

RESEARCH ARTICLE

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Modeling maximum daily temperature using a varying coefficient regression model

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Key Points:

- The relationship between water and air temperatures varies dynamically
- A varying coefficient model is developed to model the dynamical relationship
- Prediction with the model is better than commonly applied models

Supporting Information:

- Auxiliary Material FS01–03
- Readme
- Auxiliary Material TS01

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Abstract Relationships between stream water and air temperatures are often modeled using linear or nonlinear regression methods. Despite a strong relationship between water and air temperatures and a variety of models that are effective for data summarized on a weekly basis, such models did not yield consistently good predictions for summaries such as daily maximum temperature. A good predictive model for daily maximum temperature is required because daily maximum temperature is an important measure for predicting survival of temperature sensitive fish. To appropriately model the strong relationship between water and air temperatures at a daily time step, it is important to incorporate information related to the time of the year into the modeling. In this work, a time-varying coefficient model is used to study the relationship between air temperature and water temperature. The time-varying coefficient model enables dynamic modeling of the relationship, and can be used to understand how the air-water temperature relationship varies over time. The proposed model is applied to 10 streams in Maryland, West Virginia, Virginia, North Carolina, and Georgia using daily maximum temperatures. It provides a better fit and better predictions than those produced by a simple linear regression model or a nonlinear logistic model.

1. Introduction

Water temperature is a critical component of hydrologic systems [Keleher and Rahel, 1996; Caissie, 2006] and may be a determining factor in water quality and biological condition. Fish and other aquatic organisms are sensitive to extremes in temperature, as extremes affect the food sources, and the survival and distribution of organisms. Brook trout, for example, prefer cooler water found in high elevation streams, and temperatures greater than 21°C are viewed as highly stressful to the health of trout [Meisner, 1990; Beitinger et al., 2000]. Growth, reproduction, migration, and food availability are all affected by water temperature (see Caissie [2006] for a review). Factors critical to the health of aquatic systems, such as dissolved oxygen, are also dependent on temperature. Warm water tends to hold less dissolved oxygen than cold water, and dissolved oxygen levels tend to be lower in the warmer months than the cooler ones. Effects of temperature change therefore can lead to significant biological effects as more oxygen is required by fish and other organisms in summer months. Stefan et al. [2001], for example, predicts that increases in water temperature will result in increases in summer-time killing of fish in lakes. Flebbe et al. [2006] indicates that changes in temperature will result in dramatic changes in the habitat for brook trout (see also Keleher and Rahel [1996]; Minns et al. [1995]).

Models describing the change in water temperature associated with changes in air temperature are therefore critical in determining the effects of temperature change on aquatic systems, especially under climate change. Various models have been proposed to predict water temperature using air temperature data at different time scales, and the choice of a model depends on the availability of information on factors affecting water temperature, the purpose of the study, temporal and spatial aspects of the data, as well as the time step and duration of measurement [Mohseni et al., 1998; Caissie, 2006; Mayer, 2012].

Water temperature is affected by a number of physical and environmental factors [Webb, 1996], including weather conditions, flow, shading, depth, and topography [Chen et al., 1998; St-Hilaire et al., 2000]. Physical models that consider the heat transfer between the water and the surroundings environment tend to be rich in independent variables that are included in the model, have a range of time steps, and are detailed in terms of how factors influence water temperature [Sinokrot and Stefan, 1993]. The data required to

implement a full deterministic model are not always available, i.e., it is difficult to measure all factors over a reasonable time frame and incorporate them into the model through an estimation procedure.

Statistical models have been used to study the air and water temperature relationship [Benyahya *et al.*, 2007], and tend to work well for weekly mean temperature. Among different statistical methods, parametric regression models such as the linear regression model are easily implemented; all the inference tools are established and simple. Another advantage of parametric regression models is the interpretability. Parameters in the model have meaningful interpretation. Neumann *et al.* [2003], for example, developed a linear regression method to model daily maximum stream temperature in terms of maximum air temperature and other related predictors for the Truckee River in California and Nevada. The majority of the statistical models focus on weekly or greater time steps. This is partly a result of the data collection process and validity of the model. Caissie [2006] pointed out that linear regression models were more valid at weekly or monthly scales than at a daily scale. At these scales, autocorrelation tends to be less than that at a daily scale and the normality assumption is reasonable when average temperature is used. A characteristic of the water-air temperature relationship in streams that affects model choice is that water temperature often remains relatively constant when the air temperature is below 0°C. In this case, the simple parametric linear regression model might not be a good model, as the relationship becomes nonlinear. To address this weakness, nonlinear parametric models might be more applicable.

The most commonly used nonlinear parametric regression model for the air-water temperature relationship is the logistic model [Mohseni *et al.*, 1998]. The model describes the relationship between air and water temperatures as

$$W = \mu + \frac{\alpha - \mu}{1 + e^{\gamma(\beta - A)}}, \quad (1)$$

where W is the measured stream temperature, A is the measured air temperature, and α , β , γ , and μ are parameters. Compared to the linear regression model, the logistic model provides a good explanation of the flat patterns in water temperature for low (<0°C) and sometimes for high (>20°C) air temperature. The nonlinear relationship is appropriate because water temperature is less sensitive to air temperature in the cold seasons (air temperature less than 0°C) due to flow and the potential for freezing. In the warm seasons (air temperature greater than 20°C), as air temperature increases, the increase in water temperature may be small due to the high rate of evaporative cooling. As the S-shaped logistic function flattens at both ends of the range of air temperature, the logistic model easily accommodates these phenomena. A physical interpretation was also given in Mohseni and Stefan [1999]. Several recent studies have used the logistic model for modeling streams [Webb *et al.*, 2003; Mayer, 2012]. There are two potential problems that limit the use of the logistic model, especially, at the daily time scale. First, in some situations, daily water and air temperatures have high variability at certain temperatures, and this results in poor prediction (despite reasonably high goodness of fit statistics). If this variability is associated with seasonality, the standard logistic model would not address this, resulting in greater variance and weaker predictive ability. This is described as hysteresis (stream temperature being different for the same air temperature at different times of the year) in Mohseni *et al.* [1998]. Second, daily water temperatures are likely to have high autocorrelation over time. The autocorrelation affects inference and confidence in parameter estimates. This dependence across time is not taken into account by the standard logistic model, hence the variance estimates, prediction, and hypothesis testing might not be accurate at a daily time scale.

Compared to the parametric model, nonparametric regression models often provide good prediction of water temperature. The nonparametric models usually have simple assumptions and therefore are widely applicable in different situations. Modern approaches to handle temporal correlation are possible and the nonparametric models can effectively improve the prediction accuracy [Chenard and Caissie, 2008]. An example of a nonparametric model is the k -nearest neighbor method which was used to predict and forecast water temperature [Benyahya *et al.*, 2008; St-Hilaire *et al.*, 2012]. One drawback of such nonparametric models is the difficulty in interpreting the parameters in the model.

Time series models and models based on stochastic processes were designed to focus on the stochastic components of the data as well as the deterministic component [Caissie *et al.*, 1998; Cluis, 1972; Kothandaraman, 1971, 1972; Stefan and Preud'homme, 1993]. Most of the stochastic models use a daily time step and

model variation in relationships over time. Time series models might be useful for forecasting future observations and with rich data might result in accurate predictions [Cho and Lee, 2012]. One drawback of time series models is that they might not directly model the relationship between air temperature and water temperature and hence parameters in the model would not be helpful in determining the strength of the relationship and the sensitivity of water temperature to air temperature. For example, Ahmadi-Nedushan *et al.* [2007] added lagged air temperature residuals to their model of water temperature rather than actual air temperature. Cho and Lee [2012] linked air and water temperature by assuming that the ratio and/or difference of the harmonic coefficients between the air and water temperatures remained constant.

The focus of this work is to develop models relating daily maximum air and water temperatures. Daily maximum temperature was selected over weekly averages as the variable of interest because the maximum water temperature has been linked to loss of brook trout, a temperature sensitive species [Trumbo *et al.*, 2010]. This work is part of a larger study whose goal is to identify streams in southeastern United States that are likely to lose trout due to increased temperature. Hence, measuring and visualizing sensitivity of water temperature to changes in air temperature is an important goal. In this work, we propose the use of a time-varying coefficient model (VCM) to study the relationship between daily water temperature and daily air temperature (see Fan and Zhang [2008] for an overview of the VCM). The VCM is an effective tool for exploring the dynamic feature of the data and has been widely applied in different areas such as ecology [Ferguson *et al.*, 2007, 2009] and medicine [Cheng *et al.*, 2009]. The key idea of the VCM is to use a parametric model but with time-varying coefficients. The parametric property of the VCM provides meaningful interpretation of the sensitivity of stream water temperature to changes in air temperature, aids in understanding how sensitivity varies over time, and provides a way to compare sensitivity across streams.

The varying coefficient model is a useful model in situations where there is a significant amount of variability in water temperature that is not accounted for by air temperature but might be related to unmeasured factors that vary over time. For example, the natural cycle of temperature suggests that the water temperature in streams will be different for the same value of air temperature at different times of the year. Thus, an air temperature of 10°C might be associated with a different water temperature in the spring than in the fall. In this situation, both the linear regression and the nonlinear logistic regression might result in reasonable model fit statistics but may not provide accurate prediction of water temperature based on air temperature as these models overlook the time (seasonal) information in the data. For similar air temperatures at different times of the year, daily water temperature varies considerably but the resulting predictions of water temperature would be almost constant. The proposed VCM surmounts this difficulty by taking the time information into account and modeling the temporally dynamic pattern of the air-water temperature relationship through varying coefficients. Therefore, it can achieve more accurate predictions when the same air temperature occurs at different times of the year. Moreover, the proposed modeling strategy better explains the sensitivity of water temperature to the air temperature across time, providing a more comprehensive understanding of the air-water relationship in different time periods. Modeling the relationship with additional terms other than time-varying coefficients (e.g., seasonal terms) is possible but might be complicated, especially when using the logistic model, and requires choices about the number of seasonality terms to add to the model and the period associated with seasonality.

In this paper, we apply the VCM to daily maximum temperature data from 10 native brook trout streams in southeast United States and show that the VCM has predictions that are superior to the logistic or linear models. In addition, the VCM can be used to interpret the air and water temperature relationship over time.

2. Study Area and Data

As part of a study on water temperature and brook trout, paired (air and water) thermographs (HOBO Watertemp Pro v2; accuracy 0.2°C; drift < 0.1 annually) [Onset Computer Corporation, 2009] were placed at the pour point of randomly selected stream catchments in southeast USA. (The pour point or outlet of the watershed is the point in the watershed that all water flows through.) The stream catchments were selected from a statistical population of over 1000 catchments known to support brook trout. A stratified approach was used based on information on area of the catchment, elevation, forest cover, and solar radiation. Additional details on site characteristics, study design, and sampling were given in Trumbo *et al.* [2010]. All

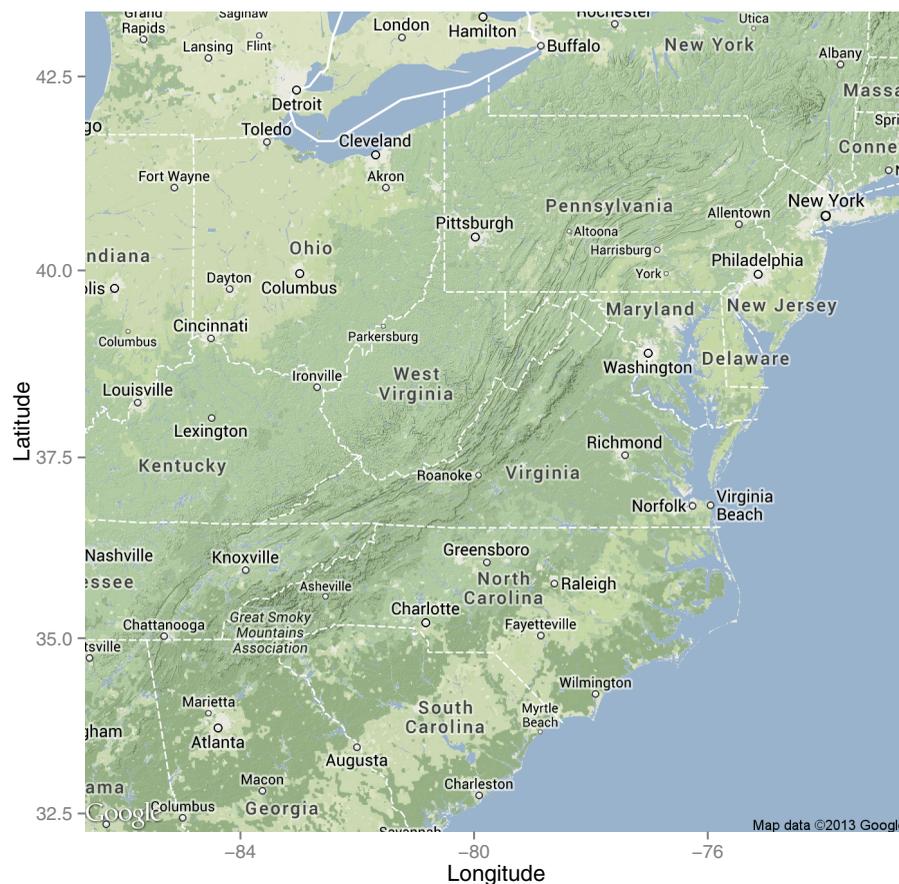


Figure 1. Location of 10 streams (black dots are the locations). From north to south, the site IDs are: Site 5, Site 6, Site 10, Site 9, Site 2, Site 1, Site 8, Site 7, Site 4, and Site 3.

thermographs were set to record every 30 min [Dunham *et al.*, 2005; Huff *et al.*, 2005] for one year starting in December 2010.

Thermographs were calibrated before and after deployment following methods summarized in Dunham *et al.* [2005]. Because stream channels may become dry during summer low flow periods, thermographs used to record water temperatures were placed near the deepest location in the stream segment when possible [Lisle, 1987]. A shield was used to reduce direct solar radiation heating on air temperature thermographs [Dunham *et al.*, 2005; Trumbo *et al.*, 2012].

We screened the raw air and water temperature series to identify outliers and other oddities resulting from thermograph malfunctions, launch/recording interval errors, or potentially dry stream beds. Preliminary analyses were also conducted to ensure data quality. Scatterplots of water and air temperatures were drawn to evaluate the joint relationship and to look for irregularities in the daily maximum air and water temperature. Index plots of lagged one-day differences were also used to identify oddities (rapid change) in temperature and potentially dry streams. For this work, 10 streams located in the states of Maryland, West Virginia, Virginia, North Carolina, and Georgia were used, and their locations are shown in Figure 1. For each site, we extracted one complete year of data with the same starting date (14 December 2010) and ending date (14 December 2011). To summarize the daily data, daily maximum values were used. The data that were input into the models consisted of 366 paired daily maximum air and water temperatures for each site.

3. Varying Coefficient Model

Let W_t be the maximum water temperature and Z_t be the maximum air temperature in day t , $t = 1, 2, \dots, T$ and $T = 366$ is the total number of days in the data set. Without loss of the generality, we use centered air

temperature, i.e., $A_t = Z_t - \bar{Z}$, where $\bar{Z} = \frac{1}{T} \sum_{t=1}^T Z_t$. We consider the following varying coefficient model for the air-water temperature relationship as

$$W_t = \theta_0(t) + A_t \theta_1(t) + \epsilon_t, \tag{2}$$

where $\theta_0(t)$ and $\theta_1(t)$ are varying intercept and slope coefficients and ϵ_t is the error term in the model. Exploratory analysis using lag-1 autocorrelation of residuals and the Shapiro-Wilk test [Kutner et al., 2004] indicated that the error terms were neither normally distributed nor independent. Levene's test [Kutner et al., 2004] indicated that the assumption of constant variance in the error terms was reasonable. Based on these analyses, we assume $E(\epsilon_t) = 0$ and $\text{var}(\epsilon_t) = \sigma^2$. Note that the proposed model has a similar format as the linear regression model $W_t = \theta_0 + A_t \theta_1 + \epsilon_t$. These varying coefficients can be interpreted as the dynamic feature of the air-water temperature relationship. That is, at different times and seasons, water temperature and sensitivity of water temperature to changes in air temperature can be different. This allows for a seasonal effect on the air-water temperature relationship. The full VCM is thus useful for following changes in the maximum water temperature over time (through the intercept) and for measuring the local sensitivity of the relationship (through the slope). Variants of the varying coefficient model can accommodate flexibility in model interpretation. For instance, one can consider a semivarying coefficient model, which has the following form

$$W_t = \theta_0 + A_t \theta_1(t) + \epsilon_t. \tag{3}$$

In model (3), the intercept θ_0 is a fixed parameter. Hereafter, we call model (2) the full VCM and model (3) the semi-VCM. The fixed intercept θ_0 in model (3) represents the average maximum water temperature for the whole period. The varying slope $\theta_1(t)$ in model (3) represents variation in slope relative to the simple linear regression. The time-varying slope provides information about the degree of deviation from a common slope. Also the times when the variation is the greatest may be relevant. Therefore, depending on the objective, one can choose either the full VCM or the semi-VCM to describe the local or global behavior of the water temperature, given the air temperature. For presentation convenience, the full VCM will be used to illustrate the details of the proposed methodology; the equations can be easily adapted to the semi-VCM.

3.1. Estimation of Coefficients

Two popular methods for estimating the varying coefficients $\theta_0(t)$ and $\theta_1(t)$ are kernel-local polynomial smoothing and smoothing spline methods [Fan and Zhang, 2008]. In this work, we adopt the penalized spline regression method as it has parsimonious parameter expression with easy interpretation [Ruppert et al., 2003]. Specifically, the penalized spline approach assumes the varying coefficients have the form

$$\theta_0(t) = \sum_{i=1}^K \alpha_i b_i(t), \tag{4}$$

$$\theta_1(t) = \sum_{i=1}^K \beta_i b_i(t), \tag{5}$$

where $\{b_1(t), \dots, b_K(t)\}$ is the set of basis functions and α_i and $\beta_i, i = 1, 2, \dots, K$ are parameters. K is the number of basis functions for each varying coefficient.

The key is to estimate the coefficients α_i and β_i such that the estimates make the series of varying coefficients $\theta_0(t)$ and $\theta_1(t)$ smooth. To achieve this purpose, we use least squares with a penalty to encourage smoothness [Hoover et al., 1998]. Specifically, we obtain the estimates by minimizing

$$\sum_{t=1}^T (W_t - \theta_0(t) - A_t \theta_1(t))^2 + \lambda \left(\int \theta_0''(t)^2 dt + \int \theta_1''(t)^2 dt \right), \tag{6}$$

where $\theta_0(t)$ and $\theta_1(t)$ were given in (4) and (5) and λ is a tuning parameter for controlling the smoothness of varying coefficients. Given the observed data, we can write the vector of water temperatures

as $\mathbf{W}=(W_1, \dots, W_T)'$ and the vector of air temperature as $\mathbf{A}=(A_1, \dots, A_T)'$. Denote $\mathbf{X}=(\mathbf{b}_1, \dots, \mathbf{b}_K, \mathbf{b}_1 \circ \mathbf{A}, \dots, \mathbf{b}_K \circ \mathbf{A})_{T \times (2K)}$, where $\mathbf{b}_i=(b_i(1), \dots, b_i(T))', i=1, \dots, T$, and \circ is the Schur product. It is easy to obtain the estimated parameter set, given λ , as

$$(\hat{\alpha}_1, \dots, \hat{\alpha}_K, \hat{\beta}_1, \dots, \hat{\beta}_K)' = (\mathbf{X}'\mathbf{X} + \lambda\mathbf{D})^{-1}\mathbf{X}'\mathbf{W}, \tag{7}$$

where \mathbf{D} is a $2K$ by $2K$ diagonal penalty matrix with diagonal elements either 0 or 1. Consequently, the estimates of the varying coefficients are $\hat{\theta}_0(t) = \sum_{i=1}^K \hat{\alpha}_i b_i(t)$ and $\hat{\theta}_1(t) = \sum_{i=1}^K \hat{\beta}_i b_i(t)$.

3.2. Tuning Parameter Selection

Note that there is a tuning parameter λ that controls the smoothness of the varying coefficients and influences the model fit. To select an optimal tuning parameter λ , one commonly used approach is leave-one-out cross-validation (LOOCV) suggested by Hoover et al. [1998]. Let $\hat{\theta}_0^{(-i)}(t)$ and $\hat{\theta}_1^{(-i)}(t)$ be the varying coefficients estimated by minimizing (6) by using data with the i th observation deleted. The LOOCV (λ) is defined as

$$LOOCV(\lambda) = \sum_{i=1}^T (W_i - \hat{\theta}_0^{(-i)}(i) - A_i \hat{\theta}_1^{(-i)}(i))^2. \tag{8}$$

One can choose the optimal tuning parameter λ_{LOOCV} as the value minimizing $LOOCV(\lambda)$. However, there are $T = 366$ data points for each site, and implementing such a method can be computationally expensive. To circumvent this difficulty, we adopt the generalized cross-validation method (GCV) [Wahba, 1990] to approximate the leave-one-out cross-validation method. Here the $GCV(\lambda)$ is defined as

$$GCV(\lambda) = (\hat{\mathbf{W}} - \mathbf{W})'(\hat{\mathbf{W}} - \mathbf{W}) / (1 - \text{tr}(\mathbf{S}_\lambda) / T), \tag{9}$$

where $\mathbf{S}_\lambda = \mathbf{X}(\mathbf{X}'\mathbf{X} + \lambda\mathbf{D})^{-1}\mathbf{X}'$ is the so-called hat matrix, $\hat{W}_t = \hat{\theta}_0(t) + A_t \hat{\theta}_1(t)$ is the fitted water temperature based on the proposed model using the entire data set and $\hat{\mathbf{W}} = (\hat{W}_1, \dots, \hat{W}_T)'$. Then the optimal tuning parameter λ_{GCV} is the one minimizing $GCV(\lambda)$. The GCV often gives a very reasonable approximation to the LOOCV and can effectively reduce the computational time [Ruppert et al., 2003].

3.3. Model Assessment: Fitting and Inference

To evaluate the goodness of fit for the proposed VCMs, the Nash-Sutcliffe coefficient (NSC) [Nash and Sutcliffe, 1970] is used as a performance measure

$$NSC = 1 - \frac{\sum_{t=1}^T (W_t - \hat{W}_t)^2}{\sum_{t=1}^T (W_t - \bar{W})^2}, \tag{10}$$

where $\bar{W} = \frac{1}{T} \sum_{t=1}^T W_t$. In the linear regression model, the NSC is equivalent to the coefficient of determination, i.e., R^2 [Rencher and Schaalje, 2008]. To compare the fit of different models, we define the relative NSC (RelNSC) using the linear regression model as the baseline, i.e.,

$$\text{RelNSC} = \frac{NSC - NSC_0}{NSC_0} \times 100\%, \tag{11}$$

where NSC_0 is the NSC of the linear regression model. A higher RelNSC means a better fit. Note that the RelNSC of the linear regression model is 0%. Here we remark that for fitting the nonlinear logistic model, we followed the two-step iterative estimation method used in Mohseni et al. [1998]: iterate the step of estimating α and μ by least squares and the step of estimating β and γ by Newton's method.

Although the VCM has a varying coefficient form, inference and testing for VCM is straightforward by using parameter estimation in (7). Similar to routine regression modeling, one can take advantage of model nesting to evaluate model fit. That is, one can conduct a statistical hypothesis test to check whether the VCM is

significant relative to the linear regression model or some other reduced model. Under such a consideration, the null hypothesis is that none of the coefficients are time varying, i.e.,

$$H_0 : \theta_0(t) = \theta_0 \text{ and } \theta_1(t) = \theta_1 \tag{12}$$

versus the alternative that at least one of the coefficients is not constant. Suppose the two models under the null and the alternative hypothesis are M_0 and M_1 , respectively

$$M_0 : W_t = \theta_0 + \theta_1 A_t + \epsilon_t, \tag{13}$$

$$M_1 : W_t = \theta_0(t) + \theta_1(t) A_t + \epsilon_t. \tag{14}$$

Because of autocorrelation and lack of normality, a standard F test is not appropriate. To test the difference between the two models, we apply a block bootstrap goodness of fit test based on the comparison of sum of the squared residuals for the varying coefficient model [Huang et al., 2002]. Note that there is no assumption of a specific distribution for ϵ_t in (2), hence bootstrap-based testing should be more robust and reliable. Suppose $\hat{\theta}_0$ and $\hat{\theta}_1$ are parameter estimates for the model M_0 , and $\hat{\theta}_0(t)$ and $\hat{\theta}_1(t)$ are parameter estimates for the model M_1 . We then can calculate the residual sum of squares for each model, respectively

$$RSS_0 = \sum_{t=1}^T (W_t - \hat{\theta}_0 - \hat{\theta}_1 A_t)^2, \tag{15}$$

$$RSS_1 = \sum_{t=1}^T (W_t - \hat{\theta}_0(t) - \hat{\theta}_1(t) A_t)^2. \tag{16}$$

Using RSS_0 and RSS_1 , we can define the test statistic $G = \frac{(RSS_0 - RSS_1)/(2K - 2)}{RSS_1/(T - 2K)}$, which is the standard F test statistic under the assumption that the error term ϵ_t 's are independent and identically normally distributed [Rencher and Schaalje, 2008]. A large value of the test statistic implies a significant difference between the two models. To assess the level of significance accurately, we adopt the block bootstrap method to compute the critical value [Huang et al., 2002]. Because water temperatures and residuals are highly autocorrelated through time, the ordinary bootstrap is not appropriate and the block bootstrap [Kunsch, 1989] is therefore more appropriate. The proposed bootstrap testing procedure is summarized as follows:

1. Calculate $G = \frac{(RSS_0 - RSS_1)/(2K - 2)}{RSS_1/(T - 2K)}$ using the original data.
2. Let

$$\hat{\epsilon}_t = W_t - \hat{\theta}_0(t) - \hat{\theta}_1(t) A_t$$

be the residual under the alternative hypothesis. Split the sample $\{\hat{\epsilon}_1, \dots, \hat{\epsilon}_T\}$ into $T - m + 1$ overlapping blocks of length m : observation 1 to m will be block 1, observation 2 to $m + 1$ will be block 2, and so on. Resample T/m blocks with replacement from the $T - m + 1$ blocks. Aligning these T/m blocks in the order they were selected will give the new sample: $\{\hat{\epsilon}_1^*, \dots, \hat{\epsilon}_T^*\}$. Note that the last block has extra points when T/m is not integer.

3. Let

$$W_t^* = \hat{\theta}_0 + \hat{\theta}_1 A_t + \hat{\epsilon}_t^*$$

be the pseudoresponses under the null hypothesis.

4. Repeat steps 2 and 3 B times to obtain B bootstrap samples.

5. From each bootstrap sample, calculate $G^b = \frac{(RSS_0^b - RSS_1^b)/(2K - 2)}{RSS_1^b/(T - 2K)}$, $b = 1, 2, \dots, B$. Reject H_0 if the value of statistic G is greater than or equal to the $\{100(1 - \alpha)\}$ percentile of G^b , where α is the significance level.

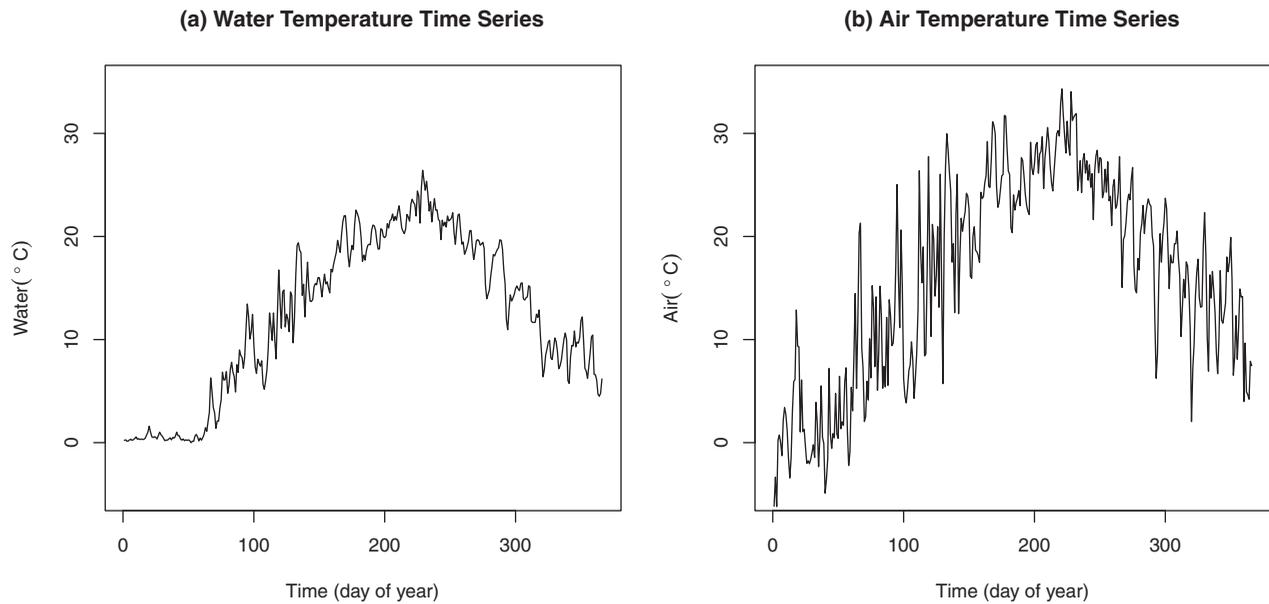


Figure 2. Plots of water and air temperatures for Site 5.

3.4. Model Assessment: Prediction

To evaluate the prediction performance of the VCM compared to the parametric models, for the data $\mathcal{X} = \{(A_t, W_t) : t = 1, \dots, T\}$ ($T = 366$) from each site, we randomly partition two-thirds of the data as the training set and the remaining as the test set. For each model compared, we calculate the root mean squared errors (RMSE) of the test set using the model estimated by the training set, which is defined as

$$RMSE = \sqrt{\frac{1}{|\mathcal{Y}| - df} \sum_{t \in \mathcal{Y}} (W_t - \hat{W}_t)^2}, \quad (17)$$

where \mathcal{Y} is the test set and $|\mathcal{Y}|$ is the number of the observations in set \mathcal{Y} . In equation (17), df is the degree of freedom in the model, where df is 14 for full VCM (there are seven bases for each of the two varying coefficients), 8 for semi-VCM (since the intercept is fixed and there are seven bases for slope), 4 for the logistic model, and 2 for the linear regression model.

4. Results

In this section, we fitted both the full VCM and semi-VCM to the data from 10 sites, respectively. The proposed methods were compared to the linear regression model and the nonlinear logistic model. The merits of the proposed VCM method will be examined through fit statistics, prediction, and interpretation of the relationship between water and air temperature. In this work, all the analyses were implemented by R software (version 2.15.3) [Hornik, 2013].

Figure 2 illustrates the data from Site 5. In Figure 2, we can see that although water and air temperature follow a similar pattern, the variation of water and air temperatures is large in spring and fall. Therefore, the prediction of the water temperature may be inaccurate if one ignores the temporal information in the model.

4.1. Basis Selection and Fitting

For fitting the data using the proposed VCM method, we need to choose the form of basis functions in (4) and (5). We considered three different polynomial bases as the candidates: linear, quadratic, and cubic splines [Ruppert et al., 2003]. Analysis of the data using these three bases resulted in similar curves for the estimated varying coefficients and also similar prediction performance. In this work, we chose to use

Table 1. Model Assessment Results: Fit Statistics and Hypothesis Tests^a

Site	Logistic ReINSC (%)	Semi-VCM ReINSC (%)	Full VCM ReINSC (%)	Semi-VCM <i>p</i> Value	Full VCM <i>p</i> Value
5	1	5	14	<0.001	<0.001
6	2	7	15	<0.001	<0.001
10	0	3	7	<0.001	<0.001
9	0	7	13	<0.001	<0.001
2	0	2	11	<0.001	<0.001
1	0	3	9	<0.001	<0.001
8	2	7	15	<0.001	<0.001
7	1	6	14	<0.001	<0.001
4	0	5	26	<0.001	<0.001
3	2	10	21	<0.001	<0.001

^aThe columns 2, 3 and 4 show the values of ReINSC fitted by using the three models (nonlinear logistic model, semi-VCM, and full VCM). The last two columns show *p* values from hypothesis testing of semi-VCM and full VCM versus a linear regression model.

quadratic splines because they resulted in smoother coefficient curves than linear splines, and had fewer parameters compared with cubic splines. Specifically, the bases we used are

$$\{1, t, t^2, (t - \zeta_1)_+^2, \dots, (t - \zeta_N)_+^2\},$$

where $\zeta_1, \zeta_2, \dots, \zeta_N$ are *N* knots and $(t - \zeta_n)_+, n = 1, 2, \dots, N$ are the splines with $(t - \zeta_n)_+ = t - \zeta_n$ if $t \geq \zeta_n$ and $(t - \zeta_n)_+ = 0$ if $t < \zeta_n$.

To select the number of knots, we fixed *N* = 4 which corresponds to four seasons. The location of the knots are evenly distributed in time, i.e., $(\zeta_1, \zeta_2, \zeta_3, \zeta_4) = (74, 147, 220, 293)$. Here numbers represent the day of the year, starting from 14 December 2010, i.e., 14 December 2010 = 1. We also estimated the proposed model and conducted prediction by using *N* = 12. It provided similar results to those using *N* = 4. Note that choosing a relatively small number of knots reduces the number of parameters in the model and reduces the curvature of the coefficient curves.

The columns 2, 3 and 4 of Table 1 show the ReINSC values for the full VCM, the semi-VCM, and the nonlinear logistic model for the 10 sites. Comparing the results with the nonlinear logistic model, both full VCM and semi-VCM have larger ReINSC values since they dynamically quantify the relationship between water and air temperatures. Moreover, the full VCM fits the data better than the semi-VCM. Note that the use of a varying intercept could further adjust the mean water temperature at each time point. Therefore, the full VCM better captures the variance of water temperature leading to higher ReINSC values.

As the proposed VCM method gives high ReINSC values, it is also important to check whether the VCM is overfitting. We applied the goodness of fit test procedure described in section 3.3 to the full VCM and semi-VCM for the 10 sites. The testing results show that both the full VCM and the semi-VCM are significantly different from the linear regression model (see the last two columns of Table 1 for *p* values) and the full VCM is significantly different from the semi-VCM (with *p* value less than 0.001 for all 10 sites) at the level $\alpha = 0.05$ for each site. Such a finding implies that the time information in the VCM is important in explaining the variation in the data.

4.2. Prediction

Both full VCM and semi-VCM have more accurate predictions compared to the linear regression model and the nonlinear logistic model. In section 3.4, we introduced a procedure for prediction validation. We repeated this procedure 250 times for each site and reported the mean and the standard deviation of predicted RMSE for the 10 sites in Table 2. Figure 3 shows boxplots for RMSEs for different models based on 250 data partition for Site 1. (Boxplots for other sites could be found in supporting materials.) From the results in Table 2 and Figure 3, the values of RMSE for the VCM methods are smaller than those for the linear regression model and the nonlinear logistic model. The full VCM also has more accurate predictions than the semi-VCM. The lower RMSEs indicate that the prediction accuracy of the VCM is improved through the ability to incorporate the seasonal trend of the water temperature. An interesting observation is that, for Site 9, the prediction of the linear regression model is slightly better than the nonlinear logistic model. An

Table 2. Predicted RMSE for 10 Sites for VCM, Logistic Model, and Linear Regression Model^a

Site	Linear	Logistic	Semi-VCM	Full VCM
1	3.24 (0.19)	3.16 (0.18)	2.83 (0.17)	1.49 (0.10)
2	2.57 (0.13)	2.43 (0.13)	2.05 (0.11)	1.01 (0.06)
3	1.66 (0.08)	1.66 (0.09)	1.44 (0.09)	1.08 (0.08)
4	1.92 (0.09)	1.90 (0.10)	1.50 (0.09)	1.09 (0.08)
5	2.68 (0.19)	2.64 (0.18)	2.46 (0.18)	1.23 (0.07)
6	2.55 (0.14)	2.52 (0.14)	2.14 (0.15)	1.04 (0.06)
7	2.85 (0.16)	2.66 (0.15)	2.19 (0.14)	0.94 (0.06)
8	2.55 (0.13)	2.44 (0.13)	2.07 (0.12)	1.11 (0.06)
9	2.71 (0.16)	2.73 (0.16)	2.44 (0.16)	0.94 (0.05)
10	3.52 (0.18)	3.37 (0.19)	2.77 (0.18)	1.23 (0.07)

^aThe mean and (standard deviation) are based on 250 different test sets for each site.

explanation is that the air temperature is not below zero for a long enough period so the logistic model does not describe the relationship as well as a linear regression.

The inaccurate predictions for the linear regression model and the logistic model could be partly explained by the large variability in water temperature with respect to fixed values of air temperature. For elaboration, we extracted 20 data points with air temperature around 20°C from the data for Site 3. Figure 4a shows the corresponding water temperatures. Clearly, there is a large variation in the water temperature with values varying from 7°C to 20°C (the circles in Figure 4a). As shown in Figures 4c and 4d, both the linear regression model and the logistic model predict the water temperature to be around 13°C. The two models ignore the time information in the data. They predict the water temperature by only using air temperature information and hence predict an almost constant value for water temperature. Taking the time information into account, the full VCM gives much more accurate predictions even at a fixed air temperature level. Figure 4b shows that the predictions given by the full VCM are very close to the true values of water temperature. Thus, although the NSC is high for the linear regression model and the logistic model, the prediction error could be large due to the ignoring of temporal information. The maximum prediction error across the 10 sites for the linear regression model and the logistic model is around 7°C. For the full VCM, it is reduced to 3°C.

4.3. Model Interpretation

The proposed VCM method not only provides accurate predictions, but also gives meaningful interpretations. In the full VCM, the varying intercept term, $\theta_0(t)$, represents the mean water temperature at time t , and the varying slope term, $\theta_1(t)$, represents the local sensitivity of water temperature to changes in air temperature at time t .

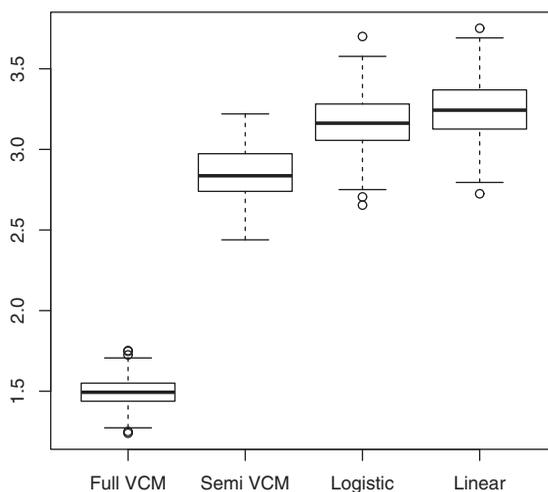


Figure 3. Boxplots of RMSEs for 250 random training and testing samples for four models for Site 1.

To elucidate, we reanalyzed the data of Site 5 for further illustration. First, we divided the data set into 12 disjoint subsets; each subset consists of about 30 data points from 30 consecutive days in a month or so. Then we analyzed these 12 monthly data sets using the linear regression model. Figure 5 shows the estimated intercept and slope for the 12 models for Site 5. The 12 intercepts and slopes were plotted at the last time point for each of the 12 subsets and were connected by straight lines to have a piecewise form. In addition, Figure 5 shows the coefficients for the full VCM, semi-VCM, and the linear regression model. For the varying intercept and the varying slope in the full VCM, we can see that the coefficients are very close to

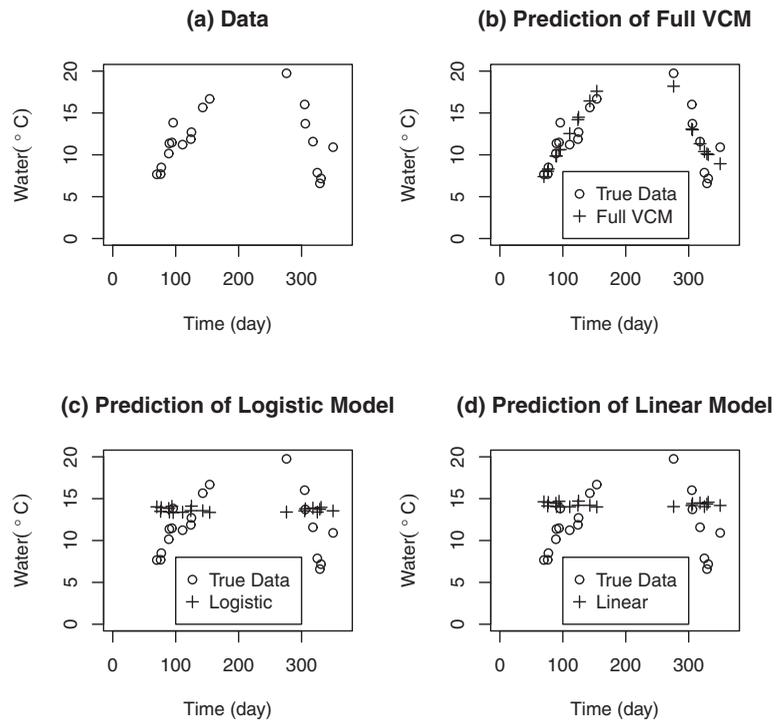


Figure 4. Prediction comparison of full VCM with linear regression model and logistic model for selected points where the air temperature is fixed around 20°C.

those in the 12 month piecewise linear regression. It shows that the full VCM can describe the local dynamic relationship between water temperature and air temperature. Therefore, the full VCM is particularly useful if one wants to study or predict water temperature in any particular season or time period over the year.

By incorporating the time information into the model, the full VCM is also able to automatically investigate hysteresis in stream water temperatures. One common cause of seasonal hysteresis is the influx of cold rain or snow melt in the spring, which results in spring water temperatures being lower than fall water

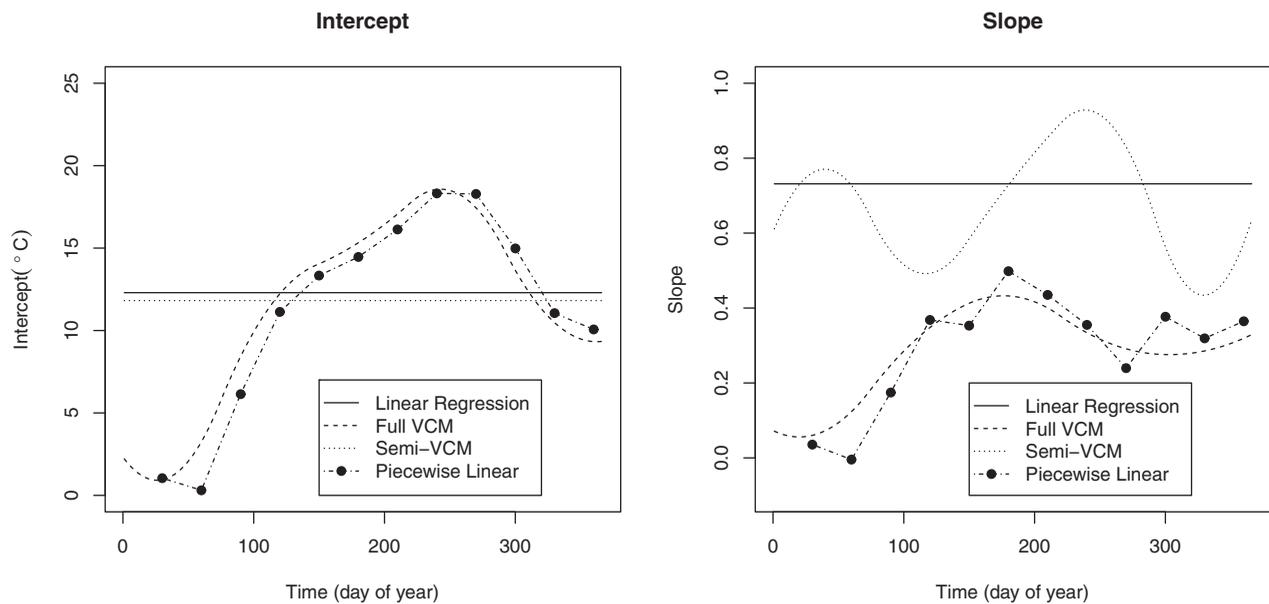


Figure 5. The intercept and the slope plot for different models for Site 5.

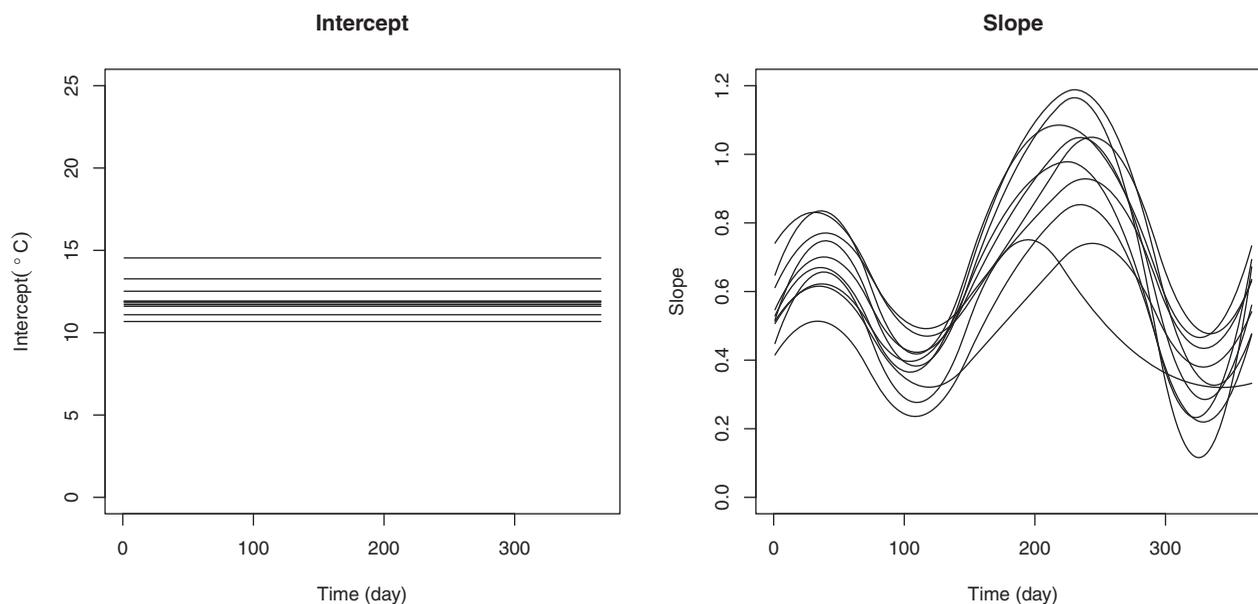


Figure 6. The intercept and the slope plot in semi-VCM for all the 10 sites.

temperatures at the same air temperature [Webb and Nobilis, 1997]. As shown in Figure 5, the estimated varying intercept in the full VCM is larger in fall than that in spring. It indicates that the mean maximum water temperature in fall is higher than the mean maximum water temperature in spring. Therefore, the full VCM gives clear evidence for the presence of hysteresis at Site 5.

For the semi-VCM, the intercept θ_0 represents a global mean daily maximum water temperature and the varying slope $\theta_1(t)$ tends to measure the ratio of the water temperature to air temperature given the mean maximum water temperature for the whole year. In Figure 5, the intercept of the semi-VCM is very close to the intercept of the linear regression model, which is the mean maximum water temperature for the year for the centered data. Because semi-VCM uses a global intercept, its slope coefficient varies around the linear regression slope. Thus the semi-VCM provides information about the global sensitivity of water temperature to changes in air temperature and how it varies over time.

To further demonstrate the properties of the semi-VCM, Figure 6 plots the intercepts and varying slopes of the semi-VCM for the 10 sites. It is clear that the values of 10 intercepts are all between 10 and 15°C. The slopes for the 10 sites tend to have a consistent pattern with a decline in spring and fall. The increased variability in air temperature results in a smaller slope in these periods. The range (the difference between the maximum and the minimum) of the slope in the semi-VCM relates to the variance of water temperature, and the location of maxima and the minima of the slope relates to the variance of the air temperature at different time points. So, by studying the slope curves in Figure 6, we obtain information about the similarity and variance in the water and air temperature relationship for all 10 sites.

The full VCM captures the relationship on a level that is more local in time than the semi-VCM. Because of the shorter focus, the slopes tend to be smaller and smoother as there is less change in temperature over shorter time periods. As indicated in Figure 5, the majority of the variability is associated with the change in the intercept of the full VCM. This is also the reason for the improved fit of the full VCM for the data sets. Therefore, we suggest using the semi-VCM when the air and water variations are small and consider using the full VCM when the air and water variations are large.

5. Discussion

The development and evaluation of the VCM require some choices which are discussed further below. These include the selection of the number of knots, selection of smoothing parameter, and the evaluation

of the VCM relative to the logistic model. The advantages of VCM and future work are also included in this section.

5.1. Smoothing Parameter Selection

In section 3.2, we introduced LOOCV and GCV as methods to select optimal smoothing parameter λ . There are other criteria that might be used, such as maximum likelihood (ML), restricted maximum likelihood (REML), and Mallows's C_p statistic [Ruppert *et al.*, 2003]. ML and REML are likelihood-based approaches and are not appropriate for the case here because the VCM in this work does not rely on an assumed distribution. GCV is approximately equal to C_p and does not require a prior estimate of the variance of the error term [Ruppert *et al.*, 2003]. Therefore, we chose GCV as the criterion for smoothing parameter selection.

5.2. Knot Selection

Besides the tuning parameter λ in (6), the number of knots also affects the smoothness of the varying coefficient curves. What is more, the number of knots determines the number of parameters in the VCM. In section 4.1, we fixed the number of knots at $N = 4$ because it provides both smooth varying coefficient curves and high NSC statistics. Two commonly used criteria for model selection are the Akaike Information Criteria (AIC) and Mallows's C_p [Ruppert *et al.*, 2003]. The AIC is a likelihood-based criterion and is not appropriate here. An approach based on a statistic such as C_p could be used as we focus more on smoothness of the coefficient curves and NSC as criteria for model selection. As part of a sensitivity analysis, we compared fits using $N = 3$ and $N = 5$ knots as well as different degrees of polynomials for the spline models and chose to use $N = 4$ knots with quadratic splines as these choices resulted in smooth curves, parsimony, and good cross-validation statistics.

5.3. Hypothesis Testing

In this work, we developed a block bootstrap hypothesis testing procedure for examining the VCM relative to the linear regression model. However, we have not constructed a testing procedure to compare the VCM with the nonlinear logistic model. Note that the logistic model is not a nested model of VCM. The usual hypothesis testing approaches, such as those based on the F-test [Rencher and Schaalje, 2008], might not be applicable. To evaluate the effect of using the VCM when the underlying model is the logistic model, we conducted a simulation study. Specifically, using air temperatures from Site 5, water temperatures are simulated based on the logistic function ($\mu=0$, $\alpha=29.2$, $\beta=12.9$, $\gamma=0.21$) with standard normal errors. Because water temperature could not be below zero, negative values in the simulated data are truncated to be zero for water temperature. We generated 1000 simulation data sets and applied the two models to each data set. The average NSC from the nonlinear logistic model was 0.97 and the average NSC from full VCM was 0.95. The results show that the VCM is comparable to the logistic model even when the true model is the nonlinear logistic model.

5.4. Advantages of VCM Over Linear Model

It is worthwhile to note that for some sites, the linear regression model could fit the data quite well (for example, NSC statistics for site 6 was 0.91). Even so, the proposed VCM method still has several merits compared with the linear regression model. First, the linear regression model is a special, degenerate case of the VCM. One could apply the goodness of fit test in section 3 to check whether the VCM is significantly different from the linear regression model. Moreover, by dynamically incorporating temporal information into the model, the VCM will always improve the prediction accuracy of the estimated model. In addition, the VCM provides a meaningful interpretation of the variation in the water-air temperature relationship over time. For sites with high NSCs, the relationship between air and water temperatures might vary due to various effects such as seasonal hysteresis. The VCM can automatically account for such variation in the air and water relationship across time.

5.5. Future Work

Further analysis techniques might be applied to better understand the power of the VCM to accurately model the air-water temperature relationship. First, point-wise or simultaneous confidence bands, constructed based on the estimated varying coefficients, could be used for predicting the range of the water temperature. Second, the estimated varying coefficients in the proposed methods could be useful for clustering different sites into groups for comparative purposes. For example, in Figure 6 we note that one slope curve had a different pattern from the others. It might be of interest if the pattern of varying coefficient

curves is connected to additional information such as elevation or solar radiation. Third, we currently build the varying coefficient model for each site separately. If spatial correlation between sites is strong, we can develop joint varying coefficient models to simultaneously consider all the sites. Fourth, this work applied the VCM to 10 streams using one year of data. More data are currently being collected using paired thermographs throughout southeast U.S. We will extend the current VCM to incorporate additional terms in the model.

6. Conclusions

We developed time-varying coefficient models for studying the relationship between daily maximum water and air temperatures for 10 stream sites in Maryland, West Virginia, Virginia, North Carolina, and Georgia. Statistical inferences using bootstrap hypothesis testing were also developed to examine the appropriateness of the proposed models. The proposed method effectively quantifies the water-air temperature relationship allowing for flexibility in local or global trend. Both the proposed full VCM and semi-VCM result in reasonably accurate prediction for the data from all 10 sites, having lower RMSEs than the linear regression model and the nonlinear logistic model. Moreover, the proposed models provide meaningful interpretations of the temporally dynamic relationship between air and water temperature.

The VCM is superior for these data sets as the effect of seasonal hysteresis is a significant determinant of water temperature. *Mohseni et al.* [1998, 1999] proposed separating the annual cycle into periods according to the warming season and the cooling season, and suggested analyzing the air-water temperature relationship separately as a way to address the problem. The full VCM is able to capture seasonal dynamics in water and air temperatures without having to separate data into different time intervals. It thus automatically accounts for the hysteresis in the streams using time-varying coefficients.

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