

Data and text mining

SciFive: a text-to-text transformer model for biomedical literature

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Abstract

Motivation: In 2019, researchers from Google released the Text-to-Text Transfer Transformer (T5) trained on the "Colossal Clean Crawled Corpus" (C4). This approach achieved state-of-the-art (SOTA) results on a diverse range of tasks related to natural language processing (NLP). In the last decade, NLP in biomedicine has become more prominent (i.e. text mining of scientific literature, analysis of electronic health records). This development has created a need for NLP methods trained on corpora of biomedical literature containing the dense technical language characteristic of scientific writing. In this report, we introduce a T5-based model that has been successfully shifted into the biomedical domain.

Results: In this report, we introduce SciFive, a domain-specific T5 model that has been pre-trained on large biomedical corpora. Our model outperforms the current SOTA methods (i.e. BERT, BioBERT, Base T5) on tasks in named entity relation, relation extraction, natural language inference, and question-answering. We show that text-generation methods have significant potential in a broad array of biomedical NLP tasks, particularly those requiring longer, more complex outputs. Our results support further research into biomedical text generation and the development of new methods in this area.

Availability: All checkpoints and pre-trained weights of SciFive are publicly available at <https://console.cloud.google.com/storage/browser/scifive>. The sources code for self-supervised and fine-tuned models is in <https://github.com/justinphan3110/SciFive>

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1 Introduction

Biomedical literature is widely accessible to the scientific community through databases such as Pubmed, PMC, and ScienceDirect. Within seconds, researchers can access millions of journal articles relating to an input query. Text generation tasks such as document summarization and question answering can allow researchers to quickly obtain important information from a large collection of papers, yet current methods generally underperform in these areas. Thus, new NLP methods are needed to parse the increasingly immense amounts of information.

1.1 Related Work

The introduction of the transformer (Vaswani *et al.*, 2017) marked a significant achievement for natural language processing. This is demonstrated by the success of transformer-based architectures such as BERT (Devlin *et al.*, 2018), which, at the time of publication, achieved state-of-the-art (SOTA) results on common NLP tasks. Furthermore, the BERT model has been extended for domain-specific tasks in NLP. Domain-specific language (i.e. biomedical language) is often challenging for NLP models because of the significant differences in vocabulary compared to standard language corpora such as Wikipedia. To solve this problem, BERT models have been pre-trained for domain-specific tasks. With this

approach, SOTA results were achieved in areas such as clinical notes, biomedical literature, and general scientific literature.

2 Approach

BERT (Devlin *et al.*, 2018) is not a unified transfer learning method because BERT-style models can only produce a single prediction for a given input. These models are simply not designed for text generation tasks such as question-answering or summarization. The text-to-text transfer transformer (T5) model proposed by Raffel *et al.* (2019) overcomes this limitation by outputting a string of text for each input, allowing for both question-answering, summarization and other tasks where a single output is generally insufficient. In this report, we introduce SciFive, a pretrained, domain-specific adaptation of the T5 model that is intended for tasks relating to biomedical literature. We here outline two primary contributions of our work.

(1) Our model achieves SOTA results on a variety of common classification tasks in biomedical NLP, including named entity recognition (NER) and relation-extraction (RE).

(2) Second, our model can be extended to tasks requiring extended outputs and achieves superior results on BioAsq question-answering challenges when compared to BioBERT, the current SOTA method to the best of our knowledge (Lee *et al.*, 2019)

3 Unlabeled Dataset

In this section we will describe our biomedical unlabeled datasets which are used in the transfer learning pre-training stage. These large datasets overcome the drawback of overfitting when building a language model in the biomedical domain. (Ruder, 2017). For SciFive, we use two different corpora of biomedical language in order to generalize our model within the domain.

PubMed Abstract¹: The PubMed database contains more than 32 millions citations and abstracts of biomedical literature. For the purpose of model pre-training, we use only the abstracts.

PubMed Central (PMC)²: PMC is a corpus of free full-text articles in the domain of biomedical and life sciences. We hypothesize that training the language model with full-text articles can improve the learning in biomedical context while still containing a generalized representation of natural language overall.

4 Methods

Here, we describe our approach to implementing the SciFive model, which retains the original structure and parameters of the T5 model (Raffel *et al.*, 2019).

4.1 T5

The text-to-text transfer transformer (T5) model (Raffel *et al.*, 2019) is highly similar to the transformer-based encoder-decoder model introduced by Vaswani *et al.* (2017). Each encoder block consists of a self-attention layer and a feed-forward neural network. Each decoder block consists of a self-attention layer, an encoder-decoder attention layer, and a feedforward neural network. There are, however, minor differences between T5 and the transformer-based encoder-decoder model. For example, layer normalization is applied between the components of each encoder block

and each decoder block. Compared to BERT (Devlin *et al.*, 2018), the addition of the decoder block allows T5 to generate outputs that are sequences of text. T5 is pre-trained with self-supervision through a learning objective called span-based language masking. (Raffel *et al.*, 2019).

4.2 SciFive

SciFive follows the sequence-to-sequence encoder-decoder architecture proposed by Vaswani *et al.* (2017) and the T5 framework³ released by Raffel *et al.* (2019). The original T5 work implemented five different model sizes - Small, Base, Large, 3B, and 11B. Due to limited computing resources, we will use only the base and large model for this study. The base and large models have 220 million parameters and 770 million parameters respectively.

Table 1. Corpus combinations for SciFive

Model	Corpus Combination
T5 Raffel <i>et al.</i> (2019)	C4
SciFive(+pubmed)	C4+pubmed
SciFive(+pmc)	C4+pmc
SciFive(+pubmed+pmc)	C4+pubmed+pmc

We first initialized SciFive with the pre-trained weights from the base T5 model. We then re-trained SciFive on various combinations of the C4 corpus (Dodge *et al.*, 2021), a corpus of PubMed abstracts, and a corpus of PMC full-text articles. We trained SciFive for extra 200k steps to optimize the pre-trained weights from T5 in the context of biomedical literature. We also trained a large version of the SciFive model, using 1.2 millions steps (200k additional steps compared to the regular model). With the provided TPU v2-8 on Google Colab, we used the self-supervised training setting recommended by Raffel *et al.* (2019) with a batch size of 128 for the base model and 64 for the large model. We used a learning rate of 0.001 and sequence length 1024 tokens for both input and target as we noticed that unlabeled biomedical text during self-supervised training is long. For the purpose of generalization of biomedical text, we train SciFive on various combinations of biomedical corpus as described in Table 1.

4.3 Input/Output Representation

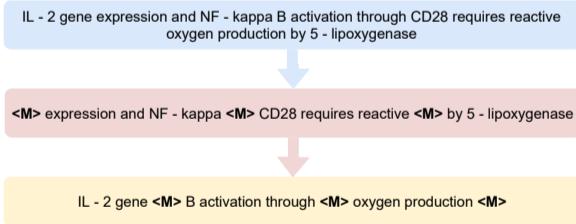


Fig. 1. An illustration on Span-based mask language modeling. For the input sentence, the set of tokens "IL", "-", "2", "gene", "expression", "and", "NF", "-", "kappa", "B", "activation", "through", "CD28", "requires", "reactive", "oxygen", "production", "by", "5", "-", "lipoxygenase" is randomly chosen for corruption, where consecutive tokens are counted as spans and replaced by a sentinel unique masked token <M>. The output sequence then consists of the concatenation of the dropped-out spans, sentinel tokens used to replace them in the input and the final sentinel token.

¹ <https://pubmed.ncbi.nlm.nih.gov>

² <https://www.ncbi.nlm.nih.gov/pmc>

³ <https://github.com/google-research/text-to-text-transfer-transformer>

Consistent with the original T5 model Raffel *et al.* (2019), SciFive converts all of the biomedical tasks into a text-to-text format. During self-supervised training, a text input sequence is given and the model will try to learn a target input going through a learning objective called span-based mask language modeling. Spans of text are randomly masked and the target sequence is predicted as a concatenation of the same sentinel tokens and the real masked spans. An illustration of span-based mask learning objective is in Figure 1.

During supervised training, a sequence of text for both input and target is given to the model for the purpose of learning to generate text. For example, when performing Named-entity recognition (NER), we generate the target sequence by prepending and appending a special token to the named entities in a sentence. The target sequence for Question Answering task is the text corresponding to the answer for a given question (the question text is the input).

4.4 Vocabulary

For every pre-trained language model (LMs), vocabulary plays a crucial role, as these models attempt to derive effective contextualized word vector representations from the training corpus. For SciFive, we use the Sentence Piece model (Kudo and Richardson, 2018) as a base vocabulary model. Sentence Piece is used in all of our SciFive models because it extracts subwords that contain the semantic meaning of a sequence. This overcomes the drawbacks of word-level tokenization and eliminates the need for an immense vocabulary set.

4.5 Multi-Task Learning

SciFive is trained with a maximum likelihood objective using "teacher forcing" (Raffel *et al.*, 2019) for all tasks, thereby enabling multi-task learning. During supervised fine-tuning, a task-specific token is prepended to the input sequence. In one example, we leverage this type of training for the Named-entity recognition task. We believe that this strategy will boost performance for biomedical NER by using the attention of each named entity across all the tasks. Figure 2 illustrates multi-task learning for our NER tasks.

4.6 Fine-Tuning SciFive

We fine-tuned SciFive on five categories of biomedical NLP tasks.

- (1) Named entity recognition (NER) involves predicting a predefined category that describes a proper noun. For example "Lupus" may be classified as "Disease".
- (2) Relation Extraction (RE) involves identifying relationships within text (i.e. gene-disease).
- (3) Natural Language Inference involves determining the validity of a hypothesis (i.e., True, False).
- (4) Document Classification involves assigning a document to a category based on the text.
- (5) Question answering involves generating an answer if given a question and a sequence of text containing the answer to that question.

We fine-tuned in both multi-tasking and single-task learning using the final checkpoints of our SciFive model, 200k steps for both base and large models. Similar to the setting during self-supervised training on TPU v2-8, we choose the batch size of 128 and 64 for the base and large respectively with learning rate 0.001. The input and output specification setting for each task is described in Table 2.

5 Results

We tested SciFive on 7 NER tasks, 5 RE asks, 1 inference task, 1 document classification task, and 3 question answering tasks. We then compared the SciFive results with the current SOTA on these tasks.

5.1 Data

We describe here the datasets and the preprocessing techniques we used. In most cases, we use the same preprocessing procedure as the current baseline models (i.e. BioBERT from Lee *et al.* (2019) and BlueBERT from Peng *et al.* (2019)).

5.1.1 Named Entity Recognition

We tested SciFive on 7 datasets commonly used for biomedical NER: NCBI disease (Doğan *et al.*, 2014), BC5CDR disease (Li *et al.*, 2016), BC5CDR chemical (Li *et al.*, 2016), BC4CHEMD (Krallinger *et al.*, 2015), BC2GM (Smith *et al.*, 2008), JNLPBA (Collier and Kim, 2004), and Species800 Pafilis *et al.* (2013). We follow the processing pipeline and the train/valid/test split similar to Lee *et al.* (2019). For all NER tasks, we evaluate the performance of SciFive based on precision (P), recall (R), and F-1 score (F).

5.1.2 Relation Extraction

We tested SciFive on 2 RE tasks: CHEMPROT (Islamaj Doğan *et al.*, 2019) and DDI (Herrero-Zazo *et al.*, 2013). We follow the same preprocessing technique as Peng *et al.* (2019). We also evaluate the F1-scores of each class in the two relation extraction corpus.

5.1.3 Natural Language Inference

To assess the NLI capabilities of SciFive, we use the MedNLI datasets from MIMIC-III (Romanov and Shivade, 2018) with the same preprocessing technique and training/testing sets.

5.1.4 Document Classification

We use SciFive to classify documents from the HoC dataset (Baker *et al.*, 2015), evaluating the F1 score on the sample average in the same manner as Zhang *et al.* (2017).

5.1.5 Question Answering

Question Answering (QA) is perhaps the most important component of our assessment, as we expect a text-to-text model to vastly outperform BERT-like models in this area. We test SciFive on the factoid questions from the BioASQ 4b, 5b, and 6b challenges Tsatsaronis *et al.* (2015). To preprocess the BioASQ data, we use the same approach as Lee *et al.* (2019).

Using the same approach as the original T5, (Raffel *et al.*, 2019), SciFive converts all problems into a text-to-text format. Therefore, we cannot use the same evaluation procedure as BioBERT. (Lee *et al.*, 2019). BioBERT determines the final answer for a question by taking the highest scoring answer across all the snippets of text corresponding to that question. Our model outputs a sequence of text, not a probability distribution, so we cannot determine our "best" answer in the same way as BioBERT. This key difference prevents us from evaluating strict accuracy as done by Lee *et al.* (2019), so we evaluate only the lenient accuracy for each task. For a single question, SciFive answers questions using a sequence of text rather than probabilities for the start and end of the answer. SciFive uses each piece of context to answer that question individually. If SciFive answers correctly using one or more of the contextual snippets, we say SciFive has answered the question correctly according to the lenient accuracy metric.

To evaluate our results, we rely on an expert assessment. SciFive outputs full-sentence answers that often do not correspond to the exact BioASQ answer provided for a given question, but, in many cases, these

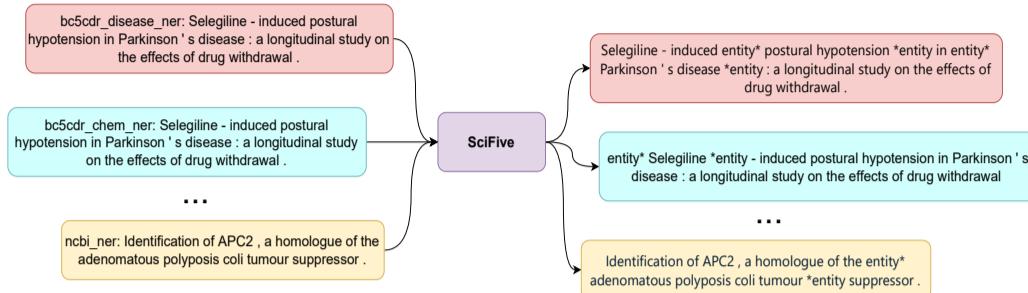


Fig. 2. An illustration about Multi-task learning in Name-entity Recognition Tasks

Table 2. The input and target sequence length settings for each Self-supervised Learning, Name-entity Recognition, Relational Extraction, and Question Answering task

Task	Dataset	Entity type	Number of entities	Task Type	Input Length	Target Length
Self-Supervise Learning	PubMed				1024	1024
	PMC				1024	1024
	PubMed+PMC				1024	1024
Name-entity Recognition	NCBI Disease	Disease	6881	Multi-Task	512	512
	BC5CDR Disease	Disease	19,665			
	BC5CDR Chem	Disease	12,694			
	BC4CHEMD	Chemical	15,411			
	BC2HM	Chemical	79,842			
Relational Extraction	JNLPBA	Gene	20,703		256	16
	Species-800	Species	3708			
Document classification	Chemprot	Protein-chemical	10,031	Single-Task	256	64
	DDI	Biomedical relation	4,920			
Inference	HoC	Biomedical Documents	1,580	Single-Task	256	12
Question Answering	BioASQ4-factoid	Biomedical QA	488	Single-Task	512	128
	BioASQ5-factoid	Biomedical QA	636			
	BioASQ6-factoid	Biomedical QA	779			

Notes: The number of entities is the sum of annotations, relations, documents, pairs, and question & answer pairs for each correspond task in the train, valid, and test sets.
The statistics from Lee *et al.* (2019), Peng *et al.* (2019), Habibi *et al.* (2017), and Zhu *et al.* (2018)

answers are still scientifically correct. For a meaningful assessment of Q/A results, the scientific accuracy must be considered rather than the phrasing of the answer. Table 4 shows several examples of SciFive answers compared to BioBERT answers. It can be easily seen from these examples that SciFive provides clearer, more complete answers than BioBERT.

5.2 Experimental Results

In Table 5, we show the results of SciFive compared to the SOTA approaches. For NER, RE, NLI, and documentation classification, we compare the F1 scores obtained by SciFive to the F1 scores obtained by the SOTA method pre-BioBERT, BioBERT Lee *et al.* (2019), BlueBERT Peng *et al.* (2019), BERT Devlin *et al.* (2018), and T5 Raffel *et al.* (2019). For the BioASQ tasks (Table 3), we compare the lenient accuracy of base SciFive only with base T5 and base BioBERT due to the time required for thorough expert assessment. It should be noted that BioBERT was the winner of these BioASQ challenges. We achieved SOTA results on 3/7 NER tasks, 2/2 RE tasks, 1/1 NLI tasks, and 3/3 question answering tasks (Table 5). We also achieved a near-SOTA result on the HoC document classification task. Based on these results, we emphasize the following point: SciFive (both base and large model) competitive results on classification tasks while

Table 3. Expert assessment result on Question Answering tasks (Lenient Accuracy)

Task	BioBERT	T5	SciFive (PubMed+PMC)	SciFive (PMC)	SciFive (Pubmed)
BioAsq 4b	57.14	85.06	87.66	85.71	88.31
BioAsq 5b	64.83	86.21	86.21	88.28	88.28
BioAsq 6b	57.52	75.82	75.16	79.08	72.55

also providing SOTA results on text generation tasks such as question-answering. This is a significant improvement over BERT-based models, which demonstrates weaker performances on question-answering tasks.

6 Discussion

We used SciFive to explore the role of text generation models in broad-spectrum biomedical NLP, achieving SOTA results on a variety of tasks. This is particularly true for question answering, where SciFive achieved SOTA results. Both T5 and SciFive significantly outperformed BioBERT, highlighting the value of text generation models in biomedical NLP. However, question answering is relatively simplistic compared to other

Table 4. Example of answer generated from SciFive and BioBERT for QA tasks

Task	Question		Text Answer
4b	What was the purpose of the FANTOM4 project?	BioBert	Mammalian Genomes 4 (FANTOM4)
		SciFive	the international functional annotation of the mammalian genomes 4 (fantom4) research collaboration set out to better understand the transcriptional network that regulates macrophage differentiation
5b	What is the RESID database?	BioBert	RESID
		SciFive	the resid database of protein modifications is a comprehensive collection of annotations and structures for protein modifications and cross-links including pre-, co-, and post-translational modifications.
6b	What is the role of gamma-secretase complex in Alzheimer's Disease?	BioBert	APH-1a
		SciFive	it cleaves a precursor to create the amyloid beta peptide
	What is the function of BAX?	BioBert	mitochondrial
		SciFive	bax, a central cell death regulator, is an indispensable gateway to mitochondrial dysfunction and a major proapoptotic member of the b-cell lymphoma 2 (bcl-2) family
	What is the function of the gene MDA5?	BioBert	RIG-1
		SciFive	melanoma differentiation-associated gene 5 (mda5) is a pattern recognition receptor that recognizes cytoplasmic viral double-stranded rna (dsrna) and initiates rapid innate antiviral responses.
	What is the function of HDAC proteins?	BioBert	Histone deacetylase
		SciFive	histone deacetylases (hdacs) prevent the relaxation of chromatin, and positively or negatively regulate transcription.

text generation tasks. To fully examine the potential of text generation models in the context of domain-specific literature, SciFive will be applied to tasks such as document summarization and abstract generation.

From our results, it can be seen that the SOTA results are split between the various versions of SciFive. While we expected the Pubmed+PMC model to have the best performances given the mixture of abstracts and full text articles, our results show that further study is needed to understand the optimal nature of biomedical corpora.

7 Conclusion

In this manuscript, we introduce SciFive, a domain-specific text-to-text model trained specifically for tasks involving biomedical literature. SciFive is effective for NER, RE, NLI, and question answering tasks, achieving SOTA or near-SOTA results in all cases. This outcome supports our conclusion that text-to-text (text generation) models are highly versatile and broadly applicable within domain-specific contexts. These models can be used for common tasks and tasks which require a longer sequence of text as an output (*i.e.* question answering). Our results suggest the need for further study of domain-specific text generation models applied to more difficult tasks such as a document summarization and abstract generation.

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Table 5. Test results in biomedical named entity recognition, relation extraction, document classification, and inference tasks

		Metrics	SOTA	Bert (base)	Base			Large								
					T5	BlueBERT	BioBERT	SciFive (PMC +PubMed)	SciFive (PubMed)	SciFive (PMC)	T5	BlueBERT	BioBERT	SciFive (PMC +PubMed)	SciFive (PubMed)	SciFive (PMC)
Disease	NCBI disease	P	84.12	87.18	-	<u>88.22</u>	88.28	86.28	88.65	87.48	-	87.70	88.10	88.52	87.64	
		R	87.19	89.93	-	91.25	89.30	89.71	<u>90.14</u>	90.14	-	89.90	90.14	89.82	89.30	
		F	88.60	85.63	88.54	-	89.71	88.79	87.96	<u>89.39</u>	88.78	-	88.79	89.11	89.17	88.46
	BC5CDR Disease	P	81.97	85.95	-	86.47	86.67	86.53	<u>86.48</u>	84.28	-	-	<u>86.73</u>	86.30	87.01	88.24
NER	BC4CHEMD	R	82.48	87.73	-	87.84	88.01	88.37	87.99	87.38	-	-	88.46	87.67	88.24	87.62
		F	86.23	82.41	86.83	86.6	87.15	87.33	<u>87.44</u>	87.23	86.31	83.8	-	87.59	86.98	87.62
	BC5CDR Chemical	P	90.94	93.30	-	93.68	93.89	94.01	<u>94.09</u>	93.44	-	93.18	94.13	93.98	93.86	
		R	91.38	93.92	-	93.26	94.80	94.69	<u>94.28</u>	95.02	-	92.09	95.39	95.36	<u>95.37</u>	
Gene/protein	Drug/chem	P	93.31	91.16	93.61	93.5	93.47	94.34	94.35	94.18	94.22	91.7	92.63	94.76	94.66	94.61
		R	91.19	90.57	-	92.80	92.50	92.71	92.01	91.19	-	93.00	92.89	92.19	91.98	
	JNLPBA	P	88.92	88.90	-	<u>91.92</u>	91.53	91.35	91.87	88.76	-	92.35	91.17	91.73	91.15	
		R	91.14	90.04	89.73	-	<u>92.36</u>	92.01	92.02	92.07	89.96	-	92.67	92.03	91.96	91.56
SPECIES	BC2GM	P	81.17	82.43	-	84.32	84.44	84.97	83.66	82.63	-	<u>84.78</u>	84.20	83.81	83.95	
		R	82.42	82.17	-	<u>85.12</u>	83.89	82.89	83.04	82.10	-	85.25	83.48	83.39	83.20	
	Species-800	P	81.69	81.79	82.29	-	<u>84.72</u>	84.16	83.92	84.29	82.36	-	85.01	83.84	83.60	83.57
		R	69.57	69.35	-	<u>72.24</u>	70.36	70.91	70.65	71.04	-	-	71.08	71.36	77.68	77.42
RE	JNLPBA	P	78.58	74.94	74.56	-	77.49	75.29	75.60	80.96	81.99	81.31	-	<u>81.62</u>	81.46	77.42
		R	69.35	72.18	-	72.80	73.47	<u>73.84</u>	72.68	72.69	-	-	<u>75.99</u>	76.08	77.55	
	ChemProt	P	74.80	76.02	81	77.02	82.59	84.24	82.35	<u>84.04</u>	-	-	72.55	73.08	74.09	
		R	56.00	71.60	89.01	75.90	91.21	93.96	92.31	86.81	-	-	81.99	81.31	83.58	
DDI	DoC	P	64.10	73.74	84.82	72.5	76.46	86.68	<u>88.83</u>	87.04	85.41	74.4	-	95.06	95.60	95.06
		R	-	-	82.68	-	-	81.96	<u>83.15</u>	82.75	83.87	-	84.22	83.88	83.00	
	HoC	P	-	-	81.41	-	-	83.04	83.15	82.33	82.84	-	82.84	<u>83.45</u>	84.27	
	NLI	MedNLI	Acc	73.5	-	83.90	84.0	-	84.88	85.30	84.25	83.8	83.8	-	86.57	86.36
		P	-	-	85.55	-	-	86.27	86.18	86.08	86.02	-	86.11	86.35	86.36	
		R	-	-	85.42	-	-	86.29	86.17	86.20	85.95	-	86.21	86.31	86.39	
		F*	81.5	-	85.22	85.3	-	85.99	85.89	85.83	85.68	87.3	-	85.87	86.03	<u>86.08</u>

Notes: P for Precision; R for Recall; F for F1 score; F* is F1 score on sample average. Best scores are in bold, second best scores are underlined. Baseline result and SOTA from Lee et al. (2019) and Peng et al. (2019)

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