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Taking climate change into account: Non-stationarity in climate drivers of ecological response

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Abstract

1. Changes in the global climate system are creating increasingly non-analogue climate conditions with expectations of non-stationarity among climate drivers. Decoupling among climate drivers complicates the assessment of ecological response to the changing climate as characteristics that could be once treated as a suite of conditions now need to be treated as potentially independent with possible synergistic effects.
2. Ecologists commonly use ordination techniques (often principal component analysis; PCA) on large climate and environmental datasets to reduce a range of variables to a few axes that are uncorrelated with each other and often explain large proportion of the variation in the original data. However, non-stationarity, with correlations among variables changing over time, can affect this approach. Here, we use a 37-year climate dataset from the Niwot Ridge Long Term Ecological Research site (Colorado, USA) to present the use of both moving window principal component analysis and moving window correlation analysis to determine non-stationarity in climate data.
3. Relationships among climate variables and between input variables and PCA axes changed over time; this obscured interpretation of relationships between PCA axes and an ecological response (plant biomass), suggesting that one-time PCA for environmental variables may lead to inappropriate inferences.
4. *Synthesis.* Care must be taken in analysing climate–ecological relationships when predictor variables exhibit non-stationarity. We present a conceptual decision-making tree to help ecologists consider when to use PCA and extract axis scores or use alternative approaches for incorporating non-stationarity into subsequent analysis, including testing variables individually to aid in interpretation, break point analyses and averaging PC scores.

KEYWORDS

axes scores, climate data, multiple regression, non-stationarity, ordination, principal component analysis

1 | INTRODUCTION

Unprecedented rates of environmental change worldwide have fuelled growing concern about how ecosystems will respond to these changes (Sala et al., 2000). However, even in well-studied cases where we have a fairly good understanding of changes over the past several decades, forecasting future dynamics and describing future states has proven difficult (Dietze et al., 2018). One key hurdle in most empirical statistical models and many process-based models is the assumption of stationarity that the current relationships among system components will hold in the future, when in many cases data actually exhibit non-stationarity (McKenzie & Littell, 2017; Turco et al., 2018; Wolkovich et al., 2014). We define non-stationarity as a change in the relationship, either in direction or magnitude (from a significant relationship to no relationship and vice versa) between variables over time. Such non-stationarity is often combined with the additional hurdle of needing multivariate statistics such as principal component analysis (PCA) to reduce the dimensionality of complex datasets.

Changes in the global climate system are creating increasingly non-analogue climate conditions (García-López & Allué, 2013), with expectations of non-stationarity among climate drivers. Highly coupled climate characteristics may begin to decouple, changing the relationships between drivers (Williams & Jackson, 2007; Williams et al., 2007; Marino et al., 2011; Deng & Wei, 2015; Cook & Wolkovich, 2016; Wu et al., 2018; Hao et al., 2019). For example, temperature and drought used to be highly coupled in Europe with drought conditions necessary for extreme heat generation; in recent decades, this relationship has been decoupled, with extreme heat events occurring without drought (Cook & Wolkovich, 2016). This sort of decoupling complicates the assessment of ecological response to the changing climate, as characteristics that could be once treated as a suite of conditions now need to be treated as potentially independent with possibilities for synergistic effects.

While we know that real-world data are rarely stationary, incorporating non-stationarity into model predictions is challenging (Wilmking et al., 2020). It has proven both difficult to find suitable alternative modelling approaches and difficult to determine which key relationships to address, as non-stationarity can occur across drivers, between a driver and response, or across responses, and these relationships may change over space or time. Many fields from meteorology (Hao et al., 2019) and hydrology (Jain & Lall, 2001; Milly et al., 2008), to ecology (Foody, 2004; da Silva Cassemiro et al., 2007; Wimberly et al., 2008), evolution (Squartini & Arndt, 2008) and dendrochronology (Wilmking et al., 2020) are beginning to address this issue. For example, Jain and Lall (2001) used moving window regressions to assess non-stationarity in flooding events over time. Yet, assumptions of stationarity remain commonplace (e.g. Cueto & Casenave, 1999; Estrada-Peña & Venzal, 2007; Jarema et al., 2009; Loarie et al., 2008; Palmer et al., 2017; Pinto et al., 2011; Short & Trembanis, 2004; Silverberg et al., 2013; Sousa et al., 2007; Voigt et al., 2003). It is thus crucial for the field of ecology, to properly analyse and interpret data, to

address this issue via discussion, awareness, education and methodological developments.

Here we explore how long time-series data can be used to identify non-stationary relationships among ecologically important climate characteristics, and how this identification of non-stationarity may affect conclusions related to ecological response to climate change. We specifically focus on long-term records of climate characteristics at the Niwot Ridge Long-Term Ecological Research site, a high elevation alpine ecosystem in the Front Range of the Rocky Mountains in Colorado. In this system, changes in temperature, precipitation and growing season length have occurred over the 37-year measurement period. We first ask whether these changes can be considered as a stationary suite of coupled characteristics relating to climate change using covariance-based analyses—moving window principal component analysis (PCA) and moving window correlations. We are not necessarily advocating for using PCA over other methods, but rather are examining the assumptions of a commonly used analysis and the potential impacts on results. We then detail the consequences of different explanatory variable approaches that treat climate changes as a suite of coupled characteristics or independently in predicting changes in alpine tundra plant biomass over time. Lastly, we discuss approaches to better understand the complexity of changes in climate variables, including the value of univariate drivers as well as breakpoint analyses, in an effort to strengthen investigations of ecological responses to climate over time.

The goal of this paper is to explore how to both incorporate the complexities of climate change into ecological analyses while also appreciating the challenges of covariance-based analyses of climate variables over time. By examining a commonly used type of covariance-based analysis, PCA, we hope to spur further discussion about these broad analytical issues. While we expect that there is no one tool or method to examine non-stationarity among co-occurring climate drivers, it is critical—from both a statistical and conceptual perspective—to treat climate change as a complex, multidimensional and likely non-stationarity phenomenon when addressing key ecological questions about how climate is driving ecological responses.

2 | MATERIALS AND METHODS

The data used in this analysis come from the Saddle Site of the Niwot Ridge Long-Term Ecological Research site in the Front Range of the Colorado Rocky Mountains (40.05°N, -105.59°W, 3,530 m elevation). Climate data have been recorded at this site since the 1950s. Here we focus on climate data from 1982 to 2018, a period with more complete data featuring additional variables not measured before the 1980s. Since this is an alpine ecosystem with a summer growing season, we mainly focus on summer (June–August) climate variables that are important for plant growth. The following nine climate variables were used in the analysis: mean summer temperature (meanT; mean of mean daily summer temperatures), growing degree days (GDD; number of degree days in June, July and August with a minimum daily

temperature above 5°C), growing season length (GSL; number of days in which the temperature never goes below −3°C for three consecutive days), ice off date (IceOff; day of year when Green Lake 4, in the valley adjacent to the Saddle Site, is clear of ice), potential evapotranspiration (PET; calculated from daily max and min temperatures and daily precipitation, Gavin, 2019), moisture deficit (MD; calculated from daily max and min temperatures and daily precipitation using the modified Thornthwaite index with a field capacity of 75, Gavin, 2019), first day since May 1 with a 5-day running max temperature above 12°C (Days12C), first day since March 1 with a 5-day running max temperature above 5°C (Days5C) and total summer precipitation (Precip). We chose the −3°C, 5°C and 12°C cut-offs as they are all biologically relevant freezing or mortality thresholds for plants, pikas and trees, respectively (Sakai & Otsuka, 1970; Sebastian et al., 2016; Stewart et al., 2015). Moisture deficit serves as a drought index and we did not use minimum or maximum temperatures as they were correlated with mean temperature and are used as inputs to calculate other variables (e.g. GSL, GDD, Days5C, Days12C). Temperature data were recorded by a thermohygrograph (1982–1986), a Campbell Instruments CR21X data logger (1986–2000), a Campbell Instruments CR23X data logger (2000–2012) and a Campbell Instruments CR1000 data logger (2012–2018). Precipitation data were recorded by a chart recorder (1982–2018). Winter precipitation was corrected for overcatch as recommended by Williams et al., (1998) with a correction factor of 0.39. Data were infilled when necessary following established methods at our site and described in Niwot Ridge LTER public datasets on the Environmental Data Initiative Website (<https://portal.edirepository.org/nis/browseServlet?searchValue=NWT>).

To ask whether relationships among these key characteristics were stationary across the 37-year time series, we conducted moving window PCA and moving window correlations. Moving window analyses involve taking a subset (window) of the dataset of a particular amount of time and then shifting the start point of the window one time point at a time until the whole dataset has been covered by the window. It thus involves performing many separate PC analyses and correlations and then plotting and examining how the results change over time. We define non-stationarity as a change in the relationship, either in direction or magnitude (from a significant relationship to no relationship and vice versa) between variables over time. We conducted PCA on scaled variables using the `rda()` function in the `VEGAN` R package (Oksanen et al., 2019). Data were checked for linearity, an assumption of PCA, by plotting all possible raw variable pairs. To assess how many components to retain, we used parallel analysis (Horn, 1965) with the `hornpa()` function in the `HORNPA` R package; the magnitude of the eigenvalues in our PCA compared to the parallel analysis suggested retaining the first two components. For correlations, we used the `cor.test()` function in the `CAR` package, using the Pearson method (Fox & Weisberg, 2019). We did not exhaustively run all pairwise correlations but rather focused on correlations between each variable and temperature (temperature strongly and consistently loaded on PC1). We conducted the PCA and correlations on the entire dataset, on 10-year windows of data, and on 15-year windows of data. We chose these window sizes to balance having enough data within each window (i.e. more years than variables)

and having enough windows to examine the trends over time. For reference, these window sizes correspond to between a half and a quarter of our total dataset and we used two window sizes to examine the consistency of the results and ensure the results are not an artefact of window size. For much longer datasets (e.g. hundreds of years tree ring data), it is recommended to use at least 30-year windows (Wilmking et al., 2020); longer window sizes are preferable because they are not so affected by outliers. We developed these methods based on consideration of the above points; there was no previous literature on methods to set window length. While the direction of a variable loading on an axis is necessary for interpretation, to analyse just the strength of the loading of a variable onto a PCA axis, we extracted the absolute value of the PC scores for each variable for each window. To formally assess the non-stationarity in variable correlations and inform sub-setting the dataset, we conducted a breakpoint analysis using the `SEGMENTED` R package (Muggeo, 2008). We also conducted breakpoint analysis on the individual climate variables over time to see whether breakpoints in the individual variables drove non-stationarity. We fit linear models using zero, one, two and three breakpoints, and compared models using the `ANOVA()` function in the `STATS` R package.

Our second objective was to determine the consequences of different explanatory variable approaches that treat climate changes as a suite of coupled characteristics or independently in predicting changes in alpine tundra plant biomass over time. Plant biomass is defined as annual net primary productivity (ANPP) and data come from 14 years of above-ground biomass clippings in five 0.2 m by 0.5 m wet meadow tundra plots also at the Saddle Site. Biomass data were not collected yearly and are thus only available for a subset of years for which we have climate data. We used linear mixed effects models implemented with the `lmer()` function in the `LME4` package (Bates et al., 2015) to assess the relationships between plant biomass and the first PCA axis (which assumes stationarity), versus relationships solely based on independent climate characteristics (temperature, growing degree days and growing season length), with plot as a random factor (to account for repeated sampling). For these mixed effects models, we report the conditional R^2 (R^2_{cond}) and marginal R^2 (R^2_{marg}) values (Nakagawa & Schielzeth, 2013) as calculated by the `r2_nakagawa()` function in the `PERFORMANCE` R package (Lüdtke et al., 2020). As a follow-up to the breakpoint analysis, we also ran separate models for the 1992–1995 time period, and 2008–2018 time period, which corresponded to periods of time in which climate variables were coupled and decoupled. We also explored the creation and effectiveness of a new PC variable by calculating a mean PC score for each year by averaging the PC scores of any moving window containing that year, which is an attempt to integrate the idea of non-stationarity into PC scores. All analyses were done in R version 3.5.3 (R Core Team, 2019).

3 | RESULTS

Principal component analysis of all 37 years of data separated the climate data into two principal axes that explained 71% (52.79% plus

18.53%) of variation in the data. The first axis generally described warming and extended growing season while the second axis described moisture stress (Figure 1). The variable loadings (displayed as vectors in Figure 1) suggested that temperature, GDD, ice off dates, evapotranspiration, and days until 5-day running 5°C and 12°C are all strongly associated with axis one while GSL was moderately associated with axis one (Table 1). Precipitation and moisture deficit were strongly associated with the second axis (Table 1).

Ten-year and 15-year moving window PCA demonstrated that temperature and GDD reliably loaded strongly onto axis one while the other variables loading on axis one in the all-years PCA did not reliably load on that axis across all moving windows (Figure 2, Figure S1). This suggests non-stationarity in these climate data, particularly between temperature/GDD and the other variables. An alternative explanation for such moving window PCA results is that, if the amount of variation explained by certain variables changes, the first and second axes in a particular window could potentially be switched, or certain variables could be strongly correlated with PC3 or other axes. Such switching is unlikely the case in our data, as temperature and GDD always loaded strongly onto axis one. The other variables sometimes loaded strongly on axis one, but this was inconsistent, suggesting non-stationary relationships between those variables and temperature or GDD. For example, across 10-year windows GSL and days to 5-day running 5°C varied from a strong loading (~0.75) in three windows to a very weak loading (~0) in three windows. The temporal patterns of PC1 score fluctuations also differed across the variables (Figure S1). Some variables (Precip, MD, Days5C) showed multiple fluctuations in their PC1 loadings while other variables (Days12C, GSL) started with high loadings which then decreased in windows starting in the 1990s before increasing again. This visual non-stationarity was further evidenced and

TABLE 1 Axes scores, loadings and correlations for the nine climate variables for the first two principal components in the full 37-year principal component analysis. The table is sorted by absolute value of PC1 score. GDD = growing degree days, Temp = mean summer temperature, PET = potential evapotranspiration, Days12C = first day since May 1 with a 5-day running max temperature above 12°C, IceOff = Green Lake 4 ice off date, GSL = growing season length, Days5C = first day since March 1 with a 5-day running max temperature above 5°C, MD = moisture deficit, Precip = summer precipitation. Loadings were calculated with the scores() function in *vegan* with scaling set to 0. Correlations between the *i*th variable and the *j*th PC were calculated with the equation $\rho_{ij} = \alpha_{ij} (\lambda_i / \sigma_{ij})^{1/2}$, where α_{ij} is the loading for the *i*th variable in the *j*th PC, λ_i is the eigenvalue associated with that PC and σ_{ij} is the variance of the *i*th variable (Cadima & Jolliffe, 1995) and can be above 1

Variable	PC1			PC2		
	Score	Loading	Correlation	Score	Loading	Correlation
GDD	1.32	0.43	1.02	-0.31	-0.17	-0.14
Temp	1.29	0.42	1.00	-0.44	-0.24	-0.20
PET	1.22	0.40	0.94	-0.21	-0.12	-0.10
Days12C	-1.17	-0.38	-0.90	-0.09	-0.10	-0.04
IceOff	-1.01	-0.33	-0.78	-0.24	-0.13	-0.11
GSL	0.90	0.29	0.69	-0.74	-0.40	-0.34
Days5C	-0.85	-0.28	-0.65	-0.42	-0.23	-0.19
MD	0.69	0.22	0.53	0.91	0.50	0.42
Precip	-0.47	-0.15	-0.36	-1.18	-0.65	-0.54

confirmed by moving window correlational analysis of temperature, GDD and GSL.

While temperature and GDD were strongly positively correlated throughout the study period (stationary relationship), the correlation between temperature and GSL changed over time (non-stationary relationship, Figure 3), becoming uncorrelated in the 1990s. The other six variables also exhibited non-stationary relationships with temperature, as correlations ranged from strong and significant to weak and non-significant over time (Figure S2). We use temperature and GDD as an example of a stationary relationship and temperature and GSL as an example of a non-stationary relationship. Breakpoint analysis identified two breaks in the temperature and GSL correlation coefficients. For the 10-year windows, breakpoints were at windows beginning in 1990 and 1997. For 15-year windows, breakpoints were at windows beginning in 1992 and 1994. Note that these breakpoints do not correspond with changes in instrumentation. We also confirmed these results with climate data from the nearby D1 climate station with more consistent instrumentation to test for the potential influence of instrument changes at the Saddle (Figure S3). Furthermore, correlation results using Spearman correlations were consistent with the Pearson correlations (Figure S4). Individually, temporal trends in temperature and days to 5-day running 12°C both exhibited breakpoints, which likely contributed to the non-stationarity in the PCA and correlations (Figure S5).

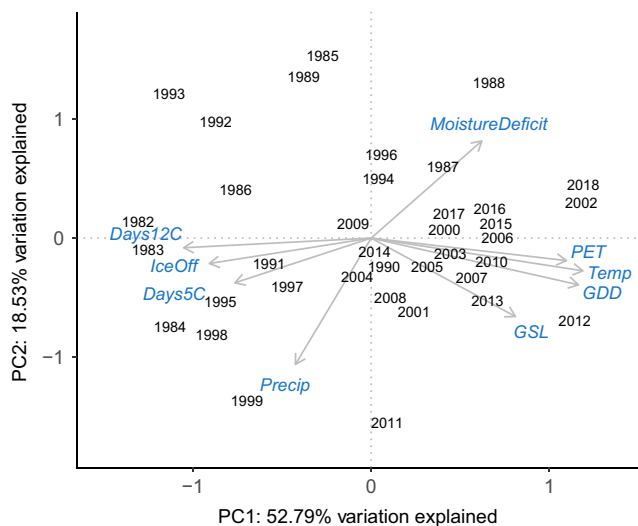


FIGURE 1 Principal component analysis of nine summer (June–August) climate variables over 37 years at Niwot Ridge, Colorado. Points are years distributed in climate space; vectors indicate the direction and extent of correlation between climate variables and each axis. Variables and their abbreviations are defined in the methods. Temp is the mean summer temperature

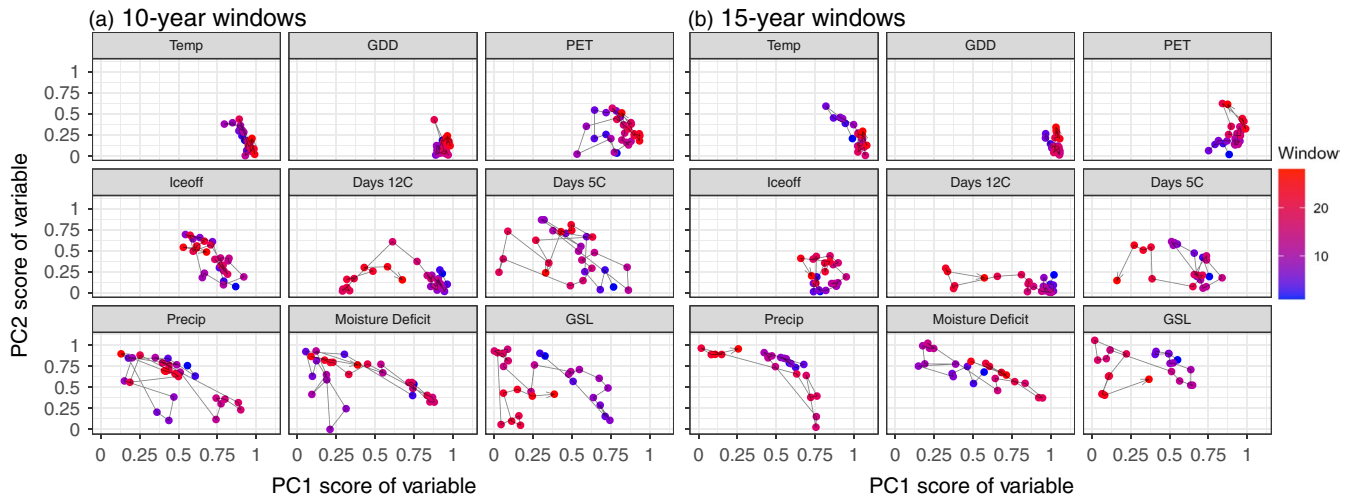


FIGURE 2 Moving window PCA of (a) 10-year windows ($n = 28$) and (b) 15-year windows ($n = 23$). The legend refers to window number, where window 1 = 1982–1991 (10-year windows) or 1982–1996 (15-year windows). To facilitate comparison of the strength of loading of the variables on each PCA axis, we show the absolute values of the first two axes scores of each variable calculated in each window. Variables that load reliably on an axis are expected to have non-stationary relationships with variables with sometimes strong and sometimes weak loadings on an axis

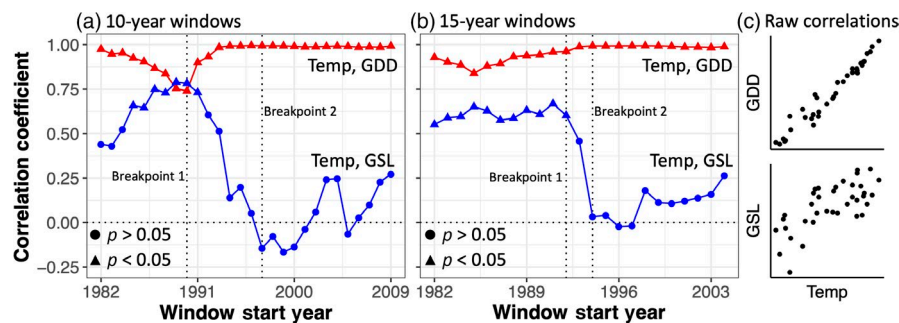
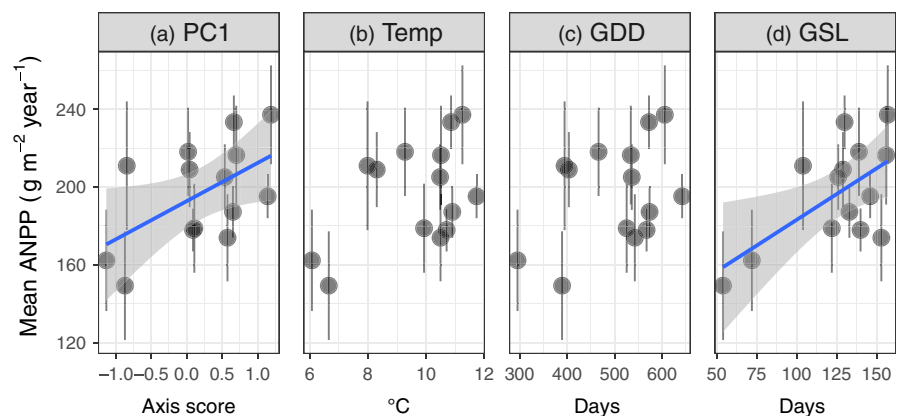


FIGURE 3 Moving window correlation analyses between mean summer temperature and either growing degree days or growing season length for (a) 10-year windows ($n = 28$) and (b) 15-year windows ($n = 23$). Panel (c) shows raw scatterplots between temperature and GSL and temperature and GDD from 1982 to 2018. Correlation coefficients are Pearson r values, and the significance of the correlations in (a) and (b) are by either triangles (significant, $p < 0.05$) or circles (not significant, $p > 0.05$). While the sample size is smaller than the whole dataset ($n = 10$ or 15 vs. $n = 37$), the trends in these graphs are not affected by sample size, as each point within each panel was calculated on the same number of samples (10 or 15). To check that the result of the correlation coefficient dropping to ~ 0 in some windows was not an artefact of the small sample size in the windows (i.e. 10 years or 15 years), we randomly selected 10 samples spread out across all decades of the dataset for 500 trials and always found that $r > 0.40$ for temperature and GSL; thus, this result is driven by correlations over consecutive years of data, not the smaller sample size

FIGURE 4 Relationship between mean ($\pm SE$) annual net primary productivity (ANPP; i.e. plant biomass) and (a) PC1, (b) mean summer temperature, (c) growing degree days and (d) growing season length. Lines are shown for significant (Linear Mixed Effects Model, $p < 0.05$) predictors. PC1 and GSL significantly predicted ANPP while temperature and GDD did not, despite strong correlations with PC1, highlighting non-stationarity and challenges with interpreting axis scores



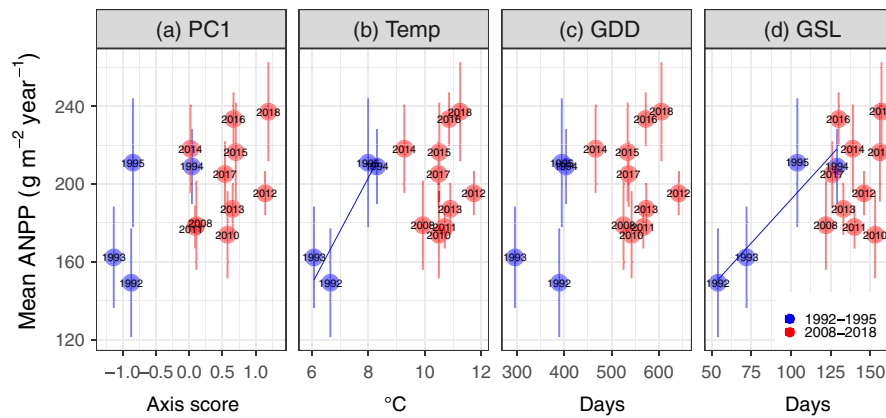


FIGURE 5 Relationship between mean (\pm SE) annual net primary productivity (ANPP; i.e. plant biomass) and (a) PC1, (b) mean summer temperature (Temp), (c) growing degree days (GDD) and (d) growing season length (GSL) for the dataset divided into two subsets (1992–1995 and 2008–2018). Lines are shown for significant (Linear Mixed Effects Model, $p < 0.05$) predictors. Temp $R^2_{\text{cond}} = 0.46$, $R^2_{\text{marg}} = 0.16$; GSL $R^2_{\text{cond}} = 0.47$, $R^2_{\text{marg}} = 0.17$. Dividing the data enables analysis of relationships between different predictor variables and a response variable for time periods during which the different predictor variables are correlated and uncorrelated with each other. The division of the data into these time periods was based on the breakpoint analysis

The purpose of examining these climate data for non-stationarity is ultimately to understand relationships between climate and ecological variables, in this case, plant production (above-ground biomass). There was a significant positive relationship between the first axis score of the PCA and plant biomass ($R^2_{\text{cond}} = 0.31$, $R^2_{\text{marg}} = 0.04$, $p = 0.01$, Figure 4). Consistent with the moving window analysis showing non-stationarity between temperature/GDD and GSL (Figure 2), plant biomass was not significantly related to either mean summer temperature ($R^2_{\text{cond}} = 0.30$, $R^2_{\text{marg}} = 0.02$, $p = 0.05$) or growing degree days ($R^2_{\text{cond}} = 0.29$, $R^2_{\text{marg}} = 0.01$, $p = 0.12$, Figure 4) but was related to growing season length ($R^2_{\text{cond}} = 0.31$, $R^2_{\text{marg}} = 0.04$, $p = 0.01$, Figure 4). When the dataset was divided into two time periods, there were significant relationships between temperature, GSL and plant biomass in the 1992–1995 timeframe and not the 2008–2018 timeframe (Figure 5).

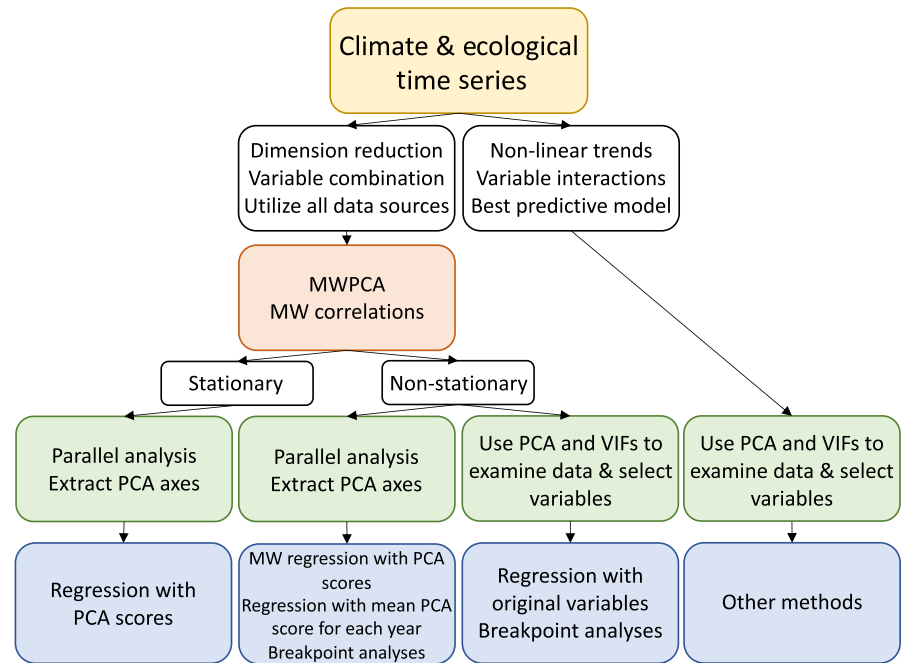
4 | DISCUSSION

Many studies in ecology involve the measurement of climatic and other environmental variables and the analysis of the relationship between those variables and the abundance, growth or distribution of organisms. Such studies are especially important now to understand how changing climate drivers are already impacting organisms and ecosystems and to predict future changes. It has become a frequent practice in ecology to conduct PCA or other covariance-based approaches on tens of climate variables to use axes scores as predictor variables in regression models with ecological responses (e.g. Cueto & Casenave, 1999; Estrada-Peña & Venzal, 2007; Jarema et al., 2009; Loarie et al., 2008; Pinto et al., 2011; Short & Trembanis, 2004; Silverberg et al., 2013; Sousa et al., 2007; Voigt et al., 2003). It is also common for climatologists to use PCA to analyse climate data (Ehrendorfer, 1987; Huth & Pokorná, 2005; Tadić et al., 2019). However, this method assumes not only linearity but

also stationarity in the climate data, an assumption that we tested in this paper. While our climate variables were linearly related, the assumption of stationarity (according to our definition, see methods) was not met and clouded important conclusions about drivers of the responses of our ecological variable, plant biomass. Below, we present a decision-making tree for considering how to best use PCA or other covariance-based approaches in temporal analyses (Figure 6).

The first thing to consider when deciding whether to use covariance-based approaches is if they are critical to helping answer the study questions or achieving the study goals, and if the data necessary to meet the requirements of the method are available (Figure 6). If the goal is to reduce the dimensionality of the dataset or develop a metric that takes multiple variables into account, extracting PCA axes scores and using them as predictor variables may be appropriate, or even necessary if a suite of variables is at play and there is no one obvious driver. For example, in our dataset, model selection with exhaustive all subsets regression showed that multiple individual predictor variables and combinations of predictor variables are very similar (within 2 AIC) in their model fits for a given response variable (Table S1). When using PCA, it is also important to conduct parallel analysis to decide how many components to contain. If the goal is to delve into nonlinear trends, examine interactions among variables or simply find the best set of predictor variables, extracting PC scores is not appropriate. In that case, PCA can still be useful for examining relationships among variables and selecting uncorrelated variables across the whole time period (Figure 6). However, as shown here, some variables may be correlated for only specific time periods so even in this case it could be beneficial to conduct moving window PCA and correlations. In our case, the goal was to develop a metric that described not just summer warming, but a hotter, drier and longer summer, to use data from both terrestrial and aquatic systems to inform this metric, and ultimately assess the effects of climate on tundra primary production. After conducting the PCA on all years of data, the first principal component emerged as a potential 'extended summer' metric, as it included

FIGURE 6 Decision-making process on how to use PCA in an analysis involving a time series of climate and ecological data. MW = moving window, VIFs = variance inflation factors. Other methods could include, but are not limited to, generalized additive models, polynomial models, random forest models, all subsets or forward or backward stepwise regressions, generalized least sum models, but it is outside the scope of this paper to compare and discuss all of these methods



temperature, growing season length, and evapotranspiration and high values on this axis corresponded to summers characterized by high values of these variables (2002, 2012, 2018).

However, it is important to appreciate that climate variables may be correlated for only specific time periods within a longer time series. Conducting moving window PCA and moving window correlations (Figure 2, Figure 3) is one approach to address this possibility. In our data, these analyses demonstrated that variables thought to be strongly correlated with a PCA axis were not always strongly correlated with that PCA axis throughout the whole course of the dataset, which could be caused by climate change and/or a combination of interannual and interdecadal variation. In particular, the relationship between growing season length and temperature was non-stationary, going from significantly correlated with relatively strong correlation coefficients between 0.5 and 0.75 to not significantly correlated with correlation coefficients near zero; this non-stationarity was confirmed with breakpoint analysis and appeared to be driven by a transition in the 1990s.

It is also important in any modelling framework to consider biological mechanisms that underpin the inclusion of a climate variable; warmer temperatures do not necessarily lead to a longer growing season length unless there are consecutive days of warmer temperatures at the start and end of the growing season. Furthermore, spring and fall temperatures may change at different rates than summer temperatures. For example, studies have shown that climate change and warming may actually increase temperature fluctuations in the spring, which can lead to frost damage in plants (Gu et al., 2008; Marino et al., 2011; Rigby & Porporato, 2008), and these types of dynamics are difficult to incorporate into models.

The issue of non-stationarity becomes especially problematic when trying to interpret a PCA-derived metric in the context of an ecological response. Thus, because of this non-stationarity, we

would either choose not to proceed with extracting axes scores and regressing them with our ecological response (Figure 6, but we have done so here for illustration) or try to incorporate the non-stationarity into the models. For example, we found that wet meadow tundra biomass increases significantly as the first axis of the all-years PCA increases, suggesting that the warmer, drier, longer summer is beneficial for plant growth in this particular ecosystem type. Without a moving window PCA, the relationship would suggest that warmer temperatures, more growing degree days, longer growing season length, earlier ice off dates, less time to reach 5 days at 5°C or 12°C and more evapotranspiration were all associated with increasing biomass, or that one or a few of these variables drove increasing biomass but could not be easily statistically isolated from the others. The moving window PCA suggests that further partitioning is both possible and advisable in light of non-stationarity, as only temperature and growing degree days reliably loaded strongly on axis one over the all of the windows. Thus, we ran individual linear regressions to see whether variables such as temperature, GDD and GSL were also significantly related to biomass. Interestingly, the two variables most strongly correlated with the first principal component, temperature and GDD, did not significantly predict plant biomass while GSL did, although R^2 values were quite low for all variables.

Alternatively, we suggest two avenues to incorporate non-stationarity into the modelling framework (a) depending on the length of the dataset, explore sub-setting the response variable into either moving windows or different time periods based on the breakpoint analysis and (b) calculating a new PC score predictor variable where the value for each year is the average value of all of the moving windows that contain that year. Note that the first method incorporates non-stationarity directly into the analysis while the second method seeks to indirectly take it into account by calculating a new variable. In our dataset, for the first method we divided the biomass data into

two timeframes—the first four years from 1992 to 1995 and the most recent years 2008–2018, and conducted the same four regressions with PC1, temperature, GDD and GSL. These subsets correspond to a time period in which temperature and GSL were decoupling, and a time period in which temperature and GSL were already decoupled. In this particular case, these subsets were driven by the gap in our data; in an ideal case with biomass data for every year, the breakpoint analysis would have suggested breaking the dataset into 1982–1990, 1991–1997 and 1998–2018 periods. The results highlighted that the trends in the data are driven by the oldest data, which contain years with two of the coldest summers (Figure 5) but also show that GSL and temperature can have the same relationship with biomass when they are more tightly coupled. Interestingly, this method also suggests non-stationarity between the predictor variable and the response variable. This concept must be considered from an ecological perspective (e.g. the relationship between temperature and biomass could be non-stationary if plant species composition has changed or if the plant species have evolved) as well as a data perspective (e.g. the range of values for different time periods). For the second method, we calculated a 'non-stationary PC1' score which is, for each year, the average PC1 score of that year across any moving windows that contained that year. This essentially provides more data input into a year's PC scores, compared to just one PCA of the whole dataset. However, regressing this new metric against biomass yielded a similar R^2 and p value as the original PC1 axis score; further work is needed to determine if this is a viable solution in other datasets.

Our results highlight the difficulties in interpreting extracted PCA axes scores and using them in subsequent analyses. In our example, we used simple variable axes loadings to interpret the first two principal components, which is the commonly used default approach (Cueto & Casenave, 1999; Dixit & Geewan, 2002; Pinto et al., 2011; Silverberg et al., 2013; Sousa et al., 2007; Voigt et al., 2003). However, when discussing PCA axis interpretation at length, researchers have cautioned against using simple axes loadings for axis interpretation (Cadima & Jolliffe, 1995; Jackson, 1991; Jolliffe, 2002; Peres-Neto et al., 2003) and have suggested calculating a correlation between an input variable and an axis score. This correlation may or may not be as strong as the axis loading because it also takes into account the variance of the input variable and the component (Cadima & Jolliffe, 1995). While this correlation is important to check, in our case the correlations match up with the variable loadings such that temperature and growing degree days are more correlated with PC1 than GSL (Table 1).

If there are certain variables of interest or a goal is to test interactions between variables, or compare multiple models, it may be better to select variables of interest and test them directly (Figure 6). This is especially true if a variable of interest strongly loads on the PCA axis. In this case, it would be best to simply run a regression between the response variable and the variable of interest. Focusing on a limited number of focal variables also facilitates easier model interpretation and allows for more effective exploration of nonlinear trends including, but not limited to, running polynomial models, generalized additive models, or broken stick regression models, or testing for interactions among variables. PCA can still be a useful tool

to examine relationships and correlations between variables and help select predictor variables for future regression analyses. For example, to find the best combination of predictor variables of plant biomass, we conducted all subsets multiple regression with the nine variables (Table S1). This would not be feasible in a dataset containing tens or hundreds of variables (for computational time, over fitting, or producing many different equally good models), so PCA could be helpful in selecting variables to input into multiple regression models. This can be achieved by examining the effective visualization of variable correlations that PCA provides and deleting variables that have similar principal component loadings or weak axes loadings. Other techniques analysing multicollinearity such as variance inflation factors (VIFs) may also be used in conjunction with PCA for deciding which variables to remove (Alin, 2010; Jolliffe, 2002; Lafi & Kaneene, 1992).

Non-stationary data are widespread in ecology, yet assumptions about stationarity are commonly violated. Part of the problem is a lack of discussion on this topic, as well as development of alternative analysis tools. Here, we have illustrated how non-stationarity among climate drivers can lead to misinterpretation of results and presented how moving window PCA, moving window correlation analyses, and breakpoint analysis can be useful for understanding the data structure and interpreting results. We have also suggested several ways to incorporate non-stationarity into the analysis. Future work should test these ideas with different datasets and expand and refine them, as we expect that each dataset will present its own complexities. We conclude that PCA or other covariance-based approaches are helpful tools for data exploration and dimension reduction, but caution must be exercised in interpreting results from models that assume a consistent relationship among variables through time. There is a critical need to predict how climate drivers will affect organisms and ecosystems. To successfully make such predictions, we must acknowledge, and take into account, that interactions among the drivers may be as complex as the interactions among the biotic responses.

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AUTHORS' CONTRIBUTIONS

C.P.B., C.T.W. and K.N.S. conceived the study; C.T.W., E.C.F. and L.M.H. processed the data; C.P.B. led the writing of the manuscript and performed the presented analyses. All authors contributed critically to the drafts and gave final approval for publication.

PEER REVIEW

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DATA AVAILABILITY STATEMENT

Raw climate and biomass data are available on the NWT LTER archives on the Environmental Data Initiative (<https://portal.edirepository.org/nis/browseServlet?searchValue=NWT>), under the following Package IDs: knb-lter-nwt.83.1, knb-lter-nwt.78.3, knb-lter-nwt.416.10, knb-lter-nwt.405.4, knb-lter-nwt.16.4. Processed data and R code are available on GitHub (<https://github.com/cliffbueno/Manuscripts/tree/master/MovingWindow>) and were released with Zenodo <https://doi.org/10.5281/zenodo.4321409> (Bueno de Mesquita et al., 2020).

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section.

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