

Sat 2024.03.09

### Improved Algorithm for Adversarial Linear Mixture MDPs with Bandit Feedback and Unknown Transition

*Long-Fei Li, Peng Zhao, Zhi-Hua Zhou*

We study reinforcement learning with linear function approximation, unknown transition, and adversarial losses in the bandit feedback setting. Specifically, we focus on linear mixture MDPs whose transition kernel is a linear mixture model. We propose a new algorithm that attains an  $\tilde{O}(\sqrt{HS^3K} + \sqrt{HSAK})$  regret with high probability, where  $d$  is the dimension of feature mappings,  $S$  is the size of state space,  $A$  is the size of action space,  $H$  is the episode length and  $K$  is the number of episodes. Our result strictly improves the previous best-known  $\tilde{O}(dS^2\sqrt{K} + \sqrt{HSAK})$  result in Zhao et al. (2023a) since  $H \leq S$  holds by the layered MDP structure. Our advancements are primarily attributed to (i) a new least square estimator for the transition parameter that leverages the visit information of all states, as opposed to only one state in prior work, and (ii) a new self-normalized concentration tailored specifically to handle non-independent noises, originally proposed in the dynamic assortment area and firstly applied in reinforcement learning to handle correlations between different states.

link: <http://arxiv.org/abs/2403.04568v1>

### ShuffleBench: A Benchmark for Large-Scale Data Shuffling Operations with Distributed Stream Processing Frameworks

*Sören Henning, Adriano Vogel, Michael Leichtfried, Otmar Ertl, Rick Rabiser*

Distributed stream processing frameworks help building scalable and reliable applications that perform transformations and aggregations on continuous data streams. This paper introduces ShuffleBench, a novel benchmark to evaluate the performance of modern stream processing frameworks. In contrast to other benchmarks, it focuses on use cases where stream processing frameworks are mainly employed for shuffling (i.e., re-distributing) data records to perform state-local aggregations, while the actual aggregation logic is considered as black-box software components. ShuffleBench is inspired by requirements for near real-time analytics of a large cloud observability platform and takes up benchmarking metrics and methods for latency, throughput, and scalability established in the performance engineering research community. Although inspired by a real-world observability use case, it is highly configurable to allow domain-independent evaluations. ShuffleBench comes as a ready-to-use open-source software utilizing existing Kubernetes tooling and providing implementations for four state-of-the-art frameworks. Therefore, we expect ShuffleBench to be a valuable contribution to both industrial practitioners building stream processing applications and researchers working on new stream processing approaches. We complement this paper with an experimental performance evaluation that employs ShuffleBench with various configurations on Flink, Hazelcast, Kafka Streams, and Spark in a cloud-native environment. Our results show that Flink achieves the highest throughput while Hazelcast processes data streams with the lowest latency.

link: <http://dx.doi.org/10.1145/3629526.3645036>

### Machine learning and information theory concepts towards an AI Mathematician

*Yoshua Bengio, Nikolay Malkin*

The current state-of-the-art in artificial intelligence is impressive, especially in terms of mastery of language, but not so much in terms of mathematical reasoning. What could be missing? Can we learn something useful about that gap from how the brains of mathematicians go about their craft? This essay builds on the idea that current deep learning mostly succeeds at system 1 abilities -- which correspond to our intuition and habitual behaviors -- but still lacks something important regarding system 2 abilities -- which include reasoning and robust uncertainty estimation. It takes an information-theoretical posture to ask questions about what constitutes an interesting mathematical statement, which could guide future work in crafting an AI mathematician. The focus

is not on proving a given theorem but on discovering new and interesting conjectures. The central hypothesis is that a desirable body of theorems better summarizes the set of all provable statements, for example by having a small description length while at the same time being close (in terms of number of derivation steps) to many provable statements.

link: <http://arxiv.org/abs/2403.04571v1>

### **Wiki-TabNER: Advancing Table Interpretation Through Named Entity Recognition**

*Aneta Koleva, Martin Ringsquandl, Ahmed Hatem, Thomas Runkler, Volker Tresp*

Web tables contain a large amount of valuable knowledge and have inspired tabular language models aimed at tackling table interpretation (TI) tasks. In this paper, we analyse a widely used benchmark dataset for evaluation of TI tasks, particularly focusing on the entity linking task. Our analysis reveals that this dataset is overly simplified, potentially reducing its effectiveness for thorough evaluation and failing to accurately represent tables as they appear in the real-world. To overcome this drawback, we construct and annotate a new more challenging dataset. In addition to introducing the new dataset, we also introduce a novel problem aimed at addressing the entity linking task: named entity recognition within cells. Finally, we propose a prompting framework for evaluating the newly developed large language models (LLMs) on this novel TI task. We conduct experiments on prompting LLMs under various settings, where we use both random and similarity-based selection to choose the examples presented to the models. Our ablation study helps us gain insights into the impact of the few-shot examples. Additionally, we perform qualitative analysis to gain insights into the challenges encountered by the models and to understand the limitations of the proposed dataset.

link: <http://arxiv.org/abs/2403.04577v1>

### **Beyond Major Product Prediction: Reproducing Reaction Mechanisms with Machine Learning Models Trained on a Large-Scale Mechanistic Dataset**

*Joonyoung F. Joun, Mun Hong Fong, Jihye Roh, Zhengkai Tu, John Bradshaw, Connor W. Coley*

Mechanistic understanding of organic reactions can facilitate reaction development, impurity prediction, and in principle, reaction discovery. While several machine learning models have sought to address the task of predicting reaction products, their extension to predicting reaction mechanisms has been impeded by the lack of a corresponding mechanistic dataset. In this study, we construct such a dataset by imputing intermediates between experimentally reported reactants and products using expert reaction templates and train several machine learning models on the resulting dataset of 5,184,184 elementary steps. We explore the performance and capabilities of these models, focusing on their ability to predict reaction pathways and recapitulate the roles of catalysts and reagents. Additionally, we demonstrate the potential of mechanistic models in predicting impurities, often overlooked by conventional models. We conclude by evaluating the generalizability of mechanistic models to new reaction types, revealing challenges related to dataset diversity, consecutive predictions, and violations of atom conservation.

link: <http://arxiv.org/abs/2403.04580v1>

### **What Cannot be Skipped About the Skiplist: A Survey of Skiplists and Their Applications in Big Data Systems**

*Venkata Sai Pavan Kumar Vadrevu, Lu Xing, Walid G. Aref*

Skiplists have become prevalent in systems. The main advantages of skiplists are their simplicity and ease of implementation, and the ability to support operations in the same asymptotic complexities as their tree-based counterparts. In this survey, we explore skiplists and their many variants. We highlight many scenarios of how skiplists are useful and fit well in these usage scenarios. We study several extensions to skiplists to make them fit for more applications, e.g., their use in the multi-dimensional space, network overlaying algorithms, as well as serving as indexes in database systems. Besides, we also discuss systems that adopt the idea of skiplists and apply the probabilistic skip pattern into their designs.

link: <http://arxiv.org/abs/2403.04582v1>

### **Unbiased Estimator for Distorted Conics in Camera Calibration**

*Chaehyeon Song, Jaeho Shin, Myung-Hwan Jeon, Jongwoo Lim, Ayoung Kim*

In the literature, points and conics have been major features for camera geometric calibration. Although conics are more informative features than points, the loss of the conic property under distortion has critically limited the utility of conic features in camera calibration. Many existing approaches addressed conic-based calibration by ignoring distortion or introducing 3D spherical targets to circumvent this limitation. In this paper, we present a novel formulation for conic-based calibration using moments. Our derivation is based on the mathematical finding that the first moment can be estimated without bias even under distortion. This allows us to track moment changes during projection and distortion, ensuring the preservation of the first moment of the distorted conic. With an unbiased estimator, the circular patterns can be accurately detected at the sub-pixel level and can now be fully exploited for an entire calibration pipeline, resulting in significantly improved calibration. The entire code is readily available from [github.com/ChaehyeonSong/discocal](https://github.com/ChaehyeonSong/discocal).

link: <http://arxiv.org/abs/2403.04583v1>

### **Learning Agility Adaptation for Flight in Clutter**

*Guangyu Zhao, Tianyue Wu, Yeke Chen, Fei Gao*

Animals learn to adapt agility of their movements to their capabilities and the environment they operate in. Mobile robots should also demonstrate this ability to combine agility and safety. The aim of this work is to endow flight vehicles with the ability of agility adaptation in prior unknown and partially observable cluttered environments. We propose a hierarchical learning and planning framework where we utilize both trial and error to comprehensively learn an agility policy with the vehicle's observation as the input, and well-established methods of model-based trajectory generation. Technically, we use online model-free reinforcement learning and a pre-training-fine-tuning reward scheme to obtain the deployable policy. The statistical results in simulation demonstrate the advantages of our method over the constant agility baselines and an alternative method in terms of flight efficiency and safety. In particular, the policy leads to intelligent behaviors, such as perception awareness, which distinguish it from other approaches. By deploying the policy to hardware, we verify that these advantages can be brought to the real world.

link: <http://arxiv.org/abs/2403.04586v1>

### **Zero-shot cross-modal transfer of Reinforcement Learning policies through a Global Workspace**

*Léopold Maytié, Benjamin Devillers, Alexandre Arnold, Rufin VanRullen*

Humans perceive the world through multiple senses, enabling them to create a comprehensive representation of their surroundings and to generalize information across domains. For instance, when a textual description of a scene is given, humans can mentally visualize it. In fields like robotics and Reinforcement Learning (RL), agents can also access information about the environment through multiple sensors; yet redundancy and complementarity between sensors is difficult to exploit as a source of robustness (e.g. against sensor failure) or generalization (e.g. transfer across domains). Prior research demonstrated that a robust and flexible multimodal representation can be efficiently constructed based on the cognitive science notion of a 'Global Workspace': a unique representation trained to combine information across modalities, and to broadcast its signal back to each modality. Here, we explore whether such a brain-inspired multimodal representation could be advantageous for RL agents. First, we train a 'Global Workspace' to exploit information collected about the environment via two input modalities (a visual input, or an attribute vector representing the state of the agent and/or its environment). Then, we train a RL agent policy using this frozen Global Workspace. In two distinct environments and tasks, our results reveal the model's ability to perform zero-shot cross-modal transfer between input modalities, i.e. to apply to image inputs a policy previously trained on attribute vectors (and

vice-versa), without additional training or fine-tuning. Variants and ablations of the full Global Workspace (including a CLIP-like multimodal representation trained via contrastive learning) did not display the same generalization abilities.

link: <http://arxiv.org/abs/2403.04588v1>

### **Embodied Understanding of Driving Scenarios**

*Yunsong Zhou, Linyan Huang, Qingwen Bu, Jia Zeng, Tianyu Li, Hang Qiu, Hongzi Zhu, Minyi Guo, Yu Qiao, Hongyang Li*

Embodied scene understanding serves as the cornerstone for autonomous agents to perceive, interpret, and respond to open driving scenarios. Such understanding is typically founded upon Vision-Language Models (VLMs). Nevertheless, existing VLMs are restricted to the 2D domain, devoid of spatial awareness and long-horizon extrapolation proficiencies. We revisit the key aspects of autonomous driving and formulate appropriate rubrics. Hereby, we introduce the Embodied Language Model (ELM), a comprehensive framework tailored for agents' understanding of driving scenes with large spatial and temporal spans. ELM incorporates space-aware pre-training to endow the agent with robust spatial localization capabilities. Besides, the model employs time-aware token selection to accurately inquire about temporal cues. We instantiate ELM on the reformulated multi-faced benchmark, and it surpasses previous state-of-the-art approaches in all aspects. All code, data, and models will be publicly shared.

link: <http://arxiv.org/abs/2403.04593v1>

### **Contrastive Continual Learning with Importance Sampling and Prototype-Instance Relation Distillation**

*Jiyong Li, Dilshod Azizov, Yang Li, Shangsong Liang*

Recently, because of the high-quality representations of contrastive learning methods, rehearsal-based contrastive continual learning has been proposed to explore how to continually learn transferable representation embeddings to avoid the catastrophic forgetting issue in traditional continual settings. Based on this framework, we propose Contrastive Continual Learning via Importance Sampling (CCLIS) to preserve knowledge by recovering previous data distributions with a new strategy for Replay Buffer Selection (RBS), which minimize estimated variance to save hard negative samples for representation learning with high quality. Furthermore, we present the Prototype-instance Relation Distillation (PRD) loss, a technique designed to maintain the relationship between prototypes and sample representations using a self-distillation process. Experiments on standard continual learning benchmarks reveal that our method notably outperforms existing baselines in terms of knowledge preservation and thereby effectively counteracts catastrophic forgetting in online contexts. The code is available at <https://github.com/lijy373/CCLIS>.

link: <http://arxiv.org/abs/2403.04599v1>

### **In-n-Out: Calibrating Graph Neural Networks for Link Prediction**

*Erik Nascimento, Diego Mesquita, Samuel Kaskio, Amauri H Souza*

Deep neural networks are notoriously miscalibrated, i.e., their outputs do not reflect the true probability of the event we aim to predict. While networks for tabular or image data are usually overconfident, recent works have shown that graph neural networks (GNNs) show the opposite behavior for node-level classification. But what happens when we are predicting links? We show that, in this case, GNNs often exhibit a mixed behavior. More specifically, they may be overconfident in negative predictions while being underconfident in positive ones. Based on this observation, we propose IN-N-OUT, the first-ever method to calibrate GNNs for link prediction. IN-N-OUT is based on two simple intuitions: i) attributing true/false labels to an edge while respecting a GNNs prediction should cause but small fluctuations in that edge's embedding; and, conversely, ii) if we label that same edge contradicting our GNN, embeddings should change more substantially. An extensive experimental campaign shows that IN-N-OUT significantly improves the calibration of GNNs in link prediction, consistently outperforming the baselines available -- which

are not designed for this specific task.

link: <http://arxiv.org/abs/2403.04605v1>

### **A Domain Translation Framework with an Adversarial Denoising Diffusion Model to Generate Synthetic Datasets of Echocardiography Images**

*Cristiana Tiago, Sten Roar Snare, Jurica Sprem, Kristin McLeod*

Currently, medical image domain translation operations show a high demand from researchers and clinicians. Amongst other capabilities, this task allows the generation of new medical images with sufficiently high image quality, making them clinically relevant. Deep Learning (DL) architectures, most specifically deep generative models, are widely used to generate and translate images from one domain to another. The proposed framework relies on an adversarial Denoising Diffusion Model (DDM) to synthesize echocardiography images and perform domain translation. Contrary to Generative Adversarial Networks (GANs), DDMs are able to generate high quality image samples with a large diversity. If a DDM is combined with a GAN, this ability to generate new data is completed at an even faster sampling time. In this work we trained an adversarial DDM combined with a GAN to learn the reverse denoising process, relying on a guide image, making sure relevant anatomical structures of each echocardiography image were kept and represented on the generated image samples. For several domain translation operations, the results verified that such generative model was able to synthesize high quality image samples: MSE: 11.50 +/- 3.69, PSNR (dB): 30.48 +/- 0.09, SSIM: 0.47 +/- 0.03. The proposed method showed high generalization ability, introducing a framework to create echocardiography images suitable to be used for clinical research purposes.

link: <http://dx.doi.org/10.1109/ACCESS.2023.3246762>

### **Strong Priority and Determinacy in Timed CCS**

*Luigi Liquori, Michael Mendler*

Building on the classical theory of process algebra with priorities, we identify a new scheduling mechanism, called "sequentially constructive reduction" which is designed to capture the essence of synchronous programming. The distinctive property of this evaluation strategy is to achieve determinism-by-construction for multi-cast concurrent communication. In particular, it permits us to model shared memory multi-threading with reaction to absence as it lies at the core of the programming language Esterel. In the technical setting of CCS extended by clocks and priorities, we prove for a large class of processes, which we call "structurally coherent" the confluence property for constructive reductions. We further show that under some syntactic restrictions, called "pivotable" the operators of prefix, summation, parallel composition, restriction and hiding preserve structural coherence. This covers a strictly larger class of processes compared to those that are confluent in Milner's classical theory of CCS without priorities.

link: <http://arxiv.org/abs/2403.04618v1>

### **MedFLIP: Medical Vision-and-Language Self-supervised Fast Pre-Training with Masked Autoencoder**

*Lei Li, Tianfang Zhang, Xinglin Zhang, Jiaqi Liu, Bingqi Ma, Yan Luo, Tao Chen*

Within the domain of medical analysis, extensive research has explored the potential of mutual learning between Masked Autoencoders(MAEs) and multimodal data. However, the impact of MAEs on intermodality remains a key challenge. We introduce MedFLIP, a Fast Language-Image Pre-training method for Medical analysis. We explore MAEs for zero-shot learning with crossed domains, which enhances the model ability to learn from limited data, a common scenario in medical diagnostics. We verify that masking an image does not affect intermodal learning. Furthermore, we propose the SVD loss to enhance the representation learning for characteristics of medical images, aiming to improve classification accuracy by leveraging the structural intricacies of such data. Lastly, we validate using language will improve the zero-shot performance for the medical image analysis. MedFLIP scaling of the masking process marks an advancement in the field, offering a pathway to rapid and precise medical image analysis without the traditional

computational bottlenecks. Through experiments and validation, MedFLIP demonstrates efficient performance improvements, setting an explored standard for future research and application in medical diagnostics.

link: <http://arxiv.org/abs/2403.04626v1>