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GRAPH LEARNING METHODS FOR CLIMATE MODELS WITH GRAPH SPARSIFICATION

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Acknowledgements

Abstract

Graph sparification techniques for graph neural networks have traditionally been used to accelerate training and inference on real-world graphs which have billions of paramaters. There are also many different climate models which use complex mathematical models to model the interactions between energy and matter over the world. Many of these models share components and the structure of these relationships is not easily found due to the complexity of these climate models. The space of all possible graphs grows super-exponentially with the number of nodes and as such any correlation or causality is difficult to find. In this paper, I attempt to quantify these relationships with graph sparsification techniques. (Talk more about climate?)

Contents

Chapter 1

Introduction

1.1 Background

The simplest climate models have existed since the 1950's with the very first computers modelling small two-dimensional climates [5]. Modern models have become increasingly more complex in part due to developments in computational techniques and the large amount of data available worldwide to train these models. [18] A common approach to studying the complex system of Earth's climate has been through sophisticated mathematical modelling with a range of temporal and spatial data [14]. One of the most important areas of study that climate science is attempting to answer is the effect of human greenhouse gas emissions on the Earth and its future. Understanding this is important as it can inform us on the potential harms to society and the environment and guide policy makers implementing change. As such, many models and "scenario runs" have been developed which predict various outcomes in temperature, precipitation, air pressure and solar radiation given a certain levels of Shared Socioeconomic Pathways (SSP). [21] These SSP's represent a broad set of possible changes in population, economic and technological growth, and urbanisation that would influence future greenhouse gas emissions. These are directly related to Representative Concentration Pathways (RCP) introduced by CMIP5 which are categorisations based on the estimated future concentrations of greenhouse gases in the atmosphere. [8]

SSP	**Description**
SSP1	Sustainability: The world shifts gradually, but pervasively, toward a more sustainable path, emphasizing more inclusive development that respects perceived environmental boundaries.
SSP2	Middle of the road: The world follows a path in which social, economic, and technological trends do not shift markedly from historical patterns.
SSP3	Regional rivalry: A resurgent nationalism, concerns about competitiveness and security, and regional conflicts push countries to increasingly focus on domestic or, at most, regional issues.
SSP4	Inequality: Highly unequal investments in human capital, combined with increasing disparities in economic opportunity and political power, lead to increasing inequalities and stratification both across and within countries.
SSP5	Fossil-fueled development: This world places increasing faith in competitive markets, innovation and participatory societies to produce rapid technological progress and development of human capital as the path to sustainable development. Global markets are increasingly integrated.

On the lower end, SSP126 assumes an increasingly sustainable world where consumption is oriented towards minimising material resource and energy usage while SSP585 assumes a worst case scenario where fossil fuel usage and an energy-intensive lifestyle intensifies. These SSPs' were the basis behind the Intergovernmental Panel on Climate Change and its 2021 IPCC sixth assessment report which published the newest generation of climate models from Coupled Model Intercomparison Project or CMIP6. [15] CMIP6 is an ensemble of models, with each base model developed by various institutions based on the ability of each group to contribute to them and as research has become far more interconnected in the modern era, many aspects such as expertise, code and literature are shared between groups. As such many of the models that contribute to CMIP6 are highly likely to be dependent. [1]. Esemble methods are more performant when the base models are diverse and independent [13] but the degree of dependence between these models is difficult to ascertain as this would require a qualitative investigation into the personel, code and references between each component of CMIP6. However, one would expect there to be some graph structure that links all models together through some dependence.
There are many different kinds of machine learning but the advent of deep learning has led to countless advancements in many practical applications. The ability of deep learning models to extract high-level, abstract features from raw data by using many layers of simple representations have developed increasingly sophisticated and near human level understanding of input. [7] The next development in neural networks came from neuroscientific principles [11] with Convolutional Neural Networks which could train models to be equivariant to translations in data and process data with grid-like structure. In recent years, Graph neural networks have become the premier method of processing data with non-cartesian structure. Much of this data exists in the world in applications such as chemical analysis [25], social networks [20]

1.2 Motivation

The goal of this thesis is to investigate whether these graph sparisifcation techniques can be used to determine some dependence structure within a graph of models which are all attempting to model the same scenario in the climate. Graph structure and dependence learning is already possible with unsupervised methods such as Variational Graph Autoencoders (VGAE) [26] but to our best knowledge, graph sparsification has not been used before as a method to infer dependence. Existing methods for determining multiple correlation such

1.3 Outline

Overview of each section and the methods of each.

Chapter 2

Methods and Related Techniques

In this chapter we will give a brief overview on how the climate works and review current standards in climate modelling along with the basics behind neural networks and the extensions towards graph neural networks.

This will basically be the section on literature review. Current methods and techniques being used etc. A lot of summaries of the papers saved in the papers folder need to be done to finish this section.

2.1 Deep Learning

Traditional machine learning techiques generally require meaningful data cleaning and feature creation which was costly to develop and often had many errors. The advent of deep learning provided algorithms that could automatically extract higher-level features from raw data. [4] The MLP The multi-layer perceptron [22] is formulated using linked layers of nodes which transforms a set of inputs into an output. The MLP attempts to approximate some ground-truth function which may also be non-linear. The single layer version of this model can be represented as

$$f(x) = \sigma(\Theta^T X) \text{ where } \Theta = \begin{bmatrix} b \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} \text{ and } X = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \tag{2.1.1}$$

Where $\sigma(.)$ is some activation function such as ReLu, hyperbolic tangent or logistic function, X is the data, Θ is the learned parameters and b represents a bias term. These parameters are set to some initial values and are iteratively updated in a back-propagation training process,

$$\theta^{t+1} = \theta^t - \eta \frac{\partial E(X, \theta^t)}{\partial \theta} \tag{2.1.2}$$

Where $E(.)$ is some loss function and η is the learning rate. The next advancement in the deep learning space came with the Convolutional Neural Network (CNN) which was a regularised MLP that could handle data with data with structure and multiple dimensions far better than the traditional MLP due to its use of weight sharing, sampling and local receptive fields. [7]
Suppose we have an image or some other kind of data in matrix form. Let $\mathbf{X} \in \mathbb{R}^{H \times W}$ be the input image and $\mathbf{W} \in \mathbb{R}^{h \times w}$ be the kernel or filter. By performing a convolution, we are effectively 'sliding' our weight matrix kernel over our input and the resulting feature map $\mathbf{Z} = \mathbf{X} * \mathbf{W}$,

$$Z_{i,j} = \sum_{u=0}^{h-1} \sum_{v=0}^{w-1} x_{i+u,j+v} w_{u,v} \tag{2.1.3}$$

The novelty of the convolutional layer compared to a linear layer is that the kernel is shared across all locations of the input and therefore if a pattern in the input moves, the corresponding output will also follow this movement. This provides shift equivariance which is something that early MLP's failed to achieve. [17]

2.2 Graph Neural Networks

Summarise the extension of GNN's from NN's and how they are useful in certain applications. When it comes to data in a graph-like structure, standard CNN's cannot be applied due to the non-euclidean nature of a graph. In an image or a matrix, our kernel is generally a $n \times n$ matrix which can be applied to the entirety of the data. In graphs this is not always possible due to the fact that any number of nodes can be connected by any number of edges. [23] The Graph Neural Network (GNN) was developed for this purpose and they can be broadly categorised into gating and attention based methods [24] and spectral or spatial methods within Graph Convolutional Network (GCN) research. [12] This propagation rule is as follows:

$$H^{(l+1)} = \sigma(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)}) \tag{2.2.1}$$

Here, $\tilde{A} = A + I_N$ is the adjacency matrix of the undirected graph $\mathcal{G}$ with self-connections from the identity matrix I_N. $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$ is the row sum of the adjacency matrix and $W^{(l)}$ is a layer trainable weight matrix. $\sigma(.)$ is an activation function such as $\text{ReLU}(.) = \max(0, .)$. $H^{(l)} \in \mathbb{R}^{N \times D}$ is the matrix of activations in the lth layer with $H^0 = X$.

2.3 Sparsification Graph Neural Network

Hornik [10] showed that in a single layer MLP and provided enough hidden neuron units, the neural network could model any smooth truth function as for each added neuron, the decision space can be segmented to conform to any response. Many experiments have also found that deep networks with many layers perform better than shallow ones [16] [19] as the usage of many layers allows deeper layers to leverage features produced by earlier layers. The noveltly of neural networks is that they do not tend to be affected greatly by overparameterisation [2], and as they generally improve with more neurons and layers these models have grown exponentially in size with some models using billions of parameters and most of these models having more parameters than training observations which has made both inference and prediction incredibly costly. (Reference some math from the number of linear decision regions and some graphs?)

The Lottery Ticket Hypothesis (LTH) [6] explored the possibility of simplifying redundant models by trainable sparse subnetworks whilst still training to full accuracy. When training a traditional neural network, this was done by instability analysis etc. etc.? (should i talk about this?)

Chen et. al. [3] extended the LTH to Graph Neural Networks by co-simplifying both the adjacentcy matrix of the graph and the weights in the network of the model. For a semi-supervised classification task, the objective function is:

$$\mathcal{L}(\mathcal{G}, \Theta) = -\frac{1}{|\mathcal{V}_{\text{label}}|} \sum_{v_i \in \mathcal{V}_{\text{label}}} y_i \log(z_i), \tag{2.3.1}$$

where $\mathcal{L}$ is the cross-entropy error of all samples and y_i is the label vector of node v_i. The Unified GNN Sparsification (UGS) framework then introduced two masks m_g and m_θ with the same shape as the adjacency matrix $\mathbf{A}$ and the weights matrix Θ, which gives the following objective function:

$$\mathcal{L}_{\text{UGS}} = \mathcal{L}(\{m_g \odot A, \mathbf{X}\}, m_\theta \odot \Theta) + \gamma_1 ||m_g||_1 + \gamma_2 ||m_\theta||_1, \tag{2.3.2}$$

where $\odot$ is the element-wise product, γ_1 and γ_2 are hyperparameters to control the shrinkage of m_g and m_θ. After training, the lowest magnitude elements in m_g and m_θ are set to zero with respect to some set values of p_g and p_θ. These sparse masks are then applied which prune $\mathbf{A}$ and Θ.

2.4 Variational Autoencoder

This section should be done with more time if the original sparsification section is completed. Show how this is an alternative in graph discovery.

Chapter 3

Framework

3.1 Climate Models

What climate models are used for etc. Use Yanan's climate papers.

Climate models are constantly being updated as many different groups and institutions implement higher spatial resolutions and new physical, chemical, biological and geological processes into these models. These models are the primary method of understanding climate change. These models often use terrabytes of data and require some of the largest supercomputers in the world to generate their predictions.

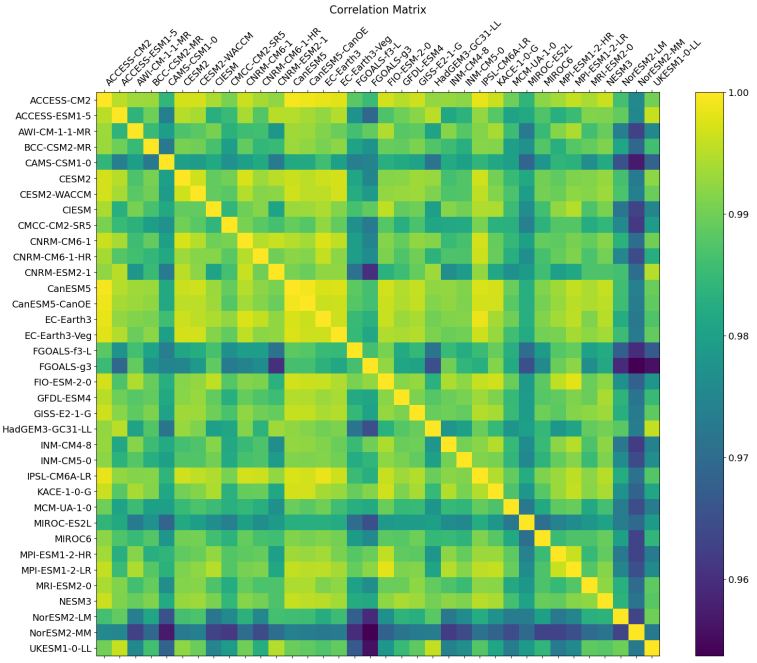
(Can we talk about how one model works?)

CMIP6 models are the premier models for this task but while it was expected to contain around 100 models, only 40 have been published so far. However, the results from these 40 models so far indicates a far greater climate sensitivity when compared to the previous generation of CMIP5 models. [9] This indicates a far greater impact from newer processes that were added in CMIP6 towards the future climate. The figure below shows general trend of a single scenario that each model estimates.

Looking at a plot of all the models, there is a clear correlation between all the models and the correlation heatmap affirms this as the correlation between each ranges from 0.96–1.

3.2 Dataset

The datasets used are from the CMIP6 scenario runs made available on the KNMI Climate Explorer website. The KNMI is part of the World Meteoriological Organization (WMO) []. The scenario runs include monthly predictions for temperature, min temperature, max temperature precipitation, radiation and pressure all over the globe in a 192×144 grid between 1850–2100 for 40 different models. Due to the time and computational limitations, this was filtered to just temperature during



the 1960–1980 period in just Australia or latitudes -44° to -12° and longtitudes 288° to 336°.

Talk a bit more about how these models in the dataset are all related by certain parts.

3.3 Problem Formulation

Maybe add this to the background section and put more of the regression, diagrams of the process and shrinkage prior stuff here that it more specific to this thesis

We define a graph as $\mathcal{G} = (\mathcal{V}, \mathbf{A})$, where $\mathcal{V}$ represents a set of verticies which contains a list of nodes $\{v_1, \ldots, v_n\}$ and $\mathbf{A} \in \mathbb{R}^{n \times n}$ the adjacentcy matrix which contains information on the graph topology. If an edge exists between two node v_i and v_j, then $\mathbf{A}_{ij} = 1$ else, $\mathbf{A}_{ij} = 0$. We also define the degree matrix as $\mathbf{D} = \sum_j A_{ij}$ where each entry on the diagonal is equal to the row sum of the adjacency matrix $\mathbf{A}$. Each node has a p-dimensional feature vector $x_i \in \mathbb{R}^p$ which describes some information about the node in the graph. By combining all n feature vectors from all nodes, we have a feature matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$. The graph also has a regression target $Y \in \mathbb{R}$ which refers to the historical temperature that each model from the graph is attempting to predict. As mentioned earlier, other variables such as precipitation, pressure and radiation are available but for simplicity, just temperature is currently being used. The two-layer GNN from [12] can be expressed as

$$f(\mathbf{A}, \mathbf{X}) = \sigma_2(\hat{\mathbf{A}}_2 \sigma_1(\hat{\mathbf{A}}_1 \mathbf{X} W^{(0)}) W^{(1)}) \tag{3.3.1}$$

where $\sigma_1(.)$ and $\sigma_2(.)$ are an activation function such as ReLU, and $\hat{A} = \tilde{D}^{-1/2}(A + I)\tilde{D}^{-1/2}$ is the symmetrically normalised adjacency matrix. The final regression problem can be formulated as

$$f : L \times X \to Y \tag{3.3.2}$$

where f denotes the learning function, L the graph, X denotes the time series input and Y the regression target.

Need to describe the math behind graph sparsification. More about shrinkage see Xiongwens.

3.4 Computational features

computation of neural network models. See georges paper

3.5 Implementation

Need to finish code to finish this section.

Chapter 4

Results

4.1 Model verification

If the VGAE section is completed, we can compared the sparsified graph with the VGAE produced graph to determine how good graph sparsification is when used for graph discovery and thereby correlation in a graph structure.

4.2 Model results

Is there some way we can test the models results depending on how sparse we make the graph etc. Research required to find some quantitative measure for this.

Some figures of the NN structure would also be helpful for this. Need to use nx or some other graph representation tool in python for this.

Chapter 5

Discussion

Chapter 6

Conclusion

Chapter 7

Appendix

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