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Chapter 1

Introduction

1.1 What is a Model?

From birth, each of us must learn to negotiate the environment that surrounds us. By experimentation we learn how to interact with our environment - we learn hot from cold, up from down. And once we gain confidence in our knowledge, we learn how to control and manipulate our surroundings. With maturity we learn that certain approaches are more effective than others - we learn right from wrong.

Thus, our world view begins with basic observations - data that we learn and remember. As data becomes more abundant, we organize these data in ways that help us remember details. The real world is a complex web of entities and relationships. Once we have sufficient data, we form relationships between entities. When we are young, we may not understand the reason for these relationships. But with education we begin to understand why these relationships exist, and learn how to use these relationships to control our environment. Finally, through experience and training, we gain sufficient wisdom to use this knowledge for our own, and perhaps society’s, betterment.

A model, then, is a representation of our environment - the observations we collect, the relationships we infer, the knowledge we gain, and the wisdom we draw upon to act. From the very beginning, we are building mental models of our environment, trying to make sense of our place on Planet Earth, and what we can do to better deal with life’s complexities.

When someone says they wish to build a model, what they are really trying to do is capture the rules by which a system operates. By explicitly stating these rules, they wish to articulate a specific mental construct of their observations, experiences and knowledge.

Many of these rules are absolute, such as the force of gravity, which can have no ambiguity. Such absolute rules can be quantified mathematically, and are called laws of nature. Other rules are less absolute, such as the path a leaf takes as it falls to the ground. While controlled by gravity, many uncertain variables - such as leaf shape, random gusts of wind, and intervening branches - affect the path in complicated ways. In these cases a statistical representation may be more useful in describing how the leaf falls.

Table 1.1: The Basis of Modeling

<table>
<thead>
<tr>
<th>Data</th>
<th>Observations of our environment, collected by design (hard data: a monitoring program, experimentation) or by circumstance (soft data: ad hoc, incidental)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Information</td>
<td>Establishing relationships between observations by interpretation of data (hard information: statistical tests), or circumstantial relationships (soft information: anecdotal)</td>
</tr>
<tr>
<td>Knowledge</td>
<td>Understanding why relationships exist - leading to the ability to predict outcomes - based on scientific principles (hard knowledge: hypothesis testing), or by experience (soft knowledge: trail and error)</td>
</tr>
<tr>
<td>Wisdom</td>
<td>Using knowledge to successfully manipulate our environment for personal or public good</td>
</tr>
</tbody>
</table>

Regardless of the approach one uses for documenting the behavior of a system, the process of model building provides the basis for documenting and communicating the specific approach used to represent a system.

In the most general sense, a model is a simplified representation of a system, where a system consists of entities and relationships between entities. Each entity is a physically or logically distinct object, such as a person or event. Relationships are the associations between entities, such as the predator-prey relationships in a food web, or an event tree in failure analysis.

Each entity and relationship has attributes, such as size, color, intensity, or severity. Parameters are used to quantify attributes, by providing quantitative or qualitative values for each entity or relationship. Parameters normally remain constant, while state variables describe attributes that change over time.

Inputs are external stimuli that cause changes to the system, where the resulting change may be instantaneous or delayed. The stimulus affects state variables as well as outputs from the system. Outputs are external responses of the system. If the response is delayed, then the maximum time required for the response to dissipate is called the memory of the system.
1.2 Reasons for Modeling

Hydrologic models are commonly used to explain and predict complex behavior associated with the management of environmental systems. Often, these models are used to evaluate the effectiveness of regulatory controls, such as for human health [49], pesticide and herbicide registration [7]; waste isolation at proposed, existing, and abandoned waste disposal sites [12], and to examine the effects of alternative regulatory policies [53].

One reason is to learn how a system operates. The process of building a model assists in data interpretation. Data collected in time and space are analyzed for the purpose of establishing relationships. These relationships, in turn, provide information about the system being modeled:

- Water levels in certain wells respond faster in one area than another;
- Floods move faster in one section of a river than another; and
- Fertilizers applied during one part of the year contaminate ground water, but not in another part of the year.

A second reason is to understand why observed relationships exist. This understanding is useful for generating knowledge. We can employ basic physics to explain that:

- The recharge rate is dependent upon the amount of rainfall and the soil moisture content;
- The flood wave velocity is a function of the channel cross-section; and
- Nutrient transport through the unsaturated zone is modified by plant root uptake.

Another reason for constructing or using a model is to identify a cause, or to assign blame. The detection of a contaminant in ground water must be the result of some release. Where was the release, who caused it, when did it occur, and why did it occur? A model is often used to reconstruct a sequence of events, constrained by available data, information, and knowledge, to assess the root cause of some observed condition.

A common reason to model is to predict the consequences of alternative actions. We are often faced with the situation that we have several options, but are not sure which course of action is best. In these cases we turn to models to help explore the possible outcomes of each alternative action. Which action is most likely to succeed? What are the possible adverse impacts of the alternatives? Given a set of options, which will cause the least amount of damage, or maximize the benefits? How can we design a system that achieves our goals?

Clearly, there are many reasons for modeling. Each application may have a different reason, thus requiring a different model - no one model can be used for all potential applications.

Different models and modeling strategies have been developed in response to these multiple modeling purposes. While scientists generally seek to remove noise and uncertainty during experiments by careful use of controls, a regulator seeks to account for uncertainty by focusing on worst-case scenarios. Engineers, as well, try to account for uncertainty by using conservative measures.

Thus, regulatory and engineering models can be readily separated from scientific models. The use of a scientific model that accounts for the myriad forms of physical, chemical and biological interactions may be fascinating for a scientist, but not useful for the design of a simple structure. In the same respect, an engineering model that grossly oversimplifies a system may provide an adequate basis for designing a structure, but ignores the components that most interest a scientist.

The regulatory model differs from the engineering model in that the engineer is not able to alter standards; the engineer designs a structure to meet a specified standard. The regulator, on the other hand, has the special obligation of standards specification.

The regulator seeks to define standards that simultaneously achieve several objectives. One objective is to safeguard the public interest. This objective often links a standard to a critical measures of exposure, which can be addressed using criteria that adequately account for uncertainties and technological capabilities.

On the other hand, standards could be so specific that only limited decision-making is given to the engineer, the result of this which is to restrain efficiency. In an ideal environment, standards should enable engineers to evaluate alternatives using measures of cost-effectiveness or reliability, without the standards placing an undo burden.

The role of regulatory modeling, therefore, should be to identify those measures of system performance that clearly represent the public interest with a minimum of interdiction by the state.

Table 1.2: General Systems Terms

<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
</tr>
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<tbody>
<tr>
<td>System</td>
<td>A set of relationships between entities</td>
</tr>
<tr>
<td>Entity</td>
<td>An object, person, or event</td>
</tr>
<tr>
<td>Relationship</td>
<td>An association between objects</td>
</tr>
<tr>
<td>Attribute</td>
<td>A quality of an entity or relationship</td>
</tr>
<tr>
<td>Parameter</td>
<td>A quantitative measure of the attribute of an entity or a relationship</td>
</tr>
<tr>
<td>State Variable</td>
<td>A measurable attribute of an entity or relationship that changes with time or space. To distinguish it from an input and output, state variables do not affect other entities or relationships.</td>
</tr>
<tr>
<td>Input</td>
<td>A measurable quantity that behaves as a stimulus an entity or relationship</td>
</tr>
<tr>
<td>Output</td>
<td>A measurable response of an entity or relationship to a stimulus.</td>
</tr>
<tr>
<td>Memory</td>
<td>The length of time that an input affects the output</td>
</tr>
</tbody>
</table>
1.2.1 Scientific Models that Describe

One objective of scientific modeling is to identify a new or unanticipated process, or to identify novel interactions between processes. Keen observation or inference is required to sort through known knowledge about previously unknown mechanisms. An additional objective is to characterize the magnitude of environmental parameters.

For both objectives, models are used in the inverse sense to identify system structure or identify parameters. A forward model is generally used only to form predictions that are compared with observed state variables or model outputs.

Several hazards arise when scientific models are used in the regulatory environment. In these cases, model uncertainties may not be explicitly quantified. Parameter distributions and uncertainties, which are minimized during a scientific experiment, may not approximate the true diversity of parameter estimates expected under natural conditions.

Because the scientific estimation problem is inverse, rather than forward, extension of modeling results from the calibration phase to the application phase is not necessarily available. That is, a model that has been constructed using focused laboratory techniques, based on sound scientific method, may never have been used to form a prediction at field scales in a way that can be verified and tested. Even when the model may have been tested for a specific field-scale experiment, the degree of agreement between model prediction and observed results is left unresolved.

While inverse models may be used in the regulatory process to assign culpability, such as when sources of pollution need to be identified for the determination of responsible parties, these inverse techniques generally lack the designed controls used in scientific studies.

Inference, in this case, is made difficult by the inherent uncertainties in defining the amount and location of contamination (i.e., source terms), subsurface material properties, and historical water levels. The exactitude of scientific hypothesis testing is further weakened by the legal requirements of liability, thus placing this type of inverse problem outside the scientific venue.

1.2.2 Engineering Models that Predict

The design of human structures may not require an advanced theoretical understanding of the components embedded within it. Engineers are most concerned about the attributes of the system that are most likely to contribute to performance and failure. Thus, those aspects of a design that affect system performance or failure require stringent characterization.

Estimating the likelihood of failure, as a function of cost and performance, are an important aspect of engineering analysis. An engineer may devote resources toward estimating a parameter, especially when the value of the parameter is near a threshold that determines failure or success. An engineer may be willing to accept a margin of error so that a minimal likelihood of failure is possible. Also, the stability of a specific parameter may be considered when designing materials or components. A more variable result generates concern, even though the value of the parameter is otherwise far from the performance threshold.

Like the scientist, the engineer relies on inverse techniques to estimate system behavior, but unlike the scientist, the engineer is satisfied with statistical certainty, rather physical certainty. Knowing that a parameter is bounded may mean more to an engineer than knowing the nature of the expected value. Because the engineer is seeking a system design for optimal operation, the specification of an absolute constant is less meaningful than knowing the worst-case possibility. By containing the behavior to desirable states, one can avoid unwanted outcomes.

The ultimate endeavor of any design effort, therefore, is to provide a system that offers predictable outcomes. The outcomes must be desirable, and they must allow for control. By evaluating alternative designs, an optimal design can be selected based upon a performance measure. The performance measure can have various forms; expected value (benefits), extreme value (worst case), expected risk (consequences), etc. Because each of these measures are incommensurate in that they generally yield different selections, some balance of these measures is used. A standard mechanism is to apply benefit-risk analyses, which balances the benefits to some against the costs to many.

Like scientific models, the use of engineering models by the regulatory community results in real dangers. Specifically, model uncertainties may not conform with regulatory intent. An engineering design that minimizes costs given a set of environmental standards may, or may not, be better than a model that is free to balance costs against standards.

An engineering model may yield an optimal solution for a specific standard, yet ignores a solution that costs insignificantly more but reduces risks substantially. Ideally, tradeoffs between alternative engineering designs are identified so that the relative merits of the alternative designs can be evaluated. Due to public perceptions of risk, the regulated and regulatory community, along with the general public, should be involved in finalizing the optimal design.

1.2.3 Regulatory Models that Control

To better understand the regulatory role of modeling, it is important to note that models often serve as the interface between data and decision-making. Few individuals are capable of making a sensible conclusion by examining large volumes of data.

Models assist in data interpretation by extracting information, and hence understanding, from data. Once experiments generate data, rules are applied via models
to gain insight into what happened where, when, why and how. The information and knowledge gained from the insight is then used to form a decision. Models are used, therefore, to improve our knowledge of the system.

Many regulators commonly employ models to help learn about processes in the environment. In this sense, the models serve as true simulators; to teach the user how the system behaves. Like pilots who use aircraft simulators to improve their performance when learning how to fly new aircraft, most modelers understand that the model they use is not an exact replication of the real system. With time, many modelers either move on to newer, more powerful codes that provide additional insight and understanding, or they bypass the simulation route by learning how to interpret data directly.

Veteran regulators acknowledge that simulation models are abstractions of reality. The abstraction is based on simplified representations of the real world. It is also recognized that model predictions are imperfect due to uncertainties. At a minimum the regulatory model should be sensitive to uncertainties, in that the performance of a system should be tested under a wide range of possible inputs, states, and material properties.

The complexity of material properties can be readily quantified if the project is limited in scale, or the magnitude of the variation is small. Unfortunately, the effects of environmental change cover a wide area and induce substantial perturbations to the environment in many ways. The complexity of the model structure can also be evaluated if the system functions deterministically, but is virtually impossible if the physical, hydraulic, chemical, thermal or biological responses are poorly known. Also, the complexity due to coupling between processes can be evaluated if the coupling are weak and limited in number, but are difficult when the system is strongly coupled, or is nonlinear in the effects of coupling.

From a regulatory viewpoint, simulation is straightforward if there are no uncertainties, but uncertainties tend to introduce ambiguity in reaching a decision. A scientific model that artificially controls or minimizes uncertainties to allow identification of relevant processes and parameters may not be useful for a decision-maker who wishes to incorporate uncertainty. The engineering design that incorporates uncertainties using conservative designs does not necessarily allow the optimum balance of risk vs. cost to be achieved. Each of these models therefore restrict the regulator in their ability to incorporate uncertainties in the decision-making process.

As noted above, a good performance measure should conform with the regulatory intent of preserving and protecting the public health and welfare. As such, regulations should protect public health, while minimizing intrusion into the design process. The ability of a performance measure to evaluate the suitability of a proposed design, or to assist in the approval of a permit, should reflect the ability of the design to meet the regulatory intent.

A regulatory policy that enhances the efficiency of the performance measure will require the use of regulatory models. These models should fully account for model and parameter uncertainties, while providing design flexibility, and also incorporate societal goals.

1.3 The Modeling Process

1.3.1 The Objective

The modeling process begins with trying to articulate the modeling objective. Is it a design objective that minimizes cost while conforming to regulatory requirements? Is it a scientific objective to understand how a system works? Is it a regulatory objective whose purpose is to establish a limit that is protective of human health and the environment? Ideally, a model should be as robust as possible (i.e., suitable for use at many locations). Also, a model that minimizes uncertainty is more useful than one which gives highly uncertain predictions.

The greatest challenge to modeling results from the confusion that commonly arises when scientists, engineers, and regulators discuss modeling. This can be expected given their disparate objectives. Simulation models vary depending upon their purpose. Scientists employ simulation models to formulate an understanding of complex systems and to identify previously unknown phenomena or processes. Engineers use simulation models to test alternate designs and to predict system behavior. Engineering models are generally coupled with prototype designs to test model assumptions. The regulatory community uses simulation models to evaluate the ability of proposed actions or activities to meet regulatory objectives. In many regulatory applications, the model is used to extract information about regulatory performance from data so that informed decisions can be made.

Clearly, an important first step is to clearly define the objectives of your modeling effort. Examples include:

Developing a Well Field for Water Supplies. Models are needed to meet an engineering objective - to provide the most efficient way to develop ground-water resources while minimizing impacts on local wells and wetlands and complying with existing environmental laws.

Establishing Liability at a Superfund Site. Models are needed to meet an identification objective - to identify the source of ground-water contamination so that responsibility for the contamination can be assigned. The models must be physically-based because of the likelihood of litigation over any liability that is assigned.

Establishing Nutrient Loading Limits. Models are needed to meet a regulatory objective - to establish an upper limit that is protective of the aquatic resource and human health. The models may be physically or statistically based. Oftentimes, sufficient information is not available to form a physically based model, so that statistical relationships are often used.

Approving a Pesticide License Application. Models are needed to meet a regulatory objective - to evaluate whether
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1.3.2 The Approach

The second step is to define the model approach. Early efforts to develop predictive models relied on scale models that reduced the size of the system to a scale that fit in the laboratory. Entire watersheds have been constructed in miniature - with dams, bridges, and miniature obstructions - for the purpose of evaluating alternative designs for channel structures. Laboratory column experiments are a type of scale model still commonly used today to evaluate the effects of contaminant transport through the subsurface.

Another early effort used resistors and capacitors to mimic the permeability and storage properties of an aquifer. These process analog models were based on the similarity between fluid flow and the flow of electricity. Heat conductivity and capacity are also analogs for water flow, and many heat flow models are commonly employed as surrogates for fluid flow.

Statistical procedures are useful when the behavior of a system is highly uncertain, such as in rainfall-runoff models. In these cases, the complexities associated with explicitly modeling the physical processes overwhelm the information available to constrain model parameters.

In other cases, the physical processes are known and appropriate parameters are readily available, so that both analytic and numeric models can be used to evaluate and predict behavior. While analytic models are usually preferred, due to their greater simplicity, site conditions may not be conducive for direct application. Instead, numerical models are used to provide greater flexibility in modeling the unique conditions at the site.

The focus of this book is to provide methods and procedures to assist in understanding the relative strengths and weaknesses these modeling approaches.

Scale Analog - Models that employ a smaller (or larger) version of the original system as an experimental tool. Examples included model airplanes, Hele-Shaw models, miniature flumes, and laboratory tests.

Process Analogs - Models that replace the flow of water with another physical or chemical process. Examples include electric-analogs, temperature-analogs, and solute-transport analogs.

Statistical Models - Models based upon information, which use observed data to identify relationships and to estimate model parameters. Examples include regression, convolution, time series, fourier, wavelet, and percolation.

Analytical Models - Models that provide analytic solutions for specific physically-based systems. The solutions are usually based on governing equations that take the form of algebraic, differential, or integral expressions.

Numerical Models - Models that provide solutions when analytic solutions for physically-based systems are not possible. Examples include iterative, Finite Difference, Finite Element, Analytic Element, and other methods.

1.3.3 The Structure

Once a general class of model has been selected, a large number of issues still need to be resolved. What processes will be considered? What are the important relationships? What state variables, inputs, outputs, and parameters can be measured? How stable are these measurements? What range of application is required?

Physical vs. Abstract - A physical model is a scaled replica of the modeled system, such as a model airplane, meant to perform identically to the original. An abstract model is a mathematical representation of the modeled system, meant to yield predictions that can be applied to the original.

Natural vs. Devised - A natural model describes the physical environment, while a devised model is one, such as law, that creates artificial rules for human conduct.

Open vs. Closed - A closed system has no input or outputs, and is entirely self-contained. An open system interacts with its external environment. Planet Earth is a closed hydrologic system, but is open with respect to energy.

Steady vs. Dynamic - A steady system is one in which there is no temporal variation in inputs, outputs, or state variables, while a dynamic system is one which changes over time.

Stable vs. Unstable - A stable system is one which can be controlled, while an unstable system is one which is difficult or impossible to control. One property of a stable system may be that, in the absence of inputs, it returns to a constant condition, while an unstable system grows or shrinks without stabilizing.

Discrete vs. Continuous - A discrete system has inputs, outputs, or state variables that take on integer values, such as the sex of a person, while a continuous system is one in which components can vary over an infinite number of conditions, such as a dimmer switch vs. an on-off switch.

Deterministic vs. Probabilistic - A deterministic system is one in which all inputs, outputs, and attributes can be described with great certainty. A probabilistic model explicitly incorporates uncertainties in the model using assumed distributions and statistical parameters.

Lumped vs. Distributed - Lumped parameters are used when an attribute of a system can be described using a single parameter or state variable. In some situations, however, a single attribute can not fully describe the variability within the system, and the entity or relationship must be divided into multiple, or distributed, components - each with their own attribute.

Causal vs. Noncausal - A causal system implies that an action at one point or time causes a response at another point or time. A noncausal system is one in which any response between two points or times is the result of a random coincidence.

Instantaneous vs. Lagged Response - An instantaneous system is one in which an input causes an immediate output,
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and there is no memory. A lagged response occurs when there is a delay between an input and a response.

**Time Variant vs. Time Invariant** - A time-variant model has parameters that change with time, while a time-invariant model has stable parameters. When faced with a problem where a parameter is time-variant, the model can be altered by specifying changing the parameter to a state variable.

**Linear vs. Nonlinear** - A linear system is one in which the magnitude of the response is a constant multiple of the magnitude of the input. That is, a doubling of the input causes a doubling of the output. A nonlinear system results when the ratio of the response to the stimulus is not constant, but varies as a function of the magnitude of the input.

The definition of the model structure is called the **conceptual model**. For some applications, this conceptual model may be uncertain, and alternative conceptual models may be required. For these cases, additional information may need to be collected to evaluate which of the alternative conceptual models is more appropriate.

**1.3.4 The Evaluation Strategy**

No phrase seems to induce greater discussion than model validation. Accurate predictions hinge on a correct model [10] [54]. While some argue that models can never be validated, due to the inability to accept a hypothesis, others argue that model validation depends upon the regulatory context. Efforts to evaluate suitability of model performance focus on the key aspects of model verification, which are used to evaluate the accuracy of coded statements (software control), and model evaluation, which focuses on the ability of the theory to replicate observed behavior. The issue of model validation comprises the core of performance assessment; risk predictions depend on accurate and precise measurements of anticipated outcomes. The performance assessments are then used for decision making, establishing regulatory policies, and for evaluating regulatory compliance.

The greatest challenge in modeling is the proper mathematical specification of the conceptual model. The identification and quantification of relevant processes can be performed using laboratory and limited-scale field experiments. In general, the mathematical equations that result are greatly simplified from the real world. The quantity, quality and types of data must be specified, both in time and space. Once data are obtained, model results are compared with experimental results to evaluate model assumptions. The conceptual model is iteratively revised until a specified performance measure is achieved. These steps do not guarantee success. The calibration and evaluation phases are both limited in areal and temporal extent. Extrapolation beyond the range of experimental testing is subject to great uncertainties, that are generally neglected when running performance assessment simulations.

The performance assessment simulations are used to develop alternative designs for a wide array of conditions, beginning with limited-scale testing under relatively controlled conditions, to extended-scale testing under open conditions. These design comparisons can be used to provide model results that limit the prototype testing to a smaller set of alternative system designs. The alternative prototype designs are then evaluated using a variety of performance measures, recognizing the uncertainties inherent in open testing. Finally, the sensitivity of model predictions to the magnitude of uncertainties is evaluated.

Confidence in the validity or appropriateness of an environmental model is enhanced if the model accurately and concisely represents the relevant physical, biological, chemical, hydrologic, geologic, and thermal processes inherent in the system being modeled. Failure to account in a meaningful way in any of these components may compromise the robustness of model predictions. Estimation of model single-phase and coupling parameters must be performed under a wide range of ambient conditions, especially those appropriate to the target environment. And finally, extended prototype testing at multiple spatial scales, time horizons, and thermal loadings is required to identify unanticipated events. Reliance on natural analogues that mimic the long-term effects of environmental disturbance, such as volcanic and meteorite-impact events are a possible mechanism for extending prototype testing.

Validation of model performance lies in the ability to quantify model uncertainties. While some model uncertainties can be quantified, many uncertainties related to model structure remain unquantifiable. Regulatory policies that rely on model predictions may not provide greater confidence than other approaches. Alternative regulatory strategies include an increased reliance on prototype testing, improved linkages between hydrologic modeling capabilities and standards, and decoupling models developed for scientific purposes from the regulatory process. In some cases, regulatory policies and simulation model capabilities may be incompatible, leading to the improper use of simulation models in the regulatory environment.

Engineers routinely establish tradeoffs between model performance and standards by incorporating margins of safety to account for uncertainties [53]. The degree of confidence reduces the need for margins of safety, and allows for economies in the design and operation of a structure. For a new design, large margins of safety are recommended, which are slowly relaxed as the understanding of the system increases. A regulatory policy that acknowledges uncertainties, or develops methods for explicitly linking uncertainties to standards, is one means for addressing incomplete understanding. Uncertainty magnitudes are especially large early in the design state, and are solidified as the prototype testing reduces unknowns.

A regulatory policy that focuses exclusively on risk minimization may fail to account for identification of unknown uncertainties. A process of uncertainty characterization and minimization can be monitored using the var-
ious performance measures addressed above. The process of testing need not be static, however. As new processes or behaviors are observed, increased surveillance and testing may be required. To define, a priori, the magnitude of uncertainty may not be possible. In fact, the magnitude will certainly be underestimated. Minimization and control of uncertainties leads to reliability of operation, the primary concern of the regulator.

1.3.5 The Limitations

A primary inadequacy of environmental models stems from their inability to provide long-term predictions with sufficient accuracy to meet regulatory requirements [49] [82] [84]. Assuring the long-term continuation of sustainable human and ecologic conditions for millions of years is difficult, given unforeseeable climate changes, human and animal interactions, geologic and astronomical instability, and other, as yet unknown, modifications of the global environment. For a regulatory requirement of predictability for only ten thousand years, many scenarios of climate change or volcanic activity could adversely affect the integrity of global systems. Incorporating the potential stresses of changes in the external environment is rendered more difficult when observed behaviors are limited by an incomplete understanding of potential future states [61].

An additional problem arises when more than a single interpretive model can be used to explain observed experimental data [37] [23] [80]. In the case of any experiment in which data are incomplete, alternative scenarios can be devised that may account for the observed distribution of state variables or measured fluxes. Thus, alternative hypotheses may not be distinguishable due to incomplete control of the experiment.

Calibration data sets and model structure substantively affect model prediction accuracy. For data sets with high multicollinearity, the parameter covariances become large, resulting in poor forecasts. Also, extrapolative models in which parameter values that lie far from the mean results in larger forecasting errors. And finally, the model shows that the objective of reducing model calibration errors can result in a poorly structured parameter covariance matrix, offsetting any reduction in forecast error.

A further confounding factor lies in the situation where a regulatory policy may not be amenable to quantitative analysis [26]. Without being specific, it may be safe to say that a quantitative definition of safe, is not scientifically possible. A policy which requires safety requires the specification of a quantifiable measure. A quantifiable measure may be the specification of a risk envelope, which is the product of the probability of an undesirable state with the likely consequence of the state, for all possible states [17]. The total risk is the sum of risks of all possible adverse events.

The total risk can be limited to specific subsets, e.g., the risk from carbon accumulation in the atmosphere. Risk calculations incorporate all outcomes, with the obvious bias due to the inability to specify the universe of outcomes. Also, the risk computation should account for risk transfers (e.g., between present and future generations), perceptions of risk (e.g., brief, high exposures may be more acceptable than chronic, low exposures given the same total consequence), and public voice (e.g., poor, minority populations may have less access to the political process than established political groups).

While mathematically simple, the use of risk as a measure of safety suffers from the inability to calculate either the likely probability of a single hazard, or even the resulting consequence for that hazard [21] [22]. The advantage of risk assessments lies in their ability to incorporate known uncertainties by coupling them with the magnitude of the consequence, yet they are biased because they fail to identify unknown processes or scenarios, or to quantify unknown uncertainties [60]. The risk measure is a relative measure, requiring the balancing of risks between alternative decisions [11]. Also, community perceptions of acceptable risks commonly differ from calculated risks [81]. And finally, risk is transferable, allowing individuals to benefit from the increased exposure of others.

The dilemma arises when a regulatory policy may not adequately incorporate model capabilities and uncertainties [60]. A model which superficially treats complex systems by using expected inputs, states, or material properties, may yield precise estimates of expected outcomes. Yet this model will undoubtedly fail to accurately represent the wide range of possible outcomes by ignoring the less likely, but still possible, alternatives.

1.4 Problems

Select a journal article of your choice that uses a model in the analysis of field data. For the model you select, identify the:

1. Modeling objectives (e.g., scientific, engineering, regulatory)
2. Processes described by the model
3. Input information used to construct the model
4. Parameters and state variables within the model
5. Outputs predicted by the model
6. Measures of model performance
7. Construct a visual diagram of the model showing the entities, relationships, parameters, state variables, inputs, outputs, feedback loops, and calibration checks.
8. Describe alternative modeling methods, and discuss how they might be useful for meeting the modeling objective.
Chapter 2

Analog Models

An analog model is an artificial physical representation of the system that is to be studied. For example, a process analog substitutes a different process, such as electricity or heat, to represent fluid flow. Another class of analog models are scale analogs which use a miniature (or perhaps an expanded) version of the system. Examples of scale analogs include miniature dams and rivers, or miniature aquifers. These models can be constructed in a laboratory so that experiments can be conducted to evaluate alternative designs.

2.1 Review

Before we launch this baby, let’s do a bit of review. I’m hoping that you’ve had (at least some of) this before. If not, please give it a try...

2.1.1 Units

The metric system is the internationally recognized system of units. All countries in the world (except for Liberia, Burma/Myanmar, and the United States) use the metric system as their official way to measure things. Mixing English with other units can result in engineering failure, such as the failure of the $125 million Mars Climate Orbiter spacecraft in 1999. In this case, two teams of scientists used two different systems of units, which were never reconciled.

Table 2.1: Metric System Units

<table>
<thead>
<tr>
<th>Mass</th>
<th>kilogram</th>
<th>kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>meter</td>
<td>m</td>
</tr>
<tr>
<td>Volume</td>
<td>liter</td>
<td>l</td>
</tr>
<tr>
<td>Time</td>
<td>second</td>
<td>s</td>
</tr>
<tr>
<td>Energy</td>
<td>joule</td>
<td>J</td>
</tr>
<tr>
<td>Power</td>
<td>watt</td>
<td>W</td>
</tr>
<tr>
<td>Force</td>
<td>newton</td>
<td>N</td>
</tr>
<tr>
<td>Pressure</td>
<td>pascal</td>
<td>Pa</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2.2: Metric System Prefixes</th>
</tr>
</thead>
<tbody>
<tr>
<td>d  deci  10^−1</td>
</tr>
<tr>
<td>c  centi  10^−2</td>
</tr>
<tr>
<td>m  milli  10^−3</td>
</tr>
<tr>
<td>µ  micro  10^−6</td>
</tr>
<tr>
<td>n  nano  10^−9</td>
</tr>
<tr>
<td>p  pico  10^−12</td>
</tr>
<tr>
<td>a  femto  10^−15</td>
</tr>
</tbody>
</table>

2.1.2 Exponents and Logarithms

The exponent is used to indicate the repeated multiplication of a number:

\[ x^3 = x \cdot x \cdot x \]  \hspace{1cm} (2.1)

A negative exponent indicates the reciprocal of the number:

\[ x^{-3} = \frac{1}{x^3} \]  \hspace{1cm} (2.2)

Non-integer exponents are also possible. For example, the exponent one-half indicates the square root of a number:

\[ x^{1/2} = \sqrt{x} \]  \hspace{1cm} (2.3)

A general rule for exponents is:

\[ x^{a/b} = (\sqrt{xa})^a \]  \hspace{1cm} (2.4)

There are two standard bases for exponents. One is the base-10 system, such that any number can be represented using:

\[ x = 10^b \]  \hspace{1cm} (2.5)

For example, \( b = 2 \) represents the number \( 10^2 = 100 \). A second base is the natural system, represented using \( e \):

\[ x = e^a \]  \hspace{1cm} (2.6)

where \( e \approx 2.71828 \).

The logarithm of a number is equal to the exponent:

\[ \log_{10} x = \log_{10}(10^b) = b \]  \hspace{1cm} (2.7)
\[
\ln(x) = \log_e x = \log_e(e^a) = a
\]

There are several basic rules of exponentials and logarithms:

\[
x \cdot y = 10^b \cdot 10^c = 10^{b+c}
\]

\[
\frac{x}{y} = 10^\frac{b}{c} = 10^{b-c}
\]

These relationships also hold for the natural system:

\[
x \cdot y = e^b \cdot e^c = e^{b+c}
\]

\[
\frac{x}{y} = e^{\frac{b}{c}} = e^{b-c}
\]

Logarithms also follow similar rules:

\[
\log(b \cdot c) = \log(b) + \log(c)
\]

\[
\log(b - c) = \frac{\log(b)}{\log(c)}
\]

for both the base-10 and natural systems. Another logarithmic relationship is:

\[
\log(ax^b) = \log(a) + b\log(x)
\]

2.2 Process Analogs

The rules that govern fluid flow are remarkably similar to those that govern heat, electrical, and solute flow. All are governed by conservation and flux equations, with similar laws and parameters.

The general conservation equation requires that any accumulation or loss in mass, heat, or current be offset by a corresponding increase or decrease in storage. The general flux law states that the rate of movement of mass, heat, or current is related to the product of a parameter with the gradient of a state variable (head, temperature, voltage, or concentration).

The ratio of the flux to the conservation parameters is termed the diffusivity, and always has units of length squared per unit time (m²/s). Thus, the flux parameter units must be paired with the conservation variable parameter so that concomitant units are used.

2.2.1 Fluid Flow

The steady and unsteady flow equations for water in the subsurface are:

\[
\vec{q} = -K \nabla h
\]

\[
\nabla \cdot \vec{q} = -S_s \frac{\partial h}{\partial t}
\]

\[
D \nabla^2 h = \frac{\partial^2 h}{\partial t^2}
\]

where \(\vec{q}\) is the flux vector, \(K\) is the hydraulic conductivity parameter, \(\nabla h\) is the gradient in the hydraulic head, \(D = K/S_s\) is the hydraulic diffusivity, \(\theta\) is the volumetric water content, and \(S_s = d\theta/dH\) is the specific storage coefficient.

2.2.2 Electricity

The corresponding equations for electricity are:

\[
\vec{i} = -\frac{\nabla V}{R}
\]

\[
\nabla \cdot \vec{i} = -C \frac{\partial V}{\partial t}
\]

\[
D \nabla^2 V = \frac{\partial V}{\partial t}
\]

where \(\vec{i}\) is the electrical flux, or amperage, vector, \(R\) is the electrical resistivity parameter, \(\nabla V\) is the gradient in the electrical potential, or voltage, \(D = 1/RC\) is the electrical diffusivity, and \(C\) is the capacitance.

In this case, the flux of electrons replaces the flux of water, the reciprocal of the resistivity replaces the hydraulic conductivity, the voltage replaces the hydraulic head, and the capacitance replaces the specific storage coefficient.

As an example, one can construct a ground-water flow model using a network of resistors. Resistors are inversely related to the hydraulic conductivity, so a low permeability aquifer would be constructed using resistors with high resistances. A voltage can be applied at any point within the network to simulate the addition or removal of water. A ground is applied at either a point, or along a line, or at multiple points to simulate the return of the water to the system.

Another means for studying fluid flow is to use electrically conductive paper. The flow domain is drawn on the paper and then the non-conducting part of the domain is cut off. An electrode is placed at one or more locations on the paper, while a second electrode is placed elsewhere. The voltage on the paper is used to simulate the resulting flow field. This analog is limited to uniform conditions, unless papers with different electrical conductivities are used.

2.2.3 Heat

The flux equation of heat is:

\[
\vec{j} = -K \nabla T
\]

\[
\nabla \cdot \vec{j} = -C_p \frac{\partial T}{\partial t}
\]

\[
D \nabla^2 T = \frac{\partial T}{\partial t}
\]

where \(\vec{j}\) is the heat flux vector, \(K\) is the thermal conductivity parameter, \(\nabla T\) is the gradient in the temperature, \(D = K/C_p\) is the thermal diffusivity, and \(C_p\) is the heat capacity.

A similar analog using heat can also be constructed. A heat-conducting surface is constructed in the shape of the system to be studied. A constant heat source is placed at one or more locations, and the resulting temperature is measured. Materials with variations in conductivity
can be used to reproduce variations in water transmitting properties.

If steady flow is desired, then only the conductance, or flux, component is needed. However, the storage must be included when modeling dynamic conditions, i.e., when there are temporal changes in the system. For the electrical analogs, capacitors must be placed alongside the resistors. For inertial components, inductors (or coils) must be used. For thermal analogs, the heat capacity of the surface should match the storage coefficient of the hydraulic system.

### 2.2.4 Solutes

The flux equation of solutes due to a concentration gradient is:

\[ \vec{J} = -D \nabla C \] 

\[ \nabla \cdot \vec{J} = -\frac{\partial C}{\partial t} \] 

\[ D \nabla^2 C = \frac{\partial C}{\partial t} \]

where \( \vec{J} \) is the solute flux vector, \( D \) is the solute diffusivity, \( \nabla C \) is the gradient in the solute concentration.

### 2.3 Scale Analogs

A scale model is a common tool for studying large systems. Like a map, the original system is reduced in size so that it fits within a laboratory or other reasonably sized structure. For a system with an original length of \( L_o \), the modeled scale, \( L_m \), is:

\[ L_m = \lambda L_o \] 

where \( \lambda \) is the model scale. Note that \( \lambda < 1 \), meaning that a smaller scale involves a larger reduction - a 1:1000 model is a smaller scale than a 1:10 model.

For example, a river with a width of 1 km, a depth of 10 m, and a length of 1000 km can be scaled down to a manageable size using a \( \lambda = 1:10,000 \) scale, so that the model river is 10 cm wide, 1 mm deep, and 100 m long. While this is still the length of a football field, model simulations might be performed within an indoor arena of sufficient size.

The features of the flowing river would also have to be reproduced. If the original bed material within the river is a sand with a diameter of 0.3 mm, then the bed material of the scale model would have to have a diameter of 30 nm, or 300 Å, which is a fine clay particle. Also, a velocity of 3 m/s in a natural setting would correspond to a velocity of 0.3 mm/s, or about 1 m/hr.

The viscosity of the fluid would also have to change because the shear stress of fluids is a function of the length scale used. As the depth of water, or any fluid, gets thinner, then the effects of viscosity increase. The Reynolds number, \( R \), describes the ratio of inertial to viscous forces:

\[ R = \frac{vL\rho}{\mu} = \frac{vL}{\nu} \] 

where \( v \) is the fluid velocity, \( L \) is the length scale, \( \rho \) is the fluid density, \( \mu \) is the dynamic viscosity, and \( \nu = \mu/\rho \) is the kinematic viscosity. For water at 4°C, \( \rho = 1 \text{ kg/L} \), \( \mu = 1 \text{ g/m/s} \), and \( \nu = 10^{-6} \text{ kg/m}^2/\text{s} \). We know that water flows is in a laminar manner if \( R < 10 \), and flows in a turbulent manner when \( R > 100 \).

The viscosity of water is a measure of its ability to flow - fluids with high viscosity flow more slowly than fluids with lower viscosity. A Newtonian fluid is one which obeys the relationship that:

\[ \Upsilon = -\mu \frac{\partial v_x}{\partial y} \] 

where \( \mu \) (Pa s), is the dynamic viscosity of water, and \( \Upsilon \) is the shear stress within the fluid, and \( \partial v_x/\partial y \) is the rate of change in the y-direction of the fluid velocity in the x-direction. The shear stress is a measure of the forces on the fluid, and turbulent flow occurs if the forces exceed a threshold value.

Thus, in order to maintain the proper flow conditions, laminar or turbulent, then the viscosity of the fluid must change at a rate equal to the product of the velocity and length scales.

### 2.3.1 Dimensional Analysis

Whenever you use an equation, pay particular attention to the units - they must balance each other on each side of the equation. For example:

\[ v \text{ (m/s)} = \frac{dx \text{ (m)}}{dt \text{ (s)}} \] 

where \( v \) is the velocity, in units of meters per second, \( dx \) is the change in distance, in units of meters, and \( dt \) is
the change in time, in units of seconds. Note how the units on the left-hand side perfectly balance those on the right. One can check the accuracy of the equation, or your calculations, by examining whether the units are correct.

When modeling a new system, one can develop a functional relationship just based on the units. For example, if we know that the velocity is based on distance and time, there is only one combination that yields a balanced set of units. So, rather than having to remember the equation, one only needs to remember the units.

Taking this one step further, the Buckingham-π theorem states that one can establish a set of possible physical relationships if the number of independent variables are known. For example, if we know that the velocity of falling water is affected by distance and time, as well as gravitational acceleration, then, by dimensional analysis, we arrive at the following possible combinations of variables:

\[
v (m/s) = f \{ g (m/s^2), dt (s) \}
\]

\[
v (m/s) = f \{ g (m/s^2), dx (m) \}
\]

\[
g (m/s^2) = f \{ v (m/s), dt (s) \}
\]

where \( g \) is the gravitational acceleration in units of m/s\(^2\). Using a bit of math, we can show that these are equivalent to:

\[
v = g dt
\]

\[
v^2 = 2g dx
\]

\[
g = \frac{dv}{dx}
\]

### 2.3.2 Example: Fractal Scaling

Some systems display self-similar behavior, meaning that it looks the same regardless of the scale of measurement. Examples include:

**Shorelines:** Length of land-ocean boundary increases as ruler length decreases

**River densities:** Number and length of waterways increases as map scale becomes finer

**Soil Physics:** Scaling of particles shifts soil-moisture characteristic curves to common shape

**Geophysical Measurements:** Bulk resistivity is not just product of resistivity and porosity

**Fractured Media:** Fracture density changes as the scale of measurement changes

We will examine tortuosity which is a commonly observed property of environmental systems. The definition of tortuosity used here (recognizing that there are several different definitions in the literature) is:

\[
\text{Tortuosity, } \tau : \text{ The ratio of the path length } \Delta s, \text{ to the ruler (straight-line) length, } \Delta x:
\]

\[
\tau = \frac{\Delta s}{\Delta x}
\]

The path length along a streamline between two points is generally unknown, however. In general, the parameters which may be measured using experimental tests are:

**Total Head Difference, } \Delta h:** The change in head between two points:

\[
\Delta h = h_b - h_a
\]

**Hydraulic Gradient, i:** The change in head, \( \Delta h \), per unit distance, \( \Delta x \):

\[
i = \frac{\Delta h}{\Delta x}
\]

**Hydraulic Conductivity, } K:** The ability of a geologic medium to transmit water, calculated using:

\[
K = \frac{q}{i}
\]

**Travel Time, } t_t:** The time required for a particle of water to move from one point to another, equal to the distance, \( \Delta x \), divided by the fluid velocity, \( v \):

\[
t_t = \frac{\Delta x}{v}
\]

**Fluid Velocity, } v:** The rate at which water moves through the aquifer, equal to the flux, \( q \), divided by the effective porosity, \( n \):

\[
v = \frac{q}{n}
\]

**Effective Porosity, } n:** The volume of voids, \( V_V \), per unit volume of geologic medium, \( V_T \):

\[
n = \frac{V_V}{V_T}
\]

The hydraulic gradient can be calculated at two scales, as a straightline gradient along \( \Delta x \), or along the curve associated with the true path described by \( \Delta s \)

\[
i_x = \frac{\Delta h}{\Delta x} \quad \text{and} \quad i_s = \frac{\Delta h}{\Delta s}
\]

It is easy to see that

\[
i_x = \frac{\Delta h}{\Delta x} = \frac{\Delta h}{\Delta s} \frac{\Delta s}{\Delta x} = i_s \tau
\]

or

\[
i_s = \frac{i_x}{\tau}
\]
The hydraulic conductivity at the experimental scale can also be related to the value at the streamline scale:

\[ K_x = \frac{q}{i_x} = \frac{q}{\tau s} = \frac{K_s}{\tau} \quad (2.48) \]

\[ K_s = \frac{q}{i_s} = \tau \frac{q}{i_x} = \tau K_x \quad (2.49) \]

For extrapolating tests from one scale, say at a field or laboratory scale of size, \( \Delta x_1 \), to a different scale, \( \Delta x_2 \), the following relationship can be used:

\[ \frac{K_1}{K_2} = \frac{i_2}{i_1} = \frac{\tau_2}{\tau_1} \quad (2.50) \]

Similar to the gradient and the hydraulic conductivity, the calculated travel time may also be affected by the scale of measurement. The travel time is defined here as the integral of the inverse velocity along a one-dimensional streamline:

\[ t_i = \int_{s_a}^{s_b} v^{-1} \, ds \quad (2.51) \]

where \( t_i \) is the fluid travel time, \( v \) is the fluid velocity along streamline, \( s \) is the distance along streamline, and \( s_a \) and \( s_b \) are the particle starting and ending positions, respectively. The fluid velocity is the volumetric flow rate per unit area (i.e., the darcian flux) divided by the porosity, or:

\[ v = \frac{q}{n} = \frac{Q}{nA} = -\frac{K_i s_i}{n} \quad (2.52) \]

where \( q = -K_i s_i \) is the fluid flux, \( n \) is the porosity, \( Q \) is the total flow, \( A \) is the cross-sectional area, \( K_s \) is the local hydraulic conductivity, and \( i_s \) is the local hydraulic gradient. By assuming constant velocity along the streamline, we obtain:

\[ t_i = \frac{\Delta s}{v} = \frac{n\Delta s}{q} = -\frac{n\Delta s}{K_i} = -\frac{n\Delta s^2}{K_s \Delta h} \quad (2.53) \]

where \( i = \Delta h/\Delta s \), and where \( \Delta s = s_b - s_a \) is the distance along the streamline, and \( \Delta h = h_b - h_a \) is the head drop along the streamline. Switching to ruler lengths, we have:

\[ t_i = -\frac{n\tau^2 \Delta s^2}{\tau K_s \Delta h} = -\frac{n\tau^2 \Delta h^2}{K_x \Delta h} \quad (2.54) \]

If the concept of fractal scaling is employed, then a relationship between the tortuosity at one scale can be related to the tortuosity at a different scale:

\[ \tau_1 = \tau_0^{\beta \Delta x_1} \quad (2.55) \]

and

\[ \tau_2 = \tau_0^{\beta \Delta x_2} \quad (2.56) \]

where \( \beta \) is a fractal scaling parameter and \( \tau_0 \) is a dimensionless fractal tortuosity parameter.

**Summary.** This example demonstrates the effect of tortuosity and the scale of measurement on the hydraulic conductivity, hydraulic gradient, and travel time. A critical parameter in this analysis is the tortuosity, a result of the geometry of the flow regime. Additional research is required related to the effects of spatial variability on tortuosity, and the relationship between scale and the estimated tortuosity.

The spatial variability of tortuosity along the streamline may or may not have significant effects on the estimated travel time. It may be possible that local fluctuations in this parameter may not significantly affect regional travel times. Also, if the tortuosity is scale invariant, then laboratory and field parameter estimates can be directly applied to regional-scale models without the need for incorporating scale effects.

### 2.4 Problems

1. **Exponents and Logarithms**

   (a) What is the range of \( e^x \) if the range of \( x \) is \(-\infty < x < \infty\)?

   (b) What is the range of \( x \) if the range of \( \log(x) \) is \(-\infty < \log(x) < \infty\)?

2. **Process Analogs** Using the provided electrical conducting paper:

   (a) Construct a fluid flow model using a simple geometry, like a stream with pools and narrows, or an aquifer with varying shape.

   (b) Attach a low-voltage electrical source to the paper - such as a 9-V battery - so that the negative terminal is connected to one end of the paper and the positive terminal is attached to the opposite end.

   (c) Map lines of constant voltage on the paper.

   (d) Discuss how one could construct a heat analog model using various metals.

   (e) Discuss the advantages and disadvantages of astronauts using swimming pools to simulate the effects of zero gravity.

3. **Scale Analogs** Consider a miniature aquifer measuring 1-m long, 10-cm wide, and 1-cm thick, in which food-coloring is added to show contaminant transport:

   (a) Discuss the effects on model results if water and a sand medium is used.

   (b) Discuss how these effects might be reduced or eliminated by using alternate materials.

4. **Tortuosity** Consider an aquifer with a tortuosity of 2.
(a) Discuss the impacts of a travel time prediction if the hydraulic conductivity was estimated using flow between two wells.

(b) Explain how the tortuosity (sometimes called the formation factor) might be estimated using electrical methods.
Chapter 3

Network Models

We are often faced with the challenge of organizing data. We start by grouping like quantities together; put all lakes in one group, all rivers in another, and all groundwater in a third. These groupings could be considered to be entities. We then try to find relationships between these entities; surface and ground water interact, rivers flow into and out of reservoirs.

This organization is called a network, in that each entity is qualitatively different from the others, and there are unique relationships between each entity. As the model develops, one may begin to distinguish between specific elements within each entity; small lakes behave differently than large lakes, surficial aquifers behave differently from confined aquifers. We then create new entities and relationships between these entities.

This chapter focuses on network models, and how they can be used to represent environmental systems.

3.1 Percolation Models

Percolation models use nodes to describe locations that have discrete values, such as occupied or vacant, on or off. They also use bonds that connect the nodes, which can be open or closed, and can have distinct attributes. In this section, we describe several types of percolation models, such as:

- Water percolating through a soil column
- Contaminants percolating a fractured rock network
- Wells connected through a layered aquifer system

These models are a function of scale and dimension:

- As distance decreases between boundaries, connected network probability changes
- For 1-d flow, only one bond needs to be broken to shut down the network, fewer bonds are needed to complete a network in higher dimension
- Fracture length strongly affects network connectivity, long fractures form a backbone

3.1.1 Frequency Distributions

There are two classes of distributions - discrete and continuous. A discrete distribution is used when only countable number of outcomes are possible, such as the tosses of a coin, or the number of students in a class. Continuous distributions are used for describing outcomes can have any fractional value, such as the monthly or annual rainfall depth.

Discrete Distributions

Examples of discrete distributions that can be used to model these problems include the uniform, binomial, and geometric distributions.

The discrete uniform distribution, as the name implies, has a constant probability for all outcomes between $x_1$ and $x_2$. The corresponding probability for each outcome, $x$, is:

$$ P(x) = \frac{1}{n} \quad (3.1) $$

where $n$ are the number of outcomes.

Another discrete distribution is the binomial, which we used earlier to predict the probability of the number of heads when a coin is repeatedly tossed $n$ times:

$$ P(x) = \binom{n}{x} p^x (1-p)^{n-x} \quad (3.2) $$

where

$$ \binom{n}{x} = \frac{n!}{x! (n-x)!} \quad (3.3) $$

is the combinatorial operator that accounts for the number of opportunities for getting the same outcome.

Another common discrete distribution is the geometric, which is used to calculate the probability of a failure after $x$ attempts:

$$ P(x) = p \ (1-p)^x \quad (3.4) $$

where $p$ is the likelihood of failure on each attempt.
CHAPTER 3. NETWORK MODELS

Continuous Distributions

Examples of continuous distributions include the uniform, normal, exponential, gamma, and Gumbel extreme value. One can increase the number of distributions by taking the logarithm of the random variable, resulting in distributions such as the log-normal, log-gamma, etc.

The continuous uniform distribution takes the form:

\[ P(x) = \frac{1}{b-a} \]

when \( a \leq x \leq b \). This is a two-parameter distribution, meaning that two numbers, \( a \) and \( b \), are sufficient to describe the distribution.

The normal distribution is another two-parameter distribution, requiring the mean and standard deviation, \( \bar{x} \) and \( s_x \), respectively. The distribution is unbounded below and above, defined using:

\[ P(x) = \frac{1}{\sqrt{2\pi} \bar{x}} e^{(z^2)/2} \]

and where

\[ z = \frac{x - \bar{x}}{\bar{x}} \]

is the standard normal variable with mean zero, \( \bar{z} = 0 \), and unit standard deviation, \( \bar{z} = 1 \).

The log-normal distribution is a two-parameter distribution obtained by setting \( y = \ln(x) \) so that \( x = e^y \) is log-normally distributed. The log-normal distribution is unbounded above, but bounded by zero on the left.

\[ P(x) = \frac{1}{\sqrt{2\pi} \ln x} e^{(z^2)/2} \]

where

\[ z = \frac{\ln x - \ln \bar{x}}{\ln x} \]

is the standard normal variable with mean zero, \( \bar{z} = 0 \), and unit standard deviation, \( \bar{z} = 1 \).

The exponential distribution has just one parameter, \( \bar{x} \), and takes the form:

\[ P(x) = \frac{1}{\bar{x}} e^{-x/\bar{x}} \]

Note that this distribution is bounded by \( 0+ \) on the left, and \( \infty \) on the right.

The gamma distribution is a two-parameter distribution that represents the sum of exponentials:

\[ P(x) = \frac{\beta^{-\alpha} x^{\alpha-1} e^{-x/\beta}}{\Gamma(\alpha)} \]

where \( \alpha = (\bar{x}/\bar{x})^2 \), \( \beta = \bar{x}^2/\bar{x} \), and \( \Gamma(\alpha) = (\alpha-1)! \) is the gamma function. The gamma function is the same as the \( \chi^2 \) distribution when \( \alpha = \nu/2 \) and \( \beta = 2 \).

The log-gamma function is also known as the Log-Pierson Type III distribution which is widely used for extreme value problems. Another common extreme-value distribution is the Gumbel:

\[ P(x) = \frac{1}{\bar{x}} e^{z} e^{-e^z} \]

where \( z = (x - \bar{x})/\bar{x} \) is the standard normal variable.

3.1.2 Markov Chains

A Markov Chain model has discrete (or finite) states, such as rainy and dry days. We can use the concept of probability to say that the sum of all states has to equal one. That is, if \( p \) is the probability that a day is rainy, and \( q \) is the probability that it is dry, then \( p + q = 1 \).

Once the states are defined, we need to define a state transition matrix, which is simply the function that indicates the probability of moving from one state to another.

<table>
<thead>
<tr>
<th></th>
<th>Rainy</th>
<th>Dry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tomorrow Rainy</td>
<td>( P_{ww} )</td>
<td>( P_{dw} )</td>
</tr>
<tr>
<td>Tomorrow Dry</td>
<td>( P_{wd} )</td>
<td>( P_{dd} )</td>
</tr>
</tbody>
</table>

where \( P_{ww} \) is the probability of a rainy day followed by rainy day, etc.

It is easy now to estimate the probability of different types of events:

- Two dry days followed by a rainy day:

\[ P(d,d,w) = P_{dd} \times P_{dw} \]  \( (3.13) \)

- \( n \) dry days followed by a rainy day:

\[ P(d,d,...,d,w) = (P_{dd})^{n-1} \times P_{dw} \]  \( (3.14) \)

- \( n \) wet days followed by a dry day:

\[ P(w,w,...,w,d) = (P_{ww})^{n-1} \times P_{wd} \]  \( (3.15) \)

Note also, the following properties:

- \( P(w) = P(w|w)P(w) + P(w|d)P(d) \)
- \( P(w) = P(w|d)/[1 - P(w|w) + P(w|d)] \)

which are forms of Bayes Theorem. Also note that:

- The transition probability decreases for increasing precipitation depths (0.01, 0.10, 1.00) because the likelihood of two days in a row with heavy rain is much less likely than days with light rain.
- \( P(w|w) \neq f(z,t) \), is relatively stable geographically and seasonally. Note that \( P(w|w) \) is the storm persistence probability, and \( P(d|w) = 1 - P(w|w) \) is the storm departure probability. If the probability is constant, this means that storm persistence is relatively uniform in space and time.
- \( P(d|d) = f(z,t) \), varies geographically and seasonally. Again, this is the drought persistence probability and \( P(w|d) = 1 - P(d|d) \) is the storm arrival probability. It is clear that desert climates have a
much lower chance of storms arriving than in a wetter climate. Also, areas with strong seasonal variation in weather, such as Monsoon and the Mediterranean climates, will have different rates of storm arrivals over the course of a year.

- Problem of persistence: extremely dry and wet weather may reinforce themselves. The solution is to add additional states that represent drought and flood conditions. This results in additional transition probabilities.

3.1.3 Discrete Event Modeling

Some things happen as distinct events - heads vs. tails, on vs. off, boy vs. girl, day vs. night. While other things happen along a gradient - shades of gray, moisture content, income. Models that describe the discrete nature of things are often easier to understand and build than ones that handle continuously changing variables.

- The roadway over a river will be flooded or dry.
- The water level in a well will drop below the bottom of the well.

3.1.4 Example: Extreme Values

The objective is to fit observed frequencies to a probability model. Extreme value distributions are commonly applied to maximum or minimum annual discharge. In this case the largest or smallest event in each year is identified. Alternatively, a data set could be constructed using all daily observations above, or below, a threshold discharge. This alternative technique is called a partial duration series.

3.2 Linear Systems Models

A system is composed of inputs, outputs, state variables, and parameters. One can draw a box with an input arrow, an output arrow, parameter boxes, and state-variable dials.

A linear system is one in which the value of the output varies linearly with the value of the input. For example:

$$y = f(x) = 2x$$  \hspace{1cm} (3.16)

is a linear system, because doubling the input, \(x' = 2x\), results in a doubling of the output \(y' = 2x'\). Yet,

$$y = f(x, b) = 2x + b$$  \hspace{1cm} (3.17)

is not a linear system because \(2y' \neq f(2x', b)\):

$$y' = f(x', b) = 2x' + b \neq 2(x' + b) = 2x' + 2b$$ \hspace{1cm} (3.18)

One can convert the non-linear system into a linear one by removing the constant, \(b\), so that \(y^o = y - b\):

$$y^o = y - b = f(x) = 2x$$ \hspace{1cm} (3.19)

which is now a linear system in \(y^o\).

---

Table 3.2: Method for Determining Return Periods

<table>
<thead>
<tr>
<th>Method</th>
<th>Exceedence Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weibull</td>
<td>( m / (n + 1) )</td>
</tr>
<tr>
<td>Hazen</td>
<td>( (m - 0.5) / n )</td>
</tr>
<tr>
<td>Cunnane</td>
<td>( (m - 0.4) / (n + 0.2) )</td>
</tr>
</tbody>
</table>

1. For discharge, and other heteroscedastic variables, transform the observations, \(x\), using the logarithm (base-10), \(y = \log x\) to make them homoscedastic.

2. Rank each observation from largest to smallest, \(m = 1, 2, \ldots, n\), where \(n\) is the number of events.

3. Calculate the exceedence probability of each observation, \(P_i\), using one of the following ranking statistics:

4. Plot the exceedence probability, \(P_i\), against the observations, \(x_i\).

5. Calculate the recurrence interval, \(T_i = 1/P_i\).

6. Plot the recurrence interval against the observations.

7. Specify a probability model (log-normal, log-gamma, etc.)

8. Estimate the sample moments and use these to estimate the model parameters.

9. Show the calculated probabilities on the above plots.

3.2.1 System Inputs

While many systems have random inputs, it is often helpful to examine the response to specific types of inputs, such as:

**Dirac Delta**

$$\delta(t_o) = \begin{cases} \infty & t = t_o \\ 0 & t \neq t_o \end{cases} \begin{array}{c} \text{continuous time} \end{array} \hspace{(3.20)}$$

**Kronecker Delta**

$$\delta(t_o) = \begin{cases} 1 & t = t_o \\ 0 & t \neq t_o \end{cases} \begin{array}{c} \text{discrete time} \end{array} \hspace{(3.21)}$$

**Heaviside (step)**

$$H(t_o) = \int_{-\infty}^{\infty} \delta(t_o) \, dt$$

$$= \begin{cases} 0 & t < t_o \\ 1 & t \geq t_o \end{cases} \hspace{(3.22)}$$
CHAPTER 3. NETWORK MODELS

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Pulse

\[ P(t_a, t_b) = H(t_a) - H(t_b) = \begin{cases} 0 & t < t_a \\ 1 & t_a \geq t < t_b \\ 0 & t_b \geq t \end{cases} \]  

Ramp

\[ R(t_a, t_b) = \frac{1}{t_b - t_a} \int_{t_a}^{t_b} P(t_a, t_b) \, dt = \begin{cases} 0 & t < t_a \\ \frac{t - t_a}{t_b - t_a} & t_a \geq t < t_b \\ 1 & t_b \geq t \end{cases} \] (3.24)

3.2.2 Convolution

Convolution is a type of mathematical operator, defined using \( y = h * x \) where \(*\) is the convolution operator and \( h \) is the unit response function. For the case where the input is a Delta function (either continuous or discrete), then \( y = h \). This means that a spike input causes an output equal to the unit response function.

Applications include:

- Rainfall-Runoff
- Soil Moisture Movement
- Contaminant Transport
- Groundwater Modeling

The convolution operator is defined using differently for the discrete and continuous cases. For the discrete case, it is:

\[ y(t) = \sum_{i=0}^{m} h(i) \, x(t - i) \]  

while for the continuous case, it is:

\[ y(t) = \int_{-\infty}^{t} h(\tau) \, x(t - \tau) \, d\tau \]  

The steps involved are:

1. Multiply unit response function, \( h(i) \), by input, \( x(t) \), for time step \( t \)
2. Shift to next hour and repeat Step 1, starting response at beginning of input interval
3. When all inputs have been multiplied by the Unit Response Function, add all responses

\[ y(i) = h(0) \, x(i) + h(1) \, x(i-1) + h(2) \, x(i-2) + h(3) \, x(i-3) + \cdots + h(n) \, x(i-n) \] (3.27)

3.2.3 Deconvolution

- An inverse method to estimate impulse response function
- Estimate \( h(\tau) \) values using linear regression, where

\[ y(i) = h(0) \, x(i) + h(1) \, x(i-1) + h(2) \, x(i-2) + h(3) \, x(i-3) + \cdots + h(n) \, x(i-n) \] (3.27)

3.2.4 Example: Unit Hydrographs

Unit hydrographs are used when the shape of a stormwater hydrograph is desired. It is used to predict the stormflow hydrograph for conditions where one unit of effective precipitation (net runoff) falls on a watershed during one time period. The duration, time to peak, and peak discharge are all represented using a unit hydrograph.

A common shape to use is the triangular unit hydrograph - where the duration of the hydrograph, \( t_c \), is the time of concentration within the watershed, and is the base of the triangle. The peak discharge, \( Q_p \), is the height of the triangle, and the maximum height occurs at the time to peak, \( t_p \).

The area of the triangle, \( Q = t_c \, Q_p / 2 \), represents the total volume of stormwater runoff. We normally set the total volume equal to one unit of runoff, hence the name unit hydrograph. Note that reducing the time of concentration requires a higher peak in order to maintain a unit runoff.

Other shapes besides a triangle can certainly be used - the only constraint is that the area under the curve must equal zero. The basic concept that a unit of runoff has a specific shape that is determined by the watershed.

3.3 Problems

1. Unit Hydrographs

- Find the outflow hydrograph for:
- An input \( x = [0, 10, 12, 3, 0, 5] \)
Table 3.3: Example convolution problem

Input, \( x = [1, 2, 3, 0, 1] \)

Response function, \( h = [0.1, 0.4, 0.3, 0.2] \)

<table>
<thead>
<tr>
<th>Time</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>t=1</td>
<td>0.1</td>
<td>0.4</td>
<td>0.3</td>
<td>0.2</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>t=2</td>
<td>0.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.6</td>
<td>0.4</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>t=3</td>
<td>0.0</td>
<td>0.0</td>
<td>0.3</td>
<td>1.2</td>
<td>0.9</td>
<td>0.6</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>t=4</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>t=5</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.1</td>
<td>0.4</td>
<td>0.3</td>
<td>0.2</td>
</tr>
<tr>
<td>SUM</td>
<td>0.1</td>
<td>1.2</td>
<td>1.2</td>
<td>2.0</td>
<td>1.4</td>
<td>1.0</td>
<td>0.3</td>
<td>0.2</td>
</tr>
</tbody>
</table>

- A response function \( h = [0.0, 0.5, 1.0, 1.3, 1.2, 0.8, 0.5, 0.2, 0.1, 0.0] \)

2. Percolation Model

- Assume that water flow through a (two-dimensional) porous medium can be represented as a finite number of nodes that are either wet or dry.
- Use an node configuration with the following transition probabilities to model water movement:

  \[
  \begin{array}{c c c c c c}
  & p_3 & & p_3 & & \\
  p_1 & p_2 & p_1 & p_2 & p_1 & \\
  & p_3 & & p_3 & & \\
  p_1 & p_2 & p_1 & p_2 & p_1 & \\
  & p_3 & & p_3 & & \\
  \end{array}
  \]

- where
  - \( p_1 = 0.4 \)
  - \( p_2 = 0.2 \)
  - \( p_3 = 0.1 \)
- The transition probabilities may need to be adjusted near boundaries.
- Assume that the drainage and wetting transitions are identical.

3. Extreme Events

- Find the median (50\textsuperscript{th} percentile), 10-year, and 100-year precipitation depths for the following data.

<table>
<thead>
<tr>
<th>Year</th>
<th>Max (inches)</th>
<th>Year</th>
<th>Max (inches)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1948</td>
<td>4.05</td>
<td>1976</td>
<td>3.27</td>
</tr>
<tr>
<td>1949</td>
<td>2.34</td>
<td>1977</td>
<td>3.83</td>
</tr>
<tr>
<td>1950</td>
<td>3.77</td>
<td>1978</td>
<td>2.86</td>
</tr>
<tr>
<td>1951</td>
<td>2.82</td>
<td>1979</td>
<td>3.36</td>
</tr>
<tr>
<td>1952</td>
<td>2.03</td>
<td>1980</td>
<td>3.67</td>
</tr>
<tr>
<td>1953</td>
<td>2.02</td>
<td>1981</td>
<td>2.71</td>
</tr>
<tr>
<td>1954</td>
<td>2.02</td>
<td>1982</td>
<td>2.21</td>
</tr>
<tr>
<td>1955</td>
<td>1.72</td>
<td>1983</td>
<td>2.74</td>
</tr>
<tr>
<td>1956</td>
<td>5.34</td>
<td>1984</td>
<td>2.39</td>
</tr>
<tr>
<td>1957</td>
<td>2.42</td>
<td>1985</td>
<td>1.66</td>
</tr>
<tr>
<td>1958</td>
<td>2.21</td>
<td>1986</td>
<td>4.31</td>
</tr>
<tr>
<td>1959</td>
<td>5.47</td>
<td>1987</td>
<td>2.99</td>
</tr>
<tr>
<td>1960</td>
<td>2.63</td>
<td>1988</td>
<td>1.94</td>
</tr>
<tr>
<td>1961</td>
<td>2.84</td>
<td>1989</td>
<td>5.43</td>
</tr>
<tr>
<td>1962</td>
<td>2.62</td>
<td>1990</td>
<td>3.16</td>
</tr>
<tr>
<td>1963</td>
<td>5.16</td>
<td>1991</td>
<td>2.54</td>
</tr>
<tr>
<td>1964</td>
<td>4.12</td>
<td>1992</td>
<td>2.38</td>
</tr>
<tr>
<td>1965</td>
<td>2.16</td>
<td>1993</td>
<td>2.42</td>
</tr>
<tr>
<td>1966</td>
<td>3.04</td>
<td>1994</td>
<td>7.34</td>
</tr>
<tr>
<td>1967</td>
<td>9.93</td>
<td>1995</td>
<td>4.32</td>
</tr>
<tr>
<td>1968</td>
<td>2.16</td>
<td>1996</td>
<td>2.11</td>
</tr>
<tr>
<td>1969</td>
<td>2.97</td>
<td>1997</td>
<td>3.80</td>
</tr>
<tr>
<td>1970</td>
<td>4.00</td>
<td>1998</td>
<td>3.51</td>
</tr>
<tr>
<td>1971</td>
<td>2.48</td>
<td>1999</td>
<td>2.20</td>
</tr>
<tr>
<td>1972</td>
<td>2.72</td>
<td>2000</td>
<td>2.11</td>
</tr>
<tr>
<td>1973</td>
<td>4.48</td>
<td>2001</td>
<td>6.22</td>
</tr>
<tr>
<td>1974</td>
<td>2.96</td>
<td>2002</td>
<td>3.54</td>
</tr>
<tr>
<td>1975</td>
<td>3.26</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Chapter 4

Statistical Models

Statistics is the science of understanding uncertainty. Will it rain today? Given that it has not rained for three months, what is the probability that it might rain in the next week? How does a dam (or ground-water pumping, wetland construction, timber harvesting) affect streamflows? What are the health risks from drinking contaminated water? These are all questions that are commonly asked.

While the goal of science is to separate fact from fiction, we are often limited to providing statistical measures of truth and error. Thus science often rests on the edge of certainty, not entirely sure, yet nor entirely unsure. Many of the early studies in statistics were performed by compulsive gamblers who wished to improve their odds of winning. Rather than accept the “roll of the dice”, these individuals wanted to better understand the risks they were taking, and place their bets in ways that maximized their likelihood of winning.

4.1 Probability and Statistics

Probability analysis is used to describe random behavior, such as the chance that an event will occur, or the likelihood that an event will exceed a certain magnitude. While much of nature is not entirely random, we can often apply probability models to natural systems. We can make these applications more readily in cases where:

- Events are independent of each other, and do not affect each other. That is, the result of one coin toss does not affect the following coin toss.
- Events are stationary - they are not a function of time. That is, heads are not more likely in the morning than in the evening.
- Events are identically distributed. That is, the variability of heads is the same under all conditions.

If these assumptions are satisfied, then we can say that the likelihood of either one event or another occurring is just the sum of the individual events:

\[ P(A \cup B) = P(A \text{ or } B) = P(A) + P(B) \]  

We can also say that the probability of two events, A and B, occurring together is just the product of the probability of each event:

\[ P(A \cap B) = P(A \text{ and } B) = P(A) \cdot P(B) \]  

For example, let us assume that the probability of landing either a heads (H) or a tails (T) when a coin is flipped are equal, so that there are two outcomes, with the probability of obtaining one or the other being \( p = 0.5 \).

When the coin is tossed twice, \( n = 2 \), there are four outcomes; \( H \cap H \), \( T \cap T \), \( H \cap T \), and \( T \cap H \). Each outcome has an equal probability because these are independent events. The probability of two heads in a row is:

\[ P(H \cap H) = p^2 = 0.25 \]
which is the same for landing two tails. The probability of landing one of each has two outcomes, so that:

\[ P((T \cap H) \cup (H \cap T)) = P(T \cap H) + P(H \cap T) \]

\[ = 2 p^2 = 0.5 \] \hspace{1cm} (4.4)

We can write this mathematically for any number of tosses, \( n \), to determine the number of heads, \( m \), and tails, \( n - m \)

\[ P(H = m, T = n - m) = \binom{n}{m} p^m (1 - p)^{n-m} \]

\[ = \binom{n}{m} p^m \] \hspace{1cm} (4.5)

where

\[ \binom{n}{m} = \frac{n!}{m! (n-m)!} \] \hspace{1cm} (4.6)

is the combinatorial operator that accounts for the number of opportunities for getting the same outcome, and where \( n! = n \times (n - 1) \times (n - 2) \times \cdots \times 1 \) is the factorial of \( n \).

For example, we can calculate the probability of getting exactly 5 heads and 5 tails in ten tosses:

\[ P(H = 5, T = 5) = \binom{10}{5} \left( \frac{1}{2} \right)^5 \left( \frac{1}{2} \right)^5 \]

\[ = \binom{10}{5} \left( \frac{1}{2} \right)^{10} = 0.246 \] \hspace{1cm} (4.7)

which means that we have a chance of only about 1 in 4 of getting an equal number of heads and tails.

If events are not independent of each other, then we can still calculate their probability using:

\[ P(A \cup B) = P(A) + P(B) - P(A \cap B) \] \hspace{1cm} (4.8)

For example, if the probability of a rainy day is thirty percent, \( P(A) = 0.3 \), the probability of snow is ten percent, \( P(B) = 0.1 \), and the probability of getting both rain and snow in a day is five percent, \( P(A \cap B) = 0.05 \), then the probability of getting either rain or snow in a day is:

\[ P(A \cup B) = 0.3 + 0.1 - 0.05 = 0.35 \] \hspace{1cm} (4.9)

Conditional probabilities arise when an event, \( A \), may be more (or less) likely given that another event, \( B \), has happened. In this case:

\[ P(A|B) = \frac{P(A)}{P(B)} \] \hspace{1cm} (4.10)

where \( P(A|B) \) means the probability of Event \( A \) given that Event \( B \) has already occurred.

For example, if the probability of rain and snow are again 30 and 10 percent, respectively, and the probability of snow given that rainfall has occurred is 20 percent, then the probability of rain given that snow has occurred is:

\[ P(A|B) = \left( \frac{0.3}{0.1} \right) 0.2 = 0.6 \] \hspace{1cm} (4.11)

or sixty percent.

### 4.1.1 Sample Statistics

We are often asked what the outcome of an uncertain event is likely to be, such as today’s expected high temperature. The expected value – equivalent to the mean or average – is calculated using:

\[ E(x) = \bar{x} = \int_{-\infty}^{\infty} x f(x) \, dx = \frac{1}{n} \sum_{i=1}^{n} x_i \] \hspace{1cm} (4.12)

where \( n \) is the number of observations, and \( f(x) \) is the frequency distribution of \( x \). The frequency distribution represents the likelihood of individual observation. Just as each observation is weighted by \( 1/n \), the distribution of individual observations will have a weight associated with them that corresponds to their frequency.

The variance of individual observations (when the expected value is unknown) is calculated using:

\[ V(x) = \bar{x}^2 = \int_{-\infty}^{\infty} (x - \bar{x})^2 \, f(x) \, dx \]

\[ = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2 \] \hspace{1cm} (4.13)

where \( \bar{x} = \sqrt{V(x)} \) is the standard deviation of the individual observations. If the expected value is known, \( E(x) = \mu \), then we have instead:

\[ V(x) = \sigma^2 = \frac{n-1}{n} \bar{x}^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)^2 \] \hspace{1cm} (4.14)

A case with a known mean is when a coin is tossed - the mean number of heads is always 1/2.
The **coefficient of variation** is the ratio of the standard deviation to the mean, \( c(x) = \bar{x}/\bar{x} \). An example would be the variation in height with age - is there more variation as people grow taller? Plotting the coefficient of variation would indicate how much variation there is as people age. Can you guess which age has the greatest variation?

A hydrologic example of the coefficient of variation is streamflow; low-flow variability is probably much smaller than under flood conditions, but their coefficient of variation may be similar.

The **covariance** between two variables is found using:

\[
C(x, y) = \int \int_{-\infty}^{\infty} (x - \bar{x}) (y - \bar{y}) f(x, y) \, dx \, dy
\]

\[
= \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x}) (y_i - \bar{y}) \tag{4.15}
\]

where \( f(x, y) \) is the joint frequency distribution between \( x \) and \( y \). The **correlation** between two variables is:

\[
r(x, y) = \frac{C(x, y)}{\sqrt{V(x) \, V(y)}}
\]

\[
= \frac{1}{\bar{x}} \sum_{i=1}^{n} \frac{(x_i - \bar{x}) (y_i - \bar{y})}{\bar{y}} \tag{4.16}
\]

Note that if \( x = y \), then \( C(x, y) = C(x, x) = V(x) \) and \( r(x, y) = r(x, x) = 1 \)

### 4.1.2 Higher Moments

Data is **skewed** when there are unbalanced high and low observations. For example, a stream may have an average discharge of 10 L/s, an extreme low flow of 1 L/s (9 L/s below the mean), and an extreme high flow of 100 L/s (90 L/s above the mean). This is an example of a positive skew, in that the larger observations are farther from the mean than the smaller observations. The skew - also called the **third moment about the mean** - is calculated using:

\[
Skew(x) = \int_{-\infty}^{\infty} (x - \bar{x})^3 f(x) \, dx
\]

\[
= \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^3 \tag{4.17}
\]

Like the coefficient of variation, the **skew coefficient**, \( G(x) \), is normalized, but rather than using the mean, we instead use the estimated standard deviation:

\[
G(x) = \frac{n}{n-2} \frac{Skew(x)}{\bar{x}^3}
\]

\[
= \frac{n}{(n-1) \, (n-2) \, \bar{x}^3} \sum_{i=1}^{n} (x_i - \bar{x})^3 \tag{4.18}
\]

This adjusts the skew by how variable the data are - one needs a greater skew when there is a greater variability to arrive at the same skew coefficient.

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>152</td>
<td>172.1</td>
<td>173.7</td>
<td>172.3</td>
<td>172.7</td>
<td>177.0</td>
<td>175.6</td>
<td>174.4</td>
</tr>
<tr>
<td>94</td>
<td>11.3</td>
<td>6.7</td>
<td>8.6</td>
<td>10.1</td>
<td>11.4</td>
<td>8.8</td>
<td>11.3</td>
</tr>
</tbody>
</table>

- \( \bar{x} = 174.0 \)
- \( \bar{\bar{x}} = 1.78 \)
- \( \bar{x} = 9.7 \)
- \( \bar{x}/\sqrt{\pi} = 1.94 \)

The **fourth-moment about the mean**, or kurtosis, is used to describe the frequency of low-probability events - both extremely high and low:

\[
Kurtosis(x) = \int_{-\infty}^{\infty} (x - \bar{x})^4 f(x) \, dx
\]

\[
= \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^4 \tag{4.19}
\]

### 4.1.3 Variation of Sample Statistics

The sample statistics calculated above were for individual observations. Once we have calculated these statistics, they may still be uncertain. For example, we may have calculated the mean and variance of daily rainfall for each month of the year. Yet the rainfall in each month varies from year to year. Clearly, there is still a variation in monthly averages.

For groups of events, the mean of the group, \( E(\bar{x}) \) should equal the mean of individual events within the
group, \( E(x) \):

\[
E(\bar{x}) = E(x)
\]  

(4.20)

but is not true if the calculated mean is biased.

Bias occurs when the average of a distribution does not converge to the true mean, usually because certain outcomes are more likely measured than others. Bias is relatively common in hydrology because we tend to sample more heavily in good weather, and avoid taking measurements when the weather is awful.

The variance of the sample mean will be different from the variance of individual events because the average behavior is commonly much less variable than the individual events.

\[
V(\bar{x}) = \frac{V(x)}{n} \quad \text{and} \quad \bar{x} = \frac{\bar{x}}{\sqrt{n}}
\]  

(4.21)

The variation in the variance is described using the \( \chi^2 \) (pronounced \( k^2 \) squared) statistic, which is mathematically equivalent to a gamma distribution (below), with \( \beta = 2 \) and \( \alpha = \nu/2 \), and where \( \nu \) (pronounced \( nu \)) are the degrees of freedom, equal to the number of observations minus the number of statistics (such as the mean and variance) that are being estimated. This is equivalent to:

\[
\chi^2(x, \nu) = \frac{2^{-\nu/2} x^{\nu/2-1} e^{-x/2}}{\Gamma(\nu/2)}
\]  

(4.22)

### 4.1.4 Hypothesis Testing

One reason for estimating statistics is to be able to make a definitive statement about a situation. Did this timber harvest cause this flooding? Did this dam destroy this habitat?

To answer a question definitively, we need some process to decide whether a chance occurrence is sufficiently unlikely that we can safely say that it is improbable. For example, we might think the number of heads and tails should be approximately equal, yet we sometimes observe twenty heads in twenty tosses. We can calculate the probability as \( 0.5^{20} = 10^{-6} \), or one chance in a million. We might suspect that this coin is not fair.

Furthermore, we might say that any coin that has a rare outcome (say, less than one chance per thousand, \( 10^{-3} \)) should not be used. Using this rejection statistic, we recommend that this coin should be rejected as being unfair. In other words, outcomes that are beyond normal expectation are rejected, while outcomes that behave normally are not rejected.

There are two errors when this method is used. Even a fair coin has a slight chance of yielding a rare outcome. Thus, by rejecting the coin, we may be making a mistake. We call the rejection of a fair coin a Type 1 Error. On the other hand, an unfair coin may still give normal results and not be detected. We call the failure to reject an unfair coin a Type 2 Error.

For example, let’s say that a river flooded following a timber cut. We observe that the flood is far worse than any observed flood, and conclude that the timber harvest caused the flood. We may then be making a Type 1 error. On the other hand, there may actually be adverse flooding from timber harvests, but the effects were too small to notice with everything else going on. This is the Type 2 error.

In statistical testing, we can assume that observations are normally distributed - the familiar bell-shaped curve. If the observation is too far from the mean, then we might think it is fundamentally different from the other observations. To check, we first find the standard normal variable:

\[
z = \frac{x - \bar{x}}{\bar{x}}
\]  

(4.23)

and then use this variable to make a decision. Using the normal distribution, we can calculate the likelihood of this variable. If the probability is too small, then we might decide that it does not belong.

### 4.2 Regression

We normally use a linear regression equation of the form:

\[
y = y_o + a x
\]  

(4.24)

where \( x \) is the column vector, \((n \times 1)\), of independent observations, \( y \) is the column vector, \((n \times 1)\) of dependent observations, \( y_o \) is the intercept, and \( a \) is the slope.

Surprisingly, this equation is not a linear function. A linear function, \( y = f(x) \), has the property that:

\[
f(2x) = 2f(x)
\]  

(4.25)

which means that if you double the input, you should double the output. To check to see if our equation, above, is linear, we have:

\[
2y = 2(y_o + ax) = 2y_o + 2ax \neq y_o + a(2x)
\]  

(4.26)

so that it is clearly nonlinear! To linearize this function, we note that:
\[ \overline{y} = E(y) = E(y_o + ax) = y_o + a\overline{x} \]  
(4.27)

We make a linear equation by subtracting this second equation from the original equation:
\[ Y = y - \overline{y} = y_o + ax - (y_o + a\overline{x}) = a(x - \overline{x}) = aX \]  
(4.28)

where the new variables, \( Y = y - \overline{y} \) and \( X = x - \overline{x} \), are just the original data with their means subtracted.

For multiple independent variables, then we can establish the multiple regression equation:
\[ y = a_o + a_1 x_1 + a_2 x_2 + \cdots + a_m x_m \]  
(4.29)

### 4.2.1 Matrices

A matrix is an organized set of numbers. For example, a simple, two-dimensional matrix may look like:
\[ u = \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \\ u_{31} & u_{32} \end{bmatrix} \]  
(4.30)

where the double underlines indicate that there are two subscripts, \( u_{ij} \), which refer to the elements in each row and column, respectively. In this case, there are three rows and two columns.

We indicate the size of the matrix using the notation, \((m, n)\), where \( m \) is the number of rows, and \( n \) is the number of columns. For our case, the size is \((3, 2)\). A three-dimensional matrix would have a size of \((m, n, p)\), where \( p \) represents the number of layers in the matrix.

The transpose of a matrix reverses the orientation of the matrix. That is, the columns are exchanged with the rows. Using the previous matrix as an example, the transpose of \( u \) is:
\[ u^T = \begin{bmatrix} u_{11} & u_{12} & u_{31} \\ u_{12} & u_{22} & u_{32} \end{bmatrix} \]  
(4.31)

where the superscript \( T \) is used to indicate the transpose. The apostrophe, \( ' \), is another symbol that is commonly used to indicate the transpose, \( u' = u^T \). The size of \( u^T \) is \((n, m)\), or \((2, 3)\) for this example. Note that one only has to switch the location of the indices, \( u'_{ij} = u_{ji} \), to obtain the transpose.

Adding, subtracting, multiply, and dividing by a constant, \( c \), to a matrix is obtained by performing the operation to every element of the matrix:
\[ c + u = \begin{bmatrix} c + u_{11} & c + u_{12} \\ c + u_{21} & c + u_{22} \\ c + u_{31} & c + u_{32} \end{bmatrix} \]  
(4.32)

\[ cu = \begin{bmatrix} cu_{11} & cu_{12} \\ cu_{21} & cu_{22} \\ cu_{31} & cu_{32} \end{bmatrix} \]  
(4.33)

Matrices can be added and subtracted if they have the same size. That is, if they have the same number of rows and columns.
\[ u + v = \begin{bmatrix} u_{11} + v_{11} & u_{12} + v_{12} \\ u_{21} + v_{21} & u_{22} + v_{22} \\ u_{31} + v_{31} & u_{32} + v_{32} \end{bmatrix} \]  
(4.34)

where the size of both \( u \) and \( v \) is \((3, 2)\). Matrix addition is also possible if one matrix has a lower dimension. For example, we can perform the operation:
\[ u + w = \begin{bmatrix} u_{11} + v_{11} & u_{12} + v_{1} \\ u_{21} + v_{2} & u_{22} + v_{2} \\ u_{31} + v_{3} & u_{32} + v_{3} \end{bmatrix} \]  
(4.35)

where the size of \( v \) is \((m) = (3)\). Note that it is also possible to add a vector with a size of \((n) = (2)\) by taking the transpose:
\[ u + w^T = \begin{bmatrix} u_{11} + v_{1} & u_{12} + v_{2} \\ u_{21} + v_{2} & u_{22} + v_{2} \\ u_{31} + v_{1} & u_{32} + v_{2} \end{bmatrix} \]  
(4.36)

Matrix multiplication is achieved by multiplying every row of the left-hand matrix by every column of the right-hand matrix. In this case, the number of columns of the left-hand matrix must equal the number of rows of the right-hand matrix, and the result has a size equal to the number of rows of the left-hand matrix and the number of columns of the right-hand matrix:
\[ (m, n) \times (n, p) = (m, p) \]  
(4.37)

\[ uv = \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \\ u_{31} & u_{32} \end{bmatrix} \times \begin{bmatrix} v_{1} \\ v_{2} \end{bmatrix} = \begin{bmatrix} u_{11}v_{1} + u_{12}v_{2} \\ u_{21}v_{1} + u_{22}v_{2} \\ u_{31}v_{1} + u_{32}v_{2} \end{bmatrix} \]  
(4.38)

For this problem, the multiplication is \((3, 2) \times (2, 1) = (3, 1)\). The identity matrix, \( I \), is defined as the matrix which when multiplied by another matrix yields the original matrix:
\[ uI = u \]  
(4.39)

where the sizes of the \( u \) and \( I \) matrices are \((m, n)\) and \((n, n)\), respectively. The identity matrix takes the form:
\[ I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]  
(4.40)

for \( n = 3 \). Note that \( I \) is always a square matrix, where the diagonal elements all equal one and all the off-diagonal elements all equal zero.

Matrix division is not possible, but we can obtain the desired solution by using the matrix inverse:
\[ u = uv \]  
(4.41)
\[
\begin{align*}
\mathbf{v}^{-1} \mathbf{w} &= \mathbf{u}^{-1} \mathbf{u} \\
\mathbf{v}^{-1} \mathbf{w} &= \mathbf{I} \mathbf{v} \\
\mathbf{v} &= \mathbf{u}^{-1} \mathbf{w}
\end{align*}
\] (4.42)

where
\[
\mathbf{u}^{-1} \mathbf{w} = \mathbf{I} \mathbf{v}
\] (4.45)

### 4.2.2 Ordinary Least Squares

In regression, we normally have a large number of observations of \(x\) and \(y\) from which we wish to estimate the regression coefficients. To do this easily we can make a set of vector equations:

\[
\mathbf{y} = \mathbf{X} \beta
\] (4.46)

where \(\mathbf{y}\) is a \((n \times 1)\) column vector of \(n\) observations of the dependent variable, \(\mathbf{X}\) is a \(n \times m\) matrix of \(n\) observations of each of the \(m\) variables, and \(\beta\) is the \((m \times 1)\) column vector of unknown regression coefficients. This is the same as:

\[
\begin{bmatrix}
Y_1 \\
Y_2 \\
\vdots \\
Y_n
\end{bmatrix} =
\begin{bmatrix}
X_{11} & X_{12} & X_{13} & \cdots & X_{1m} \\
X_{21} & X_{22} & X_{23} & \cdots & X_{2m} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
X_{n1} & X_{n2} & X_{n3} & \cdots & X_{nm}
\end{bmatrix}
\begin{bmatrix}
\beta_1 \\
\beta_2 \\
\vdots \\
\beta_m
\end{bmatrix}
\]

(4.47)

Common multiple regression uses ordinary least squares, OLS, to estimate the regression coefficients. To begin, we first pre-multiply both sides by the transpose of \(\mathbf{X}\), \(\mathbf{X}^T\):

\[
\mathbf{X}^T \mathbf{y} = \mathbf{X}^T \mathbf{X} \beta
\] (4.48)

where \((\mathbf{X}^T \mathbf{X})\) is a square matrix, diagonally dominant, and symmetric, and is closely related to the variance-covariance matrix:

Note that the variance of \(x_j\) is:

\[
V_j = \frac{1}{n-1} \sum_{i=1}^{n} X_{ij}^2
\] (4.49)

and the covariance between \(X_j\) and \(X_k\) is:

\[
C_{jk} = \frac{1}{n-1} \sum_{i=1}^{n} X_{ij} X_{ik}
\] (4.50)

so that the diagonal of the \((\mathbf{X}^T \mathbf{X})\) matrix is related to the variance of each of the variables and the off-diagonal elements are the covariances.

\[
\mathbf{X}^T \mathbf{X} = (n-1)
\begin{bmatrix}
V_1 & C_{12} & C_{13} & \cdots & C_{1m} \\
C_{21} & V_2 & C_{23} & \cdots & C_{2m} \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
C_{m1} & C_{2m} & C_{3m} & \cdots & V_m
\end{bmatrix}
\] (4.51)

and

\[
\mathbf{X}^T \mathbf{y} = (n-1)
\begin{bmatrix}
C_{1Y} \\
C_{2Y} \\
\vdots \\
C_{mY}
\end{bmatrix}
\] (4.52)

where \(C_{iY}\) is the covariance between \(X_i\) and \(Y\).

Continuing with our effort to estimate the unknown regression coefficients, \(\hat{\beta}\), we now pre-multiply both sides by the inverse of the \((\mathbf{X}^T \mathbf{X})\) matrix, \((\mathbf{X}^T \mathbf{X})^{-1}\), yielding:

\[
\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \mathbf{y})
\] (4.53)

The residuals are the difference between the estimated and observed dependent variables:

\[
e = \mathbf{y} - \hat{\mathbf{y}}
\] (4.54)

The mean of the residuals is zero, \(E(e) = \bar{e} = 0\), and the fitting error is the standard error of the residuals:

\[
V(e) = \bar{e}^2 = e^T e
\] (4.55)

The variance-covariance matrix of \(\hat{\beta}\) is:

\[
V(\hat{\beta}) = \bar{e}^2 (\mathbf{X}^T \mathbf{X})^{-1}
\] (4.56)

The variance-covariance matrix is very important because it contains information about how your model parameters are correlated. For example, if rainfall and temperature are inversely correlated, then a negative covariance is expected. Variables that are highly correlated are called colinear, and result in large values in the variance-covariance matrix. Multicolinearity is the general problem of using variables that are highly correlated to each other, causing large prediction uncertainties.

Predicted outcomes, \(\mathbf{y}_p\), for specific prediction conditions, \(\mathbf{x}_p\) (as opposed to observed conditions), is given by:

\[
\mathbf{y}_p = \mathbf{x}_p \hat{\beta}
\] (4.57)

and the prediction error is:

\[
V(\mathbf{y} - \mathbf{y}_p) = V(e) + \mathbf{x}_p V(\hat{\beta}) \mathbf{x}_p^T
\]

\[
= \bar{e}^2 + \bar{e}_p^2
\] (4.58)

which means that the total prediction error depends on the fitting errors, \(\bar{e}\), along with errors due to parameter errors, \(\bar{e}_p\).

The confidence intervals about \(\mathbf{y}_p\) are given by:

\[
\mathbf{y}_p \pm t(n, \alpha) V(\mathbf{y} - \mathbf{y}_p)^{1/2}
\] (4.59)
\[ X^T X = \begin{bmatrix} \sum_{i=1}^{n} X_{1i}^2 & \sum_{i=1}^{n} X_{1i} X_{2i} & \cdots & \sum_{i=1}^{n} X_{1i} X_{mi} \\ \sum_{i=1}^{n} X_{2i} X_{1i} & \sum_{i=1}^{n} X_{2i}^2 & \cdots & \sum_{i=1}^{n} X_{2i} X_{mi} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} X_{mi} X_{1i} & \sum_{i=1}^{n} X_{mi} X_{2i} & \cdots & \sum_{i=1}^{n} X_{mi}^2 \end{bmatrix} \]

### 4.2.3 Transformations

Ordinary least squares, the primary approach for forming a regression equation, assumes that the data are homoscedastic, meaning that the errors are constant, and are independent of the magnitude of the observation. In reality, many stream discharge measurements are variable - a function of the magnitude of the observation. These are heteroscedastic errors, which must be eliminated by transforming the data prior to performing a regression.

#### Exponential Model

A linear reservoir drains according to the following exponential equation:

\[ y = y_o \exp(-kt) = y_o e^{-kt} \tag{4.60} \]

It is common that any errors in tail are much smaller than errors near peak - that is, the magnitude of any errors are a function of the magnitude of the observation. This implies that the errors are heteroscedastic. Recall that for this exponential model, taking the log of the data eliminates heteroscedasticity:

\[ \ln(y) = \ln(y_o) - kt \tag{4.61} \]

which is now a linear model between \( \ln(y) \) and \( t \):

\[ Y = Y_o - kt \tag{4.62} \]

where \( Y = \ln y \) and \( y_o = e^{Y_o} \).

#### Log-Log Model

A non-linear reservoir model, such as a weir, has the general form:

\[ y = y_o \ x^n \tag{4.63} \]

which can be linearized by taking the logarithm of both sides:

\[ \ln y = \ln y_o + n \ln x \tag{4.64} \]

Introducing new variables, \( Y = \ln y \) and \( X = \ln x \), yields the general linear equation:

\[ Y = Y_o + n \ X \tag{4.65} \]

where \( Y_o = \ln y_o \) or \( y_o = e^{Y_o} \).

#### Polynomial Model

A general polynomial model is of the form:

\[ y = a_o + a_1 \ x + a_2 \ x^2 + a_3 \ x^3 + \cdots + a_n \ x^n \tag{4.66} \]

To make this linear, we create new variables, \( x_1 = x \), \( x_2 = x^2 \), etc., and then use these instead:

\[ y = a_o + a_1 \ x_1 + a_2 \ x_2 + a_3 \ x_3 + \cdots + a_n \ x_n \tag{4.67} \]

and estimate the coefficients using OLS.

#### Power Model

A commonly used multiplicative, or power, model is:

\[ y = a_o \ x^{a_1} \ x^{a_2} \ x^{a_3} \cdots \ x^{a_m} \tag{4.68} \]

To linearize this, we again use the logarithmic transform, \( Y = \ln y, \ X_1 = \ln x_1 \), etc., yielding:

\[ Y = A_o + a_1 \ X_1 + a_2 \ X_2 + a_3 \ X_3 + \cdots + a_m \ X_m \tag{4.69} \]

where \( A_o = \ln a_o \).

#### Examination of Residuals

One method for determining whether a transformation is needed is to examine the residuals. To begin, we first make a prediction using a linear model, \( \hat{y} = \beta x \), and then calculate the residuals, \( e = y - \hat{y} \), using the difference between the predicted and observed dependent variables. We then plot these residuals against the observed dependent variable, \( y \) vs. \( e \). Finally, we check to see if there is any correlation between \( y \) and \( e \). If so, then we must transform the \( y \) until the correlation with the residuals is eliminated.

#### Example: Watershed Characteristics

Empirical models can be used, such as the Benson model, can be used to estimate peak flows, \( Q_p \):

\[ Q_p = a \ A^b \ S^c \ S_t^d \ I_b^f \ L^g \tag{4.70} \]

where \( A \) is the watershed area, \( S \) is the main channel slope, \( S_t \) is the area of lakes and ponds, \( I_b \) is the maximum 24-hour, 10-year precipitation depth, and \( L \) is the main channel length.

Another model, proposed by Scott, is:

\[ Q_p = a \ A^b \ E_m^c \ S_t^d \ P_s^e \ I_b^f \ T^g \tag{4.71} \]
where $E_m$ is the mean altitude, $P_a$ is the average May to September precipitation depth, $I$ is the maximum 24-hour, 2-year precipitation depth, and $T$ is the mean January temperature.

And finally, the Borland model is:

$$ Q_p = a A^b E_m^c S_h^d S_t^e P_a^g P_s^h I^i L_a^j L_o^k $$

(4.72)

where $S_h$ is the watershed shape, $P_a$ is the average October to April precipitation depth, $L_a$ is the latitude, and $L_o$ is the longitude.

These models are formed by using peak stormflows at gages where watershed information is available. Normally, these models are regional - in that they can only be applied in the area where they were developed.

To form your own model, logarithmic transforms are used to linearize the equations:

$$ y = y_o + b x_1 + c x_2 + d x_3 + \cdots $$

(4.73)

where $y = \log Q_p$, $y_o = \log a$, $x_1 = \log(A)$, etc. Note that any number of factors can be added, thus improving the fitting or calibration error. Multicollinearity is a major problem with this approach, however, causing large prediction errors. One must always check the prediction uncertainties to make sure that each added parameter further decreases the prediction error.

### 4.2.4 Factor Analysis

Factor analysis, and its cousin Principal Components Analysis (PCA), are commonly used to identify the relationships between variables using the covariance or correlation matrix. If $C$ is the variance-covariance matrix, then we can form the equation:

$$ \lambda C = DC $$

(4.74)

where $\lambda$ are the eigenvalues of $C$ and $D$ are the eigenvectors, with one eigenvector per eigenvalue. The eigenvalues correspond to the relative importance of a linear set of combinations of each of the original variables in explaining the correlation between these variables.

### 4.2.5 Model Updating

We can establish the regression equation $Y = X \beta$ between model outputs, $Y$, and model inputs, $X$. Our objective in regression is to minimize the errors, $J = \sum (y_o - y_p)^2$. Note that the predicted values of $y_o$, $y_p$, are a function of model parameters, $\beta$.

A recursive estimation can be used to update the model parameters, $\beta$, as the system changes (such as happens when floods change the cross-sectional area of the channel, a dike breaks, etc.): 

$$ \Delta \beta_i = (P_i)^{-1} y_i $$

(4.75)

where

$$ P_i = P_{i-1} + (X^T X) $$

(4.76)

and

$$ g_i = \frac{\Delta J_i}{\Delta \beta} $$

(4.77)

This approach means that we update the parameters by examining what the prediction errors are and coupling that with coefficients that tell which parameters are most useful for minimizing the error.

**Kalman Filtering.** Kalman Filtering is another means for updating your model. In this case we have system outputs, $Y$, and state variables, $S$. We say that we can predict the outputs based upon predictions of the state variables, which are only approximately known, using:

$$ Y_{i,p} = H S_{i,p} $$

(4.78)

We predict the state variables for the next time step based on the state variables from the previous time step using:

$$ X_{i,p} = F S_{i-1,p} $$

(4.79)

Once we have an observation of output, $Y_i$, we find the error between that and our prediction:

$$ e_i = Y_{i,p} - Y_i $$

(4.80)

We update the state variables using:

$$ S_i = S_{i,p} + K e_i $$

(4.81)

where $K$ is the Kalman gain matrix:

$$ K_{i,p} = P_{i,p} H^T [R + H P_{i,p} H^T]^{-1} $$

(4.82)

where $R = C[e]$ and $E = C[\eta]$ in which $e = y_{i,p} - y_i$, $\eta = S_{i,p} - S_i$, and $P$ is the covariance matrix associated with the estimation error of the states, which is dynamic and is predicted using:

$$ P_{i,p} = F P + i - 1 F^T + Q $$

(4.83)

The final value of this covariance matrix is:

$$ P_i = P_{i,p} - P_{i,p} H^T [R + H P_{i,p} H^T]^{-1} H P^i_{p} $$

(4.84)

### 4.3 Time Series Analysis

A time-series model can be used to forecast variables that change with time. One can use previous observations of a time series to predict future values, called an autoregressive model. Adding previous prediction errors to the model can help improve forecasts, called a moving average model. Other variables, called external inputs often help to predict the forecast. And finally, converting the observed variables by either differencing or integrating them also can improve the prediction accuracy.
4.3.1 Autoregressive (AR)

The autoregressive model uses previous observations to predict future observations:
\[
\hat{y}(t) = y_0 + a_1 y(t-1) + a_2 y(t-2) + \ldots + a_n y(t-n)
\]
\[
= y_0 + \sum_{i=1}^{n} a_i y(t-i)
\]  
(4.85)

where \( n \) is the memory of the autoregressive system. This is often written using \( AR(n) \).

4.3.2 Moving Average (MA)

The moving-average model adds the previous prediction errors, meaning that if one is off by a certain amount on the last time step, then the error, \( e(t) = \hat{y}(t) - y(t) \), is added to the next prediction:
\[
\hat{y}(t) = y_0 + b_1 e(t-1) + b_2 e(t-2) + \ldots + b_m e(t-m)
\]
\[
= y_0 + \sum_{i=1}^{m} b_i e(t-i)
\]  
(4.86)

where \( n \) is the memory of the moving-average error. This is often written as \( MA(m) \), or \( ARMA(n,m) \) if the moving-average model is combined with the autoregressive model.

4.3.3 External Inputs (X)

Another time-series approach is to use external inputs, such as precipitation or upstream flows, to predict downstream events. This takes the form:
\[
\hat{y}(t) = y_0 + h_0 x(t) + h_1 x(t-1) + \cdots + h_p x(t-p)
\]
\[
= y_0 + \sum_{i=1}^{p} h_i x(t-i)
\]  
(4.87)

where \( p \) is the memory of the external input. This is the same as the convolution operator, where \( h_i \) is the unit response function. This is written as \( X(p) \) or \( ARMAX(n,m,p) \) when combined with the \( ARMA(n,m) \) model:
\[
\hat{y}(t) = y_0 + \sum_{i=1}^{n} a_i y(t-i)
\]
\[
+ \sum_{i=1}^{m} b_i e(t-i) + \sum_{i=1}^{p} h_i x(t-i)
\]  
(4.88)

4.3.4 Differenced (D)

Some processes are better described using their changes, such as the change in water level in a wetland. In this case, we take the first difference of the data:
\[
\Delta y(t) = y(t) - y(t-1)
\]  
(4.89)

The resulting time-series model could be a \( DAR(m) \), \( DARMA(n,m) \), or \( DARMAX(n,m,p) \), which would just use the \( \Delta y \) instead of \( y \) in the prediction equations.

4.3.5 Integrated (I)

Yet other processes might be described using cumulative observations, such as using cumulative inflows to predict reservoir volumes:
\[
Y(t) = Y(t-1) + y(t)
\]  
(4.90)

The resulting time-series model could be a \( IAR(n) \), \( IARMA(n,m) \), or \( IARMAX(n,m,p) \), which would just use the \( Y \) instead of \( y \) in the prediction equations.

Partial Correlations. Partial correlations refers to the marginal contribution of the next coefficient. For example, if you have an \( AR(t) \) model, find the net correlation of the next autoregressive term. If there is no partial correlation, and if \( r_1 = 0.9 \), then \( r_2 = r_1^2 = 0.9 \times 0.9 = 0.81 \). If we find \( r_2 > r_1^2 \), then there is a positive partial correlation. We can also say that if \( r_2 < r_1^2 \), then we have a negative partial correlation.

In general:
\[
r_{ab|c} = \frac{r_{ab} - r_{bc} r_{ac}}{\sqrt{1 - r_{bc}^2} \sqrt{1 - r_{ac}^2}}
\]  
(4.91)

For example, let \( r_{ab} = 0.79 \) and \( r_{ac} = r_{bc} = 0.9 \), then
\[
r_{ab|c} = \frac{0.79 - (0.90) \times (0.90)}{\sqrt{1 - 0.90^2} \sqrt{1 - 0.90^2}} = -0.10
\]  
(4.92)

4.3.6 Example: Salt River Project

Our objective is to determine how much water to release from three reservoirs. Data are collected every six hours and sent within a few minutes to the central office. A decision must be made whether to open up the spillways or to adjust power production. We want a prediction model for prediction horizons of 6, 12, 24 and 96-hours ahead.

We have data from ten raingages, 16 stream gages, and three reservoirs.

Based on a time-series analysis, we find that:

1. The nearest stream gage upstream of each reservoir is the best predictor for 6-hour ahead forecast.
2. Using the most upstream stream gage plus precipitation is found to provide the best 96-hour forecast.
3. One \( MA \) term was sufficient, two \( AR \) terms were generally necessary.
4. Recession flows are easier to predict than peaks.
5. Poor forecasting during cold weather often results due to lack of temperature information, which makes it difficult to distinguish between rain and snow precipitation.
4.4 Problems

1. Regression Analysis

   (a) Find and download water quality data for a minimum of five variables.

   (b) Calculate the means, standard deviations, standard errors of the means, coefficient of variation, and correlation and covariance matrices.

   (c) Select one of the variables as the dependent variable and find the regression relationship using both the original and log-transformed values. Plot the observed and predicted values against each other.

   (d) Calculate the eigenvectors and eigenvalues. Plot the two most significant eigenvectors against each other.

2. Time Series Analysis

   (a) Download three time-series from the U.S. Geological Survey water data website, preferably three stations within the same watershed.

   (b) For the most upstream location, find the AR(2) model using both the original and log-transformed discharges. Plot the predicted and observed discharges.

   (c) For the most downstream location, find the ARX(2,p) model using the other two stations. Plot the predicted and observed discharges.
Walk through the woods or down a street. Is everything the same? Do you see the clouds move? The streams flow? The fountains spout? Describing the variation in our world has always been done using words. In fact, poets have mastered the task of putting meaning into these words.

Besides poetry, another way of describing our environment uses mathematical expressions. Just as rhyming and meter are important to the poet, differential equations are the mathematical tools we use for precisely defining change. These differential equations are frequently used to formulate mathematical descriptions of our world. While algebraic equations are commonly used to relate variables to other observed values, differential equations are used to incorporate changes in observed values, such as changes in time and space.

An ordinary differential equation, ODE, describes how one or more variables change as a function of one other variable. In the previous section, the velocity is written as an ordinary differential equation, which means that the change in distance is a function of a single variable, in this case time.

For example, water levels, \( h \), may change in a linear manner with respect to time, \( t \):

\[
h = ct + b
\]

where \( c \) and \( b \) are constants. The derivative, or change in water levels, with respect to time would be:

\[
\frac{dh}{dt} = c
\]

If, instead of time, water levels change with respect to distance, \( x \), we have:

\[
h = mx + b
\]

where \( m \) and \( b \) are again constants. The derivative, in this case, would be:

\[
\frac{dh}{dx} = m
\]

If water levels in more than one aquifer are observed, then we might have multiple derivatives with respect to time or position, i.e.,

\[
\dot{h}_1 = m \dot{h}_2 \quad \text{or} \quad h_1' = m h_2'
\]

In both cases, the water levels only change as a function of time or position, but not both.

If the water level varies with both time and position, then we must write a partial differential equation, PDE:

\[
\frac{\partial h}{\partial x} = m \frac{\partial h}{\partial t}
\]

where the partial derivative means that the variable is held constant for all other variables than the one used for taking the derivative. In this case, the left-hand side is calculated for a specific time, \( t_i \), while the right-hand side is calculated at a specific position, \( x_j \):

\[
(h')_{t_i} = m \left( \frac{\dot{h}}{x_j} \right)
\]

A few basic differential rules are provided in Table 5.1.

### Table 5.1: General differentiation rules.

<table>
<thead>
<tr>
<th>Function</th>
<th>Derivative</th>
</tr>
</thead>
<tbody>
<tr>
<td>( u = f(x) )</td>
<td>( u' = du/dx )</td>
</tr>
<tr>
<td>( c )</td>
<td>0</td>
</tr>
<tr>
<td>( cx )</td>
<td>( c )</td>
</tr>
<tr>
<td>( cu )</td>
<td>( cu' )</td>
</tr>
<tr>
<td>( x^c )</td>
<td>( cx^{c-1} )</td>
</tr>
<tr>
<td>( u^c )</td>
<td>( cu^{c-1} u' )</td>
</tr>
<tr>
<td>( uv )</td>
<td>( u'v + vu' )</td>
</tr>
<tr>
<td>( u/v )</td>
<td>( (vu' - u'v)/v^2 )</td>
</tr>
<tr>
<td>( \ln u )</td>
<td>( u'/u )</td>
</tr>
<tr>
<td>( \exp u )</td>
<td>( u' \exp u )</td>
</tr>
<tr>
<td>( \sin u )</td>
<td>( u' \cos u )</td>
</tr>
<tr>
<td>( \cos u )</td>
<td>( -u' \sin u )</td>
</tr>
</tbody>
</table>

### 5.1 System Specification

#### 5.1.1 Types of Differential Equations

The general, one-dimensional equation for steady flow in saturated geologic media is given by Darcy’s law:

\[
\dot{q} = -Kh' = -K \frac{\partial h}{\partial x}
\]
which, when combined with the conservation of mass equation,
\[ \dot{q} = -\dot{\theta} \] (5.9)
yields:
\[ K \nabla^2 h = \frac{\partial \theta}{\partial t} \] (5.10)
where \( \theta \) is the water content of the aquifer. This is the same as:
\[ K \frac{\partial^2 h}{\partial x^2} = S_s \frac{\partial h}{\partial t} \] (5.11)
because \( S_s = d\theta / dh \). This can also be written as:
\[ Dh'' = \dot{h} \] (5.12)
where \( D = K / S \) is the hydraulic diffusivity.

For steady (and also for incompressible) flow this is just:
\[ Kh'' = 0 \] (5.13)
For higher dimensions, we have:
\[ \nabla \cdot \bar{q} = \nabla \cdot [-K \nabla h] = -S_s \dot{h} \] (5.14)
where \( \bar{q} \) is a second-order tensor. If \( K \) is isotropic and stationary, this reduces to:
\[ K \left[ \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right] = S_s \frac{\partial h}{\partial t} \] (5.15)
in two dimensions.

The general one-dimensional wave equation is:
\[ \frac{\partial^2 h}{\partial x^2} = \frac{\partial^2 h}{\partial t^2} \] (5.16)
These various equations can be written in general form as:
\[ ah_{ii}'' + 2bh_{ij}'' + ch_{jj}'' + dh_i' + eh_j' + fh + g = 0 \] (5.17)
where \( h_{ii} = \partial h / \partial x_i \), etc. We can determine the type of equation using the value of \( \lambda = b^2 - ac \), where:

**Hyperbolic,** \( \lambda > 0 \): A wave equation with the form \( h_{ii} = h_{jj} \).

**Parabolic,** \( \lambda = 0 \): An unsteady flow equation with the form \( h_{ii} = h_j \).

**Elliptic,** \( \lambda < 0 \): A two-dimensional flow equation with the form \( h_{ii} + h_{jj} = 0 \).

### 5.1.2 Initial and Boundary Conditions

Regardless of the type of differential equation, specific initial and boundary conditions must be prescribed to make the system uniquely defined. Failure to completely specify these conditions may make the system *ill-posed*, meaning that more than one solution may be possible for the problem.

Initial conditions refer to the values of the observed variable(s) at a prescribed time, such as \( h = h_o \) at \( t = t_o \). Boundary conditions refer to the specification of the observed variable(s) at a prescribed location, so that \( h = h_i \) at \( x = x_i \).

There is great flexibility in establishing initial and boundary conditions. Some of the many types of boundary conditions include:

- **Prescribed Head:** Used to set a single value of head, \( h \), for the boundary, such as \( h = h_i \) at \( x = x_i \).

- **Prescribed Flux:** Used to specify the flux, \( q = -Kh' \), for the boundary, such as \( q = q_i \) at \( x = x_i \). These can be either constant or change with each time step.

- **Prescribed Gradient:** Used to specify the gradient, \( h' \), such as \( h' = h'_i \) at \( x = x_i \).

- **Radiation:** Used to set the jump, \( \Delta h \), across a boundary, such as \( \Delta h = \Delta h_i \) at \( x = x_i \).

- **Mixed:** Combines the prescribed head and flux boundary conditions, \( a h_i + b h'_i = c \).

It is important to note that these initial and boundary conditions can be changed for each boundary segment for each time step, or they can remain constant.

### 5.1.3 Material Properties

The selection of the appropriate model parameters is part of the conceptual site model development process. There are a wide range of material properties that must be determined when developing the model. Specific properties include the roughness, hydraulic conductivity, transmissivity, leakance, conductance, which are descriptors of the permeability of the system. The storage terms are also important for transient problems, such as the specific yield, specific storages, storativity, water content, porosity, and specific water capacity. Combined metrics such as the aquifer diffusivity are also important.

### 5.1.4 Example: Nash Model

The Nash model is commonly used to relate stream discharge, \( Q \), to precipitation, \( P \), or to account for flood routing between two stations in a channel, \( Q_1 \) and \( Q_2 \).

We first start by defining a storage volume, \( S = A h \), where \( h \) is the depth of water, and \( A \) is the area of the
storage. We can see that the volume of water in storage increases linearly with the depth of water in storage:

\[
\frac{dS}{dh} = A
\]  

(5.18)

The change in storage over time, \( \dot{S} = \partial S/\partial t \), depends upon the relative magnitude of inflows, \( I \), and outflows, \( O \):

\[
\dot{S} = I - O
\]  

(5.19)

Combining these last two equations yields:

\[
A \dot{h} = I - O
\]  

(5.20)

as long as the area does not change with depth and time, \( A \neq f(h, t) \).

We can go a step further and assume that the outflow from the reservoir depends upon the height of water in storage:

\[
O = k h
\]  

(5.21)

which implies that the rate of outflow increases as the water depth in storage increases. Substitution yields:

\[
\dot{h} + \frac{k}{A} h = \frac{I}{A}
\]  

(5.22)

which is an ordinary differential equation.

### 5.2 Analytic Solution Methods

Many simple differential equations can be solved using a range of methods, including direct integration as well as a range of transform methods. Yet, solving PDEs for a range of initial and boundary conditions and material properties can be a challenge. This is especially true if material properties vary spatially or with time. This section focuses on analytic methods for solving relatively simple problems, while the following section introduces numerical methods that are more appropriate for more complex systems.

#### 5.2.1 Integration

The purpose of integration is to convert a differential equation into an algebraic equation that can be directly solved. A general list of integration rules are proved as Table 5.2. An excellent website for obtaining integrations, if possible, can be found at integrals.wolfram.com.

We return to the Nash model to demonstrate how a simple differential equation can be solved using integration. Recall that the linear reservoir can be described using:

\[
A \frac{dh}{dt} = I - k h
\]  

(5.23)

Table 5.2: General integration rules.

<table>
<thead>
<tr>
<th>Function</th>
<th>Integral</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c )</td>
<td>( cx )</td>
</tr>
<tr>
<td>( cx )</td>
<td>( cx^2/2 )</td>
</tr>
<tr>
<td>( x^c )</td>
<td>( (c + 1) x^{c+1} )</td>
</tr>
<tr>
<td>( cu )</td>
<td>( c \int u , dx )</td>
</tr>
<tr>
<td>( \ln x )</td>
<td>( x \ln x - x )</td>
</tr>
<tr>
<td>( \exp x )</td>
<td>( \exp x )</td>
</tr>
<tr>
<td>( \sin x )</td>
<td>( -\cos x )</td>
</tr>
<tr>
<td>( \cos x )</td>
<td>( \sin x )</td>
</tr>
</tbody>
</table>

For the case where there are no inflows, \( I = 0 \), we have:

\[
A \frac{dh}{dt} = -k h
\]  

(5.24)

Moving terms yields:

\[
\frac{dh}{h} = -\frac{k}{A} \, dt
\]  

(5.25)

Integrating both sides is:

\[
\int \frac{dh}{h} = -\frac{k}{A} \int dt
\]  

(5.26)

which is the same as:

\[
\ln h = c - \frac{k}{A} t
\]  

(5.27)

where \( c \) is the constant of integration. Taking the exponent of each side yields:

\[
h = \exp \left( c - \frac{k}{A} t \right) = Ce^{-\alpha t}
\]  

(5.28)

where \( C = \exp c \) and \( \alpha = k/A \). To identify the value of \( C \), we must have a value of \( h_i \) for a specific time, \( t_i \). In this case, we can use \( h = h_o \) when \( t = 0 \), which is an initial condition. This results in the final form:

\[
h = h_o e^{-\alpha t} \quad \text{and} \quad O = O_o e^{-\alpha t}
\]  

(5.29)

where \( O = Ah \) and \( O_o = Ah_o \) is the initial outflow.

For the case where the inflow is a non-zero constant, we have:

\[
\frac{dh}{dt} + \alpha h = \frac{I}{A}
\]  

(5.30)

where \( \alpha = k/A \). A common technique for solving ODEs of this kind is to multiply both sides by an integrating factor, \( e^{\alpha t} \):

\[
e^{\alpha t} \frac{dh}{dt} + \alpha e^{\alpha t} h = I e^{\alpha t}
\]  

(5.31)

We use the integrating factor, because the chain rule is:

\[
\frac{d(u \, v)}{dt} = u \frac{dv}{dt} + v \frac{du}{dt}
\]  

(5.32)
while one may calculate the transform directly, it is usu-
which for our case, is:
\[
\frac{d(h e^{\alpha t})}{dt} = h \alpha e^{\alpha t} + \frac{dh}{dt} e^{\alpha t}
\]  
which is exactly what we need! Substitution yields:
\[
\frac{d(h e^{\alpha t})}{dt} = \frac{I}{A} e^{\alpha t}
\]  
so that:
\[
d(h e^{\alpha t}) = \frac{I}{A} e^{\alpha t} dt
\]  
Integration yields:
\[
h e^{\alpha t} = c + \frac{1}{\alpha} \frac{I}{A} e^{\alpha t}
\]  
where \(c\) is the constant of integration. Dividing both sides
by the integrating factor, substituting \(A \alpha = k\), and inserting
initial conditions yields:
\[
h = h_0 e^{-\alpha t} + \left(1 - e^{-\alpha t}\right) \frac{I}{k}
\]  
5.2.2 Laplace Transform Methods
An alternative method for solving ordinary differential
which, for our case, is:
\[
\frac{d(h e^{\alpha t})}{dt} = h \alpha e^{\alpha t} + \frac{dh}{dt} e^{\alpha t}
\]  
which is exactly what we need! Substitution yields:
\[
\frac{d(h e^{\alpha t})}{dt} = \frac{I}{A} e^{\alpha t}
\]  
so that:
\[
d(h e^{\alpha t}) = \frac{I}{A} e^{\alpha t} dt
\]  
Integration yields:
\[
h e^{\alpha t} = c + \frac{1}{\alpha} \frac{I}{A} e^{\alpha t}
\]  
where \(c\) is the constant of integration. Dividing both sides
by the integrating factor, substituting \(A \alpha = k\), and inserting
initial conditions yields:
\[
h = h_0 e^{-\alpha t} + \left(1 - e^{-\alpha t}\right) \frac{I}{k}
\]  
 manifests Laplace transforms of some basic
\[
\text{Table 5.3: Laplace transforms}
\]  
\[
\begin{array}{ll}
 f(x) & F(s) = \mathcal{L}(f(x)) \\
 \delta(t) & 1 \\
 1 & \frac{1}{s} \\
t & \frac{1}{s} \\
\frac{t^{n-1}}{\Gamma(n)} & \frac{1}{s^n} \\
e^{at} & \frac{1}{s-a} \\
\frac{1}{a}(e^{at} - 1) & \frac{1}{s(s-a)} \\
f'(t) & sF(s) - f(0^+) \\
f''(t) & s^2 F(s) - s f(0^+) - f'(0^+)
\end{array}
\]  
Returning to the Nash model, we see that:
\[
h'(t) + \alpha h(t) = \frac{I}{A}
\]  
is the same as:
\[
[sH(s) - h_0] + \alpha H(s) = \frac{I}{As}
\]  
so that:
\[
H(s)(s + \alpha) = h_0 + \frac{I}{As}
\]  
and:
\[
H(s) = \frac{h_0}{s + \alpha} + \frac{I}{As(s + \alpha)}
\]  
Taking the inverse for each term yields:
\[
h(t) = h_0 e^{-\alpha t} - \frac{I}{A\alpha} (e^{-\alpha t} - 1)
\]  
which is equivalent to the result obtained earlier.

Laplace Transform Example
For a single linear reservoir, we have:
\[
h'(t) + \alpha h(t) = \frac{I}{A}
\]  
which is the same as:
\[
[sH(s) - h_0] + \alpha H(s) = \frac{I}{As}
\]  
so that:
\[
H(s)(s + \alpha) = h_0 + \frac{I}{As}
\]  
and:
\[
H(s) = \frac{h_0}{s + \alpha} + \frac{I}{As(s + \alpha)}
\]
Taking the inverse for each term yields:

\[ h(t) = h_o e^{-\alpha t} - \frac{I}{A\alpha} (e^{-\alpha t} - 1) \]  

(5.52)

which is equivalent to the result obtained earlier.

Let us consider the dirac (impulse) input:

\[ \delta(t_o) = \begin{cases} \infty & t = t_o \\ 0 & t \neq t_o \end{cases} \]  

(5.53)

where the dirac has the additional constraint:

\[ \int_{-\infty}^{\infty} \delta(t_o) \, dt = 1 \]  

(5.54)

For a dirac input, we have:

\[ O_1 = H_1 \ast \delta(t_o) = H_1 \]  

(5.55)

Taking the Laplace Transform of the single reservoir with a dirac input yields:

\[ O_i = H_i \ast H_{i-1} \ast \cdots \ast H_1 \]  

(5.56)

\[ h'(t) + \alpha h(t) = \frac{\delta(t_o)}{A} \]  

(5.57)

which is the same as:

\[ [sH(s) - h_o] + \alpha H(s) = \frac{1}{A} \]  

(5.58)

so that:

\[ H(s) (s + \alpha) = h_o + \frac{1}{A} \]  

(5.59)

and:

\[ H(s) = \frac{h_o + 1/A}{s + \alpha} \]  

(5.60)

Taking the inverse transform yields:

\[ h(t) = \left(h_o + \frac{1}{A}\right) e^{-\alpha t} + C \]  

(5.61)

where \( C \) is the constant of integration. Setting \( h(t) = h_o \) when \( t = 0 \) yields:

\[ C = -\frac{1}{A} \]  

(5.62)

which yields:

\[ h(t) = h_o e^{-\alpha t} + \frac{1}{A} (1 - e^{-\alpha t}) \]  

(5.63)

For a cascade of linear reservoirs, we have the response for the first reservoir:

\[ O_1 = H_1 \ast I_1 \]  

(5.64)

and for each subsequent reservoir:

\[ O_i = H_i \ast I_i \]  

(5.65)

If the outflow from reservoir 1 is the inflow to reservoir 2, then we have:

\[ O_2 = H_2 \ast O_1 \]  

(5.66)

or, in general:

\[ O_i = H_i \ast O_{i-1} \]  

(5.67)

which is the same as:

\[ O_i = H_i \ast H_{i-1} \ast \cdots \ast H_1 \ast I_1 \]  

(5.68)

5.3 Numerical Solution Methods

5.3.1 Finite Difference Methods

Numeric models are popular because they provide the flexibility for solving a broader class of problems where simple analytic answers may not be available because of variations in material properties or boundary conditions.

Numeric methods using subdivide the problem into small, homogeneous units which are individually or globally solved, and then added back together to provide the answer for the whole system.

The finite difference is, intuitively, a straightforward approach for solving differential equations. We approximate the solution using a linear approximation to the derivative:

\[ \frac{\Delta h}{\Delta t} \approx \frac{h(i+1,j) - h(i,j)}{\Delta t} \]  

(5.69)

\[ h'_{x} = \frac{\partial h}{\partial x} \approx \frac{h(i+1,j) - h(i-1,j)}{2\Delta x} \]  

(5.70)

\[ h'_{y} = \frac{\partial h}{\partial y} \approx \frac{h(i,j+1) - h(i,j-1)}{2\Delta y} \]  

(5.71)

For problems in which the second derivative is needed, we have:

\[ \frac{\Delta^2 h}{\Delta x^2} \approx \frac{h(i+1,j) - 2h(i,j) + h(i-1,j)}{(\Delta x)^2} \]  

(5.72)

\[ \frac{\Delta^2 h}{\Delta y^2} \approx \frac{h(i,j+1) - 2h(i,j) + h(i,j-1)}{(\Delta y)^2} \]  

(5.73)

Note that these approximations are better where the degree of curvature in the function is small. Clearly, taking large steps to measure the circumference of a circle is worse than taking very small steps.

We will use the notation:

\[ h(x_i, y_j, t_k) = h_{ij}^k \]  

(5.74)

to identify the time, \( t \), and location, \( (x, y) \), where \( h \) is observed. We further define the change in \( h \) with respect to \( x \) while holding \( y \) and \( t \) constant using:

\[ \frac{\Delta h}{\Delta x} = \frac{h_{ij}^k - h_{i-1,j}^k}{x_i - x_{i-1}} \]  

(5.75)
and
\[ h'_j = \frac{\Delta h}{\Delta y} = \frac{h_{i,j}^k - h_{i,j-1}^k}{y_j - y_{j-1}} \] (5.76)
\[ h^k = \frac{\Delta h}{\Delta t} = \frac{h_{i,j}^k - h_{i,j}^{k-1}}{t_j^k - t_{j-1}^k} \] (5.77)

The second derivative is calculated by taking the difference in first derivatives:
\[ h''_i = \frac{\Delta^2 h}{(\Delta x)^2} = \frac{h_{i,j}^k - h_{i,j}^k - h_{i,j+1}^k + h_{i,j+1}^k}{(x_{i+1} - x_i)^2} \] (5.78)

which corresponds to the change in the change in the function. For a constant increment, \( \Delta x \), this reduces to:
\[ h''_i = \frac{h_{i+1,j}^k - 2h_{i,j}^k + h_{i-1,j}^k}{(\Delta x)^2} \] (5.79)

Returning, yet again, to the Nash model, we can approximate the problem:
\[ \dot{h} + \alpha h = \frac{I}{A} \] (5.80)

using:
\[ \frac{h^{k+1} - h^k}{\Delta t} + \alpha h^{k+1} = \frac{I}{A} \] (5.81)

This is called the forward model because we are predicting the first derivative using existing values of \( h \). Solving for \( h^k \) yields:
\[ h^{k+1} = h^k + \left( \frac{I}{A} - \alpha h^k \right) \left( t^{k+1} - t^k \right) \] (5.82)

which, for a constant time step, \( \Delta t \), simplifies to:
\[ h^{k+1} = h^k \left( 1 - \alpha \Delta t \right) + \frac{I}{A} \Delta t \] (5.83)

We could just as easily have defined the problem using:
\[ \frac{h^{k+1} - h^k}{\Delta t} + \alpha h^{k+1} = \frac{I}{A} \] (5.84)

which yields a slightly different equation:
\[ h^{k+1} = h^k + \frac{I}{A} \Delta t \] (5.85)

This form is called the backward model because we are predicting using the future values of \( h \).

The final, and most accurate form, is the time-centered model:
\[ \frac{h^{k+1} - h^k}{\Delta t} + \alpha \left( \frac{h^{k+1} + h^k}{2} \right) = \frac{I}{A} \] (5.86)

which results in:
\[ h^{k+1} = \frac{h^k \left( 1 - \alpha \Delta t \right) + \frac{I}{A} \Delta t}{1 + \alpha \Delta t} \] (5.87)

\[ \frac{\alpha t}{A} + C = - \ln h \] (5.91)

where \( C \) is the constant of integration. This can be simplified to:
\[ h = h_o \exp(-\beta t) \] (5.92)
where $h_0 = h(t = 0)$ and $\beta = \alpha/A$. Substituting into the equation above yields:

$$Q = \alpha h = Q_o \exp(-\beta t)$$

(5.93)

where $Q_o = Q(t = 0)$. These are exponential decay equations, which means the values diminish at a slowing rate over time. Such a curve is typical of first-order streams, i.e., streams that are the smallest permanent streams in a landscape.

We can imagine a second order stream as being a second reservoir located below the first reservoir. In this case, the outflow from the first reservoir is the inflow to the second, and the outflow from the second is the inflow to the third. This series of reservoirs is called a cascade of linear reservoirs, or Nash model. The equation that describes these can be readily found using the Laplace transform method, giving a gamma function that looks just like many flood waves:

$$h(\tau) = \frac{\tau^{n-1} \beta^n \exp(-\beta \tau)}{(n-1)!}$$

(5.94)

where $n$ is the number of reservoirs in series, or, equivalently, the expected response in an $n^{th}$-order stream.

For a number of linear reservoirs in parallel, we have:

$$Q = Q_1 \exp(-\beta_1 t) + Q_2 \exp(-\beta_2 t) + Q_3 \exp(-\beta_3 t) + \cdots + Q_n \exp(-\beta_n t)$$

(5.95)

We can also consider the case when a constant input, $I$, such as upstream inflows, or precipitation, are present

$$\frac{dV}{dt} = A \dot{h} - I$$

(5.96)

where $\dot{h} = dh/dt$, so that

$$A \dot{h} + k h = I$$

(5.97)

5.5 Example: Channel Routing

5.5.1 General Routing Equation

Rather than use simple conceptual models, we can formulate a fundamental physical model that describes channel flows. Once this physical model has been constructed, we can then apply it for the routing flood flows through streams.

A common technique for solving ODEs of this kind is to multiply both sides by an integrating factor, $e^{\alpha t}$:

$$\dot{h} e^{\alpha t} + \alpha h e^{\alpha t} = \frac{I}{A} e^{\alpha t}$$

(5.98)

We use the integrating factor because the chain rule is:

$$\frac{d(u v)}{dt} = \frac{du}{dt} v + u \frac{dv}{dt}$$

(5.99)

which, for our case, is:

$$\frac{d(h e^{\alpha t})}{dt} = \dot{h} e^{\alpha t} + h (\alpha e^{\alpha t})$$

(5.100)

Substitution yields:

$$\frac{d(h e^{\alpha t})}{dt} = \frac{I}{A} e^{\alpha t}$$

(5.101)

so that:

$$d(h e^{\alpha t}) = \frac{I}{A} e^{\alpha t} dt$$

(5.102)

Integrating both sides yields:

$$h e^{\alpha t} = \frac{1}{\alpha} \frac{I}{A} e^{\alpha t} = \frac{I}{k} e^{\alpha t} + C$$

(5.103)

Dividing both sides by the integrating factor, and inserting the initial condition, $h = h_o$ at $t = 0$, yields:

$$h = h_o e^{\alpha t} + (1 - e^{\alpha t}) \frac{I}{k}$$

(5.104)
The first equation we use is the conservation of mass equation:
\[
\Delta Q = O - I = -\frac{\Delta S}{\Delta t}
\]  (5.105)

Where \(\Delta Q\) is the change in discharge along the channel, \(O\) is the channel outflow, \(I\) is the channel inflow, \(S\) is the amount of water in storage in the channel section, and \(\Delta S/\Delta t\) is the change in storage over time. This equation means that when inflows exceed outflows, the amount of water in storage must increase over time.

We can write this as a one-dimensional partial differential equation (PDE):
\[
\frac{\partial Q}{\partial x} = -\frac{\partial A}{\partial t}
\]  (5.106)

where the left-hand side represents the change in flow per unit length of channel, and the right-hand side represents the change in channel cross-sectional area, \(A\), per unit time.

We can approximately this equation using finite differences:
\[
\frac{\Delta Q}{\Delta x} = -\frac{\Delta A}{\Delta t}
\]  (5.107)

so that:
\[
\Delta Q = -\frac{\Delta S}{\Delta t}
\]  (5.108)

where \(\Delta Q = O - I\) and \(\Delta S = \Delta A \Delta x\). Note that this is identical to the original equation.

Using the original equation, we can define inflows, outflows, and storages as the averages between two times:
\[
\bar{O} = \frac{O(t + \Delta t) + O(t)}{2}
\]  (5.109)

\[
\bar{I} = \frac{I(t + \Delta t) + I(t)}{2}
\]  (5.110)

\[
\Delta S = S(t) - S(t + \Delta t)
\]  (5.111)

Substitution yields:
\[
\frac{O(t) + O(t + \Delta t)}{2} - \frac{I(t) + I(t + \Delta t)}{2} = \frac{S(t) - S(t + \Delta t)}{\Delta t}
\]  (5.112)

If we are monitoring streamflows, we have the current observations of \(I(t)\), \(O(t)\), and \(S(t)\). We can also obtain predictions for the upstream inflows, \(I(t + \Delta t)\). Solving for the future downstream outflow yields:
\[
O(t + \Delta t) = I(t + \Delta t) + I(t)
\]  (5.113)

\[-O(t) - \frac{2}{\Delta t} [S(t + \Delta t) - S(t)]
\]

But we are still have one unknown on the right-hand side of the equation, \(S(t + \Delta t)\). To eliminate this variable, we require a relationship between \(S\) and \(O\).

### 5.5.2 Nonlinear Outflow-Storage Equation

One approach is to use a nonlinear relationship between \(S\) and \(O\), which would be consistent with the weir equation, \(O = C S^n\), where \(C\) is the weir coefficient, and \(n = 3/2\) for a rectangular weir. Solving for \(S\) yields the nonlinear storage-outflow relationship, \(S = (O/C)^{2/3}\).

Substituting the storage-outflow relationship and solving for the future outflow yields:
\[
O(t + \Delta t) = I(t + \Delta t) + I(t)
\]  (5.114)

\[-O(t) - \frac{2}{\Delta t} \left(\frac{O(t + \Delta t)}{C}\right)^{m} - S(t)\]

This must be solved iteratively, using an initial estimate of \(O(t + \Delta t)\) on the right-hand side to obtain a revised estimate on the left-hand side, which is then used on the right-hand side until the value converges.

### 5.5.3 Muskingum Method

An alternative, early approach for estimating the storage function was an empirical method that splits the storage into two parts, a steady, prism storage, and a transient, wedge storage:
\[
S = S_{\text{prism}} + S_{\text{wedge}}
\]  (5.115)

where
\[
S_{\text{prism}} = C O
\]  (5.116)

\[
S_{\text{wedge}} = x C (I - O)
\]  (5.117)

where \(\tau\) is the flood wave travel time and \(x\) is a weighting factor, \(0.1 < x < 0.5\), that indicates the amount of flood attenuation. Substitution yields:
\[
S = \tau O + x \tau (I - O) = \tau [x I + (1 - x) O]
\]  (5.118)

Substituting this into the finite difference equation yields:
\[
O(t + \Delta t) = C_1 I(t + \Delta t) + C_2 I(t) + C_3 O(t)
\]  (5.119)

where
\[
C_1 = \frac{\Delta t - 2\tau x}{\Delta t + 2\tau (1 - x)}
\]  (5.120)
\[ C_2 = \frac{\Delta t + 2\tau x}{\Delta t + 2\tau (1-x)} \]  
(5.121) ... and so on. Substituting these into the original Muskingum equation yields:

\[ O(t + \Delta t) = \sum_{i=0}^{n} K_i I(t - i) \] 
(5.130) 

\[ = K_o I(t) + K_1 I(t-1) + K_2 I(t-2) + ... \]

where

\[ K_o = C_1 \] 
(5.131) 

\[ K_1 = C_1 C_3 + C_2 \] 

\[ K_2 = C_3 K_1 \] 

\[ K_n = C_3 K_{n-1} \] 

A problem with this method is that it ignores accumulating errors that might have been corrected by incorporating previous outflows. Yet another method is the SCS Convex method that is a simplification where \( C_1 = 0 \), \( C_3 = 1 - C_2 \), so that:

\[ O(t) = I_1 + C_2 [I(t - 1) - O(t - 1)] \]  
(5.132) 

The assumption that \( C_1 = 0 \) implies that \( \Delta t = 2\tau x \). This is clearly the case when \( x = 0.5 \) and \( \Delta t = \tau \). One might select a time step which satisfies this condition.

### 5.6 Problems

1. Write the Partial Differential Equations (PDEs) for:
   
   (a) Transient, surface water flow.
   
   (b) Transient, saturated, groundwater flow.
   
   (c) Transient, unsaturated, groundwater flow.
   
   (d) Transient, saturated, groundwater solute transport.

2. Solve the Nash Model for a series of Linear Reservoirs, \( Q = kH \):
   
   (a) Use Laplace Transforms to solve for a series of five linear reservoirs.
   
   (b) Use a spreadsheet to solve the equivalent system using finite differences.
   
   (c) Compare your numeric solution to the analytic solution.

3. Solve the Nash Model for a series of Non-Linear Reservoirs, \( Q = kH^{1.5} \):
   
   (a) Adjust your spreadsheet for the equivalent nonlinear system.
   
   (b) Compare your nonlinear solution to the linear solution.

4. Write the Finite Difference Equations (FDEs) for:
(a) Transient, surface water flow.
(b) Transient, saturated, groundwater flow.
(c) Transient, unsaturated, groundwater flow.
(d) Transient, saturated, groundwater solute transport.

5. Solve a one-dimensional flow equation using finite-differences.

(a) In a spreadsheet, create a time index in Column A. Label the top of the Column (Cell A1) with Time. Start with a value of zero in Cell A2, and increment each cell by 1 time step.

(b) Label the second column (cell B1) with $x = 0$. Label the columns C1:Z1 using a distance increment of 10.

(c) Put constant values of flow, say $Q = 10$, in cells B2:B50. Put different values of flow, say $Q = 5$, in cells B51:B100. These are the *upstream boundary condition*, which are prescribed head boundary conditions.

(d) Place a constant value in each of the cells in row 2, i.e., $Q = 10$ in cells B2:Y2. These are the *initial conditions*, which are also prescribed head boundary conditions.

(e) Use a prescribed head *downstream boundary condition*, say $Q = 0$, for Column Z, cells Z2:Z100.

(f) Place the time-centered flow equation in cells C3:Y100.
Chapter 6

Vectors, Complex Variables, and Quaternions

6.1 Vectors

A vector is an oriented list of numbers. A vector with two elements would look like:

\[ \vec{v} = [v_1, v_2] \]  

(6.1)

We can plot these elements on two perpendicular axes, such as the $x$- and $y$-axes of a cartesian plot. We say these axes are orthogonal, or perpendicular, to each other. The vector is oriented because, like a pointer, it has a base, located at the origin, and the tip, located at the position indicated by the list of numbers.

Another way of expressing a vector mathematically is:

\[ \vec{v} = [v_1, v_2] = i v_1 + j v_2 \]  

(6.2)

where the symbols $i$ and $j$ are just mathematical symbols to indicate the $x$- and $y$-axes. A three-dimensional vector would be:

\[ \vec{v} = [v_1, v_2, v_3] = i v_1 + j v_2 + k v_3 \]  

(6.3)

where there are now three axes, corresponding to the $x$-, $y$-, and $z$-directions. Higher order vectors are also possible, although not commonly used.

6.1.1 Algebra

Vectors addition and subtraction are performed for each element, independent of the other elements:

\[ \vec{u} + \vec{v} = [u_1, u_2] + [v_1, v_2] \]
\[ = [u_1 + v_1, u_2 + v_2] \]  

(6.4)

\[ \vec{u} - \vec{v} = [u_1, u_2] - [v_1, v_2] \]
\[ = [u_1 - v_1, u_2 - v_2] \]  

(6.5)

These operations are associative and commutative:

\[ (\vec{u} + \vec{v}) + \vec{w} = \vec{u} + (\vec{v} + \vec{w}) \]  

(6.6)

\[ \vec{u} + \vec{v} = \vec{v} + \vec{u} \]  

(6.7)

Multiplication or division of a constant, $c$, is also performed element by element:

\[ c \cdot \vec{u} = [cu_1, cu_2] \]  

(6.8)

\[ \frac{\vec{u}}{c} = \left[ \frac{u_1}{c}, \frac{u_2}{c} \right] \]  

(6.9)

Multiplication of two vectors is more complicated. In fact, there are two types of multiplication, the dot product, $\vec{u} \cdot \vec{v}$, and the cross product, $\vec{u} \times \vec{v}$. Two dimensional multiplication is defined using:

\[ \vec{u} \cdot \vec{v} = u_1 v_1 + u_2 v_2 \]  

(6.10)

\[ \vec{u} \times \vec{v} = u_1 v_2 - u_2 v_1 \]  

(6.11)

Three dimensional multiplication yields:

\[ \vec{u} \cdot \vec{v} = u_1 v_1 + u_2 v_2 + u_3 v_3 \]  

(6.12)

\[ \vec{u} \times \vec{v} = [u_2 v_3 - u_3 v_2, u_3 v_1 - u_1 v_3, u_1 v_2 - u_2 v_1] \]  

(6.13)

which is a vector. Vector multiplication is commutative for the dot product, but not for the cross-product:

\[ \vec{u} \cdot \vec{v} = \vec{v} \cdot \vec{u} \]  

(6.14)

\[ \vec{u} \times \vec{v} = -\vec{v} \times \vec{u} \]  

(6.15)

Vector division is not defined.

6.1.2 Geometry

A vector can be represented using a pointer, with the base of the pointer resting at the origin and the tip of the pointer resting at the value of the vector. Another way of representing the vector is to define the vector magnitude, $r$, of the vector using:

\[ r = \text{abs} \{ \vec{u} \} = \sqrt{u_1^2 + u_2^2} \]  

(6.16)

and a rotation angle, $\theta$, using:

\[ \theta = \text{arg} \{ \vec{u} \} = \arctan \frac{u_2}{u_1} \]  

(6.17)
The addition of two vectors, \( \vec{w} = \vec{u} + \vec{v} \), can be visualized by placing the base of the second vector at the tip of the first vector. The resulting vector is the pointer connecting the base of the first pointer to the tip of the second pointer.

\[
\begin{align*}
   r_w &= \text{abs}(\vec{w}) = \sqrt{u_1^2 + u_2^2} \\
   \theta_w &= \text{arg}(\vec{w}) = \arctan \frac{u_2 + v_2}{u_1 + v_1}
\end{align*}
\]

so that:

\[
\begin{align*}
   u_1 &= r \cos \theta \\
   u_2 &= r \sin \theta
\end{align*}
\]

The geometry of a three-dimensional vector is commonly written using two angles, \( \theta \) and \( \lambda \):

\[
\begin{align*}
   u_1 &= r \cos \theta \cos \lambda \\
   u_2 &= r \sin \theta \cos \lambda \\
   u_3 &= r \sin \theta \sin \lambda
\end{align*}
\]

### 6.1.3 Calculus

Calculus is used to describe how a function changes in space or time. Imagine an apple falling from a tree, as Newton did. He is credited with creating a branch of mathematics that describes the motion of a falling body. We also use this mathematics to describe moving liquids.

We first define the derivative of spatially variable function, \( U = f(x, y, z) \), which yields a vector:

\[
\vec{u} = \nabla U = \left[ \frac{\partial U}{\partial x}, \frac{\partial U}{\partial y}, \frac{\partial U}{\partial z} \right] = [u_1, u_2, u_3]
\]

where \( \nabla \) is the gradient, or \( \text{grad} \), operator. For two-dimensional problems, this would be:

\[
\vec{u} = \nabla U = \left[ \frac{\partial U}{\partial x}, \frac{\partial U}{\partial y} \right] = [u_1, u_2] = i u_1 + j u_2
\]

Just as there are two types of vector multiplication, the dot (\( \cdot \)) and cross (\( \times \)) products, there are also two types of vector derivatives:

\[
\nabla \cdot \vec{u} = \frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} + \frac{\partial u_3}{\partial z}
\]

\[
\nabla \times \vec{u} = \left( \frac{\partial u_2}{\partial z} - \frac{\partial u_3}{\partial y} \right) i + \left( \frac{\partial u_3}{\partial x} - \frac{\partial u_1}{\partial z} \right) j + \left( \frac{\partial u_1}{\partial y} - \frac{\partial u_2}{\partial x} \right) k
\]

and for two-dimensional vectors:

\[
\begin{align*}
   \nabla \cdot \vec{u} &= \frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial y} \\
   \nabla \times \vec{u} &= \left[ \frac{\partial u_2}{\partial y} - \frac{\partial u_3}{\partial z} \right] i + \left[ \frac{\partial u_3}{\partial x} - \frac{\partial u_1}{\partial z} \right] j
\end{align*}
\]

Note that if \( \vec{u} = \nabla U \), then:

\[
\begin{align*}
   \nabla \cdot \nabla U &= \nabla^2 U \\
   \nabla \times \nabla U &= 0
\end{align*}
\]

because \( \partial(\partial U/\partial x)/\partial y = \partial(\partial U/\partial y)/\partial x \), etc.

### 6.1.4 Tensors

A tensor is used to incorporate the variation in material properties. For example, Darcy’s law is used to account for the flow of groundwater through porous media in the subsurface. For spatially homogeneous media we have:

\[
\vec{q} = -K \nabla H = -K \vec{h}
\]

where \( q \) is the flux of water, \( K \) is the hydraulic conductivity, and \( \vec{h} \) is the groundwater gradient. In this simple example, the pointer representing the hydraulic gradient is oriented in the same direction as the groundwater flux. In some cases, however, the flux direction is not in the same direction as the hydraulic gradient. This often occurs when there is preferential flow in one direction, such as when there is bedding or geologic layers, or when joints or fractures tend to direct flow away from the direction of the hydraulic gradient. In these cases, the hydraulic conductivity is represented using a tensor:

\[
K = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}
\]

so that

\[
\vec{q} = K \vec{h} = [K_{11} h_1 + K_{12} h_2, K_{21} h_1 + K_{22} h_2]
\]

for two-dimensional flow problems. For flow in three dimensions, the tensor would be:

\[
K = \begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix}
\]
Note that $K_{12} = K_{21}$, etc., so that the hydraulic conductivity tensor is symmetric.

## 6.2 Complex Variables

A complex variable is a number composed of two parts, one called the real part and a second called the imaginary part.

$$u = u_o + i u_1$$  \hspace{1cm} (6.37)

where $i$ is used to indicate the imaginary part. We denote the real and imaginary parts using the notation:

$$\Re\{u\} = u_o$$  \hspace{1cm} (6.38)

$$\Im\{u\} = u_1$$  \hspace{1cm} (6.39)

The complex conjugate of an imaginary number is defined using:

$$\overline{u} = u_o - i u_1 = \Re\{u\} - \Im\{u\}$$  \hspace{1cm} (6.40)

### 6.2.1 Algebra

Adding two complex variables is accomplished by adding the real and imaginary parts separately:

$$u + v = (u_o + i u_1) + (v_o + i v_1) = (u_o + v_o) + i (u_1 + v_1)$$  \hspace{1cm} (6.41)

Subtraction is equivalently defined using:

$$u - v = (u_o + i u_1) - (v_o + i v_1) = (u_o - v_o) + i (u_1 - v_1)$$  \hspace{1cm} (6.42)

Note that $u + \overline{u} = 2\Re\{u\}$ and $u - \overline{u} = 2\Im\{u\}$.

Multiplication and division with a real value, $c$, where $\Im\{c\} = 0$, is allowed:

$$cu = cu_o + i cu_1$$  \hspace{1cm} (6.43)

$$\frac{u}{c} = \frac{u_o}{c} + i \frac{u_1}{c}$$  \hspace{1cm} (6.44)

Multiplication of two complex variables is achieved using term-by-term expansion:

$$uv = (u_o + i u_1)(v_o + i v_1) = (u_o v_o + i^2 u_1 v_1) + i (u_o v_1 + u_1 v_o)$$  \hspace{1cm} (6.45)

The convention is that whenever the imaginary part is multiplied by itself, the result is a real value with a negative sign, i.e.:

$$i^2 = -1$$  \hspace{1cm} (6.46)

so that:

$$uv = (u_o v_o - u_1 v_1) + i (u_o v_1 + u_1 v_o)$$  \hspace{1cm} (6.47)

### 6.2.2 Geometry

The complex number, $u$, can be written using:

$$u = r (\cos \theta + i \sin \theta)$$  \hspace{1cm} (6.52)

which is similar to the two-dimensional vector definition. It can also be shown that:

$$u = re^{i \theta}$$  \hspace{1cm} (6.53)

where:

$$e^{i \theta} = \cos \theta + i \sin \theta$$  \hspace{1cm} (6.54)

Note that $e^{i \pi} = -1$. Using the fact that multiplication of exponential functions is equivalent to the addition of the exponents yields:

$$w = uv = (ru e^{i \theta_u})(rv e^{i \theta_v}) = ru rv e^{i (\theta_u + \theta_v)}$$  \hspace{1cm} (6.55)

which means that $r_w = ru rv$ and $\theta_w = \theta_u + \theta_v$.

One can obtain a sense of what the imaginary number, $i$, represents by noting that multiplication is a rotation about the origin. Multiplying a vector by $-1$ represents a rotation of $180^\circ$ about the origin.

A rotation of $360^\circ$ involves two rotations of $180^\circ$, so the rotation requires two successive multiplications of $-1$, or $(-1) \times (-1) = 1$, which places the vector back in its original position.

With this example in mind, note that a multiplication by $i$ results in a rotation of $90^\circ$. This is because two successive multiplications (or rotations) yields $i^2$, which is the same as $180^\circ$, which is just $-1$, so that:

$$i = \sqrt{-1}$$  \hspace{1cm} (6.56)


6.2.3 Calculus

The derivative of a spatially variable (real) function, \( U = f(z) \) is found using:

\[
\nabla U = \frac{\partial U}{\partial z} = \frac{\partial U}{\partial x} \frac{\partial x}{\partial z} + \frac{\partial U}{\partial y} \frac{\partial y}{\partial z} = \nabla U \tag{6.57}
\]

where \( z = x + iy \) is the complex position, \( u = u_o + \text{i}u_1 \), and \( u_o = \partial U/\partial x \) and \( u_y = \partial U/\partial y \).

The derivative of a complex variable is handled somewhat differently. We require that the derivative of an analytic function be independent of the path of the derivative, so that:

\[
\nabla u = \frac{\partial u}{\partial x} = \frac{\partial u}{\partial 1y} \tag{6.58}
\]

This can only be true if:

\[
\frac{\partial u}{\partial x} = \frac{\partial u_o}{\partial x} + \text{i} \frac{\partial u_1}{\partial x} \tag{6.59}
\]

\[
\frac{\partial u}{\partial y} = \frac{\partial u_o}{\partial y} + \text{i} \frac{\partial u_1}{\partial y} = -\text{i} \frac{\partial u_o}{\partial y} + \frac{\partial u_1}{\partial y} \tag{6.60}
\]

which requires that:

\[
\frac{\partial u_o}{\partial y} = \frac{\partial u_1}{\partial y} \tag{6.61}
\]

\[
\frac{\partial u_1}{\partial x} = -\frac{\partial u_o}{\partial y} \tag{6.62}
\]

which are called the Cauchy-Riemann conditions. It is clear that for the case of \( \nabla = \nabla U \), we have:

\[
\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = 0 \tag{6.63}
\]

\[
\frac{\partial^2 U}{\partial x \partial y} - \frac{\partial^2 U}{\partial y \partial x} = 0 \tag{6.64}
\]

which are just \( \nabla^2 U = 0 \) and \( \nabla \times \nabla U = 0 \). These correspond to the \textit{divergence} and \textit{curl} of the gradient of \( U \) being equal to zero.

6.3 Quaternions

The quaternion is defined as a number containing four parts:

\[
u = [u_o, u_1, u_2, u_3] \tag{6.65}
\]

which forms a four-dimensional vector in a coordinate system with four orthogonal axes, equivalent to:

\[
u = u_o + u_1 \text{i} + u_2 \text{j} + u_3 \text{k} \tag{6.66}
\]

In this notation, \( u \) is the vector of the distances from the origin along one real axis and three imaginary axes \((\text{i}, \text{j}, \text{k})\). The real, \( \Re \), and imaginary, \( \Im \), components of the quaternion are defined, respectively, using:

\[
\Re(v) = u_o \quad \text{and} \quad \Im(v) = u_1 \text{i} + u_2 \text{j} + u_3 \text{k} \tag{6.67}
\]

to yield:

\[
u = \Re(v) + \Im(v) \tag{6.68}
\]

Conventional complex variables are defined so that the quaternion real axis corresponds to the real \( x \)-axis, the quaternion \( i \)-axis corresponds to the imaginary \( y \)-axis, and the quaternion \( j \) and \( k \) axes are ignored. An important advantage of quaternion variables is their ability to extend complex variable theory to include two additional dimensions.

The \textit{pure} quaternion is defined as a quaternion with only imaginary components, i.e., \( \Re(u) = 0 \), and is remarkably similar to a three-dimensional vector, \( \vec{u} \).

\[
u = \Im(u) = [u_1, u_2, u_3] = u_1 \text{i} + u_2 \text{j} + u_3 \text{k} \tag{6.69}
\]

6.3.1 Algebra

If \( u \) and \( v \) are both quaternion, then addition is performed by adding like quantities:

\[
w = u + v = (u_o + v_o) + (u_1 + v_1) \text{i} + (u_2 + v_2) \text{j} + (u_3 + v_3) \text{k} \tag{6.70}
\]

where

\[
w_o = u_o + v_o \tag{6.71}
\]

\[
w_1 = u_1 + v_1 \tag{6.71}
\]

\[
w_2 = u_2 + v_2 \tag{6.71}
\]

\[
w_3 = u_3 + v_3 \tag{6.71}
\]

It is readily shown that addition is both commutative and associative, respectively:

\[
u + v = v + u \tag{6.72}
\]

and

\[
u + (v + w) = (u + v) + w \tag{6.73}
\]

The \textit{conjugate} quaternion, \( \overline{v} \) is defined using:

\[
\overline{v} = u_o - u_1 \text{i} - u_2 \text{j} - u_3 \text{k} = \Re(v) - \Im(v) \tag{6.74}
\]

The real and imaginary parts of \( u \) can be found using:

\[
\Re(u) = \frac{1}{2}(u + \overline{u}) \quad \text{and} \quad \Im(u) = \frac{1}{2}(u - \overline{u}) \tag{6.75}
\]

The quaternion multiplication system are defined using the rules shown in Table 6.2. Note that the first row
and column are symmetric, but the remaining rows and columns are Hermitian.

These rules are equivalent to the right-hand rule of vector multiplication for a pure quaternion. Employing these rules, quaternion multiplication is:

\[
uv = (u_o + u_1 \mathbf{i} + u_2 \mathbf{j} + u_3 \mathbf{k}) (v_o + v_1 \mathbf{i} + v_2 \mathbf{j} + v_3 \mathbf{k}) = \begin{bmatrix} u_o v_o - u_1 v_1 - u_2 v_2 - u_3 v_3 \\ u_o v_1 + u_1 v_o + u_2 v_3 - u_3 v_2 \\ u_o v_2 - u_1 v_3 + u_2 v_o + u_3 v_1 \\ u_o v_3 + u_1 v_2 - u_2 v_1 + u_3 v_o \end{bmatrix}
\]

(6.77)

It can be readily shown that quaternion multiplication is both associative and distributive, respectively:

\[
u (v w) = (u v) w \quad \text{and} \quad u (v + w) = u v + u w\]

(6.78)

But quaternion multiplication is not commutative:

\[
u v \neq v u\]

(6.79)

Instead, it can be shown by expanding terms that:

\[
\overline{uv} = \overline{v} \overline{u}
\]

(6.80)

so that:

\[
u v = \overline{\overline{v} u}
\]

(6.81)

As noted previously, the pure quaternion takes the form of the traditional vector, i.e., the real part of the pure quaternion equals zero, \(\Re(u) = 0\). It is readily shown that pre- and post-multiplication of a pure quaternion, \(\vec{u}\), by any quaternion, \(\vec{v}\), always yields a pure quaternion:

\[
\vec{u} = \overline{\vec{v}} \cdot \vec{u} v
\]

(6.82)

The vector dot product corresponds to the negative of the real result of quaternion multiplication while the vector cross product corresponds to the imaginary result, such that for two pure quaternion, \(\vec{u}\) and \(\vec{v}\):

\[
\vec{u} \cdot \vec{v} = -\Re(\vec{u} \vec{v}) = u_1 v_1 + u_2 v_2 + u_3 v_3
\]

(6.83)

and

\[
\vec{u} \times \vec{v} = \Im(\vec{u} \vec{v}) = (u_2 v_3 - u_3 v_2) \mathbf{i} + (u_3 v_1 - u_1 v_3) \mathbf{j} + (u_1 v_2 - u_2 v_1) \mathbf{k}
\]

(6.84)

so that

\[
\vec{u} \vec{v} = -(\vec{u} \cdot \vec{v}) + (\vec{u} \times \vec{v}) = \begin{bmatrix} 0 & -u_1 v_1 - u_2 v_2 - u_3 v_3 \\ 0 & 0 & + u_2 v_3 - u_3 v_2 \\ 0 & -u_1 v_3 + 0 & + u_3 v_1 \\ 0 & + u_1 v_2 - u_2 v_1 & + 0 \end{bmatrix}
\]

(6.85)

where the zeros result from setting \(u_o = 0\) and \(v_o = 0\). One advantage of using quaternion variables lies in their ability to explicitly incorporate both the dot and cross product multiplications.

Division in the quaternion system is needed if we wish to solve for the quaternion \(u\) given two known quaternions, \(w\) and \(v\), defined by:

\[
w = u v
\]

(6.86)

Post-multiplication by the conjugate of \(v\), \(\overline{v}\), yields:

\[
w \overline{v} = (u v) \overline{v} = u (v \overline{v}) = u |v|^2
\]

(6.87)

where \(|v|\) is norm, or scalar length, of the quaternion. Because \(|v|\) is a scalar, we divide both sides by the squared norm of \(v\) to yield:

\[
u = \frac{w \overline{v}}{|v|^2}
\]

(6.88)

### 6.3.2 Geometry

The spatial quaternion, \(u\), can be represented using an angle quaternion, \(\phi\):

\[
\phi = \phi_o + \phi_1 \mathbf{i} + \phi_2 \mathbf{j} + \phi_3 \mathbf{k}
\]

(6.89)

with:

\[
u = e^{\phi} = \exp(\phi_o + \phi_1 \mathbf{i} + \phi_2 \mathbf{j} + \phi_3 \mathbf{k}) = \exp(\phi_o) \exp(\phi_1 \mathbf{i}) \exp(\phi_2 \mathbf{j}) \exp(\phi_3 \mathbf{k})
\]

(6.90)

Note that \(\phi_o\) is a scalar function, equal to the natural logarithm of the norm of \(u\):

\[
\phi_o = \ln |u| = \ln r
\]

(6.91)

where

\[
r = |u| = \sqrt{u_1^2 + u_2^2 + u_3^2 + u_4^2}
\]

(6.92)

so that:

\[
u = r \hat{u}
\]

(6.93)

where \(\hat{u}\) is a unit quaternion, with:

\[
\hat{u} = \exp(\phi_1 \mathbf{i} + \phi_2 \mathbf{j} + \phi_3 \mathbf{k}) = \exp(\hat{\phi})
\]

(6.94)

and

\[
\hat{u} = \mathbb{I}(\phi) = \phi_1 \mathbf{i} + \phi_2 \mathbf{j} + \phi_3 \mathbf{k}
\]

(6.95)
Conjugate Angles

The quaternion conjugate angle, \( \overline{\phi} \), is the angle of the spatial quaternion conjugate, \( \overline{\mathbf{q}} \):

\[
\overline{\mathbf{q}} = \exp \overline{\phi} = r \exp \overline{\phi}
\]

Addition of angle quaternion is associative and distributive, but not commutative because spatial quaternion multiplication is not commutative. This restriction requires the angle quaternion conjugate be defined using:

\[
\overline{\phi} = - (\phi_3 \mathbf{k} + \phi_2 \mathbf{j} + \phi_1 \mathbf{i})
\]

so that

\[
\phi + \overline{\phi} = \phi_o + (\phi_3 \mathbf{k} + \phi_2 \mathbf{j} + \phi_1 \mathbf{i}) + \phi_o - (\phi_3 \mathbf{k} + \phi_2 \mathbf{j} + \phi_1 \mathbf{i}) = 2\phi
\]

The quaternion angles can be determined by performing exponential products:

\[
\vec{\phi} = \arctan \left[ \frac{u^2 - u_3^2 - u_2^2 + u_1^2 + \beta}{2(u_3 u_2 - u_1 u_1)} \right]
\]

where

\[
v = r \cos \phi_1 \cos \phi_2 \cos \phi_3
\]

This formulation provides four equations with four unknowns, which has been solved using MAPLE to yield:

\[
\vec{\phi} = \arctan \left[ \frac{u^2 + u_3^2 + u_2^2 + u_1^2 + \beta}{2(u_3 u_2 - u_1 u_1)} \right]
\]

where

\[
\beta = \pm \sqrt{r^4 - 4(u_0 u_2 + u_1 u_3)^2}
\]

Half-Angles

Multiplication employing pure quaternion results in half-angle quaternion. Recall that the pure quaternion algebra is:

\[
\vec{\phi} = \mathbf{v} \cdot \mathbf{u} v
\]

so that the angles of \( v \) are half of a standard quaternion.

Exponential and Trigonometric Forms

We can decompose any unit quaternion into the following exponential products:

\[
\hat{u} = \exp(\phi) = \exp(\phi_1 \mathbf{i}) \exp(\phi_2 \mathbf{j}) \exp(\phi_3 \mathbf{k})
\]

which can be expanded, term-by-term, into a trigonometric form:

\[
\hat{u} = [\cos(\phi_1) + \sin(\phi_1) \mathbf{i}] [\cos(\phi_2) + \sin(\phi_2) \mathbf{j}] [\cos(\phi_3) + \sin(\phi_3) \mathbf{k}]
\]

which is the same as:

\[
\hat{u} = \left[ \begin{array}{c}
\cos \phi_1 \cos \phi_2 \cos \phi_3 - \sin \phi_1 \sin \phi_2 \sin \phi_3 \\
\sin \phi_1 \cos \phi_2 \cos \phi_3 + \cos \phi_1 \sin \phi_2 \sin \phi_3 \\
\cos \phi_1 \sin \phi_2 \cos \phi_3 - \sin \phi_1 \cos \phi_2 \sin \phi_3 \\
\cos \phi_1 \cos \phi_2 \sin \phi_3 + \sin \phi_1 \sin \phi_2 \cos \phi_3 \\
\end{array} \right] \mathbf{i}
\]

\[
\hat{u} = e^{\vec{\phi}} = \left[ \begin{array}{c}
\cos \phi_1 \cos \phi_2 \cos \phi_3 - \sin \phi_1 \sin \phi_2 \sin \phi_3 \\
\sin \phi_1 \cos \phi_2 \cos \phi_3 + \cos \phi_1 \sin \phi_2 \sin \phi_3 \\
\cos \phi_1 \sin \phi_2 \cos \phi_3 - \sin \phi_1 \cos \phi_2 \sin \phi_3 \\
\cos \phi_1 \cos \phi_2 \sin \phi_3 + \sin \phi_1 \sin \phi_2 \cos \phi_3 \\
\end{array} \right] \mathbf{k}
\]

Angle Determination

The quaternion angles can be determined by performing the following substitutions:

\[
u = v = \left[ \begin{array}{c}
1 - \tan \phi_1 \tan \phi_2 \tan \phi_3 \\
\tan \phi_1 + \tan \phi_2 \tan \phi_3 \\
\tan \phi_2 - \tan \phi_1 \tan \phi_3 \\
\tan \phi_3 + \tan \phi_1 \tan \phi_2 \\
\end{array} \right]
\]

\[
\hat{u} = e^{\vec{\phi}} = \left[ \begin{array}{c}
\cos \phi_1 \cos \phi_2 \cos \phi_3 + \sin \phi_1 \sin \phi_2 \sin \phi_3 \\
\sin \phi_1 \cos \phi_2 \cos \phi_3 - \cos \phi_1 \sin \phi_2 \sin \phi_3 \\
- \cos \phi_1 \cos \phi_2 \cos \phi_3 - \sin \phi_1 \sin \phi_2 \sin \phi_3 \\
\cos \phi_1 \cos \phi_2 \cos \phi_3 - \sin \phi_1 \sin \phi_2 \sin \phi_3 \\
\end{array} \right] \mathbf{k}
\]

and it is readily shown that:

\[
e^{-\vec{\phi}} = \left[ \begin{array}{c}
\cos \phi_1 \cos \phi_2 \cos \phi_3 + \sin \phi_1 \sin \phi_2 \sin \phi_3 \\
\sin \phi_1 \cos \phi_2 \cos \phi_3 - \cos \phi_1 \sin \phi_2 \sin \phi_3 \\
- \cos \phi_1 \cos \phi_2 \cos \phi_3 - \sin \phi_1 \sin \phi_2 \sin \phi_3 \\
\cos \phi_1 \cos \phi_2 \cos \phi_3 - \sin \phi_1 \sin \phi_2 \sin \phi_3 \\
\end{array} \right] \mathbf{k}
\]
Performing the addition and subtraction yields:

$$\cosh \vec{\phi} = \begin{bmatrix} \cos \phi_1 \cos \phi_2 \cos \phi_3 \\ \cos \phi_1 \sin \phi_2 \sin \phi_3 \\ - \sin \phi_1 \cos \phi_2 \sin \phi_3 \\ \sin \phi_1 \sin \phi_2 \cos \phi_3 \end{bmatrix} \cdot 1 + \begin{bmatrix} i \\ j \end{bmatrix} \quad \text{and} \quad \sinh \vec{\phi} = \begin{bmatrix} \sin \phi_1 \cos \phi_2 \cos \phi_3 \\ \sin \phi_1 \sin \phi_2 \sin \phi_3 \\ \cos \phi_1 \cos \phi_2 \sin \phi_3 \\ \cos \phi_1 \sin \phi_2 \cos \phi_3 \end{bmatrix} \cdot k$$

(6.113)

which is just:

$$\ddot{u} = \exp \vec{\phi} + \sinh \vec{\phi}$$

(6.114)

which is analogous to the polar form of complex numbers. The unit quaternion can also be expanded to:

$$\ddot{u} = [\cosh(\phi_1 i) + \sinh(\phi_1 i)] [\cosh(\phi_2 j) + \sinh(\phi_2 j)] [\cosh(\phi_3 k) + \sinh(\phi_3 k)]$$

(6.115)

which can be evaluated using quaternion hyperbolic identities, shown in Table 6.3, to again yield:

$$\ddot{u} = \cosh \vec{\phi} + \sinh \vec{\phi}$$

(6.116)

Table 6.3: Quaternion Hyperbolic Identities

<table>
<thead>
<tr>
<th>Identity</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>\cosh(\phi) = (e^\phi + e^{-\phi})/2</td>
<td>\sinh(\phi) = (e^\phi - e^{-\phi})/2</td>
</tr>
<tr>
<td>\cosh(\phi_1 i) = \cos(\phi_1)</td>
<td>\sinh(\phi_1 i) = \sin(\phi_1) i</td>
</tr>
<tr>
<td>\cosh(\phi_2 j) = \cos(\phi_2)</td>
<td>\sinh(\phi_2 j) = \sin(\phi_2) j</td>
</tr>
<tr>
<td>\cosh(\phi_3 k) = \cos(\phi_3)</td>
<td>\sinh(\phi_3 k) = \sin(\phi_3) k</td>
</tr>
<tr>
<td>\cosh(\phi_1 + \beta i) = \cosh(\phi_1) \cos(\beta) + \sinh(\phi_1) \sin(\beta) i</td>
<td>\sinh(\phi_1 + \beta i) = \sinh(\phi_1) \cos(\beta) + \cosh(\phi_1) \sin(\beta) i</td>
</tr>
<tr>
<td>\cosh(\phi_2 + \beta j) = \cosh(\phi_2) \cos(\beta) + \sinh(\phi_2) \sin(\beta) j</td>
<td>\sinh(\phi_2 + \beta j) = \sinh(\phi_2) \cos(\beta) + \cosh(\phi_2) \sin(\beta) j</td>
</tr>
<tr>
<td>\cosh(\phi_3 + \beta k) = \cosh(\phi_3) \cos(\beta) + \sinh(\phi_3) \sin(\beta) k</td>
<td>\sinh(\phi_3 + \beta k) = \sinh(\phi_3) \cos(\beta) + \cosh(\phi_3) \sin(\beta) k</td>
</tr>
<tr>
<td>\exp(\phi_1 i) = \cos(\phi_1) + \sin(\phi_1) i = \cosh(\phi_1) i + \sinh(\phi_1) i</td>
<td>\exp(\phi_2 j) = \cos(\phi_2) + \sin(\phi_2) j = \cosh(\phi_2) j + \sinh(\phi_2) j</td>
</tr>
<tr>
<td>\exp(\phi_3 k) = \cos(\phi_3) + \sin(\phi_3) k = \cosh(\phi_3) k + \sinh(\phi_3) k</td>
<td></td>
</tr>
</tbody>
</table>

6.3.3 Calculus

Let $s$ be a scalar variable and also let $u(s) = [u_o(s), u_1(s), u_2(s), u_3(s)]$ be a quaternion that is a continuously differentiable, single-valued function of $s$. Define the derivative of $u(s)$ with respect to $s$ as:

$$\frac{du}{ds} = \left[ \frac{du_o}{ds}, \frac{du_1}{ds}, \frac{du_2}{ds}, \frac{du_3}{ds} \right]$$

(6.117)

The derivative of the product of a quaternion function, $s \cdot (s', q)$, a quaternion constant, $q = [q_o, q_1, q_2, q_3]$, can also be shown to be:

$$(q u)' = q'u'$$

(6.119)

as long as $q' = dq/ds = 0$.

The derivative of the product of two quaternion functions, $u(s)$ and $v(s)$, both a function of $s$, can be shown to be:

$$(u v)' = u' v + u v'$$

(6.120)

Partial Derivatives

Partial derivatives are defined similarly. Let $r$ and $s$ be scalar variables and let $u(r, s)$ be a quaternion that is a continuously differentiable, single-valued function of $r$ and $s$. We define the partial derivatives of $u$ with respect to $r$ and $s$ as:

$$u'(r) = \frac{\partial u}{\partial r} = \lim_{\Delta r \to 0} \frac{\Delta u}{\Delta r} = \frac{\partial u_o}{\partial r} + \frac{\partial u_1}{\partial r} i + \frac{\partial u_2}{\partial r} j + \frac{\partial u_3}{\partial r} k$$

(6.121)

and

$$u'(s) = \lim_{\Delta s \to 0} \frac{\Delta u}{\Delta s} = \frac{\partial u_o}{\partial s} + \frac{\partial u_1}{\partial s} i + \frac{\partial u_2}{\partial s} j + \frac{\partial u_3}{\partial s} k$$

(6.122)

The derivative rules presented previously also hold for partial derivatives.

Scalar Derivative

Let $H(x)$ be a continuously differentiable, single-valued, scalar function of the quaternion position, $x = x_o + x_1 \hat{i} + x_2 \hat{j} + x_3 \hat{k}$. The gradient of this scalar function is defined using:

$$\nabla h = \frac{ \Delta H }{ \Delta x } = \lim_{\Delta x \to 0} \frac{\Delta H}{\Delta x} = \frac{\partial H}{\partial x} = \frac{\partial H}{\partial x_o} \hat{i} + \frac{\partial H}{\partial x_1} \hat{j} + \frac{\partial H}{\partial x_2} \hat{k} + \frac{\partial H}{\partial x_3} \hat{k}$$

(6.123)
which is the same as:

\[ h = \frac{dH}{dx} \frac{\bar{x}}{dx} = \frac{dH}{|dx|^2} \]  

(6.124)

This leads to the definition of the gradient operator:

\[ \partial(\cdot) = \frac{d(\cdot)}{dx} = \begin{bmatrix} \frac{\partial(\cdot)}{\partial x_0}, \frac{\partial(\cdot)}{\partial x_1}, \frac{\partial(\cdot)}{\partial x_2}, \frac{\partial(\cdot)}{\partial x_3} \end{bmatrix} \]  

(6.125)

The gradient of the product of a constant, \(c\), and a scalar function, \(H(x)\), is:

\[ \partial(cH) = \partial cH = ch \]  

(6.126)

The gradient of the product of two scalar functions, \(G(x)\) and \(H(x)\), where \(\Im(G) = 0\) and \(\Im(H) = 0\), is:

\[ \partial(GH) = G\partial H + H\partial G = G h + H g \]  

(6.127)

**Quaternion Derivative**

The derivative of a spatially variable quaternion, \(u(x)\), is obtained using:

\[ \partial u = \frac{\partial u}{\partial x_0} + \frac{\partial u}{\partial x_1} + \frac{\partial u}{\partial x_2} + \frac{\partial u}{\partial x_3} \]  

(6.128)

or, equivalently:

\[ \partial u = \begin{bmatrix} \frac{\partial u_0}{\partial x_0} + \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \\
\frac{\partial u_1}{\partial x_0} - \frac{\partial u_0}{\partial x_1} - \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \\
\frac{\partial u_2}{\partial x_0} + \frac{\partial u_1}{\partial x_1} - \frac{\partial u_3}{\partial x_2} + \frac{\partial u_0}{\partial x_3} \\
\frac{\partial u_3}{\partial x_0} - \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_3} - \frac{\partial u_0}{\partial x_2} \end{bmatrix} \]  

(6.129)

The gradient of the product of a scalar, \(H(x)\), and a quaternion, \(u(x)\), is:

\[ \partial(Hu) = h u + H \partial u \]  

(6.131)

The gradient of the product of two quaternions, \(u(x)\) and \(v(x)\), is:

\[ \partial(uv) = (\partial u)v + (\partial v)u = (\partial u + \partial v) \]  

(6.132)

Let \(H(x)\) be a continuous-differentiable, single-valued, scalar function of the quaternion position, \(x\). The quaternion derivative is defined using the gradient of the quaternion conjugate of the gradient of \(H\):

\[ \partial^2 H = \partial H = \partial (\bar{H}) = \begin{bmatrix} + h_{00} + h_{11} + h_{22} + h_{33} \\
- h_{01} + h_{10} + h_{23} - h_{32} \\
- h_{02} - h_{13} + h_{20} + h_{31} \\
- h_{03} + h_{12} - h_{21} + h_{30} \end{bmatrix} \]  

(6.133)

where:

\[ \bar{H} = \begin{bmatrix} \partial H \\
\partial x_1 \\
\partial x_2 \\
\partial x_3 \end{bmatrix} \]  

(6.134)

is the quaternion conjugate of the gradient of \(H\), and

\[ h_{ij} = \frac{\partial (\bar{H})}{\partial x_j} \]  

(6.135)

Note that if the order of differentiation is unimportant, i.e., \(h_{ij} = h_{ji}\), then \(\partial^2 H\) is a scalar:

\[ \partial^2 H = h_{00} + h_{11} + h_{22} + h_{33} \]  

(6.136)

which implies that \(\Im(\partial^2 H) = 0\).

**Angle Derivative**

It is possible to show using term-by-term expansion that the gradient of the Cartesian quaternion, \(u\), is related to the gradient of the angle quaternion:

\[ \partial u = \partial (e^{\bar{\phi}}) = (\partial \phi) \]  

(6.137)

and

\[ \partial \phi = \frac{(\partial u) \bar{u}}{u \bar{u}} = \partial \ln(u) \]  

(6.138)

which is consistent with the definition of the natural logarithm:

\[ \ln(u) = \ln(e^{\bar{\phi}}) = \phi \]  

(6.139)

**Hyperbolic Derivatives**

Note that the derivatives of the hyperbolic functions are:

\[ \begin{align*}
\frac{\partial \cosh \phi}{\partial \phi} & = -\frac{\cosh \phi}{\phi} = \sinh \phi \\
\frac{\partial \sinh \phi}{\partial \phi} & = -\frac{\sinh \phi}{\phi} = \cosh \phi
\end{align*} \]  

(6.140)

and

\[ \begin{align*}
\frac{\partial \cosh \phi}{\partial \phi} & = -k \frac{\cosh \phi}{\phi_3} = \sinh \phi \\
\frac{\partial \sinh \phi}{\partial \phi_3} & = -k \frac{\sinh \phi}{\phi_3} = \cosh \phi
\end{align*} \]  

(6.141)

but the derivatives with respect to \(\phi_2\) do not provide the desired result. Also note that the derivatives w.r.t. \(\phi_1\) require post-multiplication of the result by \(i\), while the derivatives w.r.t. \(\phi_2\) require pre-multiplication by \(k\).
CHAPTER 6. VECTORS, COMPLEX VARIABLES, AND QUATERNIONS

Integration

Let \( s \) again be a scalar variable and also let \( u(s) \) be a quaternion that is a continuously differentiable, single-valued function of \( s \). The integral of \( u \) with respect to \( s \) is defined using:

\[
\int_{s_a}^{s_b} u \, ds = \int_{s_a}^{s_b} \left[ u_a + u_1 i + u_2 j + u_3 k \right] \, ds
\]

\[
= \left[ \int_{s_a}^{s_b} u_0 \, ds + \int_{s_a}^{s_b} u_1 \, ds + \int_{s_a}^{s_b} u_2 \, ds + \int_{s_a}^{s_b} u_3 \, ds \right]
\]

(6.144)

The integral of a constant, \( c \), is:

\[
\int_{s_a}^{s_b} c \, ds = c \int_{s_a}^{s_b} ds = c (s_b - s_a)
\]

(6.145)

The integral of the gradient of a scalar, \( h = \nabla H(x) \), is:

\[
\int_{x_a}^{x_b} h \, dx = \int_{x_a}^{x_b} \nabla H \, dx = \int_{x_a}^{x_b} \frac{dH}{dx} \, dx = \int_{x_a}^{x_b} dH = H(x_b) - H(x_a)
\]

(6.146)

where the path of integration is immaterial. The integral of the gradient of a quaternion, \( \nabla u(x) \), is:

\[
\int_{x_a}^{x_b} \nabla u \, dx = u(x_b) - u(x_a)
\]

(6.147)

where the path is again immaterial. The integral of the product of a constant, \( c \), and the gradient of a quaternion, \( \nabla u(x) \) is:

\[
\int_{x_a}^{x_b} c \nabla u \, dx = c [u(x_b) - u(x_a)]
\]

(6.148)

The quaternion integral formulation is equivalent to combining Gauss’ divergence theorem with Stokes’ theorem:

\[
\int_{R_n} \vec{h} \, dR_n = \int_{R_{n-1}} \vec{H} \, dR_{n-1} = \int_{R_{n-2}} \vec{u} \, dR_{n-2} = U
\]

(6.149)

where:

- \( R_3 \) is the boundary three-dimensional volume surrounding the \( R_4 \) hypervolume;
- \( R_2 \) is the boundary two-dimensional surface surrounding the \( R_3 \) volume;
- \( R_1 \) is the boundary one-dimensional line surrounding the \( R_2 \) surface; and
- \( R_0 \) are the boundary points terminating the \( R_1 \) line segment.

6.3.4 Relationship to Vectors

The vector gradient operator of a scalar, \( \nabla H \), is related to the quaternion gradient, \( \nabla \vec{h} \), using:

\[
\nabla H = [h_1, h_2, h_3] = -\Im(\nabla \vec{h}) = \Im(\vec{h})
\]

(6.150)

The vector divergence, \( \nabla \cdot \vec{h} \), and vector curl, \( \nabla \times \vec{h} \), are related to the quaternion gradient using:

\[
\Re(\nabla \vec{h}) = \nabla \cdot \vec{h} = h_{11} + h_{22} + h_{33}
\]

(6.151)

\[
\Im(\nabla \vec{h}) = \nabla \times \vec{h} = \begin{bmatrix} h_{23} - h_{32} \\ h_{31} - h_{13} \\ h_{12} - h_{21} \end{bmatrix}
\]

(6.152)

where \( \vec{h} = [h_1, h_2, h_3] \) is a pure quaternion. The quaternion gradient can therefore be related to the divergence and curl derivatives using:

\[
\nabla \vec{h} = \left[ \nabla \cdot \vec{h}, \nabla \times \vec{h} \right]
\]

(6.153)

Note that the quaternion gradient explicitly incorporates both types of vector derivative functions (i.e., both the divergence and curl) with the additional ability to incorporate the derivative of the real part of \( h, h_c \).

The real part of the quaternion integration corresponds to Gauss’ divergence theorem:

\[
\Re \left[ \int_{R_3} \vec{u} \, dR_3 \right] = \int_{R_3} (\nabla \cdot \vec{u}) \, dR_3 = \int_{R_2} \vec{u} \cdot d\vec{R}_2
\]

(6.154)

while the imaginary part corresponds to Stokes’ Theorem:

\[
\Im \left[ \int_{R_2} \vec{u} \, dR_2 \right] = \int_{R_2} (\nabla \times \vec{u}) \cdot d\vec{R}_2 = \oint_{R_1} \vec{u} \cdot d\vec{R}_1
\]

(6.155)

6.4 The Dual

All boundary value problems share the need to define a governing equation (either differential or integral), domain properties (extent and material properties), boundary conditions, and also initial conditions for transient problems. A wide range of solution methodologies exist for using this information to provide forward predictions of hydraulic head or flux, or inverse predictions of domain properties and boundary conditions. Because boundary conditions are a vital part of the problem definition, it is critical that they are correctly formulated. While most models require that the normal component of flux boundary conditions be specified, many users fail to recognize this requirement. Instead, the flux magnitude is mistakenly used instead of the more-appropriate, normal component. The tangential component of flux relative to the boundary should always be discarded unless a complex (or, alternatively, a dual or vector) formulation is used.
6.4.1 Problem Formulation

In ground-water hydrology, Darcy’s law is used in combination with the conservation equation to specify the governing equation, domain properties are defined using homogeneous or heterogeneous distributions, and boundary and initial conditions are assigned using knowledge of the regional flow behavior. These equations are commonly solved using finite-difference or finite-element methods, and can be used for one-, two-, and three-dimensional flow problems.

For steady flow, the conservation equation can be written in differential form using the divergence of the flux vector, \( \vec{q} \):

\[
\nabla \cdot \vec{q} = 0
\]  \hspace{1cm} (6.156)

This can be combined with Darcy’s law:

\[
\vec{q} = -K \nabla h
\]  \hspace{1cm} (6.157)

to obtain:

\[
\nabla \cdot K \nabla h = 0
\]  \hspace{1cm} (6.158)

where \( h \) is the hydraulic head, and \( K \) is the hydraulic conductivity tensor. For homogeneous and isotropic \( K \), this can be simplified to just \( \nabla^2 h = 0 \).

Transient flow requires the inclusion of a storage term, resulting in:

\[
\nabla \cdot K \nabla h = S_s \frac{\partial h}{\partial t}
\]  \hspace{1cm} (6.159)

where \( S_s \) is the specific storage coefficient and \( t \) is time. This can also be written for homogenous \( S_s \) using:

\[
\nabla \cdot D \nabla h = \dot{h}
\]  \hspace{1cm} (6.160)

where \( D = K/S_s \) is the hydraulic diffusivity tensor and \( \dot{h} = \partial h/\partial t \).

External boundary conditions take the general form:

\[
\phi_b \ h(\Gamma) + \psi_b \ q_n(\Gamma) = 1
\]  \hspace{1cm} (6.161)

where \( \Gamma \) is the boundary, \( q_n \) is the normal component of the flux vector, \( \vec{q} \), and the constants (\( \phi_b \) and \( \psi_b \)) are prescribed using:

- **Prescribed head (Dirichlet)** \( \phi_b \neq 0 \) \( \psi_b = 0 \)
- **Prescribed flux (Neumann)** \( \phi_b = 0 \) \( \psi_b \neq 0 \)
- **Mixed (Cauchy)** \( \phi_b \neq 0 \) \( \psi_b \neq 0 \)

\[
\] \hspace{1cm} (6.162)

The final requirement is the specification of material properties, which can have distributed values across a finite-difference grid or finite-element mesh. For a finite-element formulation, the head and fluxes across each internal (element) boundary are specified using:

\[
h^j = h^k \quad \text{and} \quad q_n^j = -q_n^k
\]  \hspace{1cm} (6.163)

where the superscripts are used to identify neighboring boundaries (\( j \neq k \)).

It should be emphasized that that normal fluxes (i.e., \( q_n \)) are always used instead of flux magnitudes (i.e., \( |q| \)) for flux boundary conditions. Figure 6.1 presents what we mean by the normal flux and the flux magnitude. Note that the magnitude is the pythagorean sum of the normal and tangential fluxes, i.e., \( |q| = \sqrt{q_n^2 + q_t^2} \).

Also note that the tangential component of the boundary flux should be discarded. While ignoring important attributes of the system seems problematic, it arises directly from the way in which the problem is formulated.

6.4.2 Dual Formulation

The dual formulation provides a practical alternative to the classical formulation that incorporates the tangential component of the boundary flux. For anisotropic media, the problem can be posed in terms of the stream function, \( \psi \), instead of the hydraulic head and fluxes across each internal (element) boundary are specified using:

\[
\vec{q} \cdot \nabla \psi = 0
\]  \hspace{1cm} (6.170)

Figure 6.1: Diagram illustrating boundary flux components.

where the superscripts are used to identify neighboring boundaries (\( j \neq k \)).

The governing equation in this case is the curl, rather than the divergence, of the flux vector:

\[
\nabla h \cdot \nabla s = 0
\]  \hspace{1cm} (6.164)

which is equivalent to:

\[
\frac{\partial h}{\partial x} \frac{\partial s}{\partial x} + \frac{\partial h}{\partial y} \frac{\partial s}{\partial y} = 0
\]  \hspace{1cm} (6.165)

and lead to the Cauchy-Riemann conditions:

\[
\frac{\partial h}{\partial x} = \frac{\partial s}{\partial y} \quad \text{and} \quad \frac{\partial h}{\partial y} = -\frac{\partial s}{\partial x}
\]  \hspace{1cm} (6.166)

The governing equation in this case is the curl, rather than the divergence, of the flux vector:

\[
\nabla \times \vec{q} = 0
\]  \hspace{1cm} (6.167)

so that:

\[
\nabla^2 s = 0
\]  \hspace{1cm} (6.168)

The dual boundary conditions are written in terms of the tangential components of boundary flux because:

\[
\frac{\partial h}{\partial n} = \frac{\partial s}{\partial \tau} \quad \text{and} \quad \frac{\partial h}{\partial \tau} = -\frac{\partial s}{\partial n}
\]  \hspace{1cm} (6.169)

which implies that the tangential change in head equals the negative of the normal change in stream potential.

For isotropic media, the problem must be formulated in terms of the flux vector, \( \vec{q} \), instead of the hydraulic gradient, \( \nabla h \):
which is equivalent to:

\[ q_x \frac{\partial s}{\partial x} + q_y \frac{\partial s}{\partial y} = 0 \] \hspace{1cm} (6.171)

and lead to the Cauchy-Riemann conditions:

\[ q_x = \frac{\partial s}{\partial y} \quad \text{and} \quad q_y = -\frac{\partial s}{\partial x} \] \hspace{1cm} (6.172)

which again leads to \( \nabla \times \vec{q} = \nabla^2 s = 0 \) and:

\[ q_n = \frac{\partial s}{\partial n} \quad \text{and} \quad q_r = -\frac{\partial s}{\partial r} \] \hspace{1cm} (6.173)

### 6.4.3 Cauchy Integral Formulation

Alternatively, the complex variable boundary integral formulation can be used to solve steady, two-dimensional flow problems by means of the Cauchy Integral equation:

\[ w(z) = \frac{1}{2\pi i} \oint_C \frac{w(\xi)}{z - \xi} \, d\xi \] \hspace{1cm} (6.174)

where \( w \) is the complex potential:

\[ w = h + is \] \hspace{1cm} (6.175)

where \( i \) is the imaginary number \((\sqrt{-1})\), and \( z \) is the complex potential:

\[ z = x + iy \] \hspace{1cm} (6.176)

For heterogeneous media, each homogeneous region must be enclosed by a boundary and linked to surrounding homogeneous regions using matching boundary conditions:

\[ w^j = w^k \quad \text{and} \quad q^j = -q^k \] \hspace{1cm} (6.177)

where the superscripts are again used to identify neighboring boundaries \((j \neq k)\), and \( q \) is the complex flux, defined using:

\[ q = q_x + i q_y = -K \frac{\partial w}{\partial z} \] \hspace{1cm} (6.178)

where \( \bar{w} \) is the complex conjugate of \( w \). The flux can also be found using the Hadamard integral formula (Chen and Chen, 2000):

\[ q(z) = \frac{1}{2\pi i} \oint_C \frac{w(\xi)}{(z - \xi)^2} \, d\xi \] \hspace{1cm} (6.179)

### 6.4.4 References


### 6.5 Problems

#### 1. Vectors

(a) Show the results of addition, subtraction, multiplication and division of two three-dimensional vectors, \( \vec{u} = [u_1, u_2, u_3] \) and \( \vec{v} = [v_1, v_2, v_3] \)

(b) Find the gradient, \( \nabla U \), of the function, \( U = x^2 + 2xy + y^2 \). Also find the divergence, \( \nabla^2 U = \nabla \cdot \nabla U \), and the curl, \( \nabla \times \nabla U \).

(c) Find the gradient, \( \nabla U \), of the function, \( U = x^2 - 2xy + y^2 \). Also find the divergence, \( \nabla^2 U = \nabla \cdot \nabla U \), and the curl, \( \nabla \times \nabla U \).

#### 2. Complex Numbers

(a) Determine whether any or all of the mathematical operations (i.e., addition, subtraction, multiplication, and division) of complex variables is associative, commutative, and distributive.

(b) Calculate and plot the complex function \( u = x^2 \), where \( x = x_o + ix_1 \).

(c) Calculate and plot the complex function \( u = \log(x) \), where \( x = x_o + ix_1 \).

(d) If \( i \) represents a rotation of \( 90^\circ \), find the complex number which represents a rotation of \( 45^\circ \).

#### 3. Quaternions

(a) Determine whether any or all of the mathematical operations (i.e., addition, subtraction, multiplication, and division) of quaternions is associative, commutative, and distributive.

(b) Calculate and plot the function \( u = x^2 \), where \( x = x_o + ix_1 + jx_2 + kx_3 \).

(c) Calculate and plot the function \( u = \log(x) \).

(d) If \( i \), \( j \), and \( k \) represent a rotation of \( 90^\circ \), what do each of these rotations mean?.

(e) What is the difference between quaternions and latitudes-longitudes?
Chapter 7

Additional Reading

7.1 Mathematical References


7.2 Management Models


7.3 Systems/Statistical Models


7.4 Watershed/Surface Water Models


7.5 Groundwater Models


BIBLIOGRAPHY


