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Review of Forecasting Univariate Time-series Data with Application to Water-Energy Nexus Studies & Proposal of Parallel Hybrid SARIMA-ANN Model

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Problem Report submitted

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ABSTRACT

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The necessary materials for most human activities are water and energy. Integrated analysis to accurately forecast water and energy consumption enables the implementation of efficient short and long-term resource management planning as well as expanding policy and research possibilities for the supportive infrastructure. However, the integral relationship between water and energy (water-energy nexus) poses a difficult problem for modeling. The accessibility and physical overlay of data sets related to water-energy nexus is another main issue for a reliable water-energy consumption forecast. The framework of urban metabolism (UM) uses several types of data to build a global view and highlight issues of inefficiency within the network. Failure to view the whole system contributes to the inability to comprehend the complexity and interconnectivity of the issues within the system. This complexity is found in most systems, especially with systems that must be able to support and react to vacillating human interaction and behavior.

One approach to address the limitations of data accessibility and model inflexibility is through the application of univariate time-series with heterogeneous hybrid modeling addresses. Time-series forecasting uses past observations of the same variable(s) to analyze and separate the pattern from white noise to define underlying relationships to predict future behavior. There are various linear and non-linear models utilized to forecast time-series data sets; however, ground truth data sets with extreme seasonal variation are neither pure linear nor pure non-linear. This truth has propelled model building into hybrid model frameworks to combine linear and non-linear methodologies to reduce the fallacies of both model frameworks with the other's strengths. This problem report works to illustrate the limitations of complex WEN studies, build a timeline of hybrid modeling analysis using univariate time-series data, and develop a parallel hybrid SARIMA-ANN model framework to increase univariate time-series analysis capabilities in order to address previously discussed WEN study limitations. The parallel Hybrid SARIMA – ANN model performs better in comparison to SARIMA, ANN, and Series hybrid SARIMA-ANN; and shows promise for research expansion with structure flexibility to expand with additional variables.

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List of Abbreviations

ACF	Auto-Correlation Function
ADF	Augmented Dickey-Fuller
AI	Artificial Intelligence
ANN	Artificial Neural Network
ARIMA	Auto-Regressive Integrated Moving Average
DOE	Department of Energy
EIA	Energy Information Administration
kWh	kilowatt hours
LCA	Life-Cycle Analysis
LEAP	Long-range Energy Alternatives Planning
PACF	Partial Auto-Correlation Function
PHSA	Parallel Hybrid SARIMA-ANN

PP	Phillips-Perron test
SARIMA	Seasonal Auto-Regressive Integrated Moving Average
UM	Urban Metabolism
WEAP	Water Evaluation and Planning
WEN	Water-Energy Nexus

Acknowledgement

"How we live is so different from how we ought to live
that he who studies what ought to be done
will learn the way to his downfall
rather than to his preservation"
-Niccolò Machiavelli

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Chapter 1. Introduction

This problem report works for viewing urban metabolism (UM) through the scope of water-energy nexus (WEN), limiting variables to reduce the complexity of system modeling. The basic underpinnings of UM struggle with the ability to efficiently tether human interactions with the impacts on the surrounding environment in order to understand, govern, and implement resource management strategy and long-term policy. A UM model integrates and evaluates many factors from physical, technical, and social interfaces that contribute to the consumption and production of various resources and energy as well as the relationship between the resource and energy [1]. The framework of UM uses several types of data to build a global view and highlight issues of inefficiency within the network. As Kenway [1] illustrates, failing to view the system-wide issues contributes to the lack of ability to "understand the emergence of complex and wicked problems; problems which are ever-changing and are highly interconnected with action that could be taken." This complexity is found in most systems, especially with systems that must be able to support and react to vacillating human interaction and behavior. City planners and managers, traffic and civil engineers, and others must interpret complex data sets and determine solutions while taking into account ripple effects from implementing those strategies. Without a proper validating model, this process is near impossible to evaluate.

Supporting human activity in an urban environment has historically been dependent on maintaining the network of water resources. Despite advancements in technology and the design of modern infrastructure, a quarter of urban centers with a totaling $4.8 ± 0.7 trillion in economic activity, remain water stressed due to environmental and economic limitations [2]. The water-related challenges impacting the sustainability of urban areas include the lack of access to safe water and sanitation as well as acts of God such as floods and droughts [189]. Improper management has enormous consequences on human health and well-being, economic growth and development, and the environment. One of these management areas centers around the water-energy infrastructure. The integral relationship between water and energy, WEN, poses a difficult yet vital problem to model. The WEN is the relationship between the amount of water used to generate and conduct energy and the amount of energy in the collection, distribution, and processing of water [3, 4, 5]. In other words, the relationship is based on the resource production-consumption tradeoff.

1.1. Problem Statement and Needs

Modeling the links between water and energy classifies significant research and development directions, advancement possibilities for technological and management innovation, and implications of institutional decisions and actions [6, 7, 8, 9, 10]. There are many studies suggesting strategy and policy changes that would result in decreasing water-energy consumption values. However, Mitchell [11] identifies a lack of ability to accurately monitor and analyze data through case studies in Australia to measure the efficacy of those changes. Without the integration of systems—organizational networks and physical infrastructure - there is no way to precisely report system efficiency at its current capacity nor the impact of a future policy or implementation of new technology.

This issue centers around the inability to share and integrate data from these sectors. This feeds into an unsolvable loop, where change is necessary in order to effectively collect data that can be used to steer change. There have been many problems identified with data sharing in general [12], which include unstandardized data platforms and inconsistent formatting in time and spatial scales. For WEN data sharing limitations, [1] identified issues with "data detailing directional flow and linkages" for water and wastewater as well as daily population fluctuations within the boundary. The lack of coherence in water and energy sector datasets, specifically platform standardizations and physical infrastructure overlay, restrict the scope of all WEN studies.

The first step in understanding the relationship between water and energy consumption is to model and forecast the patterns of a single variable over time. This requires separating the two resources for analysis before conjoining their consumption patterns. Before the development of a complicated multivariate model, univariate time-series forecasting through a middle-out approach allows one to understand what will happen without explaining how it is happening. The resulting predictive model serves as validation for alternative models produced through top-down or bottom-up approaches. Time-series forecasting uses past observations of the same variable(s) to analyze and separate patterns from random error to define underlying relationships in order to predict future behavior [13]. Applications include: economic forecasting, material and operations planning, and model and strategy evaluations. These applications vary by time-series forecast horizon and model approach, both dependent on the data set(s) available.

There are linear and non-linear model methods utilized to forecast time-series data: engineered (simple and complex), statistical, supervised machine learning, and hybrid models. However, real-world data with extreme seasonal variation is neither purely linear nor pure non-linear. This reality has propelled the main motivation of this study. The expansion of time-series analysis model building into hybrid frameworks combines linear and non-linear methodologies in order to reduce the fallacies of both frameworks with the strengths of the other. Systems engineering requires gaining understanding through a correct approach to the data and the issues [14]. Most WEN studies fall under either top-down or bottom-up analyses and are limited to the aspects of understanding or governing decisions [1]. A middle-out model approach combats the afflictions of WEN studies data limitations and availability by reducing variables necessary for analysis to water or electricity consumption over time. The model proposed in this report addresses both of these limitations with the ability to be applied across any field of study.

1.2. Research Objective and Scope

The objective of this problem report is to explore the limitations of urban metabolism and suggest a feasible solution through the scope of WEN. In order to address the data inaccessibility and model inflexibility inherent in these studies, this document explores the possibilities of a univariate time-series model with a middle-out approach to use limited data for global conclusions. With limitations in data accessibility, a middle-out approach through univariate time-series forecasting proves to be advantageous as a first step to establish a predictive model. The limitation of model adaptability to allow for future expansion on the univariate validation model is reviewed through the implementation of heterogeneous hybrid modeling. The specific aims for this report are:

- Understand the methodologies and conclusions of past studies.
- Explore the various model approaches: top-down, bottom-up, and middle-out.
- Address the limitations of data inaccessibility and model inflexibility.
- Discuss the advantage of univariate time-series forecasting models.
- Research the development of univariate time-series forecasting models.
- Assert heterogeneous hybrid modeling of univariate time-series forecasting as the answer to limitations of past urban metabolism and WEN studies.

1.3. Report Organization

The first chapter of this report (2) will explore the study of urban metabolism and the framework used to explore the WEN issues. This will be followed by the four themes that unify research within urban metabolism: 2.1) sectoral analysis, 2.2) boundary conditions, 2.3) methodologies to quantify water-energy link, and 2.4) adaptive approaches to solutions. These themes highlight the conclusions and limitations of past studies. Chapter 3 discusses the existing models to forecast water and energy consumption broken down further into types of data and approaches available. The combined discussion of past study limitations and current existing models leads to Chapter 4 univariate time-series forecasting. The limitations discussed in previous chapters filter the model choices to heterogeneous hybrid univariate forecasting models. In Chapter 5, the parallel hybrid SARIMA-ANN model developed through this research is presented with the case study data used to illustrate the model build and performance. Future work is discussed with the possible expansion of this study with the proposed model in mind. Chapter 6 is the conclusion of this research.

Chapter 2. Urban Metabolism and Frameworks for Water-Energy Nexus Issues

Urban metabolism (UM) is "the total of the technical and socio-economic processes that occur in cities, resulting in growth, production of energy, and elimination of waste" [15]. Marx [16] first deliberated UM with his assessment of industrialization in 1883 and described metabolism as the material and energy exchanges within the environment or system. The simplest definitions consider the mass balances of all materials of the urban system [17]. The complex definition considers the city as an organism [18, 19]. Urban metabolism analysis requires quantifying the overall mass fluctuations and linkages of selected resources within a designated city boundary [17, 18, 19]. Witnessing the degradation of human wellbeing and the environment within the urban center, Wolman [18] developed the UM accounting exercise with a top-down relationship between resource consumption and the production of goods and wastes. He concludes that the expansion of a city causes a conflict of interest with the natural environment and socio-economic system. This conflict extends into the concept of urban sprawl, where Wolman's conclusion is reinforced with further studies on the impact of unrestricted, unplanned urban growth [20, 21, 22]. System friction due to increasing physical distance decreases the efficiency and stability of the system. As resource demand from the urban area periphery grows, the entire area is subjected to become a resource desert with detrimental impacts on the environment as well as the citizens within the system.

The intricate balance of resource supply-demand illustrates the magnitude of UM study, where the stability of the social fabric and political decisions are affected by the connection and management of resources—such as water and energy—within and around the city [23]. The concept of UM defines a methodical framework to help model this balance. The UM framework unifies research themes as follows: 1) categories of study to allow sectoral analysis for a hierarchical approach to research; 2) explicitly identifies the system's boundary conditions; 3) analyzes mathematical modeling approaches to integrate data for water-energy links; and 4) allows for an adaptive approach to sustainable solutions for policy and technology with respect to the consequences of implementation [24]. The following sub-chapters will break down each of these themes.

2.1. Sectoral Analysis

The complexity of UM studies propels scholars to focus on a simpler, singular flow of essential materials such as water [25, 26, 27] or energy [28, 29, 30, 31]. Although focused on a singular flow, these studies remain complex and require extensive investigation with large quantities of data. Access to water and energy is necessary for most modern human activities and general society's well-being [32]. City centers are heavily reliant on water resources and tend to pull resources from the surrounding region or periphery [33]. Resource pools of water and energy are becoming strained increasingly due to a growing population, effects of the phenomenon known as climate change and aging infrastructure. The expansion of the system to reach further into the periphery is not sustainable or resilient [21, 22]. Increases in resource distance to end-use will lead to increases of friction in the distribution of the resource and associated wastes. When accessibility to a vital resource, such as water, is constrained or damaged, ripple effects can be seen economics, environment, and social fabric of the city [34]. In order to understand the connections between societal conflict and water resources, the Pacific Institute [35] categorizes events related to water conflict through an interactive map and chronology. The integral relationship between water and energy, water-energy nexus (WEN), poses a difficult problem to understand and model; and, therefore, issues for resource governing and planning. In order to create an efficient system for tethering humanity and their interactions with the environment, a framework should integrate and evaluate numerous factors from technical and social interfaces that contribute to the consumption of water and energy.

A broad literature review of WEN study objectives illustrates the absence of detailed research and policy priorities. This spurred the development of numerous WEN studies on various scopes and scales in the early 2000s. Research in WEN has been done in the United States and Australia [1, 36, 37, 38]. Based on this research, the policy has already been implemented in at least nine states that include Arizona, California, Colorado, Connecticut, Nevada, South Dakota, Washington, West Virginia, and Wisconsin. These states have statutes that mention the annexation of water for energy production [39]. These laws mention the importance of recognizing the relationship and the need for appropriating resources accordingly.

The National Energy-Water Science and Technology Roadmap developed by the Department of Energy (DOE) outlines the efforts to remove barriers toward sustainable, efficient water and energy use, overcome current technological obstacles, and improve familiarity with the conceptual relationship between energy and water resources [40, 41]. Consequently, the Roadmap aims to establish short- and long-term water-energy security through a coordinated and integrated DOE approach. The short-term security calls for accurate mapping of resource supply-demand patterns. Long-term security requires effective implementation of policy, research, and technology for water-energy resource utilization. An Energy-Water Nexus Crosscut Team was formed in 2012 to advance this DOE approach through working on the following four areas of focus: integrated data, modeling, and analysis of the WEN; technology research development, demonstration, and deployment to support energy-efficient water systems or water-efficient energy systems; policy analysis for energy and water sustainability at the regional or national scale; and outreach and stakeholder engagement to strengthen the proposed activities.

These studies illustrate the dire need for understanding and identifying WEN but do not explain the complications. Water and energy are essential material products that have complex characteristics: storage, production, and transportation are difficult and costly. Both energy and potable water must be produced and consumed as demanded. Emergy is the available energy used directly or indirectly to produce and distribute material or service. The development of emergy metabolism allows a combination of numerous material flows into one value [42, 43, 44]. It follows that emergy values on products increase as the distance between production and consumption increases. This value quantifies why urban sprawl (unregulated expansion of the city's boundary) is unsustainable. The process of transforming various products into an emergy value is difficult and varies from study to study. The infrastructure of production, distribution, and consumption of water and energy sets the boundary of study and enables the study of how people are connected to the area.

From this end-user perspective, water efficiency measures conserve water and energy resources simultaneously [45, 46, 47, 48, 49]. From a producer perspective, the cooperation of demand management programs for water and energy utilities is much more difficult to achieve as both can be owned by several entities across varying spatial scales. The water-energy infrastructure seldomly overlaps, and management strategies have conflicting goals. According to the Energy Information Administration (EIA), utility systems are owned by private investors, federal and other public entities, or cooperatively owned [50]. This explains the difficulty in the integrated planning, development, and organization of water and energy systems, which have been historically under the control of different agencies [4, 51], as seen in **Figure 1**. Private and public stakeholders on multiple scales with different goals, ranging from economic and political gains to environmental and social wellbeing, must be presented with a variety of plans that accurately depict trade-offs for all parties [12, 52]. A politically charged process such as this would require accurate models to make justified and educated decisions.

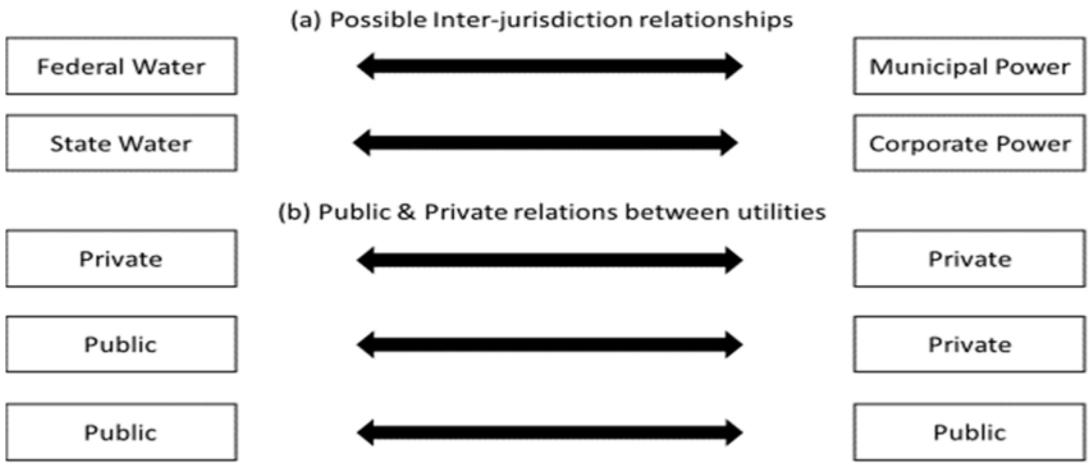

Figure 1. Arrangement of utility management. Adapted from [12].

The next scope of WEN studies is based upon circumstantial dependency. There are three established perspectives of WEN [53]:

1) Energy use of water infrastructure for water service.
2) Water use of energy infrastructure for power generation.
3) Nexus of the urban system, where system changes impact energy or water consumption.

This circumstantial dependence is the pivotal issue, creating a conflict of interest and difficult sets of trade-offs in strategy selections such as: private versus public services to supply energy and water, centralized versus decentralized infrastructure, pricing mechanisms, and facility placement. Organizational arrangements of utilities are one of the complications for data collection as well as integrated management and planning. These are issues with the first and second established perspectives. The third perspective is intricate, with multiple variables to consider. These contradictions and limitations require a simplified method of analyzing and correlating water and energy consumption data in order to step forward. The cooperation of government, industry, research, and community is necessary to address the challenges of efficient planning and implementation of the policy. This challenge of planning, funding, regulation, data management and sharing, target setting, and study requirements are summarized in **Table 1**, adapted from [1].

Table 1. Current water-energy nexus challenges and address of these challenges.

Current WEN Challenges	Addressing WEN Challenges
Management of water and energy performance is done separately. Planning, funding, regulation, and standards for water and energy are made separately; therefore, trading challenges between sectors.	Comprehensive and cooperative management of water and energy sectors through a governance framework to ensure systematic efficiency.
Methodologies for WEN studies are either inconsistent system boundary definitions or do not consider defining the system boundary.	Standardized methodologies will lead to venerated practices and policies.
Data sets and monitoring are inconsistent.	Coordinated data sets and monitoring systems enable a variety of analysis and management strategies. Management responses are cooperative, understanding how each decision impacts the other sector.
Unquantified indicators of urban performance or limited performance indicators that provide poor guidance for policy; analysis frameworks inconsistently applied.	Identification of quantified indicators that simultaneously consider water, energy, and related flows to model and implement policy.
Optimization analysis for the urban area for overall water and energy efficiency is absent.	Optimization studies will contribute to the community planning and assess the efficiency of implemented strategy and policy to allow for effective step-by-step adjustments.
Targets for urban systems are missing or unquantified.	Quantified targets for resource efficiency of cities through the joint effort of government, industry, resident, and commercial sectors.

The challenges in **Table 1** can be summarized in the inability to efficiently collect and analyze water-energy data. These originate from two main issues: 1) unstandardized data platforms between water and energy sectors and 2) inflexible model frameworks for management and efficiency evaluations [1, 11]. Further illustrated in **Figure 2**, the challenges of WEN studies provided in **Table 1** disseminates from the raw data from both sectors with inaccessible and unstandardized data platforms. These issues feed into WEN studies with inconsistent boundary definitions and lack performance indicators to determine the efficiency of implemented plans. The challenge presented by raw data feed into the WEN study and management response, wherein the data complication feed-back into the insoluble cycle.

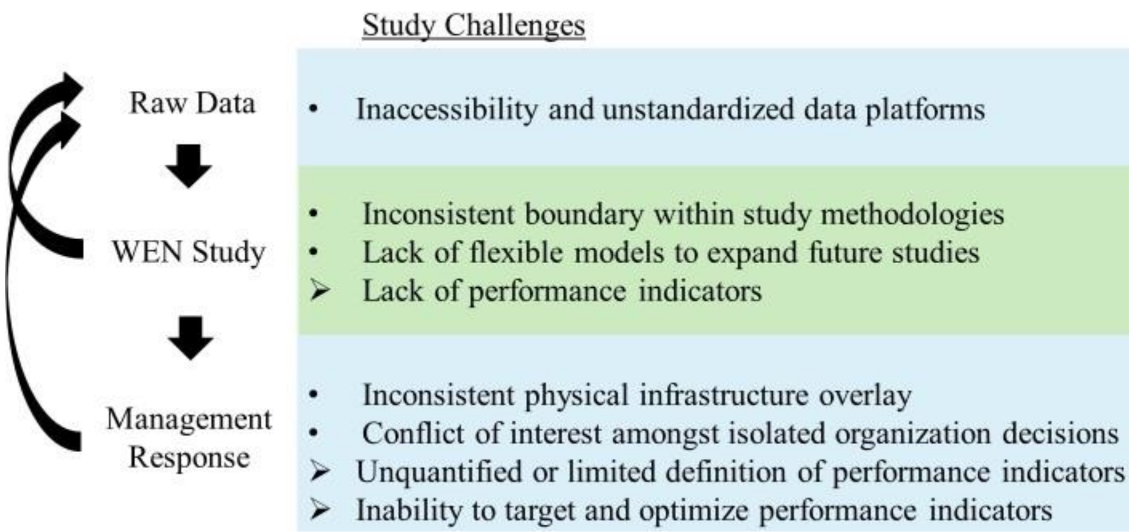

Figure 2. Dissemination of WEN study challenges

2.2. Boundary Conditions

The scope of a study relies on defining the boundary of a system. With the system boundary condition as "a critical first step to modeling analysis," there is an understanding that the scale of study defines the function and purpose of the analysis [54]. Numerous authors note the significance of system boundary to research conclusions [19, 48, 55, 56]. This helps to highlight the strength of the urban metabolism framework in a distinct system boundary leading to strong diagnostic options. The scale of the study will also reveal the data accessible and the type of framework that is applicable for such analysis. **Figure 3** illustrates how WEN studies vary from global to local scales with different functions, purposes, and types of framework. An overall review of various studies organized by dimension and scale is further discussed in the following subchapters. The following subchapters review past studies at each scale. Kenway [7] reviews each of these much more thoroughly with the methodologies utilized by each study.

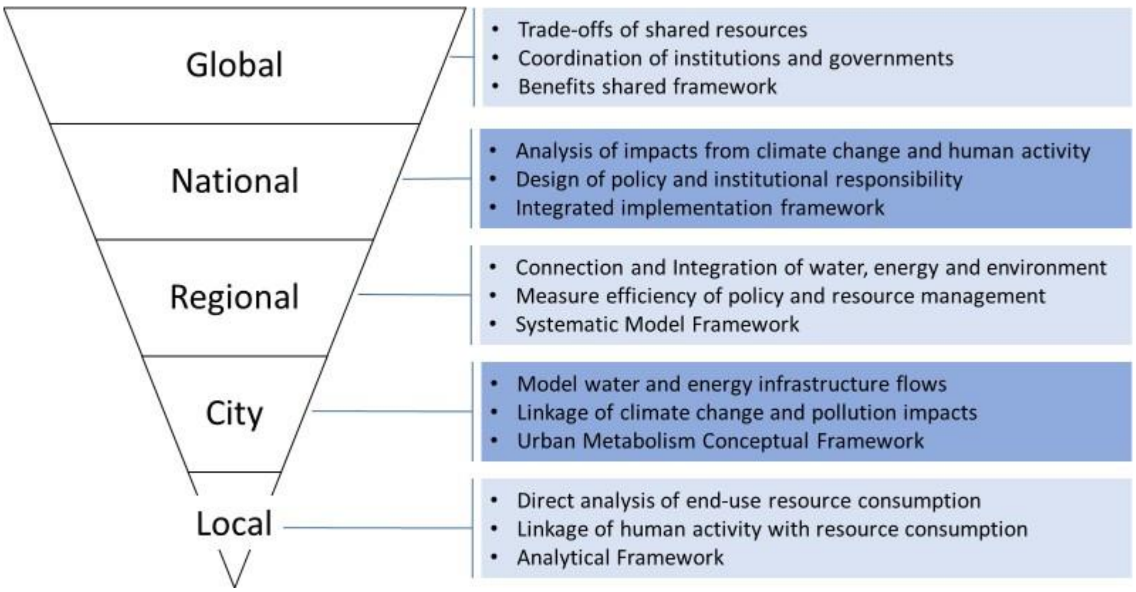

Figure 3. The scale of the study focusing on WEN. Adapted from [57].

2.2.1. Global

Resource management is complicated as resources impact multiple stakeholders or interested parties. The crux of coordinating across one or more international boundaries lies in balancing socio-economic needs and environmental sustainability for more than one ruling party [57, 58]. This is commonly done through a benefits shared framework. International WEN conflict is often found in transboundary river basins and watersheds. Examples of nexus model frameworks centered around the Mekong River Basin [58, 59, 60], Euphrates-Tigris river basin [61], and the Amu Darya Basin of Central Asia [62] were all proposed to demonstrate cost-benefit values amongst countries. These studies provide a basis for international cooperation and mediation with proposals to enacting international laws under the guise of similar interest in resources [63]. The

Trans-Pacific Partnership (TPP) is a recent attempt at incorporating economic interests with environmental regulations on water and energy sectors, among many other sectors [64].

2.2.2. National

The main goal of WEN studies at a national scale is to connect decision-making to efficiencies of water and energy resources. Policy and institutional arrangement reviews are performed to improve the management of the resources. Key challenges to be addressed in these studies at the national level include: water scarcity, irrigation pressure, climate shift, and resource stock capacity [1, 65, 66, 67, 68, 69, 70, 71, 72, 73]. The end goal for WEN studies at the national scale is for governing and management assessments for resource management. As discussed in Chapter 2.1, the National Energy-Water Science and Technology Roadmap developed by the Department of Energy (DOE) frameworks the steps to define and comprehend WEN, but there is difficulty in uniting policy through various state governments [40, 41]. Countries such as Italy, Zambia, Saudi Arabia, Australia have all made similar strides to establish national programs. The majority of programs remain in the initial stages of human and climate impact analysis with attempts toward implementing national policy and institutional changes [74, 75, 76, 77].

2.2.3. Regional

Regional-scale WEN studies investigate the connections of water and energy consumption used for urban areas and the impacts on the peripheral area. Long-term regional water and energy resources management strategies are assessed with the inclusion of the raw water source and the main areas of consumption and wastewater production. This scale allows for the connection and integration of water and energy with the surrounding environment. Stepping further than national studies, the regional scale enables policy and management strategies to be tested for efficiency. The methodological frameworks established within some of these regional studies, specifically in California and Australia, include: Water Evaluation and Planning (WEAP), Long-range Energy Alternatives Planning (LEAP), regional scale-integrated WEAP and LEAP, and the integrated model framework of New South Wales [78, 79, 82, 81]. These frameworks employ a methodical approach with the aim to support efficient policy implementation and strategy development by illustrating trade-offs [57].

2.2.4. City

The connection between the studies of UM and WEN collides at the scale of the city. The city is illustrated as a focal point of resource flows [1, 57]. Urban centers permit a representable scope for solving several problems of resource efficiency with extensive, interchanging flows of water, energy, and materials within urban areas. Cities are the center of financial and research ventures with continued redesign and development of infrastructure [1]. The loose definition of the city leads to the difficulty of using it as a proper boundary. Within the largest cities, Satterthwaite [55] identifies four different boundaries: city core, contiguous built-up area, metropolitan area, and extended planning region. The increase in population and resource demand within cities is becoming an issue for current infrastructure design. Giradet [82] states cities are only expected to grow;

> "By 2030, 60% of the world population, or 4.9 billion people, are expected to live in urban areas. In developing countries, as villagers move to the city, per capita, resource consumption typically increases fourfold. Cities located on 3-4% of the land surface use 80% of its resources, and discharge the bulk of the solid, liquid, and gaseous waste."

At the city scale, research has lacked to link resource "flows to policy frameworks at multiple scales, from local to international" [83]. Understanding the flow of material through various factors that influence innovation and development of effective sustainability policies include: "political, demographic, economic, and geographical" [83]. The city boundary provides an intermediary connection between global and local consumption. This allows an overview that includes detailed information, a method that connects policy to local implementation. Numerous studies illustrate that water is the limiting factor for the sustainability of a city [18, 19]. It is a central feature of infrastructure design that has a singular focus despite having multivariate implications. Water and energy use are inextricably linked. Water infrastructure investment in order to accommodate growing urban demand encompasses a large portion of city spending [187]. These are often massive overhauls and redesigns in the facility as well as management structure [1, 19, 81]. Restrepo [84] identifies a lack of consistency among studies for comparison in addition to a lack of knowledge in the influence of political, legal, and institutional policy on WEN efficiency. Counter to the significant WEN connection, various current energy policy positions and energy strategies disregard water matters, as water strategies likewise disregard energy matters [81].

These studies focus on climate and pollution impacts within water and energy sectors dealt with separately. This disconnect is true at a city scale, as noted by Kenway [1]:

> "In cities, management of water and energy is frequently shared across levels of government and private enterprise with little ability to communicate and analyze data. Management…is undertaken in isolation and too inconsistent boundaries."

At this scale, one can look into circumstantial dependence. A revision of the previously established perspectives of WEN through the retail water cycle provides more detail at the production scale [53]. Emerging links are confined to three categories: 1) production, 2) transportation, and 3) consumption, as seen in **Figure 4**. Production is defined by the treatment of raw water and wastewater. Transportation is defined by distribution from water resources to production and consumption nodes or connection points. Consumption is defined by end-user activities. These end-user activities can be defined by the node of consumption, buildings. Buildings are built with purpose, typically constrained by zoning code: residential, commercial, industrial, agriculture, and government/public use. Thorough studies have been completed to understand energy consumption in water production and distribution, but the consumption category remains a dynamic problem with many research sectors depending on the end-user activity. The reduction in the scale of study from a city to a local view to find these links, where measurements of water and electricity consumption over time are confined to the same boundaries, will avoid the data limitations listed above.

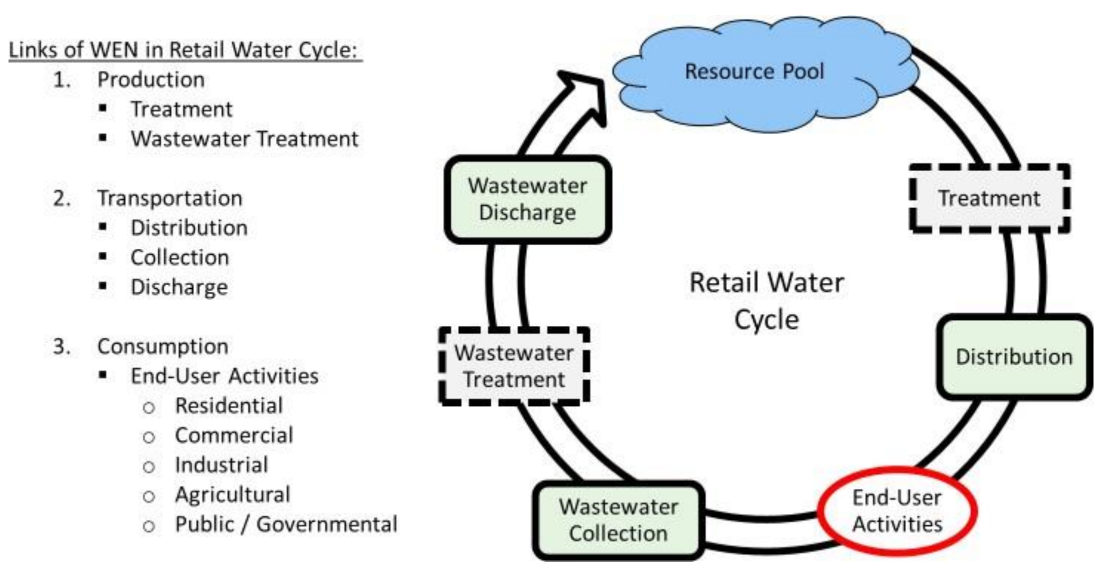

Figure 4. *The r*etail water cycle categorized into three WEN links. Adapted from [53].

2.2.5. Local

The local scale focuses on the direct analysis of the consumption category within the retail water cycle or end-user activities. The broad range of UM studies has developed the consumption category over time through varying perspectives: end-user metabolism [15, 77], industrial metabolism [30, 85, 86, 87], and household metabolism [17, 83, 88, 89]. Studies performed at the local scale provide an opportunity to study and influence the social behaviors and interactions within the boundary. For example, institutions, such as universities, provide reasonable testing grounds [90]. Bottom-up studies are composed of data sets including: building classification, HVAC systems, solar radiation exposure, energy consumption, and energy-efficiency approaches [91]. However, there has been an interest in a top-down approach to model the social and educational impacts of resource consumption on campus. Payam [92] found that the schedules of inhabitants influence the use of water and energy in a building more than any other factor, including outdoor temperature. Accurate forecasting requires a baseline maintenance consumption rate with dynamic functions representing human interaction within the building [93]. While these forecasts can provide a slew of results to guide decision-making, they require the accumulation of enormous data sets that are largely unavailable for analysis.

2.3. Mathematical Modeling Approaches for WEN

The discussion of the model approach is necessary to address the limitations in data set accessibility and model flexibility. This initiates the three-step process of building a model: specification/identification, fitting, and diagnostics [94]. The largest development in UM is the methodical framework. There are five main mathematical modeling approaches relevant to WEN: life cycle analysis, input-output modeling, mechanistic modeling, machine learning, and hybrid modeling discussed in the following chapters.

2.3.1. Life Cycle Analysis (LCA)

Life Cycle Analysis (LCA) studies the "entire life cycle of a product, from raw material extraction and acquisition, through energy and material production and manufacturing, to use and end of life treatment and final disposal" [95]. In the previous context, this would be the application of emergy in the retail water cycle. There are four phases in LCA: objective and specific aim definition, inventory examination, impact assessment, and result interpretation [95]. LCA is a methodical overview, providing a tool to examine trade-offs and complexities. Following this type of analysis, subjective discussions in the "interpretation stage" are made, shifting potential environmental and political burdens between life cycle phases or specific system processes. This analysis helps to define the WEN relationship on a large scale – global to city scales – but does not aid management optimization. This focus of WEN has been saturated with research and has expanded into other areas such as the water-energy-food nexus [96, 97]. This mathematical model requires extensive data sets to function, conflicting with the data accessibility limitation.

2.3.2. Input-Output Modeling

Developed by Wassily Leontief [98], input-output analysis (I-O) is a quantitative economic procedure based on the mutuality amongst the economic sectors. Input-output analysis is fundamentally a theory of production based on a specific type of activity. This method is frequently used to evaluate the impacts of economic shocks, whether negative or positive, and analyze the aftershocks throughout an economy. Its key relationships center around the production processes within the involved technology that produces the quantities of inputs and outputs. I-O modeling does not present a theoretical overview of either the supply or the demand side of the system of study. It does not map alternative behaviors to optimize the system. Improvement on the supply side is precluded by the assumption that the input values used are directly proportional to the output values; therein, one correct solution is attainable. Optimization of the demand side is dependent on whether the I-O model is open or closed. In the closed models, the inner workings of the system are technologically determined. In other words, the system of people is given a designated value, and therefore, does not have optimizing choices. In the open models, part of the system is designated not as products but as consumption or demand. This open system falls in line with the retail water cycle discussed in Chapter 2.2.4.

Wolman [18] developed a simple input-output linear model for urban metabolism study. Wolman relied on the system inputs going into a 'black box,' which represented all activities and transformations before becoming an output. This would be an example of a closed system. The black box requires a boundary condition around the city and does not take into account the inner workings or activities of the urban system. In more recent studies, the input-output model has been established as a strong tool investigating economic pressures on resource pools and the environment of the urban center, revealing both direct and indirect links of resource consumption [99, 100], exploring the resources pressure transfer through economic trade networks [101, 102], and distinguishing the driving force of resource consumption from an economics perspective [103, 104]. Additionally, the model can be used to examine the supply chain effects on resource consumption in an economic system by examining the linkages amid sectors [105, 106]. The linkage analysis resulting from input-output analysis is an effective approach to categorize each supplier and consumer within a sector. Duarte [105] supplemented the terms of linkage analysis with component descriptions: internal impacts, mixed supply-consumption linkages, backward linkage processes, and forward linkage processes. These descriptors help to distinguish crucial sectors from a consumption perspective.

An economic network perspective can "apply linkage analysis to a particular case of the water-energy nexus in an urban system, in order to explore the production and consumption structure of both water and energy resources, as well as the interconnected relationship between two essential resources" [107]. Many researchers, like Kenway [1] among others, have determined that "IO analysis captures big picture and more remote linkages for the entire economy; however, it is difficult to apply at city-scale" and is suited for regional or national levels. Girardet [108] proposed a cyclical urban metabolic model because "linear sequence did not accurately emulate real organisms." Duan [109] agrees with this statement in contrasting natural metabolism to urban metabolic pathways, where the urban pathways were too long, and the circulation of materials and energy was too inefficient and incomplete. Recent studies and models attempt "to move the water–nexus construct beyond an input-output relationship into the realm of resource governance" [68]. Model flexibility is necessary to shift from forecasting to optimization applications.

2.3.3. Mechanistic Modeling

Mechanistic modeling is based on the fundamental laws of natural sciences with the purpose of representing real-life events through assumptions on mechanisms or processes. This involves using experimental data sets to construct and calibrate a model then validates through data. The mechanisms are composed of simplified mathematical formulations to determine possible input-output behaviors. Analytical tools determine whether the range of possible input-output behaviors predicted by the model are consistent with experimental observations [110].

Zhang [111] redevelops the black box theory from Wolman [18], defined as inner details, or efficiencies, of system/s unknown. Zhang replaces the black box with an inner network process for urban metabolism. The metabolic process is defined with input, conversion, cycling, and output of materials and waste from a top-down perspective. This concept merges the frameworks of LCA and I-O. The object's environment and life cycle end at the boundary of the system. Exchanges across the boundary are designated as inputs and outputs, depending on the flow direction [111]. Connections between urban metabolism and spatial distribution of land-use types were extensively [112-118] analyzed in both directions- the top-down approach and the bottom-up approach. This helps to establish the need to incorporate local geographical data and geographic information system (GIS) mapping with the model. Zhang provides a thorough review that lists all the cities which have performed accounting exercises to develop an urban design [111]. All perspectives of end-user metabolisms, single metabolic flows, emergy, and spatial location-specific models have advanced early research. With this early research and accounting exercise, studies have begun to turn into tools for development.

The quantity of energy used for water services in densely settled areas depends on factors such as local topography, quality of raw water, advancement of treatment technology, and quality measurements of environmental and citizen wellbeing [37]. However, there is more to WEN than the footprint values that have been established through metrics of carbon, energy, or water consumption. The value of WEN requires socio-economic and environmental 'externalities' in order to identify opportunities for technological and management innovation as well as the implications of these investments within the city. Scholars began to develop an idea of UM and its relation to social factors.

Boyden [118] reviewed factors such as housing, air pollution, mortality, health, wellbeing, crime, and future urban development to evaluate the metabolic status of the City of Hong Kong, China. Newman used social factors such as the wellbeing of residents, employment rates, and education in order to include human opportunity and livability as measures for urban metabolism [119]. Schiller [120] established a flow linkage between energy and material with social theory by exploring potential "communicative action" to adjust "social relativity," where the idea of a bidirectional cause and effect relationship" is apparent. This shows that an accurate model requires accounting for system sensitivities and multiple effects/counter-affects. Due to the lack of connection within the city scale, the efficiency of implementing new strategies and technologies cannot be properly measured between macro and micro scales.

Mechanistic modeling conceptualizes original hypotheses for fundamental mechanisms that are generated through relatively few observations of the study focus. There is flexibility in the model's ability to be developed with small amounts of data; and, once validated, can be used as a forecasting tool where experimental data is hard to access [110]. The complexity of these models requires time for fine-tuning. For this reason, adaptability for scale and cross-study examination becomes difficult. Other disadvantages of mechanistic models are composed of oversimplified assumptions built on hypothesis; and poor prediction power. Modeling human interaction with the environment is one of the main drivers of WEN and requires a flexible, stochastic approach. This will be discussed further in Chapter 4.

2.3.4. Machine Learning

Machine learning models are applied to parse relevant inputs from large datasets for a provided output. Artificial Intelligence (AI) is the application of machine learning to solve actual problems. AI is a complex combination of computer science, physiology, and philosophy that attempts to mimic human brain learning capabilities. According to Bellman [121], "AI is the automation of activities that we associate with human thinking, activities such as decision-making, problem-solving, learning." The AI improves forecasting performance over time, learning by trial and error. This is counter to traditional model methods that rely on procedural coding based on logic, if-then rules, and decision trees [122].

There are currently two major types of AI: symbolic and computational intelligence [123]. Symbolic AI focuses on attempts to structure knowledge bases by simulating human intelligence and expertise of certain fields. The most well-known symbolic AI method is the expert system (ES). The purpose of ES is to understand the inside mechanisms of a real-life system and to predict its behavior. Expert systems provide advice and solutions to humans and appropriately use that advice and solutions to get better predictions. The advantages of ES are the ability to: 1) intake large amounts of information, 2) impute missing data, and 3) reduce the time required to solve problems. The over-reliance on large, clean datasets is a disadvantage of ES, falling into the limitation of data accessibility [123]. Computational intelligence focuses on using a computational algorithm to deal with complex, real-world. The two most common types of the computation-intelligence method are genetic algorithms (GAs) and artificial neural networks (ANN). These models are discussed in Chapters 4.4 and 4.5.

The application of AI in time-series analysis has gathered the attention of many studies proposing new ML frameworks, methodological advances, and accuracy improvements [124-130]. Many of these studies fail to provide evidence of performance versus other models. Conclusions are often condemned to three limitations [122]:

1) Report conclusions are not statistically significant, typically based on a few or even a single time-series.
2) Method forecasting time frames, or horizon, are limited to short-term or one step ahead. These forecasts do not consider alternative time frames such as medium and long-term or multiple steps.
3) Lack of benchmarks to compare the accuracy of tested ML methods with alternatives.

With these limitations, it is clear that all data sets and model goals are different. The flexibility of machine learning models makes it hard for cross-study examination. However, there is a demand for consistent results and repeatability.

2.3.5. Hybrid Modeling

Hybrid modeling is a concept of highlighting the strengths and reducing the disadvantages of two or more models. The advantage of statistical linear modeling is the ease of use and the ability to capture patterns. The major limitation is the rigid pre-assumed linear relationship with past events. A linear approach may not be adequate for real-world data. The advantage of machine learning is the flexible, non-linear modeling capability. The limitation of scalability in mechanistic techniques can be overcome with the use of machine learning. In addition, the advantages of mechanistic models can be exploited by machine learning algorithms both as temporary inputs and later as a validation model [110]. The literature on hybrid modeling was advanced by Reid [131] and Bates and Granger [132]. Clemen [133] provides a thorough review of heterogeneous hybrid models.

Supported by theoretical and empirical findings in neural network forecasting research, the combination of diverse methods can significantly and efficiently improve forecasting performance. Pelikan [135] and Ginzburg and Horn [136] proposed combining several feedforward neural networks to improve time-series forecasting accuracy. Several hybrid models composed of the autoregressive moving average (ARIMA) and artificial neural networks (ANNs)applied to time-series forecasting with improved model performance. These models will be discussed in chapter 4. The hybrid modeling technique is an attempt to address both limitations of WEN, data set accessibility, and model flexibility.

2.4. Adaptive Approaches to Solutions

The WEN studies, within the UM framework, have developed over time from an accounting exercise into a design tool. Kennedy [77] provides a further detailed chronological assessment that shows this development. The application of these design tools has branched out in various studies. Kenway [1] breaks down possible applications for UM developed into four categories: sustainability indicators, greenhouse gas accounting, policy analysis via dynamic mathematical models, and a tool for strategy and design.

The use of UM as a means of sustainability indicators is done with an analysis of the efficiency of energy and material cycles, waste management, and infrastructure of an urban system. This use is outlined by Maclaren [137] and allows for a deeper understanding of the resilience of a city. UM studies have applied greenhouse gas as a primary variable, similar to the concept of energy as the primary variable in 'emergy' discussed in chapter 2.1, where all material flows translate into a single value of greenhouse gas emissions for each activity; examples can be found in [1, 15, 138]. Policy analysis through the use of Dynamic mathematical models have been explored more extensively; for example, SIMBOX [139] and STAN [140, 141]. These dynamic mathematical models include the representation of sub- system processes, resource pools, and links within the boundary-defined system to economic modeling.

While some models are useful for accessing current resource pools and linkage flows, they can be used to simulate future changes to UM as a result of technological interventions or policies. UM models are particularly advantageous for classifying resolutions to environmental issues beyond 'end of pipe' approaches. In this respect, studies allow for analysis of technology or policy implementation. This is first shown in work by Oswald and Baccini [142] in ‘Netzstadt.’ It establishes structural and physiological tools, which can be used in the “long process of reconstructing the city,” with the recognition that the center-periphery model of cities is outdated while also recognizing current trends of expanding urbanization as unsustainable. It integrates UM by establishing four principles of redesigning cities: adaptability, sustainability, redevelopment, and accountability, as well as five criteria of urban quality: identification, diversity, flexibility, degree of self-sufficiency, and resource efficiency. Examples and uses for this are found in New Orleans after the effects of Hurricane Katrina as well as environmentally conscious designs for the city [190]. This adaptive analysis allows for the production of numerous solutions to a single issue. Identifying both physical and organizational reconstruction possibilities advance system efficiency in allocating resources. The limitation of data accessibility and model flexibility become evident with the discussion of complex design tools.

Chapter 3. Existing Models to Forecast WEN

The previous chapters have established WEN study limitations in data set accessibility and model flexibility. Therefore, exploring the model approaches and data set types determines which models are viable. The model approach is dependent on the study, whether the hypothesis is developed initially. It may also be dependent on data. The choice of modeling approach (top-down, bottom-up, or middle-up) and the specific model choice is determined by the data set type and data set availability. Type of data is discussed through load forecasting terms in order to discuss time-series analysis. Load forecasting is the foundation for establishing robust and efficient management operation schedules as well as future facility expansion [143]. The scale (or boundary) of a data set determines the proper model required for forecasting. After the appropriate model approach and data types are determined, data preprocessing is conducted to clean and standardize data sets.

3.1. Approaches: Top-down, Bottom-up, and Middle-out

The approach of model structuring is the process to define and analyze data requirements to identify a model and includes three main approaches: top-down, bottom-up, and middle-out; see **Figure 5**. The top-down approach starts with a hypothesis and builds a model with data to solve the stated issue(s) and aids in governing and policy decisions. This approach has the ability to establish system behavior constraints and performance goals within the model limits. The top-down approach generally employs stringent mathematical tools such as classical and stochastic control theory, constraint estimation, and optimization theory. The bottom-up approach is typically a mechanistic model, utilizing available data to make exploratory insights or reverse engineer a system with the parts making up the system to illustrate the system processes as a whole. The analysis tools available in the bottom-up approach are extremely efficient in describing the average system behavior. The bottom-up approach is dependent upon probability methods such as mean-field statistics and dynamical system theory. The middle-out approach focuses on a validation variable through time-series analysis. The middle-out approach is generally implemented on projects that require system improvement or optimization [144, 145].

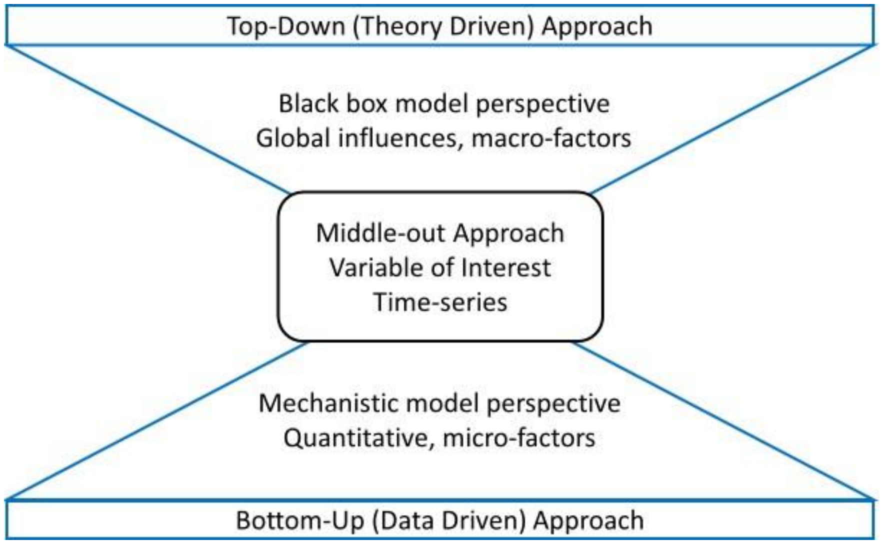

Figure 5. General analysis approaches: Top-down, Bottom-up, and Middle-Out.

3.1.1. Top-down Approach

The top-down approach treats the boundary of study as a black box or material sink and applies available datasets to describe the system. The top-down approach maintains an initial focus on information of higher-level concepts, such as identification and classification of data populations, membership rules, and relationships between such data populations. This approach allows engineers to create a system from scratch to explain an issue but requires time and resources. In the view of the WEN, the top-down approach helps to determine the impacts on water or electricity consumption due to long-term fluctuations. Variables frequently used by top-down models tend to be explanatory, including macroeconomic (i.e., GDP) and environment wellness indicators, housing construction rates, and estimates of appliance inventory within a boundary of study. The primary purpose of the top-down approach in relation to water and electricity consumption is to determine supply requirements. The strength of the top-down approach lies in the ability to rely on aggregate data—wide availability, simplicity, and reliability on historical values. In reference to the scale of the city, the census provides an abundance of available datasets. The drawback is a reliance on historical data. This does not provide a capability to model the development and implementation of new technology and policy. There is a lack of model flexibility. The simplicity of top-down modeling highlights the lack of detail regarding the activities involved in the consumption of water and energy; therefore, it eliminates the ability to designating improvements necessary to implement and critique policy and technology innovation.

3.1.2. Bottom-up Approach

In contrast to the top-down approach, the bottom-up approach calculates values through a detailed step-by-step process and aggregates the values to represent a whole system. A bottom-up approach requires an engineered modeling method with two categories: comprehensive and simple. WEN models with bottom-up approaches use physical principles and consumption behavior within the designated boundary (i.e., building, city, state, or nation). For a detailed, comprehensive model of a building's consumption, intricate formulas are utilized to determine the building baseline maintenance consumption along with variations to the baseline due to human interaction. These formulas are impacted by four factors: energy balances of indoor and outdoor climate (to be referred to as “localized artificial climatic forcing”), the physical construction of the building, utility rates linked with social interaction, and the technology that is interacted with to consume the material—water or energy. As this approach begins to reach out of the focus of this report, readers may refer to [92, 93, 146, 147, 148] for detailed energy consumption calculations and [149, 150] for detailed commercial and residential end uses of water, respectively.

3.1.3. Middle-out Approach

Both top-down and bottom-up modeling approaches require a clear definition of the variable of the study. WEN is ill-defined and varies depending on what approach is used. A middle-out approach is required in order to optimize models through both top-down or bottom-up approaches. The relationship between water and electricity consumption over time is the first step before introducing other variables, as seen in **Figure 5**. The reduction of modeling to univariate time-series establishes a flexible model able to produce validating forecasting data with limited initial training datasets. This simple forecasting model would serve as the foundation of building complex models for WEN studies. The middle-out approach focused on univariate time-series analysis addresses the fundamental problem statement of data limitations and accessibility for WEN and optimizes current models and policy decisions. Results from the middle-out approach can be used to validate models and results from top-down and bottom-up approaches. It is the best next step for WEN studies that seem to have stagnated from data inaccessibility, inconsistency between studies, and lack of optimization capabilities.

3.2. Types of Data Sets

Types of data sets for forecasting the purposes of water and electricity consumption vary from the time scales, short-term versus long-term time spans, and a number of available variables within the given time frame. These variances in data set types have different end goals. For example, the electric power load forecasting (EPLF) terms of the time-series forecasting horizon duration, which can be expanded to other resources/utilities, are as follows: short-term load forecasting (STLF), medium-term load forecasting (MTLF), and long-term forecasting (LTLF). The bounds of the horizons are one day, two weeks, and three years, respectively [151], as seen in **Figure 6**. Short-term load forecasting is an immediate analysis for demand response and scheduling. Medium-term forecasting is utilized as operation control, system planning, and resource trade. Long-term forecasting is utilized over weeks, months, and years for the purpose of capacity planning, maintenance scheduling, and policy.

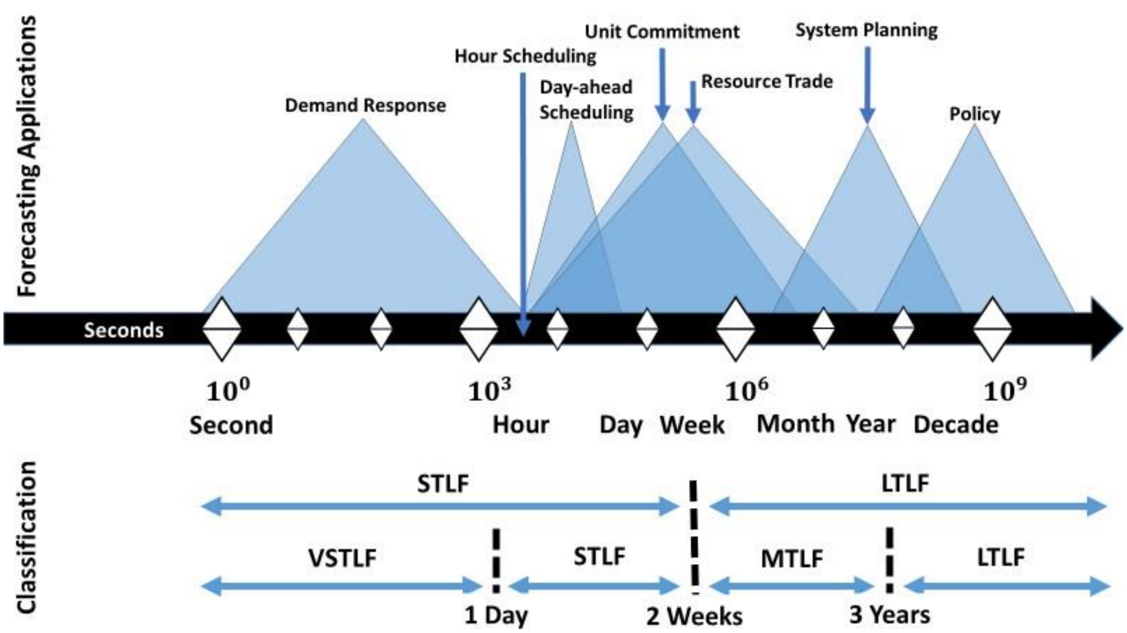

Figure 6. Forecasting capability based on the time frame of the data set. Adapted from [151].

The complexity of a model revolves around the number of input variables, either multivariate -- multiple variables or univariate -- one variable, with respect to time. Multivariate forecasting models have strength in short-term forecasting and connecting other factors. As the time scale is increased to long-term forecasting, the significance of multiple variables begins to degrade. Therefore, univariate forecasting models have strength in long-term forecasting and limited data accessibility.

There is an argument that univariate models are sufficient for short-term purposes by claiming that multiple variables put parsimony and robustness at risk [152]. This claim is formed around the reliability of the data and how it is processed; for example, incorporating models with climatic-based data sets reduces dependability to predicted climatic inputs. An additional complication to multiple variables, data processing is necessary to recognize patterns like trend and seasonality as well as white noise or randomness for various data sets. Univariate time-series analysis is of interest due to the middle-out approach's ability to address WEN limitations of data accessibility and model flexibility.

3.3. Data Preprocessing

In order to properly analyze a time-series, modeling techniques may require all observations to be independent. However, observations in a time-series are time-dependent. This requires the time-series to be stationary. A stationary time-series requires a constant variance, mean, and auto-correlation over time, as seen in **Figure 7**. To test the stationarity hypothesis, one must distinguish whether a time-series has a unit root. A unit root is evidence of more than one trend within the series. The two-unit root tests performed to determine hidden trends within specific orders of differencing are the Augmented Dickey-Fuller Test (ADF) and Phillips-Perron Unit Test.

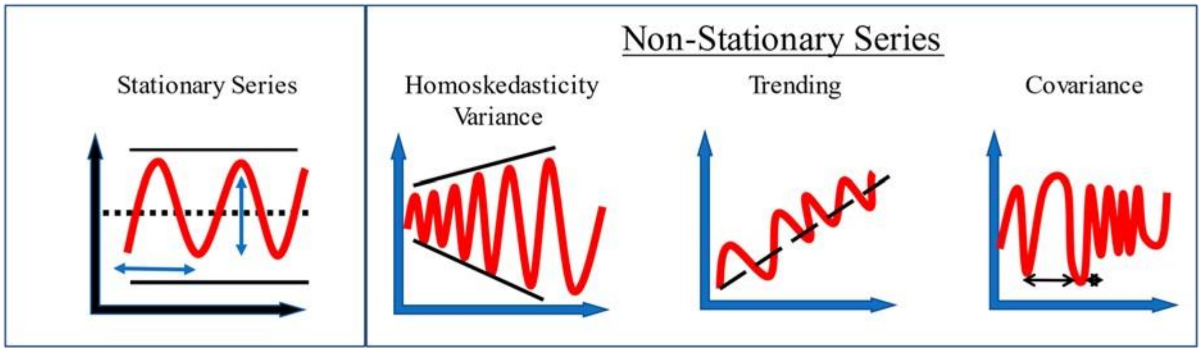

Figure 7. Examples of stationary and non-stationary time-series.

The Dickey-Fuller test is a unit root test that accesses the null hypothesis that α = 1, with α (alpha) as the coefficient of the first lag on Y.

$$y_t = c + þt + \alpha(y_{t-1}) + \hat{6}Y_{t-1} + e_t$$

where, (y_{t-1}) = lag 1-time-series; and $\hat{6}Y_{t-1}$ is first difference of time-series at the time(t-1). This is a similar null hypothesis as the unit root test. If the coefficient of (y_{t-1}) is 1, the assessment implies the existence of a unit root. If not rejected, the assessment concludes the time-series is non- stationary. The augmented Dickey-Fuller (ADF) test expands the Dickey-Fuller test equation to include the high order of the regressive process in the model [153]. The critical t-distribution values that test results should be less than (<) for the Dickey-Fuller and Phillips-Perrone tests are listed in **Table 2**.

Table 2. Critical values for the Dickey-Fuller t-distribution test.

Critical values for Dickey-Fuller t-distribution test		
	Without Trend	With Trend
Sample Size	Value at 5% confidence	Value at 5% confidence
25	-3.00	-3.60
50	-2.93	-3.50
100	-2.89	-3.45
250	-2.88	-3.43
500	-2.87	-3.42

Phillips-Perron (PP) test is similar to the ADF test, generating data for higher orders of autocorrelation [154]. The PP test is non-parametric and does not require the selection of the level of serial correlation or lag functions as in ADF. Similar to the DF test in many ways but has the ability to conduct autocorrelation and heteroscedasticity corrections. Both tests work well in large samples but are susceptible to poor results with small sample sizes.

The preprocessing options for time-series stationarity are transformation, deseasonalize, detrending, and combination. Transforming the data utilizes log or the Box-Cox [155] power transformation to achieve stationarity in the variance. If there are significant patterns in the data, autocorrelations at lag 4 or 12 may exist. Deseasonalizing the data uses the classical, multiplicative decomposition approach [156]. If there is a change in mean overtime or trending, detrending is applied to the data. A Cox-Stuart test [157] is conducted to evaluate the existence of a deterministic linear trending or exponential trending. Elimination of these trends from the data is necessary to achieve time-series stationarity. All techniques can be applied simultaneously to adjust the time-series [122].

Chapter 4. Modeling for Univariate Time-Series Forecasting

When data sets are limited to one variable over time, the choice of model is reduced to a time-series analysis. In the interest of UM and WEN studies, the data sets are specified to water and electricity consumption over time. Time-series analysis uses past observations of the same variable(s) to analyze and separate patterns from random error to define underlying relationships to predict future behavior [111]. There are two main types of time-series: deterministic and non-deterministic. Deterministic time-series are analytically expressed with no random or probabilistic aspects. By contrast, a non-deterministic time-series cannot be explained by an analytic expression as there are non-linear and random elements to the time-series.

The aim of time-series forecasting is to take real-world data composed of a mixture of both deterministic and non-deterministic time-series and forecast a sequence of observations. Since non-deterministic time-series is composed of a random element, probabilistic methods are taken into consideration. Randomness is a means of statistical terms rather than explicit mathematical relations, i.e., means and variances. A probabilistic model depends on the availability of historical data for training stages as well as on the temporal autocorrelation function of the input variables [158]. Addressing both deterministic and non-deterministic data set possibilities, models typically used for univariate time-series analyses are linear regression, ARIMA, Holts-Winter exponential smoothing, Genetic Algorithm, Artificial Neural Network, Exponential smoothing with gradient smoothing, and Hybrid SARIMA-ANN.

4.1. Linear Regression

Common types of linear regression models are simple and multiple linear regression. The simple linear regression (SLR) model relates a single independent variable to a single dependent variable, and its mathematical formation is expressed, as shown in Equation 4.1:

$$y = mx \pm c \pm e \qquad \text{Equation 4.1}$$

where y is equal to the dependent variable, x is equal to an independent variable acting as a function for the dependent variable, m is a coefficient that represents the slope of the line, c is an intercept, and e is an error term. The model approaches a perfect solution as the SLR model coefficient m approaches the value of 1. Multiple linear regression (MLR) model is an expansion of SLR by integrating more than one independent variable as a function of the single dependent variable, as shown in Equation 4.2:

$$Y(x) = k_1x_1 + k_2x_2 + k_ix_i \pm C \pm e \ , \qquad \text{Equation 4.2}$$

where Y is a dependent variable, x1, x2, ⋯⋯, xi (i = 1, 2,⋯ ,n) are independent variables, k1, k2, ⋯⋯, ki (i = 1, 2, ⋯,n) are the coefficients of a linear relationship, c is a constant, and e is an error term. To produce a more reliable model for the MLR model, multiple independent variables are filtered to select the most significant combination of variables.

The performance of the SLR model is assessed by a correlation coefficient (R), which assesses the linear relationship between two variables. The range of R is between -1 and 1. If the value of R is -1 or 1, the variables are highly negatively or positively correlated; however, if R closes to 0, the variables are not correlated. In addition, the coefficient of determination (R^2) is commonly used to assess the performance of the model. The range of R^2 is the same as that for the R-value. When R^2 is close to 1, the fitted trend-line is very close to the actual value; it is far from the actual value when R^2 is close to 0.

There are two commonly used variable selection methods: forward stepwise selection and backward stepwise selection [159]. In the forward stepwise selection method, the model begins with no independent variables in the model and then adds independent variables one at a time until no variables present strong evidence of their importance in the model. The p-value is used to select the variables based on statistical significance. Backward stepwise selection is the reverse of the forward selection method. This method starts with all potential independent variables. Variables are eliminated one at a time until the remaining variables have significant p-values.

With application to time-series, the choice between univariate and multivariate times series models determines the end goal and complexity of the model. Univariate time-series forecasting is the simplest method, using the information on the variable to be forecast. There is no attempt to discover explanatory factors of the behavior of the variable. The only goal is to determine what is happening with the variable over time. The pattern of the variable will typically be composed of trending, seasonal patterns, and white noise, or error. In this case, Equation 4.3 represents a suitable time-series forecasting equation;

$$ED_{t+1} = f(ED_t, ED_{t-i}, \ldots, \text{error}) \quad \text{Equation 4.3}$$

where t is the present day, t+1 is the next day, t−1 is the previous day, t−2 is two days ago, and so on. The prediction of the future, t+1, is based on past values of a variable. The “error” term represents a random variable and the effects of relevant variables that are not included in the model. As discussed in chapter 3.2, the univariate model has strength in long-term forecasting and limited data access.

Multivariate time-series models are much more complex, explanatory models. Multivariate time-series models use influencing factors, or predictor variables, to predict what will happen in the future and why that variable is happening. The type of variable is dependent on the approach, top-down or bottom-up. These variables are called predictor variables. For example, forecasting the daily electricity load demand (ELD), a model with predictor variables could be illustrated as;

$$LD = f(\text{TENEERATURE}, \text{ECONONIC strength}, \text{eoeulation}, \text{day of week}, \text{error}) \quad \text{Equation 4.4}$$

The normal distribution of the error illustrates no hidden patterns to be explained by an additional variable. This type of model would be found in either a top-down or bottom-up approach. Direct relationships or correlations are used to formulate an algorithm with these variables. See Chapters 3.1.1 and 3.1.2 for a review of types of data relating to the model approach. The third type of model type combines the explanatory and time-series features of the above two models. The equation would be similar to the previous Chapters 4.3 and 4.4, as seen;

$$ED_{t+1} = f(\text{TENEERATURE}, \text{eoeulation}, ED_t, ED_{t-i}, \ldots, \text{error}) \quad \text{Equation 4.5}$$

This type of “mixed model” is designated various names depending on the discipline, including dynamic regression models, panel data models, longitudinal models, transfer function models, and linear system models. These explanatory models are found in top-down or bottom-up approaches as they describe why something is happening. These mixed models are useful because they incorporate information about other variables rather than only historical values of the variable to be forecast. There are disadvantages to utilizing explanatory or mixed models. The system may not be understood properly. The data sets necessary to model an elaborate system would be extensive. If extensive datasets are accessible, accurate correlations assumed to direct the explanatory variable behavior may prove difficult to measure. Due to the varying reliability of these correlations between explanatory variables and outputs, the time-series model may provide more resilient correlations and reliable forecasts than those provided by the explanatory or mixed model. Therefore, the model to be implemented for the forecasting analysis is dependent on the model approach, dataset availability, competitive model accuracy, and model result application. The discussion advances through the various methods used for long-term univariate forecasting – as this becomes the focus of the problem statement – to address the data limitations of WEN studies: data accessibility and model flexibility.

4.2. Auto-Regressive Integrative Moving Average (ARIMA)

The auto-regressive integrative moving average (ARIMA) model is an assembly of autoregressive (AR) coefficients and moving average (MA) coefficients. The AR coefficients are multiplied by past values of the time-series and MA coefficients multiplied by past random shocks [155, 160]. The integrative term provides the differencing tool utilized to stationarize the time series. The values of the AR and MA coefficients are chosen such that the data preprocessing tests with autocorrelation function (ACF) and partial autocorrelation function (PACF) simulate the estimated ACF and PACF for the modeled time-series. ACF is an auto-correlation function that provides values of auto-correlation of a time-series series with past values. Simply, it describes the influence of lagged values on the current value. Similar to ACF, PACF finds correlations of the residuals. ARIMA modeling requires a stationary time-series (with constant mean, variance, and autocorrelations). Nonstationary time-series are assimilated into stationary time-series through simple operations and transforms, such as differencing and taking the log transform, see Chapter 3.3 for data preprocessing of nonstationary series. After this preprocessing, the ARIMA can be applied to the time-series for forecasting modeling.

Box and Jenkins [155] proposed a simple three-stage procedure for synthesizing accurate ARIMA models: 1) identification, 2) estimation, and 3) diagnostic checking. The model construction process requires data set separation where an end portion of the time-series is set aside in order to validate the forecasting accuracy. In stage 1) identification, the data preprocessing unit tests of ACF and PACF are calculated for the available time-series data. If these unit tests indicate nonstationarity, conversion of the time-series to a stationary series is performed through appropriate transforms and differencing operations. In addition, this action can be done through nonseasonal and seasonal lags. The ACF and PACF tests provide a guideline or skeleton framework for the ARIMA model to simulate the resulting stationary time-series. Tentative ARIMA models offer numerous options. The best option is a subjective part of the analysis process.

In simple terms, the ARIMA model is a time-series stationarized by integration terms (differencing or detrending) and simulated through a combination of AR and MA portions; all with the ability to include seasonal and nonseasonal patterns. The qualifications for a good forecasting model are accurate forecasts as well as parsimonious coefficients; i.e., the least number of coefficients necessary to explain the available data. In stage 2) estimation, these model coefficient values project forecasts that are then compared to actual values and adjusted to minimize a standard for the residual errors. Comparison of ARIMA model coefficient values is made through evaluating statistical quality, reduction of multicollinearity, and satisfying stationarity and invertibility restrictions [155, 161]. Once the ARIMA model fulfills all the requirements and designated standards, the resulting forecast residuals are tested for unit roots to illustrate statistical independence from random noise. This leads to stage 3) diagnostic checking, unit root tests ensure that forecast residuals are a) statistically minor, b) reduce variance, and their ACF function does not have significant short-term autocorrelations.

The seasonal auto-regressive integrative moving average (SARIMA) model is an expansion of ARIMA modeling suitable to define the linear relationship of a non-deterministic time-series with seasonal variation. The SARIMA model employs three terms to forecast univariate data: differencing term, auto-regressive (AR) term, and moving average (MA) term. Seasonality in a time-series is denoted by recurring pattern shifts that repeat over S time periods, where S defines the number of lags until the pattern repeats again. For example, monthly data typically demonstrates seasonality where patterns within the values tend to occur in particular months. In a year-to-year case, S=12 represents the time lag of months in a year. The following subchapters are presented for the discussions about the fundamental structure and identification of the best model structure.

The added differencing strengthens the traditional ARIMA model. A time-series $\{Z_t \mid t=1, 2, \ldots, k\}$ is generated by SARIMA $(p, d, q)\ (P, D, Q)_s$ model with a mean (μ) of Box and Jenkins time-series model is represented by Equation 4.6;

$$\hat{\circ}p(B)0P(Bc)(1-B)d(1-Bc)D(Zt-\mu)=8q(B)©Q(Bc)at \qquad \text{Equation 4.6}$$

where p, d, q, P, D, Q are integers; s is periodicity; $\$(B) = 1-\$_1B-\$_2B^2-\ldots-\$_pB^p$, $8(B^s) = 1-8_1B^s-8_2B^{2s}-\ldots-8_PB^{Ps}$, $8(B) = 1-8_1B-8_2B^2- \ldots -8qB^q$, and $©(B^s) = 1-©_1B^s-©_2B^{2s}- \ldots -©_QB^{Qs}$ are polynomials in B of degree p, q, P, and Q; B is the backward shift operator; d is the number of regular differences, D is the number of seasonal differences; Z_t denotes the observed value at time t, t=1, 2, …, k; and a_t is the estimated residual at time t.

The SARIMA model involves the same 3-stag iterative cycle from the ARIMA model [161]: 1) identification of the SARIMA $(p, d, q)(P, D, Q)_s$ structure; 2) estimation of the unknown parameters; and 3) diagnostic checks on the estimated residuals. This is followed by validating forecasting future outcomes based on the known data.

The random error, a_t is expected to demonstrate independence with ACF unit tests. This is shown through the normal distribution of residuals, displaying mean=0 and reduced variance a^2. The roots of $\$(Z)$=0 and $8(Z)$=0 should all lie outside the unit circle. It was suggested by Box and Jenkins that at least 50 or preferably 100 observations should be used for the SARIMA model.

Choosing the best fit model structure requires a subjective analysis. To aid in ARIMA construction, Duke University provides 13 guidelines [162]:

1) Identification of difference variable (I) and the constant:
   A. If the series presents positive autocorrelations in high lag values (10 or more), a higher-order of differencing is required and possibly indicated seasonality.
   B. If the lag-1 autocorrelation is negligible, then the series does not require a higher-order of differencing. If the lag-1 autocorrelation is -0.5 or more negative, this may be indicative of over differencing.
   C. Optimization of differencing the time-series is typically done with the focus on lowering the standard deviation. Impacts of over/under differencing may be adjusted with AR or MA terms.
   D. Stationary time-series do not require differencing. First-order differencing assumes the original time-series has a constant average trend. Second-order differencing assumes that the original time-series has a fluctuating trend.

E. Zero and first-order differencing typically involve constant terms in order to account for a non-zero mean value. In contrast, second-order differencing typically does not need to apply a constant term.

2) Identification of AR and MA coefficients:

A. If the partial autocorrelation function (PACF) of the adjusted (differenced) time-series illustrates under differencing through a sharp cutoff and/or the lag-1 autocorrelation is positive, it is possible to reduce the impact with additional AR terms to the model. The PACF test will show a cutoff lag that may indicate the AR coefficient terms required.

B. If the autocorrelation function (ACF) of the adjusted (differenced) time-series illustrates over differencing typically indicated by a sharp cutoff and/or the lag-1 autocorrelation is negative, it is possible to reduce the impact with additional MA terms to the model. The ACF test will show a lag cutoff that may indicate the MA coefficient terms required.

C. Model parsimony must be maintained, reducing the number of AR-MA terms. This is highlighted by the possibility of AR and MA terms canceling each other out.

D. If the sum of the AR coefficients is almost exactly 1-- indicating a unit root, it is recommended to reduce the number of AR terms and increase differencing.

E. If the sum of the MA coefficients is almost exactly 1 -indicating a unit root, it is recommended to reduce both the number of MA terms and the order of differencing.

F. Another unit root test for AR-MA terms is indicative in erratic or unstable long-term forecasts.

3) Identification of model seasonality:

A. The existence of strong correlations to higher lags demands the use of seasonal differencing. It is not recommended to implement more than one seasonal differencing or more than two orders of total differencing (seasonal nonseasonal).

B. When the adjusted (differenced) time-series illustrated positive at lag s in the ACF results, where s is the number of periods in a season, it is recommended to add a SAR term to the model. In contrast, when the adjusted (differenced) time-series illustrated negative at lag s in the ACF results, it is recommended to add an SMA term to the model. The SMA term is likely necessary along with seasonal differencing due to the presence of stable and logical seasonal patterns. The SAR term is likely necessary when the seasonal difference has not been used. This is only done when the seasonal pattern is erratic or fluctuating over time. Overfitting of time-series with the data must be avoided. Do not implement more than one or two seasonal parameters (SAR+SMA) within the same model.

ARIMA models have the advantage of being simple, therefore, are less likely to overfit the data in comparison to exponential smoothing and adjustment models. The calculation of confidence intervals for longer-horizon forecasts is more reliable in theory with comparison to other models. ARIMA models with constant trends retain higher confidence levels in long-term forecasts resulting in wide confidence intervals at long-term forecast horizons. Models that do not assume fluctuation in trends retain narrow confidence intervals at long-term forecast horizons [162]. The advantage of SARIMA is its ability to express the stochastic nature of time-series. Modeling multiple seasonal cycles is not a problem. However, there are disadvantages in representing only linear relationships between variables. SARIMA also becomes subjective when determining the proper order or structure [163].

4.3. Holts-Winter Exponential

The exponential smoothing method is a time-series forecasting method for univariate data with the ability to model regular trends and/or seasonal patterns. In comparison to Box-Jenkins ARIMA methodology, exponential smoothing forecasting uses weighted sums of past observations. The difference between the two models is the exponentially decreasing weight for past observations. Therefore, the exponential smoothing forecast associates higher weight to lower time lags.

The Holts-Winter Exponential Smoothing model is a triple exponential smoothing function that incorporates simulating seasonal patterns. There are several hyperparameters added to the function in order to adjust for seasonality [161]:

- Alpha -- variance
- Beta -- trending
- Gamma -- seasonal patterns
    - Trend: Additive or multiplicative
    - Dampen: Additive or multiplicative
- Phi -- Damping coefficient
    - Seasonality: Additive or multiplicative
    - Period: Time lags within the period

The *alpha* (*a*) parameter, also known as the smoothing factor, determines the rate of decay the weight influence shifts over time. The alpha parameter is set to a value between 0 and 1. A value close to 1 indicates fast learning or a recent event. Whereas a value close to 0 indicates slow learning or past observations with heavy influence. The *beta* (*b*) parameter determines the rate of decay with influence to trend overtime shifts. The *gamma* (*g*) parameter determines the influence on the seasonal component.

A damping coefficient, Phi (p), determines the rate of dampening in either: additive or multiplicative. This is dependent on the trend: linear or exponential, respectively. This model can be used for heteroscedastic time-series, but exogenic variables cannot be introduced to the model. This makes the model inflexible to additional variables. In addition, there are disadvantages of over-parameterization and a large number of starting values to estimate [163].

4.4. Genetic Algorithms (GA)

A genetic algorithm is an adaptive investigative algorithm with principles of natural selection. The genetic algorithm iteratively alters a population of individual solutions based upon strength results. GAs are a simulated natural computation, which means that species pursue suitable circumstances for survival by continuously evolving. Evolution generates new individuals through three steps: selection, crossover, and mutation. Selection develops the living environment by preserving better species and eliminating worse species. GAs mimics these processes to solve complex problems with self-organizing capabilities; therefore, it is usually used in categorization, pattern recognition, and association. GAs can solve difficult problems quickly and can interface with other models and simulations [164].

Randomness is utilized within each stage of the genetic algorithm. Individuals (data points) are selected at random from the current population (dataset) to be parents. These parents produce children (forecast) for the next generation. Over successive generations, the population "evolves" toward an optimal solution. The genetic algorithm maintains three types of restrictions within each cycle to produce the next generation [161]:

1) Selection rules
2) Crossover rules
3) Mutation rules

The first restriction is based upon how parents are selected. The second restriction is based upon how the parent passes on characteristics to the next cycle. The third restriction applies randomness to form mutations within the new cycle. In terms of data, the GA results become more robust in the presence of reasonable noise. The GA method can exploit extensive datasets with directed searches for better performance.

4.5. Artificial Neural Network (ANN)

The artificial neural network (ANN) model is appropriate to define non-linear, complex correlations within a time-series composed of multiple variables. The ANN model operates with an iterative machine learning process to produce robust results. ANN is inspired by human nervous systems and signal transmission. A neural network system uses input and output data to learn and train. It consists of many interconnected, identical basic-processing neurons. Each neuron is connected by links. During the training process, the links where are between neurons keep updating strength, and then all the experience and knowledge are saved in the links. ANN is powerful because it has a strong mathematical background and logical system. It is also able to deal with linear and complex non-linear relationships with a large number of input and output variables [164]. Due to the structure, there is model flexibility in adjusting to new variables.

4.5.1. Structure of ANN

The structure of an ANN model is built by a network of computing elements (called neurons) that adjust and work together to solve specific problems. The algorithm of the ANN model is originally inspired by the human nervous systems and signal transmission [165]. The neurons of the ANN model recognize incoming signals as input variables (e.g., X_1 and X_2), and the ANN model needs a term of bias (e.g., b) to increase the flexibility of the model. The input variables and bias are multiplied by the corresponding weights (e.g., W_1, W_2, and W_3). The weighted input variables are then formulated as an activation function, which is designed to process the input variables to an output variable (e.g., Y), which in turn becomes an input variable for the next neuron.

The ANN model is typically constructed in three layers of neurons: 1) input, 2) hidden, and 3) output, as shown in **Figure 8**. Each circle (also called node or unit) represents a neuron. A simplistic ANN model consists of one input layer, one hidden layer, and one output layer. However, multiple hidden layers are possible but tend to be avoided, typically resulting in overfitting.

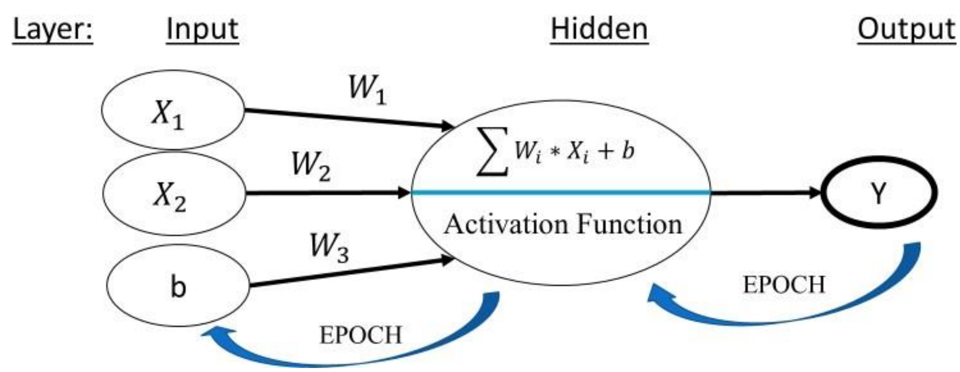

Figure 8. Structure of an artificial neural network.

There is some theoretical basis for governing the number of neurons in use. The general guidelines for determining the correct number of neurons to use in the hidden layers, such as the following [188]:

- Between the number of neurons within the input layer and output layer
- Roughly 2/3 size of the input layer, greater than the size of the output layer
- Less than twice the size of the input layer.

However, training and validating is to find the best number of hidden neurons [166]. Increasing the number of hidden layers and neurons in an ANN model increases the learning capacity. This increases the processing time and the possibility of overfitting [167]. Overfitting is a limitation of ANN, where the model tends to memorize the observations within the training set instead of extrapolating the patterns. To avoid overfitting and to fit the prescribed guidelines, an equation is recommended;

$$N_h = \frac{N_c}{(\alpha \times (N_i + N_0))} \qquad \text{Equation 4.7}$$

Where, N_h is the number of hidden neurons; N_c is the sample size of training dataset; α is an arbitrary scaling factor usually between 2-10; N_i is the number of input neurons; and N_0 is the number of output neurons.

The ANN models can be classified into feedforward and recurrent network based on the types of connections between neurons. The feedforward neural network moves only one direction, a forward path from the input layer to the output layer through the hidden layer. That is, the feedforward neural network has no connections between neurons located in the same layer. The recurrent neural network includes multidirectional network flow between the neurons in the hidden layer, as shown in **Figure 9**. It is known that feedforward neural networks are more commonly used because they are simpler and more efficient than recurrent networks [168].

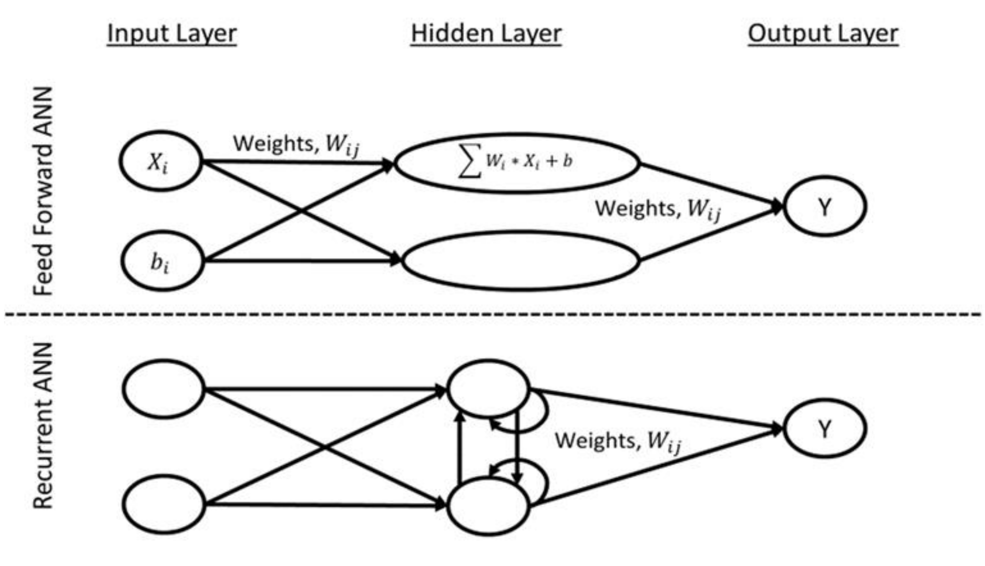

Figure 9. Structure of feedforward and recurrent neural networks.

4.5.2. Building of ANN Model

The data preprocessing to build ANN models take the first steps for data organization to detect outliers, split the data into training and validation data sets, normalize the data for the training data set, and classify input variables. The option to stationarize the data is possible (see Chapter 3.3), although there are conflicting arguments of whether machine learning models such as ANN require stationary time-series [122]. As the last proves of the ANN model building, the model validation has four steps: normalizing the input of test data, feeding normalized input test data into the model which is selected, de-normalizing the output value of the model, and comparing it to the real output value to check whether error measures (e.g., root-mean-square error (RMSE) and mean absolute error (MAE)) are satisfied. The method of modifying the weights between the network layers to reach the desired output in an ANN model is called a training or learning process [169]. ANN learning methods can be categorized as supervised, unsupervised, and reinforcement learning. The main principle of the supervised learning method analyzes the difference between the values of input and output data for a training process that adjusts the weights of the neuron connections between two different layers (e.g., input and hidden layers or hidden and output layers). The supervised learning method continues the training process until there is an acceptable output value found. The supervised learning of the ANN model is efficient in classification when the output variable is a category (e.g., "right" or "wrong") and regression when the output variable is an actual measurement (e.g., "concentration" or "weight") [170]. The unsupervised learning method has no consideration of output data for a learning process. In other words, the main purpose of the unsupervised learning method is to map inferences from input data from unlabeled responses. In general, it is used in clustering problems to searching for characteristic groupings within the dataset, such as categorizing clients by purchase patterns [171].

The reinforcement learning method is similar to the supervised learning method in its training process, but the output data is not provided to the network. The reinforcement training uses trial and error to maximize a performance index called a reinforcement signal that is to reflect the success or failure of the entire system after some sequences of actions have been performed [172]. The reinforcement signal can be positive or negative, which can refer to rewards or punishments. For example, if the robot operates well, then the learning system returns a positive value (i.e., reward), but if not, the system returns a negative value (i.e., punishment). The system takes these retunes to improve itself based on the trial-and-error process [173].

The three learning methods to utilize for training: supervised, unsupervised, and reinforcement learning. Zhou [100] finds that the supervised learning method is the most efficient in forecasting problems because the historical input and output data are available; hence, the system can directly learn from the output data and minimize the error between the future observed and predictive values. The well-known training algorithms for the supervised learning method include back-propagation network, probabilistic network, counter-propagation network, and others. The back-propagation algorithm based on the feedforward neural network is a prevalent method due to the relative simplicity [174]. The feedforward back-propagation neural network directs a one-directional signal (feedforward) from the input, hidden, and output layers. The feedforward back-propagation neural network takes three steps as follows: 1) input neurons distribute data forward through to the hidden layer; 2) data is processed through an activation function and directed into the output layer, and 3) residuals are distributed back into each neuron link to adjust weights for optimization, see **Figure 10** [173].

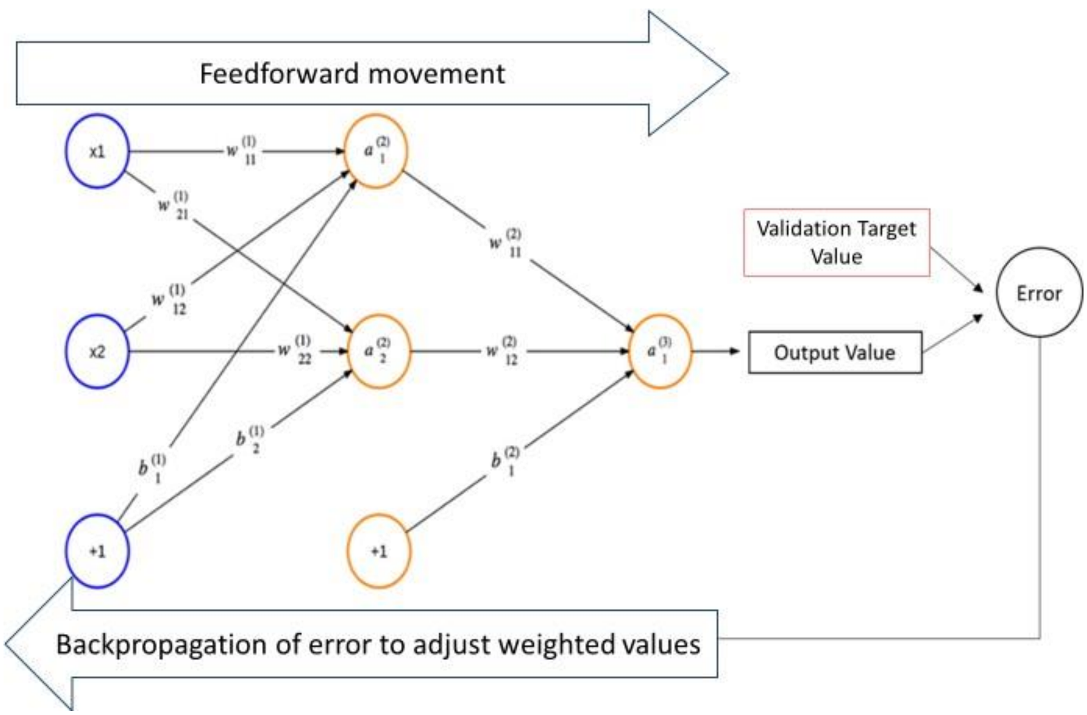

Figure 10. Example of feedforward back-propagation neural network.

Figure 10 shows the example for the feedforward and backpropagation processes that include two neurons in the input layer, two neurons in the hidden layer, and one neuron in the output layer.

The input and hidden layers also include one neuron for bias. The preliminary value of the bias neuron is assumed to be 1, but the value of biases can adjust to the other values. The links connecting any two neurons in the different layers are associated with weights. These preliminary weights are randomly selected from a given range for the neural network.

The values to the neurons (e.g., x1 and x2) and the value of the bias neuron in the input layer are proportioned by the weights assigned to the neurons in the hidden layer for the input values. The proportioned values of the input and bias neurons are then summed to generate y1 and y2 for the two neurons in the hidden layer as follows:

$$y1 = x1 \times w_{11}^{(1)} + x2 \times w_{12}^{(1)} + b_{1}^{(1)} \times 1$$ Equation 4.8

$$y2 = x1 \times w_{21}^{(1)} + x2 \times w_{22}^{(1)} + b_{2}^{(1)} \times 1$$ Equation 4.9

The weighted sums (e.g., y1 and y2) for the hidden neurons are transformed for a non-linearity property of the ANN model by one of three activation functions: logistic activation function, hyperbolic tangent activation function, and linear-activation function. The activation function is the non-linearity element of the ANN model. The logistic activation function generates all output values between 0 and 1. The logistic activation function is defined by Equation 4.10. The hyperbolic tangent activation function generates all values between -1 and 1, seen in Equation 4.11. The linear-activation function generates the same values as the input values, seen as Equation 4.12.

$$F(X) = \frac{1}{1 + e^{-s}}$$ Equation 4.10

$$F(X) = \frac{2}{(1 + e^{-2s})} - 1$$ Equation 4.11

$$F(X) = X$$ Equation 4.12

where *X* = hidden neuron inputs

Equations 4.13 and 4.14 show the transformed values (e.g. $a_1^{(2)}$ and $a_2^{(2)}$) of the weighted sums by the activation function, *fn*.

$$a_1^{(2)} = fn(y1)$$ Equation 4.13

$$a_2^{(2)} = fn(y2) \qquad \text{Equation 4.14}$$

The transformed values of the hidden neurons and the value of the bias neuron in the hidden layer are computed as the weighted sum (= y3) for the input of the neuron in the output layer as follows:

$$y3 = a_1^{(2)} \times w_{11}^{(2)} + a_2^{(2)} \times w_{12}^{(2)} + b_1^{(2)} \times 1 \qquad \text{Equation 4.15}$$

The input of the output neuron is then transformed for the final output of the ANN model as follows:

$$a_1^{(3)} = fn(y3) \qquad \text{Equation 4.16}$$

Once the feedforward process is completed, the backpropagation process first calculates the error between the final output in the output layer and an actual output value using a partial derivative. For example, the error of the transformed value, $E_{a_1^{(3)}}$, is calculated by Equation 4.17, where $Target_{a_1^{(3)}}$ is desired output value and $Out_{a_1^{(3)}}$ is given by Equation 4.12which is the output value of $a_1^{(3)}$:

$$E_{a_1^{(3)}} = Out_{a_1^{(3)}} \times (1 - Out_{a_1^{(3)}}) \times (Target_{a_1^{(3)}} - Out_{a_1^{(3)}}). \qquad \text{Equation 4.17}$$

The error, $E_{a_1^{(3)}}$, is then considered to adjust the weights of the neuron connections (e.g., $w_{11}^{(2)}$ and $w_{12}^{(2)}$) in Equation 4.15 by the following Equations 4.18 and 4.19:

$$W_{11}^{+(2)} = W_{11}^{(2)} + 5E_{a_1^{(3)}} Out_{a_1^{(2)}} \qquad \text{Equation 4.18}$$

$$W_{12}^{+(2)} = W_{12}^{(2)} + 5E_{a_1^{(3)}} Out_{a_2^{(2)}} \qquad \text{Equation 4.19}$$

In Equations 4.18 and 4.19, $W^{+(2)}_{11}$ and $W^{+(2)}_{12}$are the adjusted weights, $Out_{a_1^{(2)}}$ and $Out_{a_2^{(2)}}$ are given by Equations 4.13 and 4.14, which are output values of $a_1^{(2)}$ and $a_2^{(2)}$, respectively, in the hidden layer, and the symbol *4* represents a learning coefficient between 0 and 1, which is determined by a user. Determining the constant learning coefficient for an ANN model is usually a tedious process requiring much trial and error. If *4* is too high, the training process may become unstable and oscillate widely; if *4* is too low, the training process may take more time to converge or not converge.

The backpropagation process also calculates the errors of the transformed values in the hidden layer (e.g., $E_{a_1^{(2)}}$ and $E_{a_2^{(2)}}$), hereby Equations 4.20 and 4.21:

$$E_{(2)} = Out_{(2)} \times (1 - Out_{(2)}) \times (E_{(3)} W^{(2)}). \qquad \text{Equation 4.20}$$

a_1 a_1 a_1 a_1 11

$$E_{a_2^{(2)}} = Out_{a_2^{(2)}} \times (1 - Out_{a_2^{(2)}}) \times (E_{a_1^{(3)}} W_{12}^{(2)}). \quad \text{Equation 4.21}$$

After calculating the errors, $E_{a_1^{(2)}}$ and $E_{a_2^{(2)}}$, the weights between the input layer and hidden layer are updated (e.g., $W_{11}^{+(1)}$, $W_{12}^{+(1)}$, $W_{21}^{+(1)}$, and $W_{22}^{+(1)}$) by Equations from 4.22 to 4.25. Where In_{X1} and In_{X2} are the input values of input neurons.

$$W_{11}^{+(1)} = W_{11}^{(1)} + 5E_{a_1^{(2)}} In_{X1} \quad \text{Equation 4.22}$$

$$W_{12}^{+(1)} = W_{12}^{(1)} + 5E_{a_1^{(2)}} In_{X2} \quad \text{Equation 4.23}$$

$$W_{21}^{+(1)} = W_{21}^{(1)} + 5E_{a_2^{(2)}} In_{X1} \quad \text{Equation 4.24}$$

$$W_{22}^{+(1)} = W_{22}^{(1)} + 5E_{a_2^{(2)}} In_{X2} \quad \text{Equation 4.25}$$

The process above is just a one-time training process, also called one epoch. An epoch is one cycle of the feedforward and backpropagation to update the weights. In general, in the ANN model, this process repeatedly runs several times until the ANN model finds the minimum error [173]. There is caution in over-training the model as it will fall into overfitting the data. This is one of several limitations for the ANN model. Other limitations of ANN are: 1) bias-variance tradeoff, 2) complexity, 3) standardization of input values, 4) hidden patterns within the output values, 5) heterogeneity of data, 6) redundancy in the data, and 7) the presence of interaction and non-linearities [175].

4.6. Exponential Smoothing with Gradient Boosting

Exponential smoothing with gradient boosting is another form of hybrid modeling designed for short-term forecasting [176]. The double exponential smoothing forecasting is improved by fitting the residuals with a gradient boosting algorithm. Gradient boosting is an iterative procedure. Optimization steps are taken following each stage, with residuals from the previous step are fit using a decision tree learning method. This method is flexible and powerful but requires fine-tuning of many parameters. The issue with exponential smoothing still lingers with the inability to adjust to additional variables once a validation model is established.

4.7. Hybrid SARIMA-ANN

The idea of combining ARIMA with ANN was first introduced by Zhang [111], but this model was limited to non-seasonal data. However, future studies expanded on this research [177-179]. These studies focus on building ARIMA models and utilizing the error in the outputs, residuals, as inputs into their ANN models. Wang and Meng [179] showed promising results in energy consumption for the region of Hebei in China. Moeeni [180] pushes further with this research to predict the monthly water inflow of a dam. The data is comprised of 30 years of monthly values with evidence of extreme seasonal variance. Extreme seasonal variance is an issue not addressed by recent hybrid model studies. The Moeeni [180] framework is set up as a series with residuals of the SARIMA model feeding into the ANN model, as seen in **Figure 11**. The series Hybrid SARIMA-ANN model initially calls for the production of a linear forecast through a SARIMA model. The results are compared to a validation data set, and residuals are produced. The hybrid concept of the model routs the residuals into an ANN model to determine non-linear residual patterns that were missed by the SARIMA model. The ANN output is used as an adjustment to produce a final forecast output.

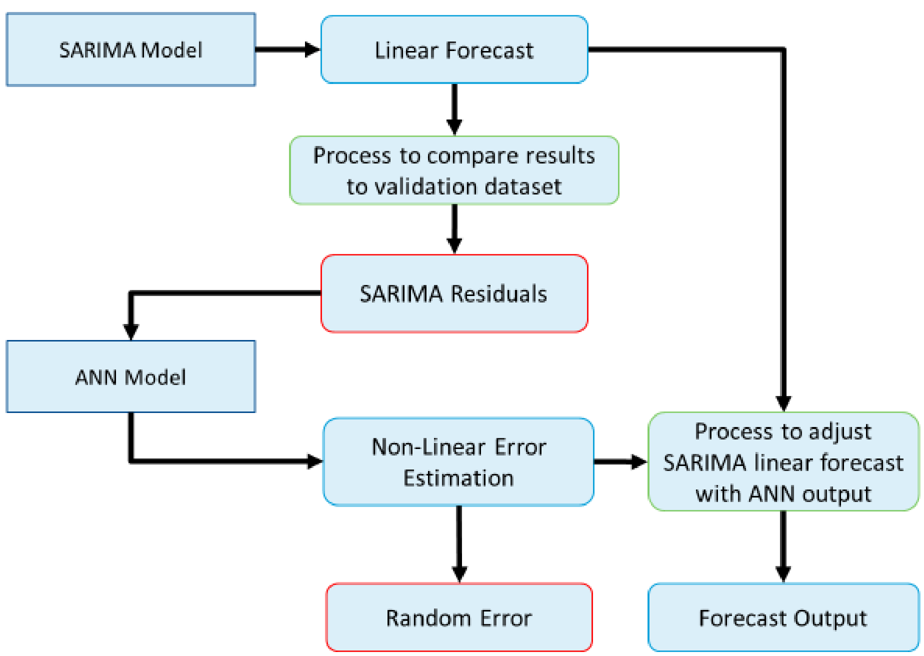

Figure 11. Series hybrid SARIMA – ANN model proposed by [180].

The hybrid SARIMA ANN model was able to capture the extreme seasonality. However, the performance fails to accurately forecast baseline values in comparison to SARIMA. This framework does not fully utilize the potential of the ANN network by providing little training data. In many past hybrid model frameworks, there is a focus on utilizing the linear residuals to use as the ANN input. This concept of hybrid model framework relies heavily on linear modeling, remaining subjective to how well one model is built. The concept also assumes that the real-world data provided is more linear in nature as it is the predominant model.

Chapter 5. Modified Model Proposal

The management of water and energy is critical to human progress and urban sustainability. Models are necessary to guide decisions and implementation of WEN systems, including resource management and institutional policy involving WEN infrastructure. The complexities of WEN studies require vast amounts of data. With data accessibility limited, the middle-out approach using the univariate time-series model serves as an initial validation model for further model building and WEN study expansion. Hybrid models have shown promise in combining the strengths of linear and non-linear modeling, highlighting the strengths of both model approaches.

5.1. Parallel Hybrid SARIMA-ANN (PHSA)

In order to improve the model performance of traditional linear modeling while gaining model flexibility, this research proposes adjusting the hybrid SARIMA-ANN model structure. The former model is set up as a series, with the SARIMA residuals feeding into the ANN model to capture non-linear patterns. The proposed parallel hybrid SARIMA-ANN model calls for two parallel models, SARIMA and ANN, where model inputs are fed the same time-series with results combined through a simple second ANN for an accurate forecast, as seen in **Figure 12**. This is different from many other current hybrid models that focus on a series framework feeding residuals of the linear model into non-linear models. The objective of the Parallel Hybrid SARIMA-ANN (PHSA) design is to forecast seasonal time-series of univariate data without overreliance on results of initial linear model results. This objective is achieved through the following specific steps:

1. Preliminary stage of data preparation
    - A. Visualize and preprocess data
    - B. Data split into training and validation datasets
2. Analyze and forecast energy consumption with univariate data analysis:
    - A. Seasonal Auto-Regression Integrated Moving Average (SARIMA)
    - B. Artificial Neural Network (ANN_0)
3. Combine linear (SARIMA) and non-linear (ANN_0) forecast into ANN_1 model

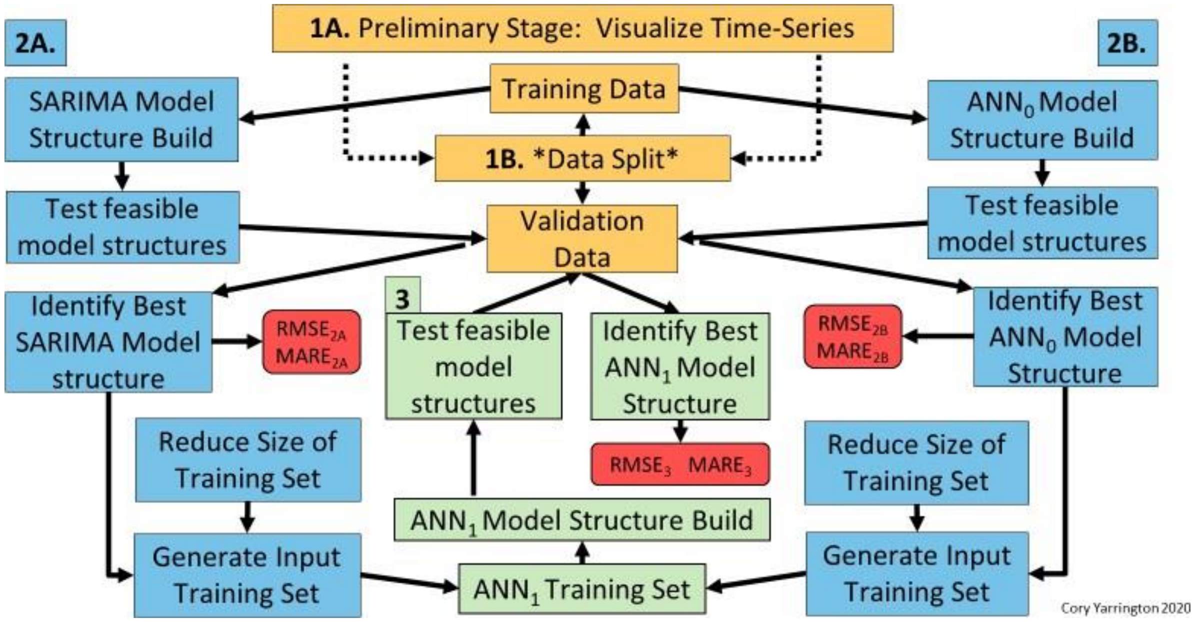

Figure 12. Parallel hybrid SARIMA-ANN model.

In comparison to SARIMA, ANN, and series Hybrid SARIMA-ANN, the proposed PHSA structure embraces the power and flexibility of ANN. The entire time-series is analyzed by the ANN model. The parallel framework retains the ANN ability to work with univariate data as well as multivariate data, another fault of the previous Hybrid SARIMA-ANN model. The PHS-A model analyzes and forecasts univariate data analysis using Seasonal Auto-Regression Integrated Moving Average (SARIMA) and Artificial Neural Network (ANN), separately; then combines the results into a second ANN to fit in outputs with higher forecast accuracy. This framework works to properly highlight the strengths of both systems and does not limit the ANN model to one variable.

5.2. Case Study: Morgantown, WV Apartment

The data within this case study is composed of monthly electricity consumption (kWh) within an apartment building from 2005-2016 in Morgantown, WV. This data set was used to demonstrate the parallel hybrid SARIMA-ANN model. Results were compared to SARIMA, ANN, and series hybrid SARIMA-ANN models.

5.2.1. Preliminary Stage (Steps 1A and 1B)

The data is preprocessed through preliminary steps 1A and 1B to have prepared the dataset for initial model builds. The preliminary step 1A enables a breakdown of the time-series to see hidden trends that need to be captured by models, see **Figure 13**. Once these trends are understood through various testing from step 1A, preprocessing of the data can be done to transform the time-series into a stationary time-series. However, it is up to the model designer to incorporate these trends within the model or transform the data before input (refer to chapter 3.3 on data preprocessing). The application of these test results guided the structure design of both SARIMA and ANN_0.

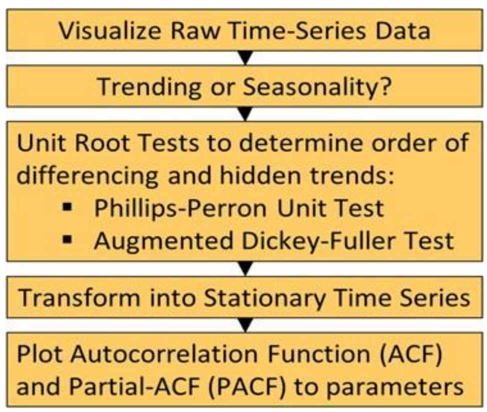

Figure 13. Preliminary stage part 1A.

Before model design specifications were attempted, the raw time-series was visualized to determine if there are any hidden trends and/or patterns of seasonality, see **Figure 14**. The increased mean over time indicated a positive trend. The month-to-month variation of values in relation to the indicates covariation issues. Both of these patterns are evidence of non-stationarity within the time-series. **Figure 15** illustrates an alternative view to the raw data with monthly max, min, and average values. This is further visual evidence of seasonal variation. Specific monthly datasets of note that will be difficult to capture in a robust model are January and September. The month of January shows the widest range between max and min values at 11,000 kWh difference. The September to October average values show the largest decrease between month averages (5,000 kWh). Capturing these monthly values in the validation model will show model resiliency to extreme seasonality trends in time-series data.

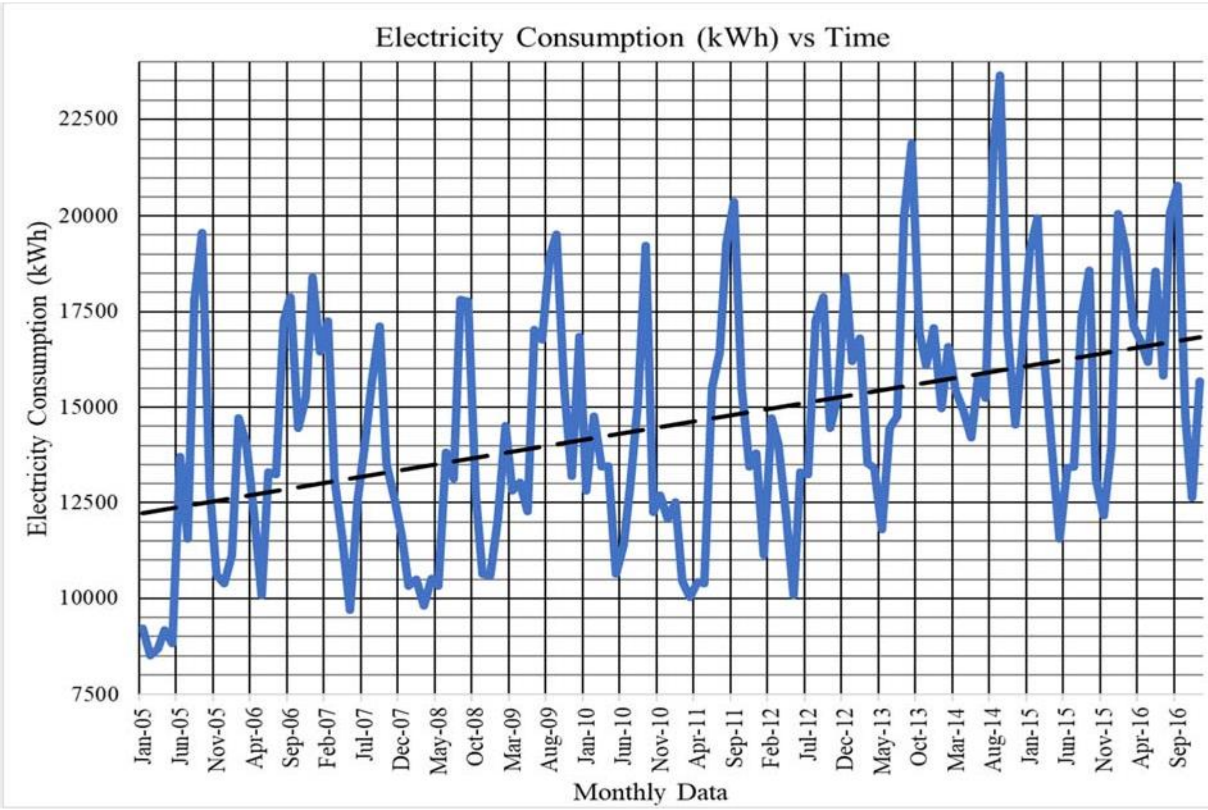

Figure 14. Visualize the raw time-series with notable trending.

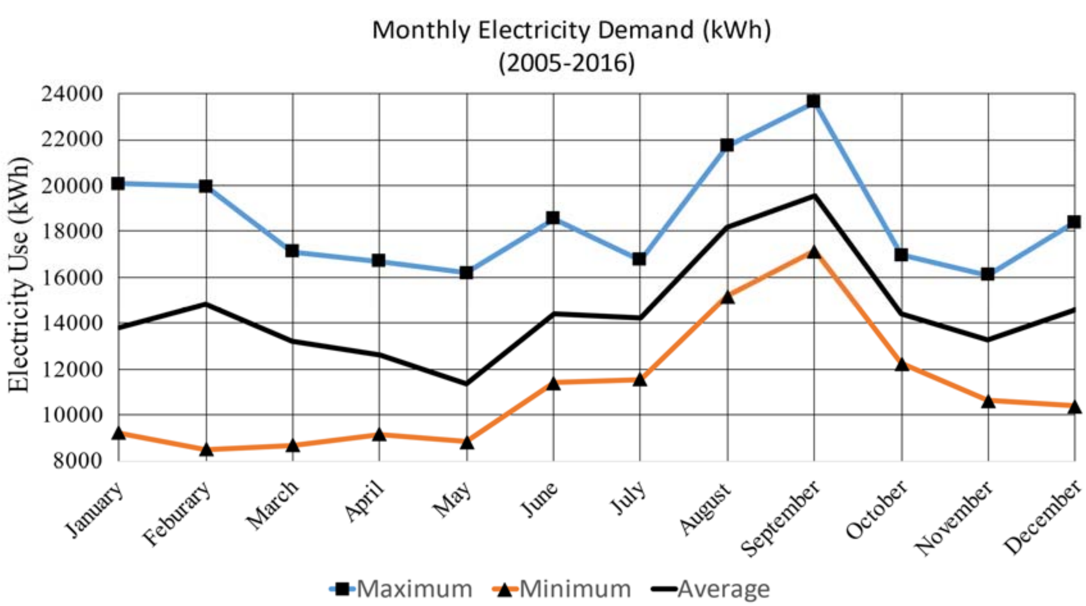

Figure 15. Time-series monthly max, min, and average showing seasonal variation.

After visualizing the time-series, it is expected to find hidden patterns within the time-series through statistical tests. Unit root testing for time-series stationarity with Phillips-Perron (PP) and Augmented Dickey-Fuller (ADF) test shows the time-series is not stationary with a 12-month lag, see **Table 3**. All t-test values pass the critical t-distribution values of < -3.45 (provided in Table 2) except for the ADF 12-month lag test value. This confirms hidden seasonal 12-month trends within the time-series, as was indicated by the analysis of **Figure 15**. The ADF lag 1 test provides an opportunity to transform the series and conduct ACF and PACF plotting to further understand the hidden trends.

Table 3. Unit root testing results.

Test	Lag	Test Value	Stationary	Result Utilization
Phillips-Perron	4	-51.36	Y	Reveal trend within 12 months
Augments Dickey-Fuller	1	- 6.48	Y	Allows ACF-PACF plot
Augments Dickey-Fuller	4	- 5.02	Y	Reveal trend within 12 months
Augments Dickey-Fuller	12	- 3.11	N	Reveal overall 12-month trend
Test value must be <-3.45 critical t-distribution value with trend and 100 samples at 95% certainty.				

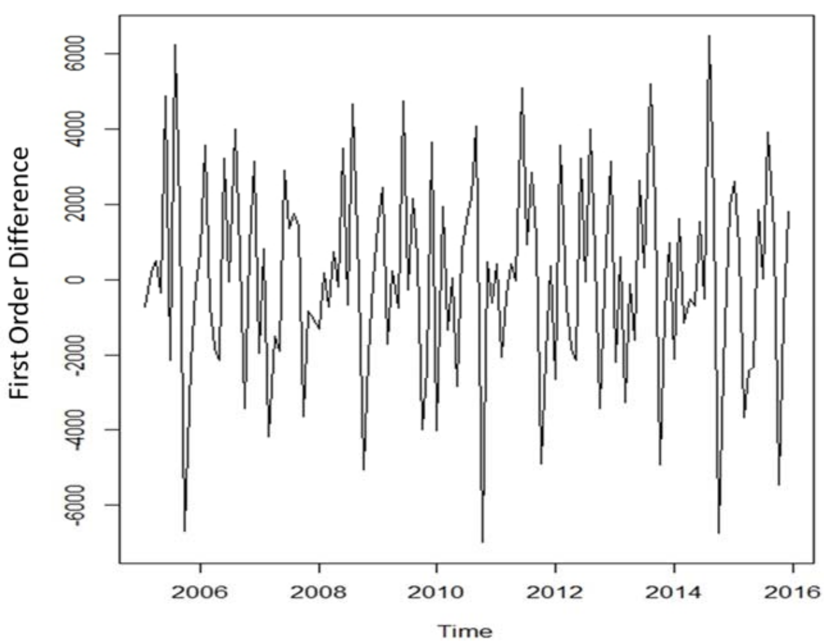

Figure 16. First-order difference of time-series.

Transformation of the time-series to remove trend was conducted through a first-order difference transformation, see **Figure 16**. There remains to be evidence of extreme seasonality with a high variation of values month to month from the mean, indicated by the large spikes followed by smaller spikes on the graph. The ACF and PACF plots confirm there is seasonality in the first-order difference time-series; see **Figures 17** and **18**. Major positive correlations are found breaching the significance guideline (indicated by the dotted line) at the seasonal lags 1, 2, and 3 in the ACF plot. There are smaller correlation patterns between the 1, 2, 3, 4, and 6 months in the ACF plot. Both of these patterns are circles in **Figure 17**. The PACF plot indicates similar patterns in **Figure 18**.

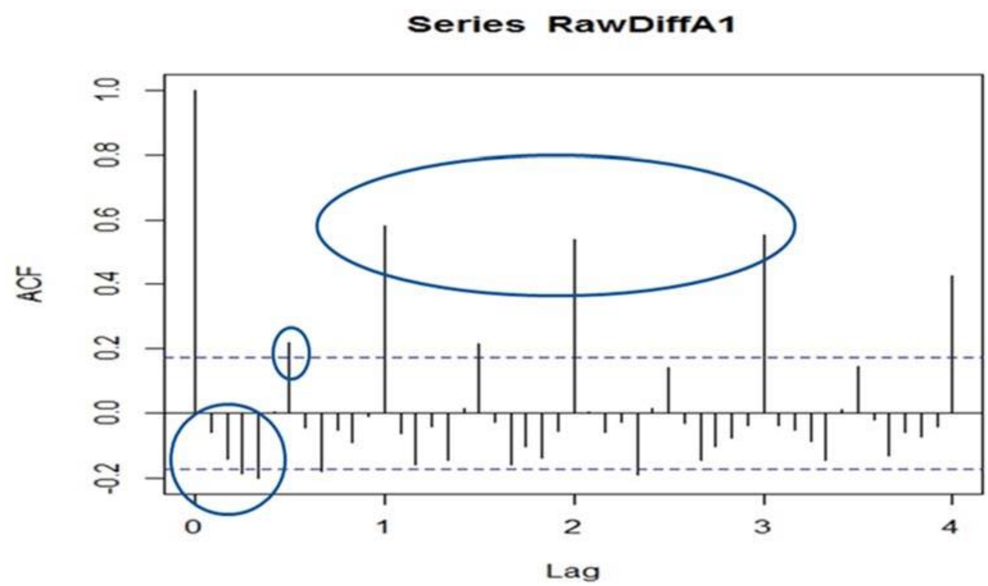

Figure 17. ACF of first-order difference time-series.

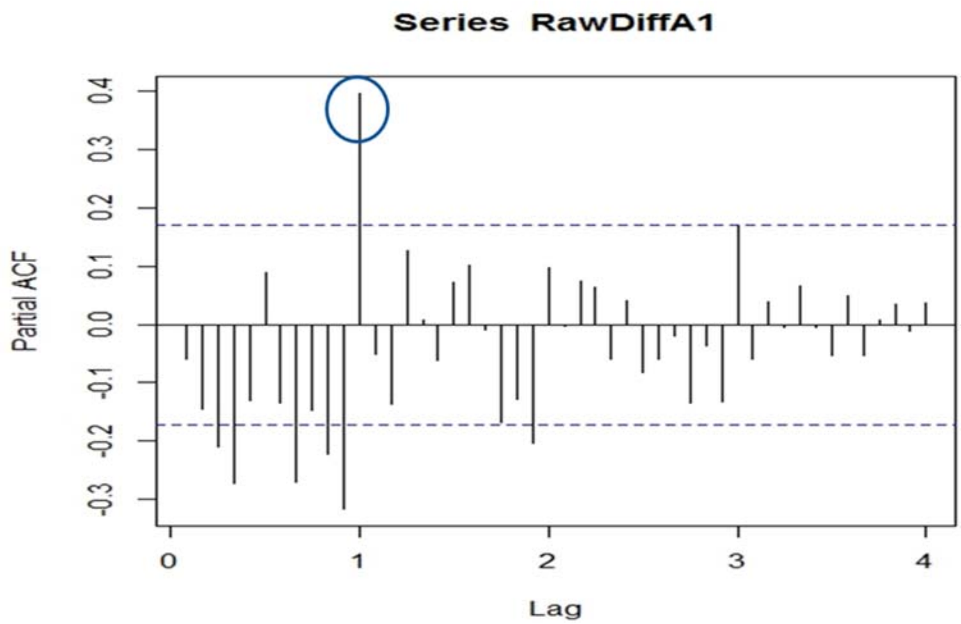

Figure 18. PACF plot of first-order difference time-series.

In order to address the seasonality in the time-series, a 12-order transformation (12 lag) was implemented, see **Figure 19**. The time-series was tested as before to be thorough. The ACF and PACF plots were done for the seasonal differenced time-series; see **Figures 20** and **21**. The guidelines to interpreting ACF and PACF plots [162] indicate: 1) positive autocorrelations out to a high number of lags requires a higher order of differencing, 2) If lag-1 autocorrelation is zero or negative, indicates higher order of difference is <u>not</u> necessary, and 3) If the lag-1 autocorrelation is -0.5 or more negative, the series may be <u>over-differenced</u>. The over-differencing can be adjusted by additional terms in the model.

Both plots indicate a non-stationary time-series with autocorrelation at lag 1. Therefore, it is understood the initial model constructed must contain a variable to capture the seasonal, 12-month autocorrelation as well as addressing correlation issues at lower lag values. The seasonal variable can be addressed by feeding the lag-12, seasonal differenced time-series into the models or by structuring models to process the seasonal correlation. Both SARIMA and ANN models have the ability to address both the seasonal and local (lag 1-4) correlations.

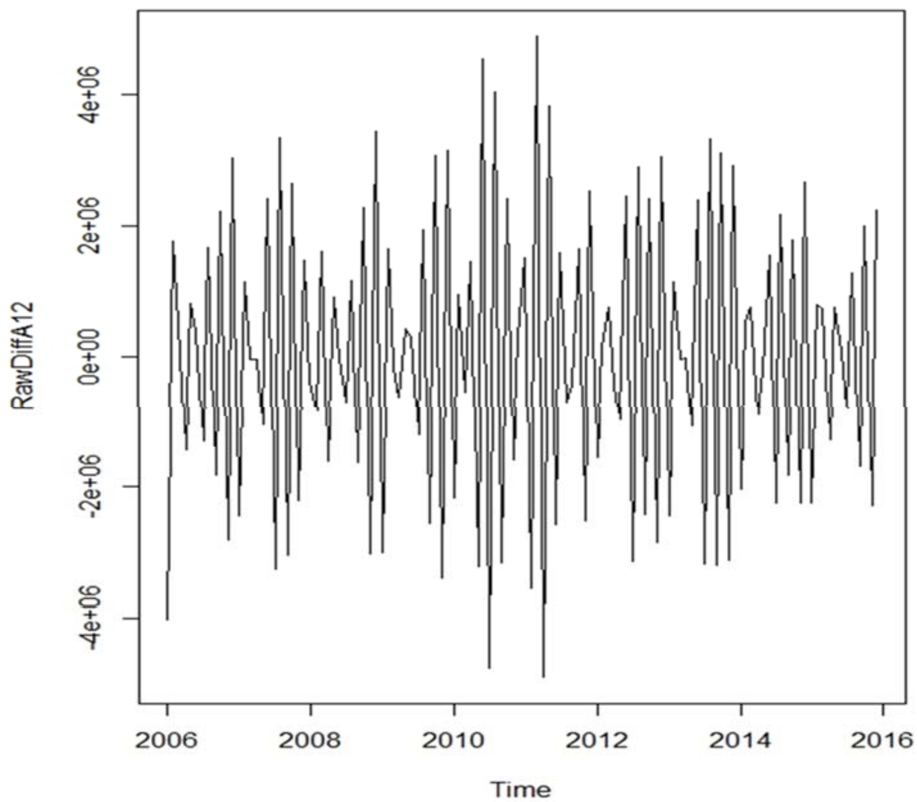

Figure 19. Seasonal (12 lag) differenced time-series.

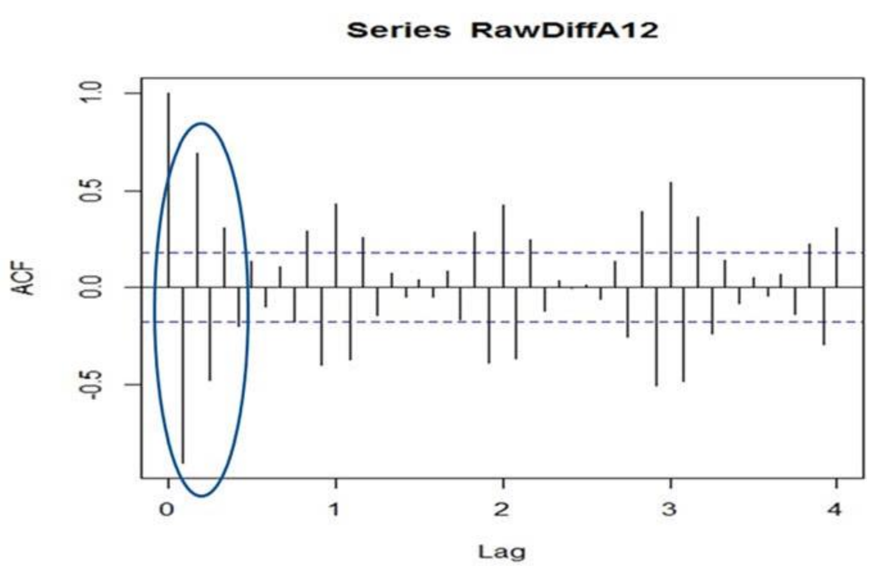

Figure 20. ACF plot of seasonal (12 lag) difference time-series.

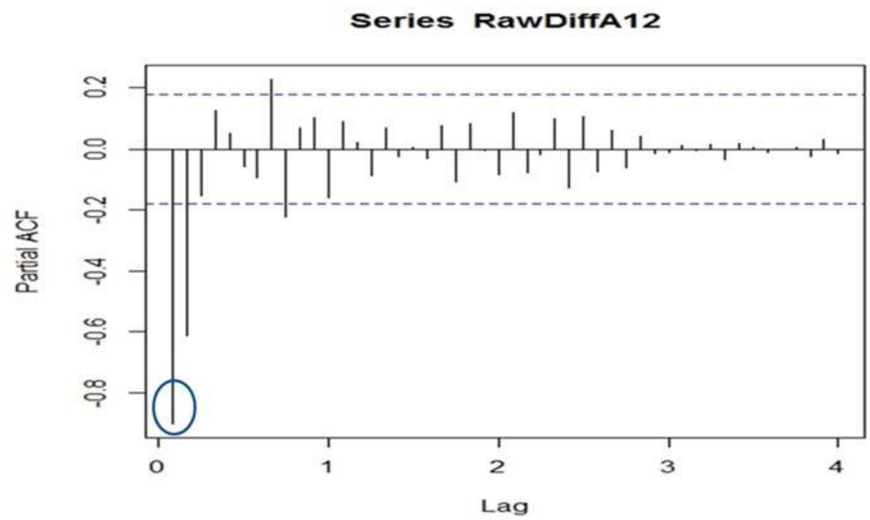

Figure 21. PACF plot of seasonal (12 lag) differenced time-series.

To finish the preliminary stage with 1B, the time-series was split into the training and final validation datasets, see **Figure 22**. The final validation dataset remained unknown to the models until final forecasts were compared. The SARIMA training dataset that retains more data points as the years of 2005-2006 were consumed by the ANN model data preprocessing, requiring the lags of 1- 4 months and 1-2 years in order to capture the autocorrelations identified in step 1A.

Model	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016
$SARIMA_0$	Training data - 132 Points 11 Year Cycles											Validation

Model	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016
ANN_{0v}	Training data - 96 Points 9 Year Cycles									Validation

Figure 22. Data split for training and final validation datasets.

5.2.2. PHSA construction (Steps 2A and 2B)

After the preliminary stage, the process continued to 2A and 2B (refer back to **Figure 12**). The unit root test results and ACF/PACF plots provide a guide to initial model structures for 2A and 2B, see **Figure 23**. Both SARIMA and ANN models must be able to capture the seasonal and local autocorrelations indicated in step 1A. The SARIMA model (1, 0, 0) $(0, 1, 0)_{12}$ assumes a seasonal value from an independent random walk. The additional non-seasonal AR-term preserves seasonal patterns and lowers the amount of differencing required. This increases the stability of the trend and response to cyclical turning points. The 7x5x1 ANN_0 structure was suggested by Zhang [111] to ensure robustness while maintaining simplicity in the model. In addition, seven is the number of inputs that seem to hold a correlation identified in step 1A. The ACF and PACF plots show peak correlations at 1, 2, 3, 4, 6, 12, and 24 months.

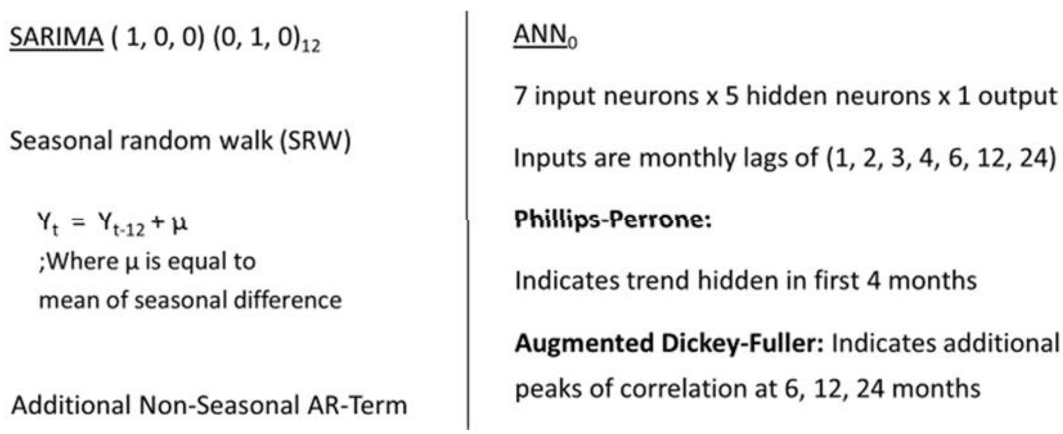

Figure 23. 2A and 2B initial model structures.

Step 2A focuses on the SARIMA build. The initial SARIMA model is the seasonal random walk (SRW); see **Figure 24**. The seasonal random walk model predicts that next year's seasonal cycle will have exactly the same shape (i.e., the same relative month-to-month changes) as this year's seasonal cycle. This is the typical initial model for SARIMA model building. However, step 1A has already shown evidence of additional terms to capture local, non-seasonal autocorrelations. The following step is to plot residential ACF. Expected failure leads to the application of 13 rules for additional optimal SARIMA parameters described in section 4.2 [162]. Multiple feasible

SARIMA models are constructed with these rules as a guide and compared using Akaike Information Criterion (AIC) and significance of coefficient.

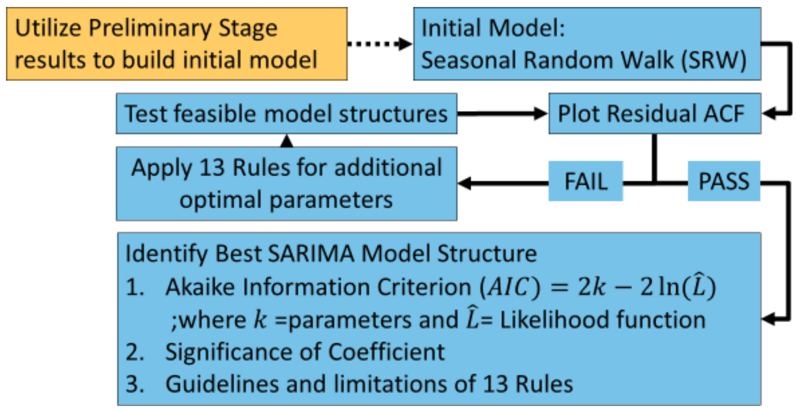

Figure 24. Fundamentals for building SARIMA model

To address this local auto-correlation, there is an additional non-seasonal AR-term to capture the month's prior influence. The initial SARIMA model (1, 0, 0) $(0, 1, 0)_{12}$ forecast results are compared to the validation dataset set aside in step 1B. The difference in forecast and validation values produces the model residuals. The residual ACF plot provides a pass-fail sequence to establish whether there is evidence of autocorrelation within the residuals of the model. If there is a pattern, or correlation, within the residuals, it indicates the need for additional terms. The tests provide an initial model for evaluation. However, variations of this model provide options with changes in non-seasonal and seasonal AR, MA, and differencing terms, see **Figure 25**. These models allow for a balance between model parsimony, optimization, and accuracy. The choice of model depends on the application of the result. Models may provide wide or narrow confidence, trending may be higher or lower, and the model may be overfitted or underfitted. Testing and applying a standard qualifying best fit model is necessary for the following step.

AutoSARIMA Model Structures		Designed SARIMA Model Structures	
$(2,0,2)(1,1,1)_{12}$	$(2,0,2)(1,1,0)_{12}$	A* $(1,0,0)\ (0,1,0)_{12}$	M $(0,0,1)\ (1,0,1)_{12}$
$(0,0,0)(0,1,0)_{12}$	$(1,0,2)(2,1,1)_{12}$	B* $(1,0,0)(2,1,0)_{12}$	N $(0,0,2)\ (1,0,1)_{12}$
$(1,0,0)(1,1,0)_{12}$	$(3,0,2)(2,1,1)_{12}$	C $(0,1,1)\ (0,1,1)_{12}$ SES	O $(0,0,1)\ (1,0,2)_{12}$
$(0,0,1)(0,1,1)_{12}$	$(2,0,1)(2,1,1)_{12}$	D $(0,1,1)\ (0,0,1)_{12}$	P $(0,0,1)\ (0,1,2)_{12}$
$(0,0,0)(0,1,0)_{12}$	$(1,0,0)(2,1,1)_{12}$	E $(1,1,0)\ (0,0,1)_{12}$	Q* $(0,0,2)\ (0,1,1)_{12}$
$(2,0,2)(0,1,1)_{12}$	$(1,0,0)(2,1,1)_{12}$	F $(1,0,1)\ (0,1,1)_{12}$	R $(0,0,2)\ (1,0,2)_{12}$
$(2,0,2)(2,1,1)_{12}$	$(1,0,0)(1,1,1)_{12}$	G $(1,1,0)\ (0,1,1)_{12}$	S $(0,0,2)\ (0,1,2)_{12}$
$(2,0,2)(2,1,0)_{12}$	$(1,0,0)(2,1,0)_{12}$	H $(0,1,1)\ (1,0,1)_{12}$	T $(0,0,2)\ (1,1,2)_{12}$
$(2,0,2)(2,1,2)_{12}$	$(1,0,0)(2,1,2)_{12}$	I $(0,1,1)\ (1,0,2)_{12}$	U $(1,0,1)\ (0,1,1)_{12}$
$(2,0,2)(1,1,0)_{12}$	$(0,0,0)(2,1,1)_{12}$	J $(0,1,0)\ (0,1,0)_{12}$	V $(0,0,1)\ (2,1,0)_{12}$
$(1,0,2)(2,1,1)_{12}$	$(2,0,0)(2,1,1)_{12}$	K $(0,1,0)\ (1,1,0)_{12}$	W $(0,0,2)\ (2,1,0)_{12}$
$(2,0,2)(2,1,2)_{12}$	$(1,0,1)(2,1,1)_{12}$	L $(0,0,1)\ (0,1,1)_{12}$	X* $(1,0,0)\ (1,1,0)_{12}$

Figure 25 Testing all feasible SARIMA structures

The feasible models were run through the process discussed in chapter 4.2. Models were compared by AIC, σ^2, and significance of variable. The Akaike Information Criteria (AIC) is a widely used measure of a statistical model to quantify the goodness-of-fit as well as the simplicity of the model. This combines model accuracy and parsimony in one indicator. When comparing the two models, the one with the lower AIC is generally "better." This is not the only deciding factor. There is a craft to ARIMA model construction with guidelines. All feasible models are reviewed with these guidelines to understand what each model structure is accomplishing with the various terms within the structure. Multiple differencing terms cause a loss of original data formatting, and multiple AR-MA terms can be conflicting in their implementation. After a thorough review of all feasible models in Figure 26, the list of feasible models is reduced to four choices, see **Figure 26**. These four models reduce differencing to one seasonal difference and rely on 1-3 additional terms to capture the other indicated correlations. Reducing the number of additional terms increases the significance of the variable, determined by the coefficient divided by the standard error. Although the AIC and σ^2 are not the best in comparison to the other four models. The model X (1, 0, 0) (1, 1, 0) provides the best fit model equation;

$$0.7467(B)(-0.5317(B)^S)(1-B^s)^D y_t = s_t \qquad \text{Equation 5.1}$$

Identification of Best SARIMA Model				
Name Model	A $(1,0,0)\ (0,1,0)_{12}$	B* $(1,0,0)(2,1,0)_{12}$	Q $(0,0,2)\ (0,1,1)_{12}$	X $(1,0,0)(1,1,0)_{12}$
AIC	2171	2097	2114	2138
Sigma^2	4054367	1684313	2217172	293992

SARIMA 'X' $(1,0,0)(1,1,0)_{12}$

Equation: $$\boldsymbol{\phi_p(B)\Phi_P(B)^S(1-B^s)^D y_t = \varepsilon_t}$$

Coefficients:	AR (ϕ_1)=	0.7467	SAR (ϕ_{12})=	-0.5317
Standard Error:		/0.0625		/0.0801
Significance of Variable:		11.947		-6.6380

Equation: $$\mathbf{0.7467(\mathit{B})(-0.5317(B)^S)(1-B^s)^D y_t = \varepsilon_t}$$

Figure 26. Identification of best-fit SARIMA model

Step 2B focuses on the ANN build. The build process is composed of data preprocessing (blue), model structure design (green), and validation process (red), see **Figure 27**. The process is similar to the process in chapter 4.5. Adjustments are made to the model structure (i x n x 1), with i representing a number of inputs and n representing a number of hidden neurons.

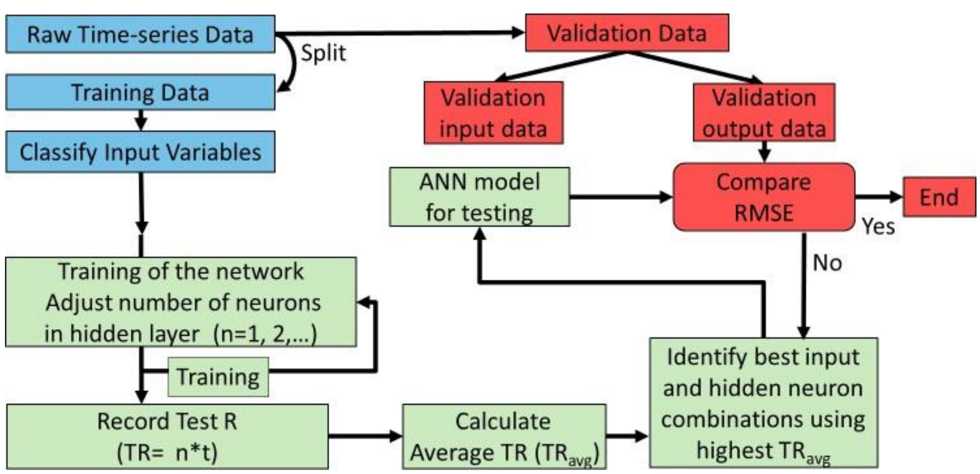

Figure 27. Fundamental process for building ANN

All feasible models are reviewed. Model structures vary by input lags, transfer functions, and the number of hidden nodes. After a thorough review of all feasible models in **Figure 28**, the list of feasible models was compared by R^2. The initial structure, 7x5x1, proved to be the best ANN model with a 0.89 R^2 and fits the guidelines discussed in chapter 4.5.1 that maintains the number of hidden nodes should be less than input nodes.

Model	**A**		**B**		**C**		**D**		**E**		**F**	
Input Lags	(1, 2, 3, 4, 6, 12, 24)		(1 ,4, 12, 24)		(4, 6, 12, 24)		(1, 2, 6, 12)		(1, 2, 4, 12, 24)		(1, 4, 6, 12, 24)	
Transfer Function	Tan	Log	Tan	Log	Tan	Log	Tan	Log	Tan	Log	Tan	Log
Hidden Nodes												
5	0.846	0.890	0.830	0.839	0.689	0.685	0.777	0.689	0.832	0.857	0.811	0.809
6	0.833	0.855	0.809	0.837	0.694	0.688	0.755	0.789	0.874	0.862	0.798	0.801
7	0.829	0.878	0.856	0.837	0.698	0.699	0.775	0.781	0.880	0.868	0.798	0.807
8	0.789	0.804	0.807	0.829	0.688	0.684	0.769	0.763	0.848	0.853	0.817	0.819
9	0.811	0.808	0.829	0.811	0.698	0.682	0.752	0.784	0.861	0.834	0.803	0.801
10	0.768	0.791	0.842	0.842	0.699	0.685	0.782	0.689	0.860	0.849	0.825	0.820

Identification of Best ANN_0 Model Structure: 7 Input x 5 Hidden x 1 Output

Transfer Function: Log Sigmoid **Input Lags:** 1, 2, 3, 4, 6, 12, 24

Figure 28. Testing all feasible ANN_0 model structures.

5.2.3. Construction of ANN_1 and forecast combination (Step 3)

After testing for the best model structure, the training datasets were reduced for both 2A and 2B; refer to **Figures 29** and **30**. In order to provide forecast residuals for the following ANN_1 model, the training data is reduced to a 6-year cycle to forecast data. This is listed as SARIMA x-11. The forecast residuals are then set aside for ANN_1 training data in step 3. The SARIMA model is linear and will produce the same results depending on the data provided. The ANN_0 model must have 100 sample runs with the training data set with an average of 100 results taken to determine the final forecast of the model. After forecasts for 2011 are set aside for the ANN_1 training set, the SARIMA training sets are increased by one year and run through a similar process. This is listed as SARIMA x-12. Each cycle increases the year of training data (SARIMA x-13,14,15); refer to **Figure 29**. This provided five years of forecasting data from 2A to be input into the simple ANN_1 model in step 3.

<table>
<tr><th>Model</th><th>2005</th><th>2006</th><th>2007</th><th>2008</th><th>2009</th><th>2010</th><th>2011</th><th>2012</th><th>2013</th><th>2014</th><th>2015</th><th>2016</th></tr>
<tr><td>SARIMA $_{x\text{-}16}$</td><td colspan="11">Training data - 132 Points
11 Year Cycles</td><td>Validation</td></tr>
<tr><td>SARIMA $_{x\text{-}11}$</td><td colspan="6">Training data - 72 Points
6 Year Cycles</td><td>Forecast
12 Points</td><td colspan="5"></td></tr>
<tr><td>SARIMA $_{x\text{-}12}$</td><td colspan="7">Training data - 84 Points
7 Year Cycles</td><td>Forecast
12 Points</td><td colspan="4"></td></tr>
<tr><td>SARIMA $_{x\text{-}13}$</td><td colspan="8">Training data - 96 Points
8 Year Cycles</td><td>Forecast
12 Points</td><td colspan="3"></td></tr>
<tr><td>SARIMA $_{x\text{-}14}$</td><td colspan="9">Training data - 108 Points
9 Year Cycles</td><td>Forecast
12 Points</td><td colspan="2"></td></tr>
<tr><td>SARIMA $_{x\text{-}15}$</td><td colspan="10">Training data - 120 Points
10 Year Cycles</td><td>Forecast
12 Points</td><td></td></tr>
</table>

Figure 29. Reduction in 2A SARIMA training dataset to produce forecast data.

<table>
<tr><th>Model</th><th>Trans. Func. / Nodes</th><th>2007</th><th>2008</th><th>2009</th><th>2010</th><th>2011</th><th>2012</th><th>2013</th><th>2014</th><th>2015</th><th>2016</th></tr>
<tr><td>ANN $_{0\text{-}16}$</td><td>Tan and Log
(4, 5, 7) x (2-6) x (1)</td><td colspan="9">Training data - 96 Points
9 Year Cycles</td><td>Validation</td></tr>
<tr><td>ANN $_{0\text{-}11}$</td><td>Log
7 x 5 x 1</td><td colspan="4"></td><td>Model
Trace</td><td colspan="5"></td></tr>
<tr><td>ANN $_{0\text{-}12}$</td><td>Log
7 x 5 x 1</td><td colspan="5">Training data - 44 Points
5 Year Cycles</td><td>Forecast
12 Points</td><td colspan="4"></td></tr>
<tr><td>ANN $_{0\text{-}13}$</td><td>Log
7 x 5 x 1</td><td colspan="6">Training data - 56 Points
6 Year Cycles</td><td>Forecast
12 Points</td><td colspan="3"></td></tr>
<tr><td>ANN $_{0\text{-}14}$</td><td>Log
7 x 5 x 1</td><td colspan="7">Training data - 68 Points
7 Year Cycles</td><td>Forecast
12 Points</td><td colspan="2"></td></tr>
<tr><td>ANN $_{0\text{-}15}$</td><td>Log
7 x 5 x 1</td><td colspan="8">Training data - 80 Points
8 Year Cycles</td><td>Forecast
12 Points</td><td></td></tr>
</table>

Figure 30. Reduction in 2B ANN$_0$ training dataset to produce forecasting data.

The process for 2B is similar to 2A. In order to provide forecast residuals for the following ANN$_1$ model, the training data is reduced to a 6-year cycle to forecast data. This is listed as ANN $_{0\text{-}11}$. The forecast residuals are then set aside for ANN$_1$ training data in step 3. The ANN model is non-linear and will produce different results with every iteration. The ANN$_0$ model must have 100 sample runs with the training data set with an average of 100 results taken to determine the final forecast of the model. After forecasts for 2011 are set aside for the ANN$_1$ training set, the ANN $_0$ training sets are increased by one year and run through a similar process. This is listed as ANN $_{0\text{-}12}$. Each cycle increases the year of training data (ANN $_{0\text{-}13,\ 14,\ 15}$); refer to **Figure 30**. This provided one year of traced data and four years of forecasting data from 2B to be input into the simple ANN$_1$ model in step 3. One of the limitations of this study is the limited dataset. The ANN$_0$ requires minimum data input. The limited data requires that the 2011 data forecast was the ANN_0 model trace of 2011 data. This means the model was provided the 2011 data in the training set. This will provide better results for the ANN_0 model in the 2011 forecast results; however, it should not have a major impact on the overall results of the study. The best way to avoid this issue would be to have an additional year for the training set. This completes the training data set for the ANN_1 model structure testing and forecasting.

The structure of the ANN_1 should remain simple. A balance of hidden neurons and restricting training iterations reduces the issues of overfitting and overcorrection of the ANN_1 model. A more dynamic ANN_1 model structure will change whether the PHSA framework is built on a 1) combined linear - nonlinear method or 2) nonlinear method. Multiple hidden neurons in the ANN_1 model increase the nonlinear computing power; therein, it is expected to increase the forecasting accuracy. **Figure 31** shows testing the structure of ANN_1 structure with two inputs and one output, 1-10 hidden node(s), and tangent/logarithmic transform function.

Number of Hidden Nodes	Average R^2	
	Tan	Log
1	0.785	0.785
2	0.785	0.784
3	0.785	0.784
4	0.784	0.784
5	0.784	0.784
6	0.784	0.785
7	0.786	0.784
8	0.785	0.785
9	0.785	0.782
10	0.783	0.785
Transform functions of the ANN_1 are designated by 'Tan' and 'Log'.		
Training repetitions limited to 10 in order to reduce overfitting.		

Figure 31. Average R^2 comparison of ANN_1 model structure test with 1-10 hidden nodes.

The comparison of models is made by running 100 simulations and taking the average R^2. Training reiterations were reduced to 10 in order to limit overfitting. There was no significant increase in model performance with additional nodes other than 0.001 increase at the hidden layer to 7 nodes with a tangent transform function. The only difference made with adding numerous nodes in the hidden layer is to define the final output of the parallel hybrid SARIMA-ANN model as a non-linear model instead of a combined linear/non-linear model. Therefore, the model structure for the ANN_1, in this case, will be a simplified ANN model (2X1X1) with log transform.

The reduction of the hidden neuron layer to one neuron reduces forecasting capability to linear with linear and nonlinear dataset inputs. The simple one hidden neuron reduces the volatility of the model and emphasizes reliance on the forecast of 2A) SARIMA and 2B) ANN_0. In accordance with the previous guidelines from chapter 4.5.1 and preserving model simplicity, ANN_1 is a simple structure (2x1x1); see **Figure 32**. This model structure is composed of: 1) two inputs of the five years of forecasting data from SARIMA and ANN_0; 2) one hidden neuron; and 3) log-sigmoid transfer function. This structure avoids overfitting and processing with the task to simply understand which model had the best fit. The forecasting points provided by 2A and 2B training dataset reduction process were submitted into the ANN_1 model structure. This is a simple ANN model, 2x1x1, that took the best points for both models to forecast a more accurate forecast. This captured the strengths of the SARIMA model and the preciseness of the ANN model.

2 Input Neurons x 1 Hidden Neuron x 1 Output

Transfer Function: Log Sigmoid

Inputs:

2A	SARIMA	5 years of Forecast (60 points)
2B	ANN_0	4 years forecast data and 1 year ANN_0 model trace (60 points)

Figure 32. Identification of best fit ANN_1 Model

The performance metrics used for the model comparisons are the root-mean-square error (RMSE) and mean average relative error (MARE). RMSE is a quadratic scoring rule that measures the average magnitude of the error; see Equation 5.2. MARE measures the average magnitude of the errors in a set of predictions without considering direction; see Equation 5.3.

$$\text{RMSE} = \sqrt{\frac{(\text{totaS CUN of error})^2}{\text{NUNBER of CANPSEC}}} \qquad \text{Equation 5.2}$$

$$\text{MARE} = \frac{\text{totaS CUN of abcoSute error}}{\text{NUNBER of CANPSEC}} \qquad \text{Equation 5.3}$$

The results of the forecasting model in comparison are provided in **Figure 33**. The validation dataset is graphed with a solid black line and all other models listed in the legend. Most models trail a similar trend in comparison to the validation data except for the months of January, May, July, and September. The ANN_0 model had a large amount of error in the September forecast. This is due to ANN models overreacting to the local maxima.

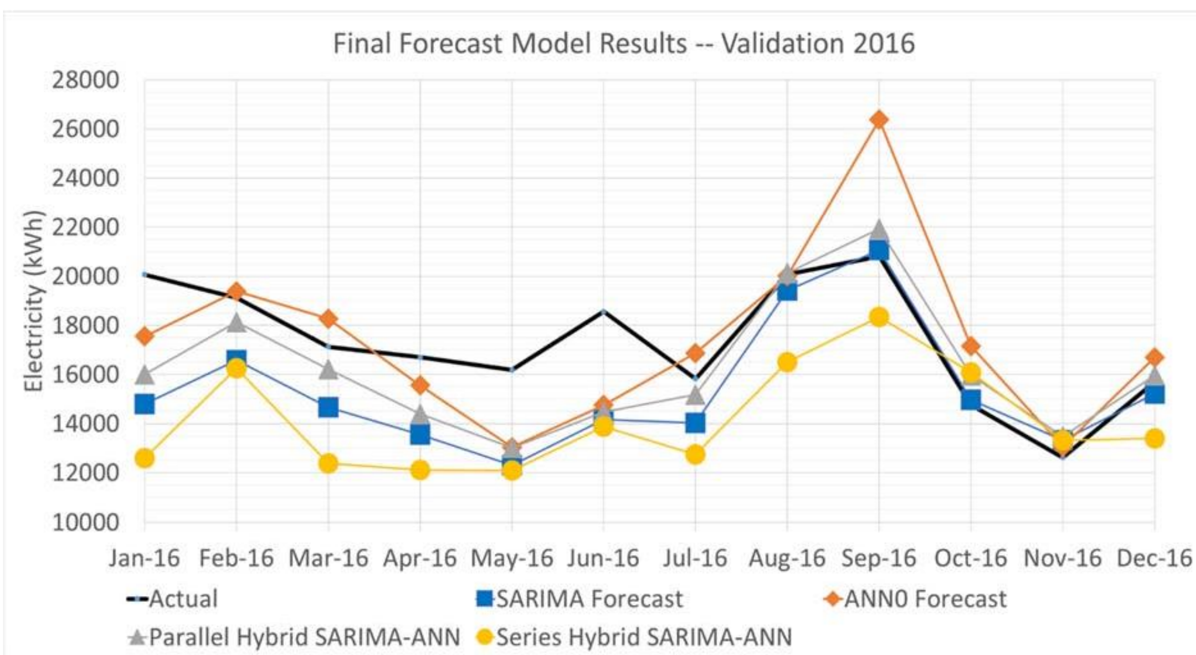

Figure 33. Forecasting validation results

The percentage of the error to the actual value for each forecast model is shown in **Figure 34**. This provides a better understanding of how the models performed month to month in comparison to the validation data set. The ANN_0 model shows its ability to outperform all other models in months (January, February, June, and November). However, the ANN_0 forecasts for the months of September and October are extreme outliers. Again, this shows the volatility of ANN models overacting to local maxima. This also shows how the parallel hybrid SARIMA-ANN model seems to act as an average function between the SARIMA and ANN function while also improving on both models in some cases. This is further discussed in Chapter 6.

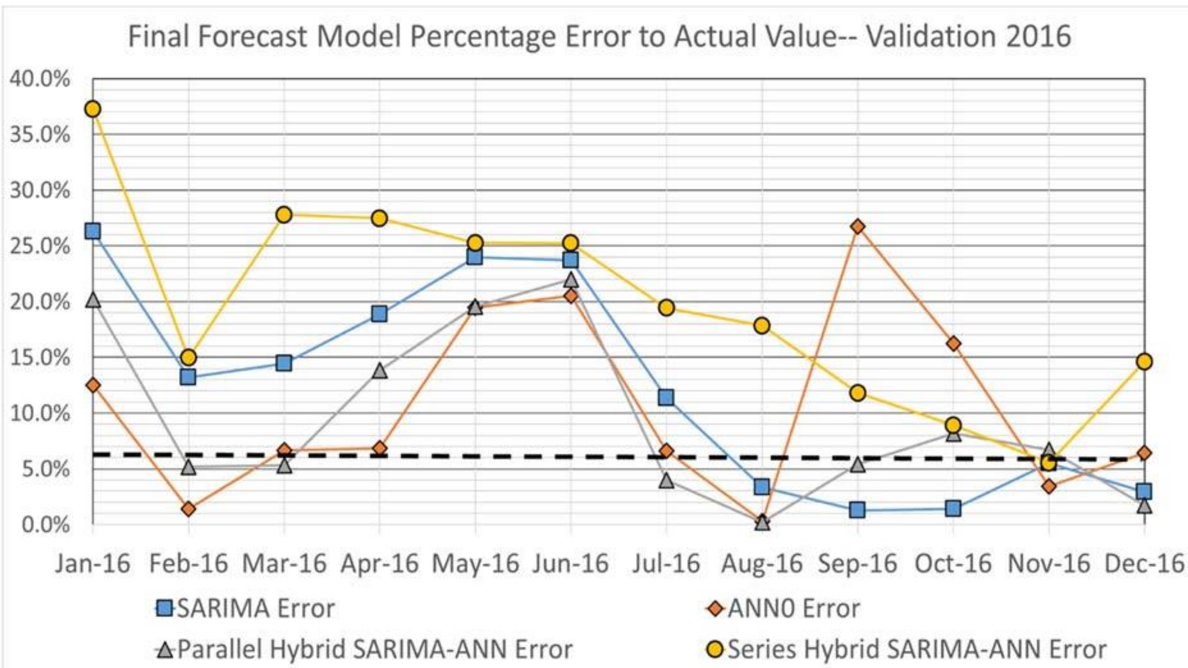

Figure 34. Forecasting validation results with percentage error to the actual value.

The performance metrics of RMSE and MARE for the final forecast models are provided in **Figure 35**. This shows the overall performance of the forecasting models. SARIMA and ANN0 models have similar performances. ANN0 is able to capture better results for a majority of months while overacting to the seasonal extremes in September and October. The parallel hybrid SARIMA-ANN model is able to combine both forecasts of the SARIMA and ANN_0 models while improving them in some cases. The absolute average error for SARIMA, ANN_0, Series, and Parallel models were 2149, 1879, 3489, and 1638, respectively. The absolute error standard deviation for SARIMA, ANN_0, Series, and Parallel models were 1674, 1584, 1734, and 1355, respectively. The error standard deviation for SARIMA, ANN_0, Series, and Parallel models were 1897, 2456, 2289, and 1846, respectively. This results in an overall better performance metric for the parallel hybrid SARIMA-ANN model. The series hybrid SARIMA-ANN performed poorly in all cases across the board.

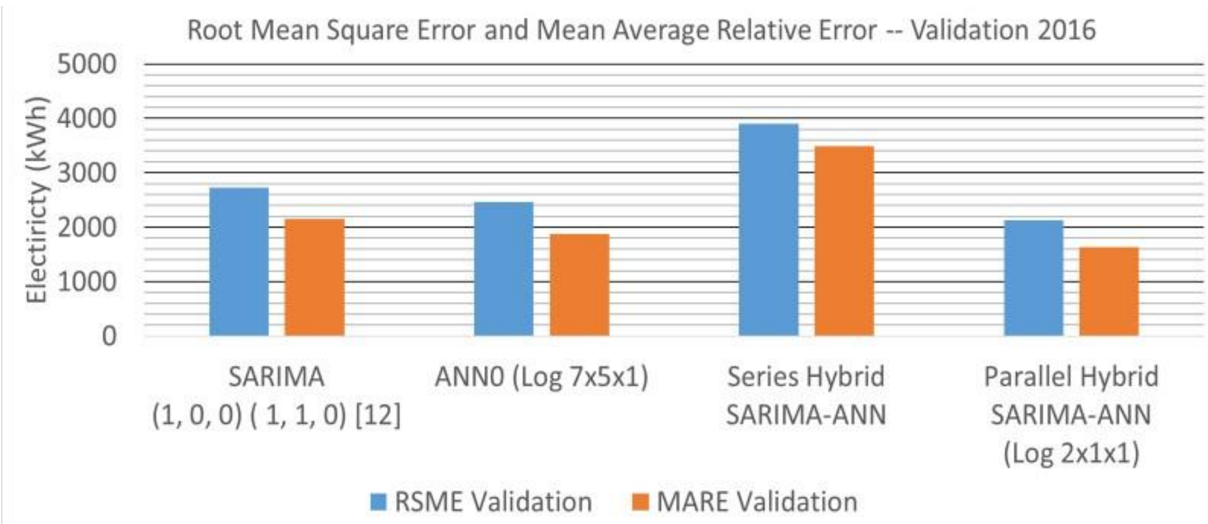

Figure 35. Performance metrics of forecast models

5.2.4. Discussion

The ANN_0 outperformed SARIMA in the first six months with the spike of inaccuracy in September 2016, reacting to local maxima but capturing extremes in January, February, April, and November. SARIMA outperformed all models in September and October. Series hybrid SARIMA- ANN did not perform well due to the need to replicate the ANN model training with forecast values, therefore consuming limited data. Parallel hybrid SARIMA-ANN (PHSA) smoothed out the ANN_0 local maxima reaction and improved seven forecasting points of ANN_0. The PHSA did improve 9 out of the 12 SARIMA model forecast points. SARIMA had slightly better results for the forecast in September and October with near 1% error, edging the parallel hybrid model by 5% error improvement. This is caused by the influence of the ANN_0 model, which is highly reactive to the September maxima. The largest error for ANN_0 is the September forecast. The PHSA was able to improve forecast when inaccuracies were similar, i.e., March, July, and December. Overall, the PHSA had the best RSME and MARE than all other tested forecast models

Expanded studies in this study would involve: 1) increasing the forecast horizon to three years in order to illustrate model reliability for long-term forecasts; 2) rearranging the years within the dataset would test model resilence to adapt to different patterns; and 3) testing additional datasets with downward and variable trends would test the reliability of the parallel hybrid SARIMA-ANN model framework. Evaluations for the best fit ANN_1 structure with changes to the number of hidden neurons require comparing long-term forecasts of 3 years with various datasets.

The previous series hybrid SARIMA-ANN model relies on preset patterns and subjective judgment of SARIMA. The PHSA model acts as a smoothing function of linear and non-linear models. The major contribution of this model is the ability to transcend into any application of research involving forecasting data. The flexibility of the ANN model allows for additional variables.

5.3. Future Work

The long-term goal of this research is focused on a robust and resilient network design of energy and water infrastructure. This is done by integrating water- energy data with organized planning. The idea is to analyze and process limited, raw water-energy data that can be incorporated into decision-making methods through GIS mapping systems. These mapping systems have the ability to evaluate infrastructure network vulnerabilities to natural and manmade disasters.

Models used in the analysis must have the flexibility to handle various factors. With social topography taken into account, network failures can be modeled to show impacts on the social and economic activity within the community. Similarly, innovations in technology and policy can be modeled to illustrate the positive social impacts. A new study framework consists of four revolving steps:

1) Collating water-energy supply and usage data sets;
2) Developing a data analysis model to map resource supply-demand patterns;
3) Delineating decision-making procedures and geopolitical boundaries (city boards, utility providers, institutions, etc.) for balancing water-energy supply-demand; and

4) Identifying and sequencing resource planning criteria. The outcomes obtained from the technical and organizational procedures will lead to resource-efficient technical and organizational practices.

This is designed to establish a dual framework that integrates resource technical and organizational procedures to homogenize the resource information flows. In order to identify and sequence resource planning criteria, two tasks are necessary. Stakeholder and critical node analysis lead to the end goal of WEN optimization at the city scale.

5.3.1. Stakeholder Analysis

After the integration of planning and decision-making processes between water and energy sectors, the development of the physical database platform for collection and investigation of water-energy issues and solutions can be done efficiently. Planning requires data; however, there needs to be a network in place to acquire and analyze data. With combined database information, one would be able to map current and future demand patterns, identify trade-offs, allocate resources, streamline the decision-making network, and provide a resilient infrastructure for future use. Siddiqi [72] considers a framework to assess the physical system integrated with social and political stakeholders. As one of the first to focus a study on the stakeholders of the WEN system at a countrywide scale, Siddiqi [72] attempts to illustrate the current management networking of the water-energy sector as well as expanding links to other sectors that can serve as collection of knowledge and evaluation exercise for decision-making activities.

It is necessary to understand the strategic linking among key stakeholders and decision-making institutions to enable impactful decision-making processes and achieve higher resource-use efficiency [52]. The analysis of the California Energy Commissions [46] shows that California can achieve "nearly all of its energy and demand reduction goals for the 2006-2008 program period by simply allowing energy utilities to realize the value of energy saved for each unit of water saved. In that manner, energy utilities can co-invest in water use reduction programs, supplementing water utilities efforts to meet as much load growth as possible through water efficiency." Stakeholder analysis works toward improving policy. In this approach, it should be recognized that policy development is a complex process in unstable and changing environments [52], building upon the thought of wicked problems identified by Kenway [1]. By taking into account the interests of the whole range of stakeholders, influence or influenced, compromise is necessary. The agglomeration of public goals and private stakeholder interests into a common objective. The only way for compromise to be met is through fluid organizational networking and data and knowledge communication.

Stakeholder Analysis, or SA, requires identifying stakeholders, assessing and comparing their interests, and examining inherent conflicts, compatibilities, and trade-offs. The term ‘Stakeholder’ is to define “any group of people, organized or unorganized, who share a common interest or stake in a particular issue or system; they can be at any level or position in society, from global, national and regional concern down to the level of household” [52]. SA is a holistic approach or procedure serving to comprehend a system and evaluate the links and influences to that system. This is done by categorizing the essential stakeholders and weighing influence within the system. Two distinct concepts are necessary to understand SA: conflicts and trade-offs. Conflicts are states of competition, where there is a fight over control of a resource. The trade-off is an alternative objective used to balance the interests among conflicting stakeholders. Trade-offs imply an opportunity cost in terms of benefits lost [52]. Conflict among stakeholders is likely to be between the influencer— ‘active stakeholder’-- and the influenced— ‘passive stakeholder.’ Intended beneficiaries are measured by importance: primary and secondary stakeholders [181]. This designation classifies a hierarchy of needs and interests. The power of influence refers to the weight certain stakeholders have over the success of a project [52, 181].

With reference to WEN and natural resource management, situations are characterized by interests and trade-offs. These are typically pulled from citizens, government departments, national and international planners, and professional advisors; and thus, particularly suited to SA [182]. In complex decision-making situations with various stakeholders using a multiple-stakeholder approach, a single solution is not the end goal. It is implemented to clarify the stakeholders' positions and identify sources of conflict to aid in developing a myriad of compromising solutions [183]. Stakeholders should be identified, weighed, and organized so that communication and representation are clearly established. Boundary spanning intermediaries, or agents, are used to mitigate dialogue. Boundary-spanning intermediary allows for the implementation of policy across different levels of decision-making [184, 185]. These intermediaries are the interface of community specialists and decision-makers, allowing knowledge to flow from the expert opinion to decision-maker understanding. This translates to the effective implementation of efficient policy and regulation [186]. By using stakeholder analysis and boundary spanning intermediaries, organizational networking can be open and transparent to identify and express the concerns and goals for all members involved.

5.3.2. Critical Node Analysis

The use of stakeholder analysis and boundary spanning intermediaries opens WEN studies to the understanding of the influence of the decision-making process. The decision-making process can be streamlined to allocate resources to projects to alleviate the needs of stakeholders on all levels while encouraging efficiency. The ability to implement technology and policy changes efficiently, however, still requires the breakdown of the physical water-energy infrastructure at the city and state scale. A clear picture of current infrastructure and demand patterns allows experts and decision-makers to identify and communicate designs and ideas. However, considering only linkages in the provision and production of water-energy perspective misses a much larger picture where only co-location of physical infrastructure and interwoven data analysis can provide a clear understanding. The only way to successfully define a water-energy nexus system based around the stakeholders and decision-makers, as well as the physical infrastructure, is through a system of nodes and links [111]:

1) Identify critical nodes in the system by the practice of an index of centrality.
2) Optimize regulation of links with the creation and destruction of pathways in order to reveal bottlenecks in the system.
3) Optimize regulation of network flows in order to track materials and links.

This methodology allows for adjusting parameters based on empirical data and testing the impact of management and technical changes. This simple framework can be expanded into a complex methodology for the breakdown, analysis, and design of both the WEN organizational (stakeholder analysis results) and physical networking (critical node analysis results) at a city scale.

5.3.3. Optimization of WEN at City Scale

Optimization of the WEN system at a city scale requires cooperation within planning, data collection, and modeling in order to support decision-makers in implementing policy and technology investment. The only way to successfully create an efficient water-energy nexus system is to organize the stakeholders and decision-makers as well as illustrate the physical infrastructure and system efficiencies. By using stakeholder analysis, organizational networking can become open and transparent with the ability to identify and express the concerns and goals as well as formal assignment and responsibility for all members involved. By using critical node analysis, physical infrastructure can be mapped to identify opportunities and assess system reliability. Mapping the data available now is limited and only allows for a glimpse into the intricate WEN relationship. With additional resources and data sharing, modeling of material flows as a result of technology or policy intermediation can be used to simulate future changes to the WEN system. The combination of data platforms between water and energy sectors will increase the efficiency of the current system as well as the modeling of a more resilient WEN system within the city.

Chapter 6. Conclusions

WEN studies have emerged across the globe, highlighting the importance of understanding the relationship between water and energy resources as well as the impact on the environment. However, there remains a gap at the city level within WEN studies due to two major limitations, data inaccessibility and model inflexibility. Traditional model approaches for analysis fall under top-down or bottom-up approaches. Both require vast datasets and require time for fine-tuning the models. A middle-out approach using univariate time-series analysis demands only one data input. Within the realm of univariate time-series forecasting, heterogeneous hybrid models composed of linear and non-linear techniques provides a symbiotic relationship between model strengths and weaknesses. In particular, the parallel Hybrid SARIMA – ANN model shows promise for research expansion as the ANN model structure flexibility allows for the possibility to expand with additional variables. The model provides a simple yet powerful forecasting tool with the ability to expand into a more complex model and design tool. The parallel hybrid SARIMA- ANN model forecast performed better overall in comparison to SARIMA, ANN, and series hybrid SARIMA-ANN model forecasts. The flexibility and performance of the parallel hybrid SARIMA-ANN model allow for the implementation of WEN data analysis in decision- making processes within the water-energy infrastructure. Future work looks to use this model to develop a dual framework that integrates resource technical and organizational procedures to homogenize the resource information flows. In order to establish a robust and resilient network design of energy and water infrastructure, a model that works with the limited data must show expansive capabilities and flexibility to new factors as research develops. The parallel hybrid model shows promise in achieving this goal. The parallel hybrid SARIMA-ANN model framework would benefit additional resiliency testing with numerous datasets, varying in trends, as well as expanding the feasible model structures of the ANN_1 in step 3.

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