CoRR, abs/1907.11692.

Tomas Mikolov, Kai Chen, Greg Corrado, and Jeffrey Dean. 2013. Efficient estimation of word representations in vector space. In 1st International Conference on Learning Representations, ICLR 2013, Scottsdale, Arizona, USA, May 2-4, 2013, Workshop Track Proceedings.

Colin Raffel, Noam Shazeer, Adam Roberts, Katherine Lee, Sharan Narang, Michael Matena, Yanqi Zhou, Wei Li, and Peter J. Liu. 2019. Exploring the limits of transfer learning with a unified text-to-text transformer. CoRR, abs/1910.10683.

Rico Sennrich, Barry Haddow, and Alexandra Birch. 2016. Neural machine translation of rare words with subword units. In Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics, ACL 2016, August 7-12, 2016, Berlin, Germany, Volume 1: Long Papers. The Association for Computer Linguistics.

Vahe Tshitoyan, John Dagdelen, Leigh Weston, Alexander Dunn, Ziqin Rong, Olga Kononova, Kristin A Persson, Gerbrand Ceder, and Anubhav Jain. 2019. Unsupervised word embeddings capture latent knowledge from materials science literature. Nature, 571(7763):95–98.

USGov. 2020. Clinicaltrials.gov.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. 2017. Attention is all you need. In Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, 4-9 December 2017, Long Beach, CA, USA, pages 5998–6008.

Alex Wang, Yada Pruksachatkun, Nikita Nangia, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel R. Bowman. 2019a. Superglue: A stickier benchmark for general-purpose language understanding systems. In Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, 8-14 December 2019, Vancouver, BC, Canada, pages 3261–3275.

Alex Wang, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel R. Bowman. 2019b. GLUE: A multi-task benchmark and analysis platform for natural language understanding. In 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019. OpenReview.net.

Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, and Jamie Brew. 2019. Huggingface’s transformers: State-of-the-art natural language processing. CoRR, abs/1910.03771.

Zhilin Yang, Zihang Dai, Yiming Yang, Jaime G. Carbonell, Ruslan Salakhutdinov, and Quoc V. Le. 2019. Xlnet: Generalized autoregressive pretraining for language understanding. In Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, 8-14 December 2019, Vancouver, BC, Canada, pages 5754–5764.