The Effect of Climatological Cycles and Storm Events on Water Quality in the National Estuarine Research Reserve Systems of the Southeastern U.S

A Final Report Submitted to

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Submitted by

Dr. Susan B. Wilde, Belle W. Baruch Institute for Marine Science, USC
Charleston, South Carolina, 29492

Dr. Don Edwards, Department of Statistics, USC
Dr. Erik Smith, Belle W. Baruch Institute for Marine Science, USC, North Inlet/Winyah Bay NERR
Dr. Elizabeth Wenner, Marine Resources Research Institute, South Carolina Dept. of Natural Resources, ACE Basin NERR
Dr. David. L. White, NOAA Hollings Marine Laboratory/JHT

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UNIVERSITY *of* NEW HAMPSHIRE

Expanded Executive Summary and Key Findings

The ultimate resource issue addressed with this investigation was detection of anthropogenic impacts on the coastal environment. The tool developed within the scope of our project was a periodicity removal and event detection analysis which allows for removal of natural cylic periodicity and known meteorological forcing on water quality parameters. Once the periodicity has been removed, there are often anomalies in the series. Unusual events in the data series are interesting sources of variability. It is important to identify and quantify events in environmental time series in order to gain a better understanding of the ecosystem. Events could be the result of natural or human influences. To try to identify their causes, detected events can be compared to known meteorological events, such as rainfall, drought, or tropical storm. Unusual events sometimes reveal processes operating at higher time or space scales. We addressed statistical procedures that are capable of lending managers the ability to discriminate between natural forcing variable and new human induced or dramatic climate forcing. These methods are superior to previously published analyses because they are more accurate and amenable to large datasets with high variability. Unfortunately, due to the overwhelming statistical challenges these data present, it was not within the scope of this project to bring this method directly to the managers in organized training sessions. We did, however, correspond with NERRs managers to guide which analyses would be most beneficial to mining these long-term water quality datasets.

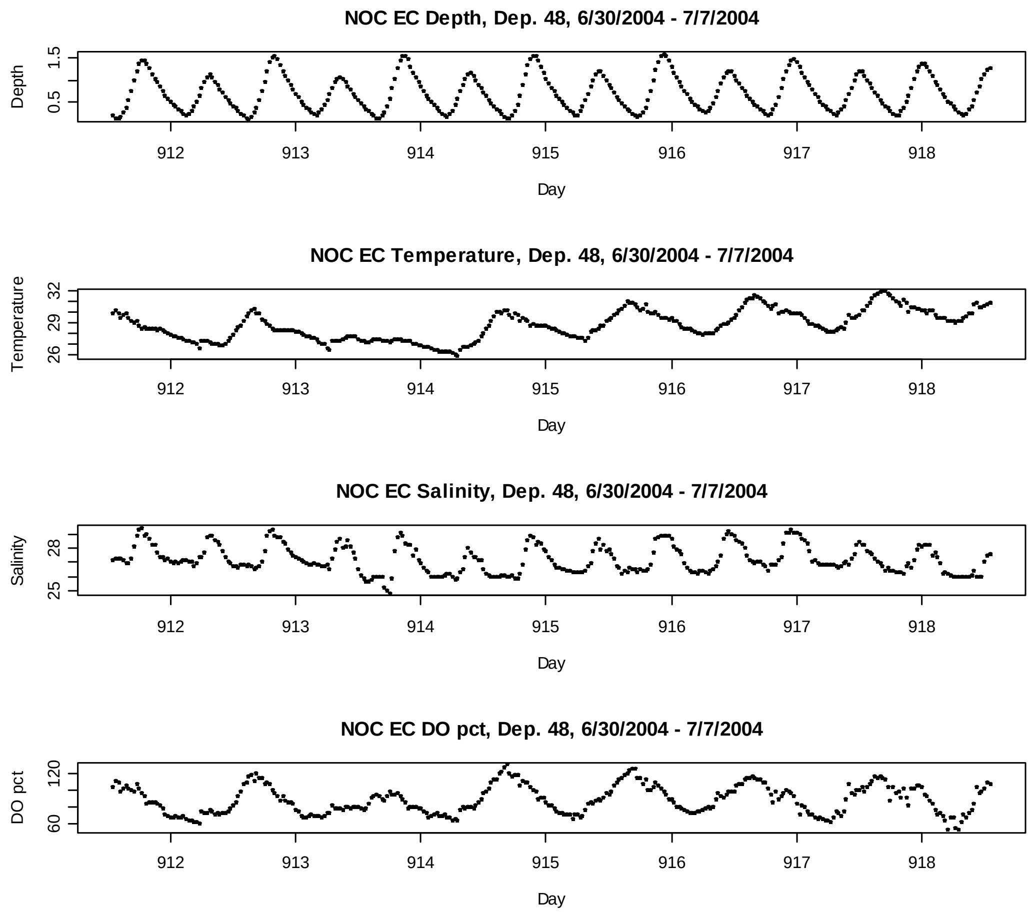
This report explores methods for modeling periodic environmental time series data from estuaries, and for detecting "events" in environmental time series. Both classical parametric and new, nonparametric methods are considered. While humans utilize and benefit from estuarine resources, they also greatly influence these ecosystems. Both human and natural influences cause estuarine habitats to be very dynamic and vulnerable ecosystems. In order to quantify human influences, it is necessary to determine baseline measures of water quality in estuarine ecosystems.

Increased awareness of the implications of both human and natural disturbances resulted in the passage of the Coastal Zone Management Act in 1972. This in turn led to the establishment of the National Estuarine Research Reserve System (NERRS). The NERRS is a network of 27 protected areas in the U.S. and Puerto Rico established for long-term research, water-quality monitoring, and education. These reserves cover over one million acres of protected estuarine waters, adjoining wetlands, and surrounding uplands (Owen and White 2005). The five reserves on the Southeastern Atlantic coast are the focus this study including North Carolina, North Inlet-Winyah Bay, ACE Basin, Sapelo Island, and Guana Tolomata Matanzas (GTM) NERRs..

In 1995, the NERRS established the System-Wide Monitoring Program (SWMP), designed to monitor a standard collection of water quality variables across all reserves. The variables that were initially chosen to be monitored beginning with Phase I in 1996 were pH, specific conductivity, temperature, turbidity, salinity, depth, and dissolved oxygen (DO; mg/L and also percent saturation, the ratio of the dissolved oxygen content to the potential capacity at that temperature and elevation, expressed as a percentage).

These particular variables were selected to measure the water quality for both estuarine species and humans. Measurements for each variable are obtained at 30-minute intervals at 2-4 sites at each of the NERRS SWMP reserves beginning January 1, 1995 (Sanger et al. 2002). These automatic data loggers relay measurements to internal memory and can run unattended for weeks at a time, after which they are removed, cleaned, recalibrated, and redeployed. As one example, Figure 2 shows the depth, water temperature, salinity, and DO (percent saturation) at the East Cribbing site of the North Carolina reserve near Wilmington, North Carolina for the 48th SWMP deployment, June 30 – July 7, 2004.

Figure 2: Water Quality Data for a Single Deployment



In these and many other environmental time series, periodicity is dominant. In the NERRS water quality data, we believe this periodicity should be modeled for the most part as signal, with deterministic origin, driven by gravitational and solar energy forces. In order to detect, measure, and understand the aperiodic influences and events in estuarine water quality data, steps should first be made to quantify and understand the effects of these natural periodic influences.

Notice the comparatively low readings of temperature, salinity, and dissolved oxygen late in day 913 in Figure 2. Since the levels of these three water quality variables appear to be lower than at the same time on other days in the deployment, this is a possible event. Once the periodicity has been removed, we can better study these series to determine if these disturbances are indeed unusual events.

The first two suggested applications of the analysis were to evaluate short-term impacts on estuarine salinity during strong rain events and named storms. Results from these analyses are also discussed within this final report and references within. While many short-term variables responded to relatively small recorded rain events, we did not detect long-term signatures within the water quality data from any of the hurricanes that were evaluated in our analyses.

Finally, all necessary statistical tools required to accomplish this effort are described in this report and are most are available free on the internet. Details of the statistical modeling efforts are contained in the University of South Carolina statistics department graduate student thesis and dissertation and pending journal articles (Autin, 2007, Li, 2007, Autin and Edwards, submitted).

Key Findings

- Generalized additive models (GAMs) are a very promising method for modeling estuarine water quality data, and more generally, for any time series with strong and potentially non-sinusoidal signals of known period.
- For the NERRS data, classical harmonic regression techniques work well for the analysis of depth data; however, they are not as satisfactory for analysis of other, less regular, water quality variables.
- The GAMs are also more automatically adaptive and require less user-intervention than the harmonic regression models.
- The ease of their use in R also makes them very appealing. Not only are they adaptive and user-friendly, but they are also non-prohibitive in terms of computation time.
- Efron’s local false discovery rate algorithm was effective is detecting events in the ACE Basin reserve water quality data.
- The model developed from the first ACE Basin site (ACEBB) suggests that small total precipitation and large mean and mean absolute deviation of landward wind results lead to a large drop in salinity.
- For the second ACE site (ACEMC), the model predicts that short rainfall duration, large total precipitation, small mean absolute deviation of precipitation and large mean absolute deviation of landward wind during rainfall period should cause a large drop in salinity.
- Hurricanes impacts on water quality parameters in NERRs site within the storm path indicated that the water quality changes were short-term and generally all parameters returned to baseline level cycles within 48 hrs.

Abstract
Determining the role of anthropogenic forces and climatic variability on estuarine water quality requires the ability to predict and distinguish effects of stochastic events (e.g., hurricanes) vs. typical estuarine periodicities, and to reveal how periodicities are influenced by large-scale, climatic variability. In these and most other environmental time series, periodicity is dominant.
In order to detect, measure, and understand the aperiodic influences and events in estuarine water quality data, steps should first be made to quantify and understand the effects of these natural periodic influences.

Our specific objectives were to remove cyclic periodicity from NERRS environmental time series as a source of variation to facilitate short-term and long-term event detection. Then using the periodicity free data, identify and quantify events in NERRS environmental time series in order to gain a better understanding of the ecosystem. To evaluate short-term storm effects, we sought to develop a statistical model of high rainfall and wind impacts upon water-quality parameters (salinity, depth) within a model estuarine ecosystem (ACE NERR site) in the southeastern US. Finally, we examine storm tracks and meteorological history of named tropical systems between 1996-2004, in order to determine the frequency, duration, and intensity of systems that potentially impacted water quality at NERR SWMP sites.

To accomplish our first objective to remove periodicity, we compare statistical methods including; harmonic regression, GAMs with cubic regression splines, and GAMs with cyclic regression splines using water quality data collected from the National Estuarine Research Reserve System (NERRS). Once the periodicity has been removed from ecological datasets, there is likely still some atypical variation, such as unusual events, in the time series. Unusual events and disturbances are important and interesting sources of variability in ecological datasets. Several methods are used in event detection including Shewhart Control Chart Method and Efron's local false discovery rate. For the third objective, rainfall and wind impact were evaluated using a SAS program, 420 rainfall events in total have been extracted from the original meteorological data at ACE Basin between July 1, 2001 and December 31, 2005. The final objective was to provide a presentation format to visualize water quality changes within NERRs sites exposed to the track of a hurricane.

We have investigated the use of classical harmonic regression models and nonparametric harmonic regression models (generalized additive models) for estuarine water quality data. For the NERRS data, classical harmonic regression techniques work well for the analysis of depth data; however, they are not as satisfactory for analysis of other, less regular, water quality variables. The GAMs show great potential for these applications. Additionally , we adapted Efron's local false discovery rate methods for detecting events in estuarine water quality data. We then used the event detection algorithm to detect events in the water quality data collected at the ACE Basin NERRS reserve. Once events are detected in a time series, causes for the events should be explored. Water quality events can be compared to known meteorological events, such as rainfall events, droughts, and El Niño/La Niña climatic cycle effects.

Introduction

Demographic pressures increasingly affect coastal resources. More than half of the nation's citizens live in coastal areas, which account for only 13% of the nation's acreage. In the next 15 years, 27 million people, (~50% of the US population increase), are predicted to move into the coastal zone (Beach 2002). Associated with these changes in population distribution, are developmental and societal practices that negatively impact ecological systems. The NERRS SWMP provides long-term monitoring of water quality, to gather baseline data for estuarine systems that may be impacted. Estuarine water quality is also influenced by the interaction of atmospheric, oceanic, watershed, and anthropogenic forces. Thus, pronounced variability occurs across a wide range of temporal and spatial scales.

The analysis of long-term, water-quality data is complicated by the uncertainty of measurements made across multiple environmental scales (i.e., climatic to estuarine). For instance, climate variability is typically recorded on global, hemispheric, and regional scales. However, to effectively manage environmental resources, it is necessary to analyze data at the ecosystem level (Preston, 2004). Determining the role of climatic variability on estuarine water quality requires the ability to predict and distinguish effects of stochastic events (e.g., hurricanes) vs. typical estuarine periodicities, and to reveal how periodicities are influenced by large-scale, climatic variability. In these and most other environmental time series, periodicity is dominant. In the NERRS water quality data, this periodicity is modeled as signal, with deterministic origin, driven by gravitational and solar energy forces. In order to detect, measure, and understand the aperiodic influences and events in estuarine water quality data, steps should first be made to quantify and understand the effects of these natural periodic influences.

In recent years, the SAB has experienced a range of both large-scale, longer-term climatological conditions and short-term storm events that have greatly impacted its estuaries. The longest drought in the past ~50 years (Waple, 2003) spanned 1998-2002, and was associated with a strong La Niña event during 1998-2001(Lawrimore, 2001; Waple, 2002). In mid-2002, the drought ended rapidly, with a dramatic rainfall increase; an El Niño event occurred from late 2002 through 2003 (Levinson, 2004). [El Niño brings moisture to the southeastern U.S., and is not conducive to hurricane formation in the Atlantic. Prolonged La Niña events are correlated with drought and increased Atlantic hurricane formation.] Superimposed upon this large-scale climatic variability, was pronounced, inter-annual variability in storm-events frequencies. In the fall of 1999, three hurricanes, including *Dennis* (Aug. 24-Sept. 5), *Floyd* (Sept. 14-17) and *Irene* (Oct. 13-16), impacted the southeast, leading to unprecedented flooding in portions of North Carolina and the northeastern coastal counties of South Carolina (Bales, 2003; Peierls, 2003).

The effects of climatic variability, across a range of scales, on estuarine water quality dynamics are thus highly relevant to the South Atlantic Bight. The development of specific, quantitative techniques to assess the effects of stochastic events and larger-scale, climatic conditions will be valuable to estuarine ecologists and coastal resource managers alike. This will provide the necessary tools for analyzing long-term water quality data sets, in order to better understand the factors affecting variability across space and time.

Objectives

The research analyses addressed complexities in evaluating effects of climatic variability by the first addressing cyclic periodicity and event detection, and then using these tools to conduct intensive investigation of short-term stochastic events including rainstorms and named tropical systems. Our analyses focused on the role of these processes at the scale of individual estuarine ecosystems (NERR sites) within the South Atlantic Bight.

Our specific objectives were to:

1. Remove cyclic periodicity from NERRS environmental time series as a source of variation to facilitate short-term and long-term event detection.
2. Identify and quantify events in NERRS environmental time series in order to gain a better understanding of the ecosystem.
3. Develop a statistical model of high rainfall and wind impacts upon water-quality parameters (salinity, depth) within a model estuarine ecosystem (ACE NERR site) in the southeastern US.
4. Examine storm tracks and meteorological history of named tropical systems between 1996-2004, in order to determine the frequency, duration, and intensity of systems that potentially impacted water quality at NERR SWMP sites.

- Objectives 1 and 2 will be used to facilitate investigation of events that could be the result of natural or human influences. To try to identify their causes, detected events are initially compared to known meteorological events, such as rainfall, drought, or tropical storm. Objectives 3 and 4 focus on rainfall, wind and named storm events on estuarine water quality parameters.
- Reports and publications generated by Objectives 1-4 are supported by implementing available web-based, analytical tools for future data modeling (Autin 2006, 2007, Li, 2007).

Methods

Objective 1. Compare methods to remove cyclic periodicity including; harmonic regression, GAMs with cubic regression splines, and GAMs with cyclic regression splines using water quality data collected from the National Estuarine Research Reserve System (NERRS).

The use of statistical models in tidal prediction is based upon the theory that all tidal components are independent and that their periods are known. The periods of the major tidal constituents (Table 1) have been calculated due to constant and astronomical forces (see e.g. Defant 1958). Semidiurnal components have a tidal cycle that consists of two high and two low tides of approximately the same height per lunar day (~24.84 hours). Diurnal components have a tidal cycle that usually consists of one high tide per day.

Classical and proposed methods for modeling periodic environmental time series are compared using data from southeastern NERRs sites. Classical harmonic regression analysis, used by physical oceanographers for decades, assumes that effects of periodic components can be modeled by weighted sums of sine waves of known periods. Generalized additive models (GAMs) allow more flexibility in the form of the regression function. They permit parametric, semiparametric, and nonparametric regression functions of the predictor variables. Applications of nonparametric harmonic regression are presented with analyses for the SWMP data from NERRs sites.

Table 1: Major Components of Tidal Forces

Designation	**Symbol**	**Period**	**Description**
Semidiurnal	M_2	12.4206012	Main lunar (semidiurnal) constituent
Semidiurnal	S_2	12.0000000	Main solar (semidiurnal) constituent
Semidiurnal	N_2	12.6583482	Lunar due to monthly variation in moon's distance
Semidiurnal	K_2	11.9672348	Soli-lunar due to changes in declination of sun and moon
Diurnal	K_1	23.9344697	Soli-lunar due to changes in declination of sun and moon
Diurnal	O_1	25.8193417	Main lunar (diurnal) constituent
Diurnal	P_1	24.0658902	Main solar (diurnal) constituent
Diurnal	S_1	24.0000000	Daily constituent
Long Period	M_1	327.858984	Moon's fortnightly constituent

Note: Period is given in solar hours.

Harmonic Regression

Harmonic regression uses the sine curve to account for periodic patterns. Multiple harmonic regression is derived from the modeling of two or more additive sine functions representing different periods. The use of multiple harmonics allows (theoretically) for any periodic function of period *p* to be arbitrarily well-approximated in this manner, given enough terms. The accuracy of the approximation improves by increasing the number of harmonics, but its scientific meaning is often unclear (Piegorsch and Edwards 2002). In practice, one or two harmonics are typically used per period for analysis of estuarine data by physical oceanographers.

Tidal components that have the same designation have periods of similar length. According to the oceanographic literature, in order to analytically separate these similar components from each other, series of ample length must be available. Specifically, according to Foreman and Henry (1989):

(1) 328 hours = 13.67 days are needed to distinguish O_1 and K_1

(2) 355 hours = 14.79 days are needed to distinguish S_2 and M_2

(3) 182 days are needed to distinguish P_1, K_1, and S_1

(4) 182 days are needed to distinguish K_2 and S_2.

In statistical terms, this inseparability of terms corresponds to severe collinearity in the multiple harmonic regression models for short series. We adopt the above guidelines in order to ensure that there will not be unacceptably strong collinearity among the similar periodic components, in both the classical and nonparametric approaches.

Generalized Additive Models

Modern generalized additive models (Hastie and Tibshirani 1990) allow more flexibility in the form of the regression function. As described in detail by Wood (2006), a univariate function $f(x)$ of the predictor x can be approximated by a spline function $g(x)$. A polynomial regression spline is a type of smoother that fits piecewise polynomials to data. The piecewise polynomials are connected at user-specified x-locations called knots, and the spline is typically required to have no discontinuity, and to be smooth, at knots. Knots must also be specified for the endpoints of the series. The difficulty in using this technique is the determination of the number and locations of knots to use.

Objective 2. Develop a data-driven event detection algorithm using Efron's (2006) idea of local false discovery rates to detect events in water quality time series.

Once the periodicity has been removed from ecological datasets, there is likely still some atypical variation, such as unusual events, in the time series. Unusual events and disturbances are important and interesting sources of variability in ecological datasets. Understanding their causes can lead to better understanding of the ecosystem. Events can be defined as sequences of observations that are improbably higher or lower than would be expected given the distribution of the "noise." In the analysis of time series data, there are two characteristics that are most important in describing an event: duration and intensity. Jassby and Powell (1990) believe that unusual events are among the most complicated, yet most crucial, phenomena that ecologists must handle effectively. The timing, frequency, length, and intensity of events may be important in determining long-term changes in ecosystem structure and function (Vernberg, 1993). Although it is important to identify and quantify these events, objective and efficient methods for doing so are not readily available for ecological data.

Allen et al. (1996) adapted quality control methods, widely used in industry, to detect and quantify unusual events in year-long data sets collected at the North Inlet-Winyah Bay Reserve in South Carolina. They used the Shewhart Control Chart Method to define four types of events according to intensity and duration. This method uses the residuals from the removal of periodicity and long-term trends from the data. Extreme residuals (or series of residuals) are flagged if they would be improbable given the magnitude of typical variability as measured by the standard deviation. Following classical industrial process control rules, Allen et al. defined four types of events, types A, B, C, and D:

(A) One point at least 3 standard deviations above or below the mean;

(B) Two out of three consecutive points at least 2 standard deviations above or below the mean;
(C) Four out of five consecutive points at least 1.5 standard deviations above or below the mean;
(D) Eight consecutive points at least 0.2 standard deviations above or below the mean.

These threshold deviation levels are standard in control chart methods, chosen such that approximately only 1 in 400 detected events are false positives under a Normal errors assumption. The Shewhart Control Chart Method used by Allen et. al. (1996) only allowed for four types of events. For each event of differing length, a new threshold criterion was defined. We would like to develop a more automated and comprehensive method for detecting events of almost any length. This gives rise to a large-scale multiple-hypothesis testing situation motivating the control of false discovery rate, discussed in the next section.

Traditionally, family-wise error rate (FWER) has been used to measure the overall error rate under the multiple-hypothesis test setting. The FWER is defined as the probability of making one or more false rejections among all tests. The significance level α is chosen such that FWER $\leq \alpha$, and then a rejection region is found that maintains level α FWER. In many circumstances, FWER is too strict, especially for a large number of tests.

Since the methods that use p-values rely on null hypothesis tail areas, they are extensions of traditional frequentist hypothesis testing. Efron (2004) presents empirical Bayes methods for large-scale false discovery rate analysis. The local false discovery rate provides a useful method for identifying "interesting" (non-null) cases. we present a data-driven event detection algorithm that utilizes Efron's local false discovery rate. The performance of this algorithm is investigated via simulation studies. The algorithm is then used to detect events in the ACE Basin reserve water quality data.

Objective 3. Develop a statistical model of high rainfall and wind impacts upon water-quality parameters (salinity, depth) within a model estuarine ecosystem (ACE NERR site) in the southeastern US.

The meteorological data has been recorded at Bennett's Point station every 15 minutes since July 1, 2001. The original yearly data sets between 2001 and 2005 have been acquired from the CDMO website. In general, we define one rainfall event like this: the starting point is when the first non-zero precipitation occurs after two consecutive hours of zero precipitation. The ending point is when the last non-zero precipitation occurs before two consecutive hours of zero precipitation. We also only consider events which last at least a half hour.

Since rainfall events which last only 15 minutes produce missing values for mean absolute deviation variables, the rainfall events project have been defined as the events whose durations are at least 30 minutes. Using a SAS program, 420 rainfall events in total have been extracted from the original meteorological data at ACE Basin between July 1, 2001 and December 31, 2005 (Li, 2007).

Objective 4. Examine storm tracks and meteorological history of named tropical systems between 1996-2004, in order to determine the frequency, duration, and intensity of systems that potentially impacted water quality at NERR SWMP sites.

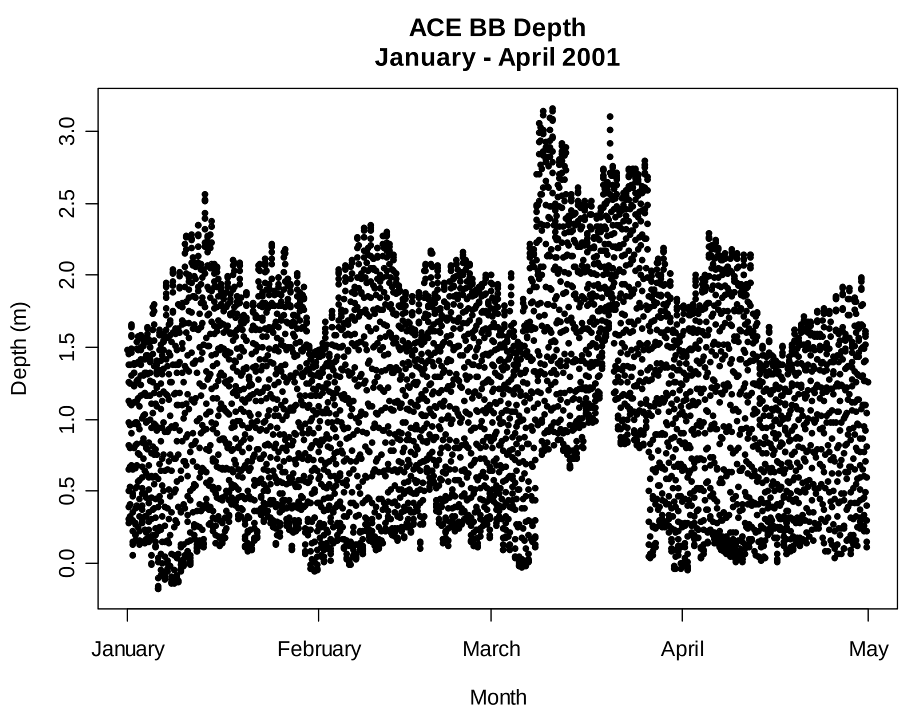
Evaluate the impact of named storms on the southeastern NERRS sites. To date, fourteen named storms have been graphically depicted in a movie format which allows simultaneous viewing of key meteorological data as forcing variables and selected responding water quality parameters.

Results

Removing periodicity from NERRS SWMP data.

This analysis focused on the NERRS reserves in the Southeast: North Carolina (NOC), North Inlet-Winyah Bay (NIW), ACE Basin (ACE), Sapelo Island (SAP), and Guana Tolomata Matanzas (GTM). All data is available on the Centralized Data Management Office website (CDMO 2007). In part because of profound shifts at redeployments (e.g. Figure 1), and in part to allow for changes in short-term periodic signals over seasons, our analysis of the water quality data from these reserves is broken into two phases. Phase I estimates and removes short-term periodic influences from each deployment of the data. Phase II estimates and removes the annual periodicity and deployment effects from the phase I residuals.

Figure 1: Raw Depth Data for Several Deployments



The most important semidiurnal and diurnal constituents are listed in Table 1. For the phase I analysis of the NERRS SWMP deployments of length 7 to 30 days, we separate and estimate four periodic signals: Diel (24-hour period = S_1), M_2, N_2, and O_1. Due to collinearity caused by limited series length, the estimated Diel signature is actually the sum of the effects of Diel + S_2 + P_1 + K_1 + K_2. At most NERRS sites, for most deployments, the Diel (D) and M_2 signals are by far the most important (Sanger et al. 2002).

The data is fit with a "floating" GAM with cyclic regression splines for each of the four periodic components:

$$y_i = \beta_0 + f_1(t_i) + f_2(Dstage_i) + f_3(M_2stage_i) + f_4(N_2stage_i) + f_5(O_1stage_i) + \varepsilon_i \,, \quad (1)$$

where t_i is time (in days) of the i^{th} observation i = 1, 2, …, n, f_1 is a slow-changing trend curve modeled with a cubic regression spline, β_0 is the intercept of the trend curve, and f_j (j = 2, 3, 4, 5) is the cyclic regression spline curve for each of the four periodic components. The errors ε_i are assumed to have mean zero. For each penalized regression spline, the user-specified dimension of the basis is one more than the maximum degrees of freedom that the term can have. After some experimentation the dimension of the basis for f_1 was set to 4 to prevent f_1 from absorbing cyclicity from other terms. For each of the cyclic regression splines, the default of 10 was used for the dimension of the basis.

As a detailed example of the phase I analysis, consider the water depth (meters) data from the East Cribbing site of the NOC reserve for the June 30 – July 7, 2004. Figure 2 shows the graphical summary of the model (1) fit: the raw data with fitted GAM, residual plot, and the profile plots of the four periodic components.

The model fits the data very well, which is typical for analyses of the depth variable. The M_2 tidal constituent is dominant, but note the asymmetry in the M_2 profile plot. As is evident here, it is often the case that the periodic components are far from being sinusoidal in shape. For this reason, we believe classical harmonic regression is not appropriate for much of the NERRS-SWMP water quality data unless a large number of harmonics are used for each period, which is not typical.

Non-sinusoidal periodic components such as the M_2 profile seen in Figure 3 are pervasive throughout the data analyses of the CICEET NERRS study. Further examples are shown in Figures 4-5. Each figure contains the raw data with the fitted GAM (1), a residual plot, and the fits for the four periodic components. Figure 3 shows the graphical summary of the phase I analysis for dissolved oxygen (measured as percent saturation) data collected during the July 18 – August 1, 2002 deployment at the St. Pierre site of the ACE Basin reserve. The M_2 component has a double-bump in the peak of the curve, and the Diel component has some slight curvature during the mid-portion of the Diel cycle.

Figure 2: Depth Phase I Analysis Example

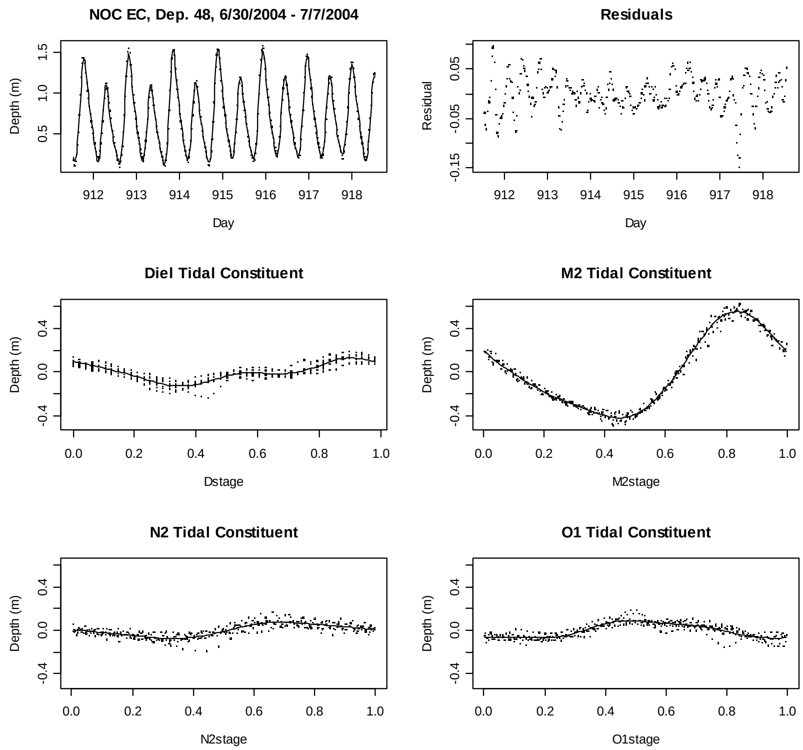
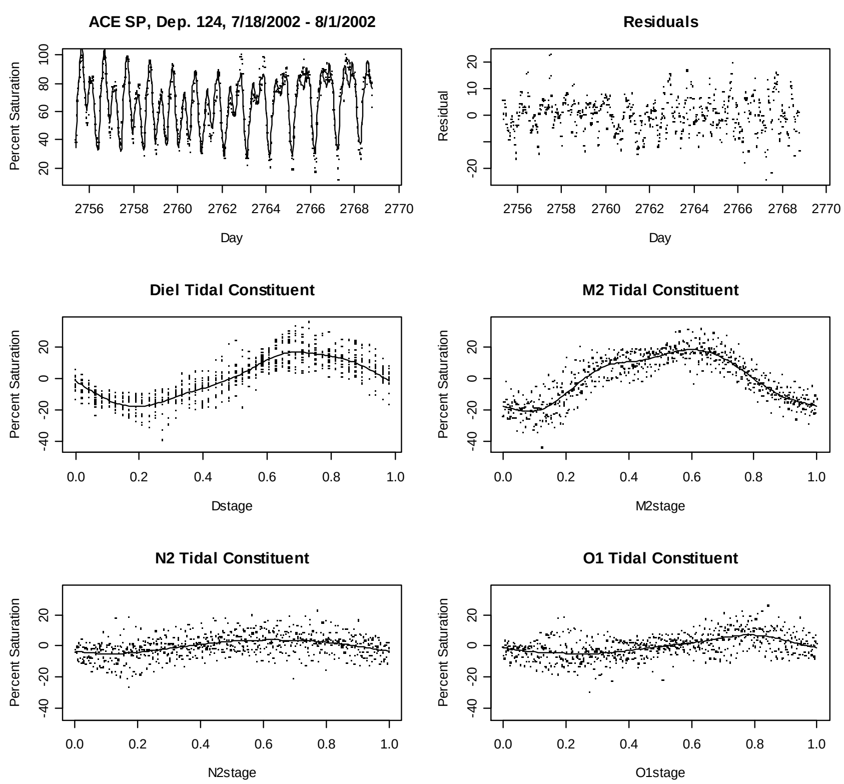
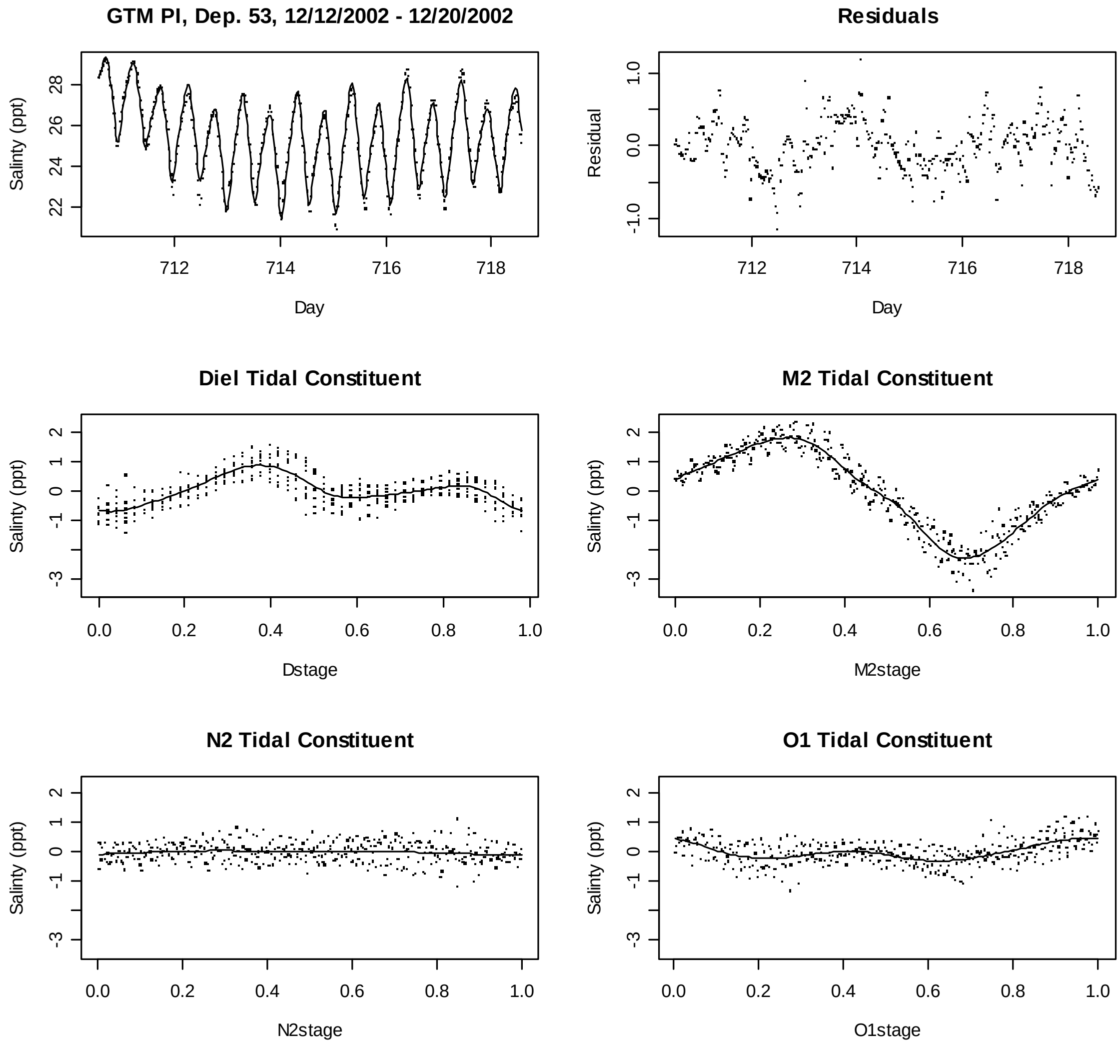


Figure 3: Percent Saturation Phase I Analysis Example



A graphical summary of a phase I analysis for salinity (parts per thousand) data is shown in Figure 4. Data was collected during the December 12-20, 2002 deployment of the Pine Island site of the GTM reserve. As with the two previous examples, the periodic components are not sinusoidal. The M_2 component, in particular, displays some curvature during the descent from peak to trough of the cycle and is almost linear from trough to peak.

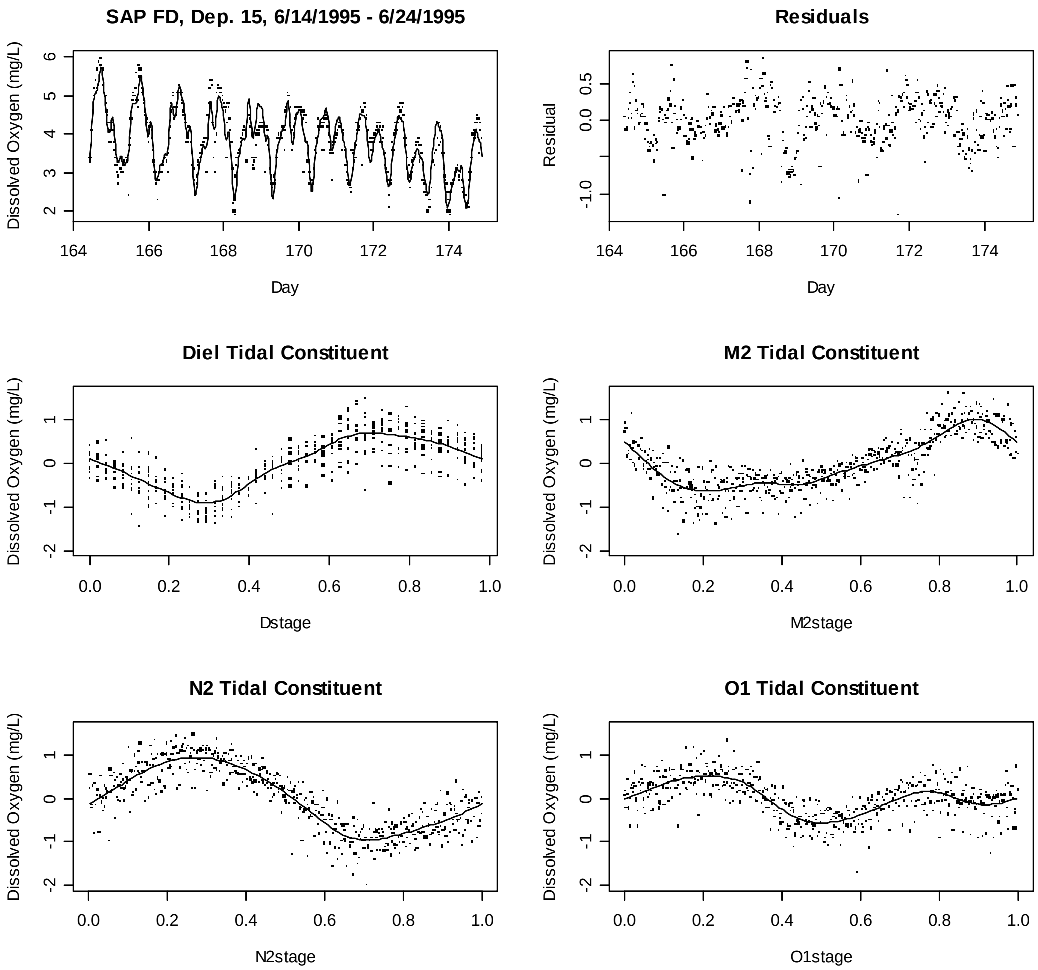
Figure 4: Salinity Phase I Analysis Example



A graphical summary of a phase I analysis for dissolved oxygen (mg/L) data is shown in Figure 5. Data was collected during the June 14-24, 1995 deployment of the Flume Dock site of the SAP reserve. Both the Diel and M_2 components have a great deal of curvature resulting in unusual shapes, especially in the M_2 component. The O_1 and N_2 constituents are unusually strong in this deployment, as is often the case at this particular site.

Since the periodic components of the water quality data often do not appear to be sinusoidal, this suggests that classical harmonic regression analysis may not be appropriate for this data. The time series for all water quality variables were fit with model (1) for each deployment containing at least seven days of data. Doing this for each site of each reserve in the CICEET study resulted in nearly 12,000 phase I analyses for the NERRS data.

Figure 5: Dissolved Oxygen Phase I Analysis Example



Phase II Analysis

In phase II analyses, one of our goals is to attempt to model annual periodicity. The trend and intercept are added back to the residuals from the phase I fit of model (1) for each deployment; these are referred to as phase I adjusted residuals. Deployment effects are removed from these by treating deployment as a factor. The GAM used for the phase II analysis is

$$y_{ij} = \beta_0 + \delta_i + f_1(t_{ij}) + f_2(YearStage_{ij}) + \varepsilon_{ij}, \tag{2}$$

where y_{ij} is the phase I adjusted residual for the j^{th} observation from deployment i, δ_i is the unknown shift for the i^{th} deployment, f_1 is a slow-changing trend curve modeled with a cubic regression spline, β_0 is the intercept of the trend curve, and f_2 is the cyclic regression spline curve for the annual periodic component (period 365.24 days). After experimentation, the dimension of the basis for f_1 was set to 3, and the dimension of the basis for f_2 was set to 5.

As an example of phase II analysis, consider the phase I adjusted residuals for the dissolved oxygen (percent saturation) data collected at the Pine Island site of the GTM reserve (2001-2004) in Figure 6. These phase I adjusted residuals were fit with model (2). Figure 7 shows the resulting estimated periodic annual component superimposed on the phase II residuals (with the estimated annual periodic component added back in).

Figure 6: Dissolved Oxygen Phase I Adjusted Residuals

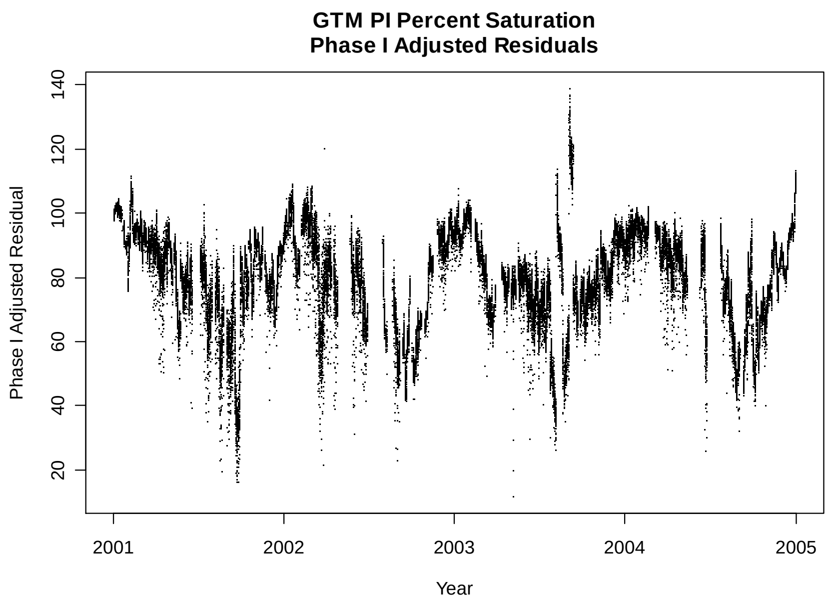
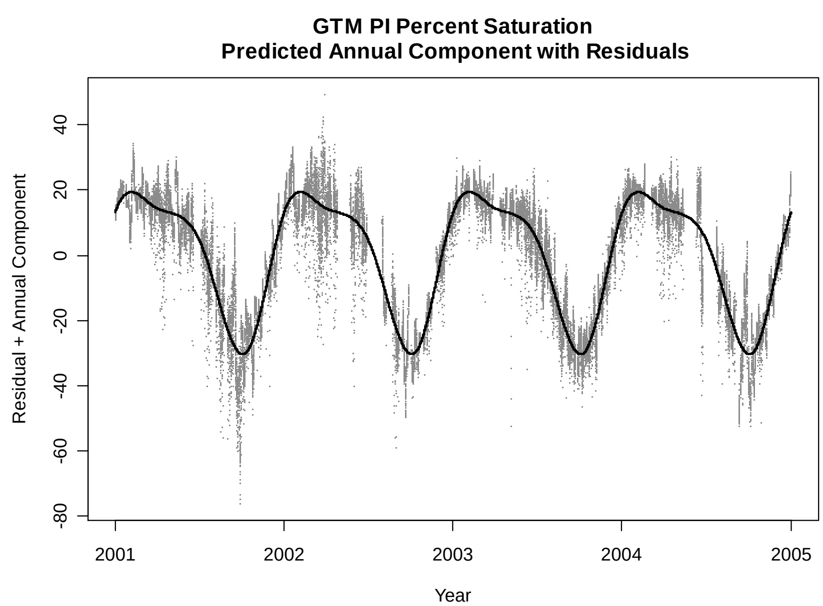


Figure 7: Dissolved Oxygen Phase II Residuals with Annual Component



As a second example of phase II analysis, consider the phase I adjusted residuals for the water temperature (degrees Celsius) data collected at the Debidue Creek site of the NIW reserve (1998-2000) in Figure 8. Figure 9 shows the estimated periodic annual component superimposed on the phase II residuals (with the estimated annual periodic component added back in), resulting from fitting the data with model.

Figure 8: Temperature Phase I Adjusted Residuals

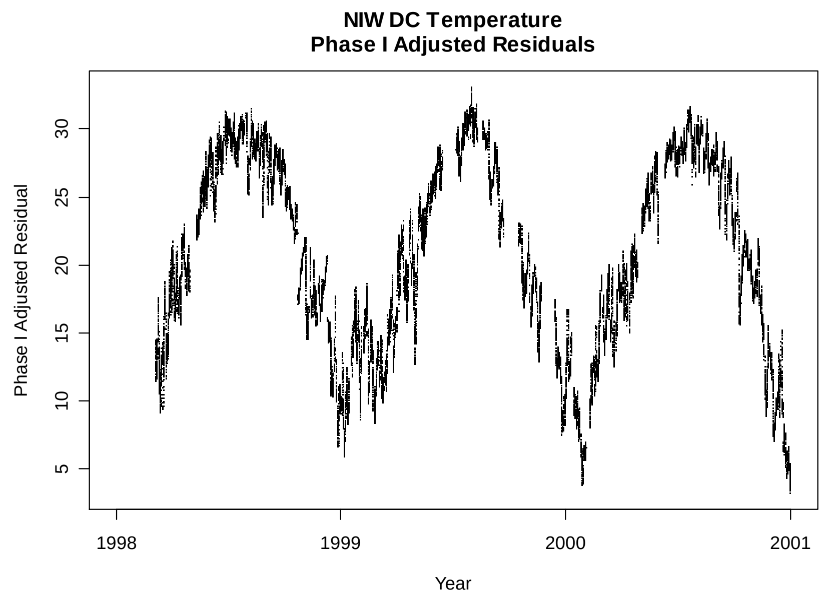
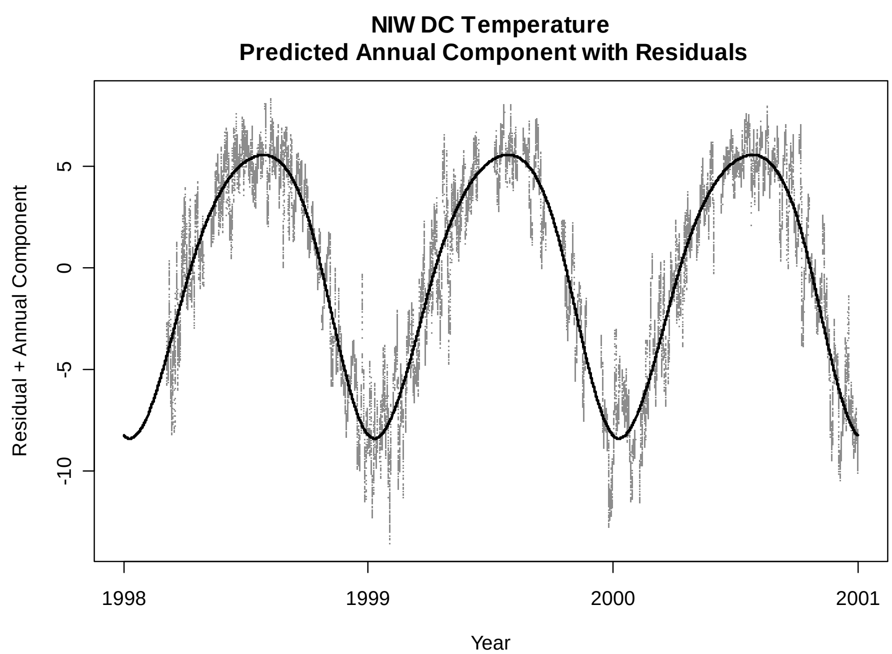


Figure 9: Temperature Phase II Residuals with Annual Component



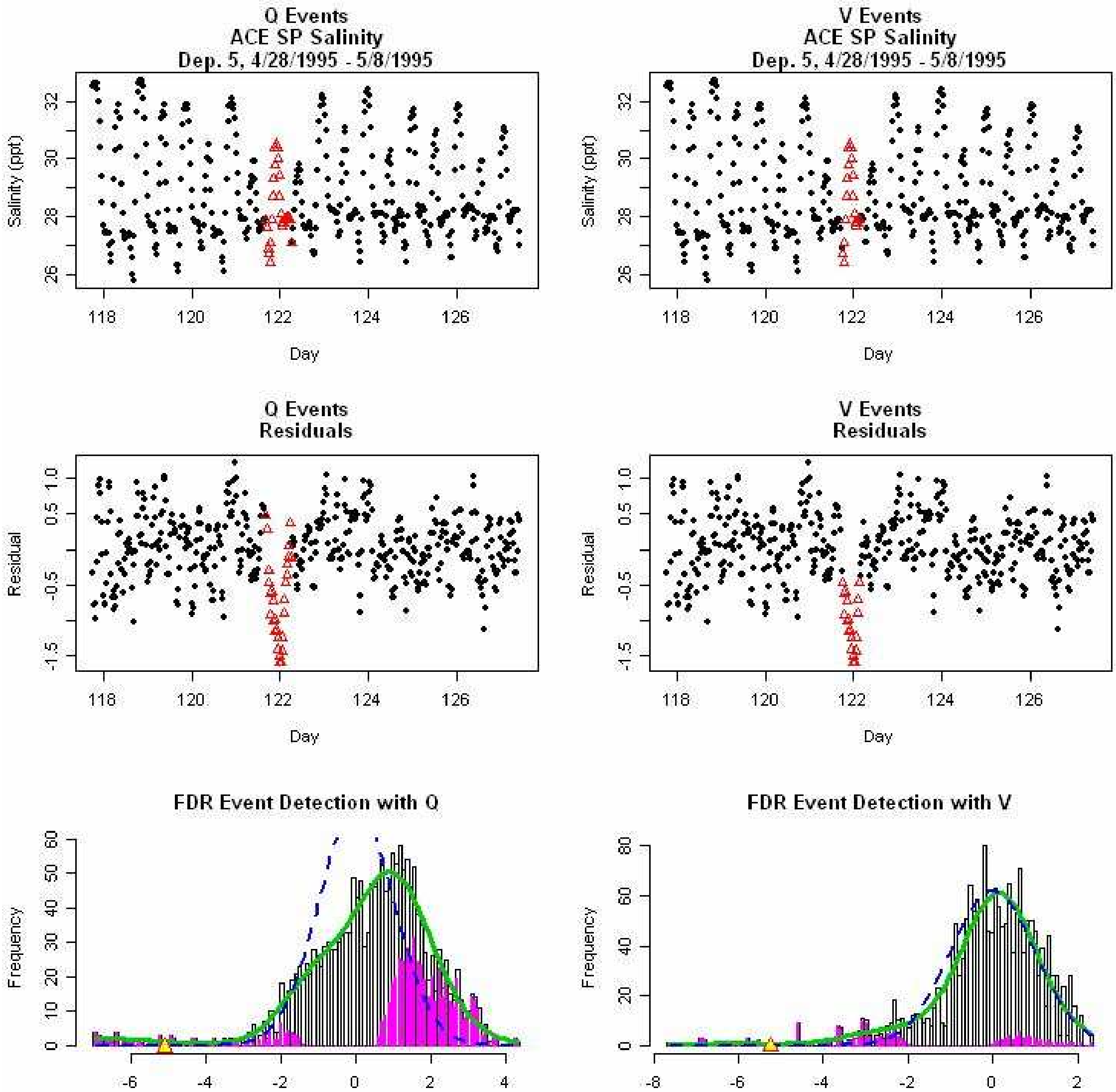
The dissolved oxygen (measured as percent saturation) annual periodic component shown in Figure 7 has an unusual, non-sinusoidal shape. Dissolved oxygen at this site is highest in late winter, and remains high in late spring before drastically dropping in the months of late summer/early autumn. The water temperature annual periodic component shown in Figure 9 is also non-sinusoidal. At this site, the higher temperatures during the summer last longer than the lower temperatures during the winter. Also, the temperature drops during autumn more quickly than it increases during spring. These periodic profiles further strengthen the premise that nonparametric harmonic regression is more appropriate for analyzing the NERRS water quality data than classical harmonic regression

2. NERRS Data Event Detection

With datasets becoming incrementally large and complex, an automated method of detection of events is required to evaluate perturbations (natural or anthropogenic). The objective here was to detect events of varying lengths in the NERRS water quality data. The analysis focused on the ACE Basin Reserve, one of the largest undeveloped estuaries on the East Coast, located just south of Charleston, South Carolina. The residuals resulting from the phase I analyses were analyzed using the event detection algorithm with $m=\{4,8,12,16\}$ and $\tau = 0.0001$. This low value of τ was chosen because higher values resulted in an implausible number of events being detected in the series. Note that the residuals used for event detection are not the phase I adjusted residuals used in phase II analysis. One problem with using the event detection algorithm for the NERRS data is the failure of the locfdr function (as mentioned in the previous section). Although there were 2114 phase I analyses completed for ACE Basin, the locfdr function succeeded (using both Q^* and V^*) in only 970 of those cases. R code used for event detection can be found in appendix of Autin (2007).

For the first example, a graphical summary of the event detection for salinity (parts per thousand) data collected during the April 28 – May 8, 1995 deployment of the St. Pierre site of the ACE Basin reserve is presented in Figure 10. The three left plots correspond to event detection using Q^*, and the three right plots correspond to event detection using V^*. The top row shows plots of raw data, with observations detected as event points plotted with triangles. The middle row shows residual plots with the detected event observations plotted with triangles. The last row contains histograms of the z-values, as well as fitted density curves $\hat{f}(z)$ (solid line) and $\pi_0 f_0(z)$ (dashed line). The colored histogram bars represent estimated non-null counts. The triangle on the x-axis indicates the z-value threshold for fdr < 0.0001. The event detection algorithm has identified an event that occurs during the late night of day 121 and early morning of day 122. However, the start and endpoints of the event differ for the two test statistics.

Figure 10: ACE SP Salinity Events (Deployment 5)



A graphical summary of the results of the detection algorithm for a deployment of dissolved oxygen (measured as percent saturation) is shown in Figure 11. This data was collected during the March 3-13 deployment at the Big Bay site of the ACE Basin reserve. Using both test statistics, the algorithm detected events at two separate times during the deployment. The first event consists of high dissolved oxygen readings during the afternoon of day 64. There is also an event of low dissolved oxygen readings during day 66. When using the *V** test statistic, a third event is detected during day 66, during which dissolved oxygen readings were higher than usual.

Figure 11: ACE BB Dissolved Oxygen Events (Deployment 1)

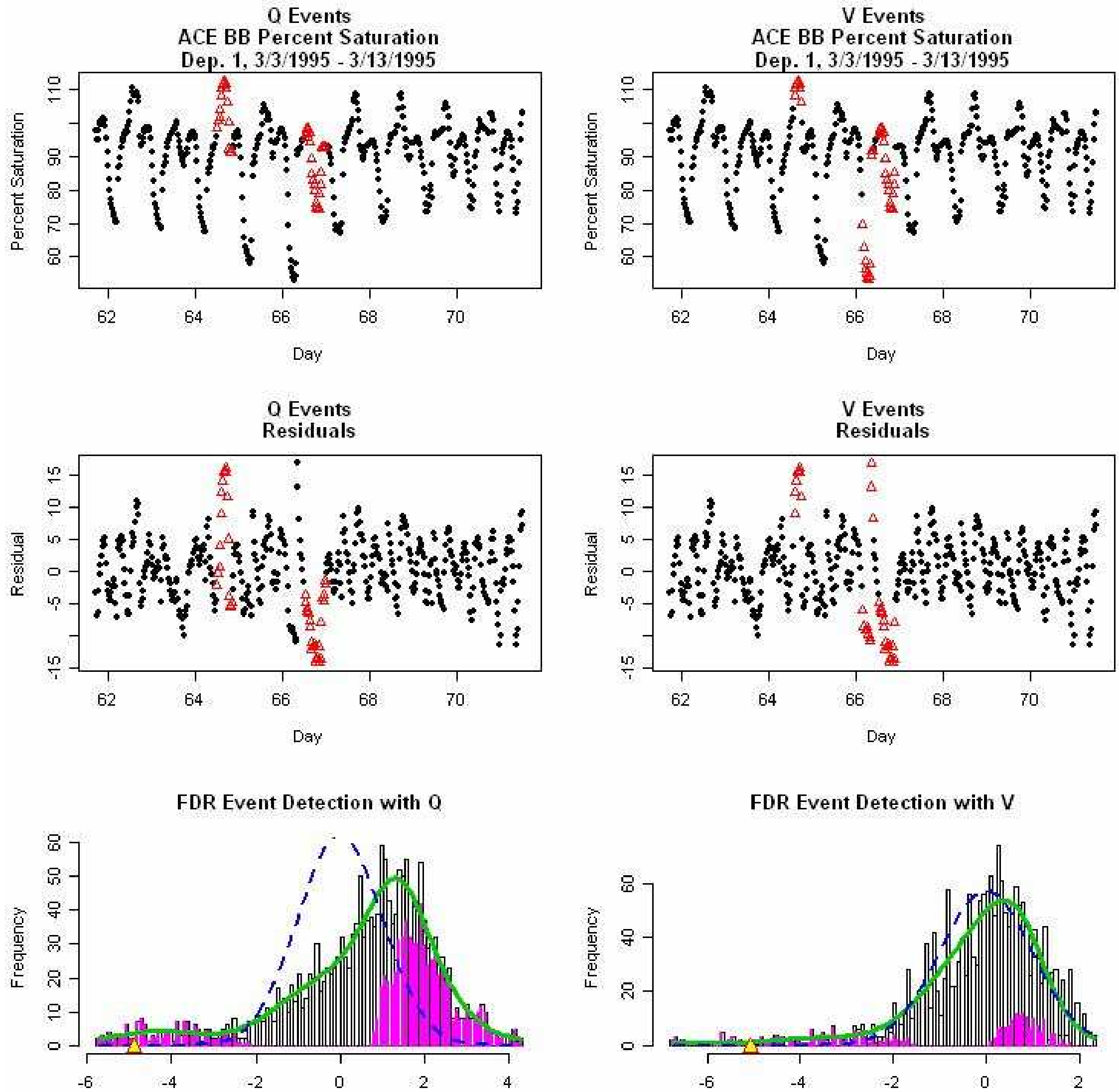
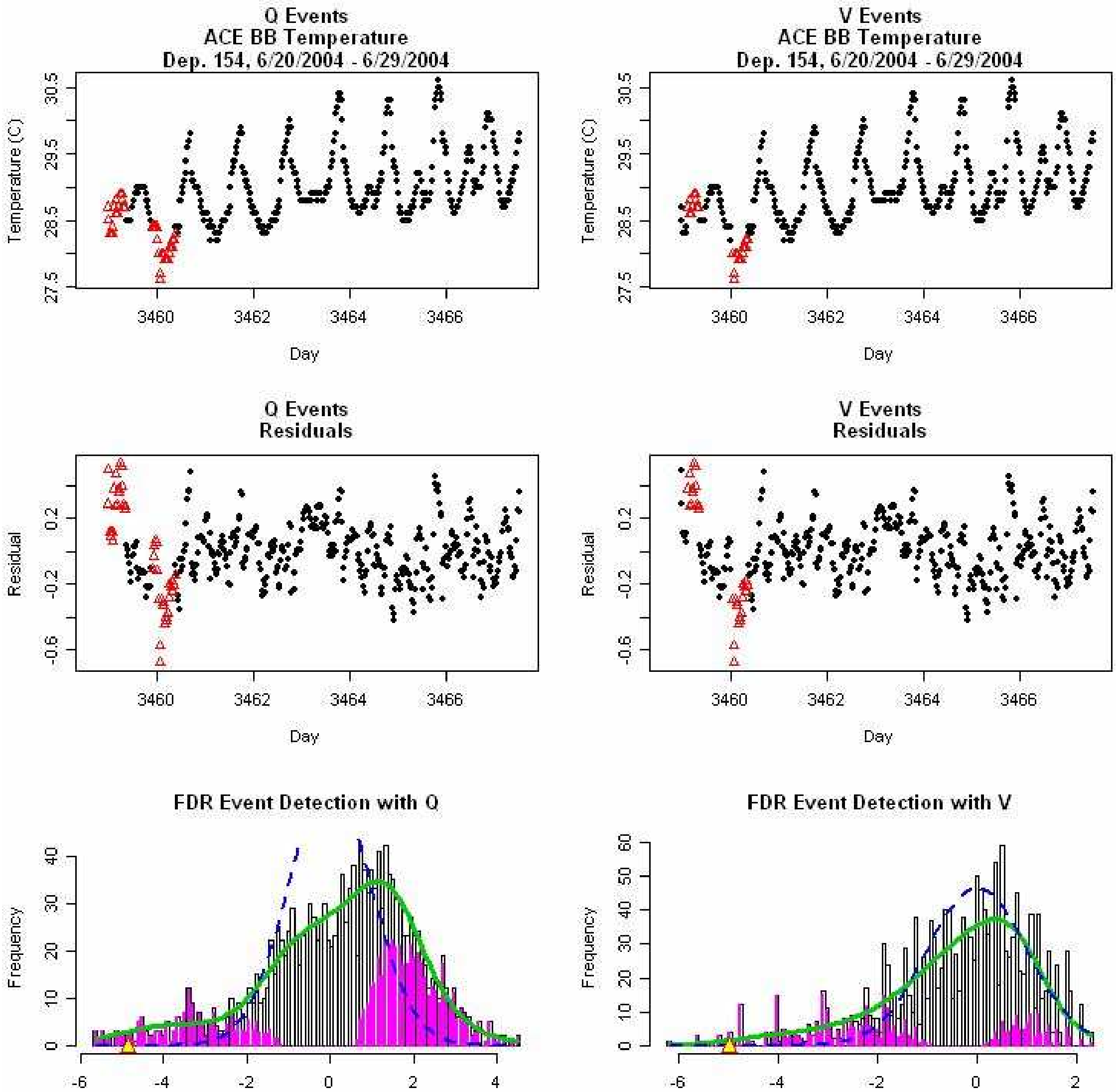


Figure 12 shows a graphical summary of the results of the event detection algorithm for a deployment of temperature (degrees Celsius) data collected during the June 20-29, 2004 deployment at the Big Bay site of the ACE Basin reserve. A higher-than-usual temperature event was detected at the beginning of the deployment using both test statistics. Similarly, a lower-than-usual temperature event was detected at the beginning of day 3460. Again, the test statistics differ in the length of the detected events, with Q^* detecting longer events.

Figure 12: ACE BB Temperature Events (Deployment 154)



3. Model high rainfall and wind impacts on ACE Basin NERRs sites.

The next step in our exploration is to investigate seasonal patterns in the rainfall event data. There are more rainfall events in summer time (May-September) than in winter time (Figure 13). In order to visually assess the relationship between rainfall events and change of water salinity at ACE Basin, the twenty eight largest rainfall events in terms of total precipitation were selected from the 420 rainfall events between July 1, 2001 and December 31, 2005. Preliminary inspections suggested that total precipitation of a rainfall event is a more significant variable than its duration. A rainfall period was defined as the time between two days before and four days after each rainfall event started. Meanwhile, the water quality sampling stations ACE Big Bay (ACEBB) and ACE Mosquito Creek (ACEMC) were selected based on data availability and their locations. ACEBB (station 1) is close to the South Carolina coast line and has the longest data record at the ACE Basin. ACEMC (station 3) is close to the ACE weather station at

Bennett's Point (station 0). The water quality data for these two locations were acquired from the official site of NERR Centralized Data Management Office.

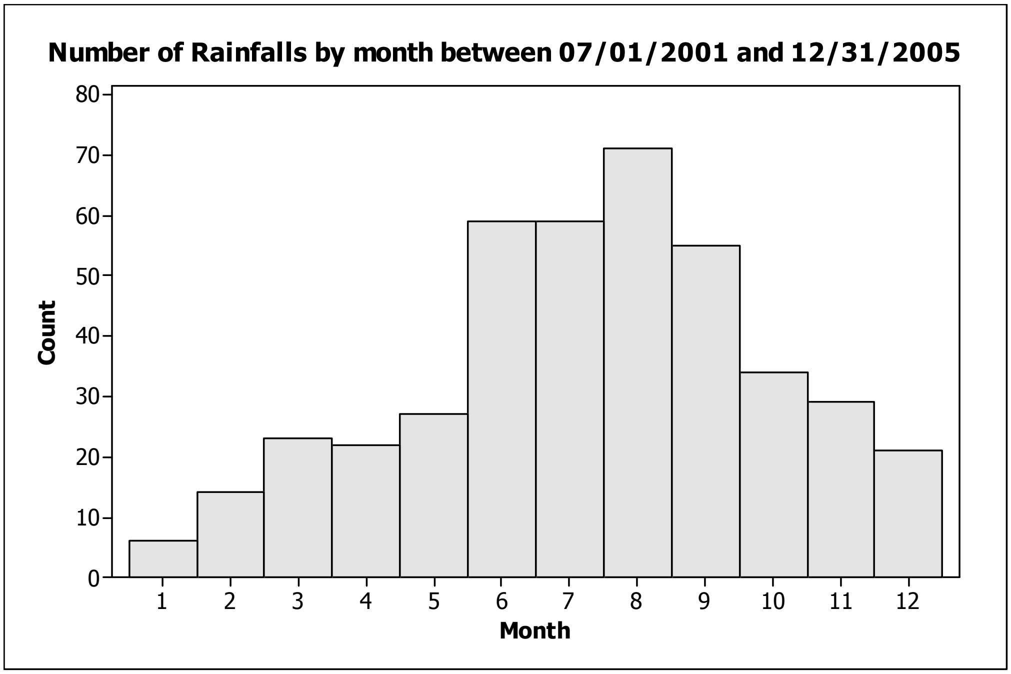


Figure 13: Number of rainfall events by month between 07/01/2001 and 12/31/2005

Scatterplots of water depth and salinity were generated for each rainfall event using Minitab. The title of each plot contains the information of water sampling station (ACEBB or ACEMC), the rainfall total precipitation ranking, rainfall precipitation (mm), rainfall duration (min) and the starting time of the event. A scatterplot of water depth is shown above the plot of water salinity in each figure to monitor tidal stage during corresponding rainfall period. All salinity plots of ACEBB and ACEMC stations have the same salinity scale from 0 to 38 ppt and from 0 to 30 ppt respectively. The left vertical reference line in each plot stands for the starting point of each rain event as the right one stands for the ending point.

ACE Big Bay Station

Scatterplots of water quality and salinity during the associated 27 largest rainfall periods were generated for ACE Big Bay station (Li, 2007). Rain 1 started in the middle of an ebbing tide. There were two large drops in salinity after the rainfall started, in synchrony with the falling tide. The overall average salinity appears to have decreased after the rainfall, and the salinity range per tidal cycle appears to have increased (Figure 14).

The information acquired from all the scatter plots of the ACEBB station is summarized in Table 2 shown below. In the table, all rainfall events are sorted by two major categories, the tide stages of rainfall onset and the types of reaction of water salinity to the rainfall events, and each category has four subcategories.

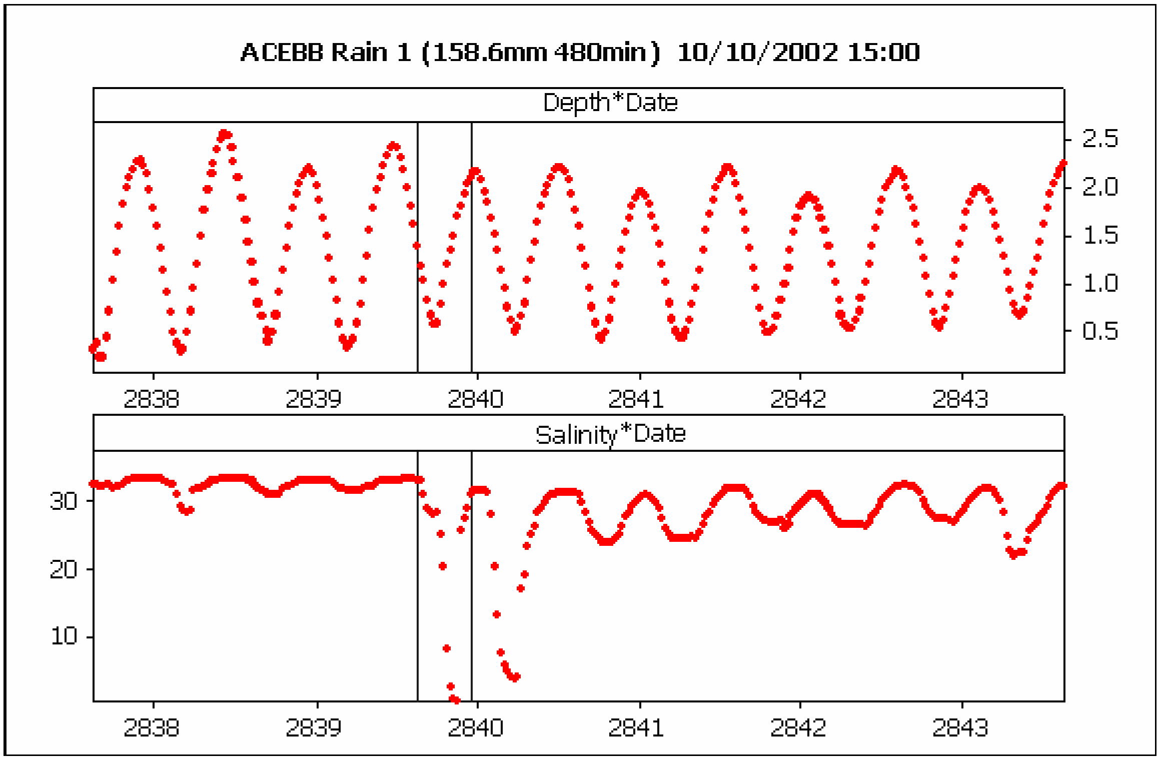


Figure 14: Scatter plot of ACEBB water depth and salinity during the rain 1 period

Table 2: Table of the rainfall events at the ACEBB station

Category		Tide stage of rainfall onset			
		High	Ebb	Low	Flood
Type of Reaction	No obvious change in salinity pattern	6, 18, 24, 25, 28	19, 23	20, 27	17
	"Lasting" drop in salinity (>4 days)	2, 3, 5, 9, 10, 11	1, 4, 12, 22	26	
	Increase in tidal range	2, 3, 5, 9, 10, 11	1, 12, 22	26	
	Temporary drop in salinity for a few tide cycles	11	1, 12, 21, 22	15, 26	7, 13, 14, 16

ACE Mosquito Creek Station

The available water quality data of ACE Mosquito Creek station, (located inland near the weather station), are dated between October 15, 2002 and December 31, 2005. There were seventeen of the largest rainfalls within this time period. The largest of these storms is depicted below to demonstrate the impact on salinity at this site. Rain 2 started at mid flood tide. The overall average salinity appears to have decreased after the rainfall, as did the tidal range for salinity (Figure 15).

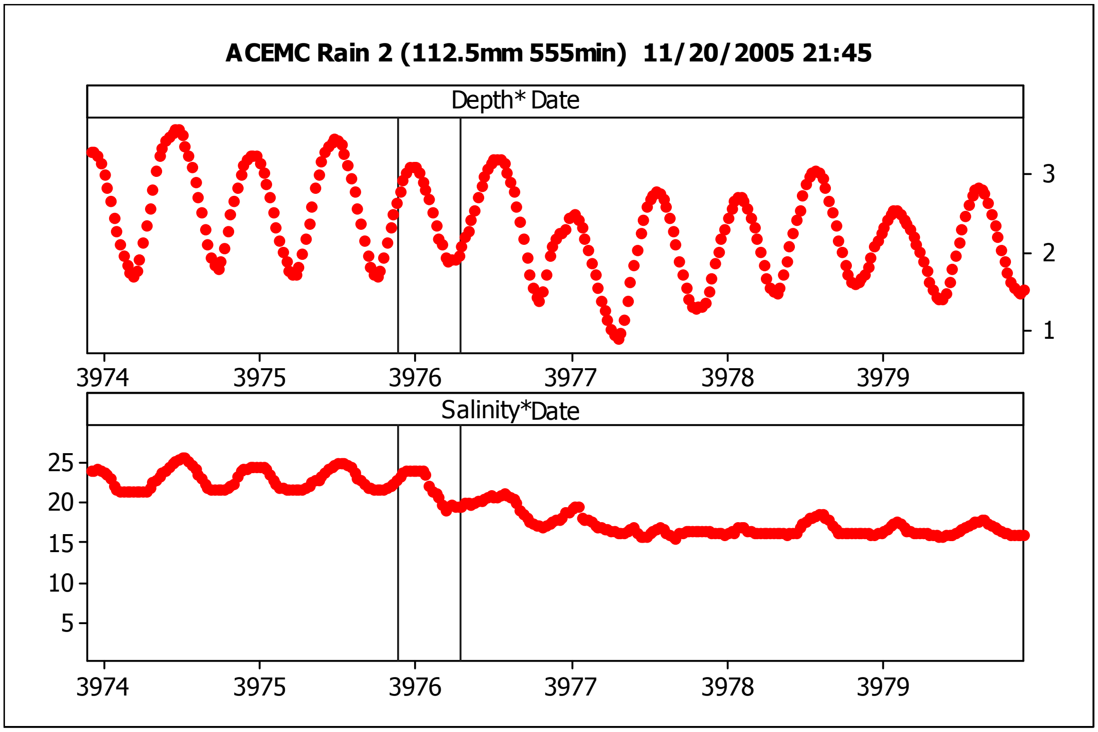


Figure 15: Scatter plot of ACEMC water depth and salinity during the rain 2 period

The information acquired from all the scatter plots of the ACEMC station is summarized in Table 3 shown below. Similar to Table 2, all rainfall events are sorted by two major categories, the tide stages of rainfall onset and the types of reaction of water salinity to the rainfall events, and each category has four subcategories.

In summary, about half of the rainfall events started at high tide at the ACEMC station, which is similar to the ACEBB station. Most of the rainfall events appear to have changed the salinity pattern after the rainfall. But unlike the ACEBB station, there was no rainfall event that caused a temporary drop in salinity for just a few cycles at the ACEMC station. Furthermore, it seems that rain 2 decreased the tidal range, which is very unusual.

The nonlinear model was fit to water salinity rainfall event data of ACEBB and ACEMC Stations using SAS PROC NLIN (Li, 2007). After checking the overlaid plots of predicted and original values, the model fits the data acceptably well for descriptive purposes, especially for ACEMC, because there were no large drops in salinity at this station. But this model does fail to predict some extreme values at both stations.

Table 3: Table of the rainfall events at the ACEMC station

Category		Tide stage of rainfall onset			
		High	Ebb	Low	Flood
Type of Reaction	No obvious change in salinity pattern	8		17	25
	"Lasting" drop in salinity (4+ days)	3, 5, 6, 9, 11, 18	4	19	2, 10
	Increase in tidal range	18, 28	23	20	
	Temporary drop in salinity for a few tide cycles				

As far as the variable change of predicted salinity ΔPS is concerned, the results of linear regression analysis from the two sampling stations are quite different from each other. For ACEBB, the model suggests that small total precipitation and large mean and mean absolute deviation of landward wind results lead to a large drop in salinity. For ACEMC, the model predicts that short rainfall duration, large total precipitation, small mean absolute deviation of precipitation and large mean absolute deviation of landward wind during rainfall period should cause a large drop in salinity. Though the variable PTOT appears in both models, it relates to the change of salinity in two different ways.

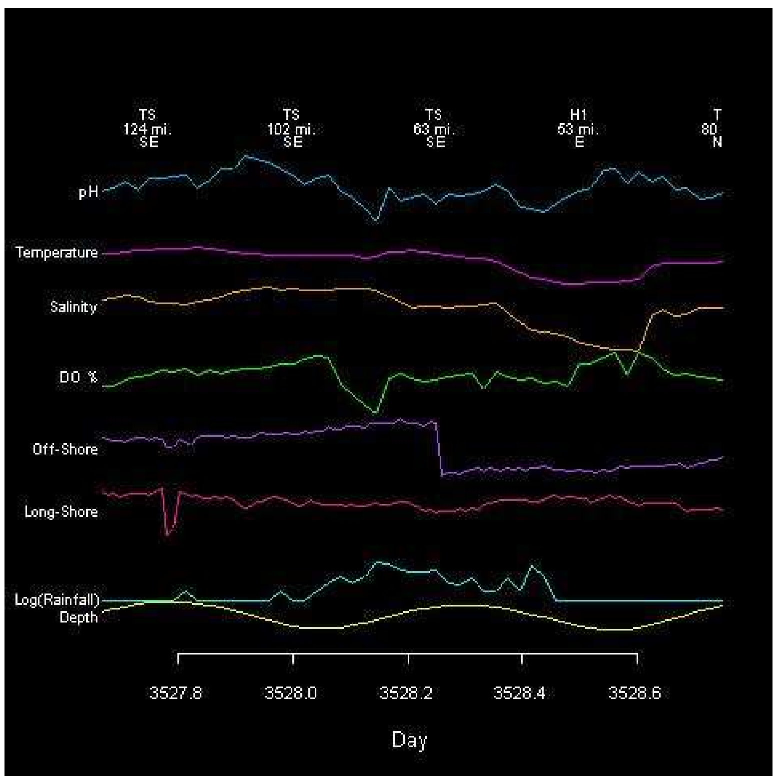
The results of regression analysis using the dependent variable $\Delta\beta_1$ are also different between the two stations. For ACEBB, the model suggests that larger mean absolute deviation of precipitation results in greater immediate drop of linear trend slope. For ACEMC, the model predicts that short rainfall duration, small mean absolute deviation of precipitation and large mean absolute deviation of long-shore wind during rainfall period should cause a greater immediate drop of slope. Though the variable PMAD appears in both models, it affects the dependent variable $\Delta\beta_1$ in opposite directions.

Finally, the third dependent variable ΔMS also has different results between the two stations. There is no common factor in the final models chosen. For ACEBB, no independent variables are significant at the 0.1 level. The significantly negative intercept suggests a drop in average salinity after the rainfalls. For ACEMC, the model suggests that small precipitation and a large mean absolute deviation of inland wind component tends to bring a greater drop in average salinity, which will typically be present given the large and negative intercept.

4. Storm tracks and impacted water quality at NERR SWMP sites.

Fourteen named storms have been graphically depicted in a movie format which allows simultaneous viewing of key meteorological data as forcing variables and selected responding water quality parameters. Deployment August 26-September, 2004 was coincident with Hurricane Gaston. The storm was within 200 miles of ACE Basin St. Pierre site from August 24-September 3, 2004. Each frame of the movie displayed one day in the time course of the hurricane event (Figure 16). At the top of the frame is the classification of the storm from TD tropical depression, TS tropical storm, H1 class X hurricane, distance from the site to the eye of the storm, and wind direction. The meteorological variables included in the graphic are off-shore winds, long-shore winds and rainfall. The water quality variables depicted have been through the Phase I periodicity removal and demonstrate divergence from baseline values.

Figure 16. Hurricane Gaston in the ACE Basin site, St. Pierre Creek. (August 28, 2004)



Discussion

Removing periodicity

We have investigated the use of classical harmonic regression models and nonparametric harmonic regression models (generalized additive models) for estuarine water quality data. We explored the performance of these models using real time series from the National Estuarine Research Reserve System.

For the NERRS data, classical harmonic regression techniques work well for the analysis of depth data; however, they are not as satisfactory for analysis of other, less regular, water quality variables. The GAMs show great potential for these applications. The cubic and cyclic regression splines are competitive with one another in terms of fit. However, in practice, the cubic regression spline often had an "edge effect" problem with the NERRS data, whereas the cyclic regression splines resulted in smoothly periodic functions. The GAMs are also more automatically adaptive and require less user-intervention than the harmonic regression models. When using harmonic regression, the user must determine the number of harmonics for each periodic term. For the NERRS data, this decision would need to be made for each variable of each deployment in phase I analysis. For the data in the CICEET NERRS project, this would result in nearly 12,000 phase I decisions. In phase II analysis, this decision would again need to be made for each variable at each site. Using GAMs to model the data is much more automated. We believe that generalized additive models are a very promising method for modeling estuarine water quality data, and more generally, for any time series with strong and potentially non-sinusoidal signals of known period. The ease of their use in R also makes them very appealing. Not only are they adaptive and user-friendly, but they are also non-prohibitive in terms of computation time; for example, phase I analyses for 150 deployments of depth data take approximately 3.5 minutes to complete on an Intel® Pentium® M 1.60 GHz processor.

Event Detection

We have adapted Efron's local false discovery rate methods for detecting events in estuarine water quality data. We used a sum of squared residuals test statistic, Q^*, as well as a more nonparametric test statistic, V^*, which is the minimum absolute error for a sequence of residuals. We developed a data-driven event detection algorithm that uses both test statistics in calculating local false discovery rates. We used the event detection algorithm to detect events in the water quality data collected at the ACE Basin NERRS reserve.

For the deployments from the ACE Basin reserve in which the locfdr function did not fail, results seem to be quite varied, even using a very low false discovery rate threshold $\tau=0.0001$. In some cases, the Q^* and V^* test statistics detected similar events that were believable. There were cases in which the two test statistics detected completely different events. In other cases, too many events were detected for the results to be believable. The reasons for these shortcomings when using the NERRS data are unclear.

Future Research

If extreme events or mid-length and long events of moderate intensity are present in a time series, this could influence the ability of the GAM to estimate the periodic components. Thus, two passes of the GAM and event detection algorithm could be employed. In the first pass, the most extreme and obvious events are removed from the dataset. In the second pass, the observations that were not detected as events are modeled with the GAM. This second pass should more accurately estimate the periodic components. The resulting residuals can then be analyzed using the event detection algorithm. Once events are detected in a time series, causes for the events should be explored. Water quality events can be compared to known meteorological events, such as rainfall events, droughts, and El Niño/La Niña climatic cycle effects. Numerical, objective detection of events is just the first step.

Utilization

This project was a development of future modeling techniques and could not be readily transferred to managers at the current stage (see future application section for plan for technology transfer).

Intellectual Property and Partnerships

The partnership between the University of South Carolina statistical professors and graduate students enhanced the quality of the analysis. Continuing this collaborative effort will yield ecological relevant information and modeling products useful to NERRs managers.

Knowledge Exchange

Presentations:

Joint Statistical Meeting. Seattle, August 2006, "Nonparametric Harmonic Regression for Estuarine Water Quality Data", Melanie Autin. She received the 2006 ASA Section on Statistics and the Environment (ENVR) JSM Presentation award.

Manuscripts:

Autin, Melanie and Don Edwards. (submitted). Nonparametric Harmonic Regression for Estuarine Water Quality Data.

Graduate students supported by this project:

Melanie Autin, PhD, Statistics Department, USC May 2007
Ross Li, MS, Statistics Department, USC. May 2007

Additional materials:

Hurricane CD: contains all water quality variable “movies” from southeastern NERRs sites during named storms.

Application

The statistical analyses summarized in this report, and detailed with the USC statistical thesis and dissertations (Li, 2007, Autin 2007) could be conducted on additional NERRs data to remove periodicity and detect events within their reserves. All the software needed, models are included in the appendix of the students’ thesis and dissertation.

Managers and scientist utilizing reserve databases could use new statistical tools to further investigate the impact of short and long term natural perturbations and anthopogenic impacts. This statistical analysis is quite advanced, however, and even with the work the students did to outline and streamline the procedure, requires analytical skills and lengthy computer time. These obstacles could be overcome if statisticians were integrated into the NERRs database management. Identifying universities who would collaborate with NERRs managers to facilitate intensive modeling efforts would encourage more utilization and investigation of the existing NERRs databases. One example of effective university/reserve collaboration is the existing relationship of the Statistical department at the University of South Carolina with ACE Basin, Sapelo Island, and North Inlet/Winyah Bay reserves.

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