Learning Spatio-Temporal Aggregations for Large-Scale **Energy** Capacity Expansion Problems

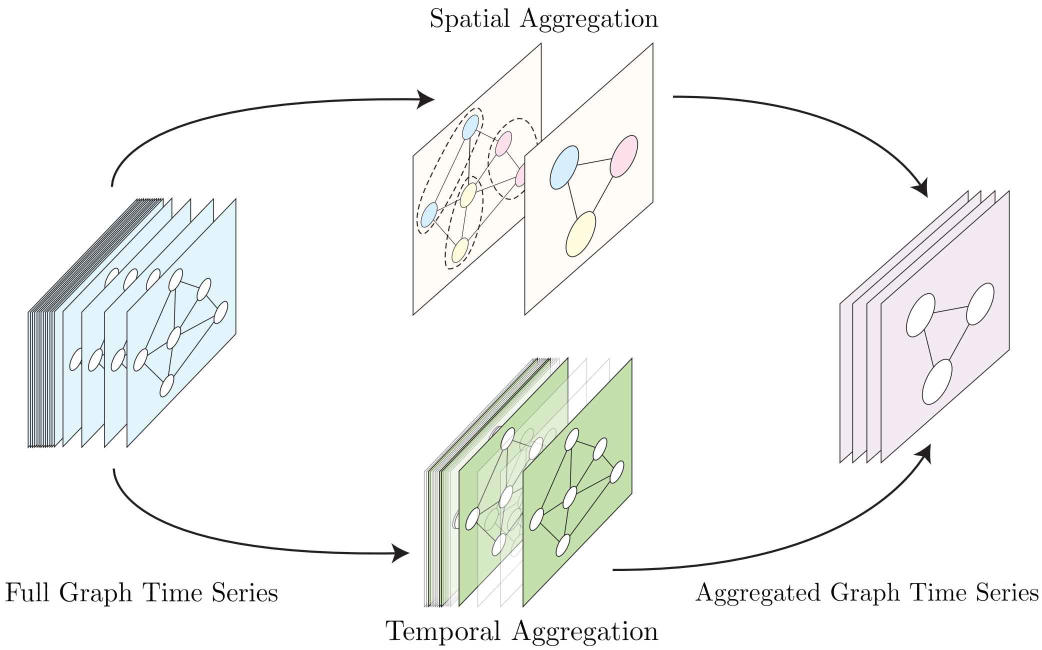

Fig. 1. Spatio-temporal aggregation is often needed to tractably solve capacity expansion problems. Spatial aggregation is applied to reduce the number of decision variables and constraints associated with individual nodes while temporal aggregation is applied to reduce the number of decision variables and constraints associated with operational periods.

Operational performance of future cyber-physical infrastructures crucially relies on the effectiveness of long-term planning decisions related to network capacity expansion. Such Capacity Expansion Problems (CEPs) quickly become intractable due to a large number of operational periods and realistic network sizes. Traditionally, this issue is tackled by selecting some representative periods and/or aggregating the network. This process often entails some rather ad hoc choices, leading to suboptimal or even infeasible solutions to the original CEP.

Here, we propose a data-driven approach to finding spatio-temporal aggregations that are useful in efficiently solving CEPs. Our approach is based on leveraging the (projected) time series of relevant supply-demand variables (e.g., nodal demand, generation capacity factors) to train a graph autoencoder model with a pooling mechanism. By minimizing the expected reconstruction loss over operational periods, we obtain data-driven spatial aggregations (i.e., clusterings of nodes). To obtain the temporal aggregation (i.e., set of representative periods), we cluster the latent representation output from the encoder. The resulting aggregations can be used to obtain high-quality solutions to large-scale CEPs. We demonstrate the efficacy of our approach by solving for generation and transmission expansion planning decisions for an interdependent power-NG model calibrated for the New England region. We also report computational results on the sensitivity of planning decisions to the extent of aggregation. Interestingly, our approach provides non-trivial upper bounds on the optimal objective of the original large-scale CEP.

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1 INTRODUCTION

Capacity Expansion Problems (CEPs) are a family of optimization formulations that aim to assist in generating high quality planning decisions for a broad range of applications in cyber-physical networks, including communication systems, water resource systems, and regional power networks [Luss 1982]. To minimize total cost of operations over a long-term horizon, CEP formulations integrate long-term investment decisions, such as production capacity expansion, facility location/decomissioning, with hour-to-hour operations, such as generation and transmission of resources. Naturally, the inclusion of these planning and operational considerations across a large network and over a multidecadal horizon makes CEP formulations powerful modeling tools. However, these features also contribute to the computational intractability of solving such problems.

To this end, it has become common practice for modelers to *aggregate* CEP formulations both spatially by grouping nodes, and also temporally by selecting a set of "representative periods" to roughly capture the distribution of demands, capacity factors, and other parameters of interest across operational periods. Given that the planning decisions depend closely on the network structure and planning horizon, the choice of aggregation can crucially impact the CEP's solution. Machine learning (ML) methods have indeed been applied previously to learn high quality temporal aggregations [Teichgraeber and Brandt 2022]. However, to the best of our knowledge, applications of ML towards learning *spatial* aggregations are yet to be explored. Motivated by the enormous potential of ML models in learning representations as well as recent developments in geometric deep learning, we propose a framework for identifying potential *spatio-temporal* aggregations using a graph convolutional autoencoder approach. We apply our framework to aggregate and solve an otherwise intractable CEP for a regional energy network. Our methodology proposes a new direction in making CEPs tractable by means of spatio-temporal aggregation and can potentially yield high quality planning decisions for sustainable and efficient operations of cyber-physical infrastructure.

Specifically, we apply our framework to address several practical and computational challenges associated with capacity expansion models (CEMs) for decarbonization of interdependent power-NG infrastructures. Classical examples of such models include the generation expansion problem (GEP) and generation and transmission expansion problem (GTEP), both of which are well-studied in the context of power systems [He et al. 2018; Li et al. 2022a]. In this paper, we focus on a GTEP formulation that determines the optimal location and timing of generation units, transmission lines, and pipelines to meet future energy demands under a range of operational and policy constraints such as joint emission constraints. In our work, we extend the model to include two main interdependencies between power and NG systems. The first interdependency captures the increasing role of gas-fired power plants in the generation mix of electricity production [(EIA) 2022; He et al. 2018]. The second interdependency reflects the *joint* emission of CO_2 in both systems.

The key *computational challenge* in solving the GTEP arises from the fact that it links long-term investment decisions (e.g. capacity and network expansion) to short-term operational ones (e.g. unit commitment, power production, and energy storage). The former decisions have a planning horizon of 10-30 years with yearly granularity, while the latter usually require hourly or sub-hourly resolution. CEPs in general, and GTEPs in particular, are usually a large-scale mixed-integer linear program (MILP), but current literature has limited success in tractably solving these problems to an adequate level of spatial and temporal resolution. In our case, the computational difficulty in solving the GTEP increases further because we model both power and NG networks. Thus, taking into account (projected) demand information on a day-to-day basis becomes prohibitively expensive from a computational viewpoint. In the classical GTEP problems for power systems, the computational challenge is addressed by aggregating power system nodes (buses) within a geographical neighborhood (power zone) to a single node [Li et al. 2022a] and by solving the GTEP for a set of representative days [Hoffmann et al. 2020]. Crucially, the new formulation instantiated on this node aggregation and representative day set must proportionately capture demand and supply patterns across the network and throughout the planning horizon.

Our work also addresses the *practical issues* arising from coarse data availability from the NG network. Firstly, we do not have access to the detailed connectivity and transmission information in the NG network while this information is readily available for the power network. Secondly, power systems typically collect demand and generation data at a fine temporal resolution (hourly or less), but this data is usually not publicly accessible for NG systems. These issues thus require us to (a) formulate network constraints based on loosely specified information on power and NG node connectivity and (b) develop an approach to leverage demand and supply data from the power system with demand data of NG system despite their different temporal resolutions.

We address the aforementioned challenges by developing a *graph convolutional autoencoder approach* that captures the physical interdependencies between power and NG networks and also handles the different granularity of data at each network. We consider demand data for both systems, and consider capacity factor (CF) data for solar and wind plants to reflect the supply pattern in the renewable-dominated future grid. We utilize graph convolutions to capture the network interactions both within and across power and NG networks, and adopt an autoencoder architecture with tuneable reconstruction losses for the respective input data. Moreover, we incorporate a graph pooling mechanism to automatically learn spatial aggregations that group together nodes that exhibit similar electricity demand behavior. We demonstrate that the resulting autoencoder models are ideally suited to learning latent embeddings of the spatio-temporal patterns in power and NG demand as well as wind and solar CF data, which can be readily incorporated into high quality spatio-temporal aggregations. Furthermore, our approach to identifying spatio-temporal aggregations can also enable an accurate estimation of the trade-off between costs (both investment and operational) and joint emissions from power and NG systems.[1]

Previous studies for spatio-temporal aggregation focus on selecting sets of representative days using variants of k-means [Barbar and Mallapragada 2022; Li et al. 2022b; Mallapragada et al. 2018; Teichgraeber and Brandt 2019], k-medoids [Scott et al. 2019; Teichgraeber and Brandt 2019], and hierarchical clustering [Liu et al. 2017; Teichgraeber and Brandt 2019]. The distance matrices used in clustering algorithms for most previous works are constructed based on a set of time series inputs such as load data and variable renewable energies (VRE) capacity factors [Hoffmann et al. 2020; Li et al. 2022a]. Notably, these approaches neither account for demand data with multiple time resolutions nor account for network interdependencies. Hence, they cannot be readily extended to address the task of extracting representative days for joint power-NG systems – an aspect that is crucial for realism and tractability in joint planning optimization models for decarbonizing these systems.

[1] We believe this capability can have a significant societal impact by lowering the barriers to investment in renewable energy resources and alleviating reliability concerns in a low-carbon energy system.

Moreover, none of these studies apply a data-driven approach to aggregating buses, which has the potential to more accurately represent heterogeneity of electricity demand behavior across nodes. We believe that our approach addresses these challenges and provides a promising path to better extract spatio-temporal aggregations in interdependent power and NG systems.

2 CAPACITY EXPANSION MODEL

Our formulation of the joint power-NG planning is based on the model proposed in [Brenner et al. 2022]. In this section, we briefly introduce the GTEP formulation for the joint power-NG system and provide its details in the Supplementary Information (SI) [SI 2022]. The problem determines the minimum investment and operational costs of co-optimizing electricity and natural gas (NG) systems for the year 2050 under various investment, operational, and policy constraints. The investment decisions for the power system include establishing new plants, transmission lines, and decommissioning existing plants, and for the NG system it includes establishing new pipelines. Our model consist of major power and NG systems' planning constraints such as minimum stable production, ramping, energy balance, flow, and storage. The interdependency between the two systems is realized through two sets of constraints. The first coupling constraint captures the flow of NG to power system to enable operation of gas-fired power plants. The second constraint imposes an economy-wide emission constraint, limiting the emission of CO_2 from both system to a pre-specified value.

To conceptualize the model, let $\boldsymbol{z}^e = (\boldsymbol{x}^e, \boldsymbol{y}^e, \boldsymbol{p})$ denote the set of variables for the power system. The integer variable $\boldsymbol{x}^e$ is the investment decision for the power system (i.e., establishing plants, decommissioning plants, and establishing new transmission lines). The continuous variable $\boldsymbol{p}$ denotes the power generation in gas-fired plants and $\boldsymbol{y}^e$ is a continuous variable that signifies all the remaining variables including power generation from non-gas-fired plants, electricity flow between nodes, storage charge/discharge, and load shedding variables. We define $\boldsymbol{z}^g = (\boldsymbol{x}^g, \boldsymbol{y}^g, \boldsymbol{f})$ to denote the NG system's variables. The variable $\boldsymbol{x}^g$ is a mixed-integer variable denoting all investment, storage, and load shedding decisions. The continuous variable $\boldsymbol{y}^g$ captures the flow inside the NG system. Finally, $\boldsymbol{f}$ denotes the flow of NG to power systems. We formulate the joint power-NG system as follows:

$$\min\ (\boldsymbol{c}_1^e\boldsymbol{x}^e + \boldsymbol{c}_2^e\boldsymbol{y}^e + \boldsymbol{c}_3^e\boldsymbol{p}) + (\boldsymbol{c}_1^g\boldsymbol{x}^g + \boldsymbol{c}_2^g\boldsymbol{y}^g + \boldsymbol{c}_3^g\boldsymbol{f}) \tag{1a}$$

$$\text{s.t. } \boldsymbol{A}^e\boldsymbol{x}^e + \boldsymbol{B}^e\boldsymbol{y}^e + \boldsymbol{D}^e\boldsymbol{p} \leq \boldsymbol{b}_1^e \tag{1b}$$

$$\boldsymbol{H}^e\boldsymbol{y}^e \geq \boldsymbol{b}_2^e \tag{1c}$$

$$\boldsymbol{A}^g\boldsymbol{x}^g + \boldsymbol{B}^g\boldsymbol{y}^g + \boldsymbol{D}^g\boldsymbol{f} \leq \boldsymbol{b}_1^g \tag{1d}$$

$$\boldsymbol{f} = \boldsymbol{E}_1\boldsymbol{p} \tag{1e}$$

$$\boldsymbol{G}_2\boldsymbol{y}^g + \boldsymbol{E}_2\boldsymbol{p} \leq \eta \tag{1f}$$

$$\boldsymbol{x}^e \in \mathbb{Z}^+, \boldsymbol{y}^e, \boldsymbol{x}^g \in \mathbb{Z}^+ \times \mathbb{R}^+, \boldsymbol{p}, \boldsymbol{y}^g, \boldsymbol{f} \in \mathbb{R}^+ \tag{1g}$$

The objective function (1a) minimizes the investment and operational costs for the power system (first term) and NG system (second term). The constraint (1b) represents all investment, and operational constraints for the power system. The constraint (1c) ensures policy considerations such as the minimum requirement for renewable portfolio standard (RPS). The NG constraints are reflected in constraint (1d), which includes technological and operational constraints such as the supply limit at each node, flow between NG nodes, and storage.

The coupling constraint (1e) ensures that gas-fired plants operate based on the gas they receive from the NG network. The economy-wide decarbonization constraint is defined by constraint (1f) and limits emissions resulting from NG consumption in electricity generation and other sectors such as heating, transportation and industry to η. The coefficient matrices $\boldsymbol{E}_1$, $\boldsymbol{G}_2$, and $\boldsymbol{E}_2$ represent the heat rate, emission factors for NG usage, and emission factor for gas-fired plants, respectively. Notice that the conceptualized model does not consider other major types of fossil-fueled plants such as coal and oil due to their declining role in the generation mix of US system

3 AGGREGATION FORMULATION

This section presents our formulation for a generation capacity expansion problem (CEP), an example of which is the GTEP considered in this paper. For ease of exposition, we only explain our method for the temporal aggregation as it can naturally be extended to spatial aggregation as well. Let $\boldsymbol{x} \in \mathbb{Z}^k$ denote the integer variables of size k associated with investment decisions. The variable $\boldsymbol{y} \in \mathbb{R}_+^n$ denotes the n continuous operational decisions whose size are subject to reduction as a result of temporal aggregation. A generic CEP can be defined as:

$$\begin{aligned} \mathcal{Z} \coloneqq \min_{\boldsymbol{x},\boldsymbol{y}} \quad & \boldsymbol{f}^\top\boldsymbol{x} + \boldsymbol{g}^\top\boldsymbol{y} \\ \text{s.t.} \quad & \begin{bmatrix} \boldsymbol{P} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Q} \\ \boldsymbol{R} & \boldsymbol{S} \end{bmatrix} \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix} \leq \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{b} \\ \boldsymbol{c} \end{bmatrix} \\ & \boldsymbol{x} \in \mathbb{Z}^k \\ & \boldsymbol{y} \in \mathbb{R}_+^n. \end{aligned}$$

where constraints $\boldsymbol{P}\boldsymbol{x} \leq \boldsymbol{a}$ and $\boldsymbol{Q}\boldsymbol{y} \leq \boldsymbol{b}$ limit $\boldsymbol{x}$ and $\boldsymbol{y}$ variables respectively, and $\boldsymbol{R}\boldsymbol{x} + \boldsymbol{S}\boldsymbol{y} \leq \boldsymbol{c}$ is a coupling constraint linking $\boldsymbol{x}$ and $\boldsymbol{y}$ variables. We assume that $\boldsymbol{Q} \in \mathbb{R}^{m_1\times n}$ and $\boldsymbol{S} \in \mathbb{R}^{m_2\times n}$ and are matrices of compatible sizes.

A temporal aggregation involves representing the entire planning horizon with a set of representative periods (i.e, representative days in energy systems). This operations results in a problem $\mathcal{Z}$ with either fewer constraints ($m' < m$) or operational variables ($n' < n$). The resulting problem can also accommodate a coefficient change for the operational variables. For example, temporal aggregation in energy problems is usually carried out by clustering and the selected operational variables are appropriately weighted to reflect the number of periods each of them represent [Teichgraeber and Brandt 2022]. From optimization perspective, temporal aggregation is the operation of removing a set of constraints and projecting the full problem to a lower dimensional space. Let a parameterized mapping $\boldsymbol{\theta} = (\boldsymbol{\Lambda}, \Sigma, \boldsymbol{\Gamma})$ be a function that carries out the temporal aggregation on the full problem where $\boldsymbol{\Gamma} \in \mathbb{R}^{m'\times m}$ is a binary matrix that specifies which constraint to retain and which one to remove. The matrix $\Sigma \in \mathbb{R}^{n'\times n}$ encodes the variable aggregation

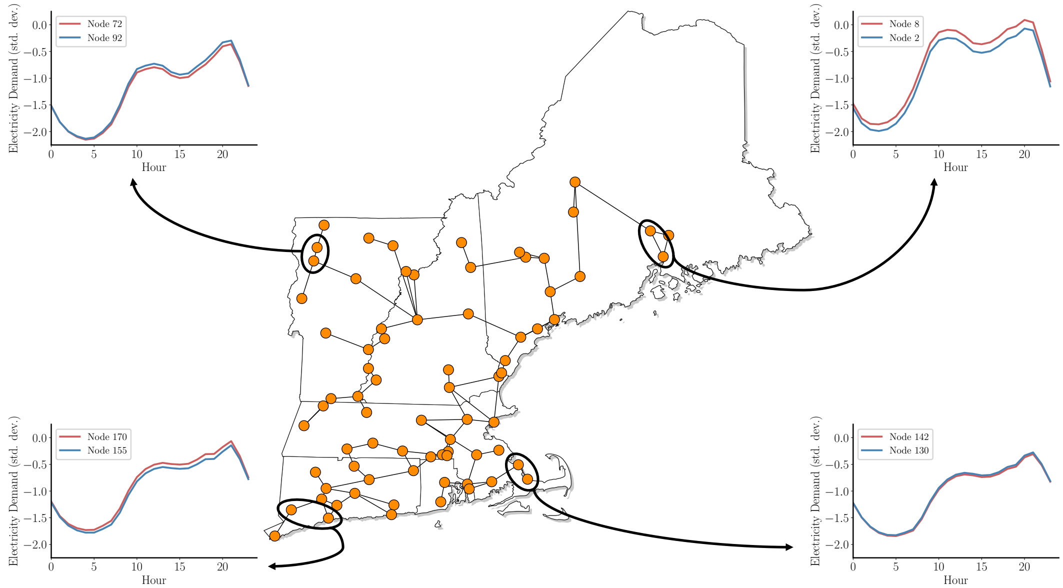

Fig. 2. Adjacent nodes in the power network demonstrate similar variations in demand over the course of the day. These spatial dependencies are modeled explicitly by graph convolutional layers in the proposed autoencoder architectures.

assignments, and $\boldsymbol{\Lambda} \in \mathbb{R}^{n' \times n'}$ is a matrix that specifies the new coefficient of variables. A variable is represented by another variable if its corresponding entry in the $\boldsymbol{\Lambda}$ is zero. Specifically, $\boldsymbol{\Gamma}_{ij} = 1$ if constraint j is kept as the i-th constraint in the aggregation; otherwise, $\boldsymbol{\Gamma}_{ij} = 0$. We define $\Sigma_{ij} = \mathbb{1}_{ij}$ where $\mathbb{1}_{ij}$ indicates whether the j-th decision variable will be kept in the aggregation as the i-th decision variable. $\boldsymbol{\Lambda}$ is a diagonal matrix with $\boldsymbol{\Lambda}_{ii}$ encoding the "weight" of the i-th variable in the aggregation. Applying $\boldsymbol{\theta}$, the full model becomes:

$$\begin{bmatrix} \boldsymbol{P} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Q} \\ \boldsymbol{R} & \boldsymbol{S} \end{bmatrix} \mapsto \begin{bmatrix} \boldsymbol{P} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Gamma Q \Sigma^\top} \\ \boldsymbol{\Gamma R} & \boldsymbol{\Gamma S \Sigma^\top} \end{bmatrix}, \quad \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{b} \\ \boldsymbol{c} \end{bmatrix} \mapsto \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{\Gamma b} \\ \boldsymbol{\Gamma c} \end{bmatrix}, \quad \boldsymbol{g} \mapsto \boldsymbol{\Lambda \Sigma g}$$

Note that be definition x variables are not subject to mapping. It is also worth noting that in practice, decision variables can be defined on a sub-period resolution. For example, while most energy system planning is expressed in term of days, the operational variables are defined on hourly basis. The generality of our exposition remain valid in such cases as one can define each operational variable of a period as a set of more granular variables. For illustrative purposes, consider a simple CEP problem with only three planning periods:

$$\begin{aligned} \mathcal{Z} := \min \quad & fx + g_1|b_1 - y_1| + g_2|b_2 - y_2| + g_3|b_3 - y_3| \\ \text{s.t.} \quad & y_1 \leq x, \quad y_2 \leq x, \quad y_3 \leq x \\ & x \in \mathbb{Z}_+ \\ & y_1, y_2, y_3 \in \mathbb{R}_+. \end{aligned}$$

where the constraints specify that production (an operational variables) of the capacity is limited by the established capacity (an investment decision). Letting b_i to be the demand in period i, the objective function wants to minimize the total cost of investment and the cost of deviations from demand at each period. Assume that period 1 is selected to represent periods 1 and 2. Then the linearized form of $\mathcal{Z}$ can be aggregated to $\mathcal{Z}_{\boldsymbol{\theta}}$ as follows:

$$\begin{array}{rl} \min & fx + g_1 z_1 + g_2 z_2 + g_3 z_3 \\ \text{s.t.} & z_1 + y_1 \geq b_1 \\ & z_1 - y_1 \geq -b_1 \\ & z_2 + y_2 \geq b_2 \\ & z_2 - y_2 \geq -b_2 \\ & z_3 + y_3 \geq b_3 \\ & z_3 - y_3 \geq -b_3 \\ & -x + y_1 \leq 0 \\ & -x + y_2 \leq 0 \\ & -x + y_3 \leq 0 \\ & x \in \mathbb{Z}^+ \\ & y_1, y_2, y_3 \in \mathbb{R}_+ \\ & z_1, z_2, y_3 \in \mathbb{R}_+ \end{array} \quad \underset{\boldsymbol{\theta}}{\mapsto} \quad \begin{array}{rl} \min & fx + 2g_1 z_1 + g_3 z_3 \\ \text{s.t.} & z_1 + y_1 \geq b_1 \\ & z_1 - y_1 \geq -b_1 \\ & z_3 + y_3 \geq b_3 \\ & z_3 - y_3 \geq -b_3 \\ & -x + y_1 \leq 0 \\ & -x + y_3 \leq 0 \\ & x \in \mathbb{Z}^+ \\ & y_1, y_3 \in \mathbb{R}_+ \\ & z_1, z_3 \in \mathbb{R}_+. \end{array}$$

Then the components of the mapping $\boldsymbol{\theta}$ become:

$$\boldsymbol{\Lambda} = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\boldsymbol{\Gamma} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

3.1 Learning Aggregations

Let $(\boldsymbol{x}^*, \boldsymbol{y}^*)$ and $(\boldsymbol{x}^*_{\boldsymbol{\theta}}, \boldsymbol{y}^*_{\boldsymbol{\theta}})$ denote the optimal solutions to $\mathcal{Z}$ and $\mathcal{Z}_{\boldsymbol{\theta}}$ respectively. Supposing that our objective for aggregation is to find a solution $\boldsymbol{x}^*_{\boldsymbol{\theta}}$ close to $\boldsymbol{x}^*$, we can formulate the aggregation objective as

$$\min_{\boldsymbol{\theta}} \|\boldsymbol{x}^* - \boldsymbol{x}^*_{\boldsymbol{\theta}}\|. \tag{3}$$

Direct optimization of this objective is impossible without knowledge of $\boldsymbol{x}^*$. Moreover, even if one somehow knew $\boldsymbol{x}^*$ a priori, aggregating $\mathcal{Z}$ would still be a combinatorially hard problem. As such, we select the parameters $\boldsymbol{\theta}$ using surrogate objectives that are easier to optimize. A natural choice for such an objective would be the clustering objective associated with operational periods (in the case of temporal aggregation) and nodal features (in the case of spatial aggregation). By grouping nodes as well as representative periods in such a way as to faithfully capture the heterogeneity of nodal demands over the planning horizon, one can hope to (indirectly) minimize (3) and parametrize an aggregation $\boldsymbol{\theta}$ that in turn yields high quality planning decisions with computational tractability.

3.1.1 Temporal Aggregation. To select a temporal aggregation, we can apply clustering to the time series data corresponding to constraints (e.g., demand data, capacity factor data). Given the number of clusters or representative periods n', we apply a clustering algorithm such as k-medoids clustering to minimize the objective function

$$\min \sum_{j \in \mathcal{S}} \sum_{i \in C_j} \|\boldsymbol{b}_i - \boldsymbol{b}_j\|_2^2 \tag{4}$$

[Hastie et al. 2001], where $\boldsymbol{b}_k$ denotes the vector of constraint features in operational period k. The set of representative days is denoted by $\mathcal{S}$, and the set of days clustered around (i.e., represented by) any day $k \in \mathcal{S}$ is denoted by C_k. Semantically, minimizing (4) can be understood as aiming to ensure that the set of representative days proportionately partitions the full set of days in the dataset by minimizing squared Euclidean distances between the time series of constraints. One might hope that in minimizing the clustering objective, the resulting set of cluster medians (i.e., representative days) and their corresponding weights proportionately capture the distribution of constraints, which will in turn yield an aggregation that is "closer" to the original formulation.

3.1.2 Spatial Aggregation. In contrast to a temporal aggregation, for which we aim to identify groups of *operational periods* with similar features (e.g., electricity demands, capacity factors), an ideal spatial aggregation would group *nodes* that demonstrate similarities in their realization of these time-varying features. With this in mind, we might hope to cluster the dataset along the spatial dimension.

3.1.3 Curse of Dimensionality. While standard clustering algorithms such as k-medoids clustering can be applied to the raw data, one might expect that such an approach would be prone to the "curse of dimensionality" due to the high dimensionality of the time series data and the large number of nodes. This is particularly true with spatial clustering, for which there are far more time series observations over the course of the planning period than there are nodes.

To resolve this challenge, we propose an autoencoder-based approach for spatio-temporal aggregation. Specifically, we learn temporal aggregations by training a graph convolutional autoencoder to reconstruct the multivariate time series corresponding to each operational period. In doing so, we are able to extract low-dimensional and denoised representations of the data, on which we can apply a clustering algorithm [Parsons et al. 2004]. Regarding spatial aggregation, we train an autoencoder with a graph pooling mechanism to reconstruct electricity demand time series data. By incorporating a pooling block, we constrain the autoencoder to identify groups of nodes that demonstrate similar electricity demands. Then, we are able to extract the learned pooling assignments as our spatial aggregations. In the following section, we elaborate on our approach for spatio-temporal aggregation.

4 GRAPH CONVOLUTIONAL AUTOENCODER APPROACH

Motivated by the ability of deep unsupervised learning methods to extract latent features from high-dimensional data, we introduce the autoencoder modeling paradigm as follows. Given a high-dimensional input such as a multivariate time series, $\boldsymbol{X} \in \mathbb{R}^p$, an autencoder can be trained to jointly learn an encoder, $g : \mathbb{R}^p \to \mathbb{R}^k$, and a decoder, $f : \mathbb{R}^k \to \mathbb{R}^p$ that minimize the reconstruction loss function $\|\boldsymbol{X} - \hat{\boldsymbol{X}}\|_2^2$, where $\hat{\boldsymbol{X}} = f(g(\boldsymbol{X}))$ is the reconstructed input. Here, $k \ll p$ denotes the dimension of the learned latent space.

Recent work on graph representation learning has facilitated the extension of deep unsupervised learning to the graph time series domain. In Sec. 4.1, we introduce relevant methods from modeling with graph neural networks. Then, in Sec. 4.2 and 4.3, we describe our exact autoencoder-based approach for spatio-temporal aggregation.

4.1 Graph Representation Learning

4.1.1 Preliminaries. We encode a graph topology with the binary adjacency[2] matrix $\boldsymbol{A}$, which we construct such that

$$\boldsymbol{A}_{ij} = \begin{cases} 0 & (i, j) \notin \mathcal{E} \\ 1 & (i, j) \in \mathcal{E}. \end{cases}$$

We also construct the diagonal degree matrix $\boldsymbol{D}$ such that $\boldsymbol{D}_{ii} = \sum_j \boldsymbol{A}_{ij}$.

4.1.2 Graph Convolutions. Our graph autoencoder approach follows [Kipf and Welling 2017] in utilizing *Chebyshev convolutional filters*, which approximate spectral convolutions to learn node embeddings as weighted local averages of embeddings of adjacent nodes. This is ideal for learning low-dimensional embeddings of energy networks as neighborhoods of nodes typically exhibit similar energy demands patterns and can thus be represented jointly (see Fig. 2). Chebyshev filters operate on the "renormalized" graph Laplacian $\tilde{\boldsymbol{L}} = \tilde{\boldsymbol{D}}^{-\frac{1}{2}} \tilde{\boldsymbol{A}} \tilde{\boldsymbol{D}}^{-\frac{1}{2}}$, where $\tilde{\boldsymbol{D}} = \boldsymbol{I} + \boldsymbol{D}$ and $\tilde{\boldsymbol{A}} = \boldsymbol{I} + \boldsymbol{A}$, and

[2]Ideally, one should construct an affinity matrix $\boldsymbol{A}$ with a Gaussian kernel such that $\boldsymbol{A}_{ij} = \exp\left(-\frac{\text{dist}(i,j)^2}{\sigma^2}\right)$ for all edges (i, j), where $\text{dist}(i, j)$ denotes the distance of edge (i, j) and σ denotes the standard deviation of distances in the network [Shuman et al. 2012]. Since we do not have access to edge distance data in our case study, we proceed with the binary adjacency matrix.

perform a form of Laplacian smoothing [Li et al. 2018; Taubin 1995]. We initialize $H^{(0)} = X$ and apply convolutional filters to learn subsequent node embeddings as follows:

$$H^{(l+1)} = \sigma(\tilde{L}H^{(l)}\Theta^{(l)}),$$

where $\Theta^{(l)}$ is a trainable weight matrix and $H^{(l)}$ is a matrix of node embeddings in layer l. $\sigma(\cdot)$ is typically a nonlinear activation function, such as ReLU or tanh.

In each layer, GCNs aggregate features from the immediate neighborhood of each node. Deep GCNs stack multiple layers with nonlinear activations to learn node embeddings as nonlinear functions of both local and global node features. In contrast, [Salha et al. 2019] propose a simpler graph autoencoder model, which they demonstrate to have competitive performances with multilayer GCNs on standard benchmark datasets despite being limited to linear first-order interactions. Shallow neural architectures are also better suited for settings where data is scarce. This is particularly significant in modeling energy systems whose data may only be available for a few historical years. Indeed, we find this shallower GCN approach to perform well for our case study.

4.1.3 Graph Pooling. Motivated by the need for dimensionality reduction and coarsening in graph-level ML tasks, multiple approaches for hierarchical graph pooling have been developed in recent years [Bianchi et al. 2020; Tsitsulin et al. 2020; Ying et al. 2018]. A typical approach to graph pooling is to train a GCN block with a softmax output activation for node cluster assignment jointly with the full GCN. Given k nodes and $k' < k$ desired node clusters, the output of this cluster assignment block is $S \in \mathbb{R}^{k\times k'}$, a matrix of soft assignments in which $S_{ij} \in (0, 1)$ encodes the degree to which node i is assigned to cluster j. To pool the node features after the l-th layer, $H^{(l)}$, we simply compute $\tilde{H}^{(l)} = S^\top H^{(l)}$. Conversely, we can disaggregate the pooled feature matrix by computing $S\tilde{H}^{(l)}$.

Intuitively, one can imagine this block as taking in a time series of electricity demands for each node and returning a "predicted" membership distribution for each node over the k' clusters. Although there is no observed membership data with which to verify node cluster assignments, the quality of the assignments is evaluated implicitly by the downstream reconstruction error, and consequently the reconstruction loss is backpropagated to the pooling block during training of the autoencoder. To minimize reconstruction loss, the pooling mechanism will learn to pool nodes that exhibit similar electricity demands in each day.

For our application, we utilize the MinCutPool operator proposed by [Bianchi et al. 2020], which corresponds to incorporating the objective

$$\min_S \mathcal{L}_u = \min_S \underbrace{-\frac{\mathrm{Tr}(S^\top \tilde{A} S)}{\mathrm{Tr}(S^\top \tilde{D} S)}}_{\mathcal{L}_c} + \underbrace{\left\| \frac{S^\top S}{\|S^\top S\|_F} - \frac{I_{k'}}{\sqrt{k'}} \right\|_F}_{\mathcal{L}_o}.$$

into the autoencoder loss function. This MinCutPool objective $\mathcal{L}_u$ is the sum of the *cut loss*, $\mathcal{L}_c$, and the *orthogonality loss*, $\mathcal{L}_o$. Minimizing the cut loss yields a cluster assignment that groups strongly connected nodes, while minimizing the orthogonality loss yields cluster assignments that are orthogonal and of similar sizes, i.e., each node is fully assigned to one cluster. The orthogonality loss term is included to discourage convergence to degenerate minima of the cut loss such as the uniform assignment of all nodes to all clusters. Consequently, to train an autoencoder with a pooling mechanism, we can minimize a weighted sum of the reconstruction loss $\mathcal{L}_r$ and the MinCutPool loss $\mathcal{L}_u$.

4.2 Temporal Aggregation Architecture

We will first present the proposed GCN architecture for temporal aggregation, which is illustrated in Fig. 3.

Variable	Interpretation	Granularity	Nodes
X_E	Electricity	Hourly	88
X_W	Wind	Hourly	88
X_S	Solar	Hourly	88
X_G	Natural Gas	Daily	18

Table 1. Notation for input variables.

We denote by $X_E \in \mathbb{R}^{d\times n_E\times t_E}$ the data tensor of electricity demands over all days d, nodes n_E, and times t_E. Similarly, we denote the natural gas data tensor by $X_G \in \mathbb{R}^{d\times n_G\times t_G}$, the wind capacity factor tensor by $X_W \in \mathbb{R}^{d\times n_W\times t_W}$, and the solar capacity factor data tensor by $X_S \in \mathbb{R}^{d\times n_S\times t_S}$ (see Table 1). Because the GTEP considers different associated costs for investment and operational decisions related to power, NG, wind, and solar, we introduce hyperparameters $\alpha_G, \alpha_W, \alpha_S$ in the autoencoder objective function to tune the trade-off between the multiple reconstruction losses. This parameter reflects the contribution of each system towards the total cost. For example, if the NG system cost is twice the power system cost, then higher values of α_G ensure that the reconstruction cost is penalized more when deviating from the data of the NG system. This gives us the following reconstruction loss function:

$$\mathcal{L}_r = \sum_{i=1}^{d} \Big(\frac{1}{dn_E t_E} \|X_E^{(i)} - \hat{X}_E^{(i)}\|_F^2 + \frac{\alpha_G}{dn_G t_G} \|X_G^{(i)} - \hat{X}_G^{(i)}\|_F^2 + \frac{\alpha_W}{dn_W t_W} \|X_W^{(i)} - \hat{X}_W^{(i)}\|_F^2 + \frac{\alpha_S}{dn_S t_S} \|X_S^{(i)} - \hat{X}_S^{(i)}\|_F^2 \Big),$$

where $\|\cdot\|_F$ denotes the Frobenius norm.

In our case study, we set $\alpha_G = 2, \alpha_S = 0.5, \alpha_W = 0.5$. However, we note that it is possible to choose the hyperparameters by evaluating the downstream GTEP objective for different values. Specifically, this can be performed using a grid search in which the quality of a combination of hyperparameters $\{\alpha_G, \alpha_W, \alpha_S\}$ is measured by GTEP objective costs given by solving the optimization model rather than the autoencoder validation loss directly.

4.2.1 Encoder. We begin by constructing the data matrix $X^{(i)}$ corresponding to day (i) as

$$X^{(i)} = \begin{pmatrix} X_E^{(i)} & X_W^{(i)} & X_S^{(i)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & X_G^{(i)} \end{pmatrix}.$$

Note that $X^{(i)} \in \mathbb{R}^{n\times t}$, where $n := n_E + n_G$ and $t := t_E + t_W + t_S + t_G$. This is because capacity factor data exists for all nodes in the power network and utilizes the same network topology. $X^{(i)}$ is then passed

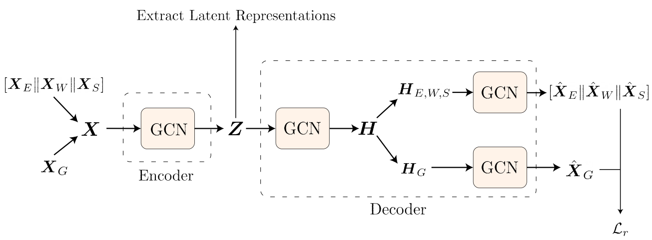

Fig. 3. The temporal aggregation autoencoder aims to learn latent embeddings as a preprocessing step for clustering the combined electric power, wind CF, solar CF, and NG time series corresponding to different days.

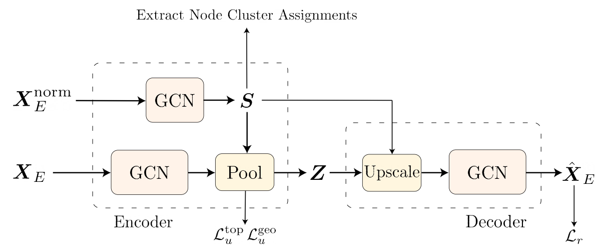

Fig. 4. The spatial aggregation autoencoder utilizes a pooling mechanism to cluster nodes based on their electricity demands.

through a GCN block to produce the low-dimensional embedding $Z^{(i)} \in \mathbb{R}^{n \times k}$. The hyperparameter k defines the bottleneck of the autoencoder architecture (i.e. the dimension of each node embedding) and consequently the tradeoff between compression and reconstruction loss.

4.2.2 Decoder. $Z^{(i)}$ is passed through a GCN block to produce the embedding $H^{(i)} \in \mathbb{R}^{n \times t}$. This reconstructed matrix is then split along the second dimension into two tensors: $H^{(i)}_{E,W,S} \in \mathbb{R}^{(n_E+n_W+n_S)\times t}$ and $H^{(i)}_G \in \mathbb{R}^{n_G \times t}$. Each tensor is then passed to a separate GCN block that maps the node embeddings in $H^{(i)}_{E,W,S}$ and $H^{(i)}_G$ respectively to the reconstructions $\hat{X}^{(i)}_{E,W,S}$ and $\hat{X}^{(i)}_G$. Finally, the tensor $\hat{X}^{(i)}_{E,W,S}$ is split into the reconstructions $\hat{X}^{(i)}_S, \hat{X}^{(i)}_W, \hat{X}^{(i)}_S$.

In our case study, we find utilizing shallow GCN blocks (one or two convolutional layers followed by a tanh activation) and setting $k = 3$ to yield a sufficient performance for our application of temporal aggregation.

4.3 Spatial Aggregation Architecture

The spatial aggregation approach differs from the temporal aggregation approach in four ways: (1) a GCN block with a pooling operator such as MinCutPool is trained jointly as part of the autoencoder to aggregate nodes; (2) a clustering algorithm is not applied to the latent embeddings; rather, the spatial aggregations are directly output by the graph pooling block in the encoder; (3) the loss that is minimized is a weighted sum of the reconstruction loss with the MinCutPool objective; (4) the autoencoder is trained using only the electricity demand data tensor X_E since the goal of the spatial aggregation is to identify groups of nodes in the power network with similar demand behaviors (and consequently, similar constraints).

4.3.1 Encoder. The encoder consists of two GCN blocks in parallel that feed into a pooling mechanism. In constructing the autoencoder architecture, the hyperparameter $k' < k$ is specified as the desired number of node clusters (i.e., nodes in the spatially aggregated formulation). Then for a given day i, the first block extracts low-dimensional features from the electricity time series $X^{(i)}_E$ while the second block outputs the node-cluster assignments $S^{(i)} \in (0, 1)^{k \times k'}$ given the normalized electricity time series. This normalization is performed to prevent the autoencoder from greedily assigning nodes to clusters based only on the magnitudes of the electricity demands; otherwise, the pooling block might assign all nodes to one cluster corresponding to days of uniformly low demand (e.g., days in winter) or another cluster corresponding to days of uniformly high demand etc. One can also include node-specific one-hot features in the normalized time series matrix, which we find to greatly increase the performance of the pooling mechanism.

Given the output of the former GCN block, $H^{(i)} \in \mathbb{R}^{k \times \eta}$, and the cluster assignment matrix $S^{(i)}$ output from the latter GCN block, the pooled feature matrix $Z^{(i)} = S^{(i)\top} H^{(i)}$ is passed to the decoder along with $S^{(i)}$.

4.3.2 Decoder. To reconstruct the input, the decoder upscales the pooled feature matrix by computing $S^{(i)} Z^{(i)} \in \mathbb{R}^{k \times \eta}$. This matrix is then passed to a final GCN block, which outputs the reconstructed electricity demand time series $\hat{X}^{(i)}_E$.

4.3.3 Geospatial and Graph Topological Clustering. It should be noted that pooling assignments that minimize the MinCutPool loss for the graph adjacency matrix occasionally assign geographically distant nodes to the same cluster. This property may be undesirable for CEP applications as geographic distance is usually regarded in conventional approaches to spatial aggregation. To resolve this, we introduce an additional objective to the loss function to penalize cluster assignments that span large geographic distances. Specifically, we construct an additional affinity matrix A^{geo} with a Gaussian kernel such that A^{geo}_{ij} encodes the geographic distance between node i and node j. Given A^{geo} and its corresponding degree matrix, we can pass a learned assignment matrix S through a MinCutPool operator to yield $\mathcal{L}^{\text{geo}}_u$, or the MinCutPool loss with respect to geographic affinities. We distinguish this loss from $\mathcal{L}^{\text{top}}_u$, or the MinCutPool loss with respect to graph topological affinities, and train the autoencoder to minimize the objective

$$\min \mathcal{L}_r + \frac{1}{2}(\mathcal{L}^{\text{top}}_u + \mathcal{L}^{\text{geo}}_u),$$

where

$$\mathcal{L}_r = \sum_{i=1}^{d} \frac{1}{d n_E t_E} \| X^{(i)}_E - \hat{X}^{(i)}_S \|^2_F.$$

4.3.4 Retrieving Spatial Aggregations. Once the autoencoder has been trained, d spatial aggregations can be retrieved by passing each of the d days through the pooling GCN block. From here, a single spatial aggregation can be chosen from the d candidates (many of which may be identical). One approach, which we chose for our case study, is to assign each node's respective cluster by taking a "vote" of cluster memberships over the d days. Another valid approach would be to weight the vote based on the learned temporal aggregation.

5 INPUT DATA

We used the input data provided in [Brenner et al. 2022]. The authors construct the New England power and NG networks by publicly available data. The power network consists of 88 nodes, located in 88 distinct locations with 338 existing and candidate transmission lines. The NG network consists of 18 NG nodes and 7 storage nodes. Each NG node is connected to two other storage nodes. Also, each power node is connected to three of its closest NG nodes. The input data consist of 12 power plants types, 5 of which existing types (e.g., "ng" which is existing gas-fired plants) and the 7 remaining are new types (e.g., CC, wind-offshore, and solar-UPV). The SI [SI 2022] provides the details of the input data for the joint power-NG planning model [SI 2022].

6 UPPER BOUND SOLUTION

To evaluate each instance of the spatio-temporal aggregation, we propose a heuristic algorithm that generates a feasible solution for the full problem (88 nodes and the entire year). The algorithm consist of three steps. The first step solves the aggregated problem and retrieves investment decisions for each spatial cluster. The second step considers the full network for only 2 days and adds sets of constraints to ensure that the sum of investment decisions over all nodes represented by a cluster equals the number of investment decisions for the cluster in the first step. For example, suppose that 5 solar plants are established in the first step for node 7, and assume that nodes 3, 6, and 44 are represented by cluster 7. Then in the second step, we set the sum of established solar plants over nodes 3, 6, and 44 to 5. The result of the second step provides investment decisions for each node. We consider the full network over the whole year in the third step and use these values instead of investment decisions. This renders the problem as a linear program with an optimal solution because the problem is feasible for any investment decisions. The solution to the third step is a feasible solution to the original problem, and consequently is an upper bound (UB).

7 RESULTS AND DISCUSSION

We consider network sizes of 6, 10, 15, and 20 for our computational study and experiment with all even representative days between 4 and 30. All instances are implemented in Python using Gurobi 9.5 and run on the MIT Supercloud system, which uses an Intel Xeon Platinum 8260 processor with up to 48 cores and 192 GB of RAM [Reuther et al. 2018]. We limit the CPU time to 3 hours for all instances, by which point all models were solved to optimality with a mixed integer gap of 1% or lower.

Fig. 6 illustrates the impact of different spatio-temporal aggregations on the total cost and various cost components. As stipulated in Section 2, the total cost consist of power and NG system's cost. The total cost of each system is comprised of different cost components including investment, fixed operation and maintenance (FOM), variable operation and maintenance (VOM) costs. Fig. 6 illustrates the change in cost components with respect to different aggregations as

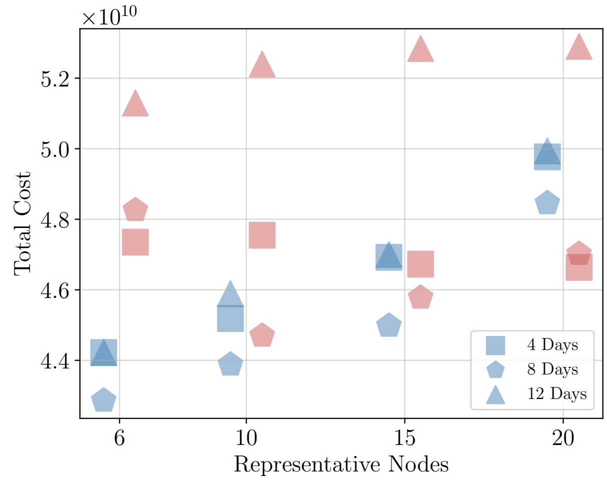

Fig. 5. The UB and objective values associated with each aggregation instance. For each value in the horizontal axis, the left hand side markers show the objective value for the aggregation instance while the markers on the right hand side represent the corresponding UB.

heatmaps (brighter colors correspond to higher costs). The horizontal axis represents the network size (spatial aggregation) while the vertical axis conveys the number of representative days (temporal aggregation). We observe that, for a given number of representative days, the total system cost increases monotonically with the network size. However, there is no obvious trend in total cost with regard to the number of representative days. The increasing total cost for larger network sizes can be explained by increased congestion in the network. Larger networks necessitate more transmission as establishing new plants, especially gas-fired plants, provides a higher capacity than the node demands. However, a large transmission of power from a node to another may not be possible due to network congestion.

As expected, the NG system's cost is almost agnostic towards the power network size. However, its variability is significant with respect to the number of representative days. For example, the NG cost for 8 days is almost twice the NG cost for 10 days. The total power system cost demonstrates a pattern similar to that of the total cost, indicating that the behavior of the total cost is largely driven by the power system cost. We observe that establishment cost increases with the network size for all representative days. A similar pattern can be observed for FOM. The VOM cost, however, sharply decreases as the network size exceeds 10. The increased establishment cost and reduction of VOM indicate that larger power network sizes tend to dispatch lower firm energies and greater renewable energies. Firm energies refer to plant types whose outputs can be changed to compensate for the load variability. Gas-fired and nuclear plants are examples of firm energies and incur variable costs, but their establishment cost is relatively low. Renewable energies such as solar and wind, in contrast, do not incur variable costs but require higher investments to provide sufficient generation.

We evaluate the UB heuristic on 4, 8, and 12 days over various network sizes and illustrate the results in Fig. 5. For each network

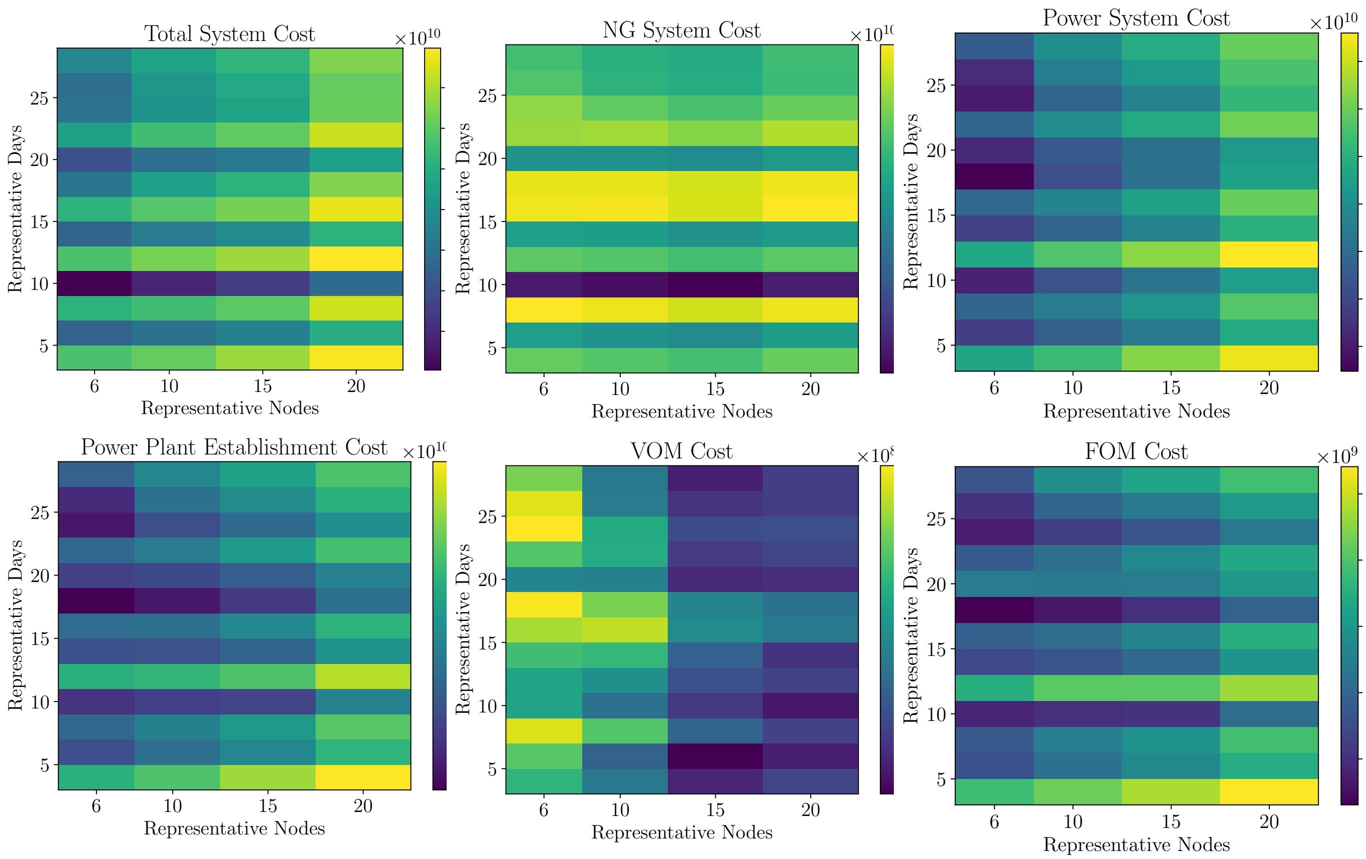

Fig. 6. Some system costs, such as VOM cost, demonstrate an obvious relationship with the resolution of spatio-temporal aggregations, while others, such as the NG system cost, do not exhibit such a clear relationship.

size, the blue markers on the left hand side correspond to the objective values for the aggregated problems while the red markers on the right hand side correspond to the UB values. Depending on the aggregation, the objective value for each aggregation can be lower or higher than the optimal objective for the original problem. For most instances, the UB yields a higher objective than that of the aggregation. However, for a network size of 15 nodes and using 4 representative days, the UB is slightly lower. This may be associated with the specific choice of representative days. If the selected days favors extreme days (i.e., days exhibiting significantly higher load than average), then the objective value of the aggregated problem may exceed the UB.

Interestingly, the analysis of the spatio-temporal aggregation results demonstrates that the *quality* of the solution does not necessarily increase with the resolution of the spatial or temporal aggregation. This is an important observation as it suggest that CEP models could be solved for highly aggregated instances without significantly compromising the solution fidelity. For instance, the best UB value is obtained in 10-node network for 8 representative days as it is shown in Fig. 5. It is also worth mentioning that, although some cost components demonstrate a clear relationship with spatio-temporal aggregations, many appear to have no discernible relationship to system costs, e.g., the seemingly random and volatile response of total system cost with regard to the number of representative days (see Fig. 6). To this end, additional investigation would be needed to understand to what degree these results are specific to our formulation and choice of aggregations as opposed to the GTEP in general.

8 CONCLUSION

In this paper, we present a graph convolutional autoencoder approach to spatio-temporal aggregation for capacity expansion problems and apply our approach to a generation transmission and expansion problem for the New England joint power-NG network. Specifically, we present two autoencoder architectures: an architecture for temporal aggregation that utilizes electricity demand, NG demand, wind CF, and solar CF data, and an architecture for spatial aggregation that uses electricity demand data to learn a node cluster assignment via graph pooling. Finally, we interpret the sensitivity of various cost components with respect to spatial and temporal aggregation resolution given a set of aggregations learned by our approach. Our analysis highlights the importance of data-driven aggregation methods and show that some highly aggregated model could provide quality solutions for capacity expansion problems.

Future studies can extend the results, methodology and observations made in this paper in several directions. For one, additional experiments can be performed with different CEP formulations to more comprehensively understand the relationship connecting aggregation resolution to both solution quality and sensitivity of the learned planning decisions. Moreover, the sensitivity of aggregations, and consequently planning decisions, with respect to changes in the dataset should be investigated. The ML technique can be tailored to reflect the characteristics of each CEP model considered.

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