Time-series aggregation for the optimization of energy systems: goals, challenges, approaches, and opportunities

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Abstract

The rising significance of renewable energy increases the importance of representing time-varying input data in energy system optimization studies. Time-series aggregation, which reduces temporal model complexity, has emerged in recent years to address this challenge. We provide a comprehensive review of time-series aggregation for the optimization of energy systems. We show where time series affect optimization models, and define the goals, inherent assumptions, and challenges of time-series aggregation. We review the methods that have been proposed in the literature, focusing on how these methods address the challenges. This leads to suggestions for future research opportunities. This review is both an introduction for researchers using time-series aggregation for the first time and a guide to "connect the dots" for experienced researchers in the field. We recommend the following best practices when using time-series aggregation: (1) Performance should be measured in terms of optimization outcome and should be validated on the full time series; (2) aggregation methods and optimization problem formulation should be tuned for the specific problem and data; (3) wind data should be aggregated with extra care; (4) bounding the error in the objective function should be considered; (5) inclusion of real "extreme days" in addition to aggregated days can often greatly improve performance.

Keywords: , Review, Clustering, Energy, Representative periods, Typical days, Optimization

1. Introduction

To reach climate targets we must radically reduce greenhouse gas emissions (1). Building an electricity system using primarily renewable energy is currently seen as the best means to achieve this goal. Minimizing the cost of such an electricity system requires complex optimization models (2). In an ideal world, these optimization models would simulate accurate power system physics, and would be solved at high geographic and temporal resolution (i.e., distribution level using sub-minute-scale supply and demand modeling). Such a model is far beyond the capabilities of current computers, so modelers always face trade-offs in how they represent the physical, spatial, and temporal details of this problem (3).

The challenge of temporal fidelity is large in energy systems optimization problems. As an example, the electricity system modeling and optimization problem faces a particularly profound challenge in the temporal domain: electric system operations depend intimately on second to sub-second alignment of supply and demand, on hourly- and daily-scale dispatch and bidding decisions, and on decadal-scale investment decisions. Thus there are linkages across 8 to 9 orders of magnitude in time scales, and second-scale operations possibilities depend directly and intimately on investment decisions made over many decades. Similar challenges arise in non-electrical models as well: we often care simultanesouly about the behavior of a system over small time instances, but that behavior is governed by larger-scale decisions that affect many many time instances.

Thus, temporal resolution of such models is the focus of this review. Because renewable energy availability varies with time and is an exogenous input to models, optimal investment solutions depend on the details of temporal data.

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This leads to optimization problems where the design and operations of the energy system must be optimized together. Many problems exhibit this characteristic, including electric system capacity expansion planning (4–15); design of local energy supply systems (16–22); and design of plants or industrial facilities for responsive operation in alignment with renewables (23–33), or more generally load-shifting and load-shedding studies for end use adaptation of demand to supply.

Even using relatively coarse hourly resolution in such a model implies 8760 time steps per year, resulting in large model sizes. In response, numerous time-series aggregation (hereafter TSA) methods have been developed over the past decade (34; 35). TSA is used to aggregate temporal data into representative periods. For example, a model may be solved for five representative days instead of a complete year of 365 days. Using TSA can reduce computation time and memory requirements by around two orders of magnitude, and thus turn an intractable problem into a tractable one.

In this work, we review TSA methods used in energy systems optimization models. We take the following general path: (1) Outline applications of TSA, (2) Discuss inherent assumptions and overall approaches, (3) outline the fundamental challenges of TSA, (4) give approaches to solve these challenges, and (5) outline best practices. Our review proceeds as follows. Section 2 discusses optimization applications and how they include time-series data. Section 3 defines goals of TSA. Section 4 outlines the general steps and inherent assumptions of TSA. Section 5 presents the challenges that need to be addressed when using TSA, and Section 6 examines approaches to deal with these challenges. Lastly, Section 7 concludes by providing best practices and future research opportunities.

2. Time series data in energy systems optimization

2.1. The role of time series data

In simplified form, the above classes of problems can often be cast as a linear program (LP), where we minimize an objective function:

$$\min_{x} : f(\mathbf{x}) = \mathbf{c}^T \mathbf{x} \tag{1}$$

subject to a set of constraints:

$$\mathbf{A}\mathbf{x} \geq \mathbf{b} \tag{2}$$

where $\mathbf{x}$ is a vector of decision variables, $\mathbf{c}$ a generalized cost or price vector, $\mathbf{A}$ a constraint body, and $\mathbf{b}$ a set of constraint conditions to be met. Time-series data can enter into any of these model elements $\mathbf{A}$, $\mathbf{b}$, $\mathbf{c}$.

The result of solving such a model is a set of optimal decision variables $\mathbf{x}^*$ and an optimal objective function value $f(\mathbf{x}^*)$. In valid solutions, the decisions $\mathbf{x}^*$ satisfy the constraints such that we are ensured that $\mathbf{A}\mathbf{x}^* \geq \mathbf{b}$. In cases where the problem cannot be readily linearized, all of the above challenges with problem size take on even more importance.

As Figure 1 illustrates, time-series data can enter this problem in various ways. Time-series data can directly enter the objective function in $\mathbf{c}$, as in the case of hourly electricity prices. Some time-series data occur in $\mathbf{A}$, the left-hand side of the constraints. For example, wind and solar availability, which yield non-dispatchable generation through multiplication by the wind and solar capacity. Lastly, some time-series data occur on the right-hand side of the constraints $\mathbf{b}$. For example, time-varying electricity demand, which may enter exogenously into $\mathbf{b}$.

The best case are LPs, where computational time in the worst-case is polynomial as a function of the number of variables and constraints (36), though often solved faster than that in practice (37). However, even for LPs, the problem can still become computationally intractable quickly. For nonlinear programs (NLPs), mixed integer linear (MILPs) programs, or mixed integer nonlinear programs (MINLPs), the computational tractability is far worse. Goderbauer et al. (38) prove that design optimization problems of energy systems that are modeled as MILPs or MINLPs are strongly NP-hard.

Using TSA to solve only a subset of the original time-series input data reduces the number of variables and constraints and thus reduces computation and memory requirements. Figure 2 compares computation times from three studies, including two LP generation capacity expansion problems and four MILP energy supply systems. Using representative periods reduces computation times by 1-2 orders of magnitude. Furthermore, the reduction in computational time is nonlinear. For example: in the studied MILPs, using 10 representative days out of the original 365 days (2.7% of the original data) reduces computational time to 0.1%-1.1% of the original problem (17; 22).
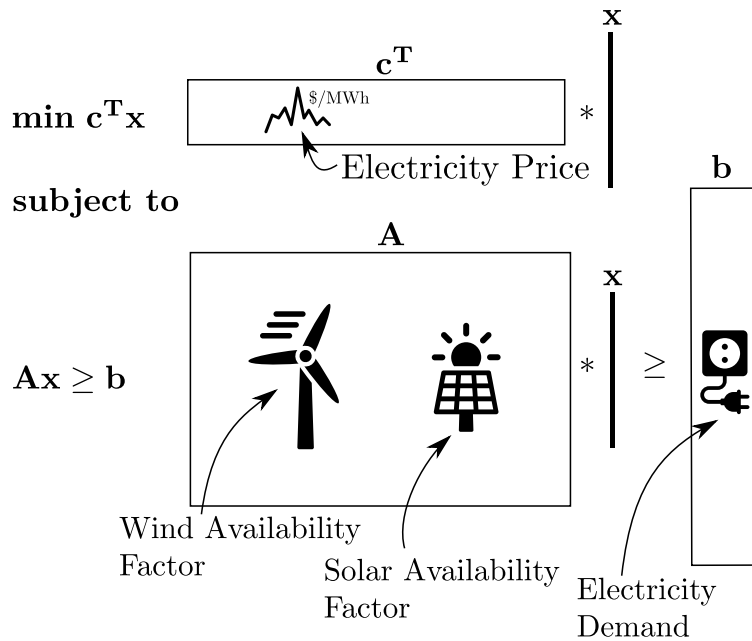
Figure 1: Time-series data can occur in different parts of the optimization problem. For a linear optimization problem, some data can occur in the objective function, some on the left-hand side of the constraints, and some on the right-hand side of the constraints. Where the data occurs influences how aggregation of these data impacts optimization outcome.
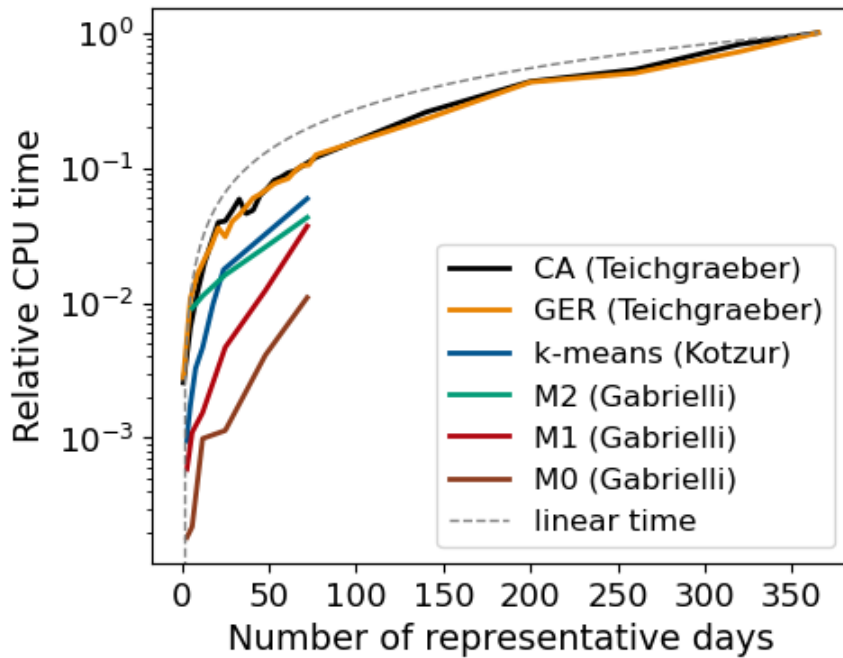

Figure 2: CPU time of energy systems optimization problems from the literature. Time-series aggregation results in reduction in computational time. Shown here is the CPU time normalized by the CPU time of the optimization problem with 365 days. We report CPU time for two LP problem formulations (Teichgraeber) and four MILP problem formulations (Kotzur (17), Gabrielli (22)). See SI for details on how the data were obtained.

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2.2. Energy systems optimization models using time-series data

The energy optimization literature contains three general classes of models where time-series data are key: (1) generation and transmission capacity expansion, (2) design and operations of local energy supply systems, and (3) design and operations of individual energy facilities or technologies.

Capacity expansion planning (CEP) (39) is used in electricity system planning over investment-scale time horizons of 20 to 30 years (40–42). CEP can include both generation capacity and transmission capacity. Due to computational limitations, generation and transmission are often modeled and solved as separate CEPs (5), but in recent years they have been more frequently combined (4; 43; 44).

The objective in CEP is to minimize overall system cost from the perspective of a central planner. Decisions include how much, where, and when to build different types of electricity generation capacity. CEP constraints require demand and supply to be equal at all times. Typical time series used in CEPs are wind and solar availability, and electricity demand.

Modeling decisions may add complexity to a CEP problem. First, multiple geographic regions are often modeled, requiring time series for each attribute for each region. The regions are then connected by transmission lines which add modeling complexity. Transmission can be modeled at various levels of physical detail (e.g., DC or AC optimal power flow) (45). Transmission line capacities can be decision variables themselves in the case of a transmission CEP, or be fixed. Environmental constraints are often added to CEP models. For example, overall CO_2 emissions may be limited. Because such a constraint links all variables over the full time horizon, it adds significant complexity to the problem (9; 46). Such constraints link all time steps together because it is the average behavior of the system over time that must be controlled, not the behavior in a given time step.

An additional complexity is storage of energy via batteries, chemicals, or pumped hydro-electric storage introduces constraints that often bind across time periods (e.g., multi-day constraints) (47; 48). In general these constraints that link time steps together limit the approaches that can be used to create representative days.

Additional modeling realism may be added by limiting ramping of thermal generators (11), by modeling thermal generators using unit commitment constraints on minimum on- and off times, minimum power generation levels, or by modeling costs as piece-wise linear functions. Some of these modeling decisions add integer variables, which make the problem an MILP and add significant computational complexity.

In addition to the classic CEP problem, local energy system (LES) models also depend on time-series data. Examples of LES models are residential energy supply systems (a house or several houses) (16–18), industrial parks (19–21) and microgrids (49) and urban regions (22). A base LES model can often be constructed similarly to a one-node CEP model (50), but LES models often couple different energy carriers, such as electricity, chemical fuels, and hot and cold streams.

Technology options in LES models consist of combined heat and power plants, gas turbines, wind turbines, solar panels, boilers, heat pumps, and batteries and heat storage tanks. Typical time series that occur in local energy supply systems are electricity demand, heating and cooling demand, wind availability, solar availability, temperature, and electricity prices.

Similar considerations occur in LES models regarding constraints that link behaviors between time steps. Features such as carbon constraints or energy storage would serve to link time steps and require care. Nonlinearities often arise in LES systems where realisim in the engineering of LES systems is aimed to be added. For example, a model of a combined heat and power system coupled to a heating and cooling network may have detailed treatment of the rates of heat loss from thermal storage and hot and cold fluid pipe networks.

A major difference between LES problems and CEPs is that the former are often connected to the (assumed to be much larger) grid which is generally modeled in an abstract fashion as a source of supply at a given price. This allows for the system to draw electricity from the grid if local production is not sufficient. Electricity prices are generally represented by an exogenous time series in this case.

Third, in individual facility or technology optimization (IFTO) models a modeler may want to evaluate the optimal design of a facility or technology under time-varying operating conditions. IFTO is a problem formulation where the objective is to maximize net present value of profits, subject to design and operating constraints, often imposed exogenously as time-series data. Individual facilities or technologies that have been optimized with representative periods are battery-storage facilities (30), gas turbines with carbon capture (23; 25; 29) and without carbon capture (30; 51), integrated solar combined cycle power plants (26; 27; 52), air separation units (53), combined heat and power
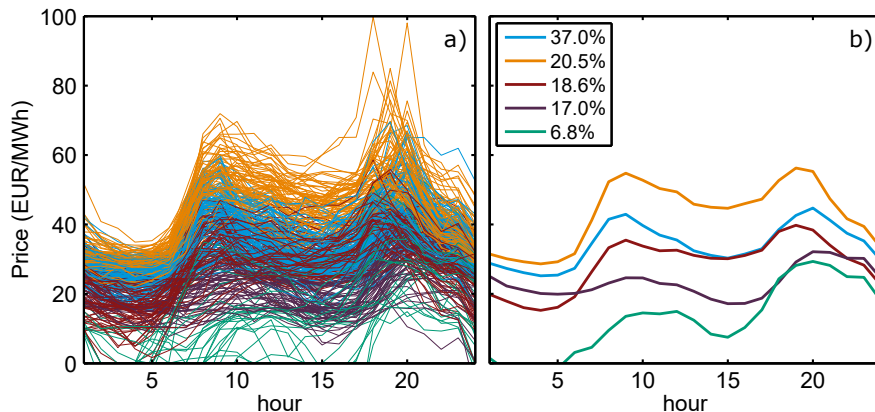
Figure 3: (a) Example full German electricity price data from 2015 and its assignments to five representative periods by color, and (b) the respective k=5 representative periods and weights. The weights signify how many out of the 365 days are represented by the respective cluster. Figure adapted from Teichgraeber and Brandt (30).

plants (54), waste-heat recovery from heavy-duty vehicles (28), volt-var optimization (55), and power consumption scheduling (56).

The time-series input data in these cases are usually electricity prices, which are present in the objective function. In some cases, additional time series are present in the constraints such as thermal properties of the fluids involved in a process (28) or incoming solar irradiance (26). Similarly to the LES cases, the more specific modeling treatment in IFTO models can require nonlinear engineering (chemistry or physics) to be implemented, further incentivizing the modeler to reduce the temporal complexity of the model.

3. Fundamental Goal

The *fundamental goal* of TSA is to create a reduced set of time-varying input data that retains all relevant characteristics of the original data set and thus results in similar optimization outcomes with less computational time and required memory.

In mathematical terms, we create a new time-series dataset that replaces some subset of $\mathbf{c}$, $\mathbf{A}$, and $\mathbf{b}$ with reduced equivalents $\hat{\mathbf{c}}$, $\hat{\mathbf{A}}$, or $\hat{\mathbf{b}}$. Ideally, when we solve our model with these new reduced inputs, we maintain relevant characteristics of our solution with little or no distortion.

What are the relevant characteristics we wish to maintain in our reduced dataset? This depends on the problem and modeling goals. Often, it is of primary importance to find optimal design decision variables in the reduced problem – call them $\hat{\mathbf{x}}^*$ – that are similar to the ones $\mathbf{x}^*$ that are found by solving the full problem. An accurate representation of the objective function by $f(\hat{\mathbf{x}}^*)$ is also desirable if profits or costs are of importance. Lastly, we also care about whether a design $\hat{\mathbf{x}}^*$ is feasible or adheres reliably to constraint reuirements.

4. Representative Periods: General Steps and Inherent Assumptions

The most common approach in TSA, and the focus of this work, is to create representative periods. In the literature, representative periods are also called typical periods (57; 58), representative days (18; 59; 60), typical days (61; 62), or time slices (6; 63). Representative periods are real or synthetic periods that represent or stand in for a larger group of similar periods. Figure 3 shows an illustrative example of representative days for electricity price data from Germany. Alternatives to creating representative periods include stochastic or sampling-based approaches, but we do not cover those here.

Figure 4 illustrates the two general steps that are taken when creating representative periods. The *original time series* consists of N consecutive time steps, each of length Δt (e.g., 1 year as N =8760 time steps of length Δt = 1 hr). Representative periods are then obtained in two general steps.

General Step 1: *Slice original time series into K operationally independent periods.*
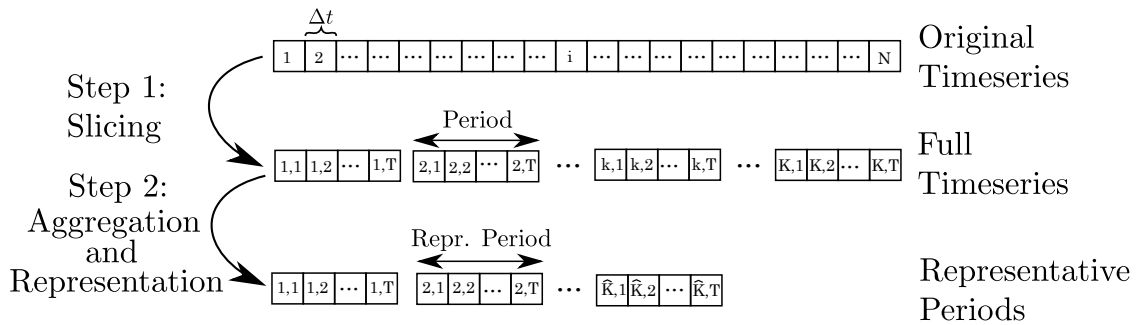
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Figure 4: Temporal representation of input data, general steps: The original problem is first sliced to obtain the original problem, and then aggregation and representation result in representative periods.

In order to obtain periods, the original time series is sliced into $K = \frac{N}{T}$ periods, where each of the K periods consists of T time steps. For example, for a year of hourly data, $K = \frac{8760}{24} = 365$. The original time series is sliced into what we call the *full time series*.

General Step 2: *Aggregate several periods and represent them by one period.*

In order to obtain representative periods, the periods of the full time series are aggregated and represented by $\hat{K} < K$ periods and their respective weights. Weights are often, but not always, proportional to the number of periods that a certain representative period represents in the full time series.

Many studies implicitly assume that neither general step above significantly affects optimization outcomes. If General Step 1 does not significantly affect optimization outcomes, it means that long-term operational interactions between periods can be neglected and that the N time steps in the original time series can be sliced into K periods of the full time series without impacting model results. If General Step 2 does not significantly affect optimization outcome, then it is possible to find $\hat{K}$ representative periods that retain all relevant characteristics of the K periods of the full time series. We will see below that these assumptions do not always hold.

5. Challenges

It is non-trivial to find representative periods that retain all relevant characteristics of the full dataset. We outline below the five major challenges for using representative periods. Figure 5 illustrates these challenges. Challenge 1 is of primary concern to the managers/decision maker. Challenges 2-5 categorize the decisions to be made by the modeler, and influence the outcome of Challenge 1.

5.1. Challenge 1: There will always be some error when using representative periods.

This first challenge is as follows: There will always be statistical error when aggregating several periods into one representative period, and this statistical error will result in at least some error in optimization outcome. However, the relationship between statistical error and error in optimization outcome is nonlinear: a large error in the statistical measure may lead to small errors in optimization outcome, and *vice versa*. Furthermore, it is important to know whether error introduced results in systematic bias in optimization results or in increased variance in optimization results.

So, when then is it appropriate to use representative periods? Ultimately, optimization models will be used to make policy, investment, and business decisions, and so "garbage in, garbage out" (64) should be avoided. The challenge is therefore to identify and avoid problem types for which the use of representative periods lead to fundamentally misleading results. This is often challenging to determine in prospect and misleading results often only become apparent in retrospective analysis.

5.2. Challenge 2: How do we measure error or success of a set of representative periods?

A second challenge then arises: There is no single, unambiguous measure of the error introduced by using representative periods. Generally, measures rely on statistical properties of the data or optimization outcomes. Because
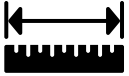
Challenges

1) There will always be some error.

2) How to measure error/success?

3) How to model temporal resolution?

4) How to find representative periods?

5) How to link representative periods?

Figure 5: We identify five challenges that the modeler should be aware of when using time-series aggregation.

long-term decisions may be made based on optimization model outcomes, measures should be aligned with the research and/or investment question asked, and measures should focus on errors or success of the optimization outcome. Because optimization models are designed to answer different questions, success can therefore be measured in numerous ways.

5.3. Challenge 3: How do we model temporal resolution?

The third challenge is that a modeler has to decide how much time series data to use (i.e. how many years of input data) and what the length of the time step Δt should be (e.g. hours). These decisions affect the performance and fidelity of the model, and also the effectiveness of TSA.

Three decisions have to be made by the modeler prior to finding representative periods. The first decision is the length of representative periods, i.e., how many time steps T a period should contain. The most common options for representative period length are days, hours, and weeks. The second decision is the number of representative periods $\hat{K}$ to select. The choice of $\hat{K}$ includes a trade-off: If $\hat{K}$ is small, the solution time and memory requirement of the optimization model is significantly reduced, but accuracy compared to the solution in using the full timeseries of K periods may be low. Whereas if $\hat{K}$ is large, we introduce less error, but the resulting problems need more solution time and memory and we obtain less benefit compared to solving the model using the full timeseries. The third decision regards data features that are important to the optimization problem. This can include original time series data or derived features such as ramp rates, and whether to use smoothed representative periods (e.g., centroids) or also extreme periods.

5.4. Challenge 4: How do we find representative periods?

Once the modeler has determined the type of representative periods to use, the fourth challenge is to find these periods. Clustering methods are the most common approach. The choice of clustering method impacts the resulting representative periods. Because the mapping from the statistical domain of the clustering algorithm to the domain of the optimal solution of the optimization problem is often highly nonlinear, it is non-trivial to pick a clustering method that retains data characteristics important to an optimization problem. If the set of representative periods is to also contain extreme days, finding these is similarly non-trivial.

5.5. Challenge 5: How do we allow for linking of periods when using representative periods?

The fifth challenge is that when slicing the N elements of the time-series data into our set of K original periods in General Step 1, modelers assume that operational interactions between periods can be neglected. However, this assumption does not always hold. An example is seasonal energy storage, which can span a longer time than the typical period length of one day. Similarly, the concept of renewable energy droughts can arise when multiple days in a row of – for example – low wind output can have detrimental impacts. In order to overcome this downside of using representative periods, methodologies have to be developed to allow for the linking or coupling of periods.

6. Approaches

In this section, we review the approaches taken to address the five challenges introduced in Section 5.

6.1. Approaches 1: There will always be some error due to using representative periods

It is critical to understand how statistical error—introduced by definition during TSA—leads to error in optimization outcomes. Because in many cases we cannot solve the optimization problem with full timeseries data made up of K periods, the resulting error is generally unknown or can only approximated by bounds.

Statistical error introduced by TSA can take several forms. The representative periods $\hat{K}$ can differ from the original periods in (1) mean, (2) within-period variance, and (3) the extreme values of the representative periods . Clustering—the most commonly used TSA technique—tends to preserve mean behavior, but to smooth time-series and thus result in lower within-period dispersion. This smoothing also result in the reduction in magnitude of extreme values (18).

Distortion in time-series means can affect optimization outcomes by affecting overall economics or performance of a system. For example, the required overall investment size or amount can be estimated poorly by the model if the representative periods $\hat{K}$ poorly represent the original mean behavior.

In contrast, error in representing within-period dispersion can affect optimization outcome because technologies such as storage or ramp-rate-constrained power generation rely on accurate representation of within-period dispersion, as well as autocorrelation of the dispersion. For example, wind availability tends to have high within-period dispersion, but aggregated wind data tend to appear more smoothed (9). System designs from using full and aggregate data can thus differ.

Lastly, distortion of extreme values in a data series can affect optimization outcomes because system infeasibility often occurs at extreme conditions. Thus if a TSA method does not reproduce extreme conditions, the reduced form design is often not reliable when operated on the full data.

The error in optimization outcome can show up in terms of error in the objective function value $f(\hat{x}^*)$, error in the optimal decision variable set $\hat{x}^*$, and error in constraint satisfaction. Zipkin (65) proves that there always exists an aggregated version (representative periods and weights) of the original input data that will perfectly reproduce the objective function value of the original problem. However, it is unclear how to find such aggregated version, and this aggregation may still result in errors in decision variable values $\hat{x}^*$ and in constraint satisfaction.

Teichgraeber and Brandt (30) show that the mapping from statistical error in the data domain to the domain of the objective function is highly nonlinear. This is true for both LPs and NLPs. They analyzed all 10,000 locally converged solutions from randomly initialized k-means and k-medoids clustering and found that a better representation in terms of clustering measure (lower statistical error) is not necessarily better in terms of objective function value of the optimization problem. Thus, error magnitudes in the statistical domain do not necessarily translate into error magnitudes in objective function value.

Merrick (66) analyzed the effect of temporal representation on the optimal design variables by looking at mis-valuation of wind and solar power generation. He shows that the marginal value of solar and wind is a function of the expected electricity prices — which is the weighted mean of the dual variables of the supply-demand balance —, the capacity factor — which is the weighted mean of solar and wind availability —, and of the covariance between the electricity prices and the solar and wind availability— which are time-varying input data. At low renewable penetrations, electricity prices are mainly influenced by electricity demand. Thus, mis-valuing of wind and solar power generation due to TSA is mainly influenced by errors in the covariance between electricity demand and wind and solar availability. Underestimating the covariance leads to undervaluation of renewables and thus less capacity built than

without aggregation, and vice versa. At high renewable energy penetrations, the error introduced by TSA depends on the covariance between electricity price and wind and solar availability, as well as the expected electricity price. Merrick further shows that the error introduced by the same aggregation can result in different system designs depending on the model parameterization. For example, depending on the capital cost of solar PV, a set of representative periods either overvalues or undervalues renewable generation. Thus, it is non-trivial to predict *a priori* how TSA affects optimization results.

In some cases, TSA introduces systematic bias. Teichgraeber and Brandt (30) prove that for optimization problems with certain structure, the optimal objective function value of the problem with aggregated input data is either an under- or overestimator of the objective function value of the problem with full input data. Similarly, Kuepper et al. (9) show this for selection of certain technology over others.

Several studies analyze simple optimization problems that can be solved for the full set of input data periods K in order to better understand the error introduced by the use of representative periods $\hat{K}$ (11; 16; 17; 30; 62; 66–70). A general result across these studies is that optimization error due to TSA is problem specific and that there is no one-size-fits-all method to reduce errors from using TSA. Many of these findings are elaborated on below.

Few generalizable insights have been found. Merrick and Weyant (71) and Weber et al. (72) provide a treatment of model appropriateness from an information theoretic point of view. Some studies have observed that error increases when the system relies more on technologies that produce power based on time-series input data (e.g. wind and solar power) and less based on dispatchable sources (9; 17; 66). In particular, wind has been found to be challenging to accurately aggregate (9).

At the heart of this lack of generalizable insights is the interrelation between the particular optimization model and the TSA method. Ideally one needs to know how input data influence the model, but if this influence were a trivial human-graspable relationship, formal computational optimization would likely not be necessary in the first place. Thus, there is a two-way interrelation between input data and models, which makes judgement on the appropriateness of using representative periods, *a priori*, inherently difficult.

6.2. Approaches 2: How do we measure error/success of a set of representative periods?

Many different error measures have been proposed for TSA. Generally, error measures use statistical properties or optimization outcome. We conclude that it is necessary to include relevant optimization outcome when measuring the success of TSA, and that statistical metrics alone are not sufficient (12; 23; 30; 66).

Many statistical error metrics have been used in TSA, either adapted from the broader clustering community or invented specifically for the application to energy systems optimization problems. Table 1 summarizes statistical error metrics used in energy systems optimization. The most common statistical error metric is the sum of squared errors (SSE) between cluster members and their cluster representative. Other metrics exist (92; 93), such as the silhouette statistic (94; 95) and the gap statistic (96).

Besides quantitative statistical metrics, visual inspection is also used. This is done by plotting each period of the full data and the representative periods and respective weights (23; 25; 26; 63; 70) (e.g. see Figure 3), or plotting heat maps of the time series (17; 62). Visual inspection allows a coarse understanding of which features of the data are captured well by the TSA method used. Visual inspection of duration curves is also used. In a duration curve, the data are sorted and plotted from the largest to the smallest value. Load duration curves have traditionally been used for electricity generation planning. In cases where only load data is aggregated, several papers (57; 61; 74) compare the load duration curve of the full input data and the aggregated input data. In cases where both load and renewable energy availability data are aggregated, duration curves can be plotted for each (6; 59; 63; 66; 75; 76). Merrick (66) and Buchholz et al. (14) show that apparently reasonable fit in duration curves may still introduce error in model output. Duration curves have two main drawbacks: 1) They present sorted data, thus neglecting the chronological order of time-series, which is important when considering ramping and storage technologies and 2) they present each attribute (e.g. load, wind, solar) individually, thus neglect connections or correlations between the various time series.

Overall, statistical error metrics or visually inspecting the data alone are not sufficient. For example, a generation capacity expansion model with certain parameter values and constraints may work well with few representative periods, but changing parameters may require the use of significantly more representative periods to reasonably approximate the behavior of the model with full data. Merrick (66) finds large impacts due to changing capital cost for PV technology, and Kuepper et al. (9) find large impacts due to tightening CO_2 constraints.

Table 1: Statistical error measures used in the literature to evaluate representative periods. Visual inspection of these measures is most commonly applied by comparing the measure for different sets of representative periods (the so-called "elbow method").

Measure	Short Description	Used in	Source
LDC	Visual inspection of the Load Duration Curve (LDC) and other duration curves	(6; 48; 57; 59; 61; 63; 66; 67; 73–80)	
ELDC	Error in Load Duration Curve Deviation compared to full data	(57; 59; 61; 73; 74; 78; 81; 82)	(61)
RDCE	Normalized root mean squared ramp duration curve error	(59)	(59)
ESE	Ratio of observed to expected squared errors for N clusters.	(57)	(83)
SSE	Sum of squared errors: Sum of intra-cluster distances	(6; 16; 23; 26; 29; 30; 41; 57; 67; 74; 81)	(84)
RMSE	Root mean squared error	(76; 79; 82; 85–89)	
Inter-cluster distance	Sum of inter-cluster distances – evaluates the separation between clusters	(57)	
Clustering dispersion indicator	Ratio of mean within-cluster distances and between-cluster distances	(41)	
Davies-Bouldin index	Balances the distances between clusters and within-cluster scatter	(61)	(90)
VarC	Covered Variance	(6; 66)	(91)
CorrE	Correlation Error	(6; 59)	(59)

These examples illustrate that considering the data alone is insufficient, and optimization-outcome based metrics need to be used. The challenge lies in the fact that the optimization problem results for the full data are often unknown.

Table 2 summarizes optimization-outcome based metrics. First, optimization outcome is often compared in terms of fidelity of the TSA-derived objective function value $f(\hat{\mathbf{x}}^*)$ to the objective function value without TSA, $f(\mathbf{x}^*)$. The absolute error in objective function is thus $|f(\hat{\mathbf{x}}^*) - f(\mathbf{x}^*)|$. The TSA-derived value can either be the objective function value of the full problem solved with aggregated input data (23; 25; 41; 66; 67; 77; 97), or the problem with fixed design decision variables determined using $\hat{K}$ periods and then operations solved on the full input data of K periods. In the case of generation capacity expansion, the problem with operations solved on full input data and fixed design decision variables is also referred to as the production cost model (22; 28; 77; 98). Comparing aggregation results based on the optimal objective function value of the full operations problem with fixed design is preferable to only using the optimal objective function value of the optimization problem with aggregated input data because it allows to evaluate how the design performs on the full time series. However, the full operations problem is sometimes itself computationally intractable. One can then use rolling horizon optimization to solve the operations problem (74).

Other authors use the relative system cost (capital and operating cost) disaggregated by design variable (17; 68) or total investment cost (41; 100), which are sub-parts of the objective function.

Besides the objective function value, the fidelity of TSA-derived design decision variables $\hat{\mathbf{x}}^*$ has been used as a metric (17; 22; 63; 66; 67; 75; 99–101). Often in energy systems optimization problems, the design decision variables are the outcome of interest (e.g., they show which capacity is built). In some cases, summary decision variable quantities such as the sum of all installed renewable energy capacity (6) have been used. Others compare generation mix by technology, which is the aggregated generation over the whole time series based on the design obtained through representative periods (6; 66).

Bahl et al. (58; 77; 106) and Baumgaertner et al. (20) develop a method to bound the error in the objective function, $|f(\hat{\mathbf{x}}^*) - f(\mathbf{x}^*)|$. In their cost minimization problem, they use the optimal objective function value of a relaxed version of the optimization problem formulation as a lower bound LB, and they use the optimal objective function value of the full operations problem with fixed design obtained through the use of representative periods as an upper bound UB. They bound the error in the objective function by setting an acceptable error ϵ, and then adding representative periods

Table 2: Error measures based on optimization outcome used in the literature to evaluate representative periods. Note that error measures that calculate the difference to D_{full}&O_{full} cannot be applied in practice when the optimization with full input data is computationally intractable, but are often used on sample optimization problems to evaluate time-series aggregation methods.

Measure	Comparison Type	Short Description	Used in
Objective function (D_{repr}&O_{repr})	Visual	Objective function of the system with representative periods	(12; 23; 25; 41; 60; 66; 67; 77; 89; 91; 97)
Objective function (D_{repr}&O_{full})	Visual	Objective function of the full operations with fixed design	(22; 28; 77; 79; 98)
Design variables	Visual	Optimal generation capacity of the technologies	(17; 22; 63; 66; 67; 73; 75; 79; 80; 82; 88; 89; 99–101)
VRE share	Visual	Sum of renewable generation capacity	(6)
Total investment cost	Visual	Capital cost associated with system design	(41; 102)
Relative investment cost by design variables	Visual	Capital cost associated with each design variable	(17; 68)
Relative system cost by cost type	Visual	Fixed and variable operating cost, investment cost, etc.	(100; 102)
Electricity Generation mix O_{repr}	Visual	Aggregated generation by technology	(6; 66; 86)
Error in objective function (D_{repr}&O_{repr})	To D_{full}&O_{full}	Difference of objective functions	(11; 16; 17; 30; 62; 66–70; 86; 87; 103–105)
Error in objective function (D_{repr}&O_{full})	To D_{full}&O_{full}	Difference of objective functions	(14; 98)
Error in optimal design	To D_{full}&O_{full}	Difference of optimal designs	(11; 14; 67; 69; 70; 86)
Root mean squared deviation in design	To D_{full}&O_{full}	Difference of optimal designs	(76)
Custom distance	To D_{full}&O_{full}	Custom distance measures integrating design and operations	(14; 66; 86)
Error in other optimization outcomes	To D_{full}&O_{full}	Difference of e.g. carbon intensity, CCGT startup	(14; 62; 86)
Optimization outcomes of the rolling horizon full operations problem	To D_{full}&O_{full}	Curtailment and non-served energy based on full operations solved with a rolling horizon	(63; 74)
Objective function error gap	Bounded error	Bound the unknown error in objective function by use of upper and lower bounds	(20; 58; 77; 102; 106; 107)

to their aggregation step by step until they reach $\frac{UB-LB}{UB} \leq \epsilon$. Figure 6 shows an example of this bounding method. Bahl et al. introduce their approach for a general two-stage optimization problem including peak-power prices (e.g. demand charges) (106), and they extend the method to two-stage optimization problems that involve storage (20; 21). Yokoyama et al. (107) also develop a bounding method. Teichgraeber and Brandt (30) present proofs that for LPs with certain structure, the objective function value of the optimization problem after TSA is a lower bound LB to the solution. Li et al. (108) extend several of these proofs to MILPs.
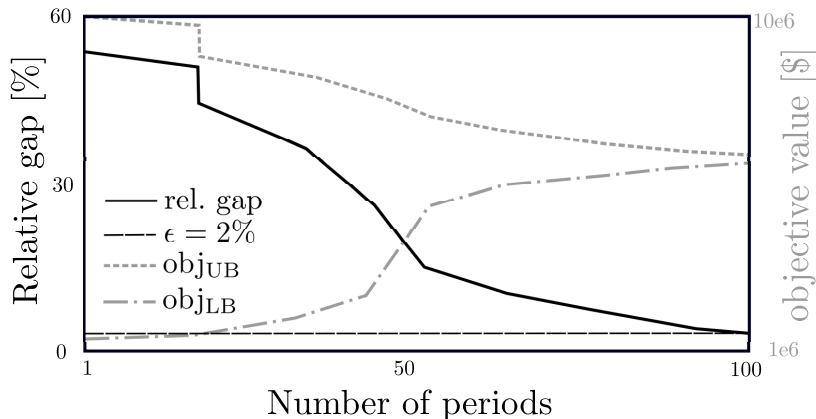
Figure 6: Bounding the error in the objective function by use of time-series aggregation. As the number of representative periods increases, the upper bound (UB) and lower bound (LB) tighten. This results in a small maximum error (relative gap) of the objective value of the found design compared to the unknown, globally optimal solution with full time-series input data. Figure adapted from Bahl et al. (106), numbers for illustrative purposes only.

6.3. Approaches 3: How to model temporal resolution?

All energy system models require decisions concerning the amount of data to be used and the time step length Δt. Historical time series are—implicitly or explicitly—used with the assumption that future conditions will be similar.

One year of historical data is a common choice (17; 30), while some studies use multiple years (6; 57; 62; 63; 76; 100; 109–111). Pfenninger (67) shows that using only one year of input data may not be enough to capture the probability distribution of wind and solar availability, and using multiple years may be required. He shows that this is especially important when using TSA. He points to the need for future research to integrate multi-decade time series into system planning. Others (31; 112–114) also evaluate system design considering time-series uncertainty. These authors also find that time-series uncertainty matters and is not accurately captured by a single year of data. Considering multiple years or in long-term planning cases decades of data is also important to capture extreme periods accurately. Extreme periods are important for planning problems and discussed in detail in Section 6.4.2.

The time step length Δt is the smallest unit at which temporal data is used in the full model. In the studies reviewed here, Δt is most commonly chosen to be one hour. This is due to many time-series data being reported at hourly resolution. Some studies also consider time step lengths of two hours (23; 58), three hours (6; 69), or 24 hours (58). Generally, time step length is a function of the characteristics of the optimization problem at hand. Priesmann et al. (115) investigate the effects of temporal resolution on model outcomes.

For TSA, several additional decisions have to be made: the length T of the periods, the number of representative periods $\hat{K}$, and more generally what features to use to select these periods.

The period length, i.e. the number of time steps T that one representative period consists of, also depends on the optimization problem at hand and its input data. Most commonly, hourly periods that span a day (e.g. $\Delta t = 1, T = 24$) are used, usually for problems that incorporate coupling constraints such as storage and ramping equations. Periods that span a single time step (e.g. $\Delta t = 1, T = 1$) are used in models without coupling constraints (19; 41; 58; 63; 66; 75; 97; 99; 101; 116). Such problems have an advantage in being able to be solved quickly due to the overall small number of decision variables, but lack the ability to track inter-step effects. is also indication that single time steps can provide good performance in models with coupling constraints (117). Several studies have tried to determine the optimal period length T (6; 17; 98). In summary, these studies conclude that T of one day is superior. On the contrary, longer period length such as 72 hours or 168 hours (1 week) result in significant increases in computational time (17) and perform worse in terms of total costs and percentage of load curtailed on an example generation capacity expansion problem (98). Methods exist to use period lengths of one day with interday storage (22; 68), described in detail in Section 6.5. These methods were found to be superior to using longer periods such as weeks.

To make the decision of period length T more systematic, Bahl et al. (58) identify periodic patterns in time series by autocorrelation (118). They calculate the autocorrelation functions per attribute, and identify periodic patterns by evaluating the normalized sum over all attributes of autocorrelation functions. They find this metric of autocorrelation

to be largest at one day and one week, which fits with known patterns of energy availability and human activity that drive energy demand and energy prices.

For a given period length T, there are also approaches to reduce the number of time steps per period. Instead of using all T time steps that a period consist of, Fazlohalli et al. (57) and Bahl et al. (58) propose to aggregate within the period so that each of them consists of $S \leq T$ segments. For example, a problem with single-day periods of length $T = 24$ one-hour time steps could be changed into periods of $S = 12$ two-hour time steps. The fewer segments one chooses, the less accurately ramp rates and within-period dispersion are represented. If these characteristics are not important, aggregating multiple time steps to segments can lead to savings in computational time without significant performance detoriation. The methods that have been developed to find within-period segments are described in Section 6.4.4.

Next, the modeler must decide how many representative periods $\hat{K}$ should be used to represent the original K periods. The number of representative periods $\hat{K}$ strongly influences computational complexity (see Figure 2). Typical numbers of representative periods are on the order of 5-30. A common approach to decide on the number of periods is using the "elbow method", where the number of periods is plotted vs. a metric of interest, and the chosen number of clusters is the point where the curve stabilizes (84). Stabilization of the curve means that adding more representative periods does not result in significant improvement in terms of the metric of interest. Commonly, the metric of interest plotted in such visual methods is a statistical error measure (SSE) (23) or optimization outcome (objective function value, design decision variables) (6; 16; 23; 25; 57; 67). Note that a stabilization in optimization outcome is not a guarantee that the optimization outcome with aggregated results actually resembles the optimization outcome with full input data. Bounding the error by use of relaxations (106) can be one way to gain more certainty in this regard (see Section 6.2 for more detail).

Lastly, the modeler must decide which features within the data are most important to represent during TSA. Most often, the original time series data are used as features (e.g., electricity prices, wind and solar availability factors). Several authors have used secondary features *derived* from the original time series data: Green et al. (62) use demand ramps as an additional feature, while Agapoff et al. (116) use price differences between nodes and Fitwi et al. (119) use moments. They also introduce hybrid features where generation, demand, and price are multiplied, and Almaimouni et al. (74) use principal component analysis to automatically extract salient features of the data for use in TSA.

6.4. Approaches 4: How do we find representative periods?

TSA is most commonly performed using clustering. Time-series data are grouped into clusters that are similar and each cluster is replaced by a single representative period. In some cases clustering is augmented by adding extreme periods (peak periods) that do not fit well within one of the clusters but whose properties may drive required investment. Including these extreme periods may be important for reliable system design.

How the relevant time series datasets enter the optimization problem has implications for TSA. Time-series data in the constraint body **A** or constraint right-hand side **b** impact the resulting design decision variables more directly (18), and the more binding the constraints with time-series data are, the more critical it is to represent these time series accurately. In those cases, inclusion of through extreme periods becomes more important. On the other hand, time-series data in the objective function coefficients **c** more directly influence the overall objective function value, and accurately representing its mean (e.g., through clustering) and variance is important.

6.4.1. Clustering

Applying clustering (120; 121) requires multiple decisions to be made, whether or not the practicioner is aware of such choices. Teichgraeber and Brandt (30) developed a framework (see Figure 7) for clustering specific to energy systems optimization that outlines these decisions. Figure 8 shows the most common choices within the framework made in the literature. The following elaborations follow the description in (30).

The three key decision steps of clustering are: (1) application of normalization, including the normalization operation and scope, (2) assignment method, including the distance measure dist(), the clustering algorithm, the center *c* selection, and (3) Representation methods, including methods to choose the representative periods and weights of each period. In the literature, authors often refer to the clustering methods they use by the name of the clustering algorithm (e.g. *k*-means clustering, *k*-medoids clustering, or hierarchical clustering). In contrast, we believe that it is important that every part of the clustering approach should be documented because every decision (implicit or explicit) can impact TSA outcomes and thereafter optimization outcomes.
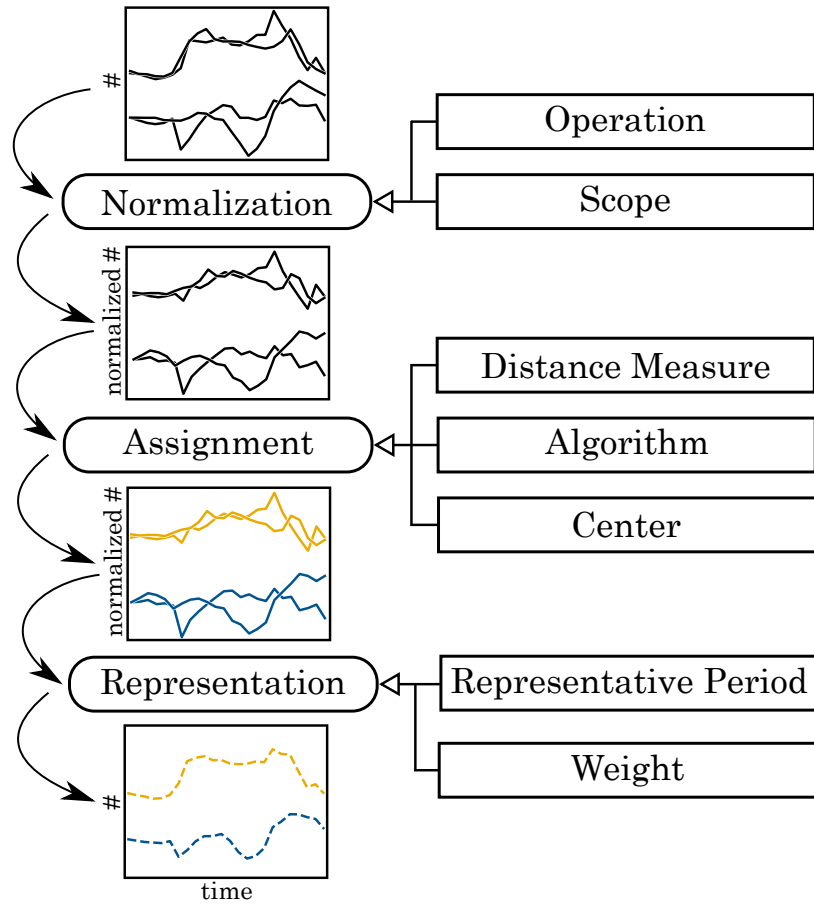
Figure 7: Framework of clustering methods for finding representative periods for the optimization of energy systems, adapted from Teichgraeber and Brandt (18). # stands for an attribute that is to be clustered (e.g. electricity price).

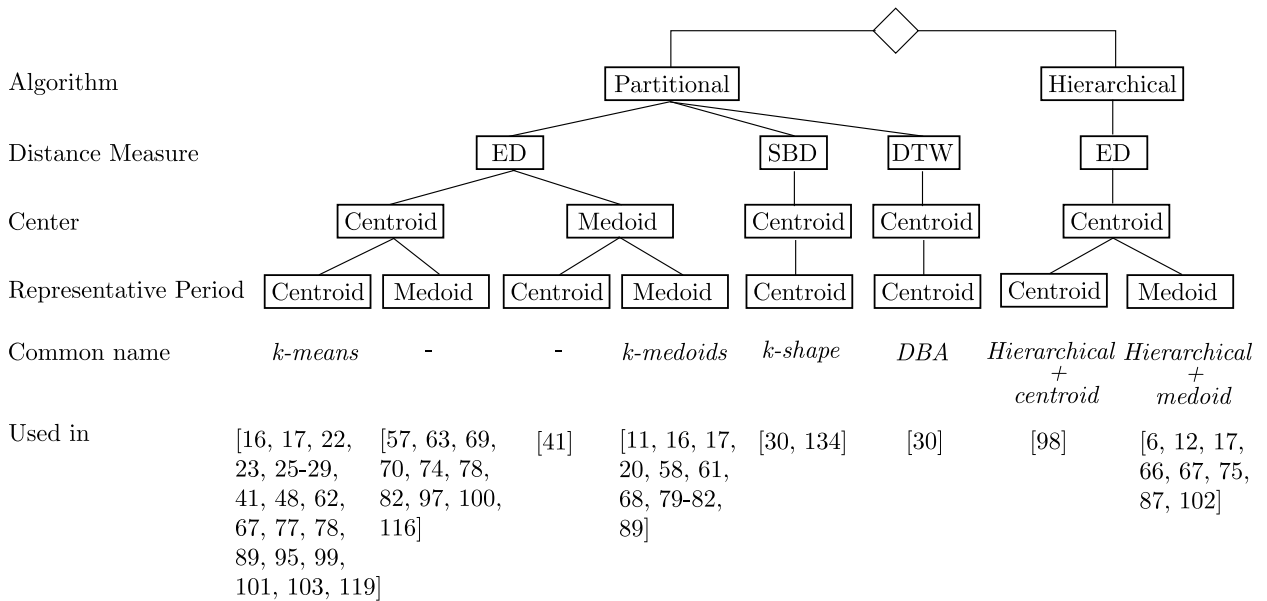|								
Algorithm			Partitional				Hierarchical	
Distance Measure		ED		SBD	DTW		ED	
Center		Centroid	Medoid	Centroid	Centroid		Centroid	
Representative Period	Centroid	Medoid	Centroid	Medoid	Centroid	Centroid	Centroid	Medoid
Common name	*k-means*	-	-	*k-medoids*	*k-shape*	*DBA*	*Hierarchical + centroid*	*Hierarchical + medoid*
Used in	[16, 17, 22, 23, 25-29, 41, 48, 62, 67, 77, 78, 89, 95, 99, 101, 103, 119]	[57, 63, 69, 70, 74, 78, 82, 97, 100, 116]	[41]	[11, 16, 17, 20, 58, 61, 68, 79-82, 89]	[30, 134]	[30]	[98]	[6, 12, 17, 66, 67, 75, 87, 102]

Figure 8: The most commonly used clustering methods in the literature categorized by choice of assignment and representative period.

The first broad set of decisions relates to timeseries dataset *normalization*. Normalization is necessary when using data with multiple attributes (e.g. wind, solar, and demand) that are often measured in different units and have quire different magnitudes. For example, clustering electricity demand measured in Wh (say, numbers of order 10^6 for an industrial facility) with solar insolation measured in W/m^2 (numbers of order 10^2 to 10^3) would result in over-weighting of demand during the clustering process due to the larger numerical magnitude of errors in fitting the data measured in Wh. For a problem with multiple time series to be co-clustered, this normalization step becomes vital. Multiple studies have investigated purposefully changing weights of different time-series attributes (9; 122), with the effectiveness of this method depending on the attributes at hand.

Three normalization operations are common: (1) no normalization, (2) normalization by the largest value, or (3) normalization to mean (μ) = 0 and standard deviation (σ) = 1 (often called *z*-normalization). See Teichgraeber and Brandt (30) for discussion of normalization methods in more detail. In addition to the operation used in normalization, one must also determine the normalization scope. There are three common options. (1) Full normalization scope (most commonly used). In this case, the full time series is normalized using a single normalization operation. For example,, one maximum or one mean and standard deviation per attribute are used to normalize the entire time series for that attribute. (2) Element-based normalization scope: each time step is normalized independently across all periods by computing the normalization operation for each data element (e.g., hour) and attribute. This will result in $T \times |\mathcal{A}|$ values for normalization operators (e.g., μ and σ). (3) Sequence-based normalization scope (also called period-based normalization scope): each period is normalized independently (e.g., resulting in 365 values of μ and σ per attribute for a year worth of data with daily periods). After the representative periods are generated, the normalization must be undone by denormalization so that the representative periods are expressed in the units of the original data (see Teichgraeber and Brandt (30) for additional details).

The second broad set of decisions to be made by the analysts regards the *assignment* of periods to clusters. Three decisions have to be made. First, each method requires a distance measure to represent goodness of fit of an observation to a cluster. For example, the Euclidean distance between an observation and the central cluster member. Second, clustering methods must use an algorithm to assign observations to clusters such as a partitional or hierarchical algorithm. Lastly, clustering methods vary in the cluster center choice with the two main options being the centroid or medoid of the cluster.

Distance measures (signified dist) compute the difference between two time-series vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^T$. The most common distance measure used is Euclidean distance (ED). ED represents distance between two time series using the l_2-norm

$$\text{dist}(\boldsymbol{x}, \boldsymbol{y}) = \text{ED}(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{\sum_{t \in \mathcal{T}} (x_t - y_t)^2} \tag{3}$$

Alternatively, one could use the Manhattan distance (based on the l_1-norm). Work has shown that optimization outcome using the Manhattan distance does not differ significantly compared to using Euclidean distance (63). Other distance measures are dynamic time warping (DTW) and shape-based distance (SBD), which take into consideration that the shape of two time-series vectors can be similar but shifted by a relatively fixed number of incremental steps. In DTW (123–125), similarity of the shape of two time series is determined by comparing stretched and contracted versions of the original time series. SBD (126) compares the shape of two time-series vectors by sliding one of them against the other. In cases where storage plays an important role, using shape-based distance measures to cluster periods can enhance performance because the shape of period variation can drive the benefits of storage systems and it is important that such patterns not get smoothed out by clustering periods together using mean-emphasizing measures like ED (30).

After the distance measure is determined, algorithms are used to assign elements to clusters. These algorithms are either partitional or hierarchical. Partitional algorithms in common use are generalizations of *Lloyd's* algorithm (127) and the *k*-means algorithm (128; 129). To begin, the cluster centers are initialized randomly. Then, the algorithm iteratively performs the following two steps until it converges (i. e., there are no changes in cluster assignments) or reaches a maximum number of iterations. (1) each period vector $\boldsymbol{x}_i$ is assigned to the closest cluster center $\boldsymbol{c}$ based on the distance measure dist:

$$C_1^* ... C_{\hat{K}}^* = \underset{C_1 ... C_{\hat{K}}}{\operatorname{argmin}} \sum_{k \in \mathcal{K}} \sum_{i \in C_k} \text{dist}(\boldsymbol{x}_i, \boldsymbol{c}_k)^2 \tag{4}$$
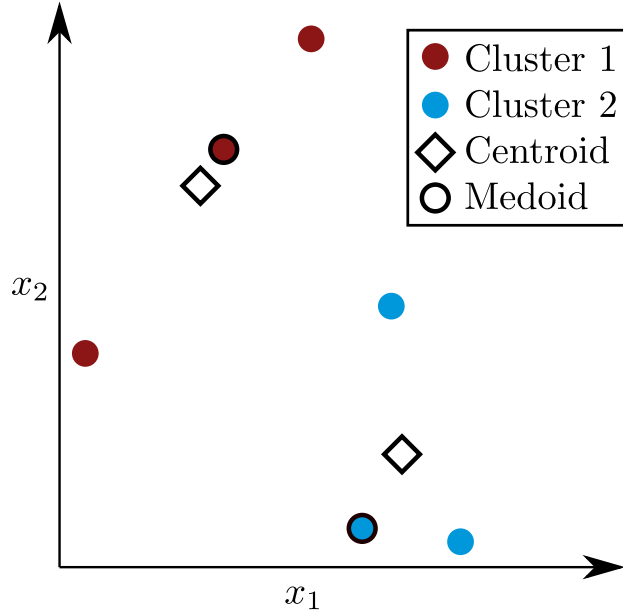
Figure 9: Illustration of cluster centroid and cluster medoid for two clusters with two-dimensional data.

Next, (2) the cluster centers c are updated in order to reflect the changes in cluster assignments. Each center is updated to the z that minimizes the within-cluster distance:

$$c_k = \underset{z}{\arg\min} \sum_{i \in C_k} \text{dist}(x_i, z)^2 \tag{5}$$

Cluster centers can be chosen as the centroid or medoid. The centroid is an artificial period $z \in \mathbb{R}^T$ that minimizes within-cluster distance, whereas the medoid is an actual period $z \in \{x_1, ..., x_N\}$ that minimizes within-cluster distance (see Figure 9 for an illustration). Partitional clustering with Euclidean distance as distance measure is commonly referred to as k-means clustering when the centroid is used as cluster center, and as k-medoids when the medoid is used as cluster center. The algorithm eventually converges and finds the cluster assignments C_k when no more updates are found that would reduce clustering error. The results from partitional methods are generally locally converged and depend on the random cluster initializations. Thus, it is usually best to initialize such processes with many starting points (e.g., by using k-means++ (130)) to ensure that a cluster assignment near the globally-best is found.

Hierarchical clustering starts with an initial assignment of $\hat{K}_0 = K$ clusters, then merges the two closest observations into one cluster, obtaining $\hat{K}_i = \hat{K}_{i-1} - 1$ clusters at iteration i. Merging two clusters is repeated until we obtain the desired number of clusters $\hat{K}$. This produces a hierarchy of cluster assignments. The hierarchy level with $\hat{K}_i$ clusters is the result of merging two clusters from the hierarchy level with $\hat{K}_{i-1}$ clusters (131). Ward's algorithm (132) is used to minimize the total within-cluster variance. In each hierarchy level, Equation 5 is used to calculate the centroid of each cluster k. Then, the Euclidean distance is calculated for all combinations of clusters and it merges the two clusters with the minimum Euclidean distanced. Hierarchical clustering is greedy, which means that it yields local solutions with sets of cluster assignments $C_1...C_{\hat{K}}$ that do not necessarily satisfy optimality in Equation 4, contrary to partitional clustering algorithms. However, hierarchical clustering is deterministic and thus reproducible. It is also computationally less expensive than partitional clustering.

The third step is *representation*. After clusters are determined, each cluster must be represented by a single representative period and an associated weight, allowing for the desired data reduction. In existing methods, both the cluster centroid and cluster medoid have been used to represent the cluster in the optimization problem. The assignment and representation steps are often connected but need not be. For example, the k-means clustering algorithm uses the cluster centroid as its center, and a natural choice is to represent the cluster with the resulting centroid. But the medoid could be used as well k-medoids.

For representative periods derived from cluster medoids, the weighted mean of the representative periods $r_1...r_k$ may be different than the mean of the full time series $x_1...x_N$. Thus, rescaling the medoid-based representations by a scaling factor s as introduced in (6; 17) is necessary in order to preserve the mean properties of the original data:

$$s = \frac{\sum_{k \in \mathcal{K}} \sum_{t \in \mathcal{T}} x_{k,t}}{\sum_{k \in \hat{\mathcal{K}}} \sum_{t \in \mathcal{T}} \omega_k \ r_{k,t}} \tag{6}$$

Many different combinations and variations of the above-mentioned normalization methods, algorithms, and representations have been applied in the literature. The most popular methods are hierarchical clustering (with the medoid as cluster representation), k-means clustering (with the centroid as the center and representation), and k-medoids clustering (with the medoid as the center and representation). Note that alternatively to being solved with the partitional clustering algorithm outlined initially, the k-medoids clustering problem can be formulated as a Binary Integer Program (BIP) as introduced by (133) and used by (61). The BIP formulation is generally NP-hard, but it can often be solved to near global optimality for real problems (30).

Kotzur et al. (17) compare k-means, k-medoids, and hierarchical clustering with medoid representation on three energy systems optimization problems and find that the choice of aggregation algorithm has only minor effect on optimal system design. But, the optimization error resulting from TSA was found to depend strongly on the system being optimized. Thus, they argue that it is important to evaluate clustering methods separately for each particular energy system model. Teichgraeber and Brandt (30) compare k-means, k-medoids, and hierarchical clustering with both centroid and medoid as the representation on operational energy system optimization problems. They show that centroid-based clustering methods represent the operational part of the optimization problem more predictably than medoid-based clustering methods. They show that using the full normalization scope is a good default for clustering and that shape-based clustering methods perform best with sequence-based normalization scope.

Two shape-based clustering methods have also been applied to energy systems optimization problems (30), dynamic time warping barycenter averaging (DBA) clustering (123; 124) and k-shape clustering (126; 134). These are partitional clustering algorithms that use less conventional distance measures – dynamic time warping and the shape-based distance – respectively. It was found that k-shape clustering can improve performance significantly over conventional clustering methods on problems that exploit intra-daily variability, such as battery energy storage problems (30). Furthermore, Liu et al. (76) introduce hierarchical clustering with minimax linkage and dynamic time warping as the distance measure to capture shape-based effects in the data of a CEP.

Table 3: Overview of extreme period inclusion methods used in the literature.

Selection process	Category	Identification measure		Calculation	Representation modification	Previously applied in
		Data type				
simple	statistical	single attribute		absolute	append	(22; 70; 135)
simple	statistical	multi attribute		absolute	append	(17; 57; 75; 79; 80; 82; 88; 89)
simple	statistical	single attribute		integral	append	()
simple	statistical	multi attribute		integral	append	(61; 67; 78)
iterative	optimization-based	infeasible periods		-	feasibility	(19; 20; 58)
iterative	optimization-based	slack variables		absolute	append	(18)
iterative	optimization-based	slack variables		absolute	feasibility	(18)
iterative	optimization-based	slack variables		integral	append	(18)
iterative	optimization-based	slack variables		integral	feasibility	(18)

6.4.2. Extreme period inclusion

In some design optimization problems, the representative periods obtained from clustering cause system designs to be unreliable (18; 46). This is true especially for optimization problems where the time-series data enter into constraints, such as cases where wind availability or solar availability strongly drive investment. In these cases, it is important to include extreme periods in order to reliably size the energy system to handle all conditions. For example,

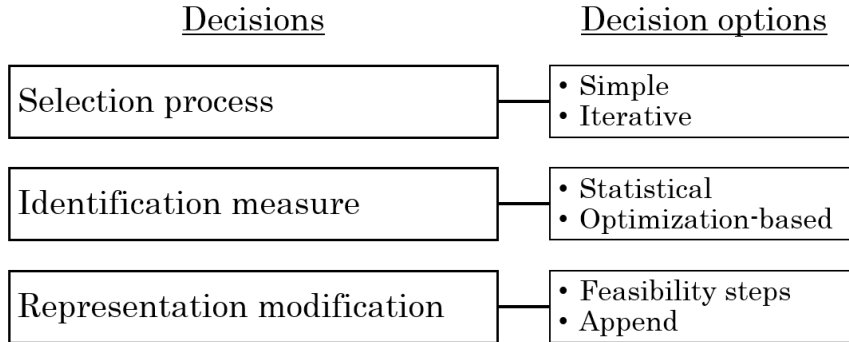| Decisions	Decision options
Selection process	• Simple • Iterative
Identification measure	• Statistical • Optimization-based
Representation modification	• Feasibility steps • Append

Figure 10: Overall framework for the inclusion of extreme periods when using clustered input data for the optimization of energy systems. There are three decision steps: the selection process, the identification measure, and the representation modification need to be chosen. Adapted from Teichgraeber et al. (18).

one might include the least windy and most windy day in the dataset to ensure that the system is feasible in those extreme days.

On the contrary, in cases where time-series input data occurs in the objective function (e.g. electricity prices) or where the constraints that input data occurs in are not strongly binding, smoothing extremes as part of a larger cluster of input data often does not significantly affect the system design (18).

Extreme events can be either added as single time steps, or as complete extreme periods with T time steps. As with representative periods in general, in the case of linkage of two successive hours (e.g. through storage or ramping constraints), it is important to consider complete extreme periods and not only extreme values. We consider complete extreme periods in the remainder of this section.

Identifying extreme periods is a *catch 22* kind of problem: Certain periods are important for accurately approximating the optimal system design of the full problem, but finding these periods requires knowledge of the optimal system design so that it is known what constraints will bind at the extremes. Thus, no non-trivial *a priori* method has been developed to find the extreme periods that are relevant for determining a sufficient system design. In place of such a general solution, iterative or approximate heuristic approaches to finding extreme days have been used instead.

Teichgraeber et al. (18) present a framework that describes the decisions to be made when using extreme periods. There are three decisions: selection process, identification measure, and representation modification. Figure 10 shows this framework and Table 3 shows the different methods that have been applied categorized by the decisions from the framework.

The selection process for extreme period inclusion can use a pre-defined number of extreme periods to be added beforehand ("simple" selection process) or iteratively add extreme periods until a criterion is met ("iterative" selection process). Criteria are often based on the optimization problem itself, e.g., that the identified system design based on the representative periods can meet demand in every time step of the full input data.

To identify extreme periods, data from the time series itself can be used, as can data from optimization results. As an example of the first approach, the time-step with the largest absolute value of the attribute of interest, e.g., the highest energy demand might be selected as a extreme day. In the case where one uses information from the optimization problem itself, one might select the day with largest demand satisfaction constraint violation.

Statistical properties used to identify extreme periods can be absolute extrema or integral extrema. An extreme period based on absolute extrema is the period that contains the maximum or minimum absolute value of the overall data within its T time steps. In contrast, an extreme period based on integral extrema is identified as the period that contains the maximum or minimum sum of values over the entirety of its T time steps. The first case may call for the highest wind hourly output in the dataset, while the second case would call for the highest overall wind output across a day.

Using information from the optimization problem itself to identify extreme periods relies on finding a system design based on the aggregated input data, and then to evaluate the performance of this design on the full input data (e.g. check if it leads to constraint violations like lost load). This is fundamentally an iterative approach.

The evaluation of the performance on the full input data can either be done based on whether there are infeasible periods within the full input data set (19; 20; 106), or based on slack variables that are additionally introduced in the problem with full input data (18; 46). Slack variables are virtual generation variables on the demand constraint that provide the unmet energy demand (also called lost load) the designed energy system cannot provide. One slack variable is added for each time-step where it can provide virtual power if needed, though at a very high cost. A possible extreme period thus can be selected as the period with the most extreme slack variable values. This is similar to finding statistical extremes: both absolute and integral extremes can be used.

Two main approaches have emerged that add extreme periods to the set of representative periods. The first is to add them with weight one in the representation (commonly referred to as "append" method (17)); the second is to add them with weight zero in the represetnation (commonly referred to as "feasibility steps" method (77)). Append adds extreme periods to the set of representative periods with a weight proportional to their occurence within the data ($\omega_k = 1$). If clustering is used to find the other periods in the set of representative periods, the clustering has to be re-performed on all periods less the extreme periods to ensure mean preservation. Adding representative periods with weight zero means that the periods are added to the set of representative periods without weight in the objective function ($\omega_k = 0$). If time series occur in the constraints, the extreme periods impact the design of the energy system through constraint satisfaction. However, there is no direct impact of the extreme periods on operating cost, and the extreme periods only indirectly impact the objective function by influencing the design decision variables. In this case, clustering only has to be performed once. Both "append" and "feasibility steps" preserve the mean of the original data:

$$\sum_{k \in \mathcal{K}} \sum_{t \in \mathcal{T}} x_{k,t} = \sum_{k \in \hat{\mathcal{K}}} \sum_{t \in \mathcal{T}} \omega_k \, r_{k,t} \tag{7}$$

Other methods proposed to find and add extreme periods are not preserving the mean and are thus not recommended (18).

Overall, different combinations of the above decisions have been used for extreme periods. It is not always clear from the literature which methods are used to include extreme periods, especially concerning the choice of absolute vs. integral extrema. The most common way to include extreme periods has been to add them through simple extreme period selection using statistical identification measures and append them to the set of representative periods, either adding one extreme period per attribute (22; 57; 61; 67; 82; 136) or only a single extreme period for electricity demand (70; 135). Several authors also use an iterative selection process with identification measures from the optimization problem itself (18–20; 58; 106; 137).

6.4.3. Other methods to find representative periods

Most of the methods to find representative periods that have been presented in the literature can be described by the frameworks for using clustering and extreme period inclusion methods that have been described above. Several authors have developed methods that aim to resolve the same challenges but are different in their general approach (59; 73; 74; 80; 82; 98; 104; 138).

Pineda and Morales (98) introduce a modified hierarchical clustering approach, with the aim to retain the chronology of the time series. The algorithm can be seen as similar to within-period segmentation, with one period for the full year, and we describe the method in more detail in the SI. Dominguez and Vitali (139) present an extension of this algorithm.

Almaimouni et al. (74; 138) apply principal component analysis (PCA) to find the relevant features within the data prior to using clustering. In time series data used as input to optimization problems, the n features are the number of time steps per period times the number of attributes, e.g. for a capacity expansion problem, n=3*24*1=72 in case of wind, solar, and demand data for clustering of daily periods with length of one hour and one region. The data is stored as a matrix $M \in R^{m \times n}$, where m are the number of periods. The idea behind PCA is to represent the data in a lower dimensional space $R^{m \times n^{Trunc}}$ by reducing the number of features that represent the data to n^{Trunc}, where $n^{Trunc} < n$. Note that this does not reduce the number of periods. In order to reduce the number of periods, clustering can then be applied on the resulting data in the lower dimensional feature space. The process is outlined in more detail in the SI. Similarly, Sun et al. (12) use Laplacian Eigenmaps to find relevant features prior to clustering.

Poncelet et al. (59) present another approach to select representative periods: an optimization based duration curve approximation. They minimize a self-defined statistical error measure that approximates the load duration curve of

each attribute, and they additionally include ramping information by considering the ramp load duration curves of each attribute. Both the representative period and the associate weight are variables in the minimization. Because the overall method works based on the load duration curve, which does not take into account temporal chronology, the approach is not applicable to systems with storage or other inter-time-step interactions. Furthermore, the authors point out that their approach requires significant implementation and computational effort compared to conventional clustering.

Another optimization-based approach was proposed by Zatti et al. (82). They find representative days and extreme days through the formulation of a mixed-integer linear program and bound the solution through a maximum deviation tolerance in terms of the load duration curve.

Recently, sampling based approaches have been proposed as well (104; 140–144). Hilbers et al. (104) propose using importance subsampling. Here, random sampling weighted by an iteratively-calculated importance based on the optimization problem itself is used to find time steps that are used for system design. The authors show good performance based on a system with 36 years of input data.

6.4.4. Within-period segmentation

Usually, temporal complexity is reduced by reducing the number of periods. Additionally, after representative periods have been identified, Fazlohalli et al. (57) and Bahl et al. (58) introduce within-period segmentation. In within-period segmentation, the T time steps within a period are aggregated to $\bar{T}_k$ segments, where $\bar{T}_k \leq T$. Note that each of the k periods can have a different number of segments, each of different length. The aggregation method developed by Pineda and Morales can also be seen as a case of within-period segementation (98). We refer to the SI for a more detailed description of these methods.

6.5. Approaches 5: How do we allow for linking of periods when using representative periods?

As noted above, the general approach to TSA assumes that the K or $\hat{K}$ time periods in a model can be treated as operationally independent. However, this assumption may not always hold, especially if long-term effects—such as seasonal storage—play an important role. In those cases, the order in which the cluster days appear matters to the overall problem, and thus the days cannot be each considered independently. Methods have been developed to maintain long-term temporal dependency within the model. In order to retain chronology, multiple approaches have been developed, such as: (1) modify the optimization problem formulation of the problem with representative periods (11; 22; 68), (2) use a so-called system states model that uses transition probabilities between different states (11), (3) use longer periods such as weeks (6; 17; 98), and (4) use a modified hierarchical clustering algorithm by only grouping neighbouring periods in order to preserve chronology (98) or by decomposition (145).

Gabrielli et al. (22) modify the optimization problem formulation by taking into account the sequence $\{k_1, k_2, ..., k_K\}$ of representative periods throughout the year, where k_i is the cluster number that period $i \in \{1...K\}$ belongs to. The core idea is that storage is modeled using all K periods, whereas all other aspects of the energy system are modeled using K representative periods. In order to do so, one has to replace the cyclic constraint that the storage state of charge (SOC) at the beginning and at the end of a representative periods have to be the same by a constraint that the SOC at the beginning and at the end of the year have to be the same. The temporal energy balance that relates charge and discharge of storage is imposed on the entire year (modeled using the index set $i \in 1...K$) instead of on each representative period ($i \in 1...\hat{K}$), and an additional constraint ensures that the SOC at the beginning of each period is the same as the SOC at the end of the previous period. This results in more operational decision variables ($SOC \in R^{K \times T}$ instead of $SOC \in R^{\hat{K} \times T}$) and more constraints and thus higher computational complexity, but it accounts for the effect that storage has on linking time periods to each other. This still will generally result in a much smaller model than one without the use of TSA where all aspects of the problem are in $R^{K \times T}$.

In another approach, Gabrielli et al. (22) recognize that binary variables are a major cause of computational complexity. In both objective and constraints, they model non-binary-related variables using representative periods, and binary-related variables using every hour of the year. The two types of decision variables are coupled using the sequence of representative periods.

Kotzur et al. (68) combine the first approach by Gabrielli et al. and the idea of multiple time grids introduced by Renaldi and Friedrich (146). Kotzur et al. use a superposition of two states to describe storage levels: the intra-period

state of charge SOC^{intra} (which is the conventionally used SOC with representative periods), and an additional inter-period state of charge SOC^{inter}. The storage constraints are modified as follows: There is one intra-period charging equation per representative period, and it remains the same as in the conventional representative period formulation:

$$SOC_{k,t+1}^{intra} = SOC_{k,t}^{intra}(1 - \eta^{self}\Delta t) + \Delta t(\eta^{char}\dot{E}_{k,t}^{char} - \frac{\dot{E}_{k,t}^{char}}{\eta^{dis}}) \tag{8}$$

where the different η are the self-discharge, charge, and discharge efficiencies of the storage technology, and $\dot{E}^{char}$ is the charging power and $\dot{E}^{dis}$ is the discharging power in a specific time step. Because the inter-period SOC accounts for long-term storage levels, the intra-period SOC is zero at the beginning of each period:

$$SOC_{k,1}^{intra} = 0 \tag{9}$$

One inter-period SOC per period of the original sequence is introduced. The inter-period SOC of each consecutive period $i + 1$ depends on the previous period i's inter-period SOC and on the intra-period state of charge at the end of the corresponding representative period k_i, which is the overall difference in SOC throughout the day:

$$SOC_{k,t+1}^{inter} = SOC_{k}^{inter}(1 - \eta^{self}\Delta t)^T + SOC_{k_i,T+1}^{intra} \tag{10}$$

Furthermore, the daily cyclic constraint is replaced by a yearly cyclic constraint:

$$SOC_{K+1}^{inter} = SOC_1^{inter} \tag{11}$$

The authors show that their approach improves performance in terms of optimization outcome, but comes at a computational cost additional to the cost of conventional representative period formulation. However, the computational cost is still significantly lower than that incurred by solving the problem with the full time series as input data.

Some studies have analyzed the effects of including longer periods such as representative weeks. Overall, longer periods come at a high computational cost that seems not to be worth the trade-off (6; 17; 98). Modifying the storage constraints of the optimization problem formulation as described above seems to be the most promising approach.

7. Conclusions, best practices, and opportunities

Time-series aggregation has been used in the context of many different applications and research questions. The goal is to create a reduced data set of time-varying input data that retains all relevant characteristics of the original data set but results in models that are much easier to solve. Representative periods are the most commonly used time-series aggregation method in the literature. We have identified the two major steps taken when using representative periods: (i) Cut the original time series into K operationally independent periods, and (ii) aggregate several periods and represent them by one. This comes with the assumptions that (i) long-term operational interactions can be neglected, and (ii) it is possible to retain all relevant characteristics of the original problem during aggregation.

Based on these assumptions, we have laid out several challenges that arise when using representative periods and approaches that have been developed in the literature to deal with these challenges. The challenges are: (1) there will always be some error due to clustering, (2) how to measure error/success of a set of representative periods, (3) how to model temporal resolution, (4) how to find the representative periods, and (5) how to allow for linking between periods.

In summary, we recommend the following best practices when using time-series aggregation:

- Performance should be measured in terms of optimization outcome.

- Performance should be validated by solving the model at least once on the full time series, if at all possible.

- Aggregation methods and optimization problem formulation should be used based on the problem and data at hand:

    - Use clustering to find several periods that form the core set of representative periods. Clustering preserves basic statistical properties of the data, such as the mean.
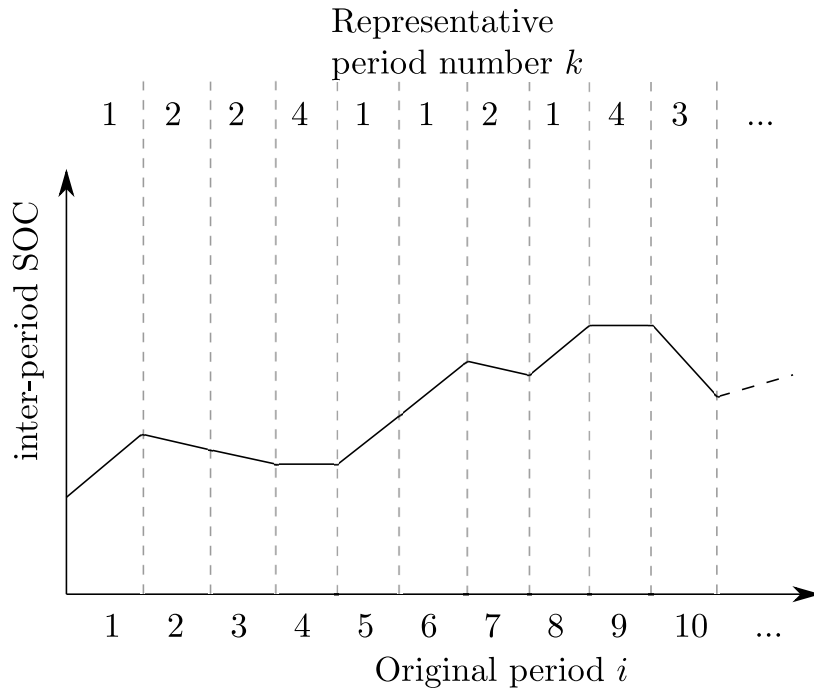
Figure 11: Seasonal storage modeling using the superposition of intra-period and inter-period states. The long term storage state of charge (inter-period SOC) of each consecutive period i depends on the previous period's inter-period state of charge and the difference in intra-period state of charge of the corresponding representative period k. Note that periods i with the same representative period k have the same slope in terms of intra-period state of charge. Figure adapted from Kotzur et al. (68), numbers for illustrative purposes only.

    – Use extreme periods when time-series data occurs in constraints and when these constraints are likely binding. This is often the case for problems that include system design.

    – Modify the aggregated formulation of the optimization problem by linking periods if storage is likely important.

- Be extra careful with wind data. Aggregation has been shown to smooth out a lot of important variability.

- Consider bounding the error in the objective function.

Time-series aggregation for the optimization of energy systems is a relatively new research area, and we have identified several opportunities based on the challenges and approaches described above:

- Developing upper and lower bounds on objective function value that bound the aggregation error in terms of optimization outcome. Developing these bounds can be both by development of general mathematical programming theorems, and application specific.

- Interconnection of different fields of research across applications. Based on the research question at hand, methods have mostly been developed individually for specific applications. However, these methods are often applicable to other applications, or similar to methods developed for other applications.

- Additional application areas. TSA methods have mostly been developed for two-stage energy systems optimization problems. There will be additional areas of application, both in terms of the specific two-stage problem at hand (e.g. electric vehicle charging infrastructure), and in terms of broader application areas such as using representative periods in operational contexts by developing operational strategies for typical days, or aggregating repetitive operating conditions for use in model predictive control.

- Use more data. Most of the work has been done using one year of data, even though systems are often designed for decades into the future. Finding representative periods from decades of historical weather data is thus beneficial for robust system design, and new methods need to be developed to do so.

- The great majority of methods is validating TSA results based on in-sample methods. The robustness and quality of decisions will be increased with the development of out-of-sample methods.

Acknowledgments

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