Two Interesting Papers on ML - a Personal Pick

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Integrating Physics-Based Modeling with Machine Learning: A Survey

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In this manuscript, we provide a structured and comprehensive overview of techniques to **integrate machine learning with physics-based modeling.** First, we provide a summary of application areas for which these approaches have been applied. Then, we describe classes of methodologies used to construct physics-guided machine learning models and hybrid physics-machine learning frameworks from a machine learning standpoint. With this foundation, we then provide a systematic organization of these existing techniques and discuss ideas for future research.

https://arxiv.org/abs/2003.04919

2 Objectives of Physics-ML Integration

2.1 Improving predictions beyond that of state-of-the-art physical models
2.2 Parameterization
2.3 Forward Solving Partial Differential Equations
2.4 Inverse Modeling
2.5 Discovering Governing Equations

3 Physics-ML Methods

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Table 1: Table of literature classified by objective and method

	Basic ML	Physics-Guided Learning	Physics-Guided Architecture	Residual Model	Hybrid Model
Improve prediction beyond physics model	[Yi and Prybutok, 1996] [Brown *et al.*, 2008] [Ham *et al.*, 2019]	[Pukrittayakamee *et al.*, 2009] [Karpatne *et al.*, 2017b] [Muralidhar *et al.*, 2018] [Doan *et al.*, 2019] [Jia *et al.*, 2019] [Read *et al.*, 2019] [Zhang *et al.*, 2019] [Erichson *et al.*, 2019] [Hu *et al.*, 2020] [Muralidhar *et al.*, 2019]	[Ling *et al.*, 2016] [Sturmfels *et al.*, 2018] [Baseman *et al.*, 2018] [Muralidhar *et al.*, 2018] [Muralidhar *et al.*, 2019] [Sadoughi and Hu, 2019] [Hu *et al.*, 2020] [Ba *et al.*, 2019b] [Muralidhar *et al.*, 2019] [Anderson *et al.*, 2019] [Park and Park, 2019]	[Xu and Valocchi, 2015] [Wan *et al.*, 2018] [San and Maulik, 2018] [Wang *et al.*, 2017]	[Goldstein *et al.*, 2014] [Solle *et al.*, 2017] [Karpatne *et al.*, 2017b] [Hamilton *et al.*, 2017] [Zhang *et al.*, 2018] [Yao *et al.*, 2018] [Paolucci *et al.*, 2018] [Chen *et al.*, 2018b] [Long *et al.*, 2018] [Vlachas *et al.*, 2018] [Yang *et al.*, 2019b] [Sadowski *et al.*, 2016] [Grover *et al.*, 2015]
Parameterization	[Chan and Elsheikh, 2017] [Gentine *et al.*, 2018] [O'Gorman and Dwyer, 2018] [Bolton and Zanna, 2019] [Rasp *et al.*, 2018]	[Beucler *et al.*, 2019]	[Beucler *et al.*, 2019]		[Krasnopolsky and Fox-Rabinovitz, 2006] [Goldstein *et al.*, 2014] [Zhang *et al.*, 2018]
Uncertainty quantification	[Xu and Valocchi, 2015] [Lakshminarayanan *et al.*, 2017] [Yang and Perdikaris, 2019b]	[Wu *et al.*, 2016] [Yang and Perdikaris, 2018] [Yang and Perdikaris, 2019a] [Zhu *et al.*, 2019] [Geneva and Zabaras, 2020]	[Daw *et al.*, 2019]		[Dong *et al.*, 2016]
Inverse modeling	[Dawson *et al.*, 1992] [Chen *et al.*, 2017] [Pilozzi *et al.*, 2018] [Lunz *et al.*, 2018]	[Raissi *et al.*, 2019b] [Biswas *et al.*, 2019]			[Parish and Duraisamy, 2016] [Hamilton *et al.*, 2017] [Jin *et al.*, 2017] [Bubba *et al.*, 2019] [Senouf *et al.*, 2019]
Discover Governing Equations	[Bongard and Lipson, 2007] [Schmidt and Lipson, 2009] [Brunton *et al.*, 2016] [Mangan *et al.*, 2016] [Rudy *et al.*, 2017]	[Raissi *et al.*, 2017a]			
Solve PDEs	[Han *et al.*, 2018] [Arsenault *et al.*, 2014] [Rudd and Ferrari, 2015] [Khoo *et al.*, 2019] [Sirignano and Spiliopoulos, 2018]	[Raissi *et al.*, 2017b] [Yang *et al.*, 2018] [Yang and Perdikaris, 2018] [Sharma *et al.*, 2018] [Meng *et al.*, 2019] [Raissi *et al.*, 2019a] [Shah *et al.*, 2019] [Zhu *et al.*, 2019] [Geneva and Zabaras, 2020] [Karumuri *et al.*, 2020] [Wu *et al.*, 2020] [de Bezenac *et al.*, 2019]	[Chen *et al.*, 2018a] [Ruthotto and Haber, 2018] [Chang *et al.*, 2019] [de Bezenac *et al.*, 2019] [Mattheakis *et al.*, 2019] [Yang *et al.*, 2019a]		
Data Generation	[Klein and Manning, 2003] [Denton *et al.*, 2015] [Oord *et al.*, 2016]	[de Oliveira *et al.*, 2017] [Bode *et al.*, 2019] [Yang *et al.*, 2019c] [Zheng *et al.*, 2019] [Kim *et al.*, 2019]	[Chen and Fuge, 2018] [Shah *et al.*, 2019]		

Semi-supervised Anomaly Detection on Attributed Graphs

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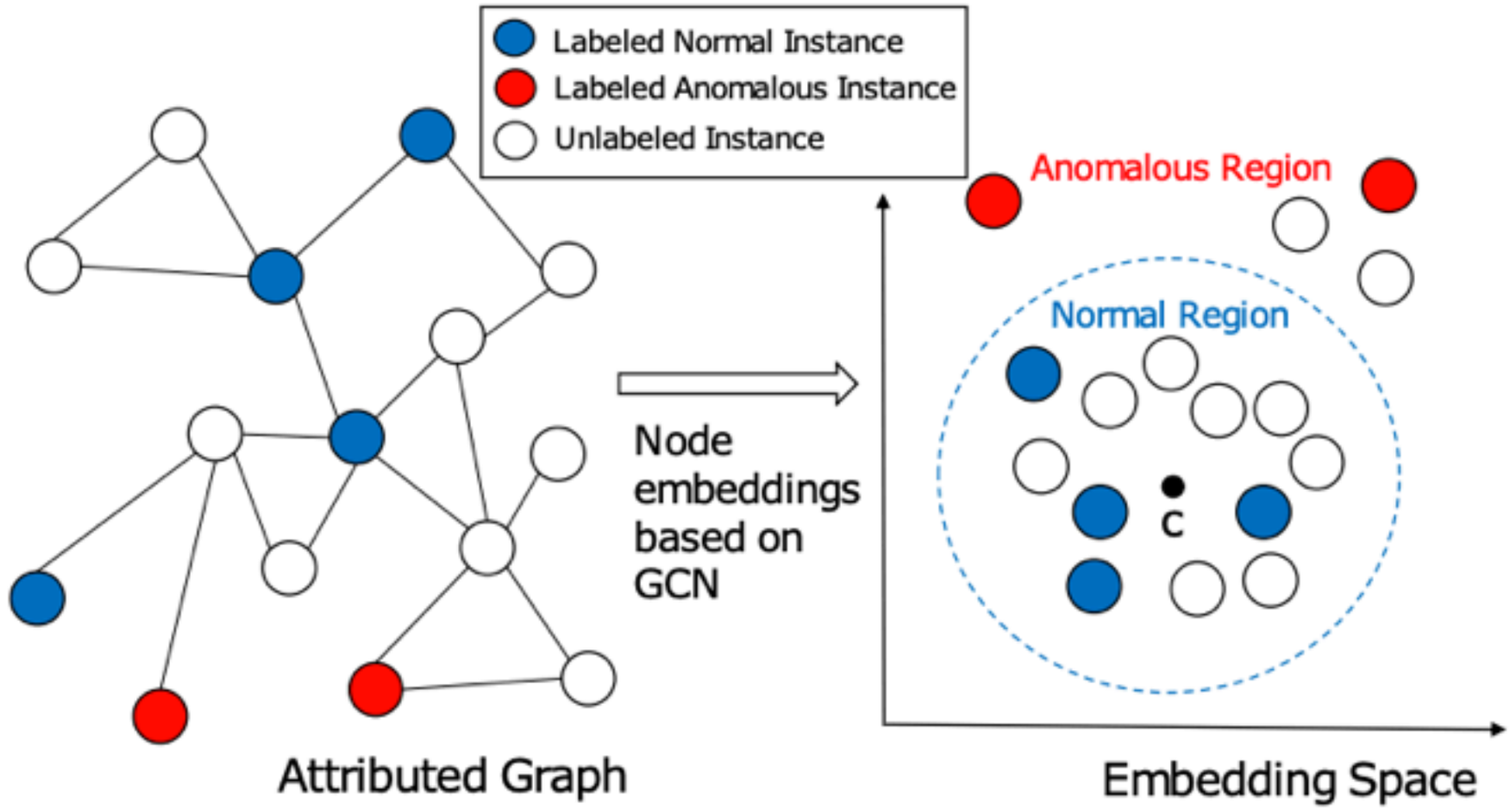
We propose a simple yet effective method for detecting anomalous instances on an attribute graph with label information of a small number of instances. **Although with standard anomaly detection methods it is usually assumed that instances are independent and identically distributed, in many real-world applications, instances are often explicitly connected with each other, resulting in so-called attributed graphs.** The proposed method embeds nodes (instances) on the attributed graph in the latent space by taking into account their attributes as well as the graph structure based on graph convolutional networks (GCNs). To learn node embeddings specialized for anomaly detection, in which there is a class imbalance due to the rarity of anomalies, the parameters of a GCN are trained to minimize the volume of a hypersphere that encloses the node embeddings of normal instances while embedding anomalous ones outside the hypersphere. This enables us to detect anomalies by simply calculating the distances between the node embeddings and hypersphere center. The proposed method can effectively propagate label information on a small amount of nodes to unlabeled ones by taking into account the node's attributes, graph structure, and class imbalance. In experiments with five real-world attributed graph datasets, we demonstrate that the proposed method achieves better performance than various existing anomaly detection methods.

https://arxiv.org/pdf/2002.12011.pdf



4.2. Comparison Methods

We evaluated two variants of the proposed method: Ours-AN and Ours-N. Ours-AN is the method explained in Section 3, which uses both anomalous and normal label information. Ours-N uses only normal label information. The proposed method was implemented by using PyTorch (Paszke et al., 2017) and PyTorch Geometric (Fey & Lenssen, 2019).

We compared the proposed method with the following nine methods.