

Adaptation of a weighted regression approach to evaluate water quality trends in an estuary

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Abstract

The increasing availability of long-term monitoring data can improve resolution of temporal and spatial changes in water quality. In many cases, the fact that changes have occurred is no longer a matter of debate. However, the relatively simple methods that have been used to evaluate trends in environmental monitoring data in estuaries are often not sufficient to disaggregate the complex effects of multiple environmental drivers, limiting the potential to relate changes to possible causes. To improve the description of long-term changes in water quality, we adapted a weighted regression approach developed to describe trends in pollutant transport in rivers to analyze a long-term water quality dataset from Tampa Bay, Florida. The weighted regression approach allows for changes in the relationships between water quality and explanatory variables by using dynamic model parameters and can more clearly resolve the effects of both natural and anthropogenic drivers of ecosystem response. The model resolved changes in chlorophyll-*a* (chl-*a*) from 1974 to 2012 at seasonal and multi-annual time scales while considering variation associated with changes in freshwater influence. Separate models were developed for each of 4 Bay segments to evaluate spatial differences in patterns of long-term change. Observed trends reflected the known long term decrease in nitrogen loading to Tampa Bay since the 1970s, such that chl-*a* concentration decreased by 32% after municipal improvements in wastewater treatment. Although trends in mean chl-*a* have remained constant since mitigation of point-sources of pollution, model predictions indicated that variation has increased in recent years for upper Bay segments, as well as an overall decrease in low productivity events for the lower Bay. Changes in model parameters for the last decade indicated that the relationship of salinity with chl-*a* was unimodal rather than continuous for upper Bay segments, such that flushing effects were observed beyond specific thresholds. Results from our analyses have allowed additional insight into water quality changes in Tampa Bay that has not been possible with traditional modeling approaches and the approach could easily be applied to other systems with long-term datasets.

Key words: chlorophyll, estuary, salinity, Tampa Bay, trend evaluation, weighted regression

1 Introduction

Eutrophication has been documented in aquatic systems worldwide and is of particular concern for coastal waters that support numerous aquatic life and human uses. Eutrophication is defined as an increase in the rate of supply of organic matter to a system (Nixon 1995) and is typically caused by elevated nitrogen or phosphorus loads. Although nutrients are necessary for the growth of primary producers, excessive anthropogenic inputs can have serious consequences for the structure and function of aquatic systems. Eutrophication of coastal systems has been associated with depletion of dissolved oxygen from the decomposition of organic matter (Diaz 2008), increases in the frequency and severity of harmful algal blooms (Glibert *et al.* 2013), and reduction or extirpation of seagrass communities (Duarte 1995, Tomasko *et al.* 2005). System-wide changes can occur as the effects of eutrophication on primary production propagate to upper trophic levels (Powers *et al.* 2005).

The effects of eutrophication are generally well understood, particularly for freshwater systems. The consequences of nutrient pollution were increasingly obvious by the 1960s such that eutrophication became a central focus of limnological research (Cloern 2001). However, the importance of understanding the relative effects of eutrophication on coastal systems were not realized until several decades later. For example, Rosenberg (1985) described the future hazards of coastal eutrophication nearly twenty years after similar issues were the focus of intense study in freshwater systems. Approaches for describing nutrient dynamics in coastal systems have relied heavily on freshwater eutrophication models that may not adequately describe idiosyncratic behaviors of individual estuaries. For example, Cloern (2001) suggests that system-specific attributes modulate coastal response to nutrient inputs, such that more appropriate conceptual

models that recognize linked changes in relevant state variables are needed. To date, empirical models that are flexible and appropriate for site-specific conditions have not been extensively applied to describe nutrient-response dynamics in estuaries.

The increasing availability of long-term, high resolution datasets has further underscored the need to develop quantitative nutrient-response models given the potential to extract detailed information on system dynamics. In many cases (e.g., [Caffrey 2003](#), [Greening and Janicki 2006](#)), long-term datasets have sufficiently described general trends in response to changing nutrient regimes or seasonal dynamics, although unambiguous and quantitative descriptions of responses have been lacking. For example, temporal variations in phytoplankton growth dynamics are often apparent by season with typical late summer blooms in temperate or tropical systems ([Cloern 1996](#)), whereas climate variation may contribute to substantial deviation in growth patterns between years ([Jassby *et al.* 2002](#)). Additionally, spatial heterogeneity in algal response to nutrients is common across salinity gradients such that effects of flux variation are most apparent near freshwater inflows ([Cloern 1996](#)). Simple statistical models that are constrained by assumptions of linearity and stationarity of variables through time may not adequately characterize subtleties in the variation of nutrient-response measures at different scales. Novel techniques that leverage the descriptive capabilities of large datasets are needed to improve our understanding of temporal and spatial variation in chlorophyll dynamics as a measure of eutrophication.

Use of simple descriptive statistics to evaluate the effects of water quality management may be ill-advised given that general trends in monitoring data may reflect both management actions and natural variation in system characteristics. [Hirsch *et al.* \(2010\)](#) developed the Weighted Regressions on Time, Discharge, and Season (WRTDS) approach to model pollutant

concentration in rivers to address these issues and shortcomings of previously-developed models. WRTDS enables a flexible interpretation of water quality changes by estimating multiple parameters that are specific to a given season, year, and discharge for individual observations across the time series. This allows for a more detailed description of water quality changes than standard regression models that characterize trends using a single set of parameters. Accordingly, the approach addresses the need to focus on descriptions of change in relation to water quality variables across time, rather than hypothesis testing. The approach has been applied to model pollutant delivery from tributary sources to Chesapeake Bay (Hirsch *et al.* 2010, Moyer *et al.* 2012, Zhang *et al.* 2013), Lake Champlain (Medalie *et al.* 2012), and the Mississippi River (Sprague *et al.* 2011). The successful applications to water quality trends in rivers suggest the approach could potentially be applied to estuaries to characterize and better understand long-term changes in water quality. Moreover, changes in pollutant sources and variation in freshwater inputs over time for many coastal systems warrant the use of novel methods for trend evaluation. Resolving these changes may improve our understanding of linkages between drivers and responses over time.

Water quality data have been collected in the Tampa Bay estuary (Florida, USA) for approximately forty years. The natural history of Tampa Bay and the corresponding data provide a useful opportunity for applying quantitative methods to model nutrient dynamics. Nitrogen loads in the mid 1970s were estimated at $8.2 \times 10^6 \text{ kg yr}^{-1}$, with approximately $5.5 \times 10^6 \text{ kg yr}^{-1}$ entering the upper bay alone (Poe *et al.* 2005, Greening and Janicki 2006). Reduced water clarity associated with phytoplankton biomass contributed to dramatic reduction in the areal coverage of seagrass (Tomasko *et al.* 2005) and development of hypoxic events causing a decline in benthic faunal production (Santos and Simon 1980). Extensive efforts to reduce nutrient loads to the Bay

occurred by the late 1970s, with the most notable being improvements in infrastructure for wastewater treatment in 1979. Improvements in water clarity and decreases in chlorophyll-*a* (chl-*a*) were observed bay-wide in the 1980s, with conditions generally remaining constant to present day. Although the nutrient management program has been successful in improving water quality, variation in water quality drivers over time suggests the WRTDS method could provide information on system dynamics that are not apparent from the observed data.

The goal of the analysis was to describe changes in algal biomass in an estuary in relation to time, season, and freshwater inputs. We adapted the WRTDS approach developed by [Hirsch *et al.* \(2010\)](#) to describe water quality trends using a multi-decadal dataset from Tampa Bay, Florida. The analysis addressed four main objectives. First, we described the weighted regression model and provided a rationale for its adaptation to estuaries. Second, we applied the model to the time series in different segments of Tampa Bay to characterize trends in both the mean response of chl-*a* and the frequency of occurrence of extreme events using quantile regression. Third, additional factors related to water quality were used to describe the unexplained variance in chl-*a* growth patterns not characterized by the model. Specifically, model residuals were compared with variation in seagrass growth, El Niño-Southern Oscillation (ENSO) effects, and nitrogen load and concentrations in the Bay. Finally, we developed informed hypotheses to explain temporal and spatial patterns in chl-*a* growth in response to large scale drivers that affect water quality. Results from the analysis provide a natural history of water quality changes in Tampa Bay that is temporally consistent with drivers of change. This analytical approach may improve our understanding of the nutrient-response paradigm in coastal systems.

2 Methods

2.1 Data

We compiled a time series of chl-*a* concentration ($\mu\text{g L}^{-1}$) in Tampa Bay using data from the Hillsborough County Environmental Protection Commission (EPC) (TBEP 2011). Data are monthly at mid-depth for each of 50 stations throughout the Bay (Fig. 1) from 1974 to 2012, producing approximately 456 observations per station ($n = 1820$, Fig. 2). Stations were visited on a rotating schedule such that one third of all stations were sampled each week. Bay segments represent management units of interest with distinct chemical and physical differences (Table 1, Lewis and Whitman 1985). Accordingly, station data were averaged by segment. In addition to chl-*a*, salinity data were obtained and used as a tracer of freshwater influence on water quality. We expected that salinity was an important factor influencing interpretation of chl-*a* trends relative to the effects of additional factors (e.g., date, nutrient load, seagrass, etc.). Salinity data were converted to dimensionless values that represent the fraction of freshwater (Dyer 1973), such that:

$$Sal_{ff} = 1 - \frac{Sal_{mea}}{Sal_{ref}} \quad (1)$$

where Sal_{mea} is the measured salinity for a given station and Sal_{ref} is salinity at the seaward reference station for each observation date. Station 94 in the Gulf (Fig. 1) was used for reference salinity. Chlorophyll concentrations below the detection limit (censored data) were set to one-half the value from the limit to zero (Gilbert 1987). Chlorophyll data were \ln -transformed because observations were skewed right, similar to a log-normal distribution. Kolomogorov-Smirnov tests indicated that the raw data were not significantly different from theoretical log-normal distributions.

2.2 *Weighted regression*

WRTDS was adapted to relate chlorophyll concentration to salinity and time:

$$\ln (Chl) = \beta_0 + \beta_1 t + \beta_2 Sal_{ff} + \beta_3 \sin (2\pi t) + \beta_4 \cos (2\pi t) + \epsilon \quad (2)$$

where the natural log of chl-*a* is related to decimal time *t*, salinity *Sal_{ff}*, and unexplained variation ϵ . Salinity and time are linearly related to chl-*a* on a sinusoidal annual time scale (i.e., cyclical variation by year). The parameters β_0, \dots, β_4 are estimated for each observed salinity at time *t* such that multiple sets of parameters are used to characterize the period of observation. Decimal time was calculated as the the year and month of each observation as an equivalent decimal (e.g., July 1974 as 1974.5). Although data were typically not collected on the first of each month, we considered the decimal time coincident with the period of observation. Additionally, quantile regression models (Cade and Noon 2003) were used to characterize trends at extreme conditional distributions of the data. Specifically, we adapted the weighted regression approach to model the conditional response at the 10th and 90th quantiles ($\tau = 0.1$, and 0.9, respectively) of the chlorophyll distribution. Quantile regression is analogous to least-squares regression such that a set of β parameters that minimizes the error term is estimated, where the minimization function is the sum of the weighted absolute deviations of the fitted values from the observed quantile. A general interpretation of the fitted values is the distribution of chl-*a* conditional upon time and salinity for low ($\tau = 0.1$) or high ($\tau = 0.9$) biomass events, rather than a characterization of ‘average’ conditions using mean models.

The WRTDS approach obtains fitted values of the response variable by estimating regression parameters for each unique observation. Specifically, a regression model was estimated

for each of 1, . . . , 456 data points for each Bay segment. Each regression model was weighted by month, year, and salinity such that a unique set of regression parameters for each observation in the time series was obtained. For example, a weighted regression for October 2003 weights other observations in the same year, month, and similar salinity with higher values, whereas observations for different months, years, or salinities receive lower weights (Fig. 3). This weighting approach allows estimation of regression parameters that vary in relation to observed conditions. [Hirsch *et al.* \(2010\)](#) used a tri-cube weighting function:

$$w = \begin{cases} \left(1 - (d/h)^3\right)^3 & \text{if } |d| \leq h \\ 0 & \text{if } |d| > h \end{cases} \quad (3)$$

where the weight w for each observation is defined by the distance d from the current observation within a window h . The weights are diminishing in relation to the current observation until the maximum window width is exceeded and a weight of zero is used. The weight for each observation is the product of all three weights assigned to month, year, and salinity. Window widths of six months, 10 years, and half the range of Sal_{ff} for each Bay segment were used (Fig. 3). Window widths were increased by 10% increments during model estimation until a minimum of 100 observations with non-zero weights were obtained ([Hirsch *et al.* 2010](#)).

The adapted WRTDS approach was used to model and interpret chl- a trends from 1974–2012 for each of the 4 bay segments. In contrast with ([Hirsch *et al.* 2010](#)), estimates were made using monthly observations rather than daily predictions given the available data for Tampa Bay. Particular attention was given to trends that have not been previously described. Following [Hirsch *et al.* \(2010\)](#), predicted values were based on interpolation matrices for each model type

(mean, 90th percentile , and 10th percentile) to reduce computation time. Specifically, a sequence of 20 salinity values based on the minimum and maximum values for each segment were used to predict chl-*a* using the observed month and year. Model predictions were then linearly interpolated from the grid using closest salinity value to the actual for each date. [Hirsch *et al.* \(2010\)](#) notes that the introduction of bias associated with using imprecise values in place of actual observations to estimate predictions was minimal. Model performance was based on coefficients of determination (R^2) for the mean regression models and pseudo- R^2 values that are specific to given quantiles ([Koenker and Machado 1999](#)). Additionally, root mean square error ($RMSE$) was calculated as an alternative measure of performance such that:

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}} \quad (4)$$

where n is the number of observations from 1, \dots , n for a given segment, y_i is the observed value of ln-chl-*a* for observation i , and \hat{y}_i is the predicted value for of ln-chl-*a* for observation i . $RMSE$ values closer to zero represent model predictions closer to observed. The performance of weighted models were compared to conventional (i.e., non-weighted) additive linear models to show potential improvements using the WRTDS approach.

A potential issue for predictions with regression models in ln-transformed space is bias associated with back-transformation ([Duan 1983](#)). Specifically, predicted values that are back-transformed by exponentiation may be biased due to variation in the concentration-salinity (or concentration-discharge) relationship through changes in residual variation across the data domain. We followed the approach in [Moyer *et al.* \(2012\)](#) that corrected for back-transformation bias using a scale parameter that is independently estimated for all regression models in the time

series. The scale parameter describes the variance of the residuals such that:

$$\hat{\sigma}_{\epsilon}^2 = \frac{\sum_{i=1}^n w_i (y_i - \hat{y}_i)^2}{\sum_{i=1}^n w_i} \quad (5)$$

where residual variance $\hat{\sigma}_{\epsilon}^2$ (scale parameter) is the weighted sum of squared errors for chlorophyll for observations $1, \dots, n$. Scale parameters were obtained for each unique regression across the time series and used to determine the correction bias in the back-transformation such that:

$$\alpha = \exp\left(\frac{\hat{\sigma}_{\epsilon}^2}{2}\right) \quad (6)$$

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$$\hat{C}hl = \alpha \exp(\beta_0 + \beta_1 t + \beta_2 Sal_{ff} + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)) \quad (7)$$

where the back-transformed chlorophyll concentration $\hat{C}hl$ is the exponentiated model prediction multiplied by the correction factor α (Moyer *et al.* 2012). Unique scale and correction bias parameters were obtained for each observation that was back-transformed. Although differences between results from bias-corrected predictions and simple exponentiation were minimal, eqs. (5) to (7) were used to create more accurate representations of chlorophyll trends in accordance with developed methods (i.e., Hirsch *et al.* 2010, Moyer *et al.* 2012).

In addition to trend description, the WRTDS approach can be used to normalize predicted values for a given explanatory variable to allow interpretation of trends in the absence of random variation. For example, water quality trends related to management actions cannot be precisely evaluated if pollutant concentrations vary with discharge. Hirsch *et al.* (2010) used the approach to normalize trends by flow, whereas our adapted approach was used to normalize by salinity

which accounts for both freshwater inputs and tidal exchange. Normalized predictions were obtained for each observation date by assuming that salinity values for the same month in each year were equally likely to occur across the time series. That is, salinity is assumed to be uniformly distributed within the range of observed values for the same month between years. For example, normalization for January 1st 1974 considers all salinity values occurring on January 1st for each year in the time series as equally likely to occur on the observed data. A normalized value for January 1st 1974 is the average of the predicted values using each of the salinity values as input, while holding month and year constant. Normalization across the time series is repeated for each observation to obtain salinity-normalized predictions.

2.3 *Evaluation of model residuals*

An advantage of the WRTDS approach is the ability to describe water quality trends by considering changes in the relationships among variables for different observation periods. Additional factors not related to time or salinity could be used to describe the unexplained variation in the models (ϵ , eq. (2)). Residuals for the mean and quantile models in each Bay segment were related to additional variables with considerable management importance: seagrass growth, ENSO climate effects by season and year, and nitrogen load and concentrations. Conventional statistics were used to obtain a general description of the relationships, such as correlation coefficients and linear regression.

Seagrass coverage in Tampa Bay has been estimated bi-annually since 1988 (Tomasko *et al.* 2005). Coverage data are based on interpretation of aerial photos to produce raster surfaces with pixels coded as continuous ($>75\%$) or patchy ($25\%–75\%$) coverage. Areal coverage of seagrass for years with available data ($n = 12$) were estimated by considering seagrass as present

(continuous or patchy) or absent within each Bay segment. ENSO data obtained from the Climate Prediction Center (CPC 2013) were based on a three year running-average of Sea Surface Temperature (SST) anomalies in the Niño 3.4 region of the Pacific Ocean (5°N–5°S, 120°–170°W). SST index values greater (less) than 0.4 (-0.4) were considered El Niño (La Niña) conditions, neutral otherwise. SST index values were categorically and quantitatively summarized by year and season using designations in Lipp *et al.* (2001): winter - January, February, March; spring - April, May, June; summer - July, August, September; fall - October, November, December. Finally, monthly loads for total nitrogen (TN, kg/mo) from 1985–2007 were obtained (Zarbock *et al.* 1994, Pribble *et al.* 2001, Poe *et al.* 2005), in addition to TN concentration from monitoring data (TBEP 2011). Nitrogen loads are based on estimated and measured contributions from nonpoint sources, point sources, atmospheric deposition, groundwater, and losses of phosphate rock and fertilizer from industrial processes.

3 Results

3.1 Observed trends in chlorophyll

Observed chl-*a* for all dates indicated mean values decreasing from Hillsborough (13 $\mu\text{g L}^{-1}$), to Old (8.8), to Middle (7.3), and to Lower Tampa Bay (3.8). Observed trends from 1974 to 2012 indicated a consistent decrease from 1974 to present as previously documented, with the most dramatic declines observed in the 1980s following wastewater treatment efforts (Fig. 2a). Percent decrease by segment based on mean concentration of chl-*a* for observations prior to and after January 1st 1980 was 53.4% for Hillsborough, 31.4% for Middle, 25.5% for Old, and 16.8% for Lower Tampa Bay. Observed trends in chl-*a* before and after treatment for the entire Bay indicated a decrease of 32.4%. Interestingly, the most dramatic declines in chl-*a* following

treatment of point sources of pollution were not observed until a few years after 1979. For example, hypereutrophic conditions persisted in Hillsborough Bay until 1984 when mean annual concentration from 1983 to 1984 decreased by 48.5%, whereas a decrease of only 28.5% was observed from 1979 to 1980. Peaks in chl-*a* have also been observed in the mid-1990s associated with El Niño effects (Greening and Janicki 2006). For example, 29.6 $\mu\text{g L}^{-1}$ of chl-*a* was observed for Old Tampa Bay in October 1995. More extreme observations have been observed for individual stations during El Niño events.

Seasonal trends in observed chl-*a* were also consistent with documented changes, primarily in response to precipitation patterns. Maximum concentrations were generally observed in late summer whereas, minimum concentrations were observed in mid winter (Fig. 2b). Mean concentrations for the entire Bay were 12.8 $\mu\text{g L}^{-1}$ for September and 4.5 for February. Trends by Bay segment were similar except that the amplitude of seasonal peaks diminished with proximity to the Gulf. For example, mean September and February concentrations for Lower Tampa Bay were 6.5 and 2.3, whereas concentrations in the same months for Hillsborough Bay were 21.9 and 8.4. Relationships of observed chl-*a* with salinity (as Sal_{ff}) indicated higher proportion freshwater was associated with higher chl-*a* (Pearson $\rho = 0.6$, $p < 0.005$, all observations). Correlations between chl-*a* and salinity by bay segment were similar (Pearson $\rho \approx 0.4$, $p < 0.005$ for all), with a slightly lower correlation in Old Tampa Bay ($\rho = 0.32$).

3.2 Predicted trends in chlorophyll

Predicted values obtained from the adapted WRTDS approach accounted for the effects of time and salinity on chl-*a* and generally followed observed trends as expected (Fig. 4). Weighted regressions were more precise than non-weighted additive linear regressions for all model types

(Table 2). Mean explained variance using R^2 for all Bay segments was 0.45, 0.44, and 0.64 for the 90th percentile, 10th percentile, and mean models, respectively, compared to 0.3, 0.3, and 0.52 for the null models. Mean error using $RMSE$ for all Bay segments was 0.61, 0.62, and 0.37 for the 90th percentile, 10th percentile, and mean models, respectively, compared to 0.69, 0.7, and 0.43 for the null models. Additionally, increases in predictive performance from a non-weighted to weighted approach were slightly higher for the quantile models as compared to the mean models. Increases in predictive performance based on R^2 for both quantile models was 0.15 averaged for all Bay segments, whereas mean models increased an average of 0.12 over standard regression models. Similar trends were observed for $RMSE$ values (Table 2).

Substantial variation in chl-*a* response from the mean predicted values was observed despite high explained variance (Fig. 4). Observed values close to the mean response were fit well by the mean model, whereas extreme observations at low or high ends of the distribution were better predicted by the quantile models. For example, Fig. 5 shows the predicted and observed values for a two year period in Hillsborough Bay such that model fit varies depending on the month of observation. Model fit for peak observed chl-*a* in September and October of 1994 is best fit by the 90th percentile models, whereas a low seasonal peak observed in the winter of 1994 was best fit by the 10th percentile model. Larger differences between the predicted values for the 90th and 10th models was also observed in earlier years of the time series, such that the period from 1974-1980 had larger variation in predicted chl-*a*, in addition to higher overall mean values (Fig. 4).

Aggregation of model results by year allowed an evaluation of annual trends for predicted and salinity-normalized concentrations (Fig. 6). Predicted values illustrated response of chlorophyll by model type, whereas salinity-normalized estimates indicated annual trends

independent of variation in tidal effects of tributary inputs by model segment. In general, trends were similar by model type such that increases or decreases in chl-*a* were similar regardless of the distribution that was characterized (i.e., mean, 0.9 τ , or 0.1 τ). Exceptions are noted for the 90th percentile models in the early years of the time series such that the frequency of high chl-*a* events were more common. Decreases in the range of chl-*a* for Lower Tampa Bay in recent years is also apparent such that the mean response is approximately the same, whereas the 90th percentile and 10th percentile models decrease in magnitude in the direction of the mean. Additionally, recent trends for Middle and Lower Tampa Bay for the 10th percentile models suggest an increase in chl-*a* such that the occurrence of low concentration events are decreasing. An annual peak in predicted chl-*a* for 1998 was observed for all Bay segments which is not apparent for the salinity-normalized data. Further aggregation of the salinity-normalized results in Table 3 illustrated trends on a decadal time scale. In particular, trends prior to treatment of point sources of pollution from 1974–1980 generally indicated high and increasing chl-*a* for all segments and model types, excluding the 10th percentile model for Hillsborough Bay which showed consistent declines for the period. In contrast, the most dramatic declines in chl-*a* were estimated from 1980 to 1990 for all Bay segments. Accordingly, mean chl-*a* concentrations from 1980–1990 were less than the previous time period. A slight positive increase for the 10th percentile model for Lower Tampa Bay in recent years is also evident on a decadal time scale.

Of potential interest is an evaluation of between-year variation for all salinity-normalized estimates. In particular, stationarity (i.e., equal variance) of chl-*a* estimates by year and model type was not observed (Table 4 and Fig. 7). Maximum within-year variation for all models was generally observed in recent years, with exceptions for models in Lower Tampa Bay where maximum variation was observed in 1993 (40.9 coefficient of variation, CV) for the mean model,

1975 (40.8) for the 90th percentile model, and 1988 (38.7) for the 10th percentile model. CV estimates between-years were also variable, with some segments and models varying more than 50% (e.g., 10th percentile model for Hillsborough Bay). Additionally, increasing variation throughout the time series was observed for the 90th percentile model for Old Tampa Bay with CV values ranging from 25.4 in 1977 to 63.4 in 2012. Variation in salinity-normalized chl-*a* estimates across seasons were comparable, although variation was reduced in summer months (Table 4). Additionally, high variation was observed for Hillsborough Bay in winter and for Lower Tampa Bay in fall.

Evaluation of model parameters across the time series provided insight into the dynamic relationships between the modelled response and predictor variables. Specifically, slope estimates for each weighted regression of each observation (multiplied by Sal_{ff} for unit conversion) were retained to evaluate the effects of salinity on chl-*a* across the time series. Changes in the response of ln-chl-*a* across salinity gradients for each Bay segment were observed based on the period of observation (Fig. 8). For example, the response of chl-*a* in Hillsborough Bay with increasing freshwater input for the first two time periods was minimal, whereas a strong positive relationship is observed from 1990–2000 followed by a unimodal response from 2000–2012. Interestingly, non-linear responses were also observed for Old and Middle Tampa Bay for the 1990–2000 and 2000–2012 periods, respectively, such that chl-*a* response reverses beyond a specific threshold. Lastly, variation in chlorophyll response to proportion freshwater by season indicated increasing trends, although less variability than between years was observed.

3.3 *Evaluation of model residuals*

Mean residual values by segment indicated that the 90th and 10th percentile models over- and under-fit the respective quantile distributions, whereas residual values for the mean models were centered at approximately zero. In other words, the 90th percentile and 10th percentile models produced residuals that were negative and positive in sign, respectively, which is expected given the definition of quantile distributions. Correlations of residuals to additional explanatory variables indicated that chlorophyll response could be attributed to factors other than time and salinity (Table 5). Not surprisingly, significant correlations were observed with TN for all segments and models, although correlations were observed for concentration rather than load. All models and segments had positive correlations with concentration except the 90th percentile model for Hillsborough, Old, and Lower Tampa Bay and the mean model for Middle Tampa Bay. Only the 90th percentile model for Old Tampa Bay was positively correlated with TN load. Correlations with seagrass coverage and ENSO index values binned by year and season were not significant (Table 5). Regression models relating residuals to ENSO categories by year and season (e.g., El Niño fall) were not significant. Regression models using continuous seasonal index values were also unable to resolve variance in the residuals, with the exception of the 10th percentile model for Lower Tampa bay such that a significant and positive relationship was observed between residuals and ENSO index values for spring dates ($F = 5.2$, $R^2 = 0.12$, $p = 0.028$).

4 Discussion

Application of the Weighted Regressions on Time, Discharge, and Season (WRTDS) model to analyze a long-term record of chl-*a* in 4 segments of Tampa Bay provided an improved quantitative description of long-term changes relative to commonly applied methods. Because the

descriptions are conceptually related to expected causes, the results enabled generation of informed hypotheses regarding ecosystem behavior and change and could suggest a potential approach for developing quantitative thresholds for water quality management. These conclusions are supported by several key aspects of the results. First, the WRTDS model provided improved predictions of chl-*a* relative to non-weighted regression, measured as both higher R^2 and lower $RMSE$ (Table 2). Second, WRTDS results for segments of the Bay that were historically most impacted by nutrient loading pointed to shifts in the response of chl-*a* to changes in freshwater inflows. These changes are temporally coherent with known changes in nutrient sources, suggesting that the WRTDS results quantify a response to changes in nutrient forcing. Finally, adaptation of WRTDS to predict quantiles in addition to the mean response provided information about long-term shifts in phytoplankton dynamics that are ecologically informative. In total, the results obtained by applying WRTDS to the Tampa Bay chl-*a* time series suggest that this model could be broadly useful for analyzing and interpreting the growing number of long-term data sets for water quality in estuaries.

4.1 Improved description of chl-*a* using WRTDS

The primary advantage of applying the WRTDS approach to the Tampa Bay dataset was an empirical description of water quality trends that accounted for the effects of freshwater variation over time. The increased predictive abilities of the WRTDS approach was apparent by comparison with unweighted linear model (Table 2). [Hirsch *et al.* \(2010\)](#) indicated similar improvements with application to Chesapeake Bay river inputs such that an increase in R^2 from 35% to 56% was observed using the weighted approach. Relative increases in predictive performance were not as dramatic for the Tampa Bay dataset, although R^2 values were higher

than those in [Hirsch *et al.* \(2010\)](#). Improved model fit results in part from more flexible parameterization. This increases the ability of the model to describe historical patterns, but reduces application to predicting future chl-*a*. If drivers of chl-*a* are changing over time, predicting future chl-*a* while assuming that drivers are not changing could be of limited value. For example, WRTDS showed that the relationship between chl-*a* and freshwater forcing changed over time, such that predictions of chl-*a* in the near future would by necessity be based on the most recent estimates of the ecosystem response to freshwater forcing rather than the long-term average response. As such, the primary use of the WRTDS is a description of historical change that can lead to formulation of hypotheses by *post hoc* reasoning. [Hirsch *et al.* \(2010\)](#) also used WRTDS to quantify changes ecological drivers, pointing to long-term changes in the strength and direction of discharge effects on nutrient concentrations in rivers. Watershed drivers of changes described by [Hirsch *et al.* \(2010\)](#) suggests similar conclusions can be made regarding drivers of observed changes in chl-*a* in Tampa Bay.

Pollutant sources for Tampa Bay have changed over time with an increasing dominance of non-point sources (??). Dominance of point-sources of pollution in the 1970s suggests that variation in salinity (i.e., freshwater inputs) has little influence on total nutrient load and consequently chl-*a* concentration. Conversely, increasing inputs from non-point sources suggests that variation in salinity should be correlated with estuarine production. Application of the WRTDS model to the Tampa Bay dataset provided evidence of these shifts in the salinity-chlorophyll relationship over time. The shifts were most apparent for Bay segments that received large tributary inputs. For example, the relationship of salinity with chlorophyll for Hillsborough Bay during earlier periods indicated no trend as expected, whereas the opposite was true for later periods. However, our measure of fraction of freshwater differs from discharge in

that the effects of tidal exchange are also implicitly included. Accordingly, fraction of freshwater only partially explains the effects of tributary inputs. [Hirsch *et al.* \(2010\)](#) developed the WRTDS approach for rivers and streams where discharge effects are considered the primary variable affecting interpretation of water quality trends. Therefore, salinity effects were included in eq. (2) as being more appropriate for estuaries that are influenced by natural variation in both tidal flow and freshwater inputs ([Cloern 1996](#)).

The final objective of the analysis was to develop informed hypotheses of temporal and spatial patterns of chl-*a* growth in response to drivers of eutrophication in Tampa Bay. The most informative indication of changes for hypothesis development is illustrated by changes in chl-*a* response over time and Bay segments (Fig. 8), particularly for Hillsborough Bay. Earlier periods (1974–1980) showed little response of chl-*a* to freshwater inputs, which is likely related to the dominance of point sources. An alternative explanation is provided by [Wofsy \(1983\)](#), such that phytoplankton growth dynamics in nutrient-saturated systems may be invariant to freshwater inputs. Biological processes, such as phytoplankton self-shading, may be more limiting for algal growth. Middle periods (1990–2000) for Hillsborough Bay showed an approximate positive and linear relationship between chl-*a* and freshwater inputs. Phytoplankton growth was likely nutrient-limited such that production and biomass may be positively correlated with river forcing that provides relief from nutrient limitation. Later periods (2000–2012) showed positive relationships with inputs related to non-point sources, followed by a specific threshold response in recent years. If nutrient concentrations associated with river flow do not stimulate phytoplankton growth sufficiently to overcome flushing, biomass could decrease in association with high flow ([Murrell *et al.* 2007](#)). Temporal dynamics for other Bay segments are also illustrative of changes in causal mechanisms. For example, Old Tampa Bay shows a distinct response to salinity changes

that may be related to variation in residence time and circulation between the Bays. Comparison to Hillsborough Bay indicated similar dynamics, although differences between concurrent periods of observation remains a question of interest.

4.2 *Changes in chl-a variability*

Most analyses of changes in water quality focus on changes in mean water quality over time. Linear models generally fit a constant seasonal cycle, a constant response to freshwater inflow, and a linear trend to describe the long-term change. The flexible parameterization of the WRTDS approach can substantially improve descriptions of water quality trends by addressing limitations of simple models. As a result, predicted values from WRTDS results are appropriate for evaluating change in direction of the response, whereas salinity-normalized values are useful for evaluating more subtle changes in variation. Direction and magnitude of change were primarily in agreement with expectations, whereas changes in variation over time have not been previously described. Salinity-normalized predictions suggested non-stationarity of chlorophyll response between-years such that variation has generally been increasing, i.e., CV values for most Bay segments have been larger than the most heavily polluted periods in the 1970s (Table 4 and Fig. 7). Differences were also observed by mean or quantile response, particularly for the 90th percentile model in Old Tampa Bay. Mechanisms describing heterogeneity of chlorophyll between years is uncertain, although increasing variation in water quality parameters is a potential indicator of ecological transition in lakes (Carpenter and Brock 2006). Variation in chlorophyll could be an indication of impending changes despite constant mean values for several decades. We further emphasize that characterization of between-year variation is only possible with methods such as WRTDS. Less complex approaches that are not data-driven may be unable to

resolve this variation (e.g., additive seasonal models, Cloern and Jassby 2010).

The inclusion of quantile models represents an important extension of the WRTDS approach by allowing insight into conditional response of chl-*a* not described by mean models. Quantile models are particularly useful for characterizing response variables that exhibit considerable heterogeneity about the mean (Terrell *et al.* 1996, Cade and Noon 2003). Practical interpretation of the quantile models are such that the 90th percentile models show variation in the occurrence of extreme events whereas the 10th percentile models show variation in low productivity events. Quantification of extreme events may provide a more informative measure of progress towards ecosystem change in response to management. For example, a previous description for developing numeric criteria for Florida waters used the 90th percentile value from cumulative distribution models of chlorophyll for multiple coastal segments (Schaeffer *et al.* 2012). Although the exact upper percentile for criteria definition is arbitrary, consistency among methods could facilitate adoption in water quality standards. Similarly, variation in low productivity events could provide information of system departure from baseline or reference conditions (e.g., Stoddard *et al.* 2006). For example, variation in the 10th percentile model for Lower Tampa Bay in recent years suggests a consistent decrease in events with low chlorophyll concentrations (Fig. 6).

4.3 Limitations and future applications

The adaptation of the WRTDS approach to quantify chl-*a* trends in estuaries shows promise, although our analysis differs in several key aspects from the original model. First, issues of spatial scale will continue to have relevance given specific research objectives. The application of the WRTDS approach to Tampa Bay considered individual segments as being most relevant

given our goal to provide a quantitative history of eutrophication that has importance for regional planning and decision-making processes. Different research objectives may warrant the use of Bay segments as inappropriate since phytoplankton growth patterns can be characterized at multiple scales. Cloern (1996) reviews spatial patterns of phytoplankton growth in estuaries such that longitudinal, lateral, and vertical dynamics are commonly observed. Growth dynamics may also be evident at scales ranging from meters to several kilometers. More subtle differences in spatial patterns are likely observed at individual stations in the Bay, which could serve as a focus for additional evaluation. Similarly, phytoplankton dynamics may be evident at different temporal scales. Hirsch *et al.* (2010) developed the WRTDS approach for daily water quality observations, although the Tampa Bay dataset prohibits analysis at time scales shorter than a month.

Additional considerations not unique to our adaption of the WRTDS approach deserve further investigation. The WRTDS method currently does not provide measures of uncertainty associated with model predictions, although development is in progress (R. Hirsch, personal communication May 2014). Lack of confidence in model predictions is a primary disadvantage of the approach that distinguishes it from alternative methods. For example, Moyer *et al.* (2012) compares the WRTDS methods with ESTIMATOR, an alternative regression-based approach (Cohn *et al.* 1992). Although WRTDS provided more accurate and precise descriptions, indications of uncertainty provided by ESTIMATOR suggested variation may be considerable in some cases. Moreover, the determination of appropriate window widths for defining model weights has been an issue of concern since initial development of the approach. A systematic evaluation of different combinations of window widths for reducing prediction error could be conducted to identify optimal widths. However, results may be specific to individual datasets and computational time may be excessive such that the increase in predictive performance may be

trivial relative to time spent defining optimum widths. Regardless, the window widths used for our analysis produced useful results and could be used for additional applications.

The lack of correlation between model residuals and additional variables was unexpected, particularly for the seagrass and ENSO data. Previous analyses have illustrated the effects of precipitation events associated with ENSO on Tampa Bay. For example, [Schmidt and Luther \(2002\)](#) described ENSO effects on salinity profiles for Tampa Bay such that high precipitation events (i.e., El Niño spring or winters) were correlated with depressed salinity profiles. Our analyses indicated that residuals were not related to ENSO variation. The WRTDS model included salinity effects such that residual variation accounts for changes in freshwater inputs, which potentially explains lack of correlation with ENSO. Lack of correlation with seagrass data may have been related to sample size such that annual averages in the residuals were evaluated based on the availability of seagrass data. Additionally, correlations between seagrass growth and chlorophyll may have been present for lags in the time series that were not evaluated. For example, high chl-*a* concentrations may have an effect on seagrass growth the following year, rather than within the same year.

4.4 Conclusions

Management over several decades has been successful in improving water quality in Tampa Bay from heavily degraded to more culturally desirable conditions ([Greening and Janicki 2006](#)). These changes have been most dramatic for Bay segments that receive a majority of nutrient pollution from tributary or point-sources, particularly Hillsborough and Old Tampa Bay. The general effects of management actions are therefore obvious, although quantitative descriptions of these changes that consider the effects of confounding variables on water quality

dynamics have been lacking. Establishing direct links between management actions and changes in water quality are critical to inform the prioritization of limited resources for future decisions. Application of the WRTDS approach to Tampa Bay has provided a novel description of eutrophication dynamics that can be evaluated in the context of observed changes over time. Conclusions from the analysis showed that 1) improved statistical performance can be obtained using WRTDS as compared to traditional regression models, 2) the results reflected dynamic relationships between chl-*a* and salinity over time that suggested temporal shifts in nutrient forcing, and 3) considerable variation in chl-*a* response can be described by quantile distributions. Overall, the ability to describe the data and aspects of long-term changes has been improved by adaptation of the WRTDS approach to Tampa Bay. Such techniques are critical for informing the nutrient-response paradigm in coastal systems, providing an incentive for validation with additional long-term datasets.

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Table 1: Summary of characteristics for Tampa Bay segments. Mean chlorophyll and salinity data for 2012 are shown. Sources: [Lewis and Whitman \(1985\)](#), [Lewis and Estevez \(1988\)](#).

Segment	Area (km ²)	Shoreline length (km)	Mean depth (m)	Watershed area (km ²)	Chlorophyll- <i>a</i> ($\mu\text{g L}^{-1}$)	Salinity
HB	105.3	128.6	3.2	3319.9	9.9	24.4
OTB	200.7	339.8	2.8	874.4	7.6	23.5
MTB	309.9	262.8	4.1	1062.7	6.1	27.1
LTB	246.6	121.6	3.8	330.5	4.1	32.2

Note: HB: Hillsborough Bay, OTB: Old Tampa Bay, MTB: Middle Tampa Bay, LTB: Lower Tampa Bay

Table 2: Model performance by bay segment comparing non-weighted and weighted regression. Performance is evaluated using R^2 for mean models, pseudo- R^2 for 90th and 10th percentile (τ) models, and $RMSE$ for all models (statistics by Bay segment).

Statistic	mean		0.9 τ		0.1 τ	
	Non-wtd	Wtd	Non-wtd	Wtd	Non-wtd	Wtd
HB						
R^2	0.54	0.66	0.32	0.47	0.31	0.45
$RMSE$	0.48	0.41	0.78	0.66	0.74	0.67
OTB						
R^2	0.54	0.65	0.29	0.45	0.34	0.47
$RMSE$	0.41	0.36	0.65	0.61	0.67	0.59
MTB						
R^2	0.60	0.71	0.34	0.51	0.38	0.51
$RMSE$	0.37	0.31	0.60	0.52	0.61	0.52
LTB						
R^2	0.40	0.51	0.26	0.37	0.18	0.34
$RMSE$	0.45	0.40	0.72	0.65	0.77	0.68

Note: HB: Hillsborough Bay, OTB: Old Tampa Bay, MTB: Middle Tampa Bay, LTB: Lower Tampa Bay

Table 3: Decadal summaries of salinity-normalized chl-*a* ($\mu\text{g L}^{-1}$) trends by Bay segment. Trends are evaluated for models fit through the mean response and the 10th and 90th percentile (τ) distributions. Mean and slope estimates are aggregated by year categories using monthly data.

Models	1974-1980		1980-1990		1990-2000		2000-2012	
	Mean	Δ chl- <i>a</i>	Mean	Δ chl- <i>a</i>	Mean	Δ chl- <i>a</i>	Mean	Δ chl- <i>a</i>
HB								
mean	24.91	0.06	18.30	-0.86***	13.00	-0.11	11.30	0.02
0.9 τ	43.51	1.56*	33.33	-2.00***	22.54	-0.10	19.23	-0.15
0.1 τ	16.41	-0.55**	10.88	-0.45***	8.10	-0.02	7.37	0.08
OTB								
mean	12.45	0.55	10.94	-0.31*	8.84	0.06	9.10	0.12
0.9 τ	19.26	0.72	17.26	-0.36*	14.91	0.12	16.30	0.16
0.1 τ	8.45	0.57**	7.32	-0.23**	5.59	0.02	6.08	0.07
MTB								
mean	10.33	0.77***	10.05	-0.34***	7.51	-0.04	6.39	0.01
0.9 τ	15.45	1.27***	16.40	-0.65***	11.61	-0.11	9.46	-0.05
0.1 τ	6.88	0.46**	6.81	-0.14	5.29	-0.05	4.57	0.05
LTB								
mean	4.68	0.33**	4.39	-0.11*	3.88	0.07	4.06	0.02
0.9 τ	8.32	0.42	8.05	-0.13	6.82	0.12	6.56	-0.12*
0.1 τ	2.84	0.22**	2.62	-0.10**	2.29	0.07**	2.75	0.07***

Note: * $p < 0.05$; ** $p < 0.01$; *** $p < 0.001$; HB: Hillsborough Bay, OTB: Old Tampa Bay, MTB: Middle Tampa Bay, LTB: Lower Tampa Bay

Table 4: Variation in chl-*a* ($\mu\text{g L}^{-1}$) for Bay segments by year and season categories. CV values are shown for salinity-normalized predictions. Trends are evaluated for models fit through the mean response and the 10th and 90th percentile (τ) distributions.

Models	1974-1980	1980-1990	1990-2000	2000-2012
HB				
mean	13.3	32.2	41.5	45.2
0.9 τ	24.2	37.2	41.4	49.1
0.1 τ	16.7	35.2	45.8	48.6
OTB				
mean	33.6	34.9	41.7	47.4
0.9 τ	26.4	30.4	43.0	54.3
0.1 τ	35.3	35.5	46.1	43.7
MTB				
mean	27.4	30.4	42.0	39.5
0.9 τ	25.0	26.4	37.5	39.1
0.1 τ	31.1	33.8	42.9	39.1
LTB				
mean	34.4	34.1	36.6	34.8
0.9 τ	37.2	31.6	34.7	33.5
0.1 τ	36.8	37.4	33.2	32.7
	winter	spring	summer	fall
HB				
mean	53.1	41.8	20.5	39.9
0.9 τ	47.9	55.6	29.4	35.5
0.1 τ	65.3	35.9	21.8	44.2
OTB				
mean	23.0	29.3	13.9	30.5
0.9 τ	23.9	25.8	20.1	31.3
0.1 τ	29.0	31.1	13.6	33.2
MTB				
mean	33.0	33.0	18.5	31.9
0.9 τ	38.0	36.4	20.6	31.4
0.1 τ	30.6	29.4	19.2	31.2
LTB				
mean	12.5	18.7	13.0	25.9
0.9 τ	17.8	16.9	17.8	28.6
0.1 τ	13.6	21.8	15.7	27.1

Note: winter: JFM, spring: AMJ, summer: JAS, fall: OND; HB: Hillsborough Bay, MTB: Middle Tampa Bay, OTB: Old Tampa Bay, LTB: Lower Tampa Bay

Table 5: Correlations between model residuals for each bay segment and potential drivers of chl-*a* ($\mu\text{g L}^{-1}$) independent of season, year, or salinity effects. Residuals were compared with seagrass area (hectares), mean ENSO index values by season and year, and total nitrogen load ($\text{kg}\cdot\text{mo}^{-1}$) and concentration ($\mu\text{g L}^{-1}$).

Models	seagrass	ENSO		TN	
		annual	season	load	conc.
HB					
mean	0.23	0.25	0.03	0.03	0.11*
0.9 τ	0.26	0.16	0.01	0.00	0.07
0.1 τ	-0.07	0.30	0.04	0.02	0.12*
MTB					
mean	-0.40	0.10	-0.04	0.00	0.11
0.9 τ	-0.24	0.06	-0.01	0.06	0.12*
0.1 τ	-0.43	0.06	-0.07	-0.06	0.12*
OTB					
mean	0.04	0.08	-0.04	0.06	0.19***
0.9 τ	0.23	0.02	-0.06	0.16**	0.11
0.1 τ	-0.03	0.07	-0.04	0.03	0.23***
LTB					
mean	0.09	0.08	0.00	0.01	0.20***
0.9 τ	0.28	0.08	0.03	0.06	0.10
0.1 τ	-0.19	0.07	-0.02	0.01	0.33***

Note: * $p < 0.05$; ** $p < 0.01$; *** $p < 0.001$; for Pearson correlations, sample size varies from 11 to 308, HB: Hillsborough Bay, MTB: Middle Tampa Bay, OTB: Old Tampa Bay, LTB: Lower Tampa Bay

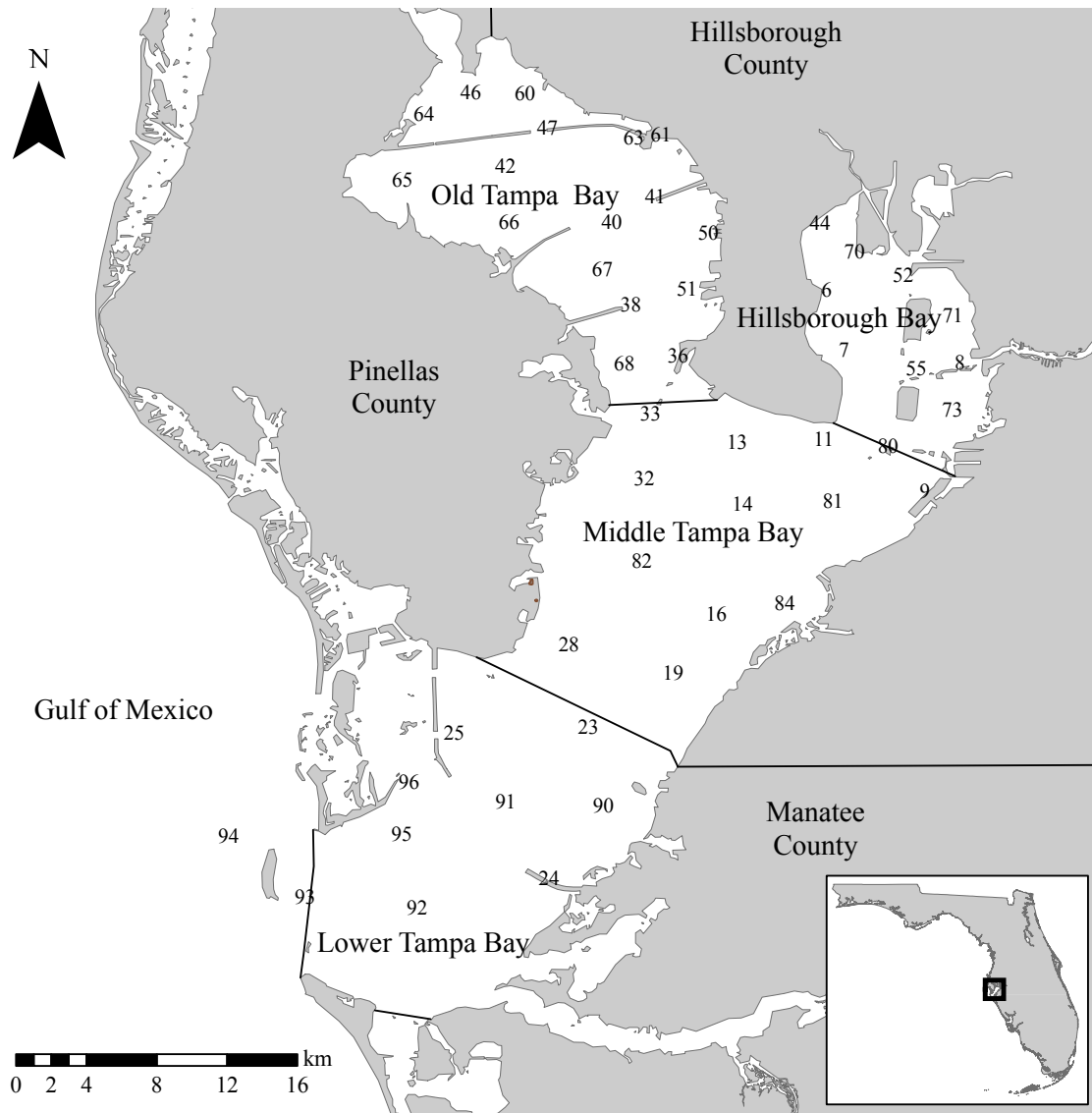


Fig. 1: The Tampa Bay estuary located on the west coast of central Florida. The Bay is separated into four segments defined by chemical, physical, and geopolitical boundaries (Lewis and Whitman 1985). Monthly water quality monitoring stations are also indicated by their identification number (Boler 2001).

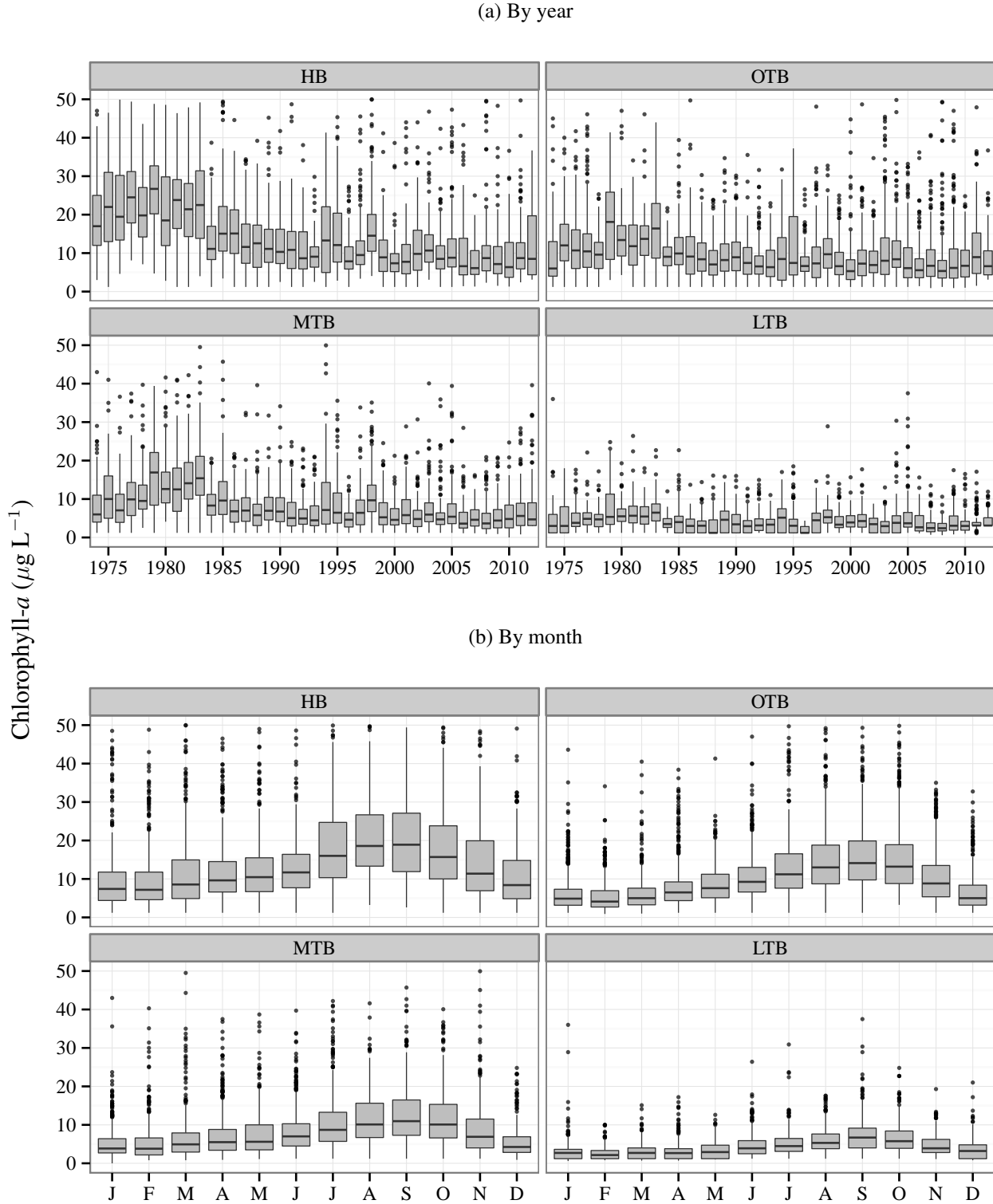


Fig. 2: Observed chl-*a* data for Tampa Bay segments by (a) year and (b) month aggregations. Each box is bisected by the median and represents the IQR (25th to 75th percentile). Outliers are present beyond whiskers (1.5·IQR) and were observed beyond 50 $\mu\text{g L}^{-1}$. HB: Hillsborough Bay, MTB: Middle Tampa Bay, OTB: Old Tampa Bay, LTB: Lower Tampa Bay.

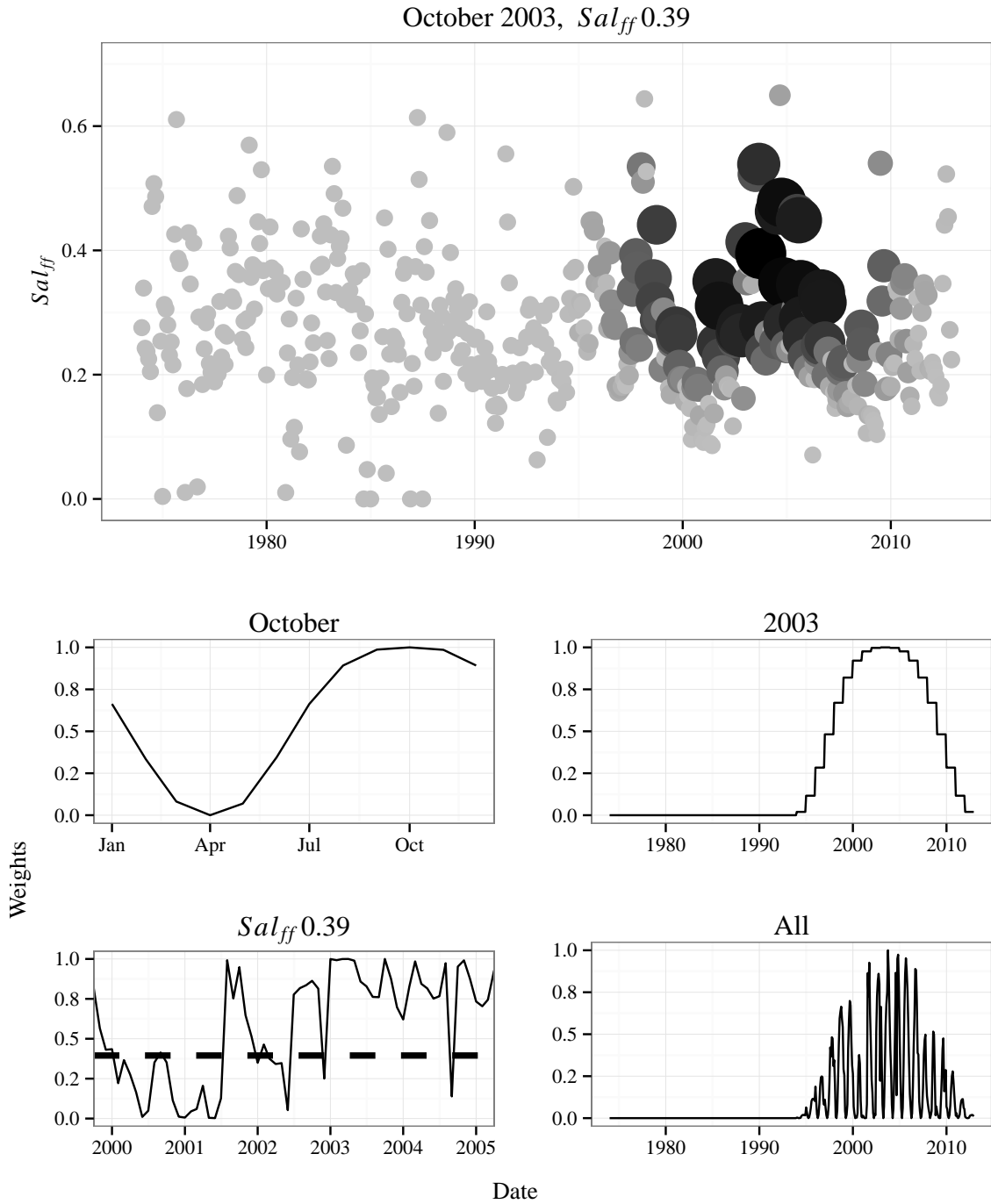


Fig. 3: Example of weighting for one observation in Hillsborough Bay. The top plot shows all data weighted for October 2003 when the proportion freshwater was 0.39. Point size and color are in proportion to weights. The bottom plots show the individual weights for month, year, proportion freshwater, and all weights combined.

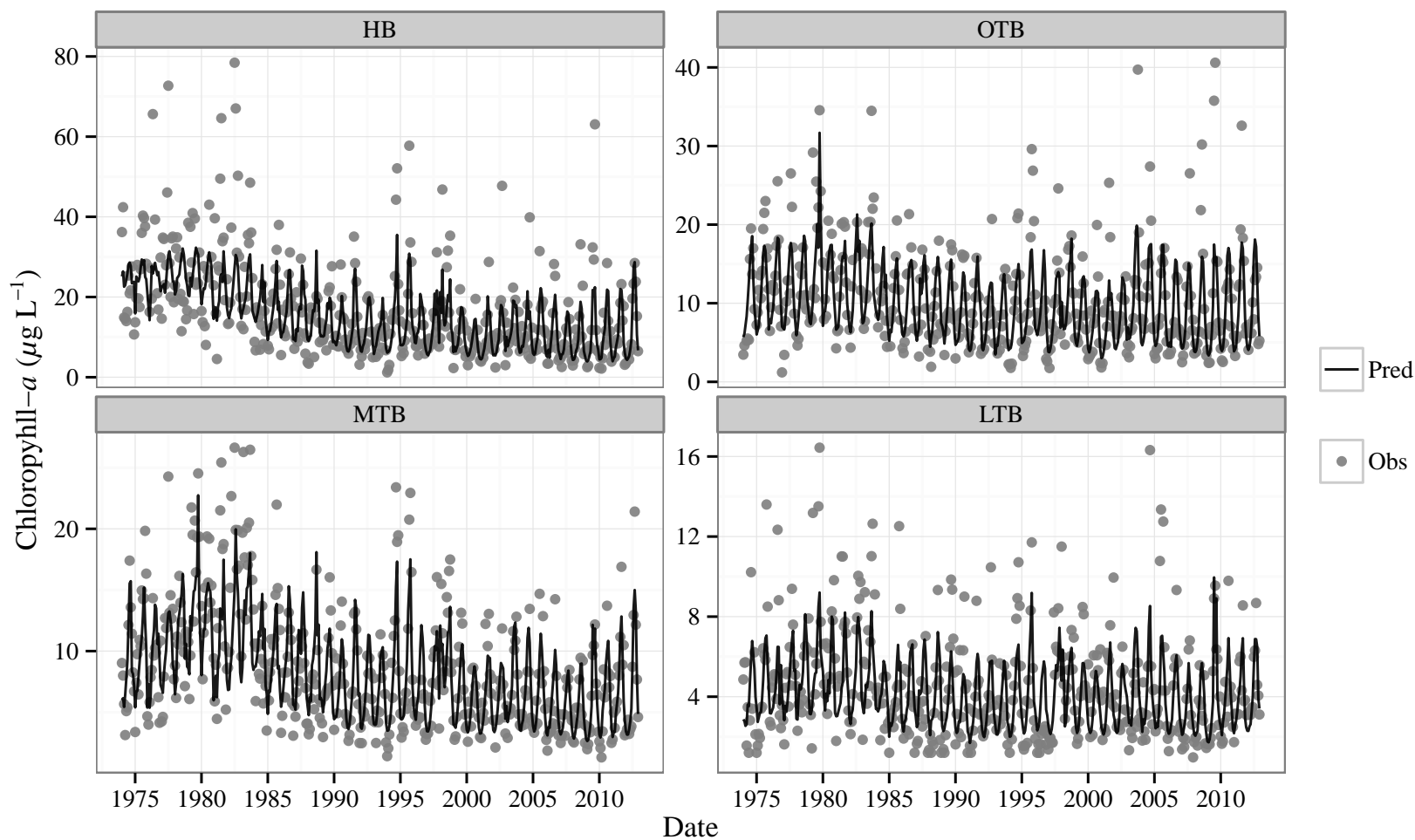


Fig. 4: Predicted and observed chl-*a* concentrations for Tampa Bay segments. Predicted values are for the weighted regression models fit through the mean response. HB: Hillsborough Bay, OTB: Old Tampa Bay, MTB: Middle Tampa Bay, LTB: Lower Tampa Bay.

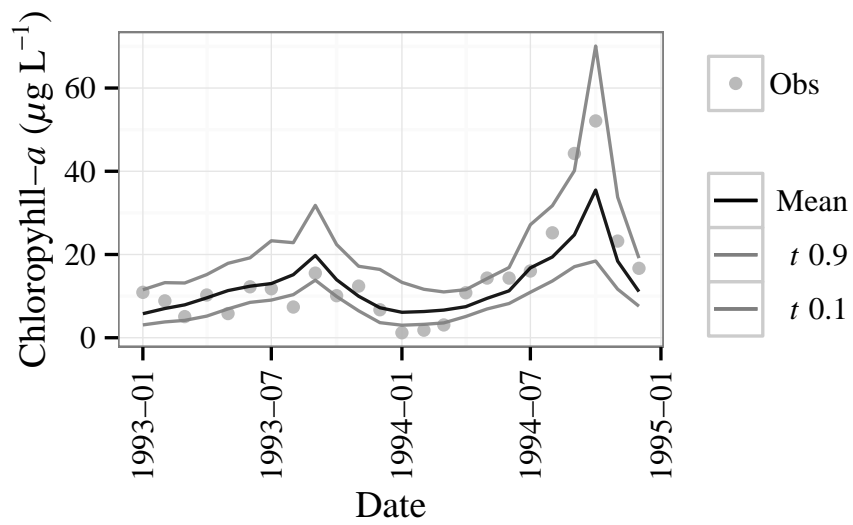


Fig. 5: Predicted and observed chl-*a* concentrations for Hillsborough Bay for 1993 to 1995 illustrating variation in model fit based on observation date. Predicted values are for the weighted regression models fit through the mean response and the 10th and 90th percentile (τ) distributions.

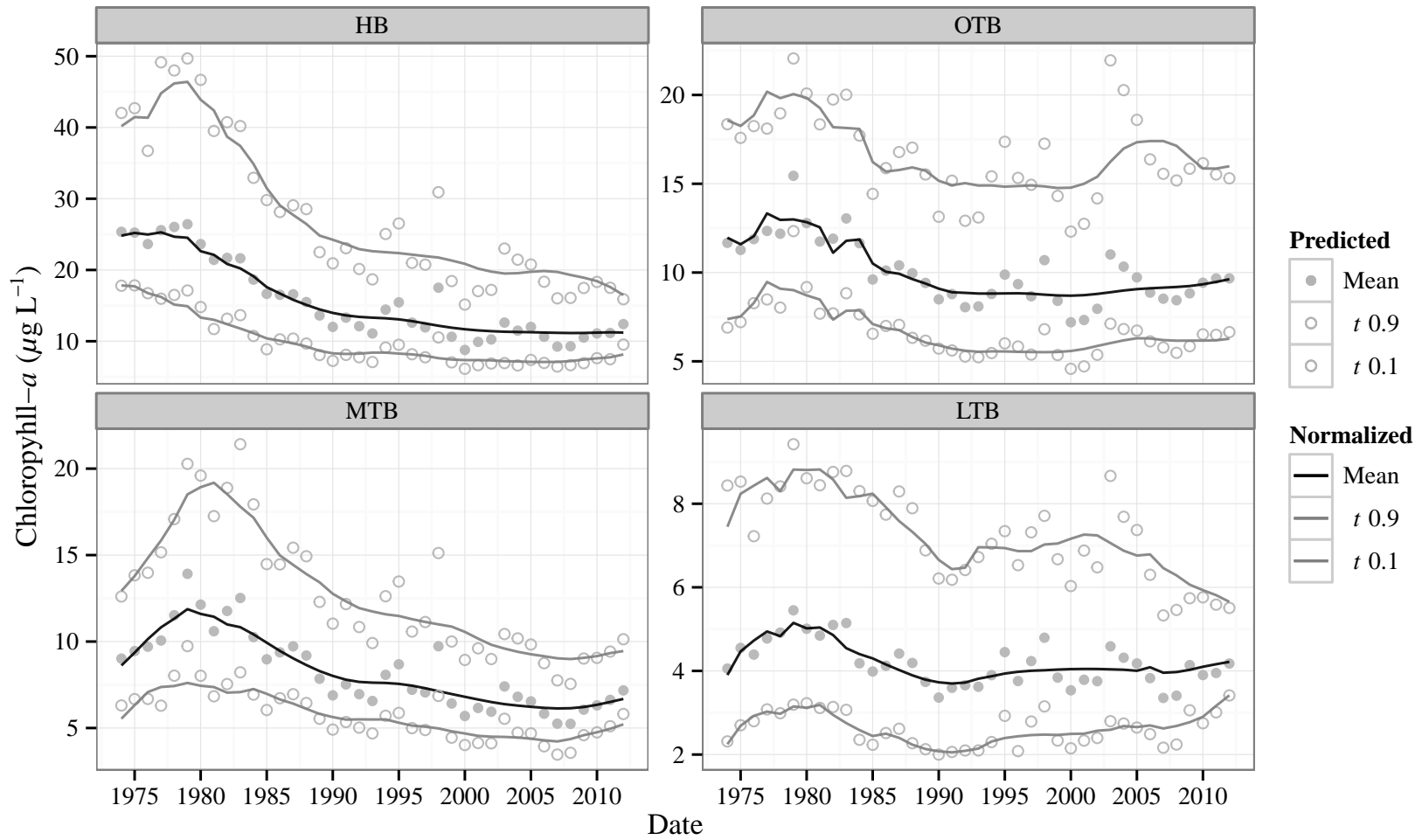


Fig. 6: Weighted regression predictions and salinity-normalized results aggregated by year for the mean response and the 10th and 90th quantile (τ) distributions. HB: Hillsborough Bay, OTB: Old Tampa Bay, MTB: Middle Tampa Bay, LTB: Lower Tampa Bay.

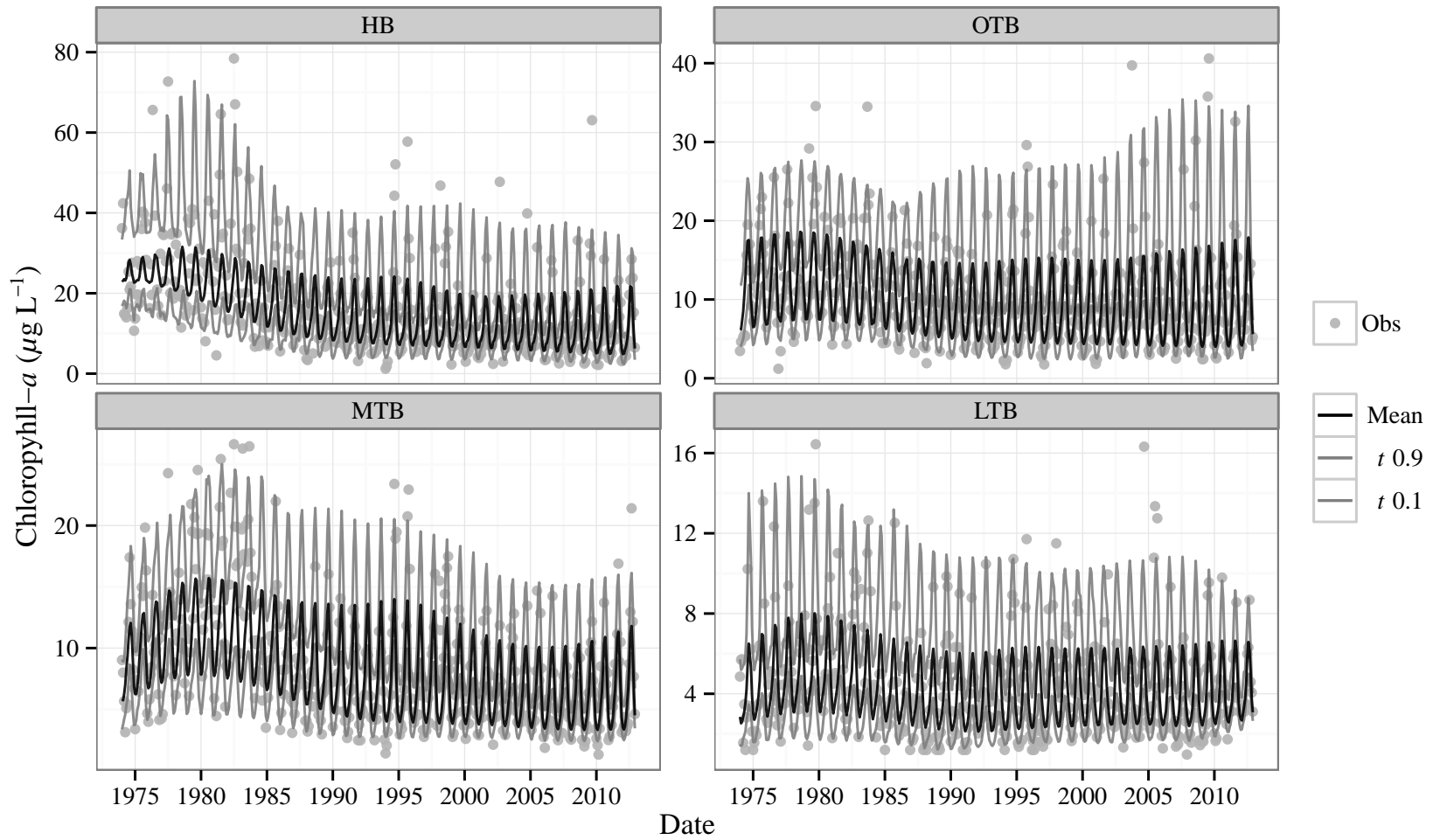


Fig. 7: Salinity-normalized results for the mean response and the 10th and 90th quantile (τ) distributions. HB: Hillsborough Bay, OTB: Old Tampa Bay, MTB: Middle Tampa Bay, LTB: Lower Tampa Bay.

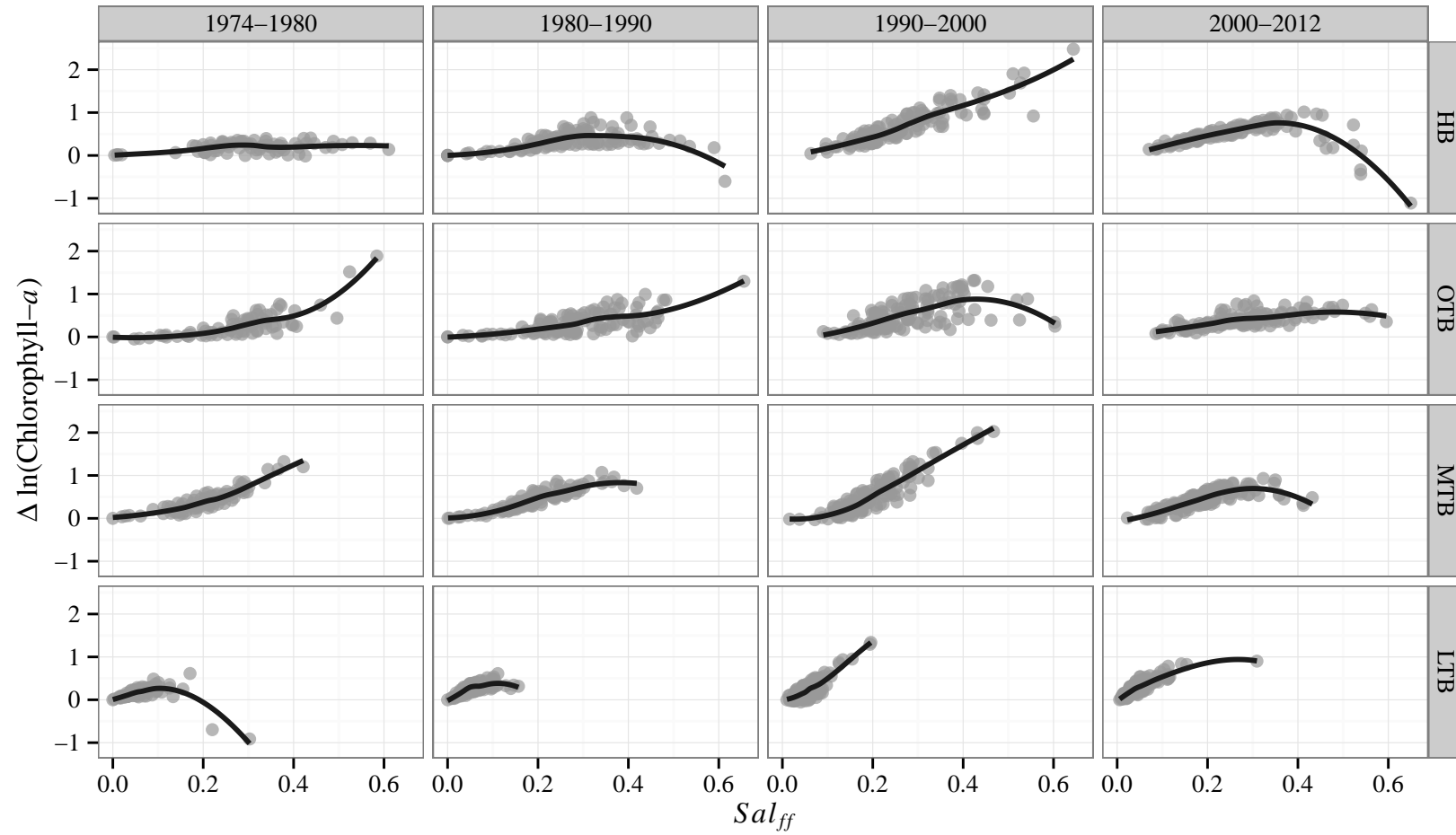


Fig. 8: Variation in the relationship between chl-*a* and salinity across the time series. Y-axis values are expected changes in ln-transformed chlorophyll for a given salinity. Expected changes are based on slope estimates for individual models over time, multiplied by the observed fraction of freshwater (Sal_{ff}). Only the mean response models are shown. Trends are approximated with loess smoothing. HB: Hillsborough Bay, OTB: Old Tampa Bay, MTB: Middle Tampa Bay, LTB: Lower Tampa Bay.