https://arxiv.org/pdf/2412.19994

ENHANCING DOMAIN KNOWLEDGE OF LLMs

Pre-training, SFT and RLHF have been the de facto way to enhance domain knowledge of LLMs.

PRETRAINING

Training on a large-scale corpus enables LLMs to capture rich language representations

SUPERVISED FINE TUNING

Pre-training on large corpus with next token prediction does not align well with users' objective, as users expect models to "follow their instructions helpfully and safely".

SFT effectively aligns LLMs with user expectations by training them on datasets consisting of (INSTRUCTION, OUTPUT) pairs

TASK SPECIFIC SUPERVISED FINE TUNING

Task-specific finetuning of LLMs has demonstrated effective prediction performances, often surpassing traditional machine learning models, particularly in low-data scenarios.

REINFORCEMENT LEARNING WITH HUMAN FEEDBACK

RLHF is a crucial step in training powerful LLMs.

While pre-training and SFT provide LLMs with domain-specific knowledge and enable them to perform specific tasks, these models are still prone to hallucination.

RLHF is the most effective method to alleviate hallucinations and build a truthful, helpful and harmless LLM.
There are many detailed algorithms to utilize human feedback, such as PPO, DPO.
Beyond human feedback, other methods for collecting preference feedback include AI feedback and environment feedback.

BENCHMARKS

Benchmarks are essential for evaluating the performance of chemistry LLMs

TRAINING

Data Diversity Training data is the foundation of LLMs.

However, most existing datasets are built from pre-existing sources.
More diverse and comprehensive datasets are required to enhance the training of LLMs and broaden their capabilities

TRAINING FOR REASONING LLMs

Chain-of-Thought reasoning is one of the most notable emergent abilities of LLMs, involving the generation of a sequence of intermediate steps leading to the final answer. LLMs often lack this critical reasoning capability due to simple training instruction pairs. Developing training data with explicit reasoning paths to effectively elicit the CoT ability in LLMs is a crucial direction for future research.

OTHER RESEARCH PAPERS

- Gpt-4 technical report.
- Towards chemical foundation models
- Flamingo: a visual language model for few-shot learning.
- Introducing claude models
- Qwen-vl: A frontier large vision-language model with versatile abilities
- Constitutional ai: Harmlessness from ai feedback.
- Autonomous chemical research with large language models.
- Sparks of artificial general intelligence: Early experiments with gpt-4.
- Towards scalable automated alignment of llms: A survey.
- Do large language models understand chemistry? a conversation with chatgpt
- Unveiling the power of language models in chemical research question answering.
- Hight: Hierarchical graph tokenization for graph-language alignment.
- Molnextr: A generalized deep learning model for molecular image recognition
- Internvl: Scaling up vision foundation models and aligning for generic visual-linguistic tasks.
- Llamp: Large language model made powerful for high-fidelity materials knowledge retrieval and distillation.
- Deep reinforcement learning from human preferences
- Unifying molecular and textual representations via multi-task language modelling

- A foundation language model for geoscience knowledge understanding and utilization
- Pre-training of deep bidirectional transformers for language understanding
- An image is worth 16x16 words: Transformers for image recognition at scale.
- Large language models open new ways of ai-assisted molecular design for chemists.
- A comprehensive multi-level chemical evaluation for large language models
- What can large language models do in chemistry? a comprehensive benchmark on eight tasks. Advances in Neural Information Processing Systems,
- Strategies for pre-training graph neural networks.
- Language is not all you need: Aligning perception with language models. Advances in Neural Information Processing Systems
- A comprehensive multi-level chemical evaluation for large language models
- Leveraging large language models for predictive chemistry
- Language models in molecular discovery. In Drug Development Supported by Informatics,
- Rlaif: Scaling reinforcement learning from human feedback with ai feedback.
- Large language models are in-context molecule learners.
- Blip-2: Bootstrapping language-image pretraining with frozen image encoders and large language models.
- From words to molecules: A survey of large language models in chemistry
- Fine-tuning large language models for chemical text mining
- Instruction tuning for large language models: A survey
- Scientific large language models: A survey on biological & chemical domains.
- Chemllm: A chemical large language model.
- Llasmol: Advancing large language models for chemistry with a large-scale, comprehensive, high-quality instruction tuning dataset.
- React: Synergizing reasoning and acting in language models
- Hallucination is inevitable: An innate limitation of large language models
- How powerful are graph neural networks?
- A systematic survey of chemical pre-trained models.
- Chain-of-thought prompting elicits reasoning in large language models
- Emergent abilities of large language models

- Scibench: Evaluating college-level scientific problem-solving abilities of large language models
- Attention is all you need
- Llama 2: Open foundation and fine-tuned chat models.
- Llama: Open and efficient foundation language models
- Galactica: A large language model for science.
- Learning to summarize with human feedback
- Scieval: A multi-level large language model evaluation benchmark for scientific research.
- Proximal policy optimization algorithms.
- Schnet–a deep learning architecture for molecules and materials.
- Neural machine translation of rare words with subword units
- Your language model is secretly a reward model
- Exploring the limits of transfer learning with a unified text-to-text transformer.
- A review of large language models and autonomous agents in chemistry
- Training language models to follow instructions with human feedback
- Augmenting large language models with chemistry tools.
- Learn to explain: Multimodal reasoning via thought chains for science question answering.
- Moleculargpt: Open large language model (llm) for few-shot molecular property prediction.
- Translation between molecules and natural language.