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ECOSYSTEMS

Toward a Standardized Method for Quantifying Ecosystem Hot Spots and Hot Moments

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ABSTRACT

Ecosystem ''hot spots'' and ''hot moments''—respectively, places and times of disproportionately high biogeochemical activity—are an important and often invoked concept in ecosystem science. Despite the popularity of the concept, there is no standard approach to quantifying hot spots and hot moments, hindering progress in understanding the phenomenon. For example, lack of a standard quantitative approach hinders advances arising from synthesis across datasets and studies potentially representing different processes, ecosystem types, places, and times. We present an approach to quantifying hot spots and hot moments based on the skewness and kurtosis of data distributions. Our approach explicitly tests for the presence of hot spots and/or hot moments, as well as identifies observations regarded as hot spots and/or hot moments. We apply our method to three case studies representing different ecosystem contexts and focal variables: soil pore space CO_2 concentrations in a humid temperate watershed; dissolved oxygen saturation in a hypereutrophic, shallow lake; and seagrass metabolism on the coast of a tropical island. A rarefaction-based sensitivity analysis showed how detection of HSHM using our methods can be sensitive to changes in spatial and temporal sampling regimes, depending on the behavior of the system. To facilitate adoption of our approach, we provide the R package ''hotspomoments'' to implement the method. Adoption of a standard quantitative approach to hot spots and hot moments would advance ecosystem science.

Key words: biogeochemistry; control points; dissolved oxygen; CO_2 efflux; net ecosystem production.

HIGHLIGHTS

- ''Hot spots'' and ''hot moments'' are key concepts but difficult to quantify
- The skewness and kurtosis of data distributions yield a quantitative approach
- Three empirical case studies demonstrate the approach in diverse contexts

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INTRODUCTION

Understanding the magnitude and drivers of spatial and temporal variability in biogeochemical rates is a central question in ecosystem ecology. Locations within a landscape or ecosystem that contain disproportionately high process rates (hot spots; HS) or periods of time during which rates are high (hot moments; HM) are important for characterizing the overall biogeochemical behavior of an ecosystem (McClain and others 2003) and understanding extremes in other ecosystem components (Batt and others 2017). These patches and periods, or control points, are driven by spatial connectivity and the movement of reactants or products over time (Bernhardt and others 2017). By definition, HS and HM (and the combination, HSHM) are spatially and temporally rare and therefore difficult to quantify. However, quantitative descriptions of this form of spatiotemporal heterogeneity are needed to improve both conceptual and numerical ecosystem models (Bernhardt and others 2017). Although rare, because HSHM are uncommonly large, they have major impacts on overall ecosystem dynamics, and hence models that account for HSHM poorly cannot provide an accurate picture of system behavior. With the advent of new sensor technologies, remote sensing, and other tools, we are well-positioned to quantify HSHM dynamics and uncover the mechanisms that generate them. However, although McClain and others (2003) formalized the HSHM concept, there is still not a widely used, statistically rigorous method for identifying HSHM in ecosystems (Bernhardt and others 2017). This impedes our ability to systematically and comparatively study the mechanisms underpinning HSHM, how these processes scale in space and time, and our ability to predict when and where HSHM occur.

Although there is currently no standard quantitative definition of HSHM (Bernhardt and others 2017; Kannenberg and others 2020), several approaches have been used, many relying on identifying extreme values from a data distribution (see Bernhardt and others 2017). For example, Kannenberg and others (2020) considered values more than two standard deviations from the mean to be HSHM; Yu and others (2013) considered observations in the 4th quartile of the distribution HSHM; and Darrouzet-Nardi and Bowman (2011) developed a mathematical definition to identify observations that are both outliers and disproportionately large. Other frameworks, such as those based on the Pareto distribution, are also useful for characterizing extreme values (for example, Carpenter and others 2015), but may require more observations than are in many ecosystem science datasets to robustly implement. One shortcoming of existing approaches is that they largely assume, rather than explicitly test, that HSHM are present in the data and instead focus on identifying which observations can be considered HSHM. Using for illustration the definition of HSHM as two standard deviations from the mean, nearly any dataset of sufficient sample size will have observations more than two standard deviations from the mean, even if these are not sufficiently large to make disproportionate contributions to the total. Hence, a widely applicable test explicitly for the presence of HSHM could improve quantification of the phenomenon by limiting qualitative or ad hoc approaches that are likely to be inconsistent across studies.

We propose an approach using the skewness and kurtosis of distributions of ecosystem measurements to detect if HSHM are present in the system, and to identify which observations constitute HSHM (Figure 1). HSHM are inherently extreme observations (McClain and others 2003), and skewness and kurtosis can be thought of as quantifying the degree to which a distribution of observations is dominated by values in the tails (extremes). Here, skewness corresponds to whether a distribution is dominated by values in the upper or lower tails: for two distributions of equal variance but unequal skewness, the more skewed will have a greater magnitude and higher density (for example, a fatter tail) of extreme values. Kurtosis can describe when more symmetric distributions have many and/or more extreme observations in both tails (that is, the distribution is leptokurtic). Considering both left- and right-skewed distributions and kurtosis accommodates process rates such as net ecosystem production (NEP), which may be positive or negative and for which a set of observations can contain extreme values in one or both directions. To move beyond simple description, we test whether skewness and/or kurtosis are significantly greater than expected if HSHM were not present by comparing against a reference distribution using a parametric bootstrapping procedure. Observations constituting HSHM can be identified by comparison to a reference distribution or other methods of identifying extreme values. Once identified, the location and timing of HSHM, and their relationships to other ecosystem variables and processes can be examined to yield inference into the underlying hydrologic, ecophysiological, and biogeochemical mechanisms of ecosystem HSHM.

Below, we present details of an approach to use distributional skewness and kurtosis for quantifying ecosystem hot spots and hot moments (HSHM) and apply it to three empirical case studies representing different ecosystem contexts and focal variables: seagrass metabolism on the coast of a tropical island, soil pore space CO_2 concentrations in a humid temperate watershed, and dissolved oxygen saturation in a hypereutrophic, shallow lake. Using the largest dataset (lake dissolved oxygen saturation), we assessed the robustness of results generated under our new method to uncertainty arising from loss of observations. Our approach is flexible to a wide range of applications and provides a standard quantitative approach to quantifying HSHM that can facilitate advances in understanding ecosystem HSHM across scales, especially through syntheses involving multiple variables, ecosystems, or time periods.

METHODS

Algorithm Implementation

Here, we present algorithms that operationalize the conceptual approach described above, using the statistical moments skewness and kurtosis of data distributions to (a) infer whether a set of biogeochemical observations contain HSHM; and (b) identify observations constituting HSHM. These algorithms are generic, and we believe they can be applied to nearly any set of biogeochemical observations, taken over space (HS), time (HM), or both (HSHM).

To infer whether a set of biogeochemical observations contains HSHM, we first test for skewness by measuring the sample skewness of the observations and assessing the statistical rarity relative to a reference distribution using a parametric bootstrapping procedure. We define sample skewness as the quantity

$$\text{skewness} = \left[\frac{n(n-1)}{n-2}\right]^{1/2}\left(\frac{\frac{1}{n}\sum_{i=1}^{n}(x_i-\overline{x})^3}{\left[\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\overline{x})^2\right]^{3/2}}\right),$$

where n is the number of observations in the dataset; x_i is the ith observation of variable x; and $\overline{x}$ is the mean (Joanes and Gill 1998). Our parametric bootstrapping procedure compares the skewness of the input data to a distribution of ''surrogate'' skewness values obtained by computing the skewness of many (say, 1000) realizations of n random deviates from a reference statistical distribution corresponding to a null model of no HSHM. Here, we use as the reference distribution the normal distribution with mean and variance equal to those of the sample x; further discussion of this choice is provided below. The rank of the skewness of the input data relative to the skewness of the surrogate datasets can then be used to assess the statistical significance of the skewness of the input data, to an acceptable level of certainty. For example, if the quantile of the empirical skewness in the distribution of surrogates is > 0.95, this could be considered statistically significant at $p < 0.05$ using a one-tailed test. Correspondingly, a quantile of < 0.05 would constitute statistical significance in left-skewed data, such as for quantities like net ecosystem exchange (NEE) or net ecosystem production (NEP) where positive/negative values indicate uptake/release (or vice versa).

If the data are not significantly left- or right-skewed, it could be the case—especially with variables for which positive/negative values indicate uptake/release or vice versa—that both uptake and release HSHM are present in the same set of observations. A leptokurtic distribution, producing proportionally more and more extreme outliers, would be consistent with this. We measure this property of excess kurtosis within a sample as,

$$\text{kurtosis} = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i-\overline{x})^4}{\left[\frac{1}{n}\sum_{i=1}^{n}(x_i-\overline{x})^2\right]^2} - 3,$$

where, as above, n is the number of observations in a sample of observations x and $\overline{x}$ is the mean of the sample. We use the same parametric bootstrapping procedure to assess the significance of excess kurtosis. Note that in this case, we focus on whether the quantile of empirical excess kurtosis in the distribution of surrogates is > 0.95 (or some other appropriate high threshold) since excess kurtosis systematically less than the reference distribution corresponds to a platykurtic distribution having proportionately few and lower-magnitude extreme values (that is, no HSHM). In practice, the choice of whether to prefer a kurtosis-based test over a skewness-based test depends primarily on whether the empirical data distribution is approximately symmetric and whether low/negative extremes of the focal variable are meaningful.

In these tests, we use normal distributions with equal mean and variance to the focal empirical dataset as the reference representing no HSHM. The normal distribution was selected because it is not skewed and has no excess kurtosis, so any skewness or kurtosis in the surrogates arises from random variation, but the mean and variance can be preserved. Although normally distributed data can contain positive and negative extreme values (its theoretical bounds are $-\infty$ to $+\infty$), we consider it an appropriate null model representing a lack of HSHM because of the rarity of those values. Considering that $< 4.6\%$ of values in a normal distribution are more than two standard deviations from the mean, and $< 0.3\%$ of values more than three standard deviations, we consider extreme values for normally distributed data too rare to disproportionately affect overall ecosystem dynamics, unlike for skewed or leptokurtic distributions which have a larger proportion of extreme values. Moreover, for finite sample sizes (typically, 10 s to 100 s of observations for ecological data), a small number of extrema consistent with a normal distribution likely should not be considered robust evidence for presence of HSHM, because poorly replicated extremes may be indistinguishable from measurement error (Hollinger and Richardson 2005). Testing against other null models might sometimes be more appropriate, and in that case, our general approach could straightforwardly be adapted to test against a different statistical distribution or data generating model. For example, if the process rate or state variable is bounded by a certain interval (for example, must be greater than or equal to zero, such as for denitrification) and the set of observations includes a substantial proportion near the lower bound, it may be useful to test against a statistical distribution that reflects this. The truncated normal distribution is one possibility.

If HSHM are detected in the data due to significant skewness or excess kurtosis, the observations constituting HSHM can be identified using an extension of the logic underpinning our test for HSHM presence. Observations constituting HSHM will be those that are more extreme than expected to occur in an appropriate reference distribution. As above, we use a normal distribution with identical mean and variance to the input data as our reference, because it has no skew or excess kurtosis. Then, we select a quantile corresponding to rarity in the reference distribution, such as 0.05 (lower tail extremes, for example, HSHM sinks) or 0.95 (upper tail extremes) and consider more extreme observations than that quantile to reflect HSHM. This approach is agnostic as to whether the extreme values reflect HS, HM, or a combination of the two. This depends in part on the sampling design or data structure. For example, some datasets contain observations through time or across space only depending on sampling regime and data pre-treatment. For datasets having both spatial and temporal resolution, whether extreme values are concentrated in space or time can signal whether HS or HM predominate in the system. Attributes of the HSHM observations and potentially data on other covariates can then be used to learn about the nature, causes, and consequences of HSHM.

An implementation of these methods for the R environment for statistical computing is available at < https://github.com/jonathan-walter/hotspomoments >.

Case Studies

We gathered three exemplary datasets from a variety of ecosystems to demonstrate the use of the algorithm described above. The example datasets are from terrestrial, freshwater, and marine ecosystems and potentially contain HS, HM, or HS and HM. The methods described above were applied to each of the data sets to test for the presence of HSHM using a normal reference distribution. Analysis code and data visualization are available at < https://github.com/jonathan-walter/hotspomoments-ms > . The details of data collection and analysis are briefly described below.

Soil pore space CO_2 concentrations

Weimer Run is a 374 ha humid, temperate watershed located in the Little Canaan Wildlife Management Area (West Virginia, USA) within the Allegheny highlands of the Appalachian Mountain chain (Atkins and others 2015). Sample plots were arranged in a factorial experimental design with three replicates of three different vegetation cover types (that is, closed-canopy, forest gap, and closed-canopy with shrub layer) at three elevation levels (that is, low = 975 m, medium = 1050 m, and high = 1170 m) for $3 \times 3 \times 3 = 27$ plots design (Atkins and others 2015). Soil pore space CO_2 concentrations were measured using the methods outlined in Pacific and others (2008) adapted from Andrews and Schlesinger (2001) using an infrared gas analyzer (IRGA) coupled with a custom in situ gas well, equilibrated with the atmosphere. Each gas well was placed at 5 and 20 cm depths in the soil. Measurements of soil CO_2 concentrations were taken using a handheld IRGA (model GM70 with M170 pump and GMP 221 CO_2 probe, Vaisala, Finland) with 2–5 min allowed for recirculation after which stabilized values were recorded (Pacific and others 2008). Soil CO_2 pore space was measured approximately weekly during the growing season (May–September) and monthly during the non-growing season from 2010 to 2012 in 27 plots located across the watershed. Because the data distribution was right-skewed, we used skewness in the test for HSHM presence and the 0.95 quantile of the reference distribution to identify HSHM observations.

Dissolved oxygen saturation in a shallow lake

Swan Lake (Iowa, USA) is a 40.5 ha, hypereutrophic lake located in a 311 ha watershed dominated by row crop agriculture (Ortiz and Wilkinson 2021). Dissolved oxygen availability is a key reactant controlling the rates of other redox-sensitive biogeochemical processes. Dissolved oxygen saturation was measured at 98 locations on Swan Lake, 17 times between day of year (DOY) 135 and 265 in 2018 (Ortiz and Wilkinson 2019). The dissolved oxygen saturation measurements were made at each sampling station 0.25 m below the surface of the water using an optical DO sensor on a YSI Pro DSS multiparameter sonde (Yellow Springs, Ohio USA) (Ortiz and Wilkinson 2021). The sensor was calibrated immediately preceding each sampling date. The spatial sampling occurred between 09:00 and 14:00 apart from the first two sampling events which lasted until 16:00. The 98 sampling stations were evenly spaced across the surface of the lake in a 65 × 65 m grid and the order of sampling (north to south) remained constant over the course of the summer. Additionally, the presence or absence of rooted submerged and floating leaf macrophytes was noted at each sampling station for each event beginning on DOY 177 when the plants were large enough to be consistently observed. The macrophyte presence data were used to generate an index ranging 0–100% based on the percentage of sampling dates that rooted macrophytes were observed at each sampling location and could be contributing to spatial and temporal heterogeneity in dissolved oxygen saturation. The macrophyte presence index was interpolated to a 25 × 25 m grid for visualization to aid in the interpretation of dissolved oxygen HSHM. Because the data distribution was right-skewed, we used skewness in the test for HSHM presence and the 0.95 quantile of the reference distribution to identify HSHM observations.

Seagrass metabolism in response to simulated grazing

Green turtles (*Chelonia mydas*) in the Caribbean exhibit a distinct foraging strategy among seagrass herbivores, in which they graze seagrass blades within an area to short heights above the substrate surface (Bjorndal 1980). To investigate the effect of this foraging strategy on ecosystem metabolism, ten plots (2 × 2 m) were set up in a shallow seagrass meadow in Little Cayman, Cayman Islands (Johnson and others 2017). Five plots were experimentally clipped to simulate grazing, and five plots served as an unclipped reference. Net ecosystem metabolism was measured weekly in each plot for 12 weeks during summer 2016 (May–August) using light and dark incubation chambers. Chambers were deployed before 11:30 each day so that incubations encompassed solar maximum, and metabolic rates were estimated from the change in dissolved oxygen (DO) concentration within chambers over the incubation period. Dissolved oxygen concentration was measured immediately following water sample collection using a YSI ProODO handheld optical DO meter (Yellow Springs Instruments, Yellow Springs, Ohio USA). Additional meadow (for example, seagrass biomass, blade length, shoot density) and environmental (for example, temperature, irradiance) characteristics were measured on a weekly or bi-weekly basis as potential drivers of variation in metabolic rates (Johnson and others 2017). Because the data distribution was approximately symmetric and the focal variable contained positive and negative values corresponding to sinks and sources, we used kurtosis in the test for HSHM presence and the 0.025 and 0.975 quantiles of the reference distribution to identify sink and source HSHM observations.

Sensitivity Analysis

Because HSHM are by definition rare events, one challenge associated with their study is that a sampling regime might fail to capture places and/or times corresponding to HSHM, and that statistical methods for their detection might be highly sensitive to the inclusion/exclusion of particular observations. An optimal method should be largely robust to changes in data density so long as the sampling regime is sufficient to capture the HSHM. To examine this, we used the Swan Lake DO data to perform a rarefaction analysis in which we iteratively and randomly removed observations from up to 2/3 of sampling locations or sampling dates, and quantified change in the detected presence of HSHM and which observations were identified as HSHM. Although the observed changes are specific to this dataset and may not fully generalize to others capturing different phenomena using a different sampling regime, an understanding of how the sampling regime interacts with ecosystem dynamics to influence detection of HSHM can aid in study design and interpretation (for example, informing repeated measures sampling, plot location, sampling intervals).

To test the sensitivity of conclusions about HSHM to spatial sampling regime, we iteratively removed observations from n randomly selected locations, where n is the set of integers ranging from 1 to 2/3 the total number of sampling locations (here, $n = 1, 2, \ldots, 65$), up to 100 times each. For each down-sampled dataset, we tested for the presence of HSHM based on distributional skewness, considering the presence of HSHM statistically significant if the quantile of the empirical down-sampled skewness exceeded that of 95% of surrogates. We also identified HSHM observations as those exceeding the 95th percentile of a normal distribution with mean and variance equal to that of the down-sampled dataset.

We evaluated consistency in the overall conclusion of whether the data reflect HSHM in terms of the proportion of down-sampled datasets in which the HSHM test was the same as, non-significant, or different (for example, significant positive skew to significant negative skew), as a function of the number of dropped sampling locations. We evaluated consistency in the identification of HSHM observations in terms of the proportion of HSHM observations identified in the full dataset that were identified in the down-sampled dataset (not counting those that were directly removed by the down-sampling procedure), as well as the ratio of the number of HSHM observations identified in the down-sampled dataset that were not included in the HSHM from the full dataset to the number of HSHM from the full dataset that were present in the down-sampled dataset.

The same procedure was used to test sensitivity to changes in the temporal spatial regime, substituting ‘‘sampling dates’’ for ‘‘locations.’’ Here, the number of dropped sampling dates $n = 1, 2, \ldots 11$.

RESULTS

Soil pore space CO_2 concentrations

Soil CO_2 concentrations at 5 cm (skewness = 6.16, $p < 0.001$) and 20 cm (skewness = 5.60, $p < 0.001$) had significantly right-skewed distributions (Figure 2a), indicating the presence of HSHM. Although more HSHM were identified at 5 cm ($n = 23$, 574 total observations than 20 cm ($n = 15$, 583 total observations), the timing and location of HSHM were generally consistent between the two depths. At both depths, HSHM were observed on 14 or more sampling dates and at no more than three plots per sampling date; however, HSHM were at least twice as common at a single low-elevation, open canopy plot than any other plot (Figure 2b). Thus, this system is characterized more so by HS of biogeochemical activity than by HM, likely a function of the strong controls on ecosystem functioning exerted by complex topography (Riveros-Iregui and McGlynn 2009; Atkins and others 2015).

Dissolved oxygen saturation in a shallow lake

The distribution of DO saturation with all sampling events and measurements pooled ($n = 1665$ measurements) was significantly skewed to the right (Figure 3a). The 8.5% of supersaturated DO values that contributed to the right-skew of the data distribution were from four sampling events, two early in the summer (DOY 142 and 156; 5.1 and 33.7% of measurements, respectively) and two mid-summer (DOY 184 and 192; 24.5 and 81.4%

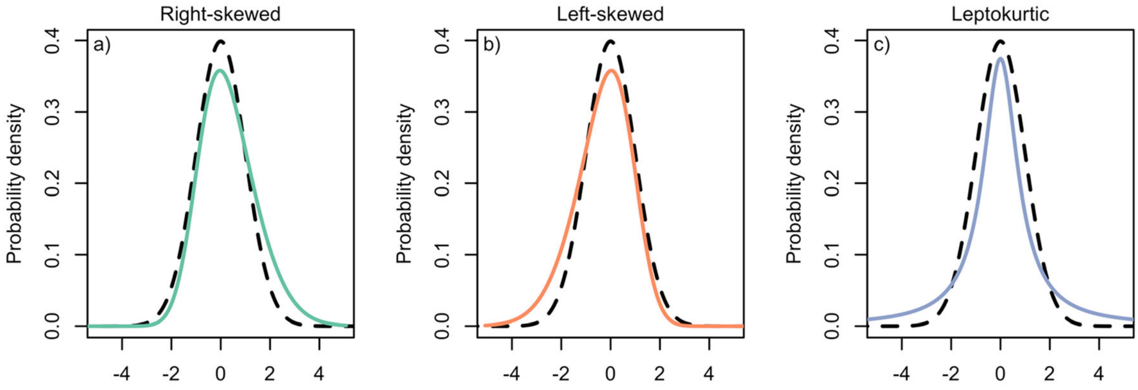

Figure 1. Illustration of **a** right-skewed (green), **b** left-skewed (orange), and **c** leptokurtic (lilac) distributions in comparison to a Gaussian (normal) distribution (dashed black).

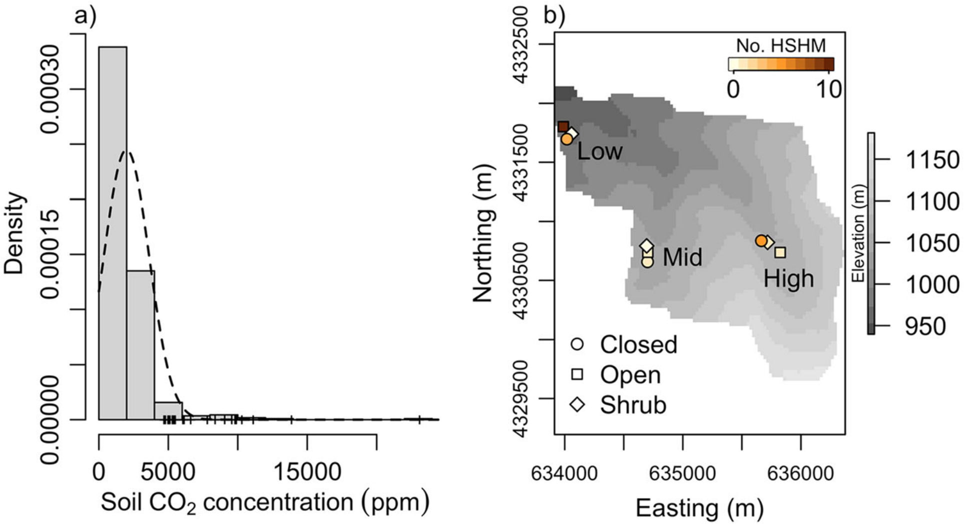

Figure 2. **a** Distribution of empirical soil CO2 pore space concentrations compared to a reference Gaussian distribution (black dashed line) with equal mean and variance. Tick marks indicate values of identified HSHM. **b** Total number of soil CO$_2$ pore space concentration HSHM identified in the Weimer Run Watershed, WV at the replicate level where each point represents three plots per elevation (as labelled) and vegetation cover combination (indicated based on point shape. The preponderance of HSHM at low elevation open canopy plots indicates that this system is best characterized by HS.

of measurements, respectively) (Figure 3b). DOY 191 was a HM of DO supersaturation in Swan Lake as 80 out of the 98 measurements contributed significantly to the right-skew of the distribution. Only measurements from the northern-most portion of the lake were not HS on this sampling date. However, the spatial heterogeneity of DO supersaturation values that contributed to the right-skew from the other three sampling events was much higher. Mapping the location of those points revealed that there were HS of DO supersaturation that coincided with areas of the lake with high rooted macrophyte occurrence (Figure 3b).

Seagrass metabolism in response to simulated grazing

The distribution of net ecosystem production (NEP) measurements (Figure 4a) across experimental plots and sampling dates ($n = 91$), was not significantly right- or left-skewed (skewness = 0.25, $p = 0.16$) nor was the distribution significantly leptokurtic (excess kurtosis = -0.53, $p = 0.87$). NEP is strongly correlated with aboveground biomass in these tropical seagrass ecosystems (Johnson and others 2017), and the approximately normal distribution of NEP data was likely driven in part by the distribution in seagrass biomass among plots. While biomass was lower in clipped plots than reference plots (a direct result of clipping), biomass varied among plots within a treatment (clipped and reference), resulting in only certain times or areas of very high or very low seagrass biomass. Despite the lack of evidence for HSHM overall, we identified negative (carbon source) and positive (carbon sink) extreme values using the HSHM identification method to illustrate how testing for HSHM presence and identification of extreme values can jointly support conclusions about HSHM. Because tests for HSHM presence were non-significant for this case study, we refer to the identified observations as 'extremes' rather than HSHM as in the other case studies. There were four instances when a plot was identified as an extreme of NEP (4.4% of measurements). Two positive (carbon sink) extremes occurred in the same reference plot (plot 10) in consecutive sampling weeks (6 and 7), while two negative (carbon source) extremes occurred during sampling week 9 (one clipped plot (plot 3) and one reference plot (plot 8); Figure 4b). Measurements in week 9 occurred on a cloudy day, resulting in decreased rates of production and reduced NEP across all plots. High sediment organic matter content in plots 3 and 8 may have fueled higher respiration rates and led to their identification as HSHM for negative NEP. Consistent with the non-significant HSHM presence tests, only a single plot was identified more than once (that is, weak evidence for HS), and on only one sampling date were there two plots identified at the same time (that is, weak evidence for HM).

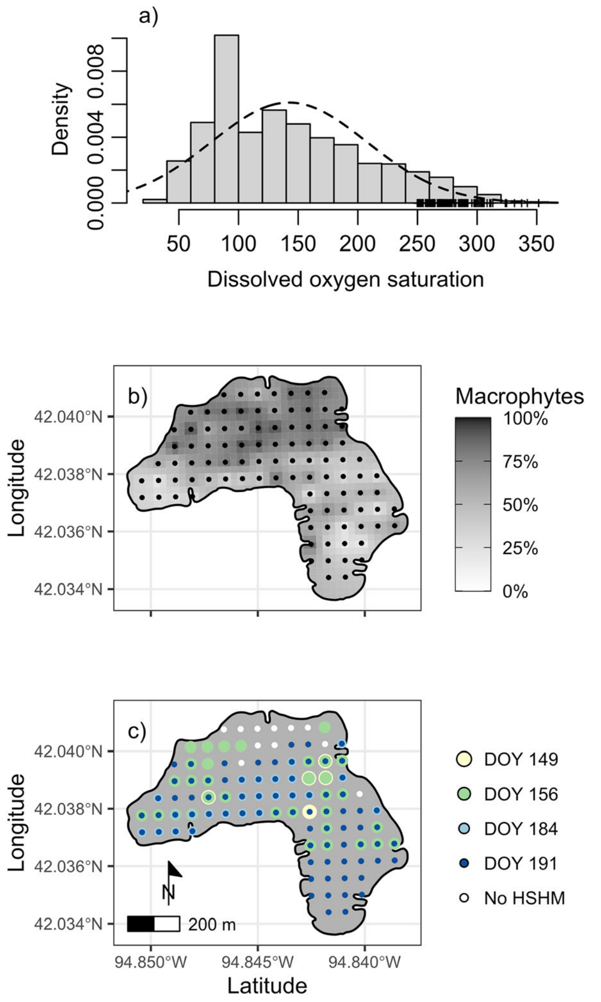

Figure 3. **a** Histogram of empirical DO saturation values overlain by a reference Gaussian distribution (black dashed line) having equal mean and variance. Black ticks indicate identified HSHM. **b** The 98 sampling locations on Swan Lake (Iowa, USA) and the associated macrophyte cover. **c** Spatiotemporal distribution of HSHM shown as circles with colors corresponding to the date when the location was identified as an HSHM. Concentric circles indicate that a sampling point was identified as an HSHM observation on multiple sampling dates. The predominance of HSHM on 4 of 17 sampling dates, combined with one or more HSHM occurring at many locations indicates that this system is characterized primarily by HM.

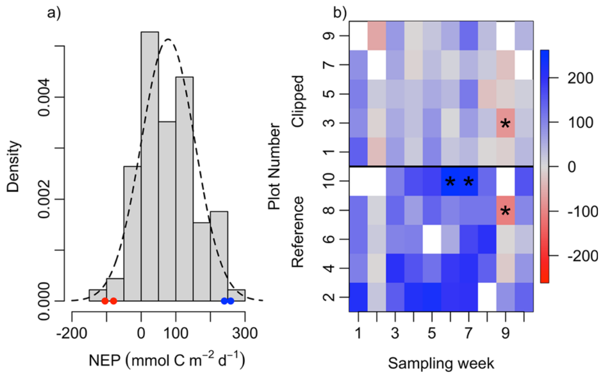

Figure 4. Seagrass metabolism (NEP, mmol C m^{-2} d^{-1}) in ten experimental plots across ten sampling weeks. **a** Histogram of empirical values overlain by a reference Gaussian distribution with equal mean and variance to the empirical distribution. Extreme negative and positive values are identified, respectively, by red and blue points. **b** NEP values across plots and sampling weeks. Extremes are indicated with an asterisk. White cells are times when metabolism measurements are missing for a given plot. The fact that no plots or sampling weeks predominate the set of extreme observations supports the conclusion from the test for HSHM presence that this case study does not reflect HSHM.

Sensitivity Analyses

Tests for whether the lake dissolved oxygen dataset contained HSHM were highly robust to removal of observations by location and by sampling date, and the identification of specific observations as HSHM was substantially robust to removal of observations by location. However, identification of specific observations as HSHM was not robust to removal of observations by sampling date, likely because this system was better characterized by the presence of HM, that is, all HSHM observations occurred on 4 of 17 sampling dates and across many locations. Thus, our approach satisfies the characteristic of an optimal quantitative method for HSHM that it be robust to data density provided that the sampling regime is sufficient to capture the dynamics of the system.

When removing observations by location, skewness of the down-sampled dataset was nearly always within ± 0.05 (95% CI = 0.63–0.73) of the original value (0.68) and the skewness of the down-sampled dataset was always greater than that of the reference distribution; thus, the conclusion that the overall data distribution reflects the presence of HSHM did not change. The proportion of HSHM observations identified in both the down-sampled and original datasets was consistently high (95% CI = 0.92–1.00) and the number of false positives relative to the number of original HSHM retained in the down-sampled dataset was consistently low (95% CI = 0.00–0.08) (Figure 5a–d).

When removing observations by sampling date, much larger differences in skewness emerged (95% CI = 0.15–1.19) and 7 of 1017 (6.9%) of down-sampled datasets had negative (left) skew; however, > 97% of down-sampled datasets were more right-skewed than the reference distribution

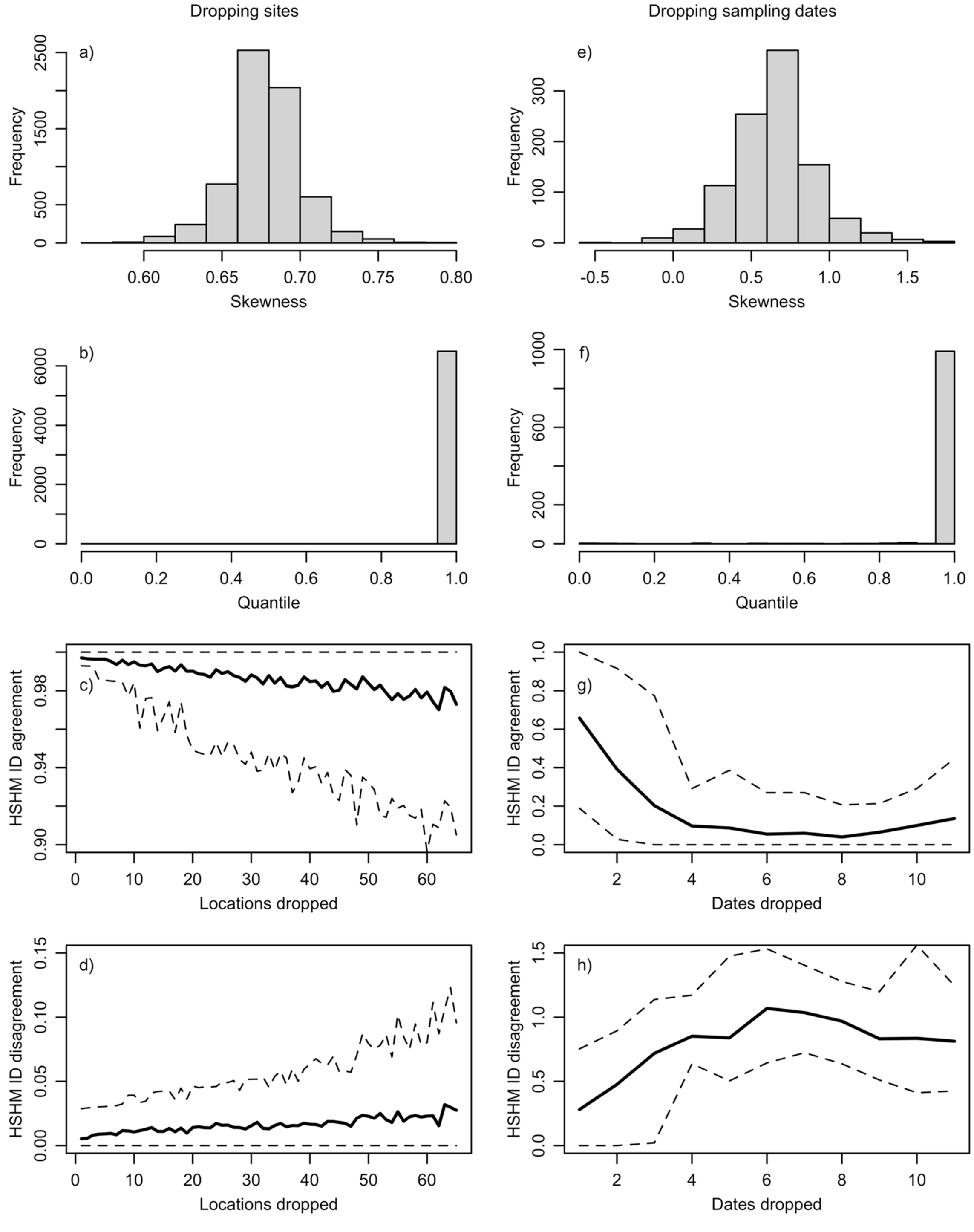

Figure 5. Sensitivity of Swan Lake dissolved oxygen HSHM results to removal of observations by site (**a–d**) and by date (**e–h**). **a**, **e** Histogram of dataset skewness when up to 2/3 of observations of sampling sites and sampling dates, respectively, are removed from the dataset. **b**, **f** Histogram of quantiles of the empirical skewness to that of surrogates, corresponding to a significance test for the presence of HSHM. **c**, **g** Proportional agreement between the original results and the results with down-sampling by site and date. The solid lines indicate the median, and the dashed lines indicate 0.05 and 0.95 quantiles. **d**, **h** Proportional disagreement between the original results and the results with down-sampling by site and date. Lines coded as in (**c**, **g**).

($\alpha = 0.05$, one-tailed test), so in general, overall conclusions about the data distribution reflecting that HSHM were present did not change. However, there was broad disagreement in which observations were identified as HSHM, as the proportion of HSHM observations identified in both the down-sampled and original datasets was commonly extremely low (median = 0.04, 95% CI = 0.00–0.79) and the number of false positives relative to the number of original HSHM retained in the down-sampled dataset often indicated more disagreement than there were original HSHM retained in the down-sampled data (median = 0.85, 95% CI = 0.01–1.45) (Figure 5e–h).

Discussion

A standard method for identifying whether hot spots and/or hot moments (HSHM) are present in a set of observations and quantifying which locations and times qualify as HSHM is necessary for improving our conceptual and quantitative models of ecosystem processes (Bernhardt and others 2017). The statistical approach presented here provides a method for systematically and comparatively studying HSHM both within and among ecosystems. Additionally, the sensitivity analysis provides information about sampling design while evaluating the robustness of HSHM identification at the spatiotemporal scales sampled. As demonstrated in three case studies, this quantitative approach to identifying if, when, and where HSHM occur can be used to advance our understanding of the underlying hydrologic and biogeochemical drivers of these rare events.

Relative to other quantitative approaches to HSHM used previously (for example, Darrouzet-Nardi and Bowman 2011; Yu and others 2013; Kannenberg and others 2020), a key advance of our approach is an explicit test for the presence of HSHM. We accomplish this by considering differences between an empirical data distribution and a reference distribution representing a null hypothesis of no HSHM. We used a normal distribution in our analyses because it has no skew or excess kurtosis but preserves the mean and variance of the empirical data. However, use of other statistical distributions or data-generating models is consistent with our approach and could be appropriate for certain applications. Other approaches common in the literature focus on identifying which observations constitute HSHM by means of identifying extreme values (for example, Darrouzet-Nardi and Bowman 2011; Yu and others 2013; Kannenberg and others 2020). We presented an approach to identifying HSHM based on extremes of the reference distribution that is logically consistent with our test for HSHM presence, but we acknowledge that different approaches to identifying extreme values can produce consistent results that results are inherently sensitive to user-specified thresholds, and that which approach is superior in a given context is not yet well-defined. We encourage further testing and comparison to support the overall goal of identifying the best standard for a quantitative definition of HSHM that can be straightforwardly applied across systems and datasets.

The HSHM behaviors in the case studies presented here were driven by a combination of hydrological and biological activity. Among the case studies, the HSHM method identified when observations were dominated by HS (soil CO_2), HM (lake dissolved oxygen), or neither (seagrass metabolism). The low elevation, open canopy plot with high CO_2 concentrations in soil pores at Weimer Run is an example of a permanent control point (sensu Bernhardt et al. 2017) where the combination of continuous hydrologic delivery of reactants and optimal environmental conditions sustained high rates of CO_2 production (Pacific and others 2009; Atkins and others 2015). Conversely, despite documented spatial heterogeneity (Ortiz and Wilkinson 2021), dissolved oxygen saturation in Swan Lake was best characterized by temporal variability. The HM of dissolved oxygen saturation in Swan Lake on DOY 191 was the result of a biological activated control point driven by a cyanobacteria bloom coinciding with the peak timing of macrophyte production (Ortiz and others 2020). This HM of dissolved oxygen availability across almost the entire lake bed likely also stimulated activated control points of internal phosphorus loading (Albright and Wilkinson 2022) driven by the spatial heterogeneity of sediment phosphorus composition (Albright and others 2022). Finally, simulated grazing of seagrass meadows by green turtles through blade clipping did not induce HS or HM of metabolism within the study meadow despite a drastic reduction in photosynthetic biomass. Although NEP was reduced in clipped plots, the observations did not skew the distribution or generate kurtotic characteristics. Based on this experiment and analysis, it is possible that green turtle grazing alone does not create HS of organic carbon remineralization and loss from seagrass sediments (Johnson and others 2017).

As these case studies illustrate, the HSHM identification method presented here can be broadly applied across ecosystems and observations. However, as with any statistical tool, it is necessary for the investigator to interpret the identified HSHM in the context of their data and knowledge of the ecosystem. The sensitivity analysis presented here was designed to aid investigators in evaluating the robustness of identifying observations as HSHM and assessing sampling design for their own study system. For example, the locations identified as HS in the Swan Lake dissolved oxygen data set were robust to the down-sampling rarefaction analysis (Figure 5c) while the HM were much more sensitive (Figure 5g). As sample days were removed, the median disagreement (between the down-sampling and full dataset) is above 50% after removing only two dates, while the removal of 2/3 of sample locations does not increase disagreement past 5%. We interpret this as further evidence that ecosystem processes resulting in extreme dissolved oxygen observations in Swan Lake are more likely to vary in time than space and that higher frequency observations may be necessary to further resolve the drivers of HM of dissolved oxygen production in the ecosystem This is one example of how the sensitivity analysis can be used by investigators to develop understanding of how the sampling regime interacts with ecosystem dynamics to influence detection of HSHM, aiding study design and interpretation.

The potential uses of standard quantitative tools, such as those presented here, for studying HSHM have major potential to advance ecosystem science. Coupled with the growing availability of data on ecosystem rates and processes, including increasingly long temporal extents, such tools can be used to answer important questions about how common HSHM are in general, and whether their occurrence is changing, potentially due to climate change or anthropogenic alterations of biogeochemical cycles. Once identified, analyses of the relationship between HSHM and variables representing, for example, meteorology and biogeochemical rates or concentrations, can shed light on the mechanisms and consequences of HSHM. In this study, we used our familiarity with these systems to make some inferences about how spatial environmental heterogeneity and other events taking place in these ecosystems may have led to occurrence of HSHM. Given the availability of data on relevant covariates, formal statistical analyses could be used to strengthen inference into mechanisms of HSHM. While linear modelling approaches common in ecosystem ecology and biogeochemistry can likely be fruitful, other less common approaches may be well-suited to the study of HSHM. For example, statistical methods suited to examining the effects of covariates on extreme values such as quantile regression (Koenker and Hallock 2001; Cade and Noon 2003), certain copulas (Ghosh and others 2020), and the partial Spearman correlation (Ghosh and others 2020) could be particularly useful since HSHM are themselves extreme values.

Biogeochemical HS spots and HM are an important, widely invoked concept in ecosystem science, but the depth and breadth of understanding of HSHM have been limited by a lack of standard quantitative definitions (Bernhardt and others 2017). Our proposed approach to testing for and identifying HSHM based on the skewness and kurtosis of data distributions could yield the standard quantitative approach the field presently lacks. One key advantage of our approach is that we provide an explicit test for the presence of HSHM, rather than assuming HSHM are present and identifying extreme values after the fact. Three case studies demonstrated how our approach can be applied to studying HSHM in a variety of ecosystems, variables, and study designs. We encourage the research community to evaluate and adopt quantitative HSHM definitions, and we provide algorithms in the form of an R package (‘‘hotspomoments’’) to facilitate uptake of the approach presented here.

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DATA AVAILABILITY

A data and code repository associated with the manuscript is available at: https://doi.org/10.5281/zenodo.7738286.

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