Transformer-based masked language models trained on general corpora, such as BERT and RoBERTa, have shown impressive performance on various downstream tasks. Increasingly, researchers are “finetuning” these models to improve performance on domain-specific tasks. Here, we report a broad study in which we applied 14 transformer-based models to 11 scientific tasks in order to evaluate how downstream performance is affected by changes along various dimensions (e.g., training data, model size, pretraining time, finetuning length). In this process, we created the largest and most diverse scientific language model to date, ScholarBERT, by training a 770M-parameter BERT model on an 221B token scientific literature dataset spanning many disciplines. Counterintuitively, our evaluation of the 14 BERT-based models (seven versions of ScholarBERT, five science-specific large language models from the literature, BERT-Base, and BERT-Large) reveals little difference in performance across the 11 science-focused tasks, despite major differences in model size and training data. We argue that our results establish an upper bound for the performance achievable with BERT-based architectures on tasks from the scientific domain.

1 Introduction

Transformer-based language models such as BERT (Bidirectional Encoder Representations from Transformers) (Devlin et al., 2019) have delivered impressive results for tasks such as named entity recognition (Hakala and Pyysalo, 2019), question answering (Qu et al., 2019; Yang et al., 2019), and sentiment classification (Gao et al., 2019). This promise has motivated the development of domain-specific scientific language models. For instance, PubMedBERT (Gu et al., 2021) is pretrained on biomedical articles; BatteryBERT (Huang and Cole, 2022) on a battery research corpus; and the multi-disciplinary SciBERT on computer science and biomedical articles. Each model has been shown to perform well on downstream tasks in its domains. Nevertheless, studies on the generalizability of domain-specific BERT-based scientific models are scarce. We hypothesize that:

H1. Models pretrained on one domain perform significantly worse (i.e., have lower F-1 scores) on tasks in a different, unrelated domain than models pretrained on that latter domain.

H2. A model pretrained on many domains does well on all domains.

In addition to their training corpus domain, extant BERT-based models differ in terms of their model size, training corpus size, and training methods. Researchers have performed some studies of how these parameters affect performance (Devlin et al., 2019; Lee et al., 2020; Gu et al., 2021; Beltagy et al., 2019; Liu et al., 2019), but not for extremely large scientific corpora or models, or in a systematic manner. We also hypothesize:

H3. A bigger model pretrained on a large corpus will outperform a model with fewer parameters pretrained on a subset of the corpus on downstream tasks.

To test these hypotheses, we collected five pretrained scientific BERT models, each trained on a corpus from one or more domains, and 11 labeled datasets that we use to define three downstream sentence classification tasks and eight downstream NER tasks, each specific to some domain(s). We also created seven new BERT-based models by increasing the size of the training corpus up to 221B tokens, an order of magnitude larger than the previous largest corpus (PubMedBERT’s 17B token dataset), and the number of parameters to 770M, more than doubling that of BERT-Large. We then conducted a systematic study of the performance of these 14 models on the 11 downstream tasks. As
we explain in detail in the sections that follow, our results tend to confirm hypothesis H2, but contradict hypotheses H1 and H3.

The major contributions of our work are:

- Analysis of BERT training performance across various model dimensions, including model size, data size, and pretraining/finetuning length.
- Two new BERT-based models, ScholarBERT and ScholarBERT-XL. At 770M parameters, ScholarBERT-XL represents (to the best of our knowledge) the largest multidisciplinary scientific language model, trained on the largest collection of scientific articles, with 225B tokens, spanning domains including Arts & Humanities, Life Sciences & Biomedicine, Physical Sciences, Social Sciences, and Technology.
- Comparisons between the original BERT models and science-focused BERT-based language models, including SciBERT, PubMedBERT, BioBERT, MatBERT, BatteryBERT, and ScholarBERT, on 11 named entity recognition, relation extraction, and sentence classification tasks spanning Biomedicine, Chemistry, Computer Science, Materials Science, Sociology and multi-disciplinary data.
- Results that demonstrate that domain-specific pretraining provides marginal performance improvements on downstream tasks within the domain, when compared to models pretrained on unrelated or more general corpora.

2 Background and Related Work

Language models for scientific tasks are typically created in two stages. In the first, pretraining stage, the model is trained on a large corpus of unlabeled text. In the second, finetuning stage, the model is initialized with weights from the pretrained model and then adapted and trained on a labeled dataset to learn a specific task. Typically, the final layer is replaced with a layer appropriate for the downstream task’s structure when finetuning a model. This method of pretraining followed by finetuning—a form of transfer learning (Weiss et al., 2016)—reduces both the need for labeled data and (when a general pretrained model can be reused) overall computational costs.

2.1 BERT Architecture

BERT models have similar architectures, along four main dimensions: casing, number of layers, hidden size, and number of attention heads. Models are either uncased, meaning the training corpus and corresponding vocabulary are converted to lowercase prior to training, or cased, where the corpus is left with its original casing. There are two canonical sizes for BERT: BERT-Base with 12 layers, a hidden size of 768, and 12 attention heads, for a total of 110M parameters; and BERT-Large with 24 layers, a hidden size of 1024, and 16 attention heads, for a total of 340M parameters. BERT-XL is also defined, with 36 layers, hidden size of 1280, and 20 attention heads.

BERT models are pretrained on unlabeled text with two pretraining objectives: 1) masked-language modeling (MLM) and 2) next-sentence prediction (NSP). At the time of conception, BERT, pretrained on English Wikipedia and the Toronto Books Corpus, achieved state-of-the-art performance when finetuned for 11 NLP tasks (Devlin et al., 2019).

BERT pretraining is performed in two phases, with maximum sequence lengths of 128 and 512, respectively. Typically, the first phase is used for the majority of pretraining steps (90% in the original BERT) because longer sequences are more expensive due to the quadratic complexity of the attention mechanism. WordPiece tokenization is used to create a vocabulary of 30,000 tokens.

In the MLM pretraining objective, 15% of tokens in the input sample are randomly masked with the [MASK] token. The model must predict the masked token given the context of the rest of the sample. When the model is later pretrained, [MASK] is not a token that typically appears in the finetuning corpus. To alleviate problems during finetuning, of the 15% of tokens selected for masking, only 80% are replaced with the [MASK] token, 10% are replaced with a random token in the vocabulary, and 10% are not changed.

The NSP task aims to improve performance in downstream tasks that use the relationship between sentences, such as question answering. Each pretraining input sample contains two sentences, where there is a 50% chance that the second sentence is the actual next sentence in the source document. Otherwise, the second sentence is a random sentence from the training corpus. For the NSP pretraining objective, the model predicts if the sec-
2.2 BERT for Science

The massive expansion in the rate of scientific publication places a tremendous cognitive burden on researchers (Teplitskiy et al., 2022), as valuable information is now being created at a rate faster than any individual researcher can process (Price, 1963; Bornmann and Mutz, 2015; Hey and Trefethen, 2003; Bell et al., 2009). Thus, the use of BERT-like transformer models for automated knowledge extraction from literature is of great interest. The original BERT model, however, was pretrained (and evaluated) on a general corpus (books and Wikipedia), the context, terminology, and writing styles of which varies considerably from that of scientific literature (Ahmad, 2012). A number of efforts have been made to adapt BERT to various science domains, primarily by pretraining new BERT models on domain-specific corpora.

For example, SciBERT (Beltagy et al., 2019) focuses on two domains: biomedical science and computer science. Four SciBERT models are available, each based on the BERT-Base architecture, and pretrained on 3.17B tokens sourced from SemanticScholar (Ammar et al., 2018) with 82% of the pretraining data coming from biomedical sources and the remaining 18% coming from computer science. The four models are cased and uncased versions of SciBERT-BaseVocab and SciBERT-SciVocab. SciBERT-BaseVocab uses the original BERT vocabulary and continues pretraining from the BERT-Base weights. SciBERT-SciVocab pretrains from scratch, using a new vocabulary built from the SciBERT pretraining corpus. The SciBERT variants outperform BERT-Base on finetuning tasks by an average of 1.66% on biomedical tasks and an average of 3.55% on computer science tasks.

BioBERT (Lee et al., 2020) is a BERT model for biomedical text. BioBERT was pretrained by extending the BERT pretraining corpus with 4.5B words from PubMed abstracts and another 13.5B words from full-text articles in PubMedCentral. At the time of writing, BioBERT’s latest version is v1.2. BioBERT shares the same architecture as BERT-Base and is trained on a cased corpus. In comparison to the original BERT model, BioBERT achieves improvements of 0.62% on biomedical named entity recognition, 2.80% on biomedical relation extraction, and 12.24% on biomedical question answering.

PubMedBERT (Gu et al., 2021), another BERT-Base model targeting the biomedical domain, is also pretrained on text from PubMed and PubMedCentral. However, unlike BioBERT, PubMedBERT is trained as a new BERT-Base model, using text drawn exclusively from PubMed and PubMedCentral. As a result, the vocabulary used in PubMedBERT varies significantly from that used in BERT and BioBERT (Gu et al., 2021). PubMedBERT is an uncased model. The pretraining corpus contains 3.1B words from PubMed abstracts and 13.7B words from PubMedCentral articles. PubMedBERT achieves state-of-the-art performance on the Biomedical Language Understanding and Reasoning Benchmark, outperforming BERT-base by 1.16% (Gu et al., 2021).

MatBERT (Trewartha et al., 2022) is a materials science-specific model pretrained on 2M journal articles (8.8B tokens). Experimental results show that it consistently outperforms BERT-Base and SciBERT models on recognizing materials science entities related to solid states, doped materials, and gold nanoparticles, with ~10% increase in F-1 score compared to BERT-Base, and a 1% to 2% improvement compared to SciBERT.

BatteryBERT (Huang and Cole, 2022) is a model pretrained on 400 366 battery-related publications (5.2B tokens). BatteryBERT has been shown to outperform BERT-Base by less than 1% on the SQuAD question answering task. For battery-specific question-answering tasks, its F-1 score is around 5% higher than that of BERT-base.

The prior literature demonstrates the efficacy of pretraining BERT models on domain-specific corpora, as significant improvements in performance on downstream tasks in that domain are observed. However, as scientific publishing continues to grow in size, pace, and diversity, pretraining new language models for each scientific domain will become prohibitively expensive. This suggests the need for larger, multi-disciplinary BERT models that harness the increased availability of diverse pretraining text available for researchers to adapt (i.e., finetune) to their unique needs. In what follows, we introduce the largest such models: ScholarBERT and ScholarBERT-XL.
3 Data and Methodology

This section outlines the pretraining dataset, related models to which we compare performance, and the architecture and pretraining process used for creating the ScholarBERT models. Moreover, we evaluate the performance of ScholarBERT and other BERT-based language models on various scientific fine-tuning tasks.

3.1 The Public Resource Dataset

We pretrain our ScholarBERT models on a dataset provided by Public.Resource.Org, Inc. ("Public Resource"), a nonprofit organization based in California. This dataset was constructed from a corpus of journal article PDF files, from which the Grobid tool, version 0.5.5, was used to extract text. Grobid is “a machine learning library for extracting, parsing and re-structuring raw documents such as PDF into structured XML/TEI encoded documents with a particular focus on technical and scientific publications” (GROBID). We used the XML/TEI encoded documents, not the underlying PDF files. Not all extractions were successful, because of corrupt or badly encoded PDF files. We successfully extracted text from 75 496 055 articles from 178 928 journals. For most articles, we also extracted metadata, such as the title, authors, a DOI, and other descriptive information. We use the journal title to categorize articles by domain and present the resulting distribution of articles in Figure 1. This non-consumptive text and data mining effort applies access and use agreements and technical measures modeled on similar services, such as the Hathi Trust Research Center (Hathi), including strict controls on sharing the dataset.

3.1.1 Pretraining Subsets

We create three pretraining subsets: PRD_1, PRD_10, and PRD_100, comprising 1%, 10%, and 100% of the Public Resource dataset, and with \(\sim10^8, 10^9,\) and \(10^{10}\) sentences, respectively. These subsets are used to understand the effect pretraining corpus size has on model performance.

We randomly sampled articles from the dataset to create each PRD subset until the target subset size is reached. For each subset, we ran WordPiece from the HuggingFace tokenizers on its articles to generate a unique vocabulary. The vocabularies generated for PRD_1 and PRD_10 differed only in 1–2% of the tokens; however, the PRD_100 vocabulary differed from PRD_10 by 15%. A manual inspection of the PRD_100 vocabulary revealed that many common English words such as “is,” “for,” and “the” were missing. These omissions were an artifact of PRD_100 being sufficiently large to cause integer overflows in the token frequency counts. HuggingFace’s tokenizers use unsigned 32-bit integers to count frequencies, and many 2-character tokens occurred more than \(2^{32}\) times in the Public Resource dataset. For example, “the” was not in the final vocabulary because the token “th” overflowed. Because WordPiece iteratively merges smaller tokens to create larger ones, the absence of tokens like “th” or “##he” means that “the” could not appear in the final vocabulary.

We modified the tokenizers library to use unsigned 64-bit integers for all frequency counts, and recreated a correct vocabulary for PRD_100. Interestingly, models trained on the PRD_100 subset with the incorrect and correct vocabularies exhibited comparable performance on downstream tasks.

3.2 Models

We consider 14 different BERT models, six of which are described in prior works: BERT-Base, BERT-Large, SciBERT, PubMedBERT, BioBERT v1.2, MatBERT, and BatteryBERT. The remaining models are the various ScholarBERT models pretrained on the different subsets of the Public Resource dataset (and, in some cases, also the Wikibooks corpus).

We distinguish these models along four dimensions in Table 1: architecture, pretraining method, pretraining corpus, and casing. For architecture, we use three BERT variants: Base, Large, and Extra-Large (XL), as described in Section 2.1. We consider two pretraining methods: standard...
BERT (Devlin et al., 2019) and the optimized RoBERTa (Liu et al., 2019) method, which speeds up training and improves downstream task performance. The various pretraining corpora, listed in Table 2, differ in size and domains covered. All models, except for PubMedBERT, are cased.

This diverse set of models allows us to evaluate the impacts of various factors on the performance achieved for a range of downstream tasks.

3.3 ScholarBERT Pretraining

Here we outline the pretraining methods (pretraining objectives, dataset preparation, hardware and software stack, and hyperparameters) used for developing the ScholarBERT models.

3.3.1 RoBERTa Optimizations

RoBERTa introduces many optimizations for improving BERT pretraining performance (Liu et al., 2019). 1) RoBERTa uses a single phase training approach whereby all training is performed with a maximum sequence length of 512. 2) unlike BERT which randomly introduces a small percentage of shortened sequence lengths into the training data, RoBERTa does not randomly use shortened sequences. 3) RoBERTa uses dynamic masking, meaning that each time a batch of training samples is selected at runtime, a new random set of masked tokens is selected; in contrast, BERT uses static masking, pre-masking the training samples prior to training. BERT duplicates the training data ten times each with a different random, static masking. 4) RoBERTa does not perform NSP during training. 5) RoBERTa takes sentences contiguously from one or more documents until the maximum sequence length is met. 6) RoBERTa uses a larger batch size of 8192. 7) RoBERTa uses byte-pair encoding (BPE) rather than WordPiece. 8) RoBERTa uses an increased vocabulary size of 50,000, 67% larger than BERT. 9) RoBERTa trains for more iterations (up to 500,000 compared to the equivalent 31,000 iterations for BERT-Base).

As indicated in the “Pretraining Method” column of Table 1, we apply most of the RoBERTa optimizations when pretraining ScholarBERT. We differ from RoBERTa in three key places. Unlike RoBERTa, we still randomly introduce smaller length samples because many of our downstream tasks use sequence lengths much smaller than the maximum sequence length of 512 that we pretrain with. We choose to pack training samples with sentences drawn from a single document, as the RoBERTa authors note that this results in slightly better performance. Finally, we use WordPiece encoding rather than BPE, as the RoBERTa authors note that BPE can result in slightly worse downstream performance.

3.3.2 Hardware and Software Stack

We perform data-parallel pretraining on a cluster with 24 nodes, each containing eight 40 GB NVIDIA A100 GPUs. In data-parallel distributed training, a copy of the model is replicated on each GPU, and, in each iteration, each GPU computes on a unique local mini-batch. At the end of the iteration, the local gradients of each model replica are averaged to keep each model replica in sync. We perform data-parallel training of ScholarBERT models using PyTorch’s distributed data-parallel model wrapper and 16 A100 GPUs. For the larger ScholarBERT-XL models, we use the DeepSpeed data-parallel model wrapper and 32 A100 GPUs. The DeepSpeed library incorporates a number of optimizations that improve training time and reduced memory usage, enabling us to train the larger model in roughly the same amount of time as the smaller model.

We perform training in FP16 with a batch size of 32,768 for ~33,000 iterations. To achieve training with larger batch sizes, we employ NVIDIA Apex’s FusedLAMB (NVIDIA, 2017) optimizer, with an initial learning rate of 0.0004. The learning rate is warmed up for the first 6% of iterations and then linearly decayed for the remaining iterations. We use the same masked token percentages as BERT. Training each model requires roughly 1000 node-hours, or 8000 GPU-hours.

Figure 2 depicts the pretraining loss for each of the ScholarBERT models. We train each model past the point of convergence and take checkpoints throughout training to evaluate model performance as a function of training time.

4 Experimental Results

We first perform sensitivity analysis across ScholarBERT pretraining dimensions to investigate the widely held belief that performance can be improved by training larger models for longer on larger datasets. We then compare the performance of ScholarBERT vs. other BERT models on various scientific tasks.
Table 1: Characteristics of the 14 BERT models considered in this study. The BERT-Base architecture has 12 layers, hidden size of 768, and 12 heads; BERT-Large has 24 layers, hidden size of 1024, and 16 heads; and BERT-XL has 36 layers, hidden size of 1280, and 20 heads. The pretraining method is either that of BERT (described in Section 2.1) or RoBERTa (described in Section 3.3). The pretraining corpora are as described in Table 2.

| Name                  | Architecture      | Pretraining Method | Casing | Pretraining Corpus          |
|-----------------------|-------------------|--------------------|--------|-----------------------------|
| BERT_Base             | BERT-Base         | BERT               | Cased  | Wiki + Books                |
| SciBERT               | BERT-Base         | BERT               | Cased  | SemSchol                    |
| PubMedBERT            | BERT-Base         | BERT               | Uncased| PubMed + PMC                |
| BioBERT_1.2           | BERT-Base         | BERT               | Cased  | PubMed + Wiki + Books       |
| MatBERT               | BERT-Base         | BERT               | Cased  | MatSci                      |
| BatteryBERT           | BERT-Base         | BERT               | Cased  | Battery                     |
| BERT_Large            | BERT-Large        | BERT               | Cased  | Wiki + Books                |
| ScholarBERT_1         | BERT-Large        | RoBERTa-like       | Cased  | PRD_1                       |
| ScholarBERT_10        | BERT-Large        | RoBERTa-like       | Cased  | PRD_10                      |
| ScholarBERT_100       | BERT-Large        | RoBERTa-like       | Cased  | PRD_100                     |
| ScholarBERT_10_WB     | BERT-Large        | RoBERTa-like       | Cased  | PRD_100 + Wiki + Books      |
| ScholarBERT-XL_1      | BERT-XL           | RoBERTa-like       | Cased  | PRD_1                       |
| ScholarBERT-XL_100    | BERT-XL           | RoBERTa-like       | Cased  | PRD_100                     |

Table 2: Pretraining corpora used by models in this study. The domains are Bio=biomedicine, CS=computer science, Gen=general, Materials=materials science and engineering, and Sci=broad scientific.

| Name       | Description                                                                 | Domain | Tokens |
|------------|-----------------------------------------------------------------------------|--------|--------|
| Wiki       | English-language Wikipedia articles (HuggingFace, 2020)                      | Gen    | 2.5B   |
| Books      | BookCorpus (Zhu et al., 2015; HuggingFace, 2020): Full text of 11038 books  | Gen    | 0.8B   |
| SemSchol   | 1.14M papers from Semantic Scholar (Cohan et al., 2019), 18% in CS, 82% in Bio | Bio, CS| 3.1B   |
| PubMed     | Biomedical abstracts sampled from PubMed (Gu et al., 2021)                   | Bio    | 3.1B   |
| PubMed     | Biomedical abstracts sampled from PubMed (Lee et al., 2020)                  | Bio    | 4.5B   |
| PMC        | Full-text biomedical articles sampled from PubMedCentral (Gu et al., 2021)   | Bio    | 13.7B  |
| MatSci     | 2M peer-reviewed materials science journal articles (Trewartha et al., 2022)  | Materials | 8.8B |
| Battery    | 0.4M battery-related publications (Huang and Cole, 2022)                     | Materials | 5.2B |
| PRD_1      | 1% of the English-language research articles from the Public Resource dataset | Sci    | 2.2B   |
| PRD_10     | 10% of the English-language research articles from the Public Resource dataset | Sci    | 22B    |
| PRD_100    | 100% of the English-language research articles from the Public Resource dataset | Sci    | 221B   |

Figure 2: Pretraining loss plots for the ScholarBERT models listed in Table 1. The vertical dashed lines indicate the approximate locations of the iteration checkpoints selected for evaluation in Table 3.
Table 3: Effect on downstream NER task performance of varying the size of the pretraining corpus (Model: 1%, 10%, and 100% of PRD) and number of ScholarBERT pretraining iterations (second column). \( SB = \) ScholarBERT.

| Model   | Iterations | Epochs | BC5CDR | JNLPBA | SciERC | NCBI-Disease | ChemDNER |
|---------|------------|--------|--------|--------|--------|--------------|---------|
| SB_1    | 900        | 4      | 65.57  | 44.52  | 16.08  | 49.10        | 61.28   |
|         | 4600       | 22     | 75.36  | 65.53  | 31.65  | 66.27        | 72.19   |
|         | 10000      | 49     | 85.67  | 71.86  | 54.36  | 82.94        | 83.13   |
|         | 23649      | 115    | 86.77  | 73.02  | 59.65  | 85.73        | 85.35   |
|         | 33250      | 165    | 87.78  | 72.45  | 60.63  | 85.90        | 84.72   |
| SB_10   | 900        | 0      | 65.31  | 44.96  | 15.41  | 48.41        | 61.17   |
|         | 4599       | 2      | 74.66  | 64.21  | 30.39  | 66.05        | 70.84   |
|         | 9999       | 4      | 85.33  | 71.82  | 55.20  | 83.73        | 82.68   |
|         | 23199      | 11     | 87.42  | 72.87  | 59.30  | 84.21        | 84.69   |
|         | 33800      | 16     | 87.82  | 73.50  | 57.64  | 87.12        | 84.91   |
| SB_100  | 900        | 0      | 64.57  | 41.90  | 18.06  | 46.60        | 59.73   |
|         | 4389       | 0      | 80.00  | 69.78  | 41.25  | 64.68        | 75.64   |
|         | 10689      | 0      | 86.39  | 73.22  | 58.13  | 80.92        | 82.15   |
|         | 22699      | 0      | 87.39  | 73.48  | 59.84  | 86.77        | 84.92   |
|         | 33900      | 1      | 87.98  | 73.51  | 58.59  | 85.34        | 84.91   |

4.1 Evaluation Tasks

We first introduce the 11 downstream tasks that we use to evaluate model performance: eight NER tasks and three sentence-level tasks. For the NER tasks, we use the following eight annotated scientific NER datasets:

1. BC5CDR (Li et al., 2016): An NER dataset identifying diseases, chemicals, and their interactions, generated from the abstracts of 1500 PubMed articles containing 4409 annotated chemicals, 5818 diseases, and 3116 chemical-disease interactions, totaling 6283 unique entities.

2. JNLPBA (Kim et al., 2004): A bio-entity recognition dataset of molecular biology concepts from 2404 MEDLINE abstracts, consisting of 21 800 unique entities.

3. SciERC (Luan et al., 2018): A dataset annotating entities, relations, and coreference clusters in 500 abstracts from 12 AI conference/workshop proceedings. It contains 5714 distinct named entities.

4. NCBI-Disease (Doğan et al., 2014): Annotations for 793 PubMed abstracts consisting of 6893 disease mentions, of which 2134 are unique.

5. ChemDNER (Krallinger et al., 2015): A chemical entity recognition dataset derived from 10 000 abstracts containing 19 980 unique chemical entity mentions.

6. MatSciNER (Trewartha et al., 2022): 800 annotated abstracts from solid state materials publications sourced via Elsevier’s Scopus-/ScienceDirect, Springer-Nature, Royal Society of Chemistry, and Electrochemical Society. Seven types of entities are labeled: inorganic materials (MAT), symmetry/phase labels (SPL), sample descriptors (DSC), material properties (PRO), material applications (APL), synthesis methods (SMT), and characterization methods (CMT).

7. ScienceExam (Smith et al., 2019): 133K entities from the Aristo Reasoning Challenge Corpus of 3rd to 9th grade science exam questions.

8. Coleridge (Coleridge Initiative, 2020): 13 588 entities from sociology articles indexed by the Inter-university Consortium for Political and Social Research (ICPSR).

The sentence-level downstream tasks are relation extraction on the ChemProt (biology) and SciERC (computer science) datasets, and sentence classification on the Paper Field (multidisciplinary) dataset:

1. ChemProt consists of 1820 PubMed abstracts with chemical-protein interactions annotated by domain experts (Peng et al., 2019).

2. SciERC, introduced above, provides 4716 relations (Luan et al., 2018).

3. The Paper Field dataset (Beltagy et al., 2019), built from the Microsoft Academic
Graph (Sinha et al., 2015), maps paper titles to one of seven fields of study (geography, politics, economics, business, sociology, medicine, and psychology), with each field of study having around 12K training examples.

4.2 Sensitivity Analysis

We first explore the impact of pretraining corpus size and number of training iterations. We train three identical ScholarBERT models on the PRD_1, PRD_10, and PRD_100 datasets until the training loss has plateaued. We select five checkpoints throughout the course of training at ∼900, 4500, 10,000, 23,000, and 33,500 iterations. We choose these iteration counts for checkpoints because they represent points of interest with respect to the pretraining loss (see Figure 2).

For each model and checkpoint, we finetune the model on the BC5CDR, JNLPBA, SciERC, NCBI-Disease, and ChemDNER datasets, to obtain a total of 3 models × 5 checkpoints × 5 datasets = 75 fine-tuned models. We then test each finetuned model on the NER task that corresponds to its finetuning dataset, to yield the results in Table 3. We observe that increasing the pretraining corpus size has no significant effect on performance for any of the five tasks. Note that the smallest dataset, PRD_1, consists of 2.2B tokens, and the original BERT model is trained on just 3.3B tokens. We infer that a model’s capacity for encoding data is inherently limited by the size of its latent space. Hence increasing the amount of data over a threshold will no longer improve the model’s performance.

With respect to number of training iterations, we observe that at the start of training, loss decreases rapidly until around 10,000 iterations, which marks the end of the “rapid learning” phase. Training longer to the point of convergence (roughly 33,000 iterations) yields small but measurable performance improvements, after which performance does not improve with further training. Therefore, the ScholarBERT models used in the following fine tuning experiments are all pretrained for 33,000 iterations.

To better exploit the magnitude of the Public Resource dataset, we trained a larger model, ScholarBERT-XL, effectively doubling the parameter space compared to ScholarBERT. Specifically, we trained two ScholarBERT-XL models, one on the smallest subset, PRD_1, and one on the entire dataset, PRD_100. The ScholarBERT-XL models performed within the run-to-run variances of the smaller ScholarBERT models. We hypothesize that these tasks are not sufficiently complex and the finetuning datasets are not sufficiently large to make use of the additional pretraining data, training time, or model parameters.

4.3 Finetuning for NER Tasks

We compare the performance of the ScholarBERT models with various state-of-the-art scientific models described in Table 1.

Model performance for NER tasks is measured by using the F-1 score, which is defined as the harmonic mean between precision and recall such that $F_1 = \frac{2 \cdot \text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$. However, as a named entity can consist of multiple tokens and there are usually multiple entity classes in an NER dataset, there are multiple ways to define the F-1 score for NER tasks (Sang and De Meulder, 2003; Nakayama, 2018). To ensure fair comparison, we download published pretrained models and finetune every model on every task with the same finetuning hyperparameters. We compute F-1 scores by using the CoNLL NER evaluation Perl script (Sang and De Meulder, 2003).

The F-1 scores for all models and datasets is presented in Table 4, and Table 5 shows the per-domain average F-1 score of each model. Each experiment is run five times and the average is reported. Unsurprisingly, the model that is trained on the same domain as the test set achieved the highest F-1 score (in bold) on the domain relevant test. However, models that are “off-domain” (i.e., pretrained on an irrelevant domain) can reach an F-1 score within a few percentage points of the relevant “on-domain” model. For example, MatBERT, trained exclusively on a Materials Science corpus, achieves an F-1 score of 83.35 on the MatSciNER task, but SciBERT, PubMedBERT and BioBERT, which are trained on Computer Science and biomedical texts, are also able to achieve an F-1 score within two percentage points of MatBERT on the same task.

4.4 Sentence classification F-1 scores

Table 6 shows the performance of each model on our three sentence-level tasks: two relation extraction (SciERC and ChemProt) and one sentence classification (PaperField). We can see that ScholarBERT-XL_100 performed best on the SciERC relation extraction task, while PubMedBERT performs best on the other two tasks. Nevertheless, we observe that the F-1 scores of off-domain models are
Table 4: NER F-1 scores for each model. Models are finetuned five times for each dataset and the average result is presented. In the first column, SB = ScholarBERT.

|          | BC5CDR | JNLPBA | NCBI-Disease | SciERC | ChemDNER | MedSciNER | ScienceExam | Coleridge | Mean  |
|----------|--------|--------|--------------|--------|----------|-----------|-------------|-----------|-------|
| BERT-Base| 85.36  | 72.15  | 84.28        | 56.73  | 84.84    | 78.51     | 78.37       | 57.75     | 74.75 |
| BERT-Large| 86.86  | 72.80  | 84.91        | 59.20  | 85.83    | 82.16     | 82.32       | 57.46     | 76.44 |
| SciBERT  | 88.43  | 73.24  | 86.95        | 59.36  | 85.76    | 82.64     | 78.83       | 54.07     | 76.16 |
| PubMedBERT| **89.34** | **74.53** | **87.91** | 59.03  | **87.96** | 82.63     | 69.73       | 57.71     | **76.11** |
| BioBERT  | 88.01  | 73.09  | 87.84        | 58.24  | 85.53    | 81.76     | 78.60       | 57.04     | 76.26 |
| MatBERT  | 86.44  | 72.56  | 84.94        | 58.52  | 86.09    | 83.35     | 80.01       | 56.91     | 76.10 |
| BatteryBERT| 87.27  | 73.06  | 85.49        | 59.00  | 86.49    | 82.94     | 78.14       | **59.87** | **76.71** |
| SB_1     | 87.69  | 73.03  | 85.65        | 58.39  | 85.80    | 80.61     | **83.24**   | 53.41     | 75.98 |
| SB_10    | 87.84  | 73.47  | 85.92        | 58.37  | 85.90    | 82.09     | 83.12       | 54.93     | 76.46 |
| SB_100   | 86.68  | 72.67  | 84.51        | 57.34  | 83.94    | 78.98     | 83.00       | 54.29     | 75.18 |
| SB_100_WB| 86.89  | 73.16  | 84.88        | 58.43  | 84.31    | 80.84     | 82.43       | 54.00     | 75.62 |
| SB-XL_1  | 87.09  | 73.14  | 84.61        | 58.45  | 85.81    | 82.84     | 81.09       | 55.94     | 76.12 |
| SB-XL_100| 87.46  | 73.25  | 84.73        | 57.26  | 85.73    | 81.75     | 80.72       | 54.54     | 75.68 |
| Best-of-SB| 87.84  | 73.47  | 85.92        | 58.62  | 85.90    | 82.84     | 83.24       | 55.94     | 76.72 |

Table 5: NER F-1 scores averaged by domain. Biomedical = {BC5CDR, JNLPBA, NCBI-Disease, ChemDNER}. CS = {SciERC}. Materials = {MatSciNER}. Sociology = {Coleridge}. Multi-Disciplinary = {ScienceExam}.

|          | Biomedical | CS           | Materials | Sociology | Multi-Disciplinary | Mean   |
|----------|------------|--------------|-----------|-----------|--------------------|--------|
| BERT-Base| 81.66      | 56.73        | 78.51     | **57.75** | 78.37              | 70.60  |
| BERT-Large| 82.60     | 59.20        | 82.61     | 57.46     | 82.32              | **72.84** |
| SciBERT  | 83.60      | **59.36**    | 82.64     | 54.07     | 78.83              | 71.70  |
| PubMedBERT| **84.94** | 59.03        | 82.63     | 57.71     | 69.73              | 70.81  |
| BioBERT  | 83.62      | 58.24        | 81.76     | 57.04     | 78.60              | 71.85  |
| MatBERT  | 82.51      | 58.52        | **83.35** | 56.91     | 80.01              | 72.26  |
| BatteryBERT| 83.43     | 59.00        | 82.94     | 59.87     | 78.14              | 72.68  |
| SB_1     | 82.77      | 58.62        | 80.87     | 55.34     | 82.75              | 72.07  |
| SB_10    | 83.04      | 58.39        | 80.61     | 53.41     | **83.24**          | 71.74  |
| SB_100   | 83.28      | 58.37        | 82.09     | 54.93     | 83.12              | 72.36  |
| SB_100_WB| 81.95      | 57.34        | 78.98     | 54.29     | 83.00              | 71.11  |
| SB-XL_1  | 82.31      | 58.43        | 80.84     | 54.00     | 82.43              | 71.60  |
| SB-XL_100| 82.66      | 58.45        | 82.84     | 55.94     | 81.09              | 71.85  |
| Best-of-SB| 83.28     | 58.62        | 82.84     | 55.94     | **83.24**          | 72.78  |
remarkably close to those of on-domain models.

4.5 Discussion

Through the experiments above, we have tested the prediction performance of existing science-focused BERT-based models on token- and sentence-level classification tasks in a variety of disciplines, and compared their performance to seven variants of the ScholarBERT model. Overall, as shown in Tables 4, 5, and 6, domain-specific models outperform other models on tasks within their respective domains. However, the performance difference measured as F-1 scores among the models is small, with most models less than two percentage points lower than the best performer. In other words, a model pretrained on a particular subject demonstrates only minimal advantage for tasks in that domain over models pretrained on corpora drawn from disparate domains. For example, PubMed-BERT, which is pretrained exclusively on biomedical text, achieves computer science NER performance just 0.3 points lower than does SciBERT, whose training corpus includes computer science articles. Moreover, the seven ScholarBERT variants also achieved similar performance, despite significant differences in their model sizes and pretraining corpora. The performance gap between models is even smaller if we take the error bars into account. We provide the standard deviation of F-1 scores for each task and model across 5 runs and visualizations with error bars in the Appendix. More parameters and larger pretraining corpus did not always lead to big increases in F-1 scores, as we had initially expected.

The reasons for these minor NER performance differences across different models could be twofold: On the one hand, finetuning can overcome missing domain-specific knowledge in pretraining. One popular motivation for pretraining language models on a specific domain is that the model learns domain-specific concepts. However, a sufficiently large finetuning dataset can allow finetuning to patch holes in domain knowledge. This was observed in our test sets, where each domain has tens to hundreds of thousands of examples for finetuning. On the other hand, the test sets used for evaluating models may not be accurate, non-biased representations of the general scientific literature. We were able to find labeled test datasets in four domains (plus one multi-disciplinary dataset) despite our best efforts, and five out of 11 datasets are in the biomedical domain. This is due to the fact that the availability of annotated datasets varies significantly across disciplines. While NLP techniques have long played an integral part in some domains (such as biomedicine (Yandell and Majors, 2002) and materials science (Tshitoyan et al., 2019)), resulting in an abundance of datasets, they are just starting to be adopted in other domains (such as social sciences (Dudeau et al., 2021; Kozlowski et al., 2019)), leading to a scarcity of labeled data. We were unable to find a comprehensive multi-disciplinary test set, and view this as an area of important future work.

5 Conclusions

We explored three hypothesises about the performance of science-focused BERT-based models. We evaluated the impact of various factors, including model size, the size and breadth of pretraining data, and pretraining and finetuning lengths. In doing so, we developed the largest and most general scientific BERT model with 770M parameters and trained on the largest collection of scientific articles, consisting of 221B tokens. To the best of our knowledge, our experiments comparing seven ScholarBERT models, five scientific BERT models, and two standard BERT models on 11 downstream scientific tasks, represent the most complete evaluation of such models performed to date.

Experimental data confirmed the hypothesis H2 by showing that ScholarBERT, pretrained on a multi-disciplinary corpus, can achieve performance on-par with domain specific models on tasks in said domain.

Our results also present the counter-intuitive finding that pretraining on the domain corresponding to a downstream task, as well as pretraining a bigger model on a larger corpus, gives the model only a marginal advantage over models trained on a different or general domain, contradicting hypotheses H1 and H3. We attribute this small performance gap to the power of finetuning, and the lack of comprehensive and non-biased labeled evaluation datasets. High costs seem likely to make the generation of a single labeled evaluation dataset(s) impractical, due to the wide variety of NLP tasks that may be undertaken in scientific fields. Instead, we believe that accurate evaluation of science-focused language models requires new methods that do not rely on labeled data; the development of such methods will be a focus of future work.
Table 6: Relation Extraction and Sentence classification F-1 scores for each model. Models are finetuned five times for each dataset and the average result is presented.

| Model            | SciERC | ChemProt | PaperField | Mean  |
|------------------|--------|----------|------------|-------|
| BERT-Base        | 74.95  | 83.70    | 72.83      | 77.16 |
| BERT-Large       | 80.14  | 88.06    | 73.12      | 80.44 |
| SciBERT          | 79.26  | 89.80    | 73.19      | 80.75 |
| PubMedBERT       | 77.45  | 91.78    | 73.93      | 81.06 |
| BioBERT          | 80.12  | 89.27    | 73.07      | 80.82 |
| MatBERT          | 79.85  | 88.15    | 71.50      | 79.83 |
| BatteryBERT      | 78.14  | 88.33    | 73.28      | 79.92 |
| SB_1             | 73.01  | 83.04    | 72.77      | 76.27 |
| SB_10            | 75.95  | 82.92    | 72.94      | 77.27 |
| SB_100           | 76.19  | 87.60    | 73.14      | 78.98 |
| SB_10 WB         | 73.17  | 81.48    | 72.37      | 75.67 |
| SB_100 WB        | 76.71  | 83.98    | 72.29      | 77.66 |
| SB-XL_1          | 74.85  | 90.60    | 73.22      | 79.56 |
| SB-XL_100        | 80.99  | 89.18    | 73.66      | 81.28 |
| Best-of-SB       | 80.99  | 90.60    | 73.66      | 81.75 |

We have published the ScholarBERT models on HuggingFace (https://huggingface.co/globuslabs). We are not permitted to share the Public Resource dataset.

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Appendix: Extended Results

Table 7 shows average F-1 scores with standard deviations (SD) for the NER tasks. The numbers are computed over five runs. Figure 3 is a visualization of the average scores with error bars. The SD and error bars for sentence classification tasks are presented in Table 8 and Figure 4. The significant overlaps of error bars for NCBI-Disease, SciERC NER, Coleridge, SciERC Sentence Classification, and ChemProt corroborates our observation in Section 4 that on-domain pretraining only provides a marginal advantage on downstream prediction performance over pretraining on a different domain or a general corpus.
Table 7: NER F-1 scores for each model. The average and standard deviation computed over five runs is reported.

|                | BCSCD-R | JNL-PBA | NCBI-Disease | SciERC |
|----------------|---------|---------|--------------|--------|
| BERT-Base      | 85.36 ± 0.189 | 72.15 ± 0.118 | 84.28 ± 0.388 | 56.73 ± 0.716 |
| BERT-Large     | 86.86 ± 0.321 | 72.80 ± 0.299 | 84.91 ± 0.229 | 59.20 ± 1.260 |
| SciBERT        | 88.43 ± 0.112 | 73.24 ± 0.184 | 86.95 ± 0.714 | 59.36 ± 0.390 |
| PubMedBERT     | 89.34 ± 0.185 | 74.53 ± 0.220 | 87.91 ± 0.267 | 59.03 ± 0.688 |
| BioBERT        | 88.01 ± 0.133 | 73.09 ± 0.230 | 87.84 ± 0.513 | 58.24 ± 0.631 |
| MatBERT        | 86.44 ± 0.156 | 72.56 ± 0.162 | 84.94 ± 0.504 | 58.52 ± 0.933 |
| BatteryBERT    | 87.42 ± 0.398 | 72.78 ± 0.190 | 87.04 ± 0.553 | 59.00 ± 1.194 |
| SB_l           | 87.27 ± 0.189 | 73.06 ± 0.265 | 85.49 ± 0.998 | 58.62 ± 0.682 |
| SB_10          | 87.69 ± 0.433 | 73.03 ± 0.187 | 85.65 ± 0.544 | 58.39 ± 1.643 |
| SB_100         | 87.84 ± 0.329 | 73.47 ± 0.210 | 85.92 ± 1.040 | 58.37 ± 1.845 |
| SB_100_WB      | 86.68 ± 0.397 | 72.67 ± 0.329 | 84.51 ± 0.838 | 57.34 ± 1.199 |
| SB_1000_WB     | 86.89 ± 0.543 | 73.16 ± 0.211 | 84.88 ± 0.729 | 58.43 ± 0.881 |
| SB-XL_1        | 87.09 ± 0.179 | 73.14 ± 0.352 | 84.61 ± 0.730 | 58.45 ± 1.014 |
| SB-XL_100      | 87.46 ± 0.142 | 73.25 ± 0.300 | 84.73 ± 0.817 | 57.26 ± 2.146 |

|                | ChemDNER | MatSciNER | ScienceExam | Coleridge |
|----------------|----------|-----------|-------------|-----------|
| BERT-Base      | 84.84 ± 0.004 | 78.51 ± 0.300 | 78.37 ± 0.004 | 57.75 ± 1.230 |
| BERT-Large     | 85.83 ± 0.022 | 82.16 ± 0.040 | 82.32 ± 0.072 | 57.46 ± 0.818 |
| SciBERT        | 85.76 ± 0.089 | 82.64 ± 0.054 | 78.83 ± 0.004 | 54.07 ± 0.930 |
| PubMedBERT     | 87.96 ± 0.094 | 82.63 ± 0.045 | 69.73 ± 0.872 | 57.71 ± 1.07 |
| BioBERT        | 85.53 ± 0.130 | 81.76 ± 0.094 | 78.60 ± 0.072 | 57.04 ± 0.868 |
| MatBERT        | 86.09 ± 0.170 | 83.35 ± 0.085 | 80.01 ± 0.027 | 56.91 ± 0.434 |
| BatteryBERT    | 86.49 ± 0.085 | 82.94 ± 0.309 | 78.14 ± 0.103 | 59.87 ± 0.398 |
| SB_1           | 85.25 ± 0.063 | 80.87 ± 0.282 | 82.75 ± 0.049 | 55.34 ± 0.742 |
| SB_10          | 85.80 ± 0.094 | 80.61 ± 0.747 | 83.24 ± 0.063 | 53.41 ± 0.380 |
| SB_100         | 85.90 ± 0.063 | 82.09 ± 0.022 | 83.12 ± 0.085 | 54.93 ± 0.063 |
| SB_100_WB      | 83.94 ± 0.058 | 78.98 ± 1.190 | 83.00 ± 0.250 | 54.29 ± 0.080 |
| SB_1000_WB     | 84.31 ± 0.080 | 80.84 ± 0.161 | 82.43 ± 0.031 | 54.00 ± 0.425 |
| SB-XL_1        | 85.81 ± 0.054 | 82.78 ± 0.190 | 87.04 ± 0.553 | 59.94 ± 0.899 |
| SB-XL_100      | 85.73 ± 0.058 | 81.75 ± 0.367 | 80.72 ± 0.174 | 54.54 ± 0.389 |

Figure 3: Visualization of NER F-1 scores from Table 7 with error bars.
Table 8: Sentence classification F-1 scores for each model. The average and standard deviation computed over five runs is reported.

| Model          | SciERC        | ChemProt       | PaperField      |
|----------------|---------------|----------------|-----------------|
| BERT-Base      | 74.95 ± 1.596 | 83.70 ± 0.472  | 72.83 ± 0.082   |
| BERT-Large     | 80.14 ± 2.266 | 88.06 ± 0.353  | 73.12 ± 0.125   |
| SciBERT        | 79.26 ± 0.498 | 89.80 ± 0.263  | 73.19 ± 0.046   |
| PubMedBERT     | 77.45 ± 0.964 | 91.78 ± 0.096  | 73.93 ± 0.099   |
| BioBERT        | 80.12 ± 0.179 | 89.27 ± 0.281  | 73.07 ± 0.074   |
| MatBERT        | 79.85 ± 0.121 | 88.15 ± 0.026  | 71.50 ± 0.135   |
| BatteryBERT    | 78.14 ± 0.550 | 88.33 ± 0.393  | 73.28 ± 0.022   |
| SB_1           | 73.01 ± 0.248 | 83.04 ± 0.150  | 72.77 ± 0.060   |
| SB_10          | 75.95 ± 0.203 | 82.92 ± 0.792  | 72.94 ± 0.182   |
| SB_100         | 76.19 ± 1.592 | 87.60 ± 0.324  | 73.14 ± 0.085   |
| SB_100 WB      | 73.17 ± 1.254 | 81.48 ± 1.705  | 72.37 ± 0.115   |
| SB_100 WB      | 76.71 ± 2.114 | 83.98 ± 0.252  | 72.29 ± 0.048   |
| SB-XL_1        | 74.85 ± 1.497 | 90.60 ± 0.246  | 73.22 ± 0.009   |
| SB-XL_100      | 80.99 ± 0.900 | 89.18 ± 0.499  | 73.66 ± 0.113   |

Figure 4: Visualization of sentence classification F-1 scores from Table 8 with error bars.