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Characterizing diurnal and interannual variability in the atmosphere through physical and stochastic models

Jonathan Michael Hobbs
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Characterizing diurnal and interannual variability in the atmosphere through physical and stochastic models

by

Jonathan Michael Hobbs

A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Co-majors: Statistics
Meteorology

Program of Study Committee:
Mark Kaiser, Co-major Professor
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Iowa State University

Ames, Iowa

2014

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DEDICATION

This dissertation is dedicated to all of my teachers, who have inspired my lifelong desire to learn.
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ABSTRACT

Mathematical models are commonplace in atmospheric science and continue to provide insight into processes across spatial and temporal scales. The study of climate dynamics relies on a spectrum of mathematical models, ranging from physical models based on the governing equations of fluid dynamics to statistical models that utilize probability to represent climate as the distribution of weather events. Hierarchical statistical models, which utilize multiple levels of conditional probability distributions, provide a framework for combining the principles or actual mathematical framework of physical models into statistical models. Development of computational tools for Bayesian analysis of hierarchical models has improved their utility, and spatio-temporal models are often implemented for climate applications. In three papers, this dissertation implements several physical and statistical models to investigate modes of variability in the climate system. The first paper develops statistical models for the diurnal cycle of relative humidity while accounting for spatial dependence in the observed realizations. The diurnal cycle varies stochastically from day to day through a dynamic model. The second study focuses on the interannual variability of large-scale stationary disturbances in the Northern Hemisphere winter circulation. The stationary waves are maintained by forcing mechanisms including anomalous heating patterns and the mean flow. Through an experiment with a numerical model, this study investigates the stationary wave response to variations in heating and the mean wind. The third component investigates the diurnal behavior of the atmospheric hydrological cycle. The study’s analysis focuses on the conditional distributions of water vapor flux divergence given neighboring values. This aids the construction of a hierarchical spatial statistical model with random condi-
tional variances. Bayesian analysis for a spatio-temporal version of the model includes posterior predictive diagnostics based on empirical conditional moments.
CHAPTER 1. GENERAL INTRODUCTION

The atmosphere is a chaotic system, yet it is characterized by processes across a large range of spatial and temporal scales that exhibit organized patterns of variability. Understanding of this complex collection of processes has been aided by the development of mathematical models that represent particular scales of processes. Each model is an approximation of the behavior of the real atmosphere, and in all cases simplifying assumptions are made to eliminate unnecessary complexity in the mathematical development and focus the investigation on the processes of interest. A model can generate data, which allows the assessment of the model’s depiction of the process against observations from the real atmosphere while accounting for important sources of uncertainty. Mathematical models in atmospheric science often involve some combination of physical and statistical depictions of the processes of interest. This dissertation develops additional mathematical tools for examining the diurnal cycle and interannual modes of variability in the atmosphere using principles from climate dynamics and spatio-temporal statistics.

1.1 Modeling Spectrum

Climate is the distribution of weather (Guttorp and Xu, 2011). This simple statement underlies a spectrum of mathematical depictions of climate and weather, collectively termed models, that add to the understanding of the climate system. Berliner (2003) identifies this spectrum of physical-statistical models as ranging from inherently deterministic models based on fluid dynamics to probabilistic descriptions of weather events.
Berliner offers a mathematical framework for connecting models along the spectrum, an appealing approach for modeling climate. Incorporating stochastic characteristics into a physical model of some aspect of the climate system provides a way to quantify and partition uncertainty with respect to the process of interest. Some examples of the models along the spectrum are outlined below and are connected to the studies that appear later in this dissertation.

The governing equations of atmospheric dynamics characterize the time-evolution of the atmospheric state variables such as temperature, wind and moisture. Climate dynamics characterize the long-term behavior of these state variables, including the mean state and the intrinsic “modes of variability” induced by the dynamics. This is the motivation behind general circulation models (GCMs), which are computer models that are capable of numerically integrating the governing equations in time. Thus, GCMs are physically-based mathematical representations of the climate system and can be made increasingly complex through enhanced spatial resolution, additional dynamical relationships, and linkage to other aspects of the climate system. GCMs are extensively evaluated against the historical observational record by simulating multiple decades of the recent past. Uncertainties arise due to resolution, external forcing and representation of small-scale processes, and combinations, or ensembles, of GCMs are used to quantify uncertainty (Taylor et al., 2012).

Since GCMs generate data for the full space-time atmospheric state, GCM experiments offer a comprehensive perspective on the climate system, which is well-suited for describing multiple climate characteristics at the global or continental scale. However, the computational demands and complexity of a GCM may inhibit the understanding of the process of interest. In addition to general numerical modeling, atmospheric science has a long history of focused investigations of simpler physical models. For example, Rossby et al. (1939) developed solutions to a basic vorticity equation to predict the behavior of large-scale atmospheric waves, and their formulation continues to facilitate
the understanding of the general circulation of the atmosphere. GCMs with simplified
dynamics, specifically a linear response to specified forcing, can provide similar insight
(Hoskins and Karoly, 1981). This approach is employed in Chapter 3 of this dissertation,
which investigates year-to-year changes in the atmospheric circulation over the Atlantic
Ocean.

Statistical models of the distribution of weather events can also focus the investigation
of an atmospheric process by abstracting weather events as stochastic processes with as-
sociated random variables. Then the stochastic model parameters inform understanding
of the atmospheric process of interest. A typical approach is to decompose the stochastic
model into systematic and random components (Nelder and Wedderburn, 1972). The
specified statistical model provides a prescription for a data-generating process, and the
statistical model can be assessed through its ability to generate data similar to observed
data (Caragea and Kaiser, 2009). Combining data with a statistical model can provide
a framework for quantifying uncertainty in the model parameters and relevant functions
of the parameters. Statistical models should incorporate sufficient complexity to be real-
istic depictions of the underlying scientific processes. Models for atmospheric processes
present some specific challenges related to the small-scale dependence present in both
space and time.

Recent years have seen substantial development of statistical models for application to
environmental data. Motivated by questions ranging from air quality to water resources
to climate change, much of the statistical development has focused on spatio-temporal
models. For complex processes, so-called hierarchical models that utilize multiple lev-
els of conditional distributions are conceptually appealing, providing a mechanism for
abstracting and combining processes that vary across space and/or time (Wikle et al.,
1998). Development of computational tools for Bayesian analysis of hierarchical models
has bolstered their utility in environmental problems. Chapter 2 of this dissertation
develops a statistical model that captures an atmospheric diurnal cycle that evolves
dynamically from day-to-day.

Cressie and Wikle (2011) outline a variety of approaches for using physical models, specifically partial differential equations (PDEs) commonly used in dynamic meteorology, as process models in a statistical model. This approach is an example of what they term scientific-statistical modeling and provides an emerging example of useful approaches in the spectrum of physical-statistical models proposed by Berliner (2003). The governing equations in climate dynamics can be well-served by this approach for a number of reasons. Stochastic components and the hierarchical model framework, with complementary tools for inference, offer a way to quantify uncertainty. In addition, statistical models can be motivated by subsets of the full PDE systems, focusing the investigation and eliminating the need for a full GCM. Chapter 4 of this dissertation investigates a PDE-inspired statistical model.

When observed atmospheric data are available, the assumptions of any model on the physical-statistical spectrum can be assessed by comparing observations to data generated from the model of interest. It is important to compare models and observations in a way that is relevant to the atmospheric process of interest and to incorporate uncertainty where appropriate. Bayesian inference offers a diagnostic framework through posterior predictive assessment (Gelman et al., 1996). This dissertation develops posterior predictive assessment tools that can be used in a variety spatio-temporal modeling applications.

1.2 Dissertation Organization

The next three chapters of this dissertation each contain a manuscript that is to be submitted to a peer-reviewed journal. The first paper, entitled “Dynamic Spatio-Temporal Models for the Diurnal Cycle,” develops several statistical models to examine characteristics of the diurnal cycle for an atmospheric variable. The approach captures
the diurnal cycle of a spatial field while accounting for spatial dependence in the observed realizations. The diurnal cycle varies stochastically from day to day through a dynamic model. Bayesian analysis for the models is illustrated for surface relative humidity fields, and model diagnostics assess the adequacy of various model components.

The second paper, “Sensitivity of North Atlantic Stationary Waves to Variability in Thermal Forcing and the Zonal Mean Flow,” focuses on the interannual variability of the North Atlantic Oscillation (NAO), a prominent climate mode in the Northern Hemisphere atmospheric general circulation. The presence of large-scale stationary disturbances in the atmosphere dictates the movement of weather systems around the globe. The stationary waves are maintained by several forcing mechanisms including the presence of mountains, anomalous heating patterns and the mean flow. This paper investigates the impact of year-to-year variations in heating and the mean flow on the characteristic wave pattern of the NAO, which is diagnosed from observed data and tested through a linear numerical model.

The third paper, “Spatio-Temporal Modeling of the Midwest Hydrological Cycle: The Roles of Mean and Variance Processes,” contains an investigation of the diurnal behavior of the atmospheric hydrological cycle. The transport of water vapor is an important dynamic mechanism in the process, with evaporation acting as a source and precipitation acting as a sink of atmospheric water vapor. Transport is characterized by water vapor flux divergence, and the paper proposes a spatio-temporal model that captures the spatially-varying diurnal cycle and the non-constant variability present in this hydrological variable. The resulting statistical model includes three spatial processes and is estimated with a Bayesian analysis. Diagnostic tools for conditionally-specified spatial models and posterior predictive assessment demonstrate the importance of non-constant variance in the hydrological cycle. Chapter 5 of this dissertation offers some concluding remarks.
References


CHAPTER 2.  DYNAMIC SPATIO-TEMPORAL MODELS FOR THE DIURNAL CYCLE

A paper to be submitted to *Mathematical Geosciences*

Jonathan M. Hobbs and Mark S. Kaiser

Abstract

Many environmental processes exhibit a characteristic day-night cycle, which can vary in complex ways in space and time. Hierarchical statistical models offer substantial flexibility for estimating this spatio-temporal behavior and its associated uncertainty. In addition these models can incorporate multiple levels of random variables to represent different environmental processes. This study incorporates these ideas into an investigation of the diurnal cycle of relative humidity over the Midwest United States. We develop models with temporally-varying diurnal cycles to account for day-to-day weather variability and a non-Gaussian response distribution to handle the constrained nature of the response. Bayesian analysis reveals that day-to-day variability in the large-scale mean and small-scale variability are noticeable in these moisture fields for the region of interest. We assess the models’ representation of the spatio-temporal processes with posterior predictive assessment of local conditional distributions.
2.1 Introduction

The earth’s climate system is driven by the sun’s energy, and the systematic differential heating of the planet on different time scales both directly and indirectly impacts weather and climate. The diurnal cycle is one such fundamental pattern, and many atmospheric variables exhibit characteristic day-night patterns. Regional diurnal cycles are governed by the global pattern but are modulated by local features such as orography and land-sea interactions as well as transient events such as the passage of weather systems. These complications present challenges for quantification of the diurnal cycle.

Fourier analysis can provide quantitative insight into the behavior of the diurnal cycle. Harmonics can be transformed to provide an amplitude and phase for the diurnal cycle, and harmonic coefficients can be estimated using a discrete Fourier transform or through regression on Fourier basis functions (Wilks, 2006). The latter approach can be computationally more intensive but can be applied to incomplete and unbalanced datasets. Harmonic analysis is commonly used in assessing the diurnal cycle of various atmospheric variables, including regional precipitation (Wallace, 1975; Higgins et al., 1997) and outgoing longwave radiation (OLR) (Hartmann and Recker, 1986). Smith and Rutan (2003) characterize the similarity of the diurnal cycle in OLR for different regions of the globe with a principal components analysis. Yang and Smith (2006) analyze regional diurnal cycles in precipitation across the tropics and subtropics and review several physical mechanisms that explain regional variation.

This study aims to extend the harmonic analysis approach to address some further fundamental challenges in quantifying the diurnal cycle. Long-run average diurnal cycles at locations over a region are often related, so it should be possible to borrow information across locations in estimating the diurnal cycle. In addition, individual observations, not just the climatology, at nearby locations often show similar variation from day-to-day or hour-to-hour. Further, the diurnal cycle itself exhibits interannual and intraseasonal
variation. Finally, atmospheric variables may exhibit diurnal cycles in their variability and small-scale spatial dependence in addition to diurnal cycles in the large-scale mean.

It would be difficult to address these issues simultaneously through data processing techniques. An alternative is to construct and fit a statistical model that includes parameters to represent the characteristics of interest. When several processes or characteristics are involved, a statistical model is often constructed through several conditional probability distributions. Often termed hierarchical modeling, this multi-level approach has been implemented for a variety of environmental processes. Wikle et al. (1998) outline a general framework for the approach and develop and fit a model for monthly averaged temperatures over the Midwest United States. In doing so, Wikle et al. introduce Fourier basis functions (harmonics) to represent the seasonally-varying climatology in the process level of the model. This modeling strategy and subsequent Bayesian analysis facilitate the estimation and uncertainty quantification under multiple sources of variability. Harmonics have been implemented in hierarchical models to estimate seasonal cycles in many environmental variables, including rainfall occurrence (Lima and Lall, 2009) and extended heat waves (Dupuis, 2012). Fuentes et al. (2005) use harmonics in a spatio-temporal model to estimate a diurnal cycle for wind speed. This study implements a similar approach for capturing the diurnal cycle in relative humidity.

Hierarchical modeling for spatio-temporal processes involves a number of choices in parameterization. This often includes how to combine the space and time dimensions. Some approaches define overall covariance structures for the spatio-temporal process, with an appropriate consideration being whether the space and time covariance structures can be separated (Cressie and Huang, 1999). Another strategy models parameters for one dimension that vary over the other dimension. Wikle et al. (1998) implement time series models with spatially-varying parameters. Stroud et al. (2001) develop spatio-temporal models with spatial process parameters that evolve dynamically.

Ultimately the scientific questions of interest can guide the hierarchical model pa-
rameterization. Here we are specifically interested in the diurnal cycle of atmospheric fields and their evolution over a short time period. We first address the diurnal behavior in a large-scale mean process but investigate other characteristics of the spatio-temporal process. A dynamic model for the diurnal cycle parameters is developed to address changes over time. The model is implemented for a sequence of surface relative humidity fields. This variable exhibits a pronounced diurnal cycle but presents unique statistical challenges.

One challenge we address is spatial modeling in a situation when a Gaussian response distribution is not suitable. This challenge has been addressed in contrasting ways in the literature. One option is to specify conditional distributions with appropriate support and combine to build a multivariate model. In the spatial context, Markov random field (MRF) models are often used for this purpose. Recent developments in this area include parameterizations that allow for interpretable large-scale structure, as in Caragea and Kaiser (2009), who model spatial dependence for dichotomous responses.

Other options incorporate latent processes with spatial structure, typically with a Gaussian process or MRF model for the latent process. Studies fall into two general groups based on the strategy for linking the Gaussian spatial process to the non-Gaussian response. One strategy is based on copula techniques, or transformation of the Gaussian process to a (potentially) location-specific non-Gaussian marginal distribution (De Oliveira et al., 1997). Specifying a non-Gaussian data model with independent observations, conditioned on the spatial process, is another strategy. Diggle et al. (1998) present examples with Poisson and binomial data models. The model presented in Section 3 resembles the latter strategy and uses a latent Gaussian MRF model.

The data source and some exploratory analysis are briefly described in Section 2. The basic statistical model and various extensions are outlined in Section 3. This is followed in Section 4 by the details of Bayesian analysis, inference and diagnostics for the models. Section 5 provides some interpretation of the results in the context of the diurnal cycle,
and Section 6 includes a discussion of potential extensions.

### 2.2 Data Source

In this article we investigate a set of hourly surface relative humidity fields over the Midwest United States. By definition, relative humidity (RH) is the ratio of actual water vapor content to the maximum possible, which is a function of temperature. Water vapor content is an important state variable for atmospheric numerical modeling and, when combined with temperature, can be expressed equivalently by several different variables, including mixing ratio, dew point, specific humidity and relative humidity. From a stochastic modeling perspective, each of these present some challenges because of the range of values they can assume. Being a proportion, relative humidity should be modeled to handle its constrained nature.

The dataset used here consists of seven days of hourly near-surface RH fields (168 hours) from the Rapid Update Cycle (RUC) analysis (Benjamin et al., 2004). The RUC is an operational data assimilation and forecast system that has been operated by the National Centers for Environmental Prediction (NCEP) since 1994. The assimilation system provides analysis fields over the contiguous United States every hour with data from a variety of surface and upper air sources. The numerical model is used operationally for short-term (up to 12 hours) mesoscale forecasting. The RUC analysis fields are convenient here because they provide fields on a regular grid at hourly intervals.

Data from a region covering $30 \times 30$ RUC grid points and the time period from 00 UTC 1 July 2007 to 23 UTC 7 July 2007 are extracted for the analysis from the NOMADS archive Rutledge et al. (2006). Figure 2.1 displays the RH fields at six-hour intervals for the first four days of the data period. Figure 2.2 provides a summary of the fields over time, treating the 900 values over space as coming from a common distribution at each point in time.
Figure 2.1 Relative humidity fields at six-hour intervals on four selected days.
Figure 2.2 Empirical distributions of hourly relative humidity fields, considering the values over space as coming from a common distribution. Solid lines depict the mean, and shaded regions represent the center 95 percent of the empirical distribution for each hour.
2.3 Spatial Models for Relative Humidity

A variety of models for representing the hourly relative humidity fields are presented in this section. These models are all variations of the same general hierarchical structure that includes a data model that assumes observations are conditionally independent given a latent spatial process and other parameters. The general model components are outlined below. The data model exhibits characteristics similar to the approach to regression for rates and proportions proposed by Ferrari and Cribari-Neto (2004). This approach models the data as random variables from conditional beta distributions, with mean parameters that are functions of large-scale parameters. The data are conditioned on a latent process that captures potential spatial dependence. Incorporating spatial dependence in a latent process versus the data model is a common choice in hierarchical modeling (Kaiser et al., 2002b,a).

2.3.1 Data Model

Let $Y(s_i, t)$ represent the relative humidity at location indexed by $s_i = (u_i, v_i)$; $u_i = 1, \ldots, U$; $v_i = 1, \ldots V$; at hour $t$. The coordinates $u_i$ and $v_i$ index the west-east and south-north position on the lattice, respectively.

$$Y(s_i, t)|\phi(t), \mu(s_i, t)) \sim \text{Beta} \left( \frac{1 - \phi(t)}{\phi(t)} \mu(s_i, t), \frac{1 - \phi(t)}{\phi(t)} (1 - \mu(s_i, t)) \right),$$

$t = 1, 2, \ldots, 168$. In this parameterization, the mean and variance of the conditional beta distribution are

$$E (Y(s_i, t)|\phi(t), \mu(s_i, t))) = \mu(s_i, t),$$

$$Var (Y(s_i, t)|\phi(t), \mu(s_i, t))) = \phi(t) \mu(s_i, t) [1 - \mu(s_i, t)].$$
### 2.3.2 Latent Spatial Process

The conditional data model mean $\mu(s_i, t)$ is related to a latent random variable $Z(s_i, t)$ through the transformation

$$\log \left( \frac{\mu(s_i, t)}{1 - \mu(s_i, t)} \right) = Z(s_i, t).$$

The field of latent variables $\mathbf{Z}_t$ for each time follow a Gaussian MRF model

$$Z(s_i, t) \mid \mathbf{z}_t(N_i) \sim \text{Gaussian } (A_{i,t}(\mathbf{z}_t(N_i)), \sigma^2_i)$$

$$A_{i,t}(\mathbf{z}_t(N_i)) = \alpha(t) + \sum_{s_j \in N_i} \eta_{i,j} \left( z(s_j, t) - \alpha(t) \right)$$

For each hour, the marginal mean of the latent process $\alpha(t)$ is the same at all locations. The conditional variances $\sigma^2_i$ and spatial dependence parameters $\eta_{i,j}$ are functions of the spatial neighborhood structure and two fixed parameters $\sigma^2$ and $\eta$. Under this general MRF model, the joint distribution for the vector $\mathbf{Z}_t$ follows a multivariate Gaussian distribution.

$$\mathbf{Z}_t \sim \text{MVN } (\mathbf{\alpha}_t, \sigma^2 \mathbf{\Sigma}(\eta))$$

The particular neighborhood structure used in this study arises from a Kronecker-product covariance structure used by Sain et al. (2011) that is particularly applicable to observations on a regular spatial lattice and can be formulated simply as a MRF model. In atmospheric science, output from climate or numerical weather prediction models or atmospheric analysis products, such as the RUC used here, have a regular lattice structure. We first consider a first-order autoregressive (AR(1)) structure for the correlations among locations along a west-east transact of the lattice, with

$$\text{Cor } (Z(s_i), Z(s_j)) = \eta^{u_i - u_j}, \{s_i, s_j : u_i = u_j\}.$$  

The collection of correlations among locations along the transect are assembled into a
$U \times U$ correlation matrix $R(\eta)$,

$$
R(\eta) = \begin{bmatrix}
1 & \eta & \eta^2 & \ldots & \eta^{U-3} & \eta^{U-2} & \eta^{U-1} \\
\eta & 1 & \eta & \ldots & \eta^{U-4} & \eta^{U-3} & \eta^{U-2} \\
\eta^2 & \eta & 1 & \ldots & \eta^{U-5} & \eta^{U-4} & \eta^{U-3} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
\eta^{U-3} & \eta^{U-4} & \eta^{U-5} & \ldots & 1 & \eta & \eta^2 \\
\eta^{U-2} & \eta^{U-3} & \eta^{U-4} & \ldots & \eta & 1 & \eta \\
\eta^{U-1} & \eta^{U-2} & \eta^{U-3} & \ldots & \eta^2 & \eta & 1 
\end{bmatrix}.
$$

Cressie and Wikle (2011) outline the corresponding AR(1) precision matrix $R^{-1}(\eta)$, which is defined as

$$
R^{-1}(\eta) = \frac{1}{1-\eta^2}
\begin{bmatrix}
1 & -\eta & 0 & \cdots & 0 & 0 & 0 \\
-\eta & 1+\eta^2 & -\eta & \cdots & 0 & 0 & 0 \\
0 & -\eta & 1+\eta^2 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1+\eta^2 & -\eta & 0 \\
0 & 0 & 0 & \cdots & -\eta & 1+\eta^2 & -\eta \\
0 & 0 & 0 & \cdots & 0 & -\eta & 1 
\end{bmatrix}.
$$

We define a $V \times V$ correlation matrix $C(\eta)$ for a south-north transect in a similar fashion. Then an overall covariance matrix $\Sigma$ for the entire lattice is formed by introducing a variance parameter $\sigma^2$ and taking a Kronecker product of the AR(1) correlation matrices,

$$
\Sigma = \frac{\sigma^2}{(1-\eta^2)^2} R(\eta) \otimes C(\eta).
$$

The resulting covariance structure in $\Sigma$ yields correlations that decay exponentially as a function of the $L_1$ norm or city-block distance,

$$
\text{Cor}(Z(s_i), Z(s_j)) = \eta^{d_1(s_i, s_j)},
$$

$$
d_1(s_i, s_j) = |u_i - u_j| + |v_i + v_j|.
$$
The corresponding full precision matrix is

$$\Sigma^{-1} = \frac{1}{\sigma^2} (1 - \eta^2)^2 R^{-1}(\eta) \otimes C^{-1}(\eta).$$

Since the components $R^{-1}(\eta)$ and $C^{-1}(\eta)$ are sparse, the Kronecker product is also sparse, suggesting that the model can be written conveniently in terms of a Gaussian MRF model. The neighborhood includes not only the four-nearest neighbors immediately to the east, west, north and south, but also four additional diagonal neighbors. Besag (1974) terms these first-order ($s_j \in N_{i,1}$) and second-order neighbors ($s_j \in N_{i,2}$), respectively. The typical configuration of neighbors is shown in Figure 2.3. In addition, the MRF conditional variances $\sigma_i^2$ and spatial dependence parameters $\eta_{i,j}$ are location-dependent. Figure 2.4 illustrates the three types of locations that have unique parameter values on a rectangular lattice. The parameters values for corner, edge and interior sites are outlined in Tables 2.1 and 2.2.

Table 2.1  Conditional variances for the Kronecker product Gaussian MRF.

<table>
<thead>
<tr>
<th>$s_i$</th>
<th>$\sigma_i^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corner</td>
<td>$\sigma^2$</td>
</tr>
<tr>
<td>Edge</td>
<td>$\frac{\sigma^2}{1+\eta^2}$</td>
</tr>
<tr>
<td>Interior</td>
<td>$\frac{\sigma^2}{(1+\eta^2)^2}$</td>
</tr>
</tbody>
</table>

Table 2.2  Dependence parameters for the Kronecker product Gaussian MRF. Neighbor locations $s_j$ are identified as either first-order ($s_j \in N_{i,1}$) or second-order ($s_j \in N_{i,2}$).

<table>
<thead>
<tr>
<th>$s_i$</th>
<th>$s_j$</th>
<th>Order</th>
<th>$\eta_{i,j}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corner</td>
<td>Edge</td>
<td>First</td>
<td>$\eta$</td>
</tr>
<tr>
<td>Corner</td>
<td>Interior</td>
<td>Second</td>
<td>$-\eta^2$</td>
</tr>
<tr>
<td>Edge</td>
<td>Corner</td>
<td>First</td>
<td>$\frac{\eta}{1+\eta^2}$</td>
</tr>
<tr>
<td>Edge</td>
<td>Interior</td>
<td>First</td>
<td>$\eta$</td>
</tr>
<tr>
<td>Edge</td>
<td>Interior</td>
<td>Second</td>
<td>$-\eta^2$</td>
</tr>
<tr>
<td>Interior</td>
<td>Edge, Interior</td>
<td>First</td>
<td>$\frac{\eta}{1+\eta^2}$</td>
</tr>
<tr>
<td>Interior</td>
<td>Corner, Edge, Interior</td>
<td>Second</td>
<td>$\frac{-\eta^2}{(1+\eta^2)^2}$</td>
</tr>
</tbody>
</table>
Figure 2.3 Configuration of first- and second-order neighbors on a regular lattice. For the location denoted as 0, first-order neighbors are denoted as 1 and second-order neighbors are denoted as 2.
Figure 2.4 Configuration of location types on a regular lattice. Corner sites (C), edge sites (E) and interior sites (I) have differing numbers of neighbors.
This spatial model on a regular lattice, which constructs a covariance structure as a Kronecker product of precision matrices on spatial transects, represents a unique combination of the two typical approaches for constructing Gaussian random field models for a fixed set of locations. As Cressie and Wikle (2011) note, Gaussian MRF models are directly tied to specification of the precision matrix $\Sigma^{-1}$ of the multivariate distribution. Usually the result is a sparse precision matrix because of the Markov assumption adopted in specifying the model. On the other hand, models constructed using covariance functions from geostatistics provide direct specification of the covariance matrix $\Sigma$. In this case an equivalent MRF can be found by inverting the covariance matrix but the resulting precision matrix will generally not have a simple analytic form. However, the Kronecker product model used here has fairly straight-forward analytic forms for both the covariance matrix and the precision matrix. This can be an advantage for parameter interpretation as well as for computing.

2.3.3 Model Variants

Using the basic data model combined with the spatial latent variable model above, several variations of the model are defined. These variations differ in their depiction of the model parameters $\alpha(t)$ and $\phi(t)$. Specifically, these parameters are simplified to be functions of other parameters that capture the diurnal cycle in some fashion. All models take the MRF spatial dependence parameter $\eta$ and conditional variance $\sigma^2$ to be constant across time.

1. Static Model

The static model assumes that the beta distribution dispersion parameter $\phi(t) = \phi$. The marginal mean of the latent spatial process follows a diurnal pattern according to

$$\alpha(t) = \beta_0 + \beta_1 \cos \left( \frac{h(t)\pi}{12} \right) + \beta_2 \sin \left( \frac{h(t)\pi}{12} \right), \quad (2.2)$$
where \( h(t) = 0, 1, \ldots, 23 \) gives the hour of the day.

2. Dynamic Large-Scale Model

This model assumes that the beta distribution dispersion parameter \( \phi(t) = \phi \).

The marginal mean of the latent spatial process follows a diurnal pattern with coefficients that vary from day to day according to

\[
\alpha(t) = \beta_{0,d(t)} + \beta_{1,d(t)} \cos \left( \frac{h(t)\pi}{12} \right) + \beta_{2,d(t)} \sin \left( \frac{h(t)\pi}{12} \right),
\]

where \( d(t) = 1, 2, \ldots, 7 \) indexes individual days. Further, the coefficients evolve dynamically over days according to

\[
\beta_{0,d(t)} = \beta_{0,d(t)-1} + w_{0,d(t)}
\]

\( w_{0,d(t)} \sim \text{Gaussian}(0, \sigma^2_{0,w}) \)

\[
\beta_{1,d(t)} = \beta_{1,d(t)-1} + w_{1,d(t)}
\]

\( w_{1,d(t)} \sim \text{Gaussian}(0, \sigma^2_{1,w}) \)

\[
\beta_{2,d(t)} = \beta_{2,d(t)-1} + w_{2,d(t)}
\]

\( w_{2,d(t)} \sim \text{Gaussian}(0, \sigma^2_{2,w}) \) \hspace{1cm} (2.4)

3. Dynamic Variability Model

This model assumes that the marginal mean of the latent spatial process follows a diurnal pattern with coefficients that vary from day to day according to the same structure as (2.3) and (2.4). The beta distribution dispersion parameter follows a diurnal pattern with coefficients that vary from day to day according to

\[
\log \left( \frac{\phi(t)}{1 - \phi(t)} \right) = \lambda_{0,d(t)} + \lambda_{1,d(t)} \cos \left( \frac{h(t)\pi}{12} \right) + \lambda_{2,d(t)} \sin \left( \frac{h(t)\pi}{12} \right),
\]

where \( d(t) \) indexes individual days as indicated above. Further, the coefficients
evolve dynamically over days according to

\[ \lambda_{0,d(t)} = \lambda_{0,d(t)-1} + v_{0,d(t)} \]
\[ v_{0,d(t)} \sim \text{Gaussian}(0, \sigma_{0,v}^2) \]
\[ \lambda_{1,d(t)} = \lambda_{1,d(t)-1} + v_{1,d(t)} \]
\[ v_{1,d(t)} \sim \text{Gaussian}(0, \sigma_{1,v}^2) \]
\[ \lambda_{2,d(t)} = \lambda_{2,d(t)-1} + v_{2,d(t)} \]
\[ v_{2,d(t)} \sim \text{Gaussian}(0, \sigma_{2,v}^2) \]  (2.6)

2.4 Bayesian Analysis

While conceptually appealing, statistical models with latent spatial processes offer substantial challenges for estimation and inference. For a model with a Gaussian response distribution combined with a latent spatial process defined by Gaussian conditional distributions or a multivariate Gaussian joint distribution, the full joint distribution of the data can be derived, making maximum likelihood estimation possible (Kaiser et al., 2002b). Maximum likelihood estimation for such models with non-Gaussian response distributions typically involves integrating out the latent variables using computational techniques such as numerical or Monte Carlo integration. Kaiser et al. (2002a) present an example of Monte Carlo maximum likelihood (MCML) estimation for a model with a latent Markov random field spatial process model.

Bayesian analysis of the models with a latent spatial process is a promising alternative. Bayesian inference relies on investigation of the posterior distribution for the model parameters given the data. The posterior distribution combines the likelihood with the prior distribution for the parameters, which reflects prior beliefs about plausible values for model parameters. The advent of Markov chain Monte Carlo (MCMC) techniques (Gelfand and Smith, 1990) makes simulation from complicated posterior distributions possible when they cannot be evaluated analytically. Bayesian inference through MCMC
has seen widespread use in hierarchical models in environmental applications (Wikle et al., 1998). Diggle et al. (1998) illustrate Bayesian analysis for a model with a latent spatial process. Their spatial process is defined using geostatistical methods, but a similar approach can be used for a conditionally-specified spatial process once the joint distribution is identified.

The following subsections describe the Bayesian analysis of the models proposed in the previous section. The prior distributions are identified for each of the models and this is followed by a brief description of the basic MCMC algorithm used for posterior simulation.

2.4.1 Prior Distributions

The relative humidity data set analyzed here has thousands of observations, so at first glance it may appear that the likelihood will dominate the posterior distribution for a variety of prior distributions that have appropriate support. However, there may actually be far less information in the likelihood for some parameters than for others, and prior choice may have a substantial impact. For all models, the spatial process conditional variance $\sigma^2$ and the spatial dependence parameter $\eta$ are constant across time, and all spatial fields inform these parameters. These parameters, along with the Beta distribution dispersion parameter $\phi$ in the dynamic large-scale model, are assigned diffuse priors that cover the support of the respective parameters.

For the models with dynamic diurnal cycle components, prior distributions for the populations of dynamic coefficients warrant the most attention. The dynamic coefficients $\beta_{k,d(t)}, \lambda_{k,d(t)}$ are defined by day, so in this dataset only seven values of these coefficients inform their population parameters $\sigma^2_{k,w}, \sigma^2_{k,v}$. This situation is not unlike that outlined by Gelman (2006) in addressing prior distributions for variance components in mixed models. We adopt one of Gelman’s recommendations and use proper uniform priors for the dynamic standard deviations $\sigma_{k,w}, \sigma_{k,v}$. All of the prior distribution choices are
Table 2.3 Model parameter prior distributions used in Bayesian analysis of three models.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Static</th>
<th>Dynamic Large-Scale</th>
<th>Dynamic Variability</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta$</td>
<td>$\text{Unif}(-1, 1)$</td>
<td>$\text{Unif}(-1, 1)$</td>
<td>$\text{Unif}(-1, 1)$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\text{Unif}(0, 1)$</td>
<td>$\text{Unif}(0, 1)$</td>
<td>$\text{Unif}(0, 1)$</td>
</tr>
<tr>
<td>$\sigma^2$</td>
<td>$\text{Inv-}\Gamma(0.001, 0.001)$</td>
<td>$\text{Inv-}\Gamma(0.001, 0.001)$</td>
<td>$\text{Inv-}\Gamma(0.001, 0.001)$</td>
</tr>
<tr>
<td>$\beta_0$</td>
<td>$\text{Gau}(0, 10^4)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(1.0, \sigma_{2,w}^2)$</td>
</tr>
<tr>
<td>$\beta_1$</td>
<td>$\text{Gau}(0, 10^4)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(1.0, \sigma_{2,w}^2)$</td>
</tr>
<tr>
<td>$\beta_2$</td>
<td>$\text{Gau}(0, 10^4)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(1.0, \sigma_{2,w}^2)$</td>
</tr>
<tr>
<td>$\beta_{0,0}$</td>
<td>$\text{Gau}(0, 10^4)$</td>
<td>$\text{Gau}(0, 10^4)$</td>
<td>$\text{Gau}(0, 10^4)$</td>
</tr>
<tr>
<td>$\beta_{1,0}$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
</tr>
<tr>
<td>$\beta_{2,0}$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
</tr>
<tr>
<td>$\theta_{0,0}$</td>
<td>$\text{Gau}(0, 10^4)$</td>
<td>$\text{Gau}(0, 10^4)$</td>
<td>$\text{Gau}(0, 10^4)$</td>
</tr>
<tr>
<td>$\theta_{1,0}$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
</tr>
<tr>
<td>$\theta_{2,0}$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
<td>$\text{Gau}(0.75, \sigma_{2,w}^2)$</td>
</tr>
<tr>
<td>$\sigma_{k,w} = \sqrt{\sigma_{k,w}^2}$</td>
<td>$\text{Unif}(0, 50)$</td>
<td>$\text{Unif}(0, 50)$</td>
<td>$\text{Unif}(0, 50)$</td>
</tr>
<tr>
<td>$\sigma_{k,v} = \sqrt{\sigma_{k,v}^2}$</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.4.2 Posterior Inference

For each of the models, the posterior distributions are not available analytically, so we simulate from the posterior distributions using Markov chain Monte Carlo (MCMC) methods. The full conditional posterior distributions are sampled successively in a Gibbs sampler. These conditional posteriors have conjugate forms and are sampled directly for some parameters, namely the variance parameter $\sigma^2$ and the large-scale coefficients $\beta_d$. Other conditional posterior distributions are sampled with Metropolis-Hastings steps. These M-H updates involve Gaussian random walk proposals, and the update is performed on a logit-transformed scale for the spatial dependence parameter $\eta$ and data model dispersion parameter $\phi$. outlined in Table 2.3.
2.4.3 Posterior Predictive Diagnostics

Assessment of any statistical model can be aided by computing appropriate diagnostic measures that characterize the model’s fit to the observed data. When a Bayesian analysis is employed, posterior predictive distributions can be used for model assessment (Gelman et al., 1996). The posterior predictive distribution is the distribution of an unknown observation from the same process given the observed data. In a general sense, the goal of posterior predictive assessment is to evaluate the “closeness” of data generated from the fitted model to the actual observed data.

Due to the complexity of spatio-temporal data, posterior predictive checking can be a challenging task. Diagnostics for a variety of data characteristics have received some attention in various studies. Cocchi et al. (2007) use a hierarchical space-time model to characterize pollutant concentration at several locations and use posterior predictive realizations to assess the model’s ability to reproduce the extreme high and low concentrations as well as the observed spatial correlation pattern. Gaetan and Grigoletto (2007) devise discrepancy measures to assess the appropriateness of an extreme value model with spatially-dependent parameters for rainfall observations.

Posterior predictive assessment can be implemented using a variety of discrepancy measures, as suggested by Gelman et al. (1996). In addition, specific characteristics of the observed data can be targeted. For example, the magnitude of spatial dependence in a spatial dataset can be compared to that from a (joint) posterior predictive distribution. For the models used here we examine some characteristics of the joint posterior predictive distribution of new realizations of the latent spatial process $z_t^*$ and data $y_t^*$. These are obtained by integrating their joint distribution over the posterior distribution of the parameters (collectively denoted as $\theta$).

$$p(z_t^*, y_t^*|y) = \int f(y_t^*|z_t^*, \theta)g(z_t^*|\theta)p(\theta|y)d\theta.$$  

In practice samples from the posterior predictive distribution can be drawn at each
iteration of the MCMC routine.

For the Bayesian analysis of each model, posterior predictive realizations of the latent spatial process \( g(z_i^* | \theta) \) are simulated using the posterior draws for the other model parameters. Posterior predictive relative humidity fields are then drawn from these spatial process realizations according to \( f(y_i^* | z_i^*, \theta) \). For both the observed fields and the posterior predictive realizations, locations are grouped according to the means of their four-nearest neighbors,

\[
\bar{y}_N(s_i, t) = \frac{1}{|N_i,1|} \sum_{j \in N_i,1} y(s_j, t).
\]

The neighbor means \( \bar{y}_N(s_i, t) \) are grouped according to similar values into \( p = 1, \ldots, P \) bins defined by lower bounds \( a_p \) and upper bounds \( b_p \). Our analysis concentrates on bins of size 0.1, so \( a_1 = 0.0, a_2 = 0.1, \ldots a_{10} = 0.9; b_1 = 0.1, b_2 = 0.2, \ldots b_{10} = 1.0 \). Let \( m_k(t) \) represent the number of locations in bin \( p \) for a spatial field,

\[
m_p(t) = \sum_{i=1}^{n} I [a_p < \bar{y}_N(s_i, t) \leq b_p]
\]

Three summaries are computed for the observations in each bin:

1. The proportion of the \( n \) locations falling in the bin

\[
T_{1,p}(t) = \frac{m_p(t)}{n}
\]

2. The mean RH value for the locations falling in the bin

\[
T_{2,p}(t) = \frac{1}{m_p(t)} \sum_{i=1}^{n} I [a_p < \bar{y}_N(s_i, t) \leq b_p] y(s_i, t)
\]

3. The variance of the RH values for the locations falling in the bin

\[
T_{3,p}(t) = \frac{1}{(m_p(t)) - 1} \sum_{i=1}^{n} I [a_p < \bar{y}_N(s_i, t) \leq b_p] (y(s_i, t) - T_{2,p}(t))^2
\]
Depictions of these quantities use the terms *conditional mean* for $T_{2,p}(t)$, the mean of RH values for locations within a bin, and *conditional variance* for $T_{3,p}(t)$, the variance of RH values for locations within a bin.

In addition the overall mean and variance for the spatial field are computed

\[
T_4(t) = \frac{1}{n} \sum_{i=1}^{n} y(s_i, t)
\]

\[
T_5(t) = \frac{1}{n-1} \sum_{i=1}^{n} (y(s_i, t) - T_4(t))^2
\]

These summaries are computed for the observed RH fields as well as posterior predictive realizations for each MCMC iteration. In the spirit of posterior predictive $p$-values, we identify where the observed statistic falls in the corresponding posterior predictive distribution. In particular the posterior predictive cumulative distribution function (CDF) value of the observed statistic is computed. As an example, consider $r = 1, \ldots, R$ posterior predictive realizations of $T_{1,p}^*(t)$. The CDF value of the observed statistic is computed as

\[
Q_{1,p}(t) = \frac{1}{R} \sum_{r=1}^{R} I[T_{1,p}(t) \leq T_{1,p}^*(t)]
\]

These diagnostics are summarized across multiple time points in the next section.

### 2.5 Results

The MCMC algorithms for the three models were run for the 168 hourly RH fields. For each model, four independent Markov chains were started from dispersed starting values. Convergence was assessed through graphical diagnosis of iteration trace plots for all fixed parameters as well as randomly selected components of the latent spatial process vectors $Z_t$. Metropolis-Hastings tuning parameters were adapted during the burn-in period and fixed beyond the burn-in. Chains were run for 50,000 iterations following burn-in of 20,000 iterations, with every 10th iteration saved for output. Draws from the posterior predictive distributions and their diagnostics were computed offline after the completion of the MCMC simulation.
In addition to the model parameters, posterior inference for some derived quantities is also of interest. Table 2.4 summarizes the posterior distributions for parameters in the three models. The variance parameter $\sigma^2$ and the spatial dependence $\eta$ in the latent spatial process are static parameters in all three models. The posterior distributions for the conditional variance $\sigma^2$ are similar for the static model and the dynamic large-scale model, but the posterior mean for this parameter is nearly cut in half in the dynamic variability model. This suggests a change in the partitioning of variability in this model versus the previous two. By allowing the beta distribution dispersion coefficient to vary with time, the dynamic variability model appears to incorporate more conditional variability in the data model at certain times when the overall field variability is large. The data model dispersion is discussed further below.

The spatial dependence parameter also contributes to the variability trade-off just mentioned. For a fixed variance parameter $\sigma^2$, a larger spatial dependence parameter yields a larger marginal variance for the process. Thus the overall variability in the spatial process can be partitioned between $\sigma^2$ and $\eta$. Indeed, the dynamic large-scale model gives the smallest posterior mean for $\eta$ and the largest value for the spatial process conditional variance $\sigma^2$. The decrease in $\eta$ from the static model to the dynamic large-scale model suggests that more variability is captured in the diurnal cycle of the large-scale mean process in the dynamic model, leaving less to be accounted for by local spatial dependence. On the other hand, the spatial dependence parameter is largest in the dynamic variability model. The added flexibility in the data model does not require spatial dependence to be compromised as the marginal variability changes with time.

Under the Kronecker-product MRF model, the spatial dependence parameter $\eta$ represents the marginal correlation within the latent spatial process for first-order neighbors. As outlined in the previous section, the Markov assumption used in all of the models involves conditioning on both first- and second-order neighbors (Table 2.2). In addition to the posterior distributions for $\eta$, Table 2.4 summarizes the posterior distributions for
location-specific dependence parameters $\eta_{i,j}$ for both first- and second-order neighbors at interior lattice sites. In all cases, the first-order dependence parameters $\eta_{i,j}$ are positive with posterior distributions concentrated between 0.49 and 0.50, and the second-order parameters are negative with posterior distributions concentrated between -0.25 and -0.24. This relationship is of course imposed by this specific spatial model, and it illustrates an important advantage the Kronecker product form can have over a four-nearest neighbor Markov assumption. The negative second-order parameters effectively allow for stronger first-order dependence, which may often be a better fit when local dependence is strong.

Gaussian MRF dependence parameters can also be interpreted in terms of partial correlations. Thus the results here suggest the spatial process yields a positive partial correlation with first-order neighbors (conditioned on all other locations) and a negative partial correlation with second-order neighbors (conditioned on all other locations). Exploratory analysis (not shown) of the RUC data and similar atmospheric reanalysis products indicates that this qualitative result is present in the data.

### 2.5.1 Dynamic Diurnal Cycle

Both the dynamic large-scale and the dynamic variability models incorporate a diurnal cycle for the large-scale mean that varies from day-to-day. The MCMC algorithm includes updates for these Fourier coefficients, $\beta_d(t)$, and their posterior distributions are readily available from the MCMC samples. Figure 2.5 provides posterior summaries for the large-scale coefficients in these two dynamic models. Posterior summaries for $\sigma^2_w$, the variances of the dynamic shocks are provided in Table 2.4. There are some subtle differences in the behavior of the large-scale coefficients between the two models, but they are generally similar. The posterior distributions for the dynamic variances indicate that day-to-day variability in the intercept ($\beta_0$) and sine ($\beta_2$) terms is more substantial than for the cosine ($\beta_1$) terms. Further, the day-to-day patterns in Figure 2.5 indicate that typically the sine and cosine terms increase and decrease in magnitude in concert.
Table 2.4  Posterior means with 95% credible intervals for Bayesian analysis of three versions of the spatio-temporal model for relative humidity.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Static</th>
<th>Dynamic Large-Scale</th>
<th>Dynamic Variability</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \eta )</td>
<td>0.8645 (0.8627, 0.8663)</td>
<td>0.8559 (0.8540, 0.8578)</td>
<td>0.8800 (0.8782, 0.8819)</td>
</tr>
<tr>
<td>( \eta_{i,j} ) : ( s_j \in N_1 )</td>
<td>0.4947 (0.4946, 0.4949)</td>
<td>0.4940 (0.4938, 0.4942)</td>
<td>0.4959 (0.4958, 0.4961)</td>
</tr>
<tr>
<td>( \eta_{i,j} ) : ( s_j \in N_2 )</td>
<td>-0.2448 (-0.2449, -0.2446)</td>
<td>-0.2440 (-0.2442, -0.2439)</td>
<td>-0.2460 (-0.2461, -0.2458)</td>
</tr>
<tr>
<td>( \phi )</td>
<td>0.001147 (0.001130, 0.001164)</td>
<td>0.001139 (0.001122, 0.001157)</td>
<td>Figure 2.6</td>
</tr>
<tr>
<td>( \sigma^2 )</td>
<td>0.01078 (0.01063, 0.01094)</td>
<td>0.01091 (0.01075, 0.01107)</td>
<td>0.00687 (0.00676, 0.00699)</td>
</tr>
<tr>
<td>( \beta_0 )</td>
<td>1.041 (1.021, 1.061)</td>
<td>Figure 2.5</td>
<td>Figure 2.5</td>
</tr>
<tr>
<td>( \beta_1 )</td>
<td>-0.825 (-0.854, -0.796)</td>
<td>0.102 (0.027, 0.332)</td>
<td>0.098 (0.026, 0.319)</td>
</tr>
<tr>
<td>( \beta_2 )</td>
<td>0.639 (0.611, 0.667)</td>
<td>0.026 (0.005, 0.088)</td>
<td>0.020 (0.004, 0.074)</td>
</tr>
<tr>
<td>( \sigma^2_{0,w} )</td>
<td>0.149 (0.040, 0.487)</td>
<td>0.141 (0.038, 0.460)</td>
<td></td>
</tr>
<tr>
<td>( \sigma^2_{1,w} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \sigma^2_{2,w} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \sigma^2_{0,v} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \sigma^2_{1,v} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \sigma^2_{2,v} )</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
This suggests that the amplitude, or the extent of the peak, of the diurnal cycle exhibits variability in time, but the phase, or the timing of the peak, remains somewhat constant. The day-to-day variability in the intercept indicates that the regional daily mean relative humidity exhibits daily fluctuations.

The dynamic variability model adds a dynamically evolving dispersion parameter in the data model. The posterior distributions of the Fourier coefficients are summarized in Figure 2.6 and the variances of the dynamic shocks are summarized in Table 2.4. As with the large-scale coefficients, the day-to-day variability in the intercept and sine terms exceeds that for the cosine term. This suggests that daily variation is present in both the regional mean small-scale variability and the amplitude of the diurnal cycle of small-scale variability. The intercept terms are consistently quite small on the logit scale, indicating that the Beta distribution dispersion parameter $\phi_t$ is generally small despite its diurnal cycle and day-to-day variability.

In the dynamic variability model, the data model conditional variance

$$\text{Var}(Y(s_i, t) | Z(s_i, t)),$$

is a function of both the dynamically-evolving large-scale mean and Beta distribution dispersion parameter. Figure 2.7 presents the posterior distribution of this conditional variance over time. Although the timing of the maximum variance (phase) changes, the maximum conditional variance is achieved near 12 UTC, often just before. This early morning period corresponds to the maximum in the large-scale mean relative humidity. A model with a constant dispersion parameter would achieve its minimum conditional variance when the large-scale mean approaches 1. This discrepancy illustrates the value of incorporating a diurnal cycle in the dispersion parameter.

### 2.5.2 Posterior Predictive Diagnostics

The MCMC procedures also include sampling from the posterior predictive distribution $p(z^*(t), y^*(t) | y)$ and computation of a variety of summary measures for the observed
Figure 2.5 Posterior summaries for $\beta$, the daily large-scale coefficients, in the two dynamic models. Points depict the posterior mean, with error bars giving the extent of 95% credible intervals.

data and posterior predictive realizations, as outlined in the previous section. Figure 2.8 summarizes $Q_4(t)$, the CDF of the observed field variance within the posterior predictive distribution. The CDF is plotted against the observed field variance for each of the 168 hours for both the dynamic large-scale and dynamic dispersion models. Both models exhibit concentrations of observed values near the extremes of the posterior predictive distribution, suggesting that both models do not entirely capture the dynamics of RH variability. The concentration near the extremes appears less pronounced in the dynamic dispersion model.
Figure 2.6  Posterior summaries for $\lambda$, the daily dispersion coefficients, in the dynamic dispersion model. Points depict the posterior mean, with error bars giving the extent of 95% credible intervals.

Figures 2.9 and 2.10 illustrate the posterior predictive distributions of the empirical conditional variances computed after binning locations according to the average of the four-nearest neighbors. Figure panels are labeled according to the lower bound $a_p$ of each bin. Figure 2.9 summarizes the posterior predictive distribution of conditional variances through the observed values’ CDF $Q_{3,p}(t)$ for the dynamic large-scale model. The lowest bins with $a_p < 0.4$ do not contain observations at all times, only capturing late-afternoon times when especially low RH values are possible. For these low-RH bins, the observed CDF values tend to be small, indicating that the posterior predictive realizations show
Figure 2.7 Posterior summaries for the data model conditional variance $\text{Var}(Y(s_i, t)|Z(s_i, t))$ in the dynamic variability model. The solid line depicts the posterior mean, and the shaded regions represent 95% credible intervals.

more variability than the observations in these bins. On the other end of the spectrum, especially for the $a_p = 0.9$ bin, the $Q_{3,p}(t)$ values are concentrated near 1. This suggests that the observations show more variability than the posterior predictive realizations in these high RH situations.

Figure 2.10 depicts the $Q_{3,p}(t)$ values for the dynamic dispersion model. For the small $a_p$ bins, the excessive variability of the posterior predictive realizations is still evident, with most $Q_{3,p}(t)$ values below 0.5, but there is some slight improvement over the dynamic large-scale model in Figure 2.9. Perhaps the strongest improvement is for the large $a_p$
bins, which exhibit a more uniform spread of CDF values for the dynamic dispersion model. This indicates that the dynamic dispersion model more adequately represents the complex mean-variance relationship in the RH fields. Even when neighbors’ average RH is high, there can be relatively substantial variability in the individual values. Since large RH occurs once daily, most commonly around 12 UTC, there is a semi-diurnal aspect to RH variability. The dynamic dispersion model is able to capture this to some extent.

Assessment of the conditional mean CDF values $Q_{2,p}(t)$ (not shown) shows minimal differences between either of the dynamic coefficient models. Both models exhibit nearly uniform $Q_{2,p}(t)$ within most neighbor average bins; even the static model performs adequately in this regard. In addition, the observed conditional means $T_{2,p}(t)$ are tightly concentrated near the center of each bin. For example, most $T_{2,p}$ fall between 0.8 and 0.9 for the $a_p = 0.8$ bin. This is a consequence of the strong spatial dependence and small conditional variability present in the RH fields, which is captured through the combination of the large-scale mean and spatial dependence in all three models.

2.6 Discussion

This study has proposed some statistical models for the diurnal cycle of an atmospheric variable in the presence of spatial dependence. We have developed a model with a latent Gaussian spatial process and a beta distribution data model that is particularly applicable to near-surface relative humidity, which exhibits a pronounced diurnal cycle over the central United States. The strong spatial dependence present in RUC analysis fields warrants a Markov random field (MRF) model resulting from a Kronecker product of AR(1) covariance structures that is well-suited for a regular lattice. Day-to-day changes in the large-scale mean relative humidity are a result of changing weather patterns and are captured in the statistical model by dynamic Fourier basis coefficients.
The large-scale behavior of relative humidity is characterized by a temporally-varying temporal process.

Aided by posterior predictive diagnostics, further investigation of the relative humidity fields revealed time-varying conditional variability that was not captured in a model with constant dispersion parameters. Specifically there are apparent semi-diurnal peaks in variability when the mean reaches both a minimum and a maximum. An alternative model with a dynamic diurnal cycle for the beta distribution dispersion parameter captures some of this behavior and exhibits improved posterior predictive characteristics. More general models that allow dynamic evolution of other parameters are possible. For example, a dynamically-evolving conditional variance for the spatial process may enhance the representation of the semi-diurnal maxima in RH variability. A diurnal cycle in spatial dependence may also be present but would likely need to be diagnosed with slightly different measures.

This general framework for modeling the diurnal cycle can potentially be extended to address emerging questions in atmospheric science. For larger spatial domains from continental to global, capturing a spatially-varying diurnal cycle is necessary. To address this, some spatial structure could be incorporated into the basis coefficients, the basis functions themselves, or both. Higher-order basis functions can also be used to capture additional semi-diurnal behavior. These extensions would be valuable in evaluating the diurnal cycle in numerical models.

Acknowledgments

The RUC analysis data used in this work were downloaded from the NOAA National Operational Model Archive and Distribution System (NOMADS). This work was partially supported by National Science Foundation grant DMS #0502347 EMSW21-RTG.
Figure 2.8 CDF of observed field variance within the posterior predictive distribution for the dynamic large-scale (top) and dynamic dispersion (bottom) models.
Figure 2.9  CDF of observed conditional variance within the posterior predictive distribution for the dynamic large-scale model. Locations are binned according to the average of the four-nearest neighbors. Each panel is labeled with the lower bound $a_p$ of neighbor averages in the bin.
Figure 2.10  CDF of observed conditional variance within the posterior predictive distribution for the dynamic dispersion model. Locations are binned according to the average of the four-nearest neighbors. Each panel is labeled with the lower bound $a_p$ of neighbor averages in the bin.
References


Abstract

The large-scale atmospheric circulation is characterized by stationary waves that have particularly large amplitude in the Northern Hemisphere during its winter season. The waves are accompanied by intensification in the zonal wind in the upper troposphere in the middle latitudes. These two characteristics of the general circulation exhibit accompanying interannual variability during extreme phases of climate modes such as the North Atlantic Oscillation (NAO). In this study, the relationship between stationary waves and the latitude-height distribution of the zonal mean zonal wind is investigated in two ways. First their primary modes of variability are related through a rotated empirical orthogonal function (EOF) analysis. Then we link them dynamically through a series of experiments with a linearized primitive equation model. These experiments characterize the stationary wave response to various diabatic heating forcing distributions under a climatological basic state and basic states with perturbed zonal mean and longwave zonal winds. Altered basic states produce an enhanced west-east contrast in stationary waves.
over the mid-latitudes in the North Atlantic, and the horizontal and vertical distribution of diabatic also impact the stationary wave response.

3.1 Introduction

The hemispheric to global atmospheric circulation in Northern Hemisphere winter has been studied extensively, from observations to simple numerical models to state-of-the-art general circulation models (GCMs). The dynamic response to complex topography and large-scale heating sources has important consequences for weather prediction, intra-seasonal weather patterns, interannual climate variability and the general circulation’s response to potential climate change. The upper-tropospheric subtropical jet and large-scale stationary disturbances exhibit interannual variability and impact the within-season and day-to-day movement of weather systems across the globe.

Two prominent characteristics of the Northern Hemisphere winter atmospheric circulation are a mid-latitude maximum in the zonal wind $u$ and the large-scale stationary eddies. Figure 3.1 displays the latitude-height cross section of the climatological zonal mean zonal wind for December, January and February (DJF), as computed from the ERA-Interim Reanalysis (Dee et al., 2011). Both hemispheres contain an upper tropospheric maximum in westerlies in the mid-latitudes. As Chen (2005) notes, the general circulation can be represented by a number of scalar fields, but the streamfunction $\psi$ represents the large-scale circulation equally well in the tropics and mid-latitudes. The stationary waves can be depicted with the average departure of the streamfunction in the upper troposphere from its zonal mean. Figure 3.2 depicts the climatology of this eddy streamfunction $\psi_E$ at 200 hPa. In the Northern Hemisphere a transition is evident near 30°N and the mid-latitudes are characterized by prominent highs over western North America and the eastern Atlantic.

Rossby et al. (1939) recognize the interaction between the zonal flow and the sta-
Figure 3.1  Latitude–height cross section of the average DJF zonal mean zonal wind. Contour interval is 10 m s$^{-1}$ and positive values are shaded.
Stationary waves in the development of the trough formula and illustrate the presence of waves in their analysis of sea-level pressure maps. Since then, the importance of forcing mechanisms such as orography and diabatic heating in maintaining stationary waves have been investigated in both diagnostic and modeling studies. Wallace (1983) presents winter stationary wave patterns in mid- and upper-tropospheric geopotential heights and sea-level pressure. The increasing availability of reanalysis datasets in recent years has facilitated more detailed analysis of the role of stationary waves in the general circulation. Chen (2005) illustrates the role of the divergent circulation in maintaining the stationary waves and identifies the differing importance of dynamic mechanisms in different parts of the Northern Hemisphere, providing a physical explanation for a subtropical transition zone observed by Wallace (1983). DeWeaver and Nigam (2000a) study the link between the stationary waves and the zonal mean zonal flow $\bar{u}$. They investigate the role of both components in the zonal mean zonal momentum budget, finding that they are connected but not attributing causality in one direction or the other. They suggest the possibility of mutual adjustment.

Figure 3.2 Average DJF eddy streamfunction $\psi_E$ at 200 hPa. Contour interval is $5 \times 10^6 \text{m}^2\text{s}^{-1}$ and positive values are shaded.
Beyond the climatological behavior, interannual variability and associated teleconnection patterns are tied to stationary waves and the zonal flow. Branstator (1984) relates intra-seasonal and interannual zonal mean perturbations to the corresponding eddy pattern shifts, finding that the strongest zonal mean departures are associated with the largest eddy anomalies. Interannual variability may be linked to previously-identified climate modes such as the North Atlantic Oscillation (NAO) and the Pacific-North America (PNA) pattern. Wallace and Gutzler (1981) extensively examine the Northern Hemisphere circulation for evidence of teleconnection patterns, defined simply as correlations in atmospheric variables at widely separated points. They outline the NAO as a seesaw between the Icelandic low and the Azores high and note its connection with weather patterns over North America and Europe. They also analyze the PNA pattern, which characterizes alternating low and high-pressure centers over the northern Pacific and western North America. DeWeaver and Nigam (2000a) identify stationary wave anomaly patterns strongly associated with both PNA and NAO and suggest that the variations could be contributed as a combination of internal variability and response to external forcing. Given the complex and highly multivariate nature of data representing the atmospheric general circulation, summarizing the relevant structures is a challenging task. Many studies in the stationary wave literature utilize empirical orthogonal functions (EOF) (DeWeaver and Nigam, 2000a; Branstator, 1984) and various extensions such as extended EOF and rotated EOF.

The advent of numerical modeling of the atmosphere and a basic conceptual model spurred substantial activity in studying the large-scale circulation. Smagorinsky (1953) investigates the atmospheric response to realistic sources of heating in a simple model, and Charney and Eliassen (1949) develop a numerical model to simulate the geopotential height response to realistic topography. Hoskins and Karoly (1981) use a linear model to study the response to both heating and topography and in the process identify a mechanism for the development of teleconnection patterns. Becker and Schmitz (2001)
explore the interaction between the zonal flow and stationary waves with a primitive equation model and prescribed diabatic heating. They suggest that a simplified GCM with prescribed heating can be a valuable experimental tool for studying the large-scale circulation.

DeWeaver and Nigam (2000b) subject a linear model to thermal forcing, forcing from sub-monthly transients and zonal-eddy coupling to investigate the dynamics of the NAO, reinforcing their earlier finding (DeWeaver and Nigam, 2000a) of a mutual adjustment between stationary waves and the zonal wind. The role of diabatic heating appears to be that of a slight negative feedback locally, but the optimal heating source region may be remote. Greatbach and Jung (2007) investigate both of these diabatic heating issues through a fully nonlinear GCM and identify a negative feedback with a role for tropical heating. The negative feedback is not present in all modeling studies, as Hoskins and Valdes (1990) find an indirect positive feedback in maintaining storm tracks, including the persistent storm track over the North Atlantic that is a dominant source of latent heat in the middle troposphere. This background on the roles of different processes in the NAO sets the stage for the investigation in the present article.

In the next section, some empirical characteristics of the link between stationary waves and the zonal wind are presented. Section 3 outlines an experiment with a linearized primitive equation model. An approach for estimating the NAO-related diabatic heating is presented in Section 4. The experimental results are detailed in Section 5, followed by some concluding remarks in Section 6.

3.2 NAO Empirical Characteristics

The climate of northern winter is characterized by the presence of a westerly jet in the upper troposphere and large-scale stationary waves. These features exhibit substantial interannual and intra-seasonal variability. Several interannual variation modes; such
as the El Niño Southern Oscillation (ENSO), Pacific-North America (PNA) pattern, North Atlantic Oscillation (NAO), and Arctic Oscillation (AO); can explain year-to-year variations in the general circulation. While it is difficult to untangle the contributions of individual modes, diagnostic analysis can reveal important aspects of the interannual variability. Empirical orthogonal function (EOF) analysis is a diagnostic tool that can aid in pattern identification of space-time data (Wilks, 2006). Outside of the geosciences, EOF analysis is also known as principal component analysis (PCA). Classical PCA examines the covariance or correlation matrix of multivariate data through an eigen decomposition. Typically patterns in the first several eigenvectors are interpreted as summary “modes” of the original data. EOF analysis for atmospheric data is similar, where spatial locations represent the multivariate components, and points in time (years in this study) represent individual cases. In this sense, the eigenvectors can actually be represented on a map and examined for spatial coherence.

In the present article the interannual variability in the eddy streamfunction patterns and zonal mean zonal wind cross sections can be characterized through separate EOF analyses, with an interest in identifying patterns that may be characteristic of the NAO. The covariance matrices to be analyzed are constructed by standardizing the multi-year data at each location and applying a latitude-weighting scheme. Locations nearer the poles have their standardized anomalies effectively down-weighted. Specifically, if $y_{t,i}$ is the data value in year $t$ at location $i$, and $\bar{y}_i$ and $s_i$ represent the multi-year average and standard deviation, respectively, the latitude-weighted anomaly

$$z_{t,i} = \frac{y_{t,i} - \bar{y}_i}{s_i} \sqrt{\cos(\phi_i)}$$

The covariance matrix of the $z_{t,i}$ is used in the EOF analysis.

An EOF analysis of the DJF anomaly fields constructed from ERA-interim data for $\psi_E$ and $\bar{u}$ was performed. The initial eigenvector patterns were rotated using varimax rotation, with the leading modes examined visually and related to the DJF average NAO index from the Climate Prediction Center (CPC). The CPC computes several Northern
Hemisphere teleconnection indices from 500 hPa height anomalies using a procedure devised by Barnston and Livezey (1987). The NAO index is oriented so that positive index values correspond to an anomalously strong Azores high with positive height anomalies in the subtropical North Atlantic. Negative index values correspond to weaker Azores high and Icelandic lows.

Figure 3.3 depicts the loading patterns for the second EOF for the eddy streamfunction $\psi_E$. The EOF time series for this mode has a correlation of 0.84 with the NAO index and explains 12.9 percent of the variance in $\psi_E$. The contrast between the mid- and high-latitudes in the Atlantic is evident in the eigenvector pattern. Figure 3.4 depicts the loading pattern for the first EOF for the vertical profile of the zonal mean zonal wind. The EOF time series for this mode has a correlation of 0.59 with the NAO index and explains 23.1 percent of the variance in the zonal mean zonal wind. The pattern is noticeably uniform vertically with the subtropic/mid-latitude/high-latitude oscillation.

This empirical link among the NAO, stationary waves and the zonal mean zonal wind motivates some further investigation of the dynamics of the NAO. This link has been investigated in a number of ways. For example, DeWeaver and Nigam (2000a) provide a momentum budget analysis to assess the role of stationary waves in maintaining the zonal wind. DeWeaver and Nigam suggest that the zonal wind and stationary waves may undergo mutual adjustment in the extreme phases of NAO. Other investigations, including DeWeaver and Nigam (2000b) and Greatbach and Jung (2007), also focus on the role of diabatic heating on stationary waves. In the next section we outline a linear model experiment to investigate the impact of the zonal wind and heating on the NAO stationary wave variability.
3.3 Primitive Equation Model

This section outlines a numerical model experiment that investigates the ability of a linearized primitive equation (PE) model to produce disturbances consistent with the extreme phases of the NAO, with a focus on the impact of varying the horizontal and vertical extent of thermal forcing as well as the role of an altered basic state zonal wind pattern. The assessment focuses on the difference in stationary wave responses under the extreme NAO phases, specifically as depicted by the eddy streamfunction $\psi_E$. A linear PE model based on the model developed by Branstator (1990) is used. The original linear model code was based on the original Community Climate Model (CCM) of the National Center for Atmospheric Research (Williamson, 1983). The CCM
dynamics use vorticity $\zeta$, divergence $\delta$, temperature $T$ and logarithm of surface pressure $q = \log(p_s)$ as state variables. The numerical scheme uses a spectral representation with triangular truncation at wavenumber 31 (T31) horizontal resolution. Briefly, the spectral scheme represents the horizontal structure of a variable as a sum of spherical harmonics. Branstator illustrates the real-coefficient representation for zonal wavenumber $m$ and meridional index $n$ as

$$\zeta = \sum_{m=0}^{M} \sum_{n=m}^{N} \zeta^c_{nm} \cos(m\lambda) P^m_n(\sin \phi) + \sum_{m=1}^{M} \sum_{n=m}^{N} \zeta^s_{nm} \sin(m\lambda) P^m_n(\sin \phi),$$

where $P^m_n$ are associated Legendre polynomials, and $M = N = 31$ represents the truncation limit. The model uses a $\sigma = p/p_s$ vertical coordinate with 12 vertical levels.
at \( \{\sigma = 0.009, 0.025, 0.060, 0.110, 0.165, 0.245, 0.355, 0.500, 0.650, 0.785, 0.875, 0.950\} \), a similar configuration to that of Hoerling and Sanford (1993).

Branstator (1990) employs the CCM numerics and linearizes about a climatological basic state. The linearization technique defines a state variable \( \zeta = \overline{\zeta} + \zeta' \) as a sum of a basic state \( \overline{\zeta} \) and a perturbation \( \zeta' \). The governing equations are rewritten in this form and simplified by retaining terms containing only a single perturbation quantity. Terms involving products of perturbation quantities are replaced by a forcing term and a damping term. This work considers a steady basic state. In the case of steady (time-invariant) forcing, the solution for the perturbation quantities can be obtained directly by solving a linear system \( LX = R \), where \( L \) is a square matrix, \( X \) represents the perturbation solution and \( R \) represents the forcing terms. Branstator notes that this characteristic can allow solutions for many forcing distributions to be computed quickly for the same basic state. This advantage allows a variety of forcing configurations to be used for the same basic state without substantial additional computational cost. Thus, the current experiment uses many forcing distributions, which are detailed below and in the next section.

The model code has a few key tasks. The elements of the matrix \( L \) are functions of the basic state variables and their horizontal gradients and vertical derivatives. Each row of the matrix corresponds to a single spectral coefficient at a single level for a particular perturbation of a state variable. This linear operator matrix \( L \) is assembled one column at a time from the basic state (Branstator, 1990; Hoskins and Karoly, 1981). In general \( L \) is a dense \( \ell \times \ell \) matrix and for T31 truncation and 12 vertical levels, \( \ell = 37,888 \). Each of the \( r \) columns of the \( \ell \times r \) forcing matrix \( R \) represents one of the specified forcing distributions for the experiment. Then the matrix \( L \) is factored and the system is solved, using the dgesv routine from the LAPACK library (Anderson et al., 1999). While assembling the operator matrix \( L \) requires some computational effort, the bulk of the overall computing cost is in factoring and solving the system.
The forcing distributions included in $R$ can represent a number of processes. As Branstator (1990) and DeWeaver and Nigam (2000b) note, time-average transient fluxes (e.g. $\overline{\mathbf{v}T'}$) are dropped from the linear model equations but can act as forcing mechanisms in the linear system for all state variables. In the thermodynamic equation, diabatic heating is a forcing mechanism, and the current experimental setup focuses on the role of diabatic heating. Other processes that are not represented in the linear formulation can explain the discrepancy between the model solution and observations and could also be considered forcing mechanisms.

With this in mind, baseline forcing distributions are defined from some composite scenarios. First let $Y_0$ be a vector containing the climatological basic state, computed from a composite of ERA-Interim DJF data. For model runs with this basic state, $L$ is constructed from $Y_0$. In a similar fashion composite basic states $Y_+$ and $Y_-$ are constructed from months with positive NAO conditions and negative NAO conditions, respectively. Negative conditions are defined as any month with the CPC NAO index at or below -0.5, and positive conditions are defined as any month with the index at or above 1.0. The values of -0.5 and 1.0 are near the 25th and 75th percentiles, respectively, of NAO indices for DJF from 1979 to 2012.

With these composite basic states assembled, define perturbations

$$X_+^* = Y_+ - Y_0,$$
$$X_-^* = Y_- - Y_0,$$

which represent the ideal perturbation solutions under positive and negative NAO conditions. If the climatological operator matrix is multiplied by each of these solutions, the ideal forcing $R_+^*, R_-^*$ under each scenario can be found,

$$R_+^* = LX_+,$$
$$R_-^* = LX_-.$$
The model experiment focuses on the impact of variability in diabatic heating on the stationary wave response. Diabatic heating forcing enters only in the temperature elements of $R$. Denoting the temperature sub-matrix as $R_T$, it is separated into contributions from diabatic heating $Q$ and from other sources $S$,

$$R_T = Q + S.$$ 

The baseline diabatic heating $Q^*_+$ and $Q^*_-\text{ are computed using a procedure outlined in the next section, and the baselines from other sources are found by taking the difference, for example,}$$

$$S^*_+ = R^*_{+,T} - Q^*_+.$$ 

In the experimental conditions outlined below, the thermal forcing is a combination of $S^*_+$ or $S^*_-\text{ and a possibly altered diabatic heating distribution.}$

### 3.3.1 Experimental Factors

The linear model experiment aims to characterize the variability in the North Atlantic stationary wave response to variations in diabatic heating and the Northern Hemisphere zonal wind. In addition, computational costs can be optimized by using relatively few different basic states and using altered forcing where possible. With this in mind, the experiment includes all combinations of three levels of each of three factors. The experimental conditions are outlined below and summarized in Table 3.1.

1. **Basic State Zonal Wind**

   Three different basic state conditions are used in the experiment in order to examine the impact of an altered zonal wind on the stationary wave response. The first basic state condition uses the climatological basic state $Y_0$. The second and third conditions use a zonal wind that is a combination of the climatological short-wave zonal wind and the NAO extreme long-wave zonal wind. In the second case,
the longwave consists of the zonal mean only (wavenumber 0). Figure 3.5 shows the latitude-height profile of the difference in zonal mean zonal wind between the NAO positive and negative scenarios. The strongest differences are evident in the northern mid-latitudes. In the third case, the longwave includes wavenumbers 0-4. Figure 3.6 illustrates the difference in the longwave zonal wind in this third case, contrasting the NAO positive and negative scenarios. As in the zonal mean only case, the distinction is focused in the northern mid-latitudes. In this third case, the largest differences are focused in the North Atlantic, with positive anomalies centered near 45°N and negative anomalies both to the north (Greenland) and to the south (subtropics).

2. Horizontal Extent of Diabatic Heating

Previous linear modeling experiments (Smagorinsky, 1953; Hoskins and Karoly, 1981) note that local heating sources can excite wave responses at remote locations, which motivates an assessment of the horizontal extent of diabatic heating in the linearized PE model experiment. On one hand, remote heating anomalies may play a role in the North Atlantic wave response, as Greatbach and Jung (2007) suggest in the case of heating in the tropics. On the other hand, local heating anomalies may impact not only the North Atlantic disturbance, but also the overall hemispheric response. These possibilities are investigated with three horizontal distributions of diabatic heating: global, North Atlantic sector only (90°W−40°E, 20°N−80°N), and extra-Atlantic (all areas outside of North Atlantic sector).

3. Vertical Extent of Diabatic Heating

The vertical distribution of diabatic heating has received differing treatment in modeling studies of the modes of variability in the general circulation. Greatbach and Jung (2007) and use a full atmospheric GCM with forcing from sea-surface temperature (SST) anomalies that produces realistic NAO variability, suggesting an
Figure 3.5  Latitude-height cross section of the difference in basic state zonal wind between NAO positive and negative scenarios under the altered zonal mean basic state condition. Contour interval is 2 m s$^{-1}$ and positive values are shaded.
Figure 3.6 Difference in 200 hPa basic state zonal wind between NAO positive and negative scenarios under the altered longwave (wavenumbers 0-4) basic state condition. Contour interval is 4 m s\(^{-1}\) and positive values are shaded.

important role for low-level heating in the oscillation. However, the linearized PE model only utilizes thermal forcing on the actual model levels and includes thermal vertical diffusion in the thermodynamic equation. DeWeaver and Nigam (2000b) argue that the inclusion of vertical diffusion makes diabatic heating redundant in the boundary layer.

In the current experiment we assess the sensitivity of the response to boundary layer heating through three vertical profiles of diabatic heating. The first condition uses diabatic heating at all vertical levels. The second condition eliminates diabatic heating in the lowest two model levels. The third condition eliminates diabatic heating in the lowest two levels and the top three levels. This last condition is introduced due to the uncertainty in estimating diabatic heating in the upper atmosphere. This uncertainty is due in part to the rapid changes in static stability near and above the tropopause. Other aspects of estimating diabatic heating are outlined in the next section.
The control condition consists of the climatological basic state $Y_0$ with global diabatic heating at all vertical levels. Other conditions are identified by the combinations of the three factors as outlined in Table 3.1. Each condition is run with both a negative and positive NAO scenario, which corresponds to separate negative NAO and positive NAO forcings, and two unique columns of $R$, for all conditions. This also implies two unique basic states for the conditions involving altered longwave zonal wind.

Table 3.1  Conditions for the linearized primitive equation model experiment. Rows and columns indicate the levels of the three factors: basic state zonal wind, horizontal extent of diabatic heating and vertical extent of diabatic heating. Cells of the table provide labels for each experimental condition.

<table>
<thead>
<tr>
<th>Diabatic Heating</th>
<th>Basic State Zonal Wind</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Climatology</td>
</tr>
<tr>
<td>Horizontal</td>
<td>Vertical</td>
</tr>
<tr>
<td>Global</td>
<td>All</td>
</tr>
<tr>
<td></td>
<td>Above PBL</td>
</tr>
<tr>
<td></td>
<td>Mid-Level Only</td>
</tr>
<tr>
<td>North Atlantic</td>
<td>All</td>
</tr>
<tr>
<td></td>
<td>Above PBL</td>
</tr>
<tr>
<td></td>
<td>Mid-Level Only</td>
</tr>
<tr>
<td>Extra-Atlantic</td>
<td>All</td>
</tr>
<tr>
<td></td>
<td>Above PBL</td>
</tr>
<tr>
<td></td>
<td>Mid-Level Only</td>
</tr>
</tbody>
</table>

3.3.2 Measured Response

The linearized PE model provides a solution $X$ that is of large dimension, and many characteristics of the solution can provide insight into the model response. Since the present article focuses on stationary waves, the analysis will center on the eddy streamfunction $\psi_E$, which can be computed from the total vorticity $\zeta = \bar{\zeta} + \zeta'$ from each model run. The difference in eddy streamfunction $\psi_{E,D}$ between the positive ($\psi_{E,+}$) and negative ($\psi_{E,-}$) NAO scenarios,

$$\psi_{E,D} = \psi_{E,+} - \psi_{E,-},$$
is emphasized in the results. As a scalar summary of the NAO response, the difference in $\psi_{E,D}$ between the Azores ($26.25^\circ W, 38.97^\circ N$) and Iceland ($22.50^\circ W, 64.94^\circ W$) is computed for each experimental run. This difference, $\psi_{E,\text{NAO}}$ quantifies the magnitude of the NAO response.

### 3.4 Forcing from Diabatic Heating

The previous section outlined the baseline forcing, $R^+_{\pm}$ and $R^-_{\pm}$, that is used in the control run of the linear model experiment. The thermal forcing includes a contribution from diabatic heating, $Q^+_{\pm}$ and $Q^-_{\pm}$. Since the experiment aims to characterize the impact of different heating distributions, the anomalous diabatic heating under positive and negative NAO scenarios will be estimated. The monthly average global distribution of diabatic heating is computed, and an empirical relationship between these heating distributions and the monthly average NAO index is estimated.

When the global values of the atmospheric state variables (indexed by longitude $\lambda$, latitude $\phi$, pressure $p$ and time $t$) zonal wind $u = u(\lambda, \phi, p, t)$, meridional wind $v = v(\lambda, \phi, p, t)$, and temperature $T = T(\lambda, \phi, p, t)$ are available, diabatic heating $Q = Q(\lambda, \phi, p, t)$ can be estimated as a residual from the thermodynamic equation (Hoerling and Sanford, 1993; Chan and Nigam, 2009). Chen and Baker (1986) provide the formulation in spherical coordinates,

$$\frac{1}{c_p} Q = \frac{\partial T}{\partial t} + \frac{u}{a \cos \phi} \frac{\partial T}{\partial \lambda} + \frac{v}{a} \frac{\partial T}{\partial \phi} - \left( \frac{RT}{c_p p} - \frac{\partial T}{\partial p} \right) \omega, \quad (3.1)$$

where $c_p$ is the specific heat of dry air and $a$ is the planetary radius. The vertical motion $\omega = \omega(\lambda, \phi, p, t)$ can be computed diagnostically using the kinematic method of O’Brien (1970), or assimilated vertical motion from reanalysis can be used if available. The latter is used here in computations using the ERA-Interim reanalysis. Using the pressure-level data at six-hour intervals, the monthly average diabatic heating is estimated for December, January and February for 1979-2012. The pressure-level heating is then
truncated to the linear model resolution of T31 and vertically interpolated to the model \( \sigma \) levels (Trenberth et al., 1993). The NAO state is quantified by the monthly mean CPC NAO index.

### 3.4.1 Regression Model

The present objective is to estimate the expected diabatic heating distribution as a function of the CPC NAO index. The response variable, diabatic heating, is a three-dimensional spatial field and the covariate, NAO index, is a scalar. In estimating the relationship, it is worthwhile to make some considerations. First, since the response is a spatial field, it may be possible to borrow strength spatially as the relationship between heating and the NAO may be similar at locations separated by short distances. Spatially-varying regression relationships have been investigated in spatio-temporal statistics. For example, Wikle and Anderson (2003) use spatially-varying regression coefficients to characterize the relationship between tornado reports in the United States and the ENSO index.

Instead of formulating a statistical model for regression coefficients, we induce spatial structure on the heating-NAO relationship through spherical harmonic analysis. The spectral truncation to T31 resolution outlined previously involves spherical harmonic analysis of the heating fields for each month using the SPHEREPACK computational library (Adams and Swarztrauber, 1999). The truncation then fixes coefficients beyond the truncation limit to zero. The nonzero spectral coefficients are saved and regressed on the NAO index. This process is repeated for all nonzero spectral coefficients and all vertical levels.

These estimates can be used to predict the spectral heating at the desired NAO index values; namely -0.50, 0.25 and 1.00; and the predicted values can be inverse-transformed to produce spatially-coherent heating fields. The baseline heating anomaly fields \( Q^*_+ \) and \( Q^*_- \) are obtained by subtracting the predicted neutral field (NAO index of 0.25)
from the predicted positive (1.00) and negative (-0.50) fields, respectively. Figure 3.7 depicts these two diabatic heating fields in the middle troposphere level of $\sigma = 0.5$. Under a positive NAO scenario, anomalous heating is focused north of $45^\circ$N between Greenland and Europe while anomalous cooling is present farther south. In the negative scenario, a positive heating anomaly extends from the southeastern United States across the Atlantic to southwestern Europe.

The regression model for each spectral coefficient can account for a wide range of relationships between heating and the NAO index. DeWeaver and Nigam (2000b) estimate a linear relationship between anomalous heating and a NAO index. In the present study possible nonlinear relationships are investigated by fitting each spectral coefficient to a small set of B-spline basis functions (Faraway, 2006). This approach allows for a smooth but possibly nonlinear relationship between the expected spectral heating and the NAO index. Figure 3.8 illustrates the approach with a scatterplot of heating versus NAO index for two locations, with the spline fit added. The spline fits have been inverse transformed, since the estimation is actually performed on the spectral coefficients.

The experimental conditions outlined in Table 3.1 utilize diabatic heating distributions characterized by their horizontal or vertical extent. Each condition contributes two columns to the matrix $Q$, consisting of $Q^*_+$ and $Q^*_-$ with the condition-specific elements set to zero. As noted in Section 3.3, the overall thermal forcing $R_T = S + Q$ combines this diabatic heating with the forcing from transients and other sources $S$. The columns of $S$ simply contain the appropriate baseline forcing, either $S^*_+$ or $S^*_-$.

3.4.2 Assessing Uncertainty

Estimation of the relationship between diabatic heating and the North Atlantic Oscillation mode is subject to several sources of uncertainty. The first is the uncertainty in quantifying the NAO state with an index; Section 3.1 identifies two approaches to constructing a NAO index and our index $\psi_{E,NAO}$ represents yet another approach. Esti-
Figure 3.7  Estimated baseline diabatic heating at $\sigma = 0.5$ under NAO extreme conditions. Top panel depicts $Q^*_+$, the anomalous heating for a positive NAO scenario, and bottom panel depicts $Q^*_-$, the anomalous heating for a negative NAO scenario. Contour interval is 2 K day$^{-1}$ and positive values are shaded.
Figure 3.8 Monthly diabatic heating $Q_c$ versus NAO Index for December, January and February from January 1979-February 2012, inclusive. Top panel depicts heating near Iceland ($22.50^\circ W, 64.94^\circ W$), and bottom panel depicts heating near the Azores ($26.25^\circ W, 38.97^\circ N$).
mation of diabatic heating introduces uncertainty due to the quantities computed, such as static stability (Gates, 1961; Nigam, 1994), and vertical interpolation (Chan and Nigam, 2009). In addition, Figure 3.8 suggests uncertainty in the estimated relationship between heating and NAO due to finite sample size and substantial residual variability. All of these sources of uncertainty can potentially propagate into the assessment of the role of heating in a numerical model.

While a comprehensive accounting of all sources of uncertainty is a challenging task, assessment of the linear model’s sensitivity to the uncertainty in the spline model estimation is a starting point. Branstator (1990) finds that a linear model can provide useful insight in the presence of random forcing. Since the computational expense of the model experiment is impacted minimally by adding columns to the forcing matrix \( \mathbf{R} \), a non-parametric bootstrap procedure is used to generate multiple estimates of the diabatic heating response under the positive and negative NAO extremes. A bootstrap dataset is assembled by randomly selecting \( J \) months with replacement from the \( J \) months in the original dataset. Then the spline regression model is fit to the spectral heating and NAO index values from this reconstructed dataset and negative, neutral and positive NAO heating distributions are computed as before. The procedure is repeated 100 times, with each realization added as a column to the forcing matrix \( \mathbf{R} \). The sensitivity of the model response is assessed primarily through the variability in the NAO stationary wave index \( \psi_{E,NAO} \) and is presented with the results in the next section.

### 3.5 Experimental Results

The control condition consists of the climatological basic state and the baseline diabatic heating distributions \( Q^*_+, Q^*_- \). Figure 3.9 shows \( \psi_{E,D} \), the difference in eddy streamfunction between positive and negative NAO scenarios, in the upper troposphere \( (\sigma = 0.245) \) for the control condition. The NAO contrast is evident over the mid-latitudes
of the Atlantic, with an enhanced low over Greenland and Iceland under a positive NAO regime and an anomalous high near the Azores. The enhanced ridging exhibits a nearly circumpolar pattern over the northern mid-latitudes with a slight northward progression across northern Europe and Asia. This is accompanied by an anomalous low and high over central Asia and the Arabian Sea, respectively.

Figure 3.9 NAO eddy streamfunction response \( \psi_{E,D} \) at \( \sigma = 0.245 \) for the control experimental condition. Contour interval is \( 2 \times 10^6 \text{m}^2\text{s}^{-1} \) and positive values are shaded.

The vertical structure of the stationary wave response over the North Atlantic exhibits slightly different characteristics under positive and negative NAO forcing. This contrast is shown in Figure 3.10, which depicts the latitude-height profile of zonally-averaged \( \psi_E \) over the North Atlantic region only. The positive NAO response yields a strong contrast in the lower troposphere between the subtropical high and the sub-Arctic low. The ridge exhibits a northward tilt and strengthening with height through most of the troposphere. In the negative NAO scenario, the upper tropospheric ridge shifts
northward and the contrast at the low levels is practically negligible, consistent with the change in orientation of storm tracks noted by Greatbach and Jung (2007).

3.5.1 Altered Basic State

Three depictions of the basic state zonal wind are included in the experiment. The control condition uses the climatological zonal wind. The second basic state depiction (U1) uses an altered zonal wind that includes the zonal mean zonal wind under positive and negative NAO scenarios. The third basic state (U2) includes the longwave zonal wind for the NAO extremes. Figure 3.11 highlights the differences in the $\psi_{E,D}$ response for these two altered basic states against the control run. Both altered basic states essentially enhance the NAO response, with the longwave zonal wind condition doing so more dramatically.

The anomalous positive $\psi_{E,D}$ that stretched from the mid-latitudes over the Atlantic to northern Europe in the control condition has a more zonal orientation in the altered basic state conditions, yielding a strong contrast between conditions in the North Sea. The combination of an altered basic state with the baseline forcing yields a stronger NAO contrast, but it has an enhanced west-east difference over the North Atlantic. In addition both basic states exhibit stronger anomalies over the Pacific, likely a result of the overall north-south shift in the jet with respect to the control simulation.

3.5.2 Diabatic Heating Distributions

Other experimental conditions address differences in the horizontal and vertical extent of diabatic heating forcing. The horizontal extent contrasts global, Atlantic only (H1), and extra-Atlantic (H2) diabatic heating. Figure 3.12 shows the effects on the NAO response for the H1 and H2 conditions conditions. For Atlantic heating only, the response is only modestly different from the control condition over the Atlantic sector and northern Europe and Asia. The most substantial differences are found over the Pacific. Previous
Figure 3.10  Latitude-height cross section of zonal mean eddy streamfunction in the Atlantic sector (60°W–15°E) for the control experimental condition. Contour interval is $4 \times 10^6$ m$^2$s$^{-1}$ and positive values are shaded. The top panel depicts the positive NAO response, and the bottom panel depicts the negative NAO response.
Figure 3.11 Differences in NAO eddy streamfunction response $\psi_{E,D}$ at $\sigma = 0.245$ for different basic state zonal wind conditions. The top panel contrasts the U1 (altered zonal mean) and control conditions, and the bottom panel contrasts the U2 (altered longwave) and control conditions. Contour interval is $2 \times 10^6 \text{m}^2\text{s}^{-1}$ (top) and $5 \times 10^6 \text{m}^2\text{s}^{-1}$ (bottom), with positive values shaded.
investigations have also found long-range teleconnection responses to localized thermal forcing (Smagorinsky, 1953; Hoskins and Karoly, 1981).

The extra-Atlantic forcing produces different stationary wave patterns at remote locations, but the strongest contrast is over eastern Atlantic. The NAO response has shifted eastward near the heating anomalies over continental Europe. The strongest anomalies present in Figure 3.7 are eliminated in the extra-Atlantic condition. Removal of the strong heating anomalies may eliminate a negative feedback, leading to an enhanced NAO response in the eastern Atlantic. Greatbach and Jung (2007) suggest a negative feedback mechanism for localized heating.

The possible negative feedback from diabatic heating may be reinforced by the effects of different vertical heating distributions. Diabatic heating is imposed at all vertical levels in the control simulation. The V1 condition removes diabatic heating in the planetary boundary layer (PBL, lowest two levels), and the V2 condition eliminates heating in the PBL and upper levels. Figure 3.13 depicts the effects of these vertical heating profiles. Both V1 and V2 have qualitatively similar effects, notably an enhanced low near Iceland and over the central Pacific. The removal of PBL heating only leads to stronger contrasts over the Pacific. The enhanced low over the North Atlantic and generally positive effects over the Atlantic mid-latitudes suggests a stronger NAO response for both V1 and V2. Once again, this would be consistent with a negative feedback.

These experimental factors may also exhibit substantial interactions, and an interaction between the horizontal and vertical distributions of heating may provide further insight into the feedback role of heating. These interactions can be explored succinctly with the scalar index \( \psi_{E,NAO} \), which is investigated next along with the role of uncertainty in estimating the diabatic heating associated with the NAO.
Figure 3.12 Differences in NAO eddy streamfunction response $\psi_{E,D}$ at $\sigma = 0.245$ for different horizontal extents of diabatic heating. The top panel contrasts the H1 (Atlantic only heating) and control conditions, and the bottom panel contrasts the H2 (extra-Atlantic heating) and control conditions. Contour interval is $5 \times 10^5 \text{m}^2\text{s}^{-1}$, with positive values shaded.
Figure 3.13 Differences in NAO eddy streamfunction response $\psi_{E,D}$ at $\sigma = 0.245$ for different vertical profiles of diabatic heating. The top panel contrasts the V1 (no boundary layer heating) and control conditions, and the bottom panel contrasts the V2 (middle troposphere heating only) and control conditions. Contour interval is $2 \times 10^5 \text{m}^2\text{s}^{-1}$, with positive values shaded.
3.5.3 Uncertainty Assessment and Interactions

We assess uncertainty in the estimated horizontal and vertical diabatic heating profiles through the bootstrap procedure outlined in Section 3.4. The estimated heating from each bootstrap dataset is used as forcing in the linear PE model, yielding a distribution of stationary wave responses for each experimental condition. The variability of the stationary wave response is summarized through the scalar NAO index $\psi_{E,NAO}$. The distributions of $\psi_{E,NAO}$ at $\sigma = 0.245$ are shown as boxplots in Figure 3.14 for the conditions with the climatological basic state.

Figure 3.14 suggests that the variability in the stationary wave response due to uncertainty in the NAO-heating relationship is fairly substantial. In addition, the variability changes with the experimental condition, particularly with the horizontal extent of heating. Variability is smallest for the Atlantic-only heating and is largest for the global heating. The distributions also reveal important interactions between the heating factors in producing the NAO stationary wave response. The extra-Atlantic heating yields the strongest NAO contrast, and the impact of the vertical heating profile is minimal without Atlantic sector heating. When heating is present over the Atlantic (global or Atlantic only), removing PBL heating results in stronger NAO contrasts. Similar distributional characteristics are found for the altered basic states (not shown), but the range of $\psi_{E,NAO}$ values change due to different orientations of the NAO stationary wave pattern induced by the different basic states.

The sources contributing to the overall variability in $\psi_{E,NAO}$ can also be partitioned quantitatively through a decomposition of sums of squares. Table 3.2 gives an analysis of variance (ANOVA) table for the combinations of experimental factors in Figure 3.14, treating the uncertainty in diabatic heating as the “error” source. Formal significance testing may not be particularly illuminating in this situation because the number of replicate runs can be arbitrarily increased. Rather, this decomposition gives a simple quantitative summary of the variability in $\psi_{E,NAO}$ from different sources. The variability
Figure 3.14  Distribution of NAO index values $\psi_{E,NAO}$ at $\sigma = 0.245$ for each experimental condition using the climatological basic state. Distributions result from estimated diabatic heating distributions for each of 100 bootstrap datasets.
induced by the bootstrap procedure accounts for over a third of the total variability in the NAO response. The horizontal extent of heating accounts for half of the variability, with the vertical extent and interaction contributing less than 10 percent each.

Table 3.2  Analysis of variance table for experimental conditions using the climatological state.

<table>
<thead>
<tr>
<th>Source</th>
<th>Sum of Squares</th>
<th>Percent of Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal Extent</td>
<td>1023.95</td>
<td>50.7</td>
</tr>
<tr>
<td>Vertical Extent</td>
<td>133.98</td>
<td>6.6</td>
</tr>
<tr>
<td>Horizontal × Vertical</td>
<td>113.70</td>
<td>5.6</td>
</tr>
<tr>
<td>Error (Bootstrap)</td>
<td>749.31</td>
<td>37.1</td>
</tr>
<tr>
<td>Total</td>
<td>2020.94</td>
<td></td>
</tr>
</tbody>
</table>

3.6  Concluding Remarks

The positive mode of the North Atlantic Oscillation is associated with a northward shift in the zonal wind, strengthening of the Icelandic low and Azores high, and corresponding northward shift in the North Atlantic storm track. This work has employed a linear primitive equation model to assess the roles of the zonal wind and diabatic heating on the dynamics of the NAO. Altered basic states with NAO-extreme zonal mean and longwave zonal wind produce enhanced NAO stationary wave patterns, particularly in the west-east contrast between the upper tropospheric trough over Greenland and ridge over northern Europe. Subjecting the linear model to various combinations of diabatic heating forcing yields important differences in the NAO stationary wave response.

In some instances, removing the diabatic heating results in an enhanced stationary wave contrast between the positive and negative NAO scenarios. This is especially true when diabatic heating over the Atlantic sector is removed and, to a lesser extent, when boundary layer diabatic heating is removed. This relationship between heating and the NAO response is suggestive of a negative feedback. Greatbach and Jung (2007) have suggested the possibility of local heating providing a negative feedback on the NAO,
which contrasts the positive feedback proposed in the self-sustaining model of storm tracks (Hoskins and Valdes, 1990). Our results are suggestive of a negative response in NAO strength to heating anomalies, but the linear model does not complete the feedback cycle. This mechanism warrants further attention in diagnostic studies and GCMs, perhaps even with coupled ocean-atmosphere simulations.

Large-scale GCM intercomparison projects (Taylor et al., 2012) are producing large quantities of simulations from ensembles of ensembles of models. This wealth of data provides another opportunity to investigate the NAO dynamics, and investigation of the dynamic links among the zonal wind, stationary waves and heating can add to the suite of tools for GCM assessment. As Boyle (2006) notes, the stationary wave characteristics in a GCM reflect a combination of model dynamics and physics, and producing realistic depictions is a difficult modeling task. A more comprehensive assessment of the NAO in modern climate runs of these GCMs can provide additional insight into the model dynamics. With an understanding of models’ depiction of the NAO under a contemporary climate, possible shifts for the future climate can continue to be investigated (Brandefelt and Kornich, 2008).

The linear model experiment conducted in this work has provided a unique opportunity to investigate the impact of uncertainty in estimating the NAO-associated diabatic heating on the variability in the stationary wave response. This assessment is made possible by the minimal computational cost in solving for many forcing distributions after factoring the model’s linear operator, an approach originally exploited by Branstator (1990). The assessment reveals that the uncertainty in estimation contributes substantially, but not overwhelmingly, to the total variability in the NAO stationary wave response. Investigation of further sources of uncertainty is warranted. In particular, a full parametric statistical model could be adopted in place of the bootstrap procedure. Uncertainty in the residual method for computing diabatic heating could be quantified as well.
Acknowledgments

The authors thank Andrew Mai for technical assistance in implementing the linear primitive equation model code. ECMWF ERA-Interim data used in this project have been provided by ECMWF and have been obtained from the ECMWF data server. The monthly NAO index data were provided by the Climate Prediction Center. We acknowledge high-performance computing support provided by NCAR’s Computational and Information Systems Laboratory, sponsored by the National Science Foundation.
References


CHAPTER 4. SPATIO-TEMPORAL MODELING OF THE MIDWEST HYDROLOGICAL CYCLE: THE ROLES OF MEAN AND VARIANCE PROCESSES

A paper to be submitted to the *Journal of Agricultural, Biological, and Environmental Statistics*

Jonathan M. Hobbs, Mark S. Kaiser and Tsing-Chang Chen

Abstract

Conservation of water vapor in the atmosphere can be summarized by a few key hydrologic processes, which vary in complex ways across space and time. Transport of water vapor by the horizontal wind redistributes moisture within the atmosphere, with transient weather systems accounting for substantial variability. Important regional processes, such as the spatially-varying diurnal cycle over the central United States, warrant attention as well. This study develops a spatio-temporal statistical model for the water vapor flux divergence to characterize these sources of variability. A mean-variance relationship is found in local empirical conditional distributions and is captured through a latent spatial model for the variance of the data-generating process, which also incorporates spatial dependence. Model assessment reveals that this flexible model reproduces key aspects of local conditional distributions more satisfactorily than a model with constant variance.
4.1 Introduction

The cycling of water vapor in the atmosphere through evaporation, transport and precipitation has profound impacts on agriculture and human life. Understanding the relationships among these processes is important in diagnosing numerical models used for both weather prediction and climate simulation on regional and global scales. The processes involved in the hydrological cycle exhibit substantial variation on a variety of spatial and temporal scales. An increasing availability of data on the water cycle presents an opportunity to investigate these sources of variation quantitatively. This article develops statistical models for the hydrological cycle along with diagnostic tools for the models’ data-generating processes.

In the atmosphere, water vapor transport from an evaporation source to an ultimate precipitation sink represents a fundamental dynamic process that is closely tied to many important aspects of the general circulation. The low-level atmospheric circulation is largely responsible for the transport of water vapor. The roles of sources and sinks of atmospheric water vapor and its transport have been investigated for the global water balance (Chen, 1985; Wong et al., 2011) as well as for regional hydrological processes such as mid-latitude cyclones (Chen et al., 1996) and intraseasonal variability of the Asian monsoon (Chen et al., 1988).

The hydrological cycle also exhibits pronounced diurnal variation, with one notable example being the central portion of North America. The Great Plains low-level jet (GPLLJ) is a frequent overnight maximum in wind speed approximately 1.5 km above the earth’s surface that transports moisture northward from the Gulf of Mexico and contributes to a nocturnal maximum in precipitation over the central United States (Wallace, 1975; Higgins et al., 1997). Moisture transport leads to the development of thunderstorm complexes, known as mesoscale convective systems (MCSs). Enhanced MCS activity has played a major role in flooding events over the central United States.
(Anderson et al., 2003; Junker et al., 1999). This region provides the setting for our development of statistical models that characterize the diurnal variation in atmospheric water vapor transport.

To date, statistical modeling for constituents of the hydrological cycle has focused on precipitation. The statistical challenges for this variable on short (i.e. daily) time scales include the frequency of zeroes and the highly skewed distribution of nonzero values. In the spatial setting, studies from Sansó and Guenni (2004) and De Oliveira et al. (1997) investigate latent Gaussian spatial processes that can be transformed via copula to marginal precipitation distributions. Berrocal et al. (2008) develop separate spatial processes for rainfall occurrence and amount in the context of probabilistic forecasting. Their approach develops a spatial model for precipitation conditioned on forecasts from numerical weather prediction (NWP) models and provides bias correction of the NWP forecast along with prediction intervals for precipitation amounts.

In addition to the value in improved prediction and uncertainty quantification in short-term prediction of precipitation, statistical models provide insight into climate, the distribution of weather events. The hydrological cycle exhibits distinct behavior in different regions of the world, and investigation of regional characteristics is bolstered by the availability of high-resolution atmospheric reanalysis products such as the North American Regional Reanalysis (Mesinger et al., 2006) and regional climate model (RCM) experiments. In examining an ensemble of RCMs, Cooley and Sain (2010) develop models for seasonal extreme precipitation using the tools from extreme value theory. Weller et al. (2012) link extreme value behavior of precipitation extremes along the Pacific coast of the United States to characteristics of the regional atmospheric circulation.

The attention these modeling approaches devote to extremes and tail behavior underscores the role of potential changes in variability of hydrologic processes across space and time. In their investigation of precipitation extremes, Cooley and Sain (2010) develop a conditional autoregressive (CAR) model for the scale parameter of a generalized
extreme value distribution. Spatio-temporal statistical models with a random variance have been investigated by Palacios and Steel (2006) and Huang et al. (2011). Palacios and Steel develop a hierarchical spatial model that includes a log-Gaussian mixing model for the location-specific variances in a Gaussian process data model, with both processes sharing a common correlation structure. Huang et al. estimate separate correlation parameters and extend to the spatio-temporal context. Yan (2007) outlines a spatial stochastic volatility model that includes Gaussian Markov random field (MRF) models for the observation process and the log variance. Non-constant variance is a focus for water vapor flux divergence, the hydrologic variable under investigation in this study.

Bayesian analysis via Markov chain Monte Carlo (MCMC) facilitates inference in many of the spatio-temporal models cited above. The Bayesian approach introduces some computational challenges but can provide a unique setting for model assessment. Gelman et al. (1996) introduce the use of model assessment through the posterior predictive distribution. Goodness of fit can be diagnosed by constructing one or several discrepancy measures that can be computed for both the observed data and replicate data generated from the posterior predictive distribution; that is, data that could have resulted from the proposed model under the same conditions. Gelman et al. illustrate examples of these realized discrepancies, some of which depend on the parameter values. In most situations, posterior predictive discrepancies can be implemented in MCMC simulation from the posterior distribution. Upon completion, the observed discrepancy’s place in the posterior predictive distribution provides an assessment of the model’s plausibility.

In the spatial setting, Kasier et al. (2012) have developed a diagnostic procedure based on realized discrepancies for Markov random field (MRF) models. MRF models are constructed by specifying a full set of compatible full conditional distributions (Besag, 1974). A Markov assumption simplifies the conditional distribution to depend on a typically small set of neighboring locations. Kasier et al. utilize the conditional specification and the imposed Markov structure to define generalized residuals based on
a probability integral transform.

Motivated by a statistical model for the water vapor flux divergence, an important hydrological variable for which statistical models have not been investigated, this paper examines a diagnostic procedure based on generalized residuals in order to detect model mis-specification due to non-constant variance. An alternative model is proposed and subsequently extended to the spatio-temporal context and its data-generating process is examined through characteristics of the posterior predictive distribution. The posterior predictive assessment utilizes moments of empirical conditional distributions and provides a new tool for the assessment of spatio-temporal models. The final spatio-temporal model provides inference for the spatially-varying diurnal cycle.

The remainder of this paper is organized as follows. In the next section, the water vapor budget and data sources are described with initial exploratory analysis that motivates subsequent statistical models. In Section 3 we consider a constant variance model for static spatial fields, essentially snapshots in time. An alternative with a spatial model for the conditional variance is developed in Section 4. These spatial models are extended to handle diurnal temporal structure in Section 5, which includes posterior predictive diagnostics based on empirical conditional distributions. Concluding remarks and potential extensions are summarized in Section 6.

4.2 Water Vapor Budget

The water vapor budget equation (Peixoto and Oort, 1992) represents the conservation of atmospheric water vapor through a set of key components that represent the dynamics of the hydrological cycle. Since fluxes to and from the earth’s surface act as sources and sinks of water vapor, the budget is often expressed in terms of a vertical atmospheric column. Thus the hydrologic variables that characterize storage and transport of water vapor in the atmosphere are integrated vertically. The constituents of the
water vapor budget at time \( t \) are computed from the zonal (eastward) wind \( U(\lambda, \phi, p, t) \), meridional (northward) wind \( V(\lambda, \phi, p, t) \), and specific humidity \( q(\lambda, \phi, p, t) \). In spherical coordinates, location is defined by longitude \( \lambda \) and latitude \( \phi \). Pressure \( p \) is the vertical coordinate.

The constituents of the water vapor budget include the precipitable water \( W \),

\[
W(\lambda, \phi, t) = \frac{1}{g} \int_{p_0(\lambda,\phi,t)}^{p_0(\lambda,\phi,t)} q(\lambda, \phi, p, t) \, dp,
\]

where \( p_0(\lambda, \phi, t) \) is the surface pressure and \( g = 9.8 \text{ m s}^{-2} \). In addition, the vertically-integrated water vapor flux vector

\[
Q(\lambda, \phi, t) = (Q_U(\lambda, \phi, t), Q_V(\lambda, \phi, t))
\]

\[
Q_U(\lambda, \phi, t) = \frac{1}{g} \int_{p_0(\lambda,\phi,t)}^{p_0(\lambda,\phi,t)} U(\lambda, \phi, p, t) \ q(\lambda, \phi, p, t) \ dp
\]

\[
Q_V(\lambda, \phi, t) = \frac{1}{g} \int_{p_0(\lambda,\phi,t)}^{p_0(\lambda,\phi,t)} V(\lambda, \phi, p, t) \ q(\lambda, \phi, p, t) \ dp
\]

characterizes the transport of water vapor through the atmosphere. The divergence (convergence) of water vapor flux serves as a sink (source) of water vapor for the location of interest. This is quantified by the water vapor flux divergence

\[
\nabla \cdot Q(\lambda, \phi, t) = \frac{1}{a \cos \phi} \left[ \frac{\partial}{\partial \lambda} Q_U(\lambda, \phi, t) + \frac{\partial}{\partial \phi} [Q_V(\lambda, \phi, t) \cos \phi] \right]
\]

The other prominent source of atmospheric water vapor is evaporation \( E(\lambda, \phi, t) \), and the other prominent sink is precipitation \( P(\lambda, \phi, t) \). The water vapor budget describes the change in precipitable water as a function of these components,

\[
\frac{\partial W(\lambda, \phi, t)}{\partial t} + \nabla \cdot Q(\lambda, \phi, t) = E(\lambda, \phi, t) - P(\lambda, \phi, t).
\]  

The water vapor budget has been utilized in global water balance studies using reanalysis (Chen, 1985) and remote sensing products (Wong et al., 2011). The regional water vapor budget over North America was investigated by Rasmusson (1968) using available station data, and Anderson et al. (2003) investigated the balance in several
regional climate models (RCMs) and in reanalyses. The contribution of atmospheric water vapor transport through the water vapor flux divergence $\nabla \cdot \mathbf{Q}(\lambda, \phi, t)$ is treated in a variety of ways depending on availability of other data. Rasmusson (1968) computed divergence using upper air observations of winds and specific humidity, and Wong et al. (2011) combined winds from reanalysis with remotely sensed water vapor to complete the calculation. Chen (1985) introduces the water vapor potential $\chi_Q$ to illustrate the divergent component of water vapor transport.

In this study we compute water vapor flux divergence from reanalysis products and develop statistical models to quantify different sources of variability in the space-time behavior of this hydrological variable. The temporal resolution of the reanalysis products is critical for estimation of the diurnal cycle. During the summer months over the central United States, water vapor flux divergence and precipitation are linked over short space and time scales, but both variables exhibit substantial local heterogeneity. Figure 4.1 illustrates precipitation fields from the Stage IV dataset (Lin and Mitchell, 2005) and water vapor flux divergence from the North American Regional Reanalysis (Mesinger et al., 2006) over a 12-hour period on July 24, 2010. Water vapor flux divergence is expressed in the same units as precipitation, in this case as a depth of water per unit time (mm hr$^{-1}$).

4.2.1 Data Sources

Two atmospheric reanalysis products are used in our data analysis. Global winds and specific humidity were obtained from the Modern-Era Retrospective Analysis for Research and Applications (MERRA) at three-hour intervals (Rienecker et al., 2011). The same variables were extracted from the North American Regional Reanalysis (NARR), also at three-hour intervals (Mesinger et al., 2006). Both reanalysis systems were developed with studies of the hydrological cycle in mind. The enhanced horizontal resolution of the NARR makes regional studies more feasible.
Figure 4.1 Precipitation rate (left panels) and water vapor flux divergence (right panels) at three-hour intervals for 23 July 2010. Areas of precipitation over 5 mm hr$^{-1}$ are shaded, and areas of water vapor flux convergence are shaded.
The vertically-integrated moisture flux vectors $Q(\lambda, \phi, t)$ were computed on each re-analysis grid. Both datasets were then re-gridded to a common 0.5° grid and merged into a single vector field, using the NARR where available and the MERRA elsewhere. Finally the divergence of the vector field was computed using spectral techniques using the SPHEREPACK library (Adams and Swarztrauber, 1999) to obtain water vapor flux divergence $\nabla \cdot Q(\lambda, \phi, t)$. Data over a region of the central United States encompassing $33 \times 33$ grid cells was extracted for statistical modeling. The subsequent analysis in this study focuses on the data from the month of July 2010.

4.2.2 Exploring Conditional Distributions

Our statistical model development will focus on the spatial characteristics of water vapor flux divergence $\nabla \cdot Q(\lambda, \phi, t)$. As noted above, this variable is particularly important for the atmospheric branch of the hydrological cycle, and existing statistical models focus primarily on precipitation. Since water vapor flux divergence can assume any value on the real line, traditional spatio-temporal models that utilize Gaussian conditional or marginal distributions will be examined initially. We will first investigate the potential for Gaussian Markov random field (MRF) models for individual spatial fields. MRF models are constructed by specifying the full conditional distributions at each location on the lattice, with a Markov assumption that the full conditional distributions are functions of a small set of neighboring locations (Besag, 1974).

Let $Y(s_i, t)$ represent the water vapor flux divergence at a location indexed by $s_i$ at time $t$. For the 0.5-degree regular lattice used here, the spatial location $s_i = (\lambda_i, \phi_i)$ is indexed by longitude $\lambda_i$ and latitude $\phi_i$. The exploratory analysis and model development below utilize two collections of neighboring values, $y_i(N_{i,1})$ and $y_i(N_{i,2})$, that Besag (1974) identifies as first-order and second-order schemes respectively. The first-order neighbors are the locations immediately east, west, north and south of the location of interest. The second-order neighbors are the next four-closest locations.
Our initial exploratory analysis constructs empirical conditional distributions from the data that emulate the conditional distributions specified in a MRF model by conditioning on neighboring values. Initial diagnostics are assembled by pairing each observed value \( y(s_i, t) \) with the average \( \bar{y}_N(N_{i,1}) \) of the values in its first-order neighborhood,

\[
\bar{y}_N(s_i, t) = \frac{1}{|N_{i,1}|} \sum_{s_j \in N_{i,1}} y(s_j, t),
\]

where \( |N_{i,1}| \) is the number of first-order neighbors for location \( s_i \). Locations on the interior of the lattice have four first-order neighbors. Locations along the edges have three, and the corner locations have two first-order neighbors.

To investigate the conditional distribution \( y(s_i, t) | \bar{y}_N(s_i, t) \), the neighborhood averages are binned together in groups with similar values. Based on the distribution of neighborhood values, the breakpoints for the bins were chosen to be -2.5, -1.5, -1, -0.5, -0.2, 0.2, 0.5, 1, 1.5, and 2.5 mm hr\(^{-1}\). This configuration places between 5% and 15% of observations in each bin. A useful initial diagnostic is a histogram of the \( y(s_i, t) \) in each of the bins. Figure 4.2 illustrates this procedure for data from July 2010. The conditional histograms suggest conditional distributions that are generally symmetric with centers that shift from negative for the smallest (negative) neighborhood averages to positive for the largest (positive) neighborhood averages. This characteristic is consistent with positive spatial dependence. Another characteristic of note is that the conditional distributions show the least spread for neighborhood averages near zero and exhibit increasing variability for averages larger in magnitude, both positive and negative.

### 4.3 Basic Spatial Model

In this section we investigate a conditionally-specified spatial model for a single water vapor flux divergence field. Even though the actual realizations of this variable are not particularly smooth, we wish to estimate a climatological mean process that is smooth.
Figure 4.2  Conditional histograms for three-hourly water vapor flux divergence for July 2010. Individual panels are characterized by the average divergence of the four nearest neighbors. Units are mm hr$^{-1}$. 
We consider a Gaussian Markov random field (MRF) model specified as

\[ Y(s_i) | y(\mathcal{N}_i) \sim \text{Gaussian} \left( \mu_{1,i}(y(\mathcal{N}_i)), \sigma_i^2 \right) \]

\[ \mu_{1,i}(y(\mathcal{N}_i)) = \alpha(s_i) + \sum_{s_j \in \mathcal{N}_i} \eta_{1,i,j} (y(s_j) - \alpha(s_j)) \] \hspace{1cm} (4.2)

This model implies a joint Gaussian distribution in which the precision matrix is determined by the parameters \( \eta_{1,i,j} \) and \( \sigma_i^2 \). A sparse precision matrix corresponds to relatively small neighborhoods \( \mathcal{N}_i \). A model in a single dimension (e.g., time or a spatial transect) that yields a sparse precision matrix is a first-order autoregressive (AR(1)) model (Cressie and Wikle, 2011, p. 169). Sain et al. (2011) use a Kronecker product of AR(1) precision matrices, one for each spatial dimension, to produce an overall precision matrix for the spatial model. The construction yields a neighborhood structure that includes both first-order neighbors \( (s_j \in \mathcal{N}_{i1}) \) and second-order neighbors \( (s_j \in \mathcal{N}_{i2}) \) in the conditional distributions. The location-specific dependence parameters \( \eta_{1,i,j} \) and conditional variances \( \sigma_i^2 \) are functions of a single autoregressive parameter \( \eta \) and variance \( \sigma^2 \). This variance is interpreted as the MRF conditional variance at one of the four corner sites on the lattice.

For a site not on the edge of the lattice, the conditional variance and dependence parameters are

\[ \sigma_i^2 = \frac{\sigma^2}{(1 + \eta^2)^2}, \] \hspace{1cm} (4.3)

\[ \eta_{1,i,j} = \frac{\eta_1}{1 + \eta_1^2}, \quad s_j \in \mathcal{N}_{i1}, \] \hspace{1cm} (4.4)

\[ \eta_{1,i,j} = -\frac{\eta_1^2}{(1 + \eta_1^2)^2}, \quad s_j \in \mathcal{N}_{i2}, \] \hspace{1cm} (4.5)

and the conditional mean is

\[ \mu_{1,i}(y(\mathcal{N}_i)) = \alpha(s_i) + \sum_{s_j \in \mathcal{N}_{i1}} \frac{\eta_1}{1 + \eta_1^2} [y(s_j) - \alpha(s_j)] - \sum_{s_j \in \mathcal{N}_{i2}} \frac{\eta_1^2}{(1 + \eta_1^2)^2} [y(s_j) - \alpha(s_j)]. \]

The marginal means \( \alpha(s_i) \) are modeled as a linear combination of a small set of
spatial basis functions

\[ \alpha(s_i) = \sum_{k=1}^{K} \beta(r_k)x_k(s_i). \]

The coefficients \( \{\beta(r_k) : k = 1, \ldots, K\} \) are unknown, and the \( x_k \) are spatial basis functions constructed from bisquare functions (Cressie and Johannesson, 2008), with a specified set of knots \( \{r_k : k = 1, \ldots, K\} \),

\[ x_k(s_i) = \begin{cases} 
(1 - \left(\frac{||s_i - r_k||}{d}\right)^2)^2, & ||s_i - r_k|| \leq d \\
0, & \text{otherwise.} 
\end{cases} \]

Figure 4.3 displays the locations of the knots for the \( K = 16 \) basis functions used in this analysis, and Figure 4.4 depicts values of the basis functions \( x_k(s_i) \).

### 4.3.1 Bayesian Analysis

We initially perform a Bayesian analysis of the constant variance model for a NARR water vapor flux field at 00 UTC on 19 July 2010. The summer of 2010 was unusually active with many areas in the Upper Mississippi River basin experiencing near record precipitation (Fenimore et al., 2011). The central United States experienced numerous mesoscale convective systems during this season, with multiple events in July in particular. A Bayesian analysis is employed for inference on the parameters \( (\eta, \sigma^2, \beta = \{\beta(r_k) : k = 1, \ldots, K\}) \). Prior distributions include uniform \((-1, 1)\) for \( \eta \), uniform \((0, 50)\) for \( \sigma = \sqrt{\sigma^2} \) and independent Gaussian \((0, 10^4)\) priors for the coefficients \( \beta(r_k) \). A Metropolis-within-Gibbs MCMC algorithm is utilized for posterior sampling, and the posterior means for each of the parameters are retained for a goodness of fit assessment. With these posterior means available as parameter estimates, the goodness of fit of the Gaussian conditionals model can be assessed using a procedure developed by Kasier et al. (2012). The assessment proceeds by separating observations into sets of non-neighboring locations termed concliques. For the Kronecker product model that results in up to eight neighbors for a location, it is feasible to divide the locations into
Figure 4.3  Spatial basis function knots $r_k$. 
Figure 4.4 Spatial basis functions $x_k(s_i)$ constructed from bisquare functions.
four concliques. Figure 4.5 shows one possible specification of the sets. The conditional distributions within each conclique can be identified using the fitted model parameters and data values in the other concliques. Then, generalized residuals are computed for each location using a probability integral transform. In this case, this is the Gaussian cumulative distribution function. Under the true model, the generalized residuals within a conclique should be uniformly distributed.

![Figure 4.5 Assignment of spatial locations to concliques for construction of generalized residuals.](image)

When this model assessment procedure is applied to water vapor flux divergence fields, a systematic pattern emerges. Figure 4.6 depicts a probability-probability (PP) plot of generalized residuals for one field that is typical of the results seen. The generalized
residuals for all concliques depict distributions that deviate substantially from uniform. This suggests that the assumption of Gaussian conditional distributions with constant conditional variance is not ideal for water vapor flux divergence fields.

Figure 4.6 Generalized residuals constructed from a Gaussian Markov random field model with constant conditional variance fit to the water vapor flux divergence field at 00 UTC 19 July 2010.
4.4 Spatial Model for Conditional Variance

The investigations based on empirical conditional distributions (Figure 4.2) and based on generalized residuals (Figure 4.6) indicate evidence of non-constant variability and heavy tails. Importantly, there is a systematic pattern to the shift in variability. When the neighborhood average is near zero, variability tends to be small and when the neighbors exhibit either strong convergence or strong divergence, variability is higher. There may be several factors contributing to this result. Strong convergence and divergence often both occur along fronts. In addition the magnitude of divergence is generally related to humidity. If more water vapor is available, both strong convergence and divergence are more likely.

The basic Gaussian MRF model should be modified to account for the relationship between the mean and variance. The modified model is termed a spatial conditional variance model, and the modifications are motivated by a few considerations.

1. The systematic change in variability with the large-scale mean should be captured by a small set of population parameters.

2. The model should produce empirical characteristics from simulated data that match observed data more closely than a constant conditional variance model.

3. The model should preserve similar interpretability of the large-scale structure as in the constant variance model.

The spatial conditional variance model specifies a unique conditional variance $\sigma^2(s_i)$ in the data model for each location on the lattice. Before developing the model for the conditional variance, we briefly consider the implications on the data model. The joint distribution for the data $y = \{y(s_i) : i = 1, \ldots, n\}$ for the $n$ locations on the lattice
given the conditional variances is

\[ y|\sigma^2, \eta_1, \alpha \sim \text{MVN}(\alpha, \Sigma), \]

\[
\Sigma = V^{1/2} \left[ \frac{1}{1 - \eta_1^2} R(\eta_1) \right] V^{1/2},
\]

\[ V^{1/2} = \text{diag}(\sigma(s_i)), \]

where \( \sigma^2 = \{\sigma^2(s_i) : i = 1, \ldots, n\} \) and \( \alpha = \{\alpha(s_i) : i = 1, \ldots, n\} \). The interpretation and support for the spatial dependence parameter \( \eta_1 \) remain the same as in the constant conditional variance model. The matrix \( R(\eta_1) \) is a matrix of correlations resulting from the Kronecker product formulation outlined in the previous section. Given the conditional variances, the conditional distributions are Gaussian with conditional means as in (4.2).

The dependence parameters for a location \( s_i \) on the interior of the lattice are

\[
\eta_{1,i,j} = \frac{\eta_1 \sigma(s_i)}{1 + \eta_1^2 \sigma(s_j)}, \quad s_j \in N_{i,1},
\]

\[
\eta_{1,i,j} = -\frac{\eta_1^2 \sigma(s_i)}{[1 + \eta_1^2 \sigma(s_j)]}, \quad s_j \in N_{i,2}.
\]

Given the relationship with the overall mean divergence and the possibility of spatial structure in the variability, a Gaussian MRF model for the logarithm of the conditional variance is

\[
Z(s_i) = \log(\sigma^2(s_i))
\]

\[
Z(s_i)|z(N_i) \sim \text{Gaussian}(\mu_{2,i}(z(N_i)), \delta_i^2),
\]

\[
\mu_{2,i}(z(N_i)) = \nu(s_i) + \sum_{s_j \in N_i} \eta_{2,i,j} (z(s_j) - \nu(s_j)),
\]

\[
\nu(s_i) = \gamma_0 + \gamma_1 [\alpha(s_i)] + \gamma_2 [\alpha(s_i)]^2.
\]

The marginal means \( \nu(s_i) \) for this process are related to the marginal means \( \alpha(s_i) \) for the data model to account for the systematic change in the expected variability with the overall mean divergence. This MRF model uses the same neighborhood structure as the data model in Section 3, with the location-specific \( \eta_{2,i,j} \) and \( \delta_i^2 \) related to a single dependence parameter \( \eta_2 \) and variance parameter \( \delta^2 \) in a similar fashion to (4.3)-(4.5).
The spatial conditional variance model is similar to the spatial stochastic volatility model developed by Yan (2007), who combined conditional autoregressive (CAR) models for the data and conditional variance. Analogs in geostatistical modeling include the spatial Gaussian-log-Gaussian model of Palacios and Steel (2006) and the spatio-temporal extension of Huang et al. (2011). The model used here uses the basis function coefficients $\beta$ in the marginal mean for both components.

4.4.1 Bayesian Analysis

Prior distributions for data model parameters remain the same as the constant variance model. Prior distributions for spatial conditional variance model parameters include uniform ($-1, 1$) for $\eta_2$, uniform $(0, 10)$ for $\delta = \sqrt{\delta^2}$ and independent Gaussian $(0, 10^4)$ priors for $\gamma_0, \gamma_1, \gamma_2$. The MCMC algorithm for the spatial conditional variance model includes sampling of the log conditional variance $z(s_i)$. The MRF specification in the data model and the spatial conditional variance model readily provides full conditional distributions, so the $z(s_i)$ are updated individually in the Gibbs sampler via Metropolis-Hastings steps.

For model assessment, the posterior means of the model parameters $(\eta_1, \eta_2, \delta^2, \beta)$ are retained, along with the posterior means of the conditional variances $\sigma^2(s_i)$. The goodness of fit procedure based on generalized residuals is then applied using these values. Figure 4.7 provides an example of the generalized residuals for the same field depicted in Figure 4.6. The residual pattern is clearly closer to uniform than for the constant variance case. This model modification is a promising alternative for characterizing water vapor flux divergence. In the next section we extend this spatial conditional variance model to a spatio-temporal setting and re-visit model assessment with additional diagnostics.
Figure 4.7 Generalized residuals constructed from a Gaussian Markov random field model with a spatial model for the conditional variance fit to the water vapor flux divergence field at 00 UTC 19 July 2010.
4.5 Spatio-Temporal Model

The spatial conditional variance model developed in the previous section is extended to include the time dimension. The spatio-temporal model will provide inference for the spatially-varying diurnal cycle of water vapor flux divergence while incorporating the local spatial characteristics identified previously. The data model assumes the same structure as the spatial conditional variance model, with the data \( Y(s_i, t) \), log conditional variances \( Z(s_i, t) \) and marginal mean processes \( \alpha(s_i, t) \) and \( \nu(s_i, t) \) now indexed in both space and time. Several of the parameters for these processes remain fixed, including spatial dependence parameters \( \eta_1 \) and \( \eta_2 \), variance parameter \( \delta^2 \) and spatial conditional variance coefficients \( \gamma = (\gamma_0, \gamma_1, \gamma_2) \).

The same set of spatial basis functions \( \{ x_k(s_i) : k = 1, \ldots, K \} \) is used, with the coefficients \( \beta(r_k, t) \) now allowed to vary in space and time as random variables. The time-varying behavior of the marginal mean process is captured through a temporal structure on the basis function coefficients. Spatial dependence among coefficients for the same time point is captured with a (third) Gaussian MRF model.

\[
\beta(r_k, t) | \beta_k(N_k) \sim \text{Gaussian} \left( \mu_{k,t}(\beta_k(N_k)), \psi_k^2 \right),
\]

\[
\mu_{k,t}(\beta_k(N_k)) = \zeta(r_k, t) + \sum_{\ell \in N_k} \omega_{k,\ell} (\beta(r_\ell, t) - \zeta(r_\ell, t)),
\]

\[
\zeta(r_k, t) = \theta_{0,k} + \theta_{1,k} \cos \left( \frac{2 \pi h(t)}{24} \right) + \theta_{2,k} \sin \left( \frac{2 \pi h(t)}{24} \right),
\]

where \( h(t) \) is the hour of the day. The spatial dependence parameters follow a similar structure to that above, being a function of a single dependence parameter \( \omega \) and the location in the lattice. Each basis function has a unique conditional variance \( \psi_k^2 \), to allow for potential regional differences in intraseasonal variability. With the layout of basis functions in Figure 4.4, this lattice is 4 × 4 in size. The Fourier coefficients \( \theta = \{ \theta_{0,k}, \theta_{1,k}, \theta_{2,k} : k = 1, \ldots, K \} \) capture the climatological diurnal cycle.

The overall spatio-temporal model is depicted graphically in Figure 4.8. Three MRF
models characterize the spatial component, with the data model for $Y(s_i, t)$ and the spatial conditional variance model for $Z(s_i, t)$ defined at the observation lattice locations. For the water vapor flux examples used here, this lattice is $33 \times 33$ cells in size. The marginal mean model for $\beta(r_k, t)$ is defined on the lattice of 16 knots ($4 \times 4$) for the spatial basis functions. The temporal structure is incorporated into the spatially-varying diurnal cycle for $\beta(r_k, t)$ via the parameters $\theta$.

Figure 4.8  Graphical depiction of the hierarchical model for water vapor flux divergence for an arbitrary point in time. Symbols enclosed with single circles represent random variables, and symbols enclosed with two circles represent fixed quantities or quantities that are deterministic functions of random variables. Shaded quantities are observed or known. Arrows represent functional dependence, with the arrow pointing toward the dependent quantity. The upper panel depicts quantities defined on the $4 \times 4$ lattice of basis function knots $r_k$. The lower panel depicts quantities defined on the $33 \times 33$ data model lattice, with locations indexed by $s_i$. 
4.5.1 Bayesian Analysis

The prior distributions used in a Bayesian analysis of the spatial conditional variance model are listed in Table 4.1. The spatial dependence parameters $\eta_1$, $\eta_2$ and $\omega$ are assigned uniform priors on (-1,1). Each of these parameters can be interpreted as the correlation between a pair of first-order neighbors for their respective processes. Fixed conditional standard deviations $\delta$ and $\psi_k$ are assigned proper uniform priors based on the results of Gelman (2006), who found posterior inference to be less sensitive using this specification as opposed to a conjugate inverse gamma prior, when implemented in hierarchical models with multiple variance components. The uniform limits for these priors are chosen to be somewhat conservative, with the upper uniform limit being an order of magnitude larger than the range of the observed data. MRF marginal mean parameters, $\gamma$ and $\theta$, are similar to regression coefficients and are assigned multivariate Gaussian priors with large variances.

Table 4.1 Prior distributions for the spatial conditional variance model parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Prior</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta_1$</td>
<td>Uniform(-1, 1)</td>
</tr>
<tr>
<td>$\eta_2$</td>
<td>Uniform(-1, 1)</td>
</tr>
<tr>
<td>$\delta = \sqrt{\delta^2}$</td>
<td>Uniform(0, 100)</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>Gaussian(0, $10^4$)</td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>Gaussian(0, $10^4$)</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>Gaussian(0, $10^4$)</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Uniform(-1, 1)</td>
</tr>
<tr>
<td>$\psi_k = \sqrt{\psi_k^2}$</td>
<td>Uniform(0, 50)</td>
</tr>
<tr>
<td>$\theta_0(r_k)$</td>
<td>Gaussian(0, $10^4$)</td>
</tr>
<tr>
<td>$\theta_1(r_k)$</td>
<td>Gaussian(0, $10^4$)</td>
</tr>
<tr>
<td>$\theta_2(r_k)$</td>
<td>Gaussian(0, $10^4$)</td>
</tr>
</tbody>
</table>

A Gibbs sampler is used to sample from the posterior distribution. The algorithm includes updates for the unknown random variables $\beta_t = \{\beta(r_k, t) : k = 1, \ldots, K\}$ and log conditional variances $z_t = \{z(s_i, t) : i = 1, \ldots, n\}$. For reference, we include some brief notes on individual steps of the overall algorithm.
• The steps for MRF marginal mean parameters $\gamma$ and $\theta$ involve conjugate multivariate Gaussian updates.

• The marginal mean MRF variances $\psi_k^2$ and dependence parameter $\omega$ are updated jointly with a Metropolis-Hastings step.

• The spatial conditional variance MRF variance $\delta^2$ and dependence parameter $\eta_2$ are updated jointly with a Metropolis-Hastings step.

• The data model MRF dependence parameter $\eta_1$ is updated with a Metropolis-Hastings step.

• The basis function coefficients $\beta_i$ at a given time are updated jointly, i.e. a single update for each time. Although the conditional posterior involves only multivariate Gaussian densities, the spatial conditional variance model is nonlinear (quadratic) in $\beta(r_k, t)$, so a conjugate form is not available and a Metropolis-Hastings step is used.

• The log conditional variances $z(s_i, t)$ are updated individually via Metropolis-Hastings updates. The MRF structures for the spatial conditional variance and data models facilitate the formulation of the individual conditional posteriors.

All Metropolis-Hastings updates use a random walk approach for the proposal distribution, and standard deviations for the proposal distributions are tuned during the MCMC burn-in to obtain reasonable acceptance rates between 20 and 40 percent (Gelman et al., 2004). The multivariate updates for $\beta_i$ require an additional correlation or covariance matrix for the proposal distribution. The covariance matrix that results from maximum likelihood estimation for a single field (e.g. Section 3) provides a reasonable depiction of the dependence among the basis coefficients and leads to adequate posterior sampling. Cressie (1993) provides the form for the MLE of marginal mean parameters such as $\beta$ in a Gaussian MRF. The Metropolis-Hastings tuning for the log conditional
variances tracks selected locations, and we find that three unique proposal standard deviations; representing corner, edge and interior sites; are sufficient for the algorithm. That is, the optimal spread of the proposal distribution depends on the number of neighbors.

The MCMC algorithm outlined above was applied to the dataset of 248 water vapor flux divergence fields (eight fields per day) during the month of July 2010. Four independent Markov chains were implemented, each initiated from dispersed starting values. Metropolis-Hastings scaling parameters were adapted periodically during burn-in, and convergence was diagnosed graphically with trace plots for all model parameters as well as $\beta(r_k, t)$ and $z(s_i, t)$ at selected spatial locations and points in time. Following burn-in, each chain was run for 50,000 iterations with every 10th iteration saved as output for subsequent inference. Computation of derived quantities and posterior predictive samples was performed offline after completion of the main MCMC procedure. For comparison, Bayesian analysis was also performed for a model with a constant data model variance $\sigma^2$. The MRF models for the basis function coefficients $\beta(r_k, t)$ and data $y(s_i, t)$ otherwise remained the same, but the MRF model for $z(s_i, t)$ was eliminated.

Posterior summaries for model parameters that do not vary spatially are provided in Table 4.2 for the constant variance and spatial conditional variance models. The data model spatial dependence parameter $\eta_1$ has a posterior mean of 0.4437 in the constant variance model and 0.4148 in the spatial conditional variance model. In the Kronecker product spatial dependence structure used in both models, this dependence parameter is the correlation between first-order neighbors. Thus the posterior distribution suggests moderately strong positive spatial dependence in both models. The spatial conditional variance model favors slightly smaller spatial dependence, which may be a result of more spatial structure being captured through the spatial process for the conditional variance.

The posterior mean for the conditional variance process dependence parameter $\eta_2$ is 0.9035, an indication of strong spatial dependence in the conditional variance process. This strong spatial dependence suggests that locations with high variability in water
vapor flux divergence are often located close to other locations with high variability. Put another way, locations with divergence that deviate substantially from their mean likely have neighbors with similarly large deviations from their means, regardless of direction. This behavior is consistent with strong convergence occurring not far from strong divergence, which can occur near fronts and mesoscale boundaries during summer in the central United States.

The quadratic relationship between the data model marginal mean $\alpha(s_i, t)$ and the conditional variance model marginal mean $\nu(s_i, t)$ is characterized on the log scale by the coefficients $\gamma_0, \gamma_1, \gamma_2$, which have posterior means of -0.505, -0.079, and 0.157 respectively. The intercept suggests conditional variances would be likely smaller than the constant variance model (posterior mean 1.311) when the mean divergence is zero. This result complements the positive value for $\gamma_2$, which indicates that the expected conditional variance increases as the square of the mean divergence increases. This quadratic relationship captures the systematic change in variability with the large-scale mean, the first modeling objective outlined at the beginning of this section.

The process model for the basis function coefficients $\beta(r_k, t)$ is also a Gaussian MRF model with a single dependence parameter $\omega$. The posterior distributions for both the constant variance and spatial conditional variance models provide evidence that $\omega$ is negative and smaller in magnitude than the other dependence parameters. The negative dependence may result from negative correlations at larger (mesoscale) distances and from the fact that the basis functions $x_k(s_i)$ overlap at many locations to ensure a smooth marginal mean. This overlap can introduce competitive dependence in estimation of the coefficients.

The conditional variances $\psi_k^2$ for the basis function coefficients vary spatially, with a unique value for each of the $K = 16$ basis functions. These parameters capture the hour-to-hour mesoscale variability in water vapor flux divergence. This is variability at a larger scale than the data model, which captures local fluctuations. The posterior distributions
Table 4.2  Posterior means with 95% credible intervals for Bayesian analysis of two spatio-temporal models for July 2010 water vapor flux divergence.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Constant Conditional Variance</th>
<th>Spatial Conditional Variance</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta_1$</td>
<td>0.4437 (0.4414, 0.4461)</td>
<td>0.4148 (0.4121, 0.4175)</td>
</tr>
<tr>
<td>$\sigma^2$</td>
<td>1.311 (1.304, 1.318)</td>
<td></td>
</tr>
<tr>
<td>$\eta_2$</td>
<td>0.9035 (0.9006, 0.9064)</td>
<td>0.9035 (0.9006, 0.9064)</td>
</tr>
<tr>
<td>$\delta^2$</td>
<td>0.0274 (0.0261, 0.0288)</td>
<td>0.0274 (0.0261, 0.0288)</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>-0.505 (-0.551, -0.458)</td>
<td>-0.505 (-0.551, -0.458)</td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>-0.079 (-0.123, -0.037)</td>
<td>-0.079 (-0.123, -0.037)</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>0.157 (0.117, 0.202)</td>
<td>0.157 (0.117, 0.202)</td>
</tr>
<tr>
<td>$\omega$</td>
<td>-0.350 (-0.386, -0.310)</td>
<td>-0.277 (-0.314, -0.240)</td>
</tr>
</tbody>
</table>

for $\psi^2_k$ are displayed in Figure 4.9. It is initially evident that the distributions are different across the region. The posterior distributions are concentrated on relatively small values for basis functions 1-5, which are centered over the Gulf coast states. Areas farther north and east favor larger values of $\psi^2_k$, indicating more hourly variability in July 2010.

The other noticeable feature of Figure 4.9 is the stark contrast between the posterior distributions for the two models for some components, especially $k = 11$ (eastern Iowa). This result is another indication that variability is partitioned differently in the two models. The spatial variance model allows the local variability to increase when mean convergence is strong, as it often was in the Upper Mississippi River basin during the summer of 2010. In addition the model allows spatial structure in this local variability. On the other hand, the constant variance model lacks these features and “compensates” with larger variability in the basis function coefficients in those areas. This distinction between the two models has important implications for inference on the diurnal cycle parameters $\theta$. The posterior variability for these parameters is related to the basis coefficient conditional variance $\psi^2_k$, so the diurnal cycle is estimated more precisely in the spatial conditional variance model than in the constant conditional variance model. Although this posterior precision comparison is not shown, further inference for the diurnal cycle is discussed below.
Figure 4.9 Comparison of posterior distributions for basis coefficient conditional variances $\psi^2$ under the constant variance and spatial variance models. Points depict the mean and error bars enclose the central 95% of the posterior distribution.
4.5.2 Diurnal Cycle

Capturing the spatially-varying diurnal cycle is one modeling objective for this study. The spatio-temporal model incorporates a mean diurnal cycle $\zeta(r_k, t)$ for the basis function coefficients $\beta(r_k, t)$ through the parameters $\theta(r_k, t)$. Since some characteristics of the data model are conditioned on the basis function coefficients, this diurnal cycle induces a diurnal cycle for characteristics of the data model and the conditional variance model, most notably in the expected marginal means of these Gaussian MRF models. The expected marginal mean for the data model is a useful illustration of the spatially-varying diurnal cycle. Formally this local diurnal cycle is

$$E(\alpha(s_i, t)) = \sum_{k=1}^{K} \zeta(r_k, t)x_k(s_i).$$

The local diurnal cycle $E(\alpha(s_i, t))$ is a spatio-temporal process and can be illustrated in a number distinct ways (Cressie and Wikle, 2011). In dynamic meteorology the governing equations, including the water vapor budget, are formulated to give the time evolution of the state variables, which are functions of spatial location. This formulation motivates illustrating the diurnal cycle as a temporally-varying spatial process. Figure 4.10 depicts this view of the posterior mean of the local diurnal cycle for the spatial conditional variance model. The eight panels provide the posterior mean field for the times of day when NARR data are available. This view reveals the complex structure of the diurnal cycle during July 2010. Parts of Missouri and Illinois have posterior mean convergence at all times, with the strongest from 06-09 UTC. Moving farther northwest, eastern Nebraska, western Iowa and western Minnesota see a peak in divergence from 00-06 UTC and transition to mean convergence by 12 UTC. South Dakota and western Nebraska see peak convergence from 00-06 UTC and transition to divergence from 15-21 UTC.

The perspective provided by Figure 4.10 reveals rich information about the regional variation of the diurnal cycle, but it is difficult to highlight local characteristics and to
Figure 4.10  Posterior mean of local marginal expectations for July 2010. The local marginal expectation is defined as \( E(\alpha(s_i, t)) = \sum_{k=1}^{K} \mu(r_k, t)x_k(s_i) \). The contour interval is 0.1 mm hr\(^{-1}\) and negative values are shaded. Separate panels depict different hours of the day (UTC).
summarize the uncertainty in the estimates. These properties can be captured by an alternative perspective on the spatio-temporal process, as a spatially-varying temporal process. This view, illustrated in Figure 4.11, arises from considering a time series at a specific location with the understanding that the local time series characteristics change across space. Figure 4.11 provides the posterior mean and 95% credible intervals for the local diurnal cycle at the locations of the basis function knots, $s_i = r_k$, for the spatial conditional variance model applied to the July 2010 data. This view reinforces some of the behaviors noted previously, including the consistent mean convergence in Missouri (basis function $k = 7$) and the overnight transition in western Iowa (basis function $k = 10$). This view highlights broad differences in the amplitude and phase of the diurnal cycle, and the west-to-east phase transition from the southern Great Plains to the southeast is evident.

The visualization approaches used in Figures 4.10 and 4.11 provide complementary inference about the spatially-varying diurnal cycle of water vapor flux divergence. The temporally-varying spatial perspective of Figure 4.10 easily illustrates the spatial extent and locations of transitions in the diurnal evolution and gives a comprehensive spatial perspective that is not feasible otherwise. On the other hand, the spatially-varying temporal perspective of Figure 4.11 provides detailed quantitative information at an individual locations and offers an opportunity to illustrate the uncertainty associated with the estimated diurnal cycle.

4.5.3 Posterior Predictive Assessment

The goodness of fit assessment based on the generalized spatial residuals of Kasier et al. (2012) was illustrated in previous sections for both a constant variance model and the spatial conditional variance model. Here we turn to posterior predictive assessment to investigate the characteristics of the empirical conditional distributions the conditional variance model produces and how they relate to those from the observed data. The
Figure 4.11 Posterior distribution of diurnal cycle at basis function knot locations \( s_i = r_k \) for July 2010. Solid lines depict the posterior means and shaded regions provide 95% credible intervals for the local diurnal cycle given by

\[
E(\alpha(s_i, t)) = \sum_{k=1}^{K} \zeta(r_k, t)x_k(s_i).
\]
spatio-temporal model and time sequence of water vapor flux divergence fields are well-suited for diagnosing the systematic change in variability observed in Figure 4.2. This pattern emerges over time as the variability associated with passing weather systems provides a wide range of observed water vapor flux divergence.

For posterior predictive assessment, we return to the neighbor averages $\bar{y}_N(s_i, t)$ constructed for the exploratory analysis in Section 4.2.2. With MCMC samples available from the posterior distribution of the model parameters, posterior predictive realizations for the three MRF components $\beta^*$, $z^*$, and $y^*$ can be sampled sequentially and the resulting posterior predictive sample $y^*$ is stored for each MCMC iteration. Since this posterior predictive distribution is of high dimension, a smaller set of summary statistics are typically computed and their posterior distributions examined (Gelman et al., 1996). The posterior predictive distributions are then compared to the same summary statistics computed from the observed data. The summary statistics are defined below for the observed data $y$, but the same procedure is used for any posterior predictive realization $y^*$. Our procedure follows the exploratory analysis by grouping locations into one of $P = 9$ bins according to the average of first-order neighbors $\bar{y}_N(s_i, t)$. Let $a_p$ and $b_p$ be the lower and upper bounds of values contained in each bin. The lower bounds are $a_1 = -2.5, a_2 = -1.5, \ldots, a_P = 1.5$ and the upper bounds are $b_1 = -1.5, b_2 = -1.0, \ldots b_P = 2.5$. Then define $m_p$ as the number of observations contained in each bin

$$m_p = \sum_{t=1}^{T} \sum_{i=1}^{n} I [a_p < \bar{y}_N(s_i, t) \leq b_p]$$

Our posterior predictive assessment will focus on the empirical moments of the distribution of values within each of the $P$ bins. The bin means should change systematically due to the positive spatial dependence present in the data. The bin variances should also change systematically, with large variance for the first and last bins and small variances for the center bins. The bin skewness may also change systematically across bins. Finally, excess kurtosis should be generally positive, reflecting the heavy-tailed behavior.
of the empirical conditional distributions. Palacios and Steel (2006) note that kurtosis can be large in their scale mixture of Gaussian processes model for spatial heteroscedasticity. For reference, a Gaussian distribution has zero excess kurtosis. Specifically these empirical moments are

- **Mean**
  \[ T_{1,p} = \frac{1}{m_p} \sum_{t=1}^{T} \sum_{i=1}^{n} I(a_p < \bar{y}_N(s_i, t) \leq b_p) y(s_i, t) \]

- **Variance**
  \[ T_{2,p} = \frac{1}{m_p - 1} \sum_{t=1}^{T} \sum_{i=1}^{n} I(a_p < \bar{y}_N(s_i, t) \leq b_p) [y(s_i, t) - T_{1,p}]^2 \]

- **Skewness**
  \[ T_{3,p} = \frac{1}{m_p - 1 [T_{2,p}]^{3/2}} \sum_{t=1}^{T} \sum_{i=1}^{n} I(a_p < \bar{y}_N(s_i, t) \leq b_p) [y(s_i, t) - T_{1,p}]^3 \]

- **Excess Kurtosis**
  \[ T_{4,p} = \left[ \frac{1}{m_p - 1 [T_{2,p}]^2} \sum_{t=1}^{T} \sum_{i=1}^{n} I(a_p < \bar{y}_N(s_i, t) \leq b_p) [y(s_i, t) - T_{1,p}]^4 \right] - 3 \]

The posterior predictive assessment was implemented for both the spatial conditional variance model and the constant variance model. In the latter case, the posterior samples of \( \sigma^2 \) used in place of simulation of realizations of \( z^* \). Figures 4.12-4.15 summarize the posterior predictive distributions of empirical conditional moments \( T_{1,p}, T_{2,p}, T_{3,p}, T_{4,p} \) computed after binning observations according to their neighbor averages \( \bar{y}_N(s_i, t) \). In each case the horizontal axis is ordered by bin from strong convergence to strong divergence from left to right. The summary statistic for the observed data from July 2010 is also displayed for reference. The posterior predictive distributions for the conditional mean \( T_{1,p} \) (Figure 4.12) are similar between the two models and generally comparable to the observations and exhibit the general pattern of positive spatial dependence.
Contrasts between the two models emerge when examining the posterior predictive distribution of the empirical conditional variance $T_{2,p}$ (Figure 4.13). The constant variance model performs as advertised, exhibiting a nearly constant value across all conditioning bins, with modest increases in the most extreme bins. The spatial variance model shows changes in variability across the spectrum. For the center bins with generally weak divergence or convergence, the spatial variance model captures the relatively small variability well. The change in variability in the spatial variance model does not “ramp up” in the same way as the observed values, and both models under-represent the observed variability in the most extreme bins.

Important aspects of the shape of the empirical conditional distributions are revealed through the skewness $T_{3,p}$ (Figure 4.14) and excess kurtosis $T_{4,p}$ (Figure 4.15). The conditional distributions shift from left-skewed in the presence of strong convergence to symmetric to right-skewed under strong divergence. The spatial variance model produces this behavior in a noticeable way. As speculated in the exploratory analysis, the observed empirical conditional distributions have heavy tails, yielding positive excess kurtosis. The spatial conditional variance model produces this characteristic in a similar fashion, but the constant variance model has exclusively Gaussian tail characteristics. This heavy-tailed behavior is noted by Palacios and Steel (2006) in scale mixtures of spatial Gaussian processes.

Overall the spatial variance model meets the modeling objective of producing empirical characteristics consistent with the observed data. This is particularly true for the skewness and kurtosis of the empirical conditional distributions and for the general pattern in the variance. The magnitude of the ramp-up in empirical conditional variance does not match the observations.
Figure 4.12  Comparison of posterior predictive distributions of empirical conditional means under the constant variance and spatial variance models. Points depict the mean and error bars enclose the center 95% of the posterior predictive distribution.
Figure 4.13  Comparison of posterior predictive distributions of empirical conditional variances under the constant variance and spatial variance models. Points depict the mean and error bars enclose the center 95% of the posterior predictive distribution.
Figure 4.14 Comparison of posterior predictive distributions of empirical conditional skewness under the constant variance and spatial variance models. Points depict the mean and error bars enclose the center 95% of the posterior predictive distribution.
Figure 4.15  Comparison of posterior predictive distributions of empirical conditional excess kurtosis under the constant variance and spatial variance models. Points depict the mean and error bars enclose the center 95% of the posterior predictive distribution.
4.6 Discussion

The hydrological cycle of the central United States is a highly dynamic system, and a spectrum of processes contribute to its variability in space and time. These include the day-to-day passage of weather systems and their interaction with the day-night cycle of the low-level circulation. This study has developed a spatio-temporal model for the water vapor flux divergence to provide a simplified stochastic representation of these different sources of variability. The components of the statistical model include a spatially-varying climatological diurnal cycle and random mesoscale basis function coefficients that define a smooth mean divergence field. The data model incorporates spatial dependence at the observation level along with a spatially-structured random process for the data-level variability.

Bayesian analysis reveals evidence of moderate positive spatial dependence for the data model, which was anticipated from exploratory analysis of empirical conditional distributions. An intriguing result from the posterior inference was that the spatial dependence in the conditional variance model was very strong. This indicates that observations that have large deviations from their mean tend to be located near observations with similarly large deviations, regardless of sign. This is physically plausible, since small concentrations of strong divergence and convergence can occur close together in the presence of fronts and mesoscale boundaries. An extension to this work would be the development of posterior predictive diagnostics that characterize the spatial dependence in variability, which would aid the understanding of the realization of this strong dependence in data.

The posterior predictive assessment based on empirical conditional moments identified key distinctions between the constant variance model and the spatial conditional variance model. The spatial conditional variance model captures a systematic change in the local variability based on the neighbors’ average divergence, yielding small variability
when neighboring values are near zero and large variability in the presence of strong divergence or convergence. However, the conditional variance model does have some room for improvement on this metric, which could be addressed with a more flexible function than the quadratic polynomial used in the marginal mean process for the conditional variance MRF model. The spatial conditional variance model also depicts changes in conditional skewness seen in the observed data and peaks up on the consistently large excess kurtosis present in the empirical conditional distributions.

The spatial conditional variance model provides adequate precision to estimate a spatially-varying diurnal cycle in water vapor flux divergence. Changes in the overall mean, amplitude and phase are evident in analysis of data from July 2010, a particularly wet and active period in the Upper Mississippi River basin. The spatio-temporal model could be applied to a drought period to identify important differences in model parameters during two hydrological extremes. This could also be extended to a more comprehensive analysis that includes interannual variability. The spatio-temporal model is general enough that it could be applied to gridded regional climate model (RCM) output and provide additional insight for hydrological processes in RCMs, complementing work on the RCM water vapor budget (Anderson et al., 2003) and precipitation extremes (Cooley and Sain, 2010).

Another key extension to the spatio-temporal model for water vapor flux divergence would be a multivariate model that includes other constituents of the water vapor budget, especially precipitation. For processes like mesoscale convective systems, water vapor flux divergence and precipitation are strongly coupled, and a statistical model that captures this multivariate relationship that may have have interesting lags in time would have broad utility. The application to climate models would be useful in this case as modeled precipitation is the result of a combination of grid-scale and parameterized processes, whereas divergence would be strongly (but not entirely) governed by grid-scale dynamics. This study has underscored the importance of non-constant variability in statistical
modeling of the hydrological cycle and should be a key consideration moving forward.

Acknowledgments

NARR data was accessed from the NOAA/ESRL Physical Science Division, Boulder Colorado from their Web site at http://www.esrl.noaa.gov/psd/. MERRA data was accessed from the NASA Goddard Earth Sciences Data and Information Services Center.
References


CHAPTER 5. GENERAL CONCLUSION

5.1 Summary

This dissertation has implemented a variety of mathematical models to aid the understanding of key modes of variation in the climate system, particularly the diurnal cycle and the year-to-year variability. These models, like most used in atmospheric science, utilize some combination of physical and statistical modeling. Physical models rely on the governing equations of fluid dynamics and often involve numerical integration of discretized versions of the governing equations. Climate dynamics investigates the distribution of states induced by the underlying physical models. Statistical models abstract weather events by associating them with random variables with specified probability distributions. The model parameters characterize the atmospheric processes of interest.

Chapter 2 adopted a statistical model to characterize the diurnal cycle of relative humidity. A regional diurnal cycle was captured in the model’s large-scale structure through Fourier coefficients. Additionally, these large-scale coefficients followed a dynamic stochastic process in time, yielding a temporally-varying temporal process for the large-scale mean. A more complex version of the model also revealed that the small-scale variability has a diurnal cycle as well, whereas small-scale spatial dependence remains constant in time. The paper utilized Bayesian inference in a spatio-temporal model and developed posterior predictive diagnostics to assess the model’s capability in producing local conditional distributions with characteristics like the observed data.

Chapter 3 used a physically-based model to investigate the roles of the zonal wind
and diabatic heating in producing variability in winter stationary waves over the North Atlantic Ocean. The model utilized a general circulation model (GCM) dynamical core linearized about a basic state with a steady forcing, producing a linear system to be solved for a perturbation about the basic state. The simplified dynamics provided computational efficiency and the opportunity to test specific forcing hypotheses. A model experiment revealed that stationary wave responses were sensitive to both the horizontal and vertical extent of diabatic heating. In addition modified basic state zonal winds produced a stronger west-east contrast in the North Atlantic response. The versatility of the linear model allowed further demonstration of the propagation of uncertainty in the diabatic heating distribution to the stationary wave response.

Chapter 4 implemented a spatio-temporal statistical model that was motivated by the water vapor budget, a succinct physical model of the conservation of water vapor in the atmosphere. The statistical model focused on water vapor flux divergence, which quantifies transport of water vapor within the atmosphere. Diagnostics of an initial spatial model revealed evidence of heavy-tailed behavior in empirical conditional distributions, and a model with random conditional variance demonstrated improved model representation of this observed behavior. The spatio-temporal version of the model included a spatially-varying diurnal cycle that quantified the nighttime maximum in convergence of water vapor flux over portions of the central United States.

5.2 Future Research

The three papers presented in Chapters 2-4 of this dissertation have outlined some possible extensions to the application of the models developed in each case. Extensions to the dynamic model for the diurnal cycle include a spatially-varying large-scale structure with dynamic evolution and additional diagnostics for the correlation structure in local conditional distributions. The NAO stationary wave response in coupled GCM
simulations should be investigated, and the roles of additional sources of uncertainty in diabatic heating is possible with a linear model. Statistical modeling of the hydrological cycle can be extended by combining the model for water vapor flux divergence with approaches previously developed for precipitation, providing a quantitative link between these two important variables.

In a broader context, the opportunities for methodological development along the spectrum of physical-statistical models in atmospheric science are numerous. The hierarchical statistical modeling framework allows a mathematically convenient distinction between data models and process models, linked through conditional probability. In this context the methodological development of process models is continuing to evolve and encompasses a range from actual discretized partial differential equations to complex spatio-temporal models. Development of statistical approximations to the PDE-implied dynamics is important in both the time and space dimensions. In addition it would be valuable to investigate the uncertainty introduced in using different choices of process models, involving a range of physical and statistical approaches.

This dissertation also emphasized the use of diagnostic tools, particularly to assess a model’s ability to produce characteristics present in observations. Since both physical (e.g. GCMs) and statistical models generate data, these diagnostic approaches are appropriate along the modeling spectrum. When Bayesian inference is implemented, posterior predictive assessment is a natural option. However, the choice of diagnostic is not straightforward in a complex model. Several diagnostics have been implemented in this dissertation, and each has addressed a specific aspect of the model in question. Development of additional diagnostics for spatio-temporal statistical models would be essential for evaluating further model characteristics, such as the temporal correlation structure or the spatially-varying mean structure. A tailor-made diagnostic is ideal for any proposed model, but the development of a general suite of posterior predictive diagnostics for spatio-temporal models could offer widespread value.