Improving estimates of ecosystem metabolism computed from dissolved oxygen time series

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Abstract

In aquatic ecosystems, time series of dissolved oxygen (DO) have been used to compute {acro:DO} estimates of integrated ecosystem metabolism. Central to this open water or "Odum" method is the assumption that the dissolved oxygen time series is a Lagrangian specification of the flow field. However, most DO time series are collected at fixed locations, such that the method must assume changes in dissolved oxygen principally reflect ecosystem metabolism and that effects due to advection or mixing can be neglected. A statistical model using weighted regression was applied to separate variability in DO associated with metabolism from tidal variation or other advection in estuaries, thereby helping to partially relax this assumption and improve estimates of ecosystem metabolism. The method was developed and tested using a simulated DO time series with known biological and physical components, and then applied to one year of continuous monitoring data from four water quality stations within the National Estuarine Research Reserve System. Overall, the approach is a useful way to reduce variability in estimates of ecosystem metabolism caused by advection, particularly when the magnitude of tidal influence is high and correlations between tidal change and solar cycling are low. By reducing the effects of physical transport on metabolism estimates, there may be increased potential to empirically relate metabolic rates to causal factors on times scales of several days to several weeks. Estimates of variability associated with physical advection may also be more interpretable, since convolution of physical and biological effects can be reduced.

Introduction

{intro}

Time series of dissolved oxygen are increasingly used to estimate ecosystem metabolism (Kemp and Testa 2012, Needoba et al. 2012). Integrated measures of metabolism describe the balance between production and respiration processes that create and consume organic matter, respectively. Although metabolic rates vary naturally at different spatial and temporal scales (Ziegler and Benner 1998, Caffrey 2004, Russell and Montagna 2007), anthropogenic nutrient sources are often contributing factors that increase rates of production (Nixon 1995, NRC 2000). Inputs of limiting nutrients beyond background concentrations may decrease the resilience of an ecosystem such that higher rates of production are coupled with higher biological oxygen demand (Yin et al. 2004, Kemp et al. 2009). Cultural eutrophication is frequently linked to declines in water quality through lower levels of dissolved oxygen, degradation in aquatic vegetation habitat, and increased frequency of harmful algal blooms (Cloern 1996, Short and Wyllie-Echeverria 1996, Rabalais et al. 2002, Diaz and Rosenberg 2008). Reliables estimates of ecosystem metabolism are critical for measuring both background rates of production and potential impacts of human activities on ecosytem condition.

Open-water techniques have been used for decades to infer metabolic rates using *in situ* measurements from continuous monitoring data (Odum 1956). Daily integrated measurements of metabolism represent the balance between daytime production and nighttime respiration. The open-water method uses the diel fluctuation of dissolved oxygen to estimate ecosytem metabolism, after correcting for air-water gas exchange (Kemp and Testa 2012). As with any method, the ability to accurately estimate whole system metabolism depends on the degree to which assumptions of the theory are met. The fundamental assumption is that the time series of {acro:DO} dissolved oxygen (DO) represents a Lagrangian specification of the flow field that describes the same water mass over time (Needoba et al. 2012). The Lagrangian specification assumes that the time series characterizes individual fluid parcels regardless of location, as in a parcel of water moving with the tide. In reality, most DO time series are collected at fixed locations such as a mooring or dock, which is characteristized by an Eulerian specification of the flow field. Time series at fixed locations may characterize water masses with different metabolic histories if water particles are transported by physical advection. A Lagrangian flow field is often assumed, such that estimates of metabolism may be inaccurate if substantial variation in water column mixing occurs throughout the period of observation (Kemp and Boynton 1980, Russell and Montagna 2007). Given this critical challenge, the open-water method has been used with varying success in lakes (Staehr et al. 2010, Coloso et al. 2011, Batt and Carpenter 2012) and estuaries (Caffrey 2004, Russell and Montagna 2007, Caffrey et al. 2013). Appropriate placement of monitoring sondes, sampling frequency and duration, and reliability of data from single stations have been relevant issues in applying the open-water method to systems influenced by physical mixing (Russell and Montagna 2007, Staehr et al. 2010). Application of the method to estuaries is a particular concern as physical mixing caused by tidal currents may confound the biological variation in DO time series (Kemp and Boynton 1980, Caffrey 2003, Nidzieko et al. 2014). Individual sampling stations near bay inlets or along major tidal axes may produce DO time series that fail to meet the assumptions of the open-water method.

Although numerous studies have shown that application of the open-water method to lakes or estuaries may be problematic (Ziegler and Benner 1998, Caffrey 2003, Coloso et al. 2011, Batt and Carpenter 2012, Nidzieko et al. 2014), very few quantitative approaches have been developed to address potential bias or noise in DO signals from physical advection. For example, an extensive analysis by Caffrey (2003) applied the open-water method to estimate metabolism at 28 continuous monitoring stations at 14 US estuaries. A significant portion of the production and respiration estimates were negative (3 - 69% depending on site), suggesting advection of water masses was a likely factor influencing the DO time series. These 'anomalous' values are typically omitted from the analysis (Caffrey 2003, Collins et al. 2013), which may upwardly bias estimates of metabolism (Murrell et al. 2013). Further, Nidzieko et al. (2014) evaluated the effects of tidal advection on metabolism estimates in a mesotidal estuary. Estimates from a single location were strongly correlated with the spring-neap cycle such that net heterotrophy was more common during spring tides, whereas metabolism was generally balanced during neap tides. A control-volume approach was used by impounding a section of the upper estuary to understand how physical processes contribute to biological variability. Although useful as an *in situ*, site-specific approach, more accessible statistical methods specific to time series are needed given the increasing availability of continuous monitoring data. For example, Batt and Carpenter (2012) explored the use of a Kalman filter (Harvey 1989) to remove process and observation uncertainty from DO time series in lakes. Similar approaches have not been developed for estuaries, particularly those that address potential effects of tidal advection.

This article describes the development and application of a method for improving estimates of ecosytem metabolism computed from DO time series. Specifically, the apparent effects of tidal advection on DO observations are removed to improve the fidelity of open-water metabolism estimates derived from continuous water quality data. We used a weighted regression approach originally developed to resolve trends in pollutant concentrations in streams and rivers (Hirsch et al. 2010). The weighted regression approach creates dynamic predictions of DO as a function of time and tidal height change, which are then used to filter, or detide, the DO signal.

The model is based on the recognition that daily fluctuations in DO are caused by metabolism associated with the solar cycle, whereas other fluctuations in estuaries are likely associated with water level changes that generally exhibit pregression relative to the solar cycle. The weighted regression model was applied, rather than methods commonly used for detiding in physical oceanography, to allow for the complex and dynamic patterns of DO changes relative to advection. First, we used simulated DO time series with known characteristics to evaluate ability of the weighted regression to remove the simulated effects of a tidally-advected DO gradient. Second, the simulation results informed the application of the method to four case studies chosen from the National Estuarine Research Reserve System (NERRS, Wenner et al. 2004). In all examples, tidal height is used as a proxy for lateral water movements that may influence DO observations. In the absence of quantitative data describing lateral DO variation (e.g., contemporaneous stations along a tidal axis), we assume tidal height is an appropriate characterization of lateral variation. Accordingly, 'tidal variation' or 'changes in tidal height' are used throughout in reference to assumed lateral DO gradients that are carried past monitoring sensors by tidal currents.

Materials and Procedures

Weighted regression for modelling and filtering DO time series

For this study, we adapted a weighted regression model to filter DO time series for apparent tidal effects. This model relied heavily on concepts used to develop the weighted {acro:WRTI regression on time, discharge, and season (WRTDS) method for estimating pollutant concentrations in streams and rivers (Hirsch et al. 2010). The functional form of the model is:

$$DO_{obs} = \beta_0 + \beta_1 t + \beta_2 H \tag{1}$$ {funform}

where DO_{obs} is a linear function of time t and tidal height H. Time is a continuous variable for the day and time of each observation as a proportion of the number of total observations added to each day. The beginning of each day was considered the nearest thirty minute observation to sunrise for the location. Our model differed from the original WRTDS method that included parameters to estimate variation of the response variable on a sinuisoidal period. DO variation was not modeled using this approach to avoid constraining parameter estimates by periodic, diel components.

Weighted regression was implemented as a moving window that allowed for estimation of DO throughout the time series by adapting to variation through time as a function of tide. Regression models were estimated sequentially for each observation in the time series using dynamic weight vectors that change with the center of the window. Weight vectors quantified the relevance of observations to the center of the window in respect to time, hour of the day, and tidal height. Specifically, weights were assigned to each variable using a tri-cube weighting function (Tukey 1977, Hirsch et al. 2010):

$$w = \begin{cases} \left(1 - (d/h)^3\right)^3 & \text{if } |d| \leq h \\ 0 & \text{if } |d| > h \end{cases} \tag{2}$$

where the weight w of each observation is inversely proportional to the distance d from the center of the window such that observations more similar to the point of reference are given higher importance in the regression. Weights exceeding the maximum width of the window h are equal to zero. The tri-cube weighting function is similar to a Gaussian distribution such that weights decrease gradually from the center until the maximum window width is reached. Regressions that use simpler windows (e.g., boxcar approach) are more sensitive to influential observations as they enter or leave the window, whereas the tri-cube function minimizes their effect through gradual weighting of observations from the center (Hirsch et al. 2010). The final weight vector for each observation is the product of three separate weight vectors for time (day), hour, and tidal height. Windows for time and hour weight observations based on distance (time) from the center of the window. The window for tidal height weights observations based on the difference from the center as a proportion of the total tidal height range. For example, a half-window width of 0.5 means that observations are weighted proportionately within +/- 50% the total range referenced to the tidal height in the center of the window. A low weight is given to an observation if any of the three weighting values were not similar to the center of the window since the final weight vector is the product of three weight vectors for each variable (see the link in the multimedia section for graphical display of different weights).

The choice of window widths for weight vectors strongly affects the model results. Excessively large or small window widths may respectively under- or over-fit the observed data. Accordingly, appropriate window widths depend on the objective for using the model. The weighted regression approach can be used for both predicting observed DO and filtering the observed time series to remove the variance that coincided with the tidal cycle. Window widths that minimize prediction error or fit to the observed data are typically smaller than widths that would be used for filtering tidal effects. Similarly, window widths that more effectively filter the DO signal may produce imprecise predictions for the observed data. Evaluations of the weighted regression method with simulated DO time series, described below, used multiple window widths to evaluate the ability of the model to filter the DO signal. The ability to predict observed DO was not a primary objective such that the window widths were evaluated only in the context of removing tidal variation from the DO time series.

The approach to filter physical advection from the observed DO time series differs slightly from methods in Hirsch et al. (2010). The previous approach used a two-dimensional grid predicted for stream pollutant concentrations across the time series and the range of discharge values observed in the study system (Hirsch et al. 2010). Normalized or discharge-independent values for pollutant concentration were obtained by averaging grid predictions across the discharge values that were likely to occur on a given day. Rather than creating a two-dimensional grid of DO related to time and tidal height change, the normalized time series herein were the model predictions conditional on time and constant tidal height set to the mean:

$$DO_{nrm} = f(DO_{obs} | \bar{H}, t) \tag{3}$$ {do_nrm}

such that the normalized time series represents DO variation related to biological processes. The term ‘filter’ is used in reference to the removal of a specific variance component from the time series, while maintaining the structure of the biological component. Although the approach shares similarities with common filtering techniques, a distinction is noted such that weighted regression has a specific purpose rather than the more generic objectives of common filters (e.g., moving window averages or local smoothers, Shumway and Stoffer 2011).

Assessment

Simulation of DO time series

To test the ability of the weighted regression to filter the DO signal for apparent tide effects, multiple time series with known characteristics were simulated and filtered. A simulation approach was used prior to application with real data given that the true biological signal can be created as a known component for comparison with the filtered results from weighted regression. The following describes the theoretical basis for developing the simulated time series. Observed DO time series were simulated as the sum of variation from biological processes and physical effects related to tidal advection:

$$DO_{obs} = DO_{bio} + DO_{adv} \qquad (4) \qquad \{\texttt{do\_obs}\}$$

Biological DO signals are inherently noisy (Batt and Carpenter 2012) and variance can be further described as:

$$DO_{bio} = DO_{die} + DO_{unc} \qquad (5) \qquad \{\texttt{do\_bio}\}$$

$$DO_{unc} = \epsilon_{obs} + \epsilon_{proc} \qquad (6) \qquad \{\texttt{do\_unc}\}$$

where the biological DO signal (DO_{bio}) is the sum of diel variation (DO_{die}) plus uncertainty or noise (DO_{unc}). Total uncertainty in the biological DO signal is described as variation from observation and process uncertainty (ϵ_{obs} and ϵ_{pro}, Hilborn and Mangel 1997). Multiple time series at 30 minute time steps over 30 days were created by varying the relative magnitudes of each of the components of observed DO in eqs. (4) to (6) to test the effectiveness of weighted regression under different scenarios. Accordingly, observed DO was generalized as the additive combination of four separate time series (Fig. 1):

$$DO_{obs} = DO_{adv} + DO_{die} + \epsilon_{obs} + \epsilon_{pro} \tag{7}$$ {do_obs_a

Each component of the simulated time series was created as follows. First, the diel component, DO_{die}, was estimated (Cryer and Chan 2008):

$$DO_{die} = \alpha + \beta \cos\left(2\pi f t + \Phi\right) \tag{8}$$ {do_sin}

such that the mean DO (α) was 8, amplitude (β) was 1, f was 1/48 to represent 30 minute intervals, t was the time series vector and Φ was the x-axis origin set for an arbitrary sunrise at 630. The diel signal was increasing during the day and decreasing during the night for each 24 hour period and ranged from 7 to 9 mg L^{-1}. Uncertainty was added to the diel DO signal as the sum of observation and process uncertainty:

$$DO_{unc,n} = \epsilon_{obs,n} + \int_{t=1}^{n} \epsilon_{pro,t} \tag{9}$$ {do_unc_n

where observation and process uncertainty (ϵ_{obs}, ϵ_{pro}) were simulated as normally distributed random variables with mean zero and standard deviation varying from zero to an upper limit, described below. Process uncertainty was estimated as a serially correlated variable using the cumulative sum of n observations plus random variation added at each time step for $t = 1, ..., n$. The total uncertainty, DO_{unc}, was added to the diel DO time series to create the biological DO time series (eq. (5) and Fig. 1).

A semidiurnal tidal series was simulated with a period of 12.5 hours to represent the principal lunar component (Foreman and Henry 1989). The amplitude was set to 1 meter and centered at 4 meters. The tidal time series simulated DO changes with advection, DO_{adv} (eq. (7) and Fig. 1). Conceptually, this vector represents the rate of change in DO as a function of horizontal water movement from tidal advection such that:

$$\frac{\delta DO_{adv}}{\delta t} = \frac{\delta DO}{\delta x} \cdot \frac{\delta x}{\delta t} \tag{10}$$ {deltdo}

$$\frac{\delta x}{\delta t} = k \cdot \frac{\delta H}{\delta t} \tag{11}$$ {deltx}

where the first derivative of the tidal time series, as change in height over time $\delta H/\delta t$, is multiplied by a constant k, to estimate horizontal tidal excursion over time, $\delta x/\delta t$. The horizontal excursion is assumed to be associated with a horizontal DO change, $\delta DO/\delta x$, such that the product of the two estimates the DO change at each time step from advection, DO_{adv}. In practice, the simulated tidal signal was used to estimate DO_{adv}:

$$DO_{adv} \propto H \tag{12}$$ {do_advp}

$$DO_{adv} = 2 \cdot a + a \cdot \frac{H - \min H}{\max H - \min H} \tag{13}$$ {do_adv}

where a is analogous to k in eq. (11) and is chosen as the transformation parameter to standardize change in DO from tidal height change to desired units. For example, $a = 1$ will convert H to a scale that simulates changes in DO from tidal advection that range from +/- 1 mg L^{-1}. The final time series for observed DO was the sum of biological DO and advection DO (eq. (4) and Fig. 1).

Evaluation of weighted regression with simulated DO time series

Multiple time series were simulated by varying the conditions in eq. (7) (Fig. 2) to evaluate weighted regression under difference conditions. Specifically, the simulated data varied in the relative amount of noise in the measurement (e_{pro}, e_{obs}), relative amplitude of the diel DO component (DO_{die}), and degree of association of the tide with the DO signal (DO_{adv}). Three levels were evaluated for each variable: relative noise as 0, 1, and 2 standard deviations for both process and observation uncertainty, amplitude of diel biological DO as 0, 1, and 2 mg L^{-1}, and DO change from tidal advection as 0, 1, and 2 mg L^{-1}. A total of 81 time series were created based on the unique combinations of parameters (Fig. 2). Half-window widths (day, hour of day, and tide height) for the weighted regressions were evaluated for each time series: time as 1, 3, and 6 days, time of day as 1, 3, and 6 hours, and tidal height as 0.25, 0.5, and 1 as a proportion of the total range given the height at the center of the window. The window widths were chosen based on preliminary assessments that suggested a large range in model performance was described by these values. In total, 27 window width combinations were evaluated for each of 81 simulated time series, producing results for 2187 weighted regressions.

The filtered DO time series were compared to the simulated data to evaluate the ability of weighted regression to characterize the biological DO time series in eq. (4). Comparisons were made using Pearson correlation coefficients and the root mean square error (RMSE). Overall, the {acro:RMSE weighted regressions produced filtered time series that were similar to the 'true' biological time series regardless of the simulation parameters (Table 1) or window widths (Table 2, results for each simulation can be viewed using the link in the multimedia section). The median correlation between the filtered and biological values for all time series and window widths was 0.63, with values ranging from 0.05 (very poor) to 1.00 (perfect). Mean error was 1.02, with values ranging from 0 (perfect) to 2.12 (very poor). Simulations with very poor performance were those those with the DO signal composed entirely of noise from observation uncertainty. As expected, simulations with no biological or tidal influence had filtered time series that were identical to the true time series (e.g., correlation of one, RMSE of zero).

Characteristics of DO time series that contributed to improved model performance were increasing amplitude of the diel DO component (DO_{die}) and increasing process error (e_{pro}), whereas increasing observation error contributed to decreased performance (Table 1 and Fig. 3). Model performance was not significantly affected by increasing tidal effects (i.e., increasing magnitude of DO_{adv}). Model performance was not substantially affected by variation in half window widths relative to characteristics of the DO time series (Table 2 and Fig. 4). Graphical summaries of model performance averaged by simulation parameters (Fig. 3) and half window widths (Fig. 4) support the general trends described by Tables 1 and 2.

Validation of weighted regression with case studies

Results from the simulated time series were used to inform the validation of weighted regression with real data, specifically with respect to choosing half-window widths described below. Continuous monitoring data from the National Estuarine Research Reserve System was used to validate the weighted regression model by evaluating estimates of ecosytem metabolism obtained from observed and filtered DO time series. NERRS is a federally-funded network of 28 protected estuaries established for long-term research, water-quality monitoring, education, and coastal stewardship (Wenner et al. 2004). Continuous water quality data have been collected at NERRS sites since 1994 through the System Wide Monitoring Program (SWMP, CDMO 2014).

In addition to providing a basis for trend evaluation, data from SWMP provides an ideal opportunity to evaluate long-term variation in water quality parameters from biological and physical processes. Continuous SWMP data can be used to describe DO variation at sites with different characteristics, including variation from ranges in tidal regime (Sanger et al. 2002) and rates of ecosystem production (Caffrey 2003, 2004). We selected sites from the SWMP database that had desirable characteristics for validating weighted regression. Specifically, four macrotidal sites were chosen based on apparent relationships between DO and tidal changes (Fig. 5 and Table 3): Vierra Mouth station at Elkhorn Slough (California, 36.81°N, 121.78°W), Bayview Channel at Padilla Bay (Washington, 48.50°N 122.50°W), Middle Blackwater River station at Rookery Bay (Florida, 25.93°N 81.60°W), and Dean Creek station at Sapelo Island (Georgia, 31.39°N 81.28°W).

The weighted regression model was applied to continuous DO time series and water level measurements from January 1st to December 31st 2012 at the four sites. Tide predictions were obtained for each site using harmonic regression applied to the sonde depth data (`oce` package in R, Foreman and Henry 1989, RDCT 2014). The stations were generally semidiurnal or mixed semidiurnal and net heterotrophic on an annual basis (Table 3). Net heterotrophy (i.e., respiration exceeding production) is typical for shallow water systems at temperate latitudes (Caffrey 2003), although values in Table 3 were from observed DO time series that were strongly correlated with water level height.

Estimates of ecosystem metabolism before and after filtering {met_sec}

The weighted regression method was applied to the annual data for each station to obtain a filtered DO time series for estimating metabolism. Ecosystem metabolism was estimated using the open-water technique (Odum 1956) as described in Caffrey et al. (2013). The method is used to infer net ecosystem metabolism using the mass balance equation:

$$\frac{\delta DO}{\delta t} = P - R + D \tag{14}$$ {metrate}

where the change in DO concentration (δDO, g O_2 m^{-3}) over time (δt, hours) is equal to photosynthetic rate (P, g O_2 m^{-3} hr^{-1}) minus respiration rate (R, g O_2 m^{-3} hr^{-1}), corrected for air-sea gas exchange (D, g O_2 m^{-3} hr^{-1}) (Caffrey et al. 2013). D is estimated as the difference between the DO saturation concentration and observed DO concentration, multiplied by a volumetric reaeration coefficient, k_a (Thébault et al. 2008). The diffusion-corrected DO flux estimates were averaged during day and night for each 24 hour period in the time series, where flux is an hourly rate of DO change. Respiration rates were assumed constant during the night and substracted from daily net production estimates to yield gross production (Table 3).

Unlike the simulated data, the true biological DO signal was unknown for the case studies. The selection of half-window widths for filtering the DO time series was based on a weight-of-evidence approach using four performance metrics to evaluate the results. First, the regression results were evaluated using correlations of DO and metabolism estimates with tidal height before and after application of the model. Daily metabolism estimates before and after filtering were compared to the mean rate of tidal height change (i.e., first derivative of the predicted tidal height) for each day during separate solar periods. Production rates were compared to mean rates of tidal height change during the day and respiration rates were compared to mean rates of change during the night. The second and third performance metrics evaluated changes in the mean and standard error of annual metabolism estimates before and after filtering. We assumed that mean values that represent annual aggregations would be unchanged because tidal variation is primarily diurnal, whereas the variance (i.e., standard error) would be reduced after filtering. Finally, results were evaluated based on the occurrence of 'anomalous' daily production or respiration estimates, where anomalous was defined as negative production during the day and positive respiration estimates during the night. Anomalous values have been previously attributed to the effects of physical processes on DO time series (Caffrey 2003). Although anomalies could be caused by processes other than tidal advection, e.g., abiotic dark oxygen production (Pamatmat 1997), we assumed that physical processes were the dominant sources of these values given the tidal characteristics at each site.

Multiple combinations of half-window widths were evaluated for the case studies. Specifically, half-window widths of 1, 3, 6, 9, and 12 days, 1, 3, 6, 9, and 12 hours, and 0.2, 0.4, 0.6, 0.8, and 1 tidal height proportions were evaluated, producing a total of 125 unique combinations. Half-window widths that maximized the four performance metrics for each case study were chosen as the 'optimal' values. Accordingly, the optimal half-window widths were 12, 6, and 0.8 (days, hours, tidal height) for Elkhorn Slough, 3, 6, and 0.6 for Padilla Bay, 3, 1, and 0.6 for Rookery Bay, and 3, 1, and 0.6 for Sapelo Island. Filtering had significant effects on the correlations between water level changes, DO time series, and daily integrated metabolism estimates (Table 4, see the link in the multimedia section for graphical results of each case study). Correlations of observed DO time series with predicted tidal height were positive at all sites, except Padilla Bay where increases in water level were associated with decreases in DO concentration. The filtered DO time series had correlations with tidal height close to zero. Similarly, metabolic rates (production, respiration) estimated from the filtered DO time series had significantly reduced correlations with tidal height change.

The proportion of daily integrated metabolism estimates that were anomalous (negative production, positive respiration) were significantly reduced for all sites after filtering (Table 5), perhaps indicating the relative effects of water movement. Before filtering, anomalous values ranged from 0.09 (as a proportion of the total estimates, Rookery Bay) to 0.22 (Padilla Bay) for production and 0.08 (Rookery Bay) to 0.21 (Elkhorn Slough) for respiration. Anomalous values were reduced to near zero for all case studies, particularly Rookery Bay and Sapelo Island. Metabolism estimates using filtered DO time series had decreased mean production (-63.1 % change from the annual mean) and respiration (-62.6 %) for Elkhorn Slough, increased mean production (17.8 %) and respiration (18.8 %) for Padilla Bay, and generally unchanged mean production and respiration for Rookery Bay and Sapelo Island (Table 5). Changes in mean estimates based on filtered DO time series suggests that the weighted regression removed variation attributed to both biological and physical processes. The implications of these undesirable results are described below. Decreases in the standard erorr for all metabolism estimates were observed for all cases after filtering.

An example from Sapelo Island illustrates the effects of weighted regression on DO and metabolism estimates (Figs. 6 to 8). A two-week period in February showed when the tidal cycles were both in and out of phase with the diel cycling, where phasing describes synchronicity between maximum tide heights and day/night periods (Nidzieko et al. 2014). That is, maximum tide heights were generally out of phase with the diel cycle during the first week when low tides were observed during the middle of the night and the middle of the day (Fig. 6), whereas tide heights were in phase during the second week when the maximum tide height occured during the day and night (Fig. 7). The effects of tidal height change on the observed DO time series are visually apparent in the plots. The first week illustrates a strong negative bias (less respiration, less production) in the observed DO signal from low tides at mid-day and mid-night, whereas the second example illustrates a strong positive bias (more respiration, more production) in the observed DO from high tides. These biases are apparent in the metabolism estimates using the observed data (Fig. 8). Anomalous estimates occur when low tides are in phase with the solar cycle (week one), whereas metabolism estimates are likely over-estimated when high tides are in phase with the solar cycle (week two). The filtered time series shows noticeable changes given the direction of bias from the phasing between tidal height and diel period. DO values were higher after filtering when low tides occurred during night and day periods, whereas DO values were lower after filtering when high tides occurred during day and night periods (Figs. 6 and 7). Changes in metabolism estimates after filtering were also apparent, such that the anomalous values were removed during the first week and the positive bias in the second week is decreased (Fig. 8).

Accuracy of results and effects of aggregation

A point of concern is the period of observation within which observed DO is affected by tidal height changes and the extent to which this affects the interpretation of ecosystem metabolism. The effects of tidal variation on daily estimates may not be of concern if seasonal or annual aggregations (e.g., mean annual metabolism) remove this potential bias. The example from Sapelo Island in the previous section highlights this point given that mean production and respiration estimates before and after filtering were generally unchanged for the two-week period. Alternatively, annual averages of production and respiration estimates were significantly different for Elkhorn Slough and Padilla Bay but not Rookery Bay and Sapelo Island (Table 5). Therefore, an evaluation of weighted regression to filter the effects of tidal variation on ecosystem metabolism for different periods of observation is critical for its application. Specifically, does the period of observation affect the ability of weighted regression to remove physical variation in the time series? When should filtering be applied if aggregation of observed data on longer time periods removes potential bias? The first question is addressed by evaluating collinearity between tidal change and solar periods. The second question is addressed by comparing observed and filtered estimates that are aggregated over different periods of observation.

Collinearity between tidal height change and solar cycling likely affected the ability of weighted regression to quantify the variation in DO time series. Model parameterization may be unreliable if, for example, tidal height follows diurnal periods by increasing during the day or decreasing during the night. Nidzieko et al. (2014) found that such covariation is common in Elkhorn Slough during the summer months when high tides always occurred during the night. Given that the phasing between tidal height change and diurnal cycling is variable, the ability of weighted regression to quantify variation attributed to both is also expected to vary. The correlation between sun angle and tidal change (measured as an angular rate) was evaluated using a moving window approach for each case study. This approach is analogous to weighted regression by providing an indication of when collinearity may occur as a function of the moving window. Weighted regression can be expected to effectively characterize biological and physical variation during periods when the correlation between tidal height change and diurnal cycling is low within the window. Fig. 9 suggests that collinearity between sun angle and tidal height change can exceed +/-0.2 for Elkhorn Slough and Padilla Bay, whereas correlations were much smaller regardless of the period of observation for Rookery Bay and Sapelo Island. Given the change in mean annual metabolism using the filtered DO time series and the relatively high collinearity between tidal change and solar cycling, the results for Elkhorn Slough and Padilla

Bay may not be accurate. The results may only be interpretable when correlations are close to zero (e.g., April and October for Elkhorn Slough).

The observed and filtered daily estimates were averaged by month for each case study to evaluate effects of aggregation on mean production and respiration, in addition to the mean annual estimates in Table 5. Significant variation in aggregated production and respiration estimates was observed for each case study (Fig. 10). Filtered production and respiration estimates for Padilla Bay and Rookery Bay exhibited monthly variation that was more characteristic of expected trends during warmer months. Specifically, metabolism estimates based on observed DO were substantially muted for both Padilla Bay and Rookery Bay during summer months, whereas values were significantly higher after filtering. Results for Sapelo Island suggested that aggregated estimates were similar before and after filtering, although winter and summer months were slightly under- and over-estimated, respectively, using the observed data. Results for Elkhorn Slough varied significantly such that production and respiration were significantly reduced after filtering, which may have been related to collinearity. Overall, these trends emphasize the importance of considering different aggregation periods for interpreting metabolism estimates. Each case study showed differences in observed and filtered values at monthly aggregations, suggesting tidal variation may influence metabolism estimates at relatively long time scales Table 5).

Discussion

The weighted regression approach was developed to improve estimates of ecosystem metabolism by removing variation associated with tidal change in observed DO time series. The application to simulated DO time series with known characteristics and extension to continuous monitoring data from selected NERRS sites suggested the approach can isolate and remove variation in observed DO from tidal change. Further, aggregation of metabolism estimates using the filtered DO time series were significantly different than those using the observed data, particularly for relatively long periods of observation depending on location. These results suggest that previous estimates may not accurately reflect true metabolic signals if the effects of tidal variation confound biological signals in observed DO time series. Additionally, variation of aggregated metabolism estimates were substantially reduced after filtering, suggesting greater confidence in interpreting estimates even if the mean values are similar.

Comparisons between filtered and biological DO time series from the simulations indicated that weighted regression can reduce the effects of tidal variation for a range of characteristics of DO time series. An examination of scenarios that produced abnormal results can provide additional insight into factors that affect the performance of weighted regression. For example, poor performance was observed when the observation uncertainty (ϵ_{obs}) was high and both process uncertainty (ϵ_{pro}) and tidal advection (DO_{adv}) were low. These examples represent time series with excessive random variation, no auto-correlation, and no tidal influence. Poor performance is expected because the weighted regression models a non-existent tidal signal in a very noisy DO time series. These results were observed even for time series with a large diel component of the biological DO signal, suggesting that the model will produce random results in microtidal systems with high noise and no serial correlation. From a practical perspective, weighted regression should not be applied to noisy time series if there is not sufficient evidence to suggest the variation is related to tidal changes. Alternative approaches, such as the Kalman filter (Harvey 1989, Batt and Carpenter 2012), may be more appropriate if random variation is the primary source of uncertainty. Similarly, results with perfect or near-perfect correlations between filtered and biological DO time series were observed when observation uncertainty and tidal effects were not components of the simulated time series. Although there is no need to apply weighted regression to time series with no apparent tidal influences, the results will not be incorrect. We emphasize that the weighted regression should only be applied to time series for which specific conditions apply, as described in the recommendations below.

For all case studies, weighted regression was generally successful in reducing the variation in the DO time series that was caused by physical advecttion. In particular, the reduction of anomalous metabolism estimates after filtering was observed. Negative production and positive respiration estimates suggest assumptions of the open-water method are violated (Needoba et al. 2012), although 'normal' estimates (positive production and negative respiration) may still include a significant source of bias from physical advection by providing over-estimates of true values. For example, Nidzieko et al. (2014) observed that net metabolism at Elkhorn Slough was strongly heterotrophic during spring tides that occurred at nighttime such that inundation of salt marshes during the night following by draining with low tide during the day lead to inflated respiration values. Synchrony between solar and tidal cycles is a critical concern for interpreting metabolism estimates such that collinearity between the two may diminish the performance of weighted regression.

The weighted regression approach makes no assumptions as to the relationships between DO and tidal variation over time. Although the functional form of the model is a simple linear regression with only two explanatory variables (eq. (1)), the moving window approach combined with the adaptive weighting scheme allows for quantification of complex tidal effects that may not be possible using alternative approaches. A similer approach by Batt and Carpenter (2012) uses a Kalman filter to improve estimates of ecosystem metabolism in lakes. The approach minimizes uncertainty in observed DO using a filter that combines information about the data generation process and the manner in which the data are observed (Harvey 1989). Although a similar approach could be used for estuaries, it may not be effective given that the effects of tidal advection are not related to process or observation uncertainty. Additionally, results from the case studies illustrated the ability of the weighted regression approach to model changes over time in the relationships between tidal change and DO. Results for Padilla Bay and Rookery Bay suggested that filtering had the largest effect during the summer, whereas the results for cooler months were not significantly different from the observed. The weighted regression method produced filtered time series that accommodated seasonal variation in DO conditional on tidal height change, whereas moving window filters or standard regression techniques would likely not have characterized these dynamic relationships.

Comments and recommendations

Results from the simulations and case studies suggested that weighted regression can be a practical approach for filtering DO time series. However, application may only be appropriate under specific situations. The case studies were chosen based on the relatively high proportion of metabolism estimates that were anomalous and the strength of correlation between the observed DO time series and tidal height. Despite these similarites, filtering had variable effects on metabolism estimates. The results for Elkhorn Slough and Padilla Bay are of particular concern given that mean annual estimates were substantially different compared to those from the observed DO time series. Although the correlation of DO and tidal height was reduced for both cases, in addition to a reduction of anomalous estimates, collinearity between tidal change and solar cycling likely contributed to the relative change in mean metabolism before and after filtering. Evaluating collinearity, as in Fig. 9, is an important diagnostic for characterizing the expected performance of weighted regression and choosing appropriate window widths. These plots should indicate whether weighted regression is appropriate for the whole time series (e.g., Sapelo Island) or only for specific periods when collinearity is low (e.g., April and October at Elkhorn Slough). A weight-of-evidence approach should also be used such that application of weighted regression should reduce anomalous metabolism estimates, minimize correlations between observed DO and tide height, and reduce clear visual patterns of tide change on DO. In general, a pragmatic approach is emphasized such that results should be evaluated based on the preservation of diel variation from production while exhibiting minimal changes with the tide. Such an approach, combined with further validation, will support informed management decisions through more accurate estimates of ecosystem metabolism.

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Figures

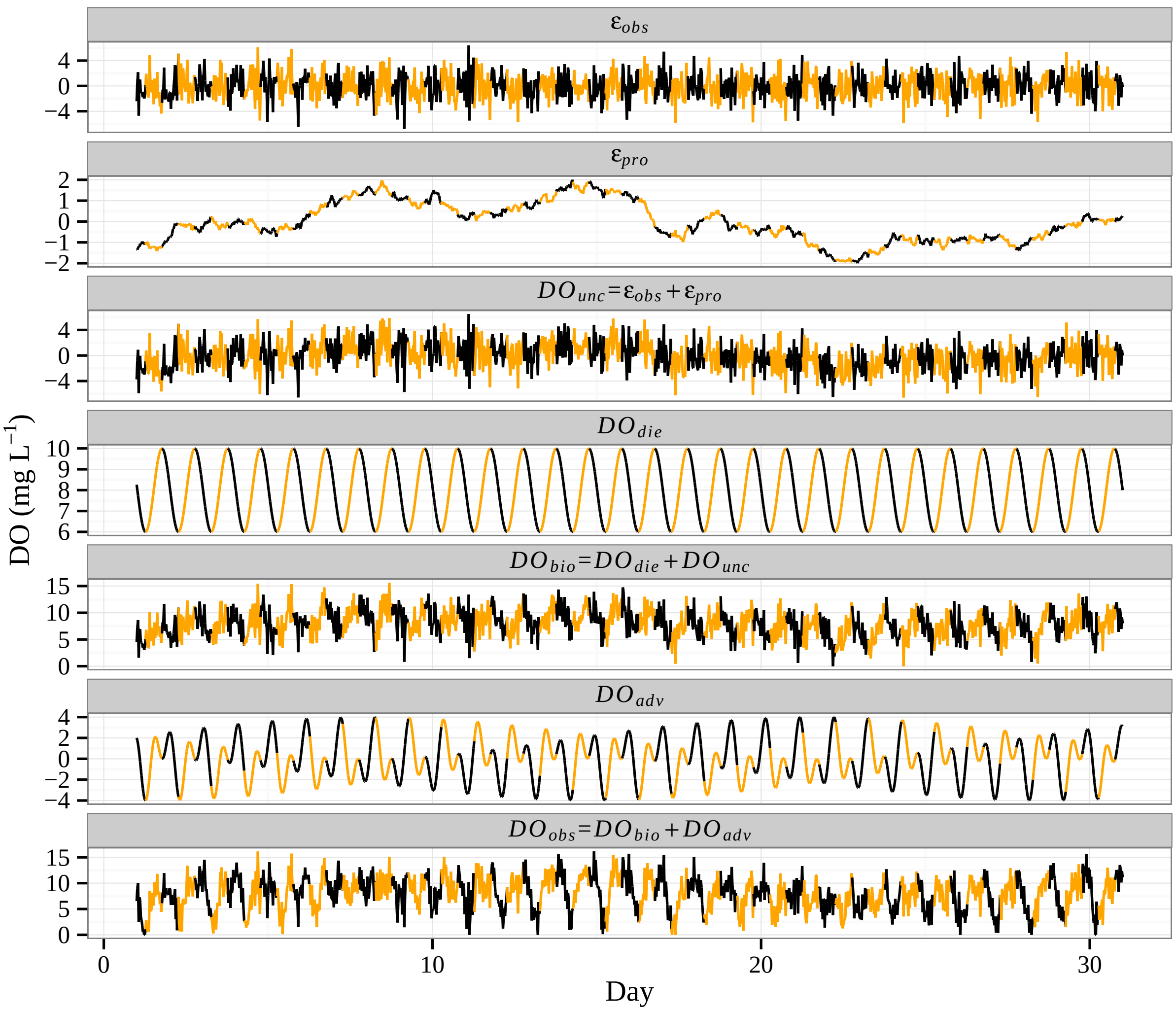

Fig. 1: Example of each component of a simulated DO time series for testing weighted regression. The time series were created using eqs. (4) to (13). Yellow indicates a twelve hour daylight period beginning at 630 each day. fig:do_sim

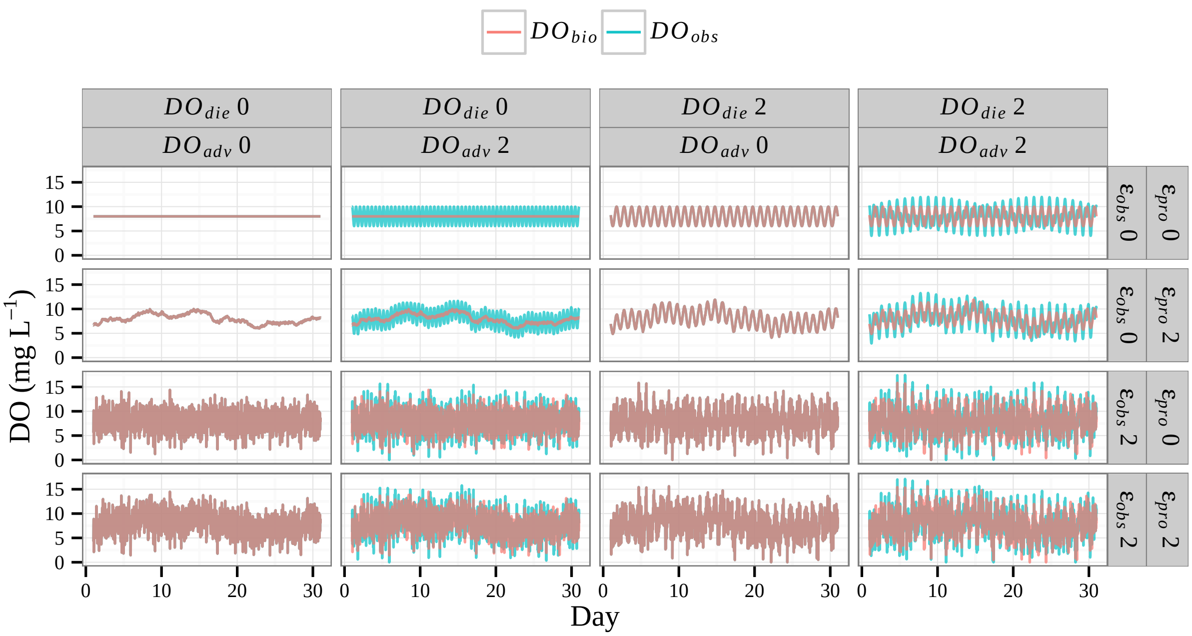

Fig. 2: Representative examples of simulated time series of observed DO (DO_{obs}, blue lines) and biological DO (DO_{bio}, as a component of observed, red lines) created by varying each of four parameters: strength of tidal association with DO signal (DO_{adv}), amount of process uncertainty (ϵ_{pro}), amount of observation uncertainty (ϵ_{obs}), and strength of diel DO component (DO_{die}). Parameter values represent the minimum and maximum used in the simulations as mg L^{-1} of DO. fig:sim_ex

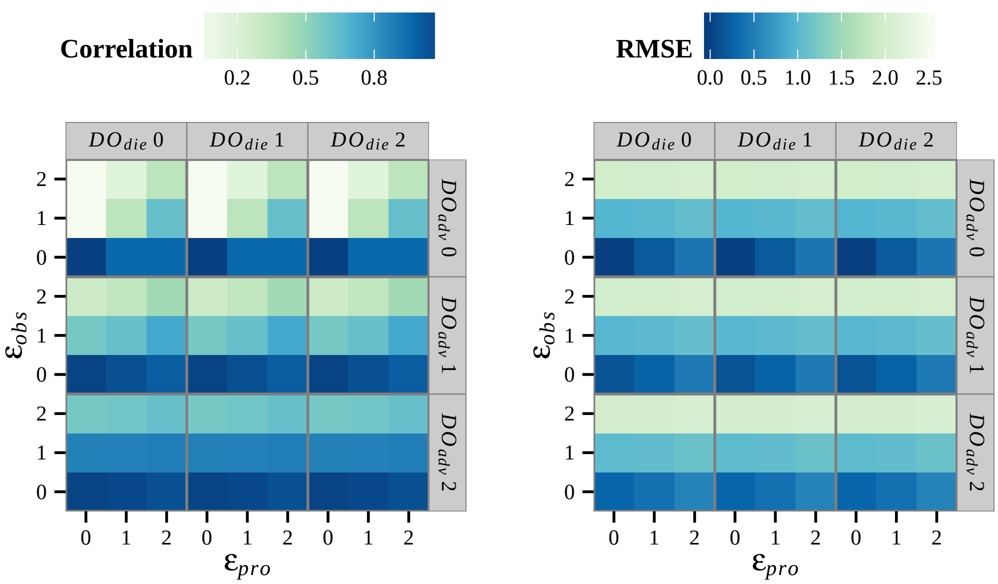

Fig. 3: Heat maps of correlations and errors (RMSE) for filtered DO time series (DO_{dtd}) from weighted regression with 'true' biological DO (DO_{bio}) for varying simulation parameters: strength of tidal association with DO signal (DO_{adv}), amount of process uncertainty (ϵ_{pro}), amount of observation observation uncertainty (ϵ_{obs}), and strength of diel DO component (DO_{die}). Each tile represents the correlation or error from results for a given combination of simulation parameters averaged for all window widths (Fig. 4). fig:err_surf1

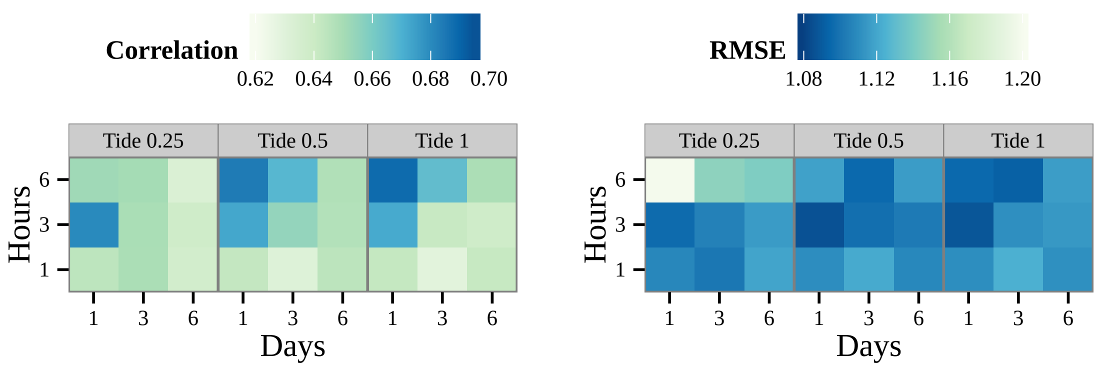

Fig. 4: Heat maps of correlations and errors (RMSE) for filtered DO time series (DO_{dtd}) from weighted regression with 'true' biological DO (DO_{bio}) for varying half window widths: days, hour of day, and proportion of tidal range. Each tile represents the correlation or error from results for a given combination of window widths averaged for all simulation parameters (Fig. 3). fig:err_surf2

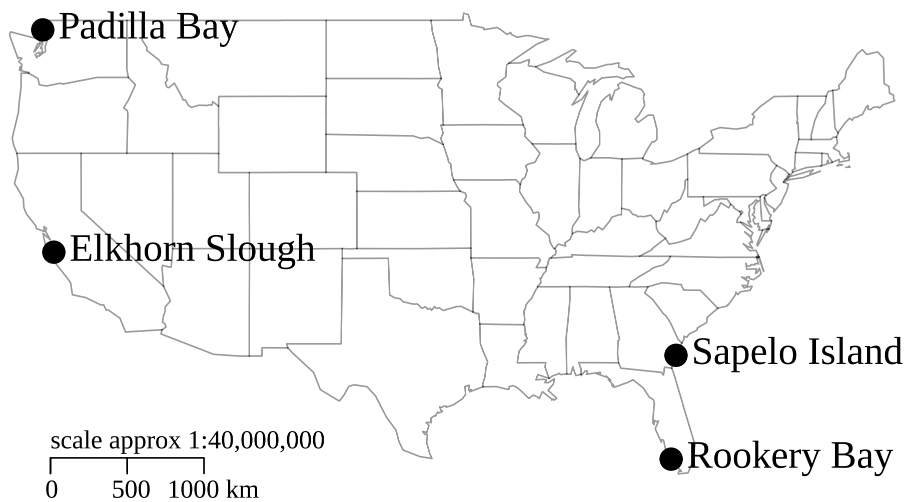

Fig. 5: Locations of NERRS sites used as case studies to validate weighted regression. Stations at each reserve are ELKVM (Vierra Mouth at Elkhorn Slough), PDBBY (Bayview Channel at Padilla Bay), RKBMB (Middle Blackwater River at Rookery Bay), and SAPDC (Dean Creek at Sapelo Island). fig:case_map

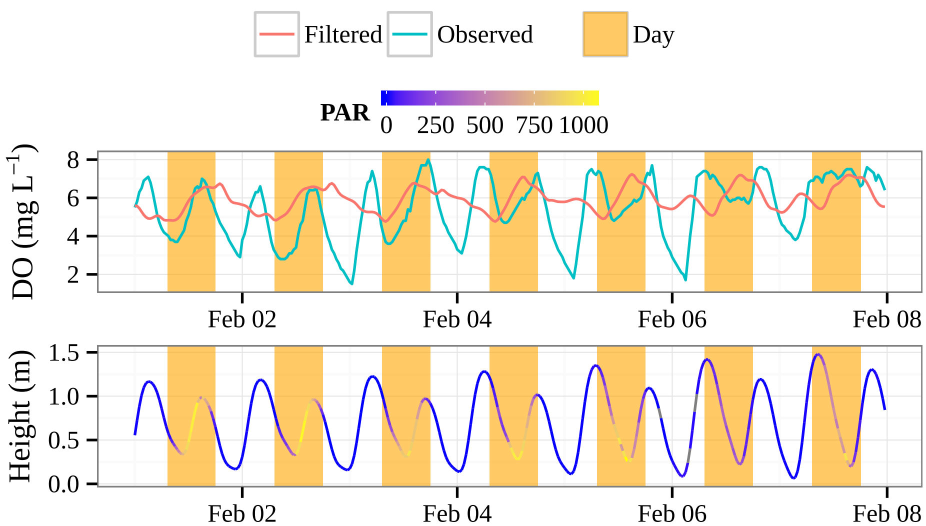

Fig. 6: Continuous DO time series before (observed) and after (filtered) filtering with weighted regression (top) and tidal height (m) colored by total photosynthetically active radiation (bottom, mmol m^{-2}). Results are for the Sapelo Island station for a seven day period when high tide events were out of phase with diel periods, creating lower than expected observed DO during night and day periods. Filtered values are based on a weighted regression with half window widths of six days, one hour within each day, and tidal height proportion of one half.fig:phase_out

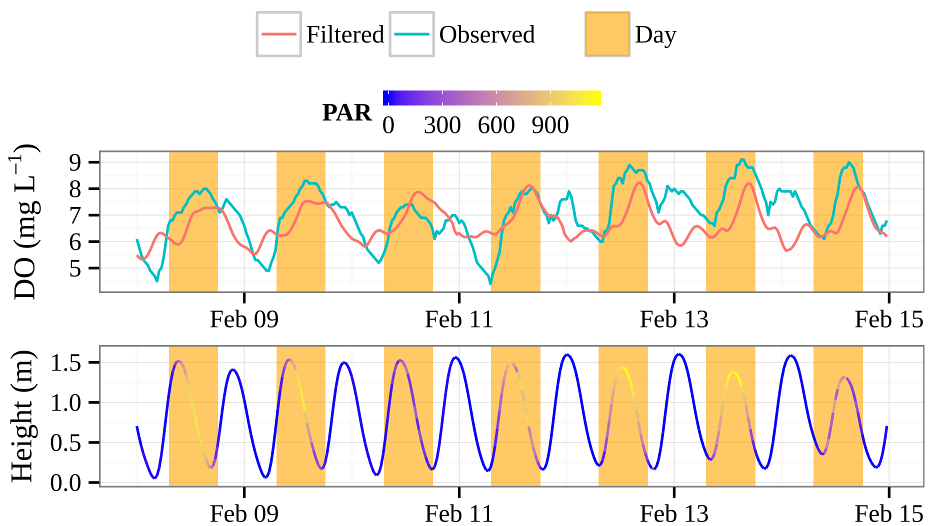

Fig. 7: Continuous DO time series before (observed) and after (filtered) filtering with weighted regression (top) and tidal height (m) colored by total photosynthetically active radiation (bottom, mmol m^{-2}). Results are for the Sapelo Island station for a seven day period when high tide events were in phase with diel periods, creating higher than expected observed DO during night and day periods. Filtered values are based on a weighted regression with half window widths of six days, one hour within each day, and tidal height proportion of one half. fig:phase_in

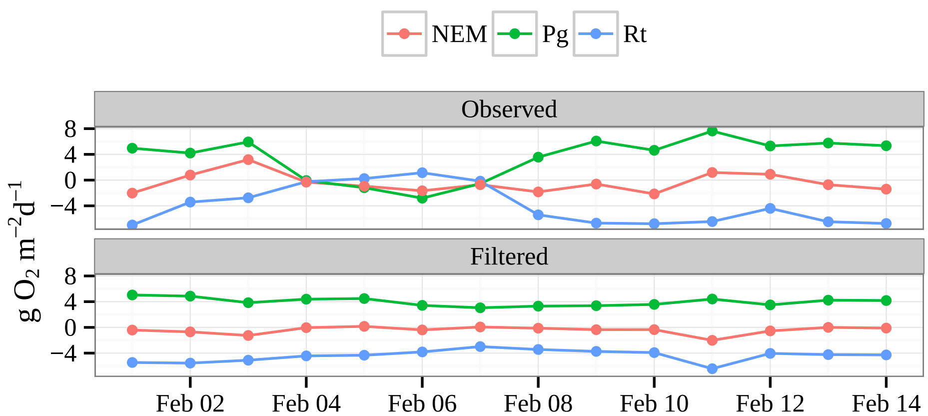

Fig. 8: Example of daily mean metabolism (net ecosystem metabolism, gross production, and total respiration) before (observed) and after (filtered) filtering with weighted regression. Results are for the Sapelo Island station for a two week period in February, 2012 when high tide was out of phase with the diel cycle during the first week (Fig. 6) and in phase during the second week (Fig. 7). fig:case_ex

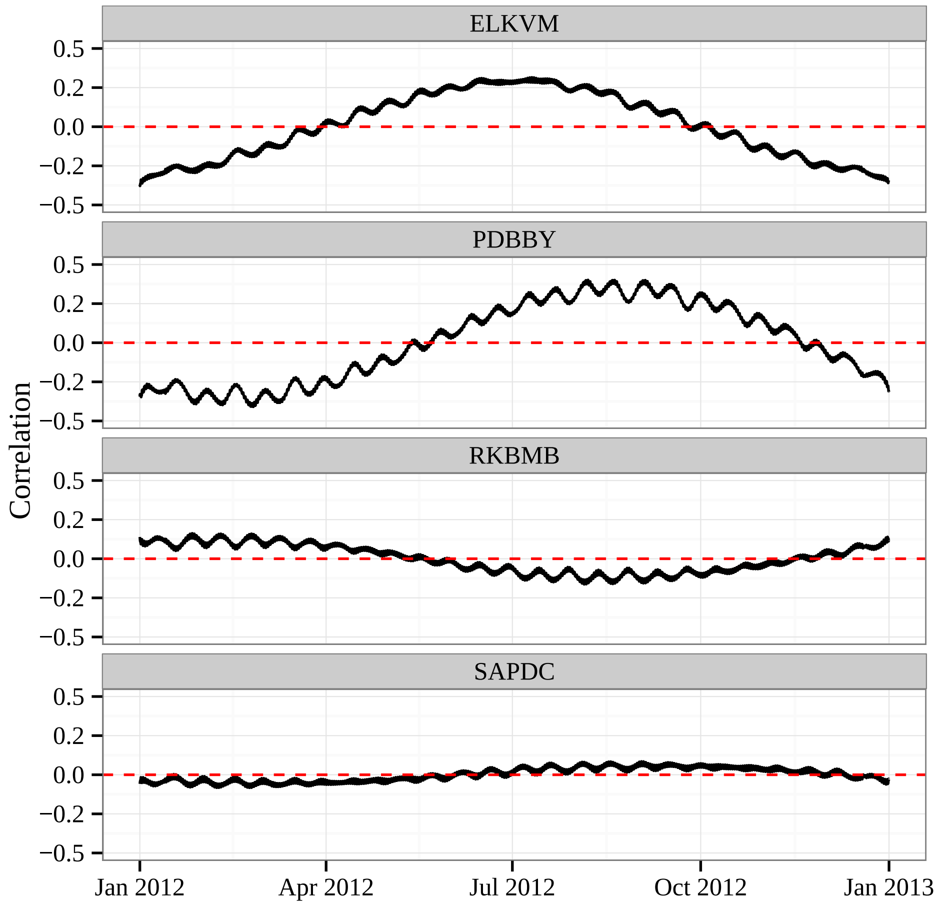

Fig. 9: Correlations of sun angle with tidal change (as an angular rate) using a half-window width of 12 days. Correlations larger or smaller than zero are periods when weighted regression may not effectively quantify variation from biological and physical sources in DO time series due to collinearity.fig:move_corrs

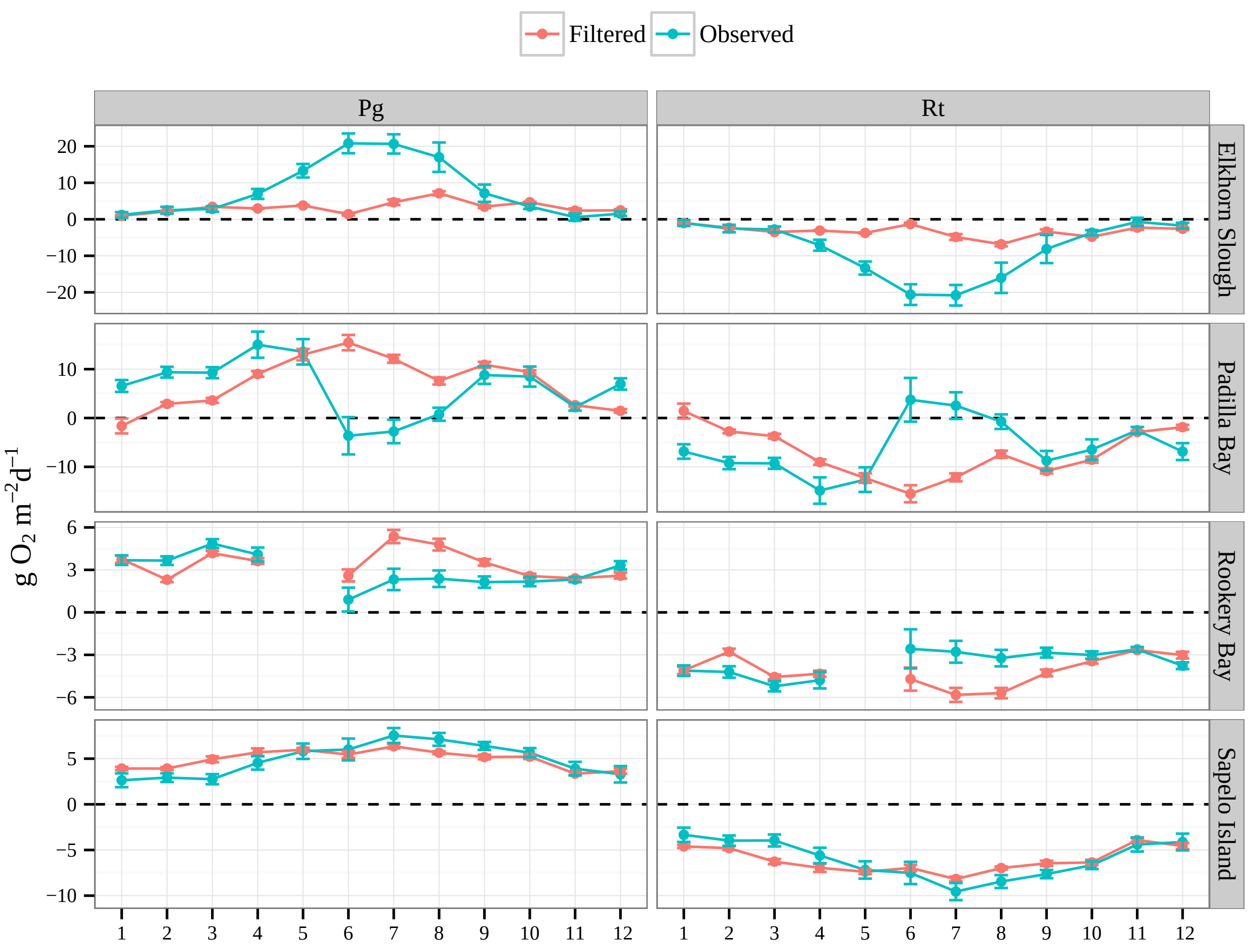

Fig. 10: Means and standard errors of daily metabolism estimates (gross production, total respiration) aggregated by month. Aggregated estimates are shown for observed and filtered DO time series. May was removed from Rookery Bay because of incomplete data. fig:metab_sum

Tables

Table 1: Summary (range, median, quartiles) of correlations and error estimates comparing filtered and biological DO time series for different simulation parameters (DO_{die}, DO_{adv}, ϵ_{pro}, ϵ_{obs}). Values represent averages from multiple simulations with common parameters (e.g., row one is a summary of all simulations for which the diel DO component was zero). tab:dtd_perf1

Parameter	**Correlation**					**RMSE**				
	Min	25th	Median	75th	Max	Min	25th	Median	75th	Max
$\boldsymbol{DO_{die}}$										
0	0.05	0.20	0.41	0.86	1.00	0.00	0.33	1.01	1.96	2.05
1	0.28	0.44	0.61	0.93	1.00	0.02	0.42	1.02	1.96	2.06
2	0.55	0.60	0.81	0.96	1.00	0.05	0.52	1.06	1.99	2.12
$\boldsymbol{DO_{adv}}$										
0	0.05	0.42	0.63	0.93	1.00	0.00	0.46	1.02	1.97	2.12
1	0.05	0.42	0.63	0.93	1.00	0.00	0.46	1.02	1.97	2.12
2	0.05	0.42	0.63	0.93	1.00	0.00	0.46	1.02	1.97	2.12
$\boldsymbol{\epsilon_{pro}}$										
0	0.05	0.31	0.58	0.99	1.00	0.00	0.23	0.99	1.95	2.11
1	0.16	0.37	0.61	0.93	0.99	0.10	0.33	1.02	1.97	2.11
2	0.34	0.58	0.69	0.89	0.98	0.19	0.56	1.10	2.01	2.12
$\boldsymbol{\epsilon_{obs}}$										
0	0.80	0.93	0.97	0.99	1.00	0.00	0.17	0.29	0.46	0.84
1	0.05	0.56	0.62	0.81	0.84	0.97	1.00	1.02	1.08	1.28
2	0.05	0.31	0.38	0.57	0.63	1.93	1.97	1.98	2.01	2.12

Table 2: Summary (range, median, quartiles) of correlations and error estimates comparing filtered and biological DO time series for simulations using different half window widths in the weighted regressions (days, hours, and proportion of tidal range). Values represent averages from multiple simulations with common window values (e.g., row one is a summary of all simulations for which the half window width was one day). tab:dtd_perf2

Window	**Correlation**					**RMSE**				
	Min	25^{th}	Median	75^{th}	Max	Min	25^{th}	Median	75^{th}	Max
Days										
1	0.07	0.44	0.66	0.96	1.00	0.00	0.43	1.02	1.96	2.12
3	0.07	0.41	0.62	0.93	1.00	0.00	0.45	1.02	1.97	2.08
6	0.05	0.37	0.61	0.88	1.00	0.00	0.51	1.02	1.97	2.08
Hours										
1	0.07	0.38	0.61	0.89	1.00	0.00	0.51	1.02	1.97	2.05
3	0.06	0.42	0.63	0.95	1.00	0.00	0.43	1.02	1.97	2.05
6	0.05	0.44	0.64	0.95	1.00	0.00	0.48	1.04	1.96	2.12
Tide										
0.25	0.05	0.42	0.62	0.92	1.00	0.00	0.47	1.03	1.97	2.12
0.5	0.07	0.42	0.63	0.94	1.00	0.00	0.45	1.02	1.96	2.04
1	0.07	0.42	0.63	0.94	1.00	0.00	0.44	1.02	1.97	2.04

Table 3: Summary statistics of tidal component amplitudes (m), selected water quality parameters (DO mg L^{-1}, chlorophyll-a μg L^{-1}, salinity psu, water temperature °C) and metabolism estimates (gross production, respiration, and net ecosystem metabolism as g m^{-2} d^{-1}) for each case study. Tidal components are principal lunar semidiurnal (O1, frequency 25.82 hours), solar diurnal (P1, 24.07 hours), lunar semidiurnal (M2, 12.42 hours), and solar semidiurnal (S2, 12 hours) estimated from harmonic regressions of tidal height (`oce` package in R, Foreman and Henry 1989, RDCT 2014). Water quality data are averages for the entire period of record for each site. Metabolism estimates are means of daily integrated values. tab:case_att

Site	**Tidal amplitude**				**Water quality**				**Metabolism**[a]		
	O1	P1	M2	S2	DO	Chl	Sal	Temp	Pg	Rt	NEM
ELKVM	0.24	0.12	0.48	0.13	7.87	3.87	32.43	13.78	8.14	-8.19	-0.05
PDBBY	0.46	0.23	0.63	0.15	8.97	2.24	29.17	10.44	5.95	-5.90	0.05
RKBMB	0.13	0.04	0.36	0.10	4.48	4.50	30.53	25.85	3.02	-3.62	-0.60
SAPDC	0.10	0.02	0.54	0.07	4.96	5.98	27.30	21.77	4.89	-6.04	-1.16

[a]Pg: gross production, Rt: respiration, NEM: net ecosystem metabolism

Table 4: Correlations of tidal changes at each site with continuous DO observations and metabolism estimates (gross production, respiration) before (observed) and after (filtered) filtering with weighted regression. Values are averages of monthly correlations. DO values are correlated with predicted tidal height at each observation, whereas metabolism estimates are correlated with mean tidal height change between observations during day or night periods for production and respiration, respectively. tab:cor_res

Site	DO	Pg[a]	Rt
ELKVM			
Observed	0.44	0.43	0.43
Filtered	-0.04	0.04	-0.01
PDBBY			
Observed	-0.49	-0.11	-0.29
Filtered	0.01	-0.05	0.00
RKBMB			
Observed	0.45	0.26	0.34
Filtered	0.02	-0.04	0.03
SAPDC			
Observed	0.62	0.47	0.64
Filtered	0.00	-0.04	0.07

[a] Pg: gross production, Rt: respiration, NEM: net ecosystem metabolism

Table 5: Summary of metabolism estimates (gross production, respiration) for case studies using DO time series before (observed) and after (filtered) filtering with weighted regression. Means and standard errors are based on daily integrated metabolism estimates. Anomalous values are the proportion of metabolism estimates that were negative for gross production and positive for respiration. tab:case_res

Site	**Pg**[a]			**Rt**		
	Mean	Std. Err.	Anom	Mean	Std. Err.	Anom
ELKVM						
Observed	8.14	0.67	0.19	-8.19	0.69	0.21
Filtered	3.00	0.13	0.07	-3.06	0.14	0.07
PDBBY						
Observed	5.95	0.69	0.22	-5.90	0.74	0.19
Filtered	7.01	0.40	0.05	-7.01	0.40	0.06
RKBMB						
Observed	3.02	0.14	0.09	-3.62	0.15	0.08
Filtered	3.46	0.10	0.01	-4.07	0.11	0.01
SAPDC						
Observed	4.89	0.23	0.13	-6.04	0.25	0.11
Filtered	4.94	0.09	0.00	-6.13	0.10	0.00

[a]Pg: gross production, Rt: respiration

Multimedia

{multi}

The supporting information for this manuscript includes a graphical illustration of the weighting scheme described in the material and procedures section (http://spark.rstudio.com/beckmw/weights_widget), results for each simulation (http://spark.rstudio.com/beckmw/detiding_sims), and results for each case study (http://spark.rstudio.com/beckmw/detiding_cases). Each link is a graphical summary of data based on interactive inputs to support the results in the manuscript.