Replies to the Anonymous Referees

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We thank the editors and anonymous reviewers for their input and devoted time to our work. The detailed revisions were very helpful and have allowed us to improve the manuscript greatly. The major changes in the new version of the manuscript include:

- Adding results and analysis of the principal component 3 to the manuscript.
- A revised introduction picking up all research questions that appear later in the manuscript.
- A better explanation of what differentiates the present study from other studies using PCA.
- An expanded "Hysteresis" section, with an improved and more intuitive explanation.
- Move some of the results from the appendix into the main text.
- Many other revisions.

We have addressed all concerns in detail below, reviewers' comments are in normal font, replies are in *italics and blue*. Additionally, many small improvements have been made to the manuscript and many errors have been corrected. For a full list of changes, please see the attached document at the end of this document. We hope that with all these changes the manuscript meets the high quality standards of the journal.

Kind regards,

The Authors

1 Anonymous Referee #1

1.1 General Remarks

I appreciated reading the discussion paper Summarizing the state of the terrestrial biosphere in few dimensions by Guido Kraemer and colleagues. The paper presents an approach for summarizing key variables on the terrestrial biosphere into fewer independent components using established multi-variate methods. They exemplify their approach by showing several trajectories across space and time and by highlighting some major anomalies visible in their data. While the work is well presented and scientifically sound, I have some major concerns regarding the publication of the manuscript in its current form.

We thank the reviewer for his positive and very thorough review and the helpful comments. We have now addressed the open issues as we will show below. We especially thank the reviewer for the detailed review of the overall structure of the manuscript and pointing out the many small details that have been improved in the new version of the manuscript.

1.2 Concerns

1) The number of dimensions

The authors state that the first two components explain large parts of the variance and that the 'knee' is reached with the second component. However, inspecting Figure 1a, it seems that the 'knee' is reached with the third component, which still explains 9% of the variance. I was a little confused that the third component was disregarded throughout the whole manuscript, without giving a strong justification. Figure 2b indicates that the third component might be strongly connected to albedo. I encourage the authors to either expand their analysis to also include the third component, or to give a very strong argument for its exclusion. As it stands now, the decision to only inspect the first two components is very subjective.

The reviewer is right that the 3rd principal component still contains important information. Therefore, we included results and analysis of component 3 in the manuscript. Accordingly, we have implemented the following changes:

- *Added axis 3 to the manuscript (for details, see the attached document showing all changes).*
- *Flipped axis 3 so that higher values for PC3 mean higher albedo.*

We think that the addition of the third component improved the manuscript substantially and want to thank the reviewer for recommending this.

2) Scientific novelty and usefulness

I am missing a strong discussion/conclusion on how the manuscript advances scientific progress. Putting it into simple terms, the authors apply PCA – a widely used and established method – to a set of existing data sets. As such, it is not really a novel methodological development, but rather a demonstration of what could be done with global datasets as provided though the Earth System Data Lab. While this is not a deal-breaker per sé, the authors could greatly advance their manuscript by explaining how this approach can be used by other scientists, that is how it will advance the science of the terrestrial biosphere.

Thank you for this critique and comment which can be viewed from several angles. At first glance, the reviewer is right: we simply applied a PCA to a highly curated global data set—a data cube contained in the Earth system data lab. But, although the method is similar to EOFs in climatology, where the matricization (the flattening of the 4th order tensor, variables $\times$ time $\times$ longitude $\times$ latitude, to a matrix) happens maintaining time. We are maintaining both, space and time and reduce only over the variables, as far as the authors are aware, this has not been done on global data.

This is in our view an innovation, as we account, for the first time, for the many redundancies in high-dimensional Earth observations. We have carefully reviewed the literature, but do not find a study that has investigated the global covariations of multiple Earth observation data streams. This is the main novelty of our work, to better explain our approach in more depth, we have added some explanations to better explain these differences to the reader.

Also, the use of a simple PCA algorithm is not incidental here: we seek for a method that learns a data transformation that is invertible, and allows us to measure/compute the reconstruction error in meaningful physical units. This cannot be done with more complicated/sophisticated nonlinear machine learning methods, where the (probably more accurate) transform is hard to analyze.

3) Too many results in the appendix

Many of the results are buried in the Appendix but never picked-up in the main text. In fact, Figure A1, B1, D1 and C1 were never referenced in the main text. The authors thus present many results in the Appendix that are not discussed in the main manuscript and thus the reader is left alone with her own interpretation. As some of the results are quite crucial for evaluating the method (e.g., the errors presented in B1), I strongly encourage the authors to thoroughly discuss them in their manuscript.

Thank you for the observation! We fully agree that we have a lot of results in the appendix, some of them very relevant for the discussion. Following the suggestion, we moved parts of the appendix into the main text and have also added references to the figures into the text:

- *Moved the section "Reconstruction Error" from the appendix to the text.*
- *Moved figure C1 ("Bowen Ratio") into the text.*
- *We added the corresponding references into the text.*

4) Writing

The writing needs improvement for turning this already good manuscript into an excellent manuscript. For example, the authors often describe their figures, instead of the results (Figure X shows...). It would be much more interesting to read about the main result instead (A influences B (Figure X)). I am sure the senior authors of this manuscript can do a great job in revising the manuscript to make it more accessible and exciting for the reader.

We thank the reviewer for the pointing this out and have revised many aspects of the paper, see the marked up manuscript version showing all changes. We hope that we have corrected the manuscript accordingly.

5) Spelling/grammar

There are some wording and spelling/grammar issues, some of which listened below:

Thanks for the thorough revision provided. We have corrected all suggested minor changes, and commented further on the critical ones below.

L. 16: Suggest removing 'the' before 'global'.

Thank you, changed.

L. 27: Spring is not a phenological event. Could use onset of bud-flush or similar.

Thanks for catching this detail.

L. 74: Not clear how standardization accounts for differences in scales. What scales? Spatial? Temporal?

Indeed, the wording is a bit ambiguous. We have changed it to make clear that we mean scale in a statistical sense here.

L. 138: The breakpoint detection comes out of the blue. Why is this done? What was the rational behind? This needs a decent introduction.

The reviewer is right that we do breakpoint detection without properly introducing it, we mentioning the topic in the introduction now.

L. 142: Same as above. The term hysteresis is never introduced before, but then explained in the results section (L. 239). As a reader, I would love to hear the details upfront, instead of reading about them in the results/discussion.

This was missing from the introduction, we thank the reviewer for noticing this, we have remedied the situation.

L. 148: Maybe include an example figure here, instead of referencing to the results already.

The hysteresis may be a complex topic for people not familiar with it, we thank the reviewer for pointing this out and have added a conceptual figure to the "Methods" section that hopefully makes the concept easier to understand.

L. 151: 'We see that…' is not a good opener. Directly describe the result, be precise and upfront (e.g., The first two components explained 73% of the variance (Figure 1a))

Removed "We see that".

L. 160: What is the pre-imaging problem? Please do not assume that the reader reads up the details in the reference provided. Either avoid naming it or give a brief description.

Again we thank the reviewer for pointing out that this is a topic that the target audience may not be acquainted to. We have improved the description and hopefully made the concept understandable to everyone.

L. 162: Again, not the best opener. The first sentence of a paragraph should summarize the main point of the paragraph (topic sentence), allowing the reader to skim through the manuscript. This sentence just describes where the reader can find a result, but nothing about the result itself.

Thanks for pointing this out, we have have removed the sentence.

L. 164: Odd formulation (two times related).

Thank you for noticing! We have changed the sentence accordingly.

L. 174ff: his paragraph actually described the indicators used and does not discuss the results. This could go into the methods description or should be more clearly related to the actual results.

This paragraph describes PC2 and discusses how the variables that make up PC2 are related, therefore we have decided to leave it in, as a discussion of PC2.

Figure 2: What are 'some points'? How were they chosen?

It says so in the caption: "The trajectories were chosen to fill a large area in the space of the first two principal components."

L. 139: As said before, this is rather introduction than results/discussion. I would have very much appreciated reading this in the introduction.

This is the wrong line number, the reviewer is probably referring to the description of the Bowen ratio as this should be mentioned in the introduction, indeed. We have added the Bowen ratio to the introduction and changed the paragraph to highlight the main result.

L. 258: rephrase: … and can therefore be interpreted…

Thank you for finding this, we have rephrased the sentence.

L. 282: Again, put the result in the spotlight, not the figure showing the result.

The reviewer is right, this also counts for some of the other paragraphs describing that figure, thank you for pointing this out. We hope to have remedied the situation with the changes made to the paragraphs referring to the same figure.

L. 305: Occur instead of occurring.

Changed, thanks.

L. 312: Move 'especially' after 'showed'.

Changed, thank you.

L. 313: Repeats methods.

Thanks for noticing, we have removed the phrase and added "... patterns of trends ..." to the next sentence.

L. 320: Why did you calculate the trends from the full data? Would it have been better to use the growing season as well to facilitate comparison? Please give a reasoning why you do it differently.

The reviewer is right, that usually these kind of analyses are made on the growing season only. Because of simplicity of the analysis, we opted to do the analysis this way, just as with the breakpoints we did not want to develop complicated methods for detecting the growing season from PC1 because this is not the scope of this paper. The analyses on the resulting indicators are simple and straightforward because of their exploratory nature. The next question would have been, how to limit PC2 and PC3? Use the wet/dry season for PC2 because it shows water, and summer/winter for PC3, or also use the growing season? Using growing season data only, we probably could have found stronger trends in PC1, but this could be an interesting topic for future research.

L. 324: Something odd with the sentence starting with 'Inside...'.

Thanks for finding this one, fixed!

L. 327: Remove 'a' before 'browning'.

Removed, thank you.

L. 349: The breakpoints are actually never shown, nor discussed. The conclusion is thus not really based on data here.

The reviewer is right, we have added the breakpoints at several places throughout the manuscript. Thank you for pointing this out.

L. 352: in, not 'ina'.

Changed, thank you.

2 Anonymous Referee #2

2.1 General Remarks

2.1.1 General assessment

This is a very interesting paper addressing some important issues of big data analysis for ecology studies. It is rich in analyses and provides some new views on an old method (PCA). I particularly liked the analysis of trajectories that I found quite powerful, notably for case studies.

The authors thank the reviewer for the positive review, his time and thorough comments. We think that the comments allowed us to greatly improve the manuscript. We have addressed all of the reviewer's concerns as detailed below.

2.1.2 Key research question

Yet I found it difficult to understand what key research questions are addressed in this paper. This is important to clarify at the end of the introduction as the authors is providing us with a suit of analyses that may resemble (for non PCA-expert) an attempt of addressing many (all?) questions without real rationale. The readers need to have a clear (concise) view of the objectives of this paper, and they need to be guided through the analyses by referring back to the main research questions.

Thank you for pointing this out. The reviewer is right in that the paper may appear to try to solve too many problems. We have done some major revisions and hope that thate focus of the paper is clearer now. Thanks for the comment.

The main motivation and goal of this paper is a lack of a systematic data-driven approach to explain the main features in Earth system data cubes in the literature. We first introduce a novel way of applying PCA as a method to create such summarizing indicators, then we apply the method to a global set of representative variables describing the biosphere. Finally, to prove the effectiveness of the method, we give interpretations of the resulting set of indicators and explore the information contained in the indicators by analyzing them in different ways and relating them to well known phenomena. We have explicitly declared such motivation and approach at the end of the "Introduction" section.

2.1.3 Input data may cause the resulting axes

In addition, I also have a major concern related to the set of inputs data used to feed the PCA. I agree that PCA is a powerful tool to deal with correlated variables, yet I have difficulties understanding why the authors have decided to include variables that are obviously highly correlated. To my opinion, vegetation productivity proxies are overrepresented as well as those related to water availability and stress. It puts some doubts in my head as to whether the finding of PC1 (primary productivity) and PC2 (surface hydrology) driving the state of the biosphere in space and time is truly original (or just purely mathematical). It is therefore important for the authors to justify the set of original variables. A suggestion could also be to decrease the number of input variables (removing obvious redundant proxies) as the amount of data to be condensed is mainly coming from the 8days interval used for the analysis.

PCA extracts uncorrelated components, therefore the resulting axes will not change much if more or less variables are added that represent a certain aspect of the ecosystem. Intuitively, adding correlated variables in the analysis means that geometrically they point in the same direction in the feature space and do not change much the selection of the corresponding principal component. What does change are the explained variances of the resulting axes, i.e. including more variables that are proxies for primary productivity will cause this axis to explain more variance. The set of covariates we chose constitutes a large complementary and representative set that describes the exchange of mass and energy of the biosphere with the atmosphere. We have added a justification for the variables used to the "Data" section.

2.2 Detailed comments

Finally I also have other comments and concerns - notably related to the structure of the manuscript - that would need to be addressed by the authors prior publication of their research (see attached report for details).

(1) Abstract

The authors start off the abstract by mentioning the importance of detecting abrupt and gradual changes in terrestrial ecosystem but do not develop further in the introduction. In the method section, the detection of breakpoints reappears but no results are presented or discussed (except for the appendix A). The authors should decide whether to consider the detection of abrupt changes as a real research question for this study.

The reviewer is right, do not really go into detail in the analysis of breakpoints. To remedy this, we have changed the first sentence and made it clear that there is a proof of concept analysis in the appendix.

(2) Introduction

As stated in my main comment, I find that there is somewhat a mismatch between the introduction and the method section. In the introduction, the authors touch upon many issues related to assessing and attributing changes of biosphere properties. However apart from creating a new set of independent, 'essential' variables, they do not clearly mention what other research questions this study is going to address; whereas in the methods they mention PCA, trend and breakpoints analyses. Clearly stating the research questions for this study would help the readers to understand the rationale behind each analysis.

The reviewer is right, therefore we have also extended the "Introduction" section to contain all research questions.

(3) Data and methods

Better description of the data The description of the data slightly too minimalistic, including in the appendix F. Mentioning the input data (satellite, climate or others) feeding into each dataset would be helpful. The observation period used for this study is also not mentioned.

We thank the reviewer for pointing this out. We have added the limits of the time dimension and the type of grid in the "Data" section and have extended the descriptions of the variables in the appendix.

L. 75, Mention projection This statement is not always valid (e.g. in the case of equal-area projection). The sentence would be clearer if the authors would mention the projection system used here.

We thank the reviewer for pointing this out. See previous response.

L77. Better explanation of PCA The authors mentioned that they used a modified PCA, reading from the description given in the following lines, the PCA applied here seems to be standard. Could the authors provide some explanations to why / how the PCA has been modified? It should also clarify whether they applied the PCA in s or t-mode.

We have clarified the PCA analysis by discussing it in the context of frameworks describing PCA in the context of climatology and ecology and hope that this will help with the understanding of the method.

- *The PCA is a decomposition of the correlation matrix.*
- *Building the correlation matrix is not standard due to the big data aspects, and the spatial extension, both of which require a lot of care in the calculation of the covariance matrix, which is described in the "Methods" section.*
- *We summarize the dimensions in a novel way, there are a number of different frameworks (S- vs. T-mode in climatology, Q- vs. R-mode in ecology and multivariate statistics, and primal vs. dual modes in machine learning) that describe standard applications of PCA, none of which give an exact description of the analysis done here. We have added a section ("Relations to other PCA-type analyses") describing the relation of the present analysis with these frameworks.*

Per-pixel analysis It would be nice here to make a link to the (extended – see comment above) research questions in order to understand directly the rationale for such analyses.

The link was really unclear, we have added more research questions to the introduction (see previous replies) and are now mentioning the research questions.

(4) Results

General comment: I highly suggest to split the results and discussion into two separate sections. It will facilitate the reading and will allow the authors to emphasise better the originality of their work. Example: L155-161, L164-173, L175-182, L235-246, etc. should not be in a results section s.s., but would rather belong to a discussion (or even introduction or method). Please consider at least moving all methods description and introduction to new concepts to the respective adequate sections.

We thank the reviewer for this suggestion, but we think that a joint results and discussions section is a better choice, as it allows for the results and their discussions to be closer and easier to follow.

L153 and Figure 1 The authors mentioned that there is a knee at component 2. I believe it is rather at component 3. This component still contribute to the total variability to a share of almost 10%, therefore the authors should either include it in the rest of the analysis or provide an adequate justification not to. Also I generally miss a figure presenting together the temporal and the spatial patterns for the main PCs. This could be put as supplementary material. In the caption of Fig.1 I would recommend to change the term axis 1 and 2 by PC1 and 2. The comment also applies to the text itself (Ex. L190).

The third component was missing to simplify the analysis. Looking back at this decision, we fully agree with the reviewer that it should be included for the sake of completeness. We have added it to the paper now, we thank the reviewer for pointing this out, as it improved the manuscript substantially. The spatiotemporal figure was also missing and we have added it, this was an oversight of our part and we corrected it. We have also unified the terminology, axis is now never used to describe principal components.

- *We have added the third component to the manuscript.*
- *Added an appendix with joint time and space patterns.*
- *Removed the term axis when in designated a component in the entire manuscript.*

L183 Please describe in the first sentence what the triangle is made of.

Thank you for noticing. We have provided a better description of the figure.

L203 'movement of a spatiotemporal pixel in variable space', please rephrase. A pixel cannot be moving spatiotemporally, like in a sliding puzzle.

The pixel is moving in the vector space of the principal components, this formulation was easily misunderstood and thereore we have changed it. We thank the reviewer for pointing this out.

L221-224 This should be described in the methods section and should be linked to a key research questions.

We thank the reviewer for pointing out this oversight. We have added a definition of the means seasonal cycle to the methods and link to it in the introduction.

(5) Conclusion

L341 The results of the breakpoints analyses were not reported or discussed in the main text, therefore the statement 'To monitor gradual and abrupt changes in times of global change' do not hold.

We thank the reviewer for pointing this out and hope that we have remedied the situation. We have changed the beginning of the conclusion to: "To monitor the complexity of the changes occurring in times of an increasing human impact on the environment . . . "

Appendixes Some results presented in the appendixes do not appear in the main text, e.g. Figures A1 and B1. The authors should maybe decide on the key results to be presented here and maybe save some others for a follow-up paper?

We thank the reviewer for pointing this out and all appendices should be referenced in the text now.

(6) Two final comments for reflexion:

Legacy effects: The authors have applied PCA on time series of 8 day variables without considering any lag or accumulation effect in the response of a given variable. Would it be fair to say that legacy effects might not be captured adequately by such analysis?

The method ignores lag and memory effects, lag effects may still be captured implicitly in the components but there will probably not be a "memory axis". Something like this may be captured using a combination of more advanced machine learning algorithms (e.g. autoencoders and recurrent neural networks) but as far as the authors know, no one ever attempted an analysis like this.

Operationalization: The authors refer to the MEI in the introduction as an example of a successful PCA-based indicator. Could the authors elaborate on the requirement for operationalising their methods (e.g. if one would like to use the new indicators operationally, how frequently should the PCA be updated?).

Applying a trained PCA is very simple and computationally efficient. The trained PCA should also be quite stable and therefore we assume that updates do not have to happen frequently. The implementation with `WeightedOnlineStats.jl` would theoretically allow a very efficient *update with every step, but we assume that this will not be necessary. For a real time application of the method, the most important limitation is that only real time data can be used. This limits the type of data that that can be used, as most of the data we used here are created years after collecting the satellite or field observations.*

3 Anonymous Referee #3

3.1 General Remarks

This manuscript entitled "Summarizing the state of the terrestrial biosphere in few dimensions" is well-thought and well-written, and fits the scope of Biogeosciences, so overall, I am favourable to get it published there. I do have some concerns which I would like to see addressed by the authors, and I also have several recommendations to improve the manuscript before getting it published. Please find these points below.

We thank the reviewer for the positive comment and hope that we can address all mentioned concerns and recommendations.

3.2 Better explanation for the interpretation

My first point regards the interpretation of the first to PCA components. Having the first related to productivity and the second to water availability is indeed interesting and useful to summarize that state of vegetation. However, I believe some more effort is needed to more clearly separate these 2 in their interpretation. Productivity is inevitably dependent on water availability, so in principle, one wonders why these would be the first 2 components, which by definition should be orthogonal and 'unrelated'. I suppose this is perhaps because these refer to signals at different scales, PC1 describing an overall general state of potential productivity of the system at that location, while PC2 describes more events of water shortages and or excesses that are not directly related to the stationary potential productivity. Am I correct? Could you please clarify/elaborate on this to help readers better understand how these two axes should be 'read'.

Much related to the previous point, isn't it surprising that the 2 first principal components have such similar spatio-temporal patterns in Figure 3? These seem very highly correlated, which is something I would not have expected from the first two components which explain the maximum of variance in two orthogonal direction. Can you help me grasp this apparent paradox? In a way having such similar patterns make me wonder how useful having 2 PC is instead of only 1? Of course you do show the value of the 2D space in figure 2, but even there, much of the variation goes along the PC1 axis. Your selected cases in the anomalies in Figure 5 also generally go in the same direction of lower productivity coinciding with dryer conditions (Russian heatwave, droughts in Amazon), or vice versa (Floods in horn of Africa). Perhaps a stronger focus in general throughout the paper should be made on highlighting the much more specific cases where the two PCs give different but complementary information rather that going in the same direction.

While the reviewer is right that ecosystem productivity is dependent on water availability, the availability of water can be restricted due to several reasons which are reflected by PC2. We have added extensive descripitons to the text.

3.3 Explain component 3

I think you should also explore the third component. It does represent 9% of the variance, which is not so little, but above all it seems to be quite different from the first 2 in that it reacts much more to the albedo, which you hardly mention in the entirety of the manuscript. Could this be related to biophysical effects that vegetation could have on the climate? E.g. to understand where radiative vs non-radiative mechanisms dominate their effect on local temperature, for instance.

This is really a good suggestion and we added component three and a comprehensive interpretation.

3.4 Include static variables?

The behavior of the biosphere is much related to the elevation. While I know the effect of elevation should be reflected in the other variables, this is still dependent of modelling assumptions that may end up diluting the effect of elevation. Yet elevation is a variable that is very well measured, and which could contribute to summarizing the terrestrial biosphere. So why not including such a variable in the PCA? I know changes in elevation are minimal (and probably very difficult to detect) and having a static variable with respect to all the other dynamic ones you propose is a bit odd, but still, what are your arguments for not doing so? I think some discussion on this is warranted.

We thank the reviewer for this suggestion, but we are only including variables that are affected by the biosphere, it is true that elevation has a strong effect *on the biosphere, the biosphere has no impact on elevation (excluding long term effects, such as erosion).*

3.5 General structure

The paper generally could be improved by curating more the structure. Several points on this:

We thank the reviewer for these suggestions and hope that we have addressed satisfactorily.

- Section 3.2 could benefit from some introduction naming what you intend to calculate first (get trends, test significativity, get breakpoints, hysteresis) before going in the details. This part could also be more pedagogic, providing more rational on why you do these things.

  We have done extensive restructuring of the text and hope that this solved this problem.

- Parts of the 'discussion' should be much further after the 'results', such as lines 155-162 which should come in some kind of 'caveats and perspective about the method' section

  We have done a lot of text reorganization and hope that we have addressed this issue.

- Section 3.2 is very unbalanced with respect to 3.1. Probably best to reorganize to avoid 'sub-sub-sections' and have subsections from 3.1 to 3.5

  We have done a lot of reorganization of the text and hope that the text is better balanced now.

- Parts describing concepts, such as Hysteresis (lines 235-246) should not appear in the results but before, either in methods or introduction.

  We have moved the description of hysteresis into the "Methods" section, see comments to previous reviewer.

3.6 Minor stuff

Lines 74, 75: how do you manage intermittent gaps in the data? Does this affect your averages and your normalization? Also, please clarify if the normalization is based on the entire data cube for each variable, or is the normalization done per time frame?

This was not entirely clear in the original text, we thank the reviewer for pointing this out. Normalization for each variable is done globally, pixels with missing values are ignored. We have added an explanation to the "Data"-section.

Line 182: don't you mean sensible heat instead of latent heat?

Yes, thank you for noting this, changed.

Figure 1: caption could be more instructive, perhaps somehow say there what the reader should understand/read from the "rotation matrix".

Thank you for pointing out that the term rotation matrix may not be understood by everyone. We have changed the caption to be more instructive.

Figure 7: surprised to see the strong pattern in Eastern Australia. Is this corroborated in other studies?

This is indeed interesting, we added a paragraph describing the reasons for this particular trend to the "Trends in Trajectories" section: "In eastern Australia we find a strong wetness and greenness trend which is due to Australia having a "milennium drought" since the mid nineties with a peak in 2002 (Nicholls, 2004; Horridge et al., 2005) and extreme floods in 2010–2011 (Hendon et al., 2014)."

Mention the time period for trend analysis. Regarding all trend analyses, make sure you more clearly mention in the captions the extend of the period you are considering, as these are not long-term trends and could thus be misinterpreted.

Good point, added the year to the captions of the figures related to trends.

Add contour for coast lines For clarity and readability, figures with maps could benefit from either a dark background on the oceans or a line vector showing the coasts, as many of the colour scales use very light colours which are confounded with the white background.

Done, improved the figures quite a bit, thanks for the suggestion!

Move breakpoint detection to SI, including description I wonder if the breakpoint detection is really useful if it is not more mentioned and elaborated in the main text and just left in appendix. I would recommend to bring it in as a main figure if something strong can be extracted from there, and otherwise remove it entirely from the methods. Eventually you could include it in supplementary, but then include the description of the breakpoint methodology only there.

The breakpoint detection is an example analysis that showcases one of the possible set of changes that can occur and that can be detected, therefore we think it has it's place in the paper as an example what can be possible, without going into too much detail.

Move Fig C1 into the main text On the other hand, I would strongly recommend to integrate the Figure C1 in the main text as you do talk in detail about the Bowen ratio and how the 2 PCs do characterize it well.

Thank you for the good suggestion, we have moved the figure into the main text.

Unify scale ranges for fig D1 Figure 1D I have a bit of a hard time to make good use of it as it is. Are the values in normalized units or absolute values? Would it not be prefereable to have the same scale for MSC min and MSC max? Do you refer to this figure in the main text.

Thank you for this suggestion, but this figure is entirely about showing, that very different ecosystems can be very similar at certain points in time, for this, we don't need to compare across subfigures and therefore a single scale won't help for this, they will just remove contrast, especially across MSC min and MSC max.

Typos There are some typos in several places. Make sure to address them.

We have fixed many and hope we did not forget any.

4 Anonymous Referee #4

4.1 General remarks

The authors present a well-written manuscript on the analysis of two principal components derived from a set of biosphere variables, one related to vegetation productivity and the other one related to water stress. The trajectories of those components over time reveal interesting seasonal patterns, inter-annual changes and anomalies, and can be used to track extreme events and state shifts of ecosystems/biomes. Therefore, I believe that this is a novel and relevant contribution to Biogeosciences.

The authors thank the reviewer for the his time and thorough comments, we think that the comments greatly improved the manuscript. We have addressed them below.

4.2 Major concern

4.2.1 Advantage of PCA

My major concern lies in the fact that the authors select mainly variables related to productivity and water availability, and thus not surprisingly the PCA shows those two major axes. I wonder whether just selecting for example GPP and evaporative stress for the analysis of time trajectories would give the same results, but it might be easier to interpret than principal components representing a mix of variables. Can the authors elaborate in more depth what is the advantage of using PCs in this context?

There are multiple advantages,

- *Having to observe less dimensions: We can quantify the number of dimensions we have to measure. If we simply take GPP, we don't know how much of the variance of the dataset we are explaining.*
- *Information on the covariance structure of the covariates.*
- *If some event happens only on one of the variables driving a component, then it can still be observed in the final component.*
- *Directional information, when observing extremes.*

4.2.2 More data streams

For describing the state of the terrestrial biosphere, I think the authors are missing a very important component related to biodiversity, habitat quality, intactness, forest degradation and fragmentation. These aspects are crucial to describe the state of the terrestrial biosphere. There is still research needed to develop these as operational data streams, but a few examples are available at least at one point in time, e.g. Global Habitat Heterogeneity from EarthEnv, datasets from Global Forest Watch, Dynamic Habitat Indices DHI from Silvislab. This might not be sufficient (in terms of temporal resolution) to include it for this analysis, but the results from this study could be compared to those datasets (especially the DHI) and the need and relevance of global biodiversity and habitat intactness/quality information should be discussed.

We think that the reviewer has a very relevant point here, we would have loved to include more data streams that are relevant to the biosphere. The major problem is the availability of relevant of open data streams at a sufficiently high resolution in space and time which is currently very limited. As we want to track the change of the indicators over time, including static variables did not really make sense in this analysis. Including variables that have a yearly temporal resolution would require to aggregate our data by year which would also have made for a very interesting analysis but outside of the scope of this study.

4.3 Minor comments

L18: new satellite missions, add: Schimel, D., Schneider, F., Bloom, A., Bowman, K., Cawse-Nicholson, K., Elder, C., . . . Zheng, T. (2019). Flux towers in the sky: global ecology from space. New Phytologist, nph.15934. `https://doi.org/10.1111/nph.15934`

added

L25: green revolution, add: Chen, C., Park, T., Wang, X., Piao, S., Xu, B., Chaturvedi, R. K., . . . Myneni, R. B. (2019). China and India lead in greening of the world through land-use management. Nature Sustainability, 2(2), 122–129. `https://doi.org/10.1038/s41893-019-0220-7`

added

L27: changes are not only occurring in the onset of spring, but also browning trends, see:

- Garonna, I., de Jong, R., de Wit, A. J. W., Mücher, C. A., Schmid, B., & Schaepman, M. E. (2014). Strong contribution of autumn phenology to changes in satellite-derived growing season length estimates across Europe (1982 - 2011). Global Change Biology, 20(11), 3457–3470. `https://doi.org/10.1111/gcb.12625`
- Garonna, I., de Jong, R., & Schaepman, M. E. (2016). Variability and evolution of global land surface phenology over the past three

decades (1982-2012). Global Change Biology, 22(4), 1456–1468. https://doi.org/10.1111/gcb.13168

Thanks for the suggestion, we have added the suggesting changes.

L35: if a principal component is a mix of productivity measures, I don't necessarily think it's more intuitive to interpret than a simple GPP map.

Thanks for pointing this out, changed the sentence to:

The rationale is that dimensionality reduction only retains the main data features, which makes them easier accessible for analysis.

L63: What do you mean by "of parts"? Parts of what?

We have changed "parts" to "observations" to clarify the sentence.

L75: Isn't this dependent on the coordinate system and/or projection? What is the coordinate system used? And why not try to use an equal-area projection (e.g. equal earth projection)?

We have added the coordinate system, thank you for pointing out this oversight.

L152: So what is contributing to the third component. It's still 9% of explained variance!

Thank you for pointing this out, we have added the third component to the manuscript.

L162: Figure 1b is not very intuitive to me. What exactly does it show and how do you read from this that the first component represents productivity and the second hydrology? The figure doesn't seem to show any clear patterns to me. Could you also show the biplots of PC1 and 2, and PC2 and 3?

As biplots are the "standard" way do describe this type of information, we have thought about adding biplots, but decided against it for the following reasons: 1) Biplots don't really contain any information that is not already contained in fig 2b and fig. 4. 2) The number of observations is so high that it would be impossible to add all the observations to a plot: we worked our way around this by showing bivariate histograms as a background shading in fig. 4, and 3) the manuscript contains too many figures already and adding even more would hamper readability.

L177/178: check spelling

Thanks for finding this, fixed!

Figure 2: Very interesting figure! A degraded or stressed system might show different trajectories, could you somehow visualize the difference between intact and degraded ecosystems?

Thank you for the positive comment, in this figure we are trying to show trajectories that are diverse. You can see a comparison between a degraded and non-degraded trajectory in fig. 9a.

L258: check spelling

Thanks for finding this one. This sentence was changed in reply to another comment.

Figure 5: third line, the effects of the drought

Changed drought → floods. Thank you for finding this mistake.

Figure 6: This figure is a bit confusing to me. Could you improve the legends? I don't see an increase in seasonal amplitude in 6a, but maybe I just don't read this figure correctly. (b-c-d) seem to show the mean seasonal cycle and an event, but what do we see in 6a?

Thank you for pointing out that this may be confusing, we have added an explanatory sentence to the caption.

L305: changes that occurring?

Thank you for finding this, this sentence was changed in reply to another comment.

L340: Additional research is needed to better represent biodiversity, habitat quality and intactness, forest degradation and fragmentation, etc. . . See:

- Jetz, W., Cavender-Bares, J., Pavlick, R., Schimel, D., Davis, F. W., Asner, G. P., . . . Ustin, S. L. (2016). Monitoring plant functional diversity from space. Nature Plants, 2(3), 16024. `https://doi.org/10.1038/nplants.2016.24`
- Chiarucci, A., & Piovesan, G. (2019). Need for a global map of forest naturalness for a sustainable future. Conservation Biology, 00(0), cobi.13408. `https://doi.org/10.1111/cobi.13408`

- Nicholas C. Coops, Michael A. Wulder, (2019). Breaking the Habit(at), Trends in Ecology & Evolution, Volume 34, Issue 7, https://doi.org/10.1016/j.tree.2019.04.013.

We think that the reviewer has a very valid point here, it would be very desirable to include these variables into the analysis. Unfortunately these variables do not exist, yet.

L352: detected ina a similar fashion

Thanks for finding this one.

References

Harry H. Hendon, Eun-Pa Lim, Julie M. Arblaster, and David L. T. Anderson. Causes and predictability of the record wet east Australian spring 2010. *Climate Dynamics*, 42(5):1155–1174, March 2014. ISSN 1432-0894. doi: 10.1007/s00382-013-1700-5.

Mark Horridge, John Madden, and Glyn Wittwer. The impact of the 2002–2003 drought on Australia. *Journal of Policy Modeling*, 27(3):285–308, April 2005. ISSN 0161-8938. doi: 10.1016/j.jpolmod.2005.01.008.

Neville Nicholls. The Changing Nature of Australian Droughts. *Climatic Change*, 63(3):323–336, April 2004. ISSN 1573-1480. doi: 10.1023/B:CLIM.0000018515.46344.6d.

Summarizing the state of the terrestrial biosphere in few dimensions

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Abstract. In times of global change, we must closely monitor the state of the planet in order to understand ~~gradual or abrupt changesearly on~~the full complexity of these changes. In fact, each of the Earth's subsystems—i.e. the biosphere, atmosphere, hydrosphere, and cryosphere—can be analyzed from a multitude of data streams. However, since it is very hard to jointly interpret multiple monitoring data streams in parallel, one often aims for some summarizing indicator. Climate indices, for example, summarize the state of atmospheric circulation in a region. Although such approaches are also used in other fields of science, they are rarely used to describe land surface dynamics. Here, we propose a robust method to create global indicators for the terrestrial biosphere using principal component analysis based on a high-dimensional set of relevant global data streams. The concept was tested using 12 explanatory variables representing the biophysical ~~states~~ state of ecosystems and land-atmosphere water, energy, and carbon fluxes. We find that ~~two~~ three indicators account for ~~73~~82% of the variance of the state of the biosphere in space and time across the globe. While the first indicator summarizes productivity patterns, the second indicator summarizes variables representing water and energy availability. The third indicator represents mostly changes in albedo. Anomalies in the indicators clearly identify extreme events, such as the Amazon droughts (2005 and 2010) and the Russian heatwave (2010), they also allow us to interpret the impacts of these events. The indicators ~~also reveal changes in the seasonal cycle, e. g.~~ can also be used to detect and quantify changes in seasonal dynamics. Here we report for instance increasing seasonal amplitudes of productivity in agricultural areas and ~~in~~ arctic regions. We assume that this generic approach has great potential for the analysis of land-surface dynamics from observational or model data.

1 Introduction

Today, humanity faces ~~the~~ negative global impacts of land use and land cover change (Song et al., 2018), global warming (IPCC, 2014), and associated losses of biodiversity (IPBES, 2019), to only mention the most prominent transformations. Over the past decades, new satellite missions ~~(Berger et al., 2012)~~(e.g. Berger et al., 2012; Schimel and Schneider, 2019), along with the continuous collection of ~~more~~ ground based measurements ~~(Baldocchi et al., 2001; Baldocchi, 2008)~~(e.g. Wingate et al., 2015; Nasahara a , and the ~~generation of model data to anticipate future dynamics in the Earth system (Eyring et al., 2016)~~ integration of both (Papale et al., 2015; Babst et al., 2017; Jung et al., 2019) have increased our capacity to monitor the Earth's surface enormously. However, there are still large knowledge gaps limiting our capacity to monitor and understand the current ~~changes~~

transformations of the Earth system ~~(Rockström et al., 2009). Regional trends of vegetation greeningand browning that have~~ (Steffen et al., 2015; Rosenfeld et al., 2019; Yan et al., 2019; Piao et al., 2020).

Many of recent changes due to increasing anthropogenic activity are manifested in long-term transformations. One prominent example is “global greening” that has been attributed to fertilization effects~~on the one hand,~~ , temperature increases, and ~~long-term climate change on the other, need to be understood (de Jong et al., 2011; Zhu et al., 2016; Wright et al., 2017). Changes in the seasonal cycles of primary production, e. g. decreased seasonal amplitudes in~~ land-use intensification (de Jong et al., 2011; Zhu et al., . It is also known that phenological patterns change in the wake of climate change (Schwartz, 1998; Parmesan, 2006). However, these phenological patterns vary regionally. In “cold” ecosystems one may find decreased seasonal amplitudes on primary production due to warmer winters (Stine et al., 2009)~~or increased seasonal amplitude~~ . Elsewhere, seasonal amplitude may increase e.g. in agricultural areas due to the so called “green revolution” ~~, are expected (Zeng et al., 2014). In general, phenological patterns are changing in the wake of climate change , leading primarily to changes in the onset of spring (Schwartz, 1998; Parmesan, 2006) . Additionally, we are confronted with cascading effects induced by today’s~~ (Zeng et al., 2014; Chen et al., 2019). Another change in terrestrial land-surface dynamics is induced by increasing frequencies and magnitudes of extreme events (Barriopedro et al., 2011; Reichstein et al., 2013)~~which are~~ . The consequences for land-ecosystems have yet to be fully understood ~~(Flach et al., 2018; Sippel et al., 2018). The question~~ (Flach et al., 2018; Sippel et al., 2018), and require novel detection and attribution methods tailored to the problem (Flach et al., 2017; Mahecha et al., 2007a). While extreme events are typically only temporary deviations from a normal trajectory, ecosystems may changes their qualitative state permanently. Such shifts or tipping points can be induced by changing environmental conditions or direct human influence, and pose yet another problem that needs to be considered (Lenton et al., 2008). The question we address here is, how to uncover and summarize ~~effects of this kind from the wealth of available~~ changes in land-surface dynamics in a consistent framework. The idea is to simultaneously take advantage of a large array of global data streams~~? Do we need to develop specific solutions for every observed phenomenon or can we develop a single~~ , without addressing each observed phenomenon in a specific domain only. We seek to develop an integrated approach to uncover ~~a wide variety of phenomena.~~ changes in the land-surface dynamics based on a very generic approach.

The problem of identifying patterns of change in high dimensional data streams is not new. Extracting the dominant ~~dynamics~~ features from high-dimensional observations is a well-known problem in many disciplines. ~~In climate science, for example~~One approach is to manually define indicators that are know to represent important properties such as the “Bowen Ratio” (Bowen, 1926), another one consists in using machine learning to extract unique, and ideally independent features from the data. In the climate sciences, for instance, it is common to summarize atmospheric states using Empirical Orthogonal Functions (EOF), also known as Principal Component Analysis (PCA; Pearson, 1901). The rationale is that dimensionality reduction only retains the main data features, ~~but makes them better accessible to intuitive interpretations~~which makes them easier accessible for analysis. One of the most prominent examples is the description of the El Niño Southern Oscillation (ENSO) dynamics in the multivariate ENSO index (MEI; Wolter and Timlin, 2011), an indicator describing the state of the regional circulation patterns at a certain point in time. The MEI is a very successful index that can be easily interpreted and used in a variety of ways, most basically it provides a measure for the intensity and duration of the different quasi-cyclic ENSO events but it can also be associated with its characteristic impacts: E.g. seasonal warming, changes in seasonal temperatures and overall dryness in the Pacific Northwest of the United States (Abatzoglou et al., 2014), drought related fires in the Brazilian Amazon (Aragão et al., 2018), and crop yield anomalies (Najafi et al., 2019).

In plant ecology, indicators based on dimensionality reduction methods are used to describe changes to species assemblages along unknown gradients ~~(Legendre and Legendre, 1998; Mahecha et al., 2007a).~~ (Legendre and Legendre, 1998; Mahecha et al., 2007a) . The emerging gradients can be interpreted using additional environmental constraints, or based on internal plant community dynamics (van der Maaten et al., 2012). It is also common to compress satellite based Earth Observations via dimensionality reduction to get a notion of the underlying dynamics of terrestrial ecosystems. For instance, Ivits et al. (2014) showed that one can understand the impacts of droughts and heatwaves based on a compressed view of the relevant vegetation indices. In general, dimensionality reduction is the method of choice to compress high-dimensional observations in a few (ideally) independent components with little loss of information (Van Der Maaten et al., 2009; Kraemer et al., 2018).

Understanding changes in land-atmosphere interactions is a complex problem, as all aforementioned ~~changes~~ patterns of change may occur and interact: Land cover change may alter biophysical properties of the land surface such as albedo with consequences for the energy balance. Long-term trends in temperature, water availability, or fertilization may impact productivity patterns and biogeochemical processes. In fact, these land surface dynamics have ~~multidimensional implications~~ implications on multiple dimensions and require monitoring of biophysical state variables such as leaf area index, albedo, etc., as well as associated land-atmosphere fluxes of carbon, water, and energy.

Here, we aim to summarize these high-dimensional surface dynamics and make them accessible to subsequent interpretations and similar analyses as the original variables, such as mean seasonal cycles (MSC), anomalies, trend analyses, breakpoint analyses, and the characterization of ecosystems. Specifically, we seek a set of ~~independent~~uncorrelated, yet comprehensive, state indicators. We want to have a set of very few indicators that represent the most dominant features of the above described temporal ecosystem dynamics. These indicators should also be uncorrelated, so that one can study the system state by looking and interpreting each indicator independently. The approach should also give an idea of the general complexity contained in the available data streams. If more than a single indicator is required to describe land surface dynamics accurately, then these indicators shall describe very different aspects. While one indicator may describe global patterns of change, others could be only relevant in certain regions, for certain types of ecosystems, or for specific types of impacts. The indicators shall have a number of desirable properties: (1) Representing the overall state of ~~parts~~ observations comprising the system in space and time. (2) Carrying sufficient information to allow for reconstructing the original observations faithfully from these indicators. (3) Being of much lower dimensionality than the number of observed variables. (4) Allowing intuitive interpretations.

In this work, we first introduce a method to create such indicators, then we apply the method to a global set of variables describing the biosphere. Finally, to prove the effectiveness of the method, we interpret the resulting set of indicators and explore the information contained in the indicators by analyzing them in different ways and relating them to well known phenomena.

2 Methods

2.1 Data

Table 1. Variables used describing the biosphere, for a description of the variables, see ~~appendix~~ Appendix A.

Variable	Details	Source
Black Sky Albedo	Directional reflectance	Muller et al. (2011)
Evaporation	$[\mathrm{mm\,day^{-1}}]$	Martens et al. (2017)
Evaporative Stress	Modeled water stress	Martens et al. (2017)
fAPAR	fraction of absorbed photosynthetically active radiation	Disney et al. (2016)
Gross Primary Productivity (GPP)	$[\mathrm{gCm^{-2}day^{-1}}]$	~~Tramontana et al. (2016)~~Tramontana et al. (2016
Latent energy (LE)	$[\mathrm{Wm^{-2}}]$	~~Tramontana et al. (2016)~~Tramontana et al. (2016
Net Ecosystem Exchange (NEE)	$[\mathrm{gCm^{-2}day^{-1}}]$	~~Tramontana et al. (2016)~~Tramontana et al. (2016
Root-Zone Soil Moisture	$[\mathrm{m^3m^{-3}}]$	Martens et al. (2017)
Sensible Heat (H)	$[\mathrm{Wm^{-2}}]$	~~Tramontana et al. (2016)~~Tramontana et al. (2016
Surface Soil Moisture	$[\mathrm{mm^3mm^{-3}}]$	Martens et al. (2017)
Terrestrial Ecosystem Respiration (TER)	$[\mathrm{gCm^{-2}day^{-1}}]$	~~Tramontana et al. (2016)~~Tramontana et al. (2016
White Sky Albedo	Diffuse reflectance	Muller et al. (2011)

Table 1 gives an overview of the data streams used in this analysis (for a more detailed description ~~in appendix~~ see Appendix A). For an effective joint analysis of more than a single variable, the variables have to be harmonized and brought to a single grid in space and time. The Earth System Data Lab (ESDL; www.earthsystemdatalab.net; Mahecha et al., 2019) curates a comprehensive set of data streams to describe multiple facets of the terrestrial biosphere and associated climate system. The data streams are harmonized as analysis ready data on a common spatiotemporal grid (equirectangular 0.25° grid in space and 8 days in time, 2001–2011), forming a 4d hypercube, which we call a ~~*data cube*~~"data cube". The ESDL not only curates Earth system data, but also comes with a toolbox to analyze this data efficiently. For this study we chose all variables available in the ESDL v1.0 (the most recent version available at the time of analysis), divided the available variable into meteorological and biospheric variables and discarded the atmospheric variables. We also discarded variables with distributions that are badly suited for a linear PCA (e.g. burnt area contains mostly zeros) and variables with too many missing values. The only dataset that was added post hoc was fAPAR which represents an important aspect of vegetation which was not available in the data cube at the time on analysis (it is part of the most recent version of the data cube).

In this study, each variable was normalized globally to zero mean and unit variance to account for the ~~differences in scales.Because the~~ different units of the variables, i.e. transform the variables to have standard deviations from the mean as the common unit. Because in the equirectangular coordinate system used by the ESDL the area of the pixel changes with latitude, the pixels were weighted according to the represented surface area. Spatiotemporal pixels with missing values were ignored in the calculation of the covariance matrix.

2.2 Dimensionality Reduction with PCA

As a method for dimensionality reduction, we used a modified principal component analysis ~~(PCA)~~ to summarize the information contained in the observed variables. PCA transforms the set of d centered and, in this case, standardized variables into a subset of p~~(~~, $1 \leq p \leq d$~~)~~, principal components (PCs). Each component is uncorrelated with the other components, while the first PCs explain the largest fraction of variance in the data.

The data streams consist of ~~d~~ $d = 12$ observed variables at the same time and location. Each observation is defined in a d-dimensional space, $\mathbf{x}_i \in \mathbb{R}^d$, and we define the dataset by collecting all samples in the matrix ~~$\mathbf{X} = [\mathbf{x}_1 | \cdots | \mathbf{x}_n] \in \mathbb{R}^{d \times n}$~~ $\mathbf{X} = [\mathbf{x}_1 | \cdots | \mathbf{x}_n] \in \mathbb{R}$ The observations are repeated in space and time and lie on a grid of lat$\times$lon$\times$time~~, which in our caseare $n = \#\text{lat} \times \#\text{lon} \times \#\text{time} = 720 \times$~~ ~~where # denotes the length~~. In our case, we have $n = |\text{lat}| \times |\text{lon}| \times |\text{time}| = 720 \times 1440 \times 506 = 524,620,800$ observations, where $|\cdot|$ denotes the cardinality of the dimension. Note that the actual number of observations was lower, ~~$n = 106360156$~~ $n = 106,360,156$ because we considered land points only and removed missing values.

~~To derive the PCs, we used an eigendecomposition of the covariance matrix,~~

~~$\mathbf{Q} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T \in \mathbb{R}^{d \times d}$.~~

~~The covariance matrix, in this case, is equal to~~ The fundamental idea of PCA is to project the data to a space of lower dimensionality that preseserves the covariance structure of the data. Hence, the ~~correlation matrix because we standardized the variables to unit variance. $\mathbf{\Lambda}$ is a diagonal matrix with the the eigenvalues, $\lambda_1, \ldots, \lambda_d$, in the diagonal in decreasing order and $\mathbf{V} \in \mathbb{R}^{d \times d}$, the matrix with the corresponding eigenvectors in columns. $\mathbf{V}$ can project the new incoming input data $\mathbf{x}_i$ (centered and standardized) onto the PCs:~~

~~$\mathbf{y}_i = \mathbf{V}^T \mathbf{x}_i \in \mathbb{R}^d$,~~

~~where $\mathbf{y}_i$ is the projection of the observation $\mathbf{x}_i$ onto the d PCs.~~

~~Because the observations were centered~~ fundament of a PCA is the computation of a covariance matrix, $\mathbf{Q}$. When all variables are centered to global zero mean and normalized to unit variance, the covariance matrix can be ~~calculated by using a simple formula~~ in principle estimated as

$$\mathbf{Q} = \frac{1}{n-1}\mathbf{X}\mathbf{X}^T = \frac{1}{n-1}\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^T. \tag{1}$$

~~Given that~~ However, in our case the data cube lies on a regular 0.25° grid ~~,~~ and estimating $\mathbf{Q}$ as above would lead to overestimating the influence of dynamics in relatively small pixels of high latitudes compared to lower latitudes where each data point represent ~~largers~~ larger areas. Hence, ~~we used~~ one needs a weighted approach to calculate the covariance matrix,

$$\mathbf{Q} = \frac{1}{w}\sum_{i=1}^{n} w_i \mathbf{x}_i \mathbf{x}_i^T, \tag{2}$$

where $w_i = \cos(\text{lat}_i)$ and lat_i is the latitude of observation i~~.~~, $w = \sum_{i=1}^{n} w_i$ is the total weight, and n the total number of observations. Equation (2) has the additional property that it can be computed sequentially on very big ~~data sets~~datasets, such as our Earth ~~system data cube, by~~ System Data Cube, by an consecutively adding observations to an initial estimate.

~~The~~ Note that the actual calculation of the covariance matrix ~~was~~ is even more complicated, because summing up many floating-point numbers ~~one by one~~ one-by-one can lead to large inaccuracies due to precision issues of floating-point numbers and instabilities of the naive algorithm (Higham, 1993; the same ~~goes~~ hols for the implementations of the `sum` function in most software used for numerical computing). Here, we used the Julia package `WeightedOnlineStats.jl`[1] (implemented by the first author of this paper)~~is used~~, which uses numerically stable algorithms for summation, higher precision numbers, and a map-reduce scheme that further minimizes floating point errors.

Based on this weighted and numerically stable covariance matrix, the PCA can be computed used an eigendecomposition of the covariance matrix,

$$\mathbf{Q} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T \in \mathbb{R}^{d\times d}. \tag{3}$$

In this case, the covariance matrix $\mathbf{Q}$ is equal to the correlation matrix because we standardized the variables to unit variance. $\mathbf{\Lambda}$ is a diagonal matrix with the the eigenvalues, $\lambda_1,\ldots,\lambda_d$, in the diagonal in decreasing order and $\mathbf{V} \in \mathbb{R}^{d\times d}$, the matrix with the corresponding eigenvectors in columns. $\mathbf{V}$ can project the new incoming input data $\mathbf{x}_i$ (centered and standardized) onto the retained PCs,

$$\mathbf{y}_i = \mathbf{V}^T\mathbf{x}_i \in \mathbb{R}^d, \tag{4}$$

where $\mathbf{y}_i$ is the projection of the observation $\mathbf{x}_i$ onto the d PCs.

The canonical measure of the quality of a PCA is the fraction of explained variance ~~, calculated as~~ by each component, σ_i^2, calculated as

$$\sigma_i^2 = \frac{\lambda_i}{\sum_{i=1}^{d}\lambda_i}. \tag{5}$$

~~where λ_i is the i-th eigenvalue of the covariance matrix $\mathbf{Q}$.~~ To get a more complete measure of the accuracy of the PCA, we used the "reconstruction error" in addition to the fraction of explained variance. PCA allows a simple projection of an observation onto the first p PCs and a consecutive reconstruction of the observations from this p-dimensional projection. This is achieved by

$$\mathbf{Y}_p = \mathbf{V}_p^T\mathbf{X} \in \mathbb{R}^{p\times n} \text{ and } \mathbf{X}_p = \mathbf{V}_p\mathbf{Y}_p \in \mathbb{R}^{d\times n}, \tag{6}$$

where $\mathbf{Y}_p$ is the projection ~~on~~ onto the first p PCs, $\mathbf{V}_p$ the matrix with columns consisting of the eigenvectors belonging to the p largest eigenvalues, and $\mathbf{X}_p$ the observations reconstructed from the first p PCs.

The reconstruction error, $\mathbf{e}_i$, was calculated for every point, $\mathbf{x}_i$ in the ~~space-time-domain~~ space–time domain based on the reconstructions from the first p principal components:

$$\mathbf{e}_i = \mathbf{V}_p\mathbf{V}_p^T\mathbf{x}_i - \mathbf{x}_i \in \mathbb{R}^d. \tag{7}$$

[1]DOI: 10.5281/zenodo.3360311, repository: https://github.com/gdkrmr/WeightedOnlineStats.jl/

As this error is explicit in space, time and variable, it allows for disentangling the contribution of each of these domains to the total error. This can be achieved by estimating e.g. the (weighed) mean square error

$$\mathrm{MSE} = \frac{1}{w}\sum_i w_i \mathbf{e}_i^2$$

~~where $w_i = \cos(\mathrm{lat}_i)$, lat_i the latitude of $\mathbf{e}_i$, $w = \sum_i w_i$ the total weight. Therefore, this~~

$$\mathrm{MSE} = \frac{1}{w}\sum_i w_i \mathbf{e}_i^2. \tag{8}$$

This approach can give a better insight into the compositions of the error than a single global error estimate based on the eigenvalues.

2.3 Pixel-wise analyses of time series

~~When calculating slopes using measured data, ordinary least squares regression is not the optimal choice because outliers can significantly change the estimator. One possible solution is using the Theil-Sen estimatorwhich is robust~~ The principal components estimated as described above are ideally low-dimensional representations of the land-surface dynamics that require further interpretation. These components have a temporal dynamics that needs to be understood in detail. One crucial question is how the dynamics of a system of interest deviates from it's expected behaviour at some point in time. A classical approach is inspecting the "anomalies" of a time series, i.e. the deviatiosn from the mean seasonal cycle at a certain day of year.

Another key description of such system dynamics are trends. We estimated trends of the indicators as well as of their seasonal amplitude using the Theil–Sen estimator. The advantage of the Theil–Sen estimator is its robustness to up to 29.3% of outliers (Theil, 1950; Sen, 1968), while ordinary least squares regression is highly sensitive to such values. The calculation of the estimator consists simply on computing the median of the slopes spanned by all possible pairs of points

$$\mathrm{slope}_{ij} = \frac{z_i - z_j}{t_i - t_j}, \tag{9}$$

where z_i is the value of the response variable at time step i and t_i the time at time step i. In our experiments, we computed the slopes separately per pixel and principal component ~~where time is~~ with time as the predictor and the value of the principal component ~~is~~ as the response variable.

To test the slopes for significance, we used the Mann-Kendall statistics (Mann, 1945; Kendall, 1970) and adjusted the resulting p-values with the Benjamini-Hochberg method to control for the false discovery rate (Benjamini and Hochberg, 1995). Slopes with an adjusted $p < 0.05$ were deemed significant.

~~For the calculation of the number of~~ To identify disruptions in trajectories, breakpoint detection provides a good framework for analysis. For the estimation of breakpoints, the generalized fluctuation test framework (Kuan and Hornik, 1995)~~was used to test for the presence of breakpoints~~. The framework uses recursive residuals (Brown et al., 1975) ~~, and~~ such that a breakpoint is identified when the mean of the recursive residuals deviates from zero. We used the implementation in Zeileis et al. (2002). For practical reasons, here we only focus on the ~~biggest~~ largest breakpoint.

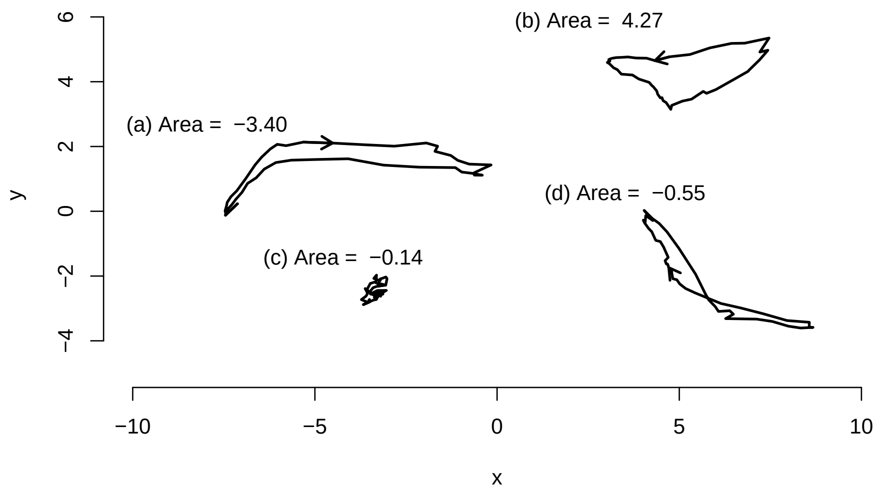

Figure 1. Example polygons and their areas, Eq. 10, the arrows indicate the directionality. (a) Clockwise polygon, has a negative area. (b) Counterclockwise polygon, has a positive area. (c) Chaotic polygon, has a very low area. (d) Polygon with a single intersection, has both a clockwise and counterclockwise portion. The clockwise portion is slightly larger than the counterclockwise portion, therefore the area is slightly negative.

~~Hysteresis was calculated as the area,~~

A very different type of dynamic is considering bivariate relations. In the context of oscillating signals it is particularly instructive to quantify their degree of phase shift and direction—even if booth signals are not linearly related. A “hysteresis” would be such a pattern describing that the pathways $A \to B$ and $B \to A$ between states A ~~,~~and B differ (Beisner et al., 2003). We estimated hysteresis by calculating the area inside the polygon formed by the mean seasonal cycle of ~~PC1 and PC2~~

$$\cancel{A = \frac{1}{2}\sum_{i=1}^{n} x_i(y_{i+1} - y_{i-1}),}$$

the combinations of two components (PC$_1$ to PC$_3$).

$$\text{Area} = \frac{1}{2}\sum_{i=1}^{n} x_i(y_{i+1} - y_{i-1}), \tag{10}$$

where $n = 46$, the number of time steps in a year, x_i and y_i the mean seasonal cycle of ~~PC$_1$ and PC~~two of PC$_1$ to PC$_{\cancel{2}3}$ at time step i, respectively. The polygon is circular, i.e. the indices wrap around the edges of the polygon so that $x_0 = x_n$ and $x_{n+1} = x_1$. This formula gives the actual area ~~of the polygon~~ inside the polygon only if it is non-self-intersecting and the vertices run counterclockwise. If the vertices run clockwise, the area is negative. If the polygon is shaped ~~as~~ like an 8, the clockwise and counterclockwise parts will cancel each other (partially) out~~, e. g. the green trajectory in fig. 4b. Trajectories that cover a larger range~~. Trajectories that have a larger amplitudes will also tend to have larger areas ~~.~~as illustrated in fig. 1.

3 Results and Discussion

In the following we first briefly present and discuss the quality of the global dimensionality reduction (Sect. 3.1), we then interpret the individual components from an ecological point of view (Sect. 3.2), before we turn to summarize the global dynamics we can uncover in the low-dimensional space (Sect. 3.3) and characterize the contained seasonal dynamics (Sect. 3.4), including spatial patterns of hysteresis (Sect. 3.5). We then describe global anomalies of the identified trajectories (Sect. 3.6), and discuss the identified anomalies in depth based on local phenomena (Sect. 3.7). Finally, we turn to global trends and their breakpoints (Sect. 3.7).

3.1 ~~The~~ Quality of the PCA~~embedding~~

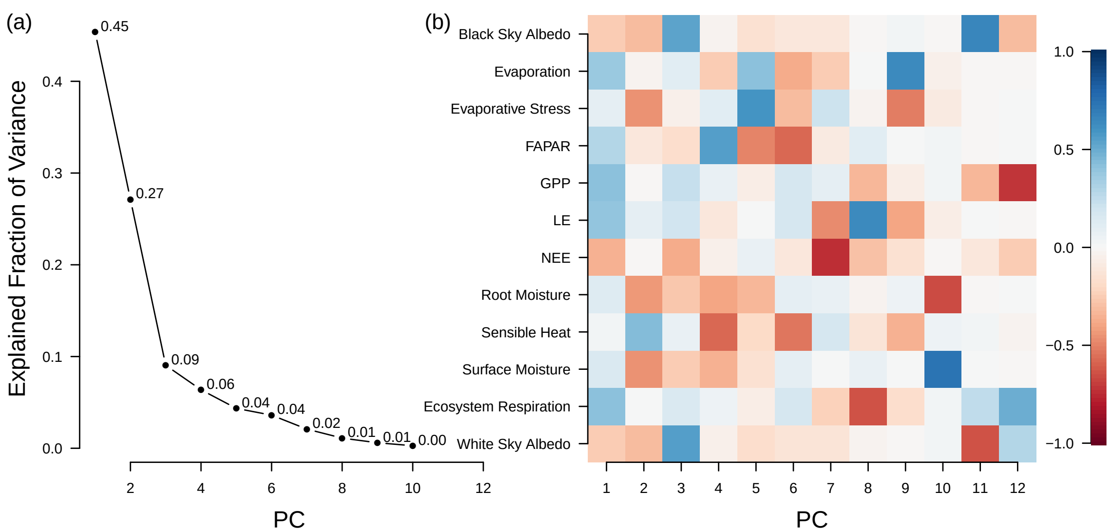

Figure 2. (a) Fraction of explained variance of the PCA by component. ~~Components~~ Knee at component three suggest that components four and higher do not ~~conrtibute~~ contribute much to total variance. (b) Rotation matrix of the global PCA model (also called *loadings*, ~~axis one describes~~ eq. 4). The columns of the rotation matrix describe the linear combinations of the (centered and standardized) original variables that make up the principal components. PC_1 is dominated by primary productivity related variables, ~~axis~~ PC_2 two ~~describe~~ by variables describing water availability, PC_3 by variables describing albedo.

Figure 2a shows the explained fraction of variance (Eq. 5) for the global PCA based on the entire data cube. ~~We see that the first two~~ The two leading components explain 73% of the variance from the 12 variables; additional components contribute ~~little < 10% explained variance~~ relatively little additional variance (PC_3 contributes 9%, all subsequent PCs less than 7%) each. This results in a "knee" at component ~~2~~3, which suggests that two indicators are sufficient to capture the major global dynamics of the terrestrial land surface~~and therefore we focus on these~~, but we will also consider the third components in the following analyses ~~.~~ (Cattell, 1966).

~~Using PCA as a method for dimensionality reduction means that we are assuming linear relations among features. A nonlinear method could possibly be more efficient in reducing the number of variables, but would also have significant disadvantages. In particular: nonlinear methods typically require tuning of specific parameters, objective criteria are often lacking, a proper weighting of observations is difficult, and it is harder to interpret the resulting indicators due to their nonlinear nature (Kraemer et al., 2018).The salient feature of PCA is that an inverse projection is well defined and allows for a deeper inspection of the errors, which is not the case for nonlinear methods due to the pre-imaging problem (Mika et al., 1999; Arenas-Garcia et al. .~~

~~The contributions of each variable to the resulting indicators can be understood from the rotation matrix (Eq. 4, fig. 2b). The~~ We estimated the reconstruction error sequentially up to the first three principal components (fig. 3). Regions that do not fit the model well show a higher reconstruction error. Considering one component only, highest reconstruction errors appear in high latitudes but decrease strongly with each additional component and nearly vanish if the third component is included.

3.2 Interpretation of the PCA

The first PC summarizes variables that are closely related to ~~vegetation primary productivity~~ to primary production (GPP, LE, NEE, fAPAR)~~. These variables are related because they are all directly related to primary productivity.~~ , and therefore highly interrelated (see fig. 2b). The energy for photosynthesis comes from solar radiation, and fAPAR is an indicator for the fraction of light used for photosynthesis~~is given by fAPAR. Photosynthesis fixes carbon from gaseous CO_2 producing sugars to~~ . The available photosynthetic radiation is used by photosynthesis to fix CO_2 and producing sugars that maintain the metabolism of ~~plants, this~~ the plant. The total uptake of CO_2 is reflected in GPP~~. However, the CO_2 uptake is~~ , whiche is also closely related to water consumption. The actual uplift of water within the plant is not only essential to enable photosynthesis, but also drives the transport of nutrients from the roots and is ultimately reflected in transpiration—together with evaporation from soil surfaces one can observe the integrated latent energy needed for the phase transition (LE). However, ecosystems also respire~~and hence~~ ; CO_2 is produced by plants in energy consuming processes as well as by the decomposition of dead organic materials via soil microbes and other heterotrophic organisms. This total respiration can be observed as terrestrial ecosystem respiration (TER). The difference between GPP and TER is the net ecosystem exchange (NEE) rate of CO_2 between ecosystems and the atmosphere (Chapin et al., 2006), and both variables are also well represented by the first dimension.

~~On the second axis we observe variables that are~~ The second component represents variables related to the surface hydrology of ecosystems ~~.~~ (see fig. 2b). Surface moisture, evaporative stress, root-zone soil moisture, and sensible heat, are all essential indicators for the state of plant available water. While surface moisture is a rather direct measure, evaporative stress is a modeled quantity summarizing the level of plant stress~~, a~~ : A value of zero means that there is no water available for transpiration, while a value of one means that transpiration equals the potential transpiration (Martens et al., 2017). Root-zone soil moisture is the moisture content of the root zone in the soil, the moisture directly available for root uptake. If this quantity is below the wilting point, there is no water available for uptake by the plants. Sensible heat is the exchange of energy by a change of temperature, if there is enough water available, then most of the surface heat will be lost due to evaporation (latent heat), with decreasing water availability more of the surface heat will be lost due to ~~latent~~ sensible heat, making this also an indicator of dryness.

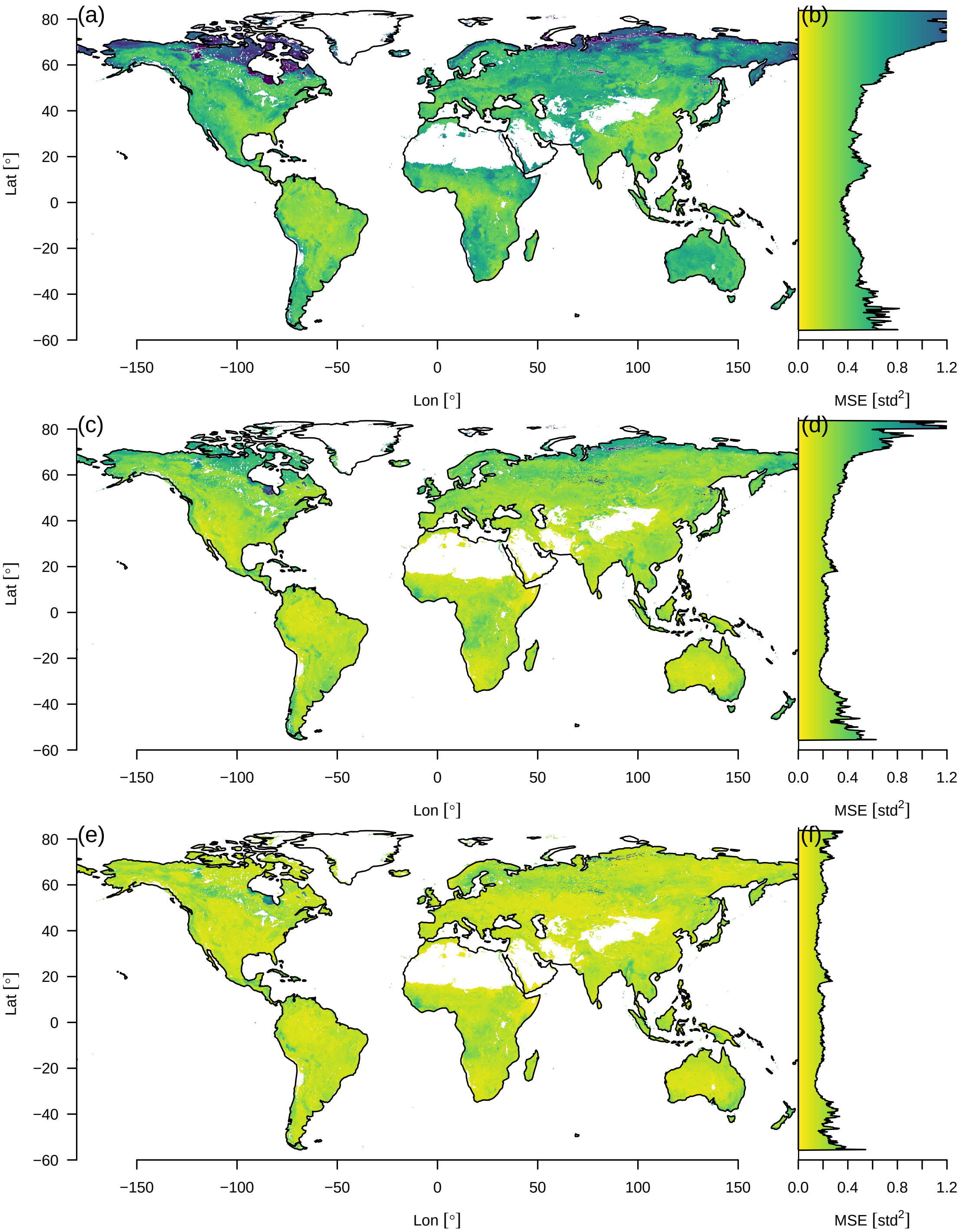

Figure 3. Reconstruction error of the data cube using varying numbers of principal components aggregated by the mean squared error. Reconstruction errors aggregated over all time steps and variables are shown in the left column: (a) Using only the first component; (c) Using the first two; (e) Using the first three. Corresponding right plots (b, d, f) show the mean reconstruction error aggregated by latitudes.

We observe that the third component is most strongly related to albedo (fig. 2b). Albedo describes the overall reflectiveness of a surface. Light surfaces, such as snow and sand, reflect most of the incoming radiation, while surfaces that have a high liquid water content or active vegetation absorb most of the incoming radiation. Local changes to albedo can be caused by a large array of reasons, e.g. snow fall, vegetation greening/browning, or land use change.

The relation of PC_3 to productivity and hydrology is opposite to what we would expect from an albedo axis. Because vegetation uses radiation as an energy source, albedo is negatively correlated with the productivity of vegetation, hence the negative correlation of albedo with PC_1. Given that water also absorbs radiation we can observe a negative correlation of albedo with PC_2 (see fig. 2b). We observe that PC_1 and PC_2 are positively correlated with PC_3 on the positive portion of their axes (see fig. 4d and f), which means counterintuitively that the index representing albedo is positively correlated with primary productivity and moisture content. Finally we can observe that PC_1 and PC_2 have a much higher reconstruction error in snow covered regions, which is strongly improved by adding PC_3 (see fig. 3f). Therefore the third component should be regarded mostly as binary variable that introduces snow cover, as the other information that is usually associated with albedo is already contained in the first two components.

~~The~~

3.3 Distribution of points in PCA space

The bivariate distribution of the first two principal components form a ~~triangle~~ “triangle” (gray background in fig. 4~~). On one edge of the first principal component we find ecosystems in a~~ a). At the high end onf PC_1 we find one point of the triangle in which ecosystems have a high high state of primary productivity (high values of GPP, fAPAR, LE, TER, and evaporation), mostly limited by radiation~~, while on~~ . On the lower end of the principal component one we find ~~states of low productivity. Ecosystem~~ the other two points of the triangle describing two alternative states of low productivity~~are further separated by~~ : These can happen either when the second principal component ~~: Low productivity can coincide with radiation~~ coincides with temperature limitation (the negative extreme of the second principal component) as seen in the lower left corner of the distribution in fig. 4a and b or ~~with~~ due to water limitation (~~the~~ positive extreme of the second principal component, the upper left corner in fig. 4a). This pattern reflects the two essential global limitations of GPP in terrestrial ecosystems (Anav et al., 2015).

~~Both axes form the space~~

Both components form a subspace in which most of the variability of ecosystems takes place. ~~Axis~~ Component one describes productivity and ~~axis~~ component two the limiting factors to productivity. Therefore, we can see that most ecosystems with high values on ~~axis~~ component one (a high productivity) are at the approximate center of ~~axis~~ component two. When ecosystems are found outside the center of ~~axis~~ component two, they have lower values on ~~axis~~ component one (lower productivity) because they are limited by water or temperature (see fig. 4b).

~~Heat transfer~~

To further interpret the “triangle” we analyze how the Bowen ratio embeds into the space of the first two dimensions. Energy fluxes from the surface into the atmosphere can ~~happen either by~~ either represent a radiative transfer (sensible heat) or

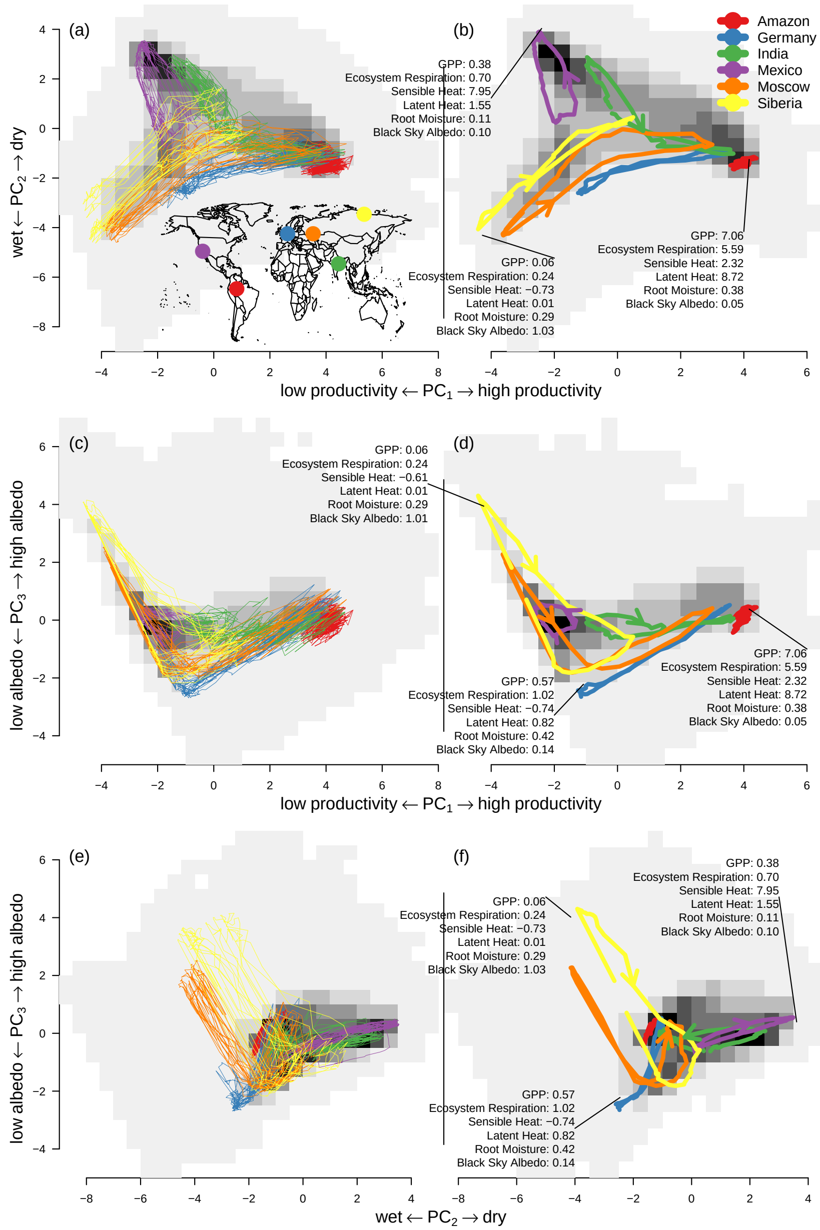

Figure 4. Trajectories of some points (colored lines) and the area weighted density over principal components one and two (the gray background shading shows the density) for (left column) the raw trajectories and (right column) the mean seasonal cycle. The trajectories are shown in the space of PC_1–PC_2 (first row), PC_1–PC_3 (second row), and PC_2–PC_3 (third row). The trajectories were chosen to cover a large area in the space of the first two principal components. Some of the trajectories have an arrow indicating the direction. The numbers illustrate the value of some variables, for units see tab. 1. Description of the points: Red: Tropical Rainforest, 67.625°W, 2.625°S; Blue: Maritime climate, 7.375°E, 52.375°N; Green: Monsoon climate, 82.375°E, 22.375°N; Purple: Subtropical, 117.625°W, 34.875°N; Orange: Continental climate, 44.875°E, 52.375°N; Yellow: Arctic climate, 119.875°E, 72.375°N.

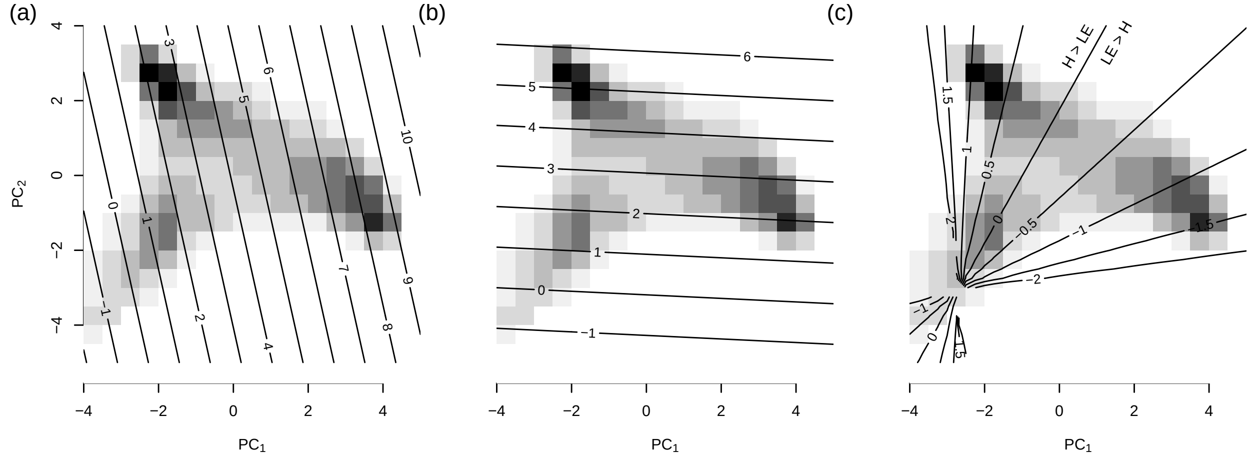

Figure 5. The background shading show the distribution of the mean seasonal cycle of the spatial points (see fig. 4). The contour lines represent the reconstruction of the variables from the first two principal components. The reconstructed variables are (a) Latent Heat (LE), (b) Sensible heat (H), and (c) $\log_{10}\left(\frac{\text{Sensible Heat}}{\text{Latent Heat}}\right)$, the $\log_{10}$ of the Bowen ratio. Note that the LE and H have been considered in the construction of the PCs, and hence are a linear function of the PCs. The Bowen ratio, instead, was not considered here and clearly responds in a nonlinear form.

evaporation (latent heat). Their ratio is the “Bowen ratio”, ~~$B = \frac{\text{LE}}{\text{H}}$~~ $B = \frac{\text{H}}{\text{LE}}$, (Bowen, 1926; see also fig. 5)~~, if there is enough moisture, then~~. When water is available most of the available energy will be dissipated by evaporation, $B < 1$, resulting in a high latent heat flux~~, but when the surface does not contain much moisture the~~. Otherwise, the transfer by latent heat will be low and most of the incoming energy has to be dissipated via sensible heat, $B > 1$. In higher latitudes, there is ~~not much~~ relatively limited incoming radiation and ~~the~~ temperatures are low, therefore there is not much energy to be dissipated and both heat fluxes are low. A high sensible heat flux is an indicator for water limitation~~and both low sensible and latent heat flux are indicators for ecosystems that are limited by low temperatures and low amounts of incoming radiation. We can see that the bowen ratio embedds well into the space spanned by the first two PCs.~~.

3.4 ~~Trajectories~~

~~Trajectories of some points (colored lines) and the area weighted density over principal components one and two (the gray background shading shows the density) for (a) the raw trajectories and (b) the mean seasonal cycle. The trajectories were chosen to fill a large area in the space of the first two principal components. Some of the trajectories in (b) have an arrow indicating the direction. The numbers illustrate the value of some variables, for units, see tab. 1. Description of the points: Red: Tropical Rainforest, 67.625°W, 2.625°S; Blue: Maritime climate, 7.375°E, 52.375°N; Green: Monsoon climate, 82.375°E, 22.375°N; Purple: Subtropical, 117.625°W, 34.875°N; Orange: Continental climate, 44.875°E, 52.375°N; Yellow: Arctic climate, 119.875°E, 72.375°N;~~

~~The principal components may be used to summarize the movement of~~

3.4 Seasonal Dynamics

The leading principal components represent most of the variability of the space spanned by the observed variables, summarizing the state of a spatiotemporal pixel ~~in variable space, so that they represent the current state of the ecosystem at a certain location in space and~~ efficiently. This means that the PCs track the state of a local ecosystem over time (fig. 4 ~~a) ortime of year of~~ left column) or, in case of the mean seasonal cycle~~of the pixel~~, time of the year (fig. 4 ~~b).~~ right columns). For a representation of the state of the first three components in time and space, see appendix fig. B1.

~~Because the underlying data are 8-daily resolution, we can observe the seasonal variability and find that the~~

A first inspection reveals a substantial overlap of seasonal cycles of very different regions of the world~~can substantially overlap. We~~. We also see that very different ecosystems may reach very similar states in the course of the season, even though their seasonal dynamics are very ~~distinct~~different. For instance, a mid-latitude ~~areas~~ pixel (blue trajectory in fig. 4) ~~show~~ shows very similar characteristics to tropical forests during ~~their~~ peak growing season~~because their patterns of~~. This indicates that the an ecosystem of the a mid-latitude can reach similar levels of productivity and water availability ~~are similar~~ than a tropical rain forest (see also SI fig. C1). Likewise, on the first two components, many high latitude areas show similar characteristics to ~~mid-latitude~~ midlatitude areas during winter on the (low latent and sensible energy release as well as low GPP) and many dry areas such as deserts show similar characteristics to areas with a pronounced dry season, e.g. the Mediterranean.

~~Ecosystems states~~ Depending on their position on Earth, ecosystem states can shift from limitation to growth during the year (fig. 4b, e.g. Forkel et al., 2015). For example, the orange trajectory in fig. 4, an area close to Moscow, shifts from a temperature limited state in winter to a state of very high productivity during summer. Other ecosystems remain in a single limitation state with only slight shifts, such as the red trajectory in fig. 4. In the corner of maximum productivity of the distribution, we find tropical forests characterized by a very ~~shallow~~ low seasonality. We also observe that very different ecosystems can have very similar characteristics during their peak growing season, e.g. green (located in north east India), blue (north west Germany), and orange (located close to Moscow) trajectories have very similar characteristics during peak growing season compared to the red trajectory.

3.4.1 ~~The Mean Seasonal Cycle of Trajectories~~

The third components shows a different picture. Due to a consistent winter snow cover in higher latitudes the albedo is much higher and the amplitude of the mean seasonal cycle is much larger than in other ecosystems. Other areas show comparatively little variance on the third component and their relation to productivity and moisture content is even positively correlated to the third component, which is the opposite of what is expected from an albedo axis.

~~As with ordinary variables, we can compute the Mean Seasonal Cycle (MSC) of the principal components summarizing the average state of the ecosystem during the course of the year. Removing year-to-year variability and long-term trends reveals a general characterization of the local ecosystem (cf. fig. 4b).~~

~~The global main~~ The global pattern of the first principal component follows the productivity cycles during summer and winter (fig. 6, left column) of the northern hemisphere, with positive values (high productivity, green) during summer and

~~Mean seasonal cycle of the first principal component during the year. Left column: first principal component. Right column: second Principal Component. Rows from top to bottom: equally spaced intervals during the year.~~

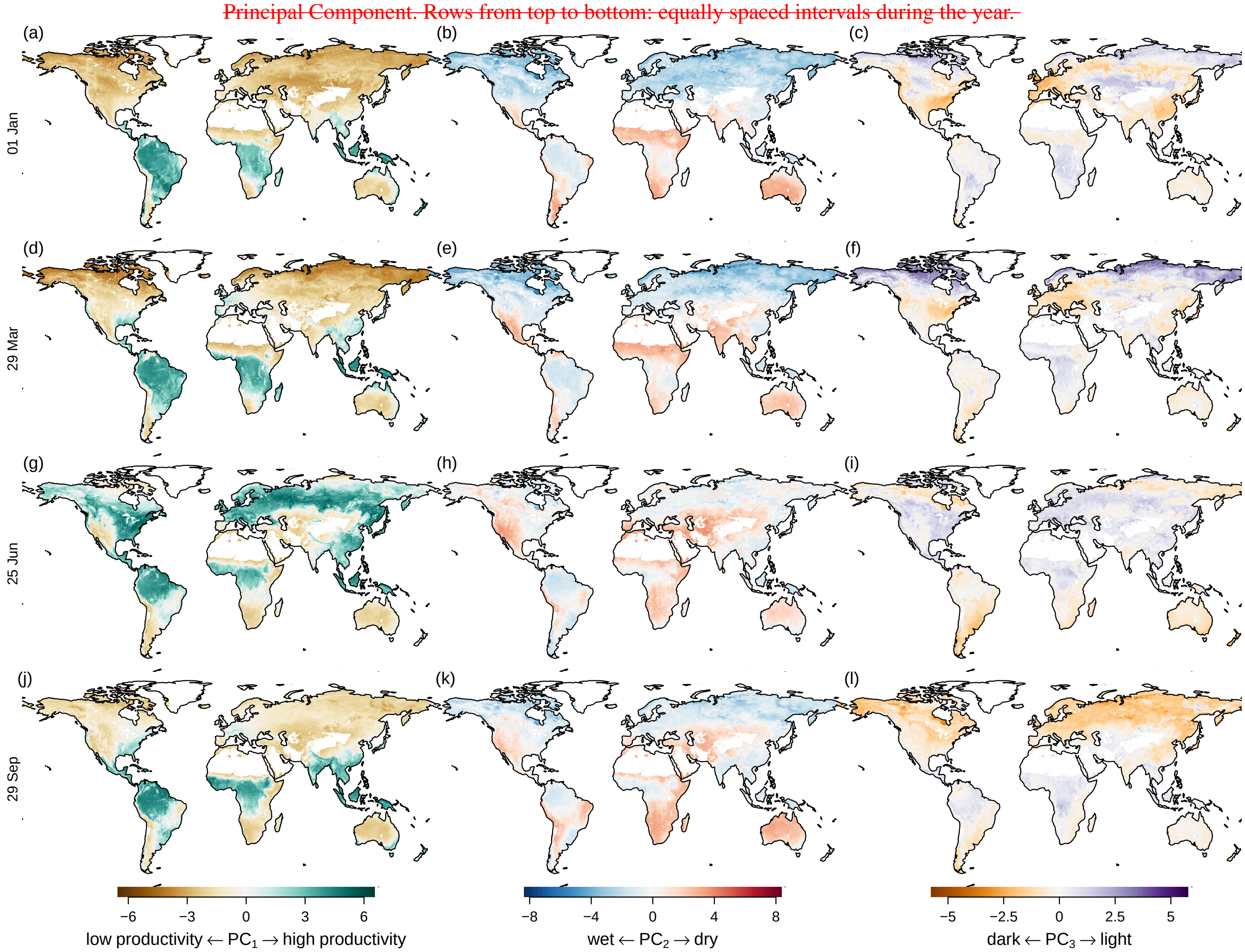

Figure 6. Mean seasonal cycle of the first three principal components (in columns) during the seasons (in rows). Left column: first principal component. Middle column: second principal component. Right column: third principal component. Rows from top to bottom: equally spaced intervals during the year.

negative values (low productivity, brown) during winter. The tropics show high productivity all year. The global pattern shows the well known green wave (Schwartz, 1994, 1998) because the first dimension integrates over all variables that correlate with plant productivity.

The second principal component (fig. 6, ~~right~~ middle column) tracks water deficiency: red and light red values indicate water deficiency, light blue values excess water, and dark blue water growth limitation due to cold. Areas which are temperature limited during winter but have a growing season during summer, such as boreal forests, change from dark blue in winter to light blue during the growing season. Areas which have low productivity during a dry season change their coloring from red to light red during the growing season, e.g the north west of Mexico/south west of the United States.

The third principal component (fig. 6, right column) tracks surface reflectance. Therefore we can see the highest values in the arctic region during winter, other areas vary much less in their reflectance throughout the year. Again, the third component shows a counterintuitive behavior in midlatitudes, as it is positively correlated with productivity and therefore shows the opposite behaviour of what would be expected from an indicator tracking albedo.

Although the principal components are globally uncorrelated, they covary locally (see fig. D1). Ecosystems with a dry season have a negative covariance between PC_1 and PC_2 while ecosystems that cease productivity in winter have a positive covariance. Cold arid steppes and boreal climates show a negative covariance between the PC_1 and PC_3, while other ecosystems that have a strong seasonal cycle show a positive correlation, many tropical ecosystems don't show a large covariance. A very similar picture paints the covariance between PC_2 and PC_3, boreal and and steppe ecosystems show a negative covariance, while most other ecosystems show a more or less pronounced positive covariance, again depending on the strength of the seasonality.

Observing the mean seasonal cycle of the principal components gives us a tool to characterize ecosystems and may also serve as a basis for further analysis, such as a global comparison of ecosystems ~~(Metzger et al., 2013; Mahecha et al., 2017)~~ (Metzger et al., 2013; Mahecha et al., 2017).

3.4.1 ~~Hysteresis~~

3.5 Hysteresis

~~Hysteresis in ecology means that the pathways $A \to B$ and $B \to A$ between stable states A and B can be different (Beisner et al., 2003~~ ~~. These alternative paths~~ The alternative return path between ecosystem states forming the hysteresis loops arise from the ecosystem tracking seasonal changes in the environmental condition, e.g. summer–winter or dry–rainy seasons (fig. 4b)~~).~~

. Hysteresis is a common occurrence in ~~ecology, e. g. in community ecology it is often cited as the reason why communities may not recover after a disturbance, it is usually attributed to memory and lag effects (Folke et al., 2004; Blonder et al., 2017; Renner et al.,~~ ~~.~~ ecological systems (Folke et al., 2004; Blonder et al., 2017; Renner et al., 2019). For instance, a hysteresis loop can be found when plotting soil respiration against soil temperature (Tang et al., 2005). The sensitivity of soil respiration to soil temperature changes seasonally due to changing soil moisture and photosynthesis (by supplying carbon to the rhyzosphere) producing a seasonally changing hysteresis effect (Gaumont-Guay et al., 2006; Richardson et al., 2006; Zhang et al., 2018). Biological variables also show a hysteresis effect in their relations with atmospheric variables, e.g. Mahecha et al. (2007b) found a hysteresis effect between seasonal NEE, temperature, and a number of other ecosystem and climate related variables.

~~Looking at some~~ Here we look at the mean seasonal cycles of ~~trajectories, e.g. the~~ pairs of indicators and the area they enclose.

The orange trajectory (area close to Moscow) in fig. 4b shows that the paths between maximum and minimum productivity can be very different, in contrast to the blue trajectory located in the north west of Germany which also has a very pronounced yearly cycle but shows no such effect. Fig. 4 also indicates that the area inside the means seasonal cycles of PC_1–PC_2 and

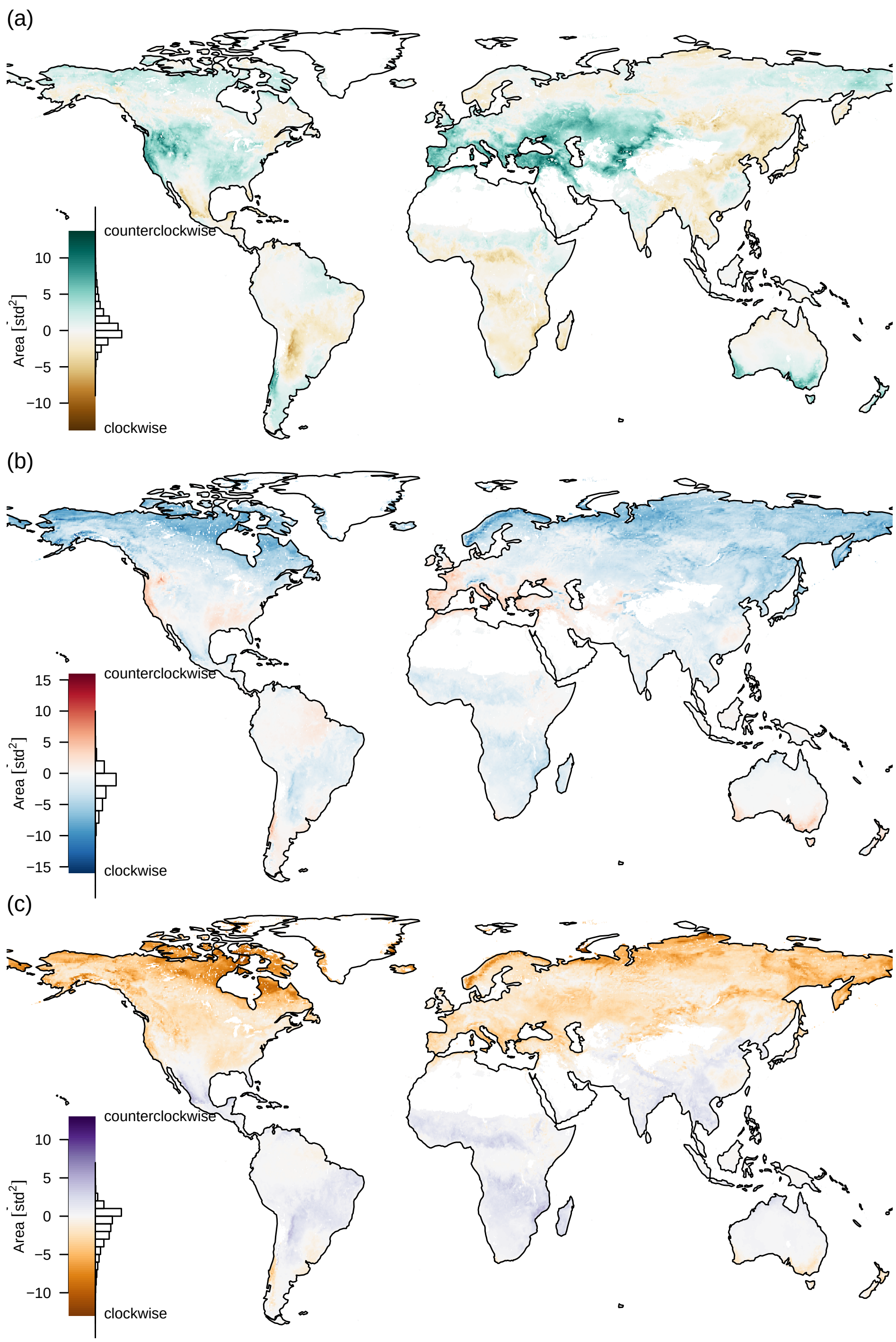

Figure 7. The area inside the mean seasonal ~~cycle~~ cycles of ~~PC1 and PC2~~(a) PC_1–PC_2, (b) PC_1–PC_3, and (c) PC_2–PC_3. The area is positive if direction is counterclockwise and negative if the direction is clockwise. ~~We can observe that most~~ Most of the trajectories need a ~~pronounced~~ strong seasonal cycle to show a pronounced hysteresis effect. ~~E~~If the mean seasonal cycle intersects, the areas cancel each other out, e.g. the green trajectory of 4b~~does not show up here, because it is shaped like an 8 and therefore the clockwise and counterclockwise parts cancel each other out~~.

PC_1–PC_3 show important characteristics while hysteresis in PC_2–PC_3 is a much less pronounced feature, i.e. we can only see a pronounced area inside the yellow curve in fig. 4f.

The trajectories that show a more pronounced ~~hysteresis effect seem to have~~ anticlockwise hysteresis effect in PC_1–PC_2 (fig. 7a) are areas with a warm and temperate climate and partially those that have a snow climate with warm summers, i.e. areas that have pronounced growing, dry, and wet seasons and therefore shift their limitations more strongly during the year, i.e. the moisture reserves deplete during growing season and therefore the return path has higher values on the second principal component (the climatic zones are taken from the Köppen–Geiger classification; Kottek et al., 2006). We can also see that ~~most trajectories that show hysteresis turn counterclockwise for the same reason (see~~ areas with dry winters tend to have a clockwise hysteresis effect, e.g. many areas in East Asia, due to the humid summers there is no increasing water limitation during the summer months which causes a decrease on PC_2 instead on an increase. Other areas with clockwise hysteresis can be found in winter dry areas in the Andes and the winter dry areas north and south of the African rainforests. Tropical rainforests do not show any hysteresis effect due to their low seasonality. In general we can say that the area inside the mean seasonal cycle trajectory of PC_1–PC_2 depends mostly on water availability in the growing and non-growing season, i.e. the contrast of wet summer and dry winter vs. dry summer and wet winter.

The hysteresis effect on PC_1–PC_3 (fig. 7~~)~~b) shows a pronounced counterclockwise MSC trajectory mostly in warm temperate climates with dry summers, while it shows a clockwise MSC trajectory in most other areas, again tropical rainforests are an exception due to their low seasonality. The most pronounced clockwise MSC trajectories are are found in tundra climates in arctic latitudes, where there is a consistent winter snow cover and a very short growing period. The lower end of PC_3 is positively correlated with ecosystem productivity, but there are still enough differences to PC_1 to distinguish the start and the end of the growing season and show different trajectories. A counterclockwise rotation can be found in summer dry areas, such as the Mediterranean and and California, but also some more more humid areas, such as the south east United States and the south east coast of Australia. In these areas we can find a decrease on PC_3 in during the non-growing phase which probably corresponds to a drying out of the vegetation and soils.

The hysteresis effect on PC_2–PC_3 (fig. 7c) mostly depends on latitude, there is a large counterclockwise effect in the very northern parts, due to the large amplitude of PC_3, the amplitude gets smaller further south until the rotation reverses in winter dry areas at the the northern and southern extremes of the tropics and disappears on the equatorial humid rain forests.

We can see that the hysteresis of pairs of indicators represents large scale properties of climatic zones. Not only the area enclosed gives interesting information, but also the direction of the rotation. Hysteresis can give information on the seasonal availability of water, seasonal dry periods or snowfall. With the method presented here, we can not observe intersecting trajectories, which would probably give even more interesting insights (e.g. the green trajectory in fig. 4b). ~~Usually plant growth starts when there is enough water available (low values on component 2) , leading to increasing values on the first component. At the end of the growing season waterresources deplete (increasing values on component 2)and productivity decreases (decreasing values on component 1).~~

3.5.1 ~~Anomalies of the Trajectories~~

3.6 Anomalies of the Trajectories

The deviation of the trajectories from their mean seasonal cycle should reveal anomalies and extreme events. These anomalies have a directional component ~~and can be therefore be interpreted~~ which makes them interpretable the same way as the original PCs~~which contain information of the underlying variables that were affected. In this sense, ,~~ , therefore one can infer the state of the ecosystem during an ~~anomalous state~~anomaly. For instance the well-known Russian heatwave in summer 2010 (Flach et al., 2018) appears in fig. 8 as a dark brown spot in the southern part of the affected area, indicating lower productivity, and as a thin green line in the northern parts, indicating an increased productivity. This confirms earlier reports ~~that~~ in which only the southern agricultural ecosystems were negatively affected by the heatwave, while the northern predominantly forest ecosystems rather benefited from the heatwave in terms of primary productivity (Flach et al., 2018).

Another example of an extreme event that we find in the PCs is the very wet November rainy season of 2006 in the Horn of Africa after a very dry rainy season in the previous year. This event was reported to bring heavy rainfall and flooding events which caused an emergency for the local population but also an increased ecosystem productivity (Nicholson, 2014). The rainfall event appears as green and blue spots in fig. 8b and c, preceded by the drought events which appear as red and brown spots.

~~Fig. 8e and 8f~~ Figures 8f and g also show the strong drought events in the Amazon, particularly the droughts of 2005 and 2010 (Doughty et al., 2015; Feldpausch et al., 2016) appear strongly north and south of the Amazon basin. The central Amazon basin does not show these strong events, because the observable response of the ecosystem was buffered due to the large water storage capacity in the central Amazon basin.

3.6.1 ~~Single Trajectories~~

Another extreme event that can be seen is the extreme snow and cold event affecting Central and South China in January 2008, causing the temporary displacement of 1.7 million people and economic losses of approximately US $ 21 billion (Hao et al., 2011). This event shows up clearly on PC_2 and PC_3 as cold and light anomalies respectively (see fig. 8k and f).

3.7 Single Trajectories

Observing single trajectories can give insight into past events that ~~happen~~ happened at a certain place, such as extreme events or permanent changes in ecosystems. The creation of trajectories is an old method used by ecologists, mostly on species assembly data of local communities, to observe how the composition changes over time (e.g. Legendre et al., 1984; Ardisson et al., 1990). In this context, we observe how the states of the ecosystems inside the grid-cell shift over time, which comprises a much larger area than a local community but is probably also less sensitive to very localized impacts than a community level analysis. One of the main differences of the method applied here to the classical ecological indicators is that the trajectories observed here are

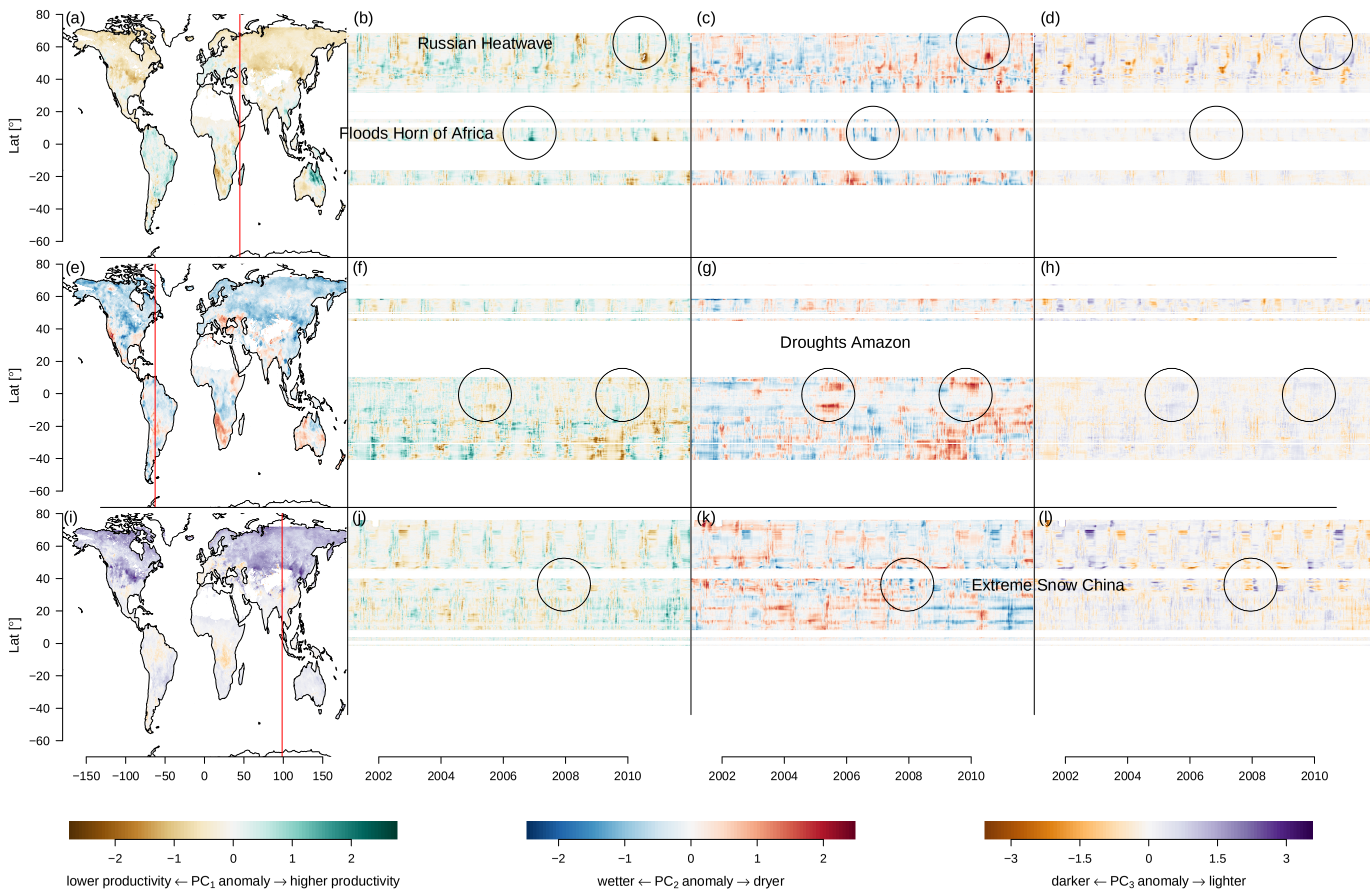

Figure 8. Anomalies of the first ~~two~~ three principal components; ~~Brown-green~~ Brown–green contrast shows the anomalies on ~~PC1~~PC_1, a relative low productivity or greening respectively. ~~Blue-green~~ Blue–red contrast shows the anomalies on ~~PC2~~PC_2, a relative wetness or dryness respectively. Brown–purple contrast shows the anomaly on PC_3, a relative deviation in albedo. (a)~~Map~~ , (e), and (i) are map showing the ~~PC1~~ anomalies of PC_1–PC_3 on the 1/1/~~2001.~~ 2001 respectively. (b)~~and~~ , (c), and (d) show longitudinal cuts of ~~PC1 and PC2~~ PC_1–PC_3 at the red vertical line in sub-figure (a) respectively. The effects of of the ~~drought~~ floods on the Horn of Africa (2006) and the Russian heatwave (2010) are highlighted by circles. (~~d~~f)~~Map showing the PC2 anomalies on the 1/1/2001.~~ , (~~e~~g), and (~~f~~h) show longitudinal cuts of ~~PC1 and PC2~~ PC_1–PC_3 at the red vertical line in sub-figure (~~d~~e) respectively. Strong droughts in the Amazon during 2005 and 2010 can be observed as large red spots on the fringes of the Amazon basin (highlighted by circles). (j), (k), and (l) show longitudinal cuts of PC_1–PC_3 at the red vertical line in sub-figure (i) respectively. A strong snowfall event affecting Central and Southern China is marked in circles.

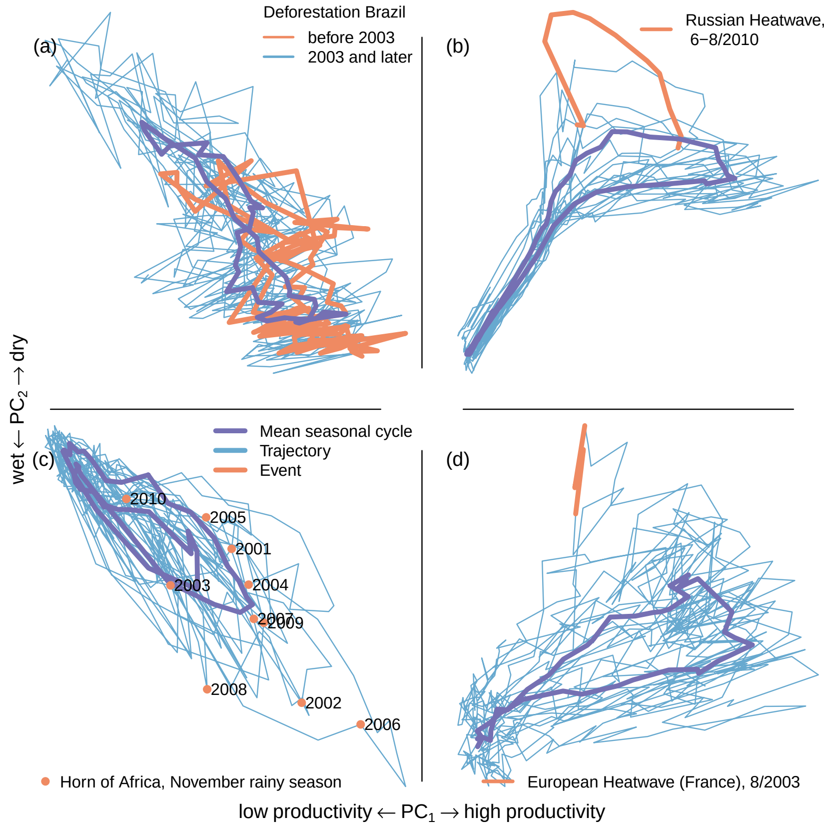

Figure 9. Trajectories of the first two Principal Components for single pixels. (a) Deforestation increases the seasonal amplitude of the first two PCs (Brazilian rainforest, 9.5°S 63.5°W). The red line shows the trajectory before 2003, the blue line the trajectory 2003 and later, a strong increase in seasonal amplitude can be observed after 2003. (b) The heatwave is clearly visible in the trajectory (red, Russian heatwave, summer 2010, 56°N 45.5°E). (c) Rainfall in the short raining season (November/December) influences agricultural yield and can cause flooding (extreme flooding after drought, 11/2006, 3°N 45.5°E). (d) European heatwave in Summer 2003 was one of the strongest on record (France, 47.2°N 3.8°E). The mean seasonal cycle of the trajecotries is shown in purple.

embedded into the space spanned by a single global PCA and therefore we can compare a much broader range of ecosystems directly.

The seasonal amplitude of the trajectory in the Brazilian Amazon increases due to deforestation and crop growth cycles. Figure 9a shows an area in the Brazilian Amazon in Rondônia (9.5°S, 63.5°W) which ~~has been~~ was affected by large scale land use change and deforestation. It can be seen that the seasonal amplitude increases strongly after the beginning of 2003. Reasons for this increased amplitude could lie in any of the following reasons or a combination of them: Deforestation decreases water storage capability and dries out soils causing larger variability in ecosystem productivity. Therefore, during periods of no rain, large scale deforestation can cause a shift in local scale circulation patterns causing lower local precipitation (Khanna et al., 2017). Crop growth and harvest causes an increased amplitude in the cycle of productivity. An analysis of the trajectory can point to the nature of the change, however finding the exact causes for the change requires a deeper analysis.

~~Figure~~The 2010 Russian heatwave has a very clear signal in the trajectories, fig. 9b shows the deviation of the trajectory during the Russian heatwave (red line) in an area east of Moscow (56°N 45.5°E). In the southern grass- and croplands, the heatwave caused the productivity to drop significantly during summer due to a depletion of soil moisture. In the northern forested parts affected, the heatwave caused an increase in ecosystem productivity during spring due to higher temperatures combined with sufficient water availability. This shows the compound nature of this extreme event (see fig. 8a and Flach et al. 2018). The analysis of the trajectory points directly towards the different types of extremes and responses that happened in the biosphere during the heatwave.

Variability of rainfall during the November rainy season in the Horn of Africa (3°N 45.5°E, fig. 9c) shows the trajectory and points in November of the observed time. The November rain has implications for food security because the second crop season depends on it. In 2006, the rainfall events were unusually strong and caused widespread flooding and disaster but also higher ecosystem productivity (cf. also fig. 8). This was especially devastating because it followed a long drought that caused crop failures. Note also the two rainy seasons in the mean seasonal cycle (purple line if fig. 9c).

The 2003 European heatwave is reflected in the trajectories just a the 2010 Russian heatwave. Figure 9d shows the trajectory during the August 2003 heat wave in Europe (France, 47.2°N 3.8°E). The heatwave was unprecedented and caused large scale environmental, health, and economics losses (Ciais et al., 2005; García-Herrera et al., 2010; Miralles et al., 2014). The 2010 heatwave was stronger than the 2003 heatwave but the strongest parts of the 2010 heatwave were in eastern Europe (cf., fig. 8), while the center of the 2003 heatwave was located in France.

As we have seen here, observing single trajectories in reduced space can give us important insights into ecosystem states and changes that ~~occurring~~occur. While the trajectories can point us towards abnormal events, they can only be the starting points for deeper analysis to understand the details of such state changes.

3.7.1 ~~Trends in Trajectories~~

3.8 Trends in Trajectories

The accumulation of CO_2 in the atmosphere should cause an increase in global productivity of plants due to CO_2 fertilization, while ~~large~~ larger and more frequent droughts and other extremes may counteract this trend. Satellite observations and models have shown that during the last decades the world's ecosystems have greened up during growing seasons. This is explained by CO_2 fertilization, nitrogen deposition, climate change and land cover change (Zhu et al., 2016; Huang et al., 2018; Anav et al., 2015). Tropical forests ~~especially showed~~ showed especially strong greening trends during growing season.

~~To find local trends, we used the Theil-Sen estimator to calculate robust slopes on the trajectories. Figure 10 shows positive and negative trends of the principal components over time. General patterns~~ General patterns of trends that can be observed are a positive trend (higher productivity) on the first principal component in ~~the arctic regionsand higher temperatures~~many arctic regions, many of these regions also show a wetness trend, with the notable exception of the western parts of Alaska which have

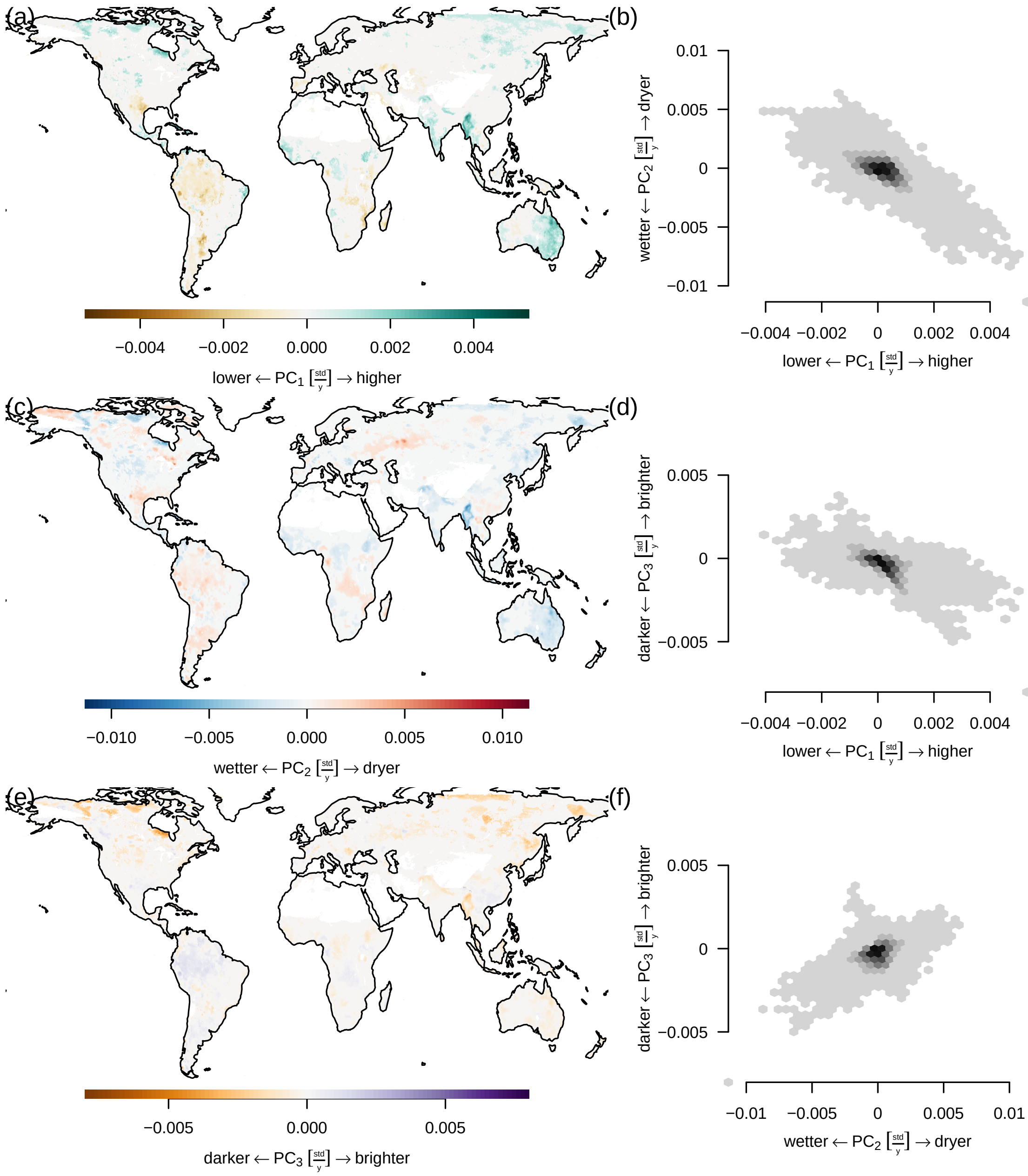

Figure 10. (a), (c), (e) Trends in ~~PC1 and PC2 indicators~~PC_1–PC_3 respectively (2001–2011). (b), (d), (f) Bivariate distribution of trends. Trends were calculated using the ~~Theil-Sen~~ Theil–Sen estimator~~.~~, (a)~~The spatial distribution of slopes~~, ~~only significant slopes are shown~~ (~~$p < 0.05$, Benjamini-Hochberg adjusted~~c)~~. The maximum cutoff for the legend limits was set symmetrically around zero to the maximum absolute value of the 0.1~~, and ~~0.9 quantiles.~~ (~~b~~e) ~~Distribution of spatial points in the space of the first two PCs. The colors correspond to the ones used in~~ show significant trends only (~~a~~$p < 0.05$, Benjamini–Hochberg adjusted).

become dryer, this is important, because wildfires play a major role in these ecosystems (Jolly et al., 2015; Foster et al., 2019), these changes are also accompanied by a decrease on PC_3 due to a loss in snow cover. A large scale dryness trend can also be observed across large parts of western Russia. Increasing productivity can also be observed on ~~almost the entire~~ large parts of the the Indian subcontinent and eastern Australia. Negative trends in the first component can also be observed: they are generally smaller and appear in regions around the Amazon and the Congo basin, but also in parts of western Australia. The main difference from previous analyses on the observations presented here is that e.g. Zhu et al. (2016) looked only at trends during the growing season while this analysis uses the entire time series to calculate the slope.

In the Amazon basin, we find a dryness trend accompanied by a decrease in productivity and a slight increase in PC_3; In the Congo basin, we find a wetness trend and an increasing productivity in the northern parts, while the southern part and woodland south of the Congo basin show a strong dryness trend with decreased productivity. This is different to the findings of Zhou et al. (2014), who found a widespread browning of vegetation in the entire Congo basin for the April-May-June seasons during the period 2000–2012. The finding of Zhou et al. (2014) is not reflected in our data, especially compared to the areas surrounding the Congo basin, we can find only minor browning effects ~~. Inside~~ inside the basin and our findings are more in line with the global greening (Zhu et al., 2016), which show a browning mostly outside the Congo basin.

~~Almost the entire~~ In eastern Australia we find a strong wetness and greenness trend which is due to Australia having a “milennium drought” since the mid nineties with a peak in 2002 (Nicholls, 2004; Horridge et al., 2005) and extreme floods in 2010–2011 (Hendon et al., 2014).

Large parts of the Indian subcontinent shows a trend towards higher productivity and an overall wetter climate. The greening trend in India happens mostly over irrigated cropland~~, however~~ . However browning trends over natural vegetation have been observed but do not ~~show up~~ emerge in our analysis (Sarmah et al., 2018). A very notable greening and wetness trend can be observed in Myanmar due to an increase in intense rainfall events and storms, although the central part experienced some strong droughts at the same time (Rao et al., 2013). In Myanmar we also find one of the strongest trends in PC_3 outside of the Artic.

In large parts of the Arctic, a ~~general~~ trend towards higher productivity can be observed, vegetation models attribute this general increase in productivity to CO_2 fertilization and climate change. The changes also cause changes to the characteristics of the seasonal cycles (Forkel et al., 2016). Stine et al. (2009) found a decreased seasonal amplitude of surface temperature over norther latitudes due to winter warming.

The seasonal amplitude of atmospheric CO_2 concentrations has been increasing due to climate change causing longer growing seasons and changing vegetation cover in northern ecosystems (Forkel et al., 2016; Graven et al., 2013; Keeling et al., 1996). Therefore we checked for trends in the seasonal amplitude, but because each time series only consists of 11 values (one amplitude per year), after adjusting the p-values for false discovery rate, we could not find a significant slope. However, there were many significant slopes with the unadjusted p-values, see the appendix, fig. E1.

Another way to detect changes to the biosphere consists in the detection of breakpoints, which has been applied successfully to detect changes in global NDVI time series (de Jong et al., 2011; Forkel et al., 2013), or generally to detect changes in time series (Verbesselt et al., 2010). A proof of concept analysis can be found in fig. F1, we hope that applying this method to indicators instead of variables can detect a wider range of breakpoints analyzing a single time series.

3.9 Relations to other PCA-type analyses

One of the most popular applications of PCA in meteorology are EOFs, which applies PCA typically on a single variables, i.e. on a data set with the dimensions lat $\times$ lon $\times$ time, although EOFs can be calculated from multiple variables. EOFs can be calculated in S-mode and R-mode. If we matricize our data cube so that we have time in rows and lat $\times$ lon $\times$ variables in columns, then S-mode PCA works on the correlation matrix of the combined variable and space dimension. In T-mode, the PCA works on the correlation matrix formed the time dimension (Wilks, 2011). The PCA presented here works slightly different: (1) We did a different matricization (lat $\times$ lon $\times$ time in rows and variables in columns) and then (2) the PCA works on the correlation matrix formed by the variables, therefore in this framework we could call this a V-mode PCA.

Ecological analyses use PCA usually with matrices of the shape object $\times$ descriptors, when calculating the PCA on the correlation matrix formed by the objects, then it is called a Q-mode analysis, when the PCA is applied on the correlation matrix formed by the variables, then it is called an R-mode analysis (Legendre and Legendre, 1998). The PCA done in this study is closest to an R-mode analysis, in the present case the descriptors are the various data streams and the objects are the spatiotemporal pixels.

Using PCA as a method for dimensionality reduction means that we are assuming linear relations among features. A nonlinear method could possibly be more efficient in reducing the number of variables, but would also have significant disadvantages. In particular: nonlinear methods typically require tuning specific parameters, objective criteria are often lacking, a proper weighting of observations is difficult, the methods are often not reversible, and it is harder to interpret the resulting indicators due to their nonlinear nature (Kraemer et al., 2018). The salient feature of PCA is that an inverse projection is well defined and allows for a deeper inspection of the errors, which is not the case for nonlinear methods which learn a highly flexible transformation that is hard to invert. Therefore interpretability of the transform in meaningful physical units in the input space is often not possible. In the machine learning community, this problem is known as the "pre-imaging problem" (Mika et al., 1999; Arenas-Garcia et al., 2013) and is a matter of current research.

4 Conclusions

To monitor ~~gradual and abrupt changes~~ the complexity of the changes occurring in times of ~~global change~~an increasing human impact on the environment, we used PCA to construct indicators from a large number of data streams that track ecosystem state in space and time on a global scale. We showed that a large part of the variability of the terrestrial biosphere can be summarized using two indicators. The first emerging indicator represents carbon exchange, while the second indicator shows the availability of water in the ecosystem, the third indicator represents mostly a binary variable that indicates the presence of snow cover. The distribution in the space of the first two principal components reflects the general limitations of ecosystem productivity. Ecosystem production can either be limited by water or energy.

The first ~~two~~ three indicators can detect many well-known phenomena without analyzing variables separately due to their compound nature. We showed that the indicators are capable of detecting seasonal hysteresis effects in ecosystems, as well as breakpoints, e.g., large scale deforestation. The indicators can also track other changes to the seasonal cycle such as patterns of changes to the seasonal amplitudes and trends in ecosystems. Deviations from the mean seasonal cycle of the trajectories indicate extreme events such as the large scale droughts in the Amazon during 2005 and 2010 and the Russian heat wave of 2010. The events are detected ~~ina~~ in a similar fashion as with classical multivariate anomaly detection methods while directly providing information on the underlying variables.

Using ~~compound~~ multivariate indicators we gain a high level overview of phenomena in ecosystems and the method therefore provides an interesting tool for analyses where it is required to capture a wide range of phenomena which are not necessarily known a priori. Future research should consider nonlinearities, ~~and~~ adding data streams that represent different aspects (e.g. biodiversity, and habitat quality), and work to include different subsystems, such as the atmosphere or the anthroposphere.

Code and data availability. The data are available and can be processed at https://www.earthsystemdatalab.net/index.php/interact/data-lab/, last accessed 28 June 2019

Appendix A: ~~Breakpoints in Trajectories~~

~~Breakpoint detection, (a) on PC1, (b) on PC2, the color indicates the year of the biggest breakpoint if a significant breakpoint was found, grey if there was no significant breakpoint found.~~

~~As the environmental conditions change, due to climate change and human intervention, the local ecosystems may change gradually or abruptly. Detecting these changes is very important for monitoring the impact of climate change and land use change onto the ecosystems. We applied breakpoint detection on the trajectories (fig. F1).~~

~~Breakpoints on the first component were found in the entire Amazon and the largest breakpoint is dated in the year 2005 during the large drought event. The entire eastern part of Australia shows its largest breakpoint towards the end of the time series because of a La Niña event, which caused lower temperatures and higher rainfall than usual during the years 2010 and 2011.~~

Appendix A: ~~Reconstruction Error~~

~~The reconstruction error of the first two pca dimensions aggregated over variables an time by the mean of the square error. The right plot shows the mean reconstruction error aggregated over latitudes.~~

~~In order to find ecosystems that do no fit well your model of two indicators, we calculated the reconstruction error of the first two PCA axes. Ecosystems that do not fit our model well show a higher reconstruction error, see fig. 3. Higher reconstruction errors appear in extreme latitudes, areas with especially high reconstruction error are at the southern part of the Hudson Bay area. Very limited regions in central and eastern Russia and northern Siberia.~~

Appendix A: ~~Bowen Ration~~

~~The background shading show the distribution of the mean seasonal cycle of the spatial points (see fig. 4). The contour lines represent the reconstruction of the variables from the first two principal components. The reconstructed variables are (a) Latent Heat, (b) Sensible heat, and (c) $\log_{10}\left(\frac{\text{Latent Heat}}{\text{Sensible Heat}}\right)$, the $\log_{10}$ of the Bowen Ratio.~~

Appendix A: ~~Mean Seasonal Cycle Extrema~~

~~Shows the minimum (left column) and maximum (right column) mean seasonal cycles of GPP (upper row), Latent Heat (middle row), and Sensible heat (lower row). This illustrates the similarity of possibly very different ecosystems in terms of productivity and limitations. During peak growing season, many mid latitude areas have a similar productivity and latent energy release as tropical rainforests (subfigure b and d). The highest maximum seasonal sensible heat loss can be found in dry areas around the world and is lowest in areas with a wet climate such as tropical rainforests and maritime climates (subfigure f).~~

Appendix A: ~~Changes in the Seasonal Amplitude~~

~~Trends in the amplitude of the yearly cycle, Theil-Sen estimators only significant slopes ($p < 0.05$), *unadjusted*, are shown. Because there is only a single amplitude per year and therefore only 11 data points per time series, the adjusted significances are not significant.~~

Appendix A: Description of variables

Variables used describing the biosphere can be found in tab. 1, here we provide a more complete description of all variables:

Black Sky Albedo is the reflected fraction of total incoming radiation under direct hemispherical reflectance, i.e. direct illumination (Muller et al., 2011). This dataset is derived from the SPOT4-VEGETATION, SPOT5-VEGETATION2, and the MERIS satellite sensors.

White Sky Albedo is the reflected fraction of total incoming radiation under bihemispherical reflectance, i.e. diffuse illumination (Muller et al., 2011). Together with black sky albedo it can be used to estimate the albedo under different illumination conditions. This dataset is derived from the SPOT4-VEGETATION, SPOT5-VEGETATION2, and the MERIS satellite sensors.

Evaporation $[\mathrm{mm/day}]$ is the amount of water evaporated per day~~(Martens et al., 2017)~~, depends on the amount of available water and energy. This dataset is based on the GLEAMv3 model (Martens et al., 2017), using satellite data from ESA CCI and SMOS to derive a number of variables.

Evaporative Stress modeled water stress for plants, zero means that the vegetation has no water available for transpiration and one means that transpiration equals potential transpiration~~(Martens et al., 2017)~~. This dataset is based on the GLEAMv3 model (Martens et al., 2017), using satellite data from ESA CCI and SMOS to derive a number of variables.

fAPAR the fraction of absorbed photosynthetically active radiation, a proxy for plant productivity (Disney et al., 2016). This dataset is based on the GlobAlbedo dataset (http://globalbedo.org) and the MODIS fAPAR and LAI products.

Gross Primary Productivity (GPP) $[\mathrm{gCm^{-2}day^{-1}}]$ the total amount of carbon fixed by photosynthesis (Tramontana et al., 2016). This dataset is derived from upscaling eddy covariance tower observations to a global scale using machine learning methods.

Terrestrial Ecosystem Respiration (TER) $[\mathrm{gCm^{-2}day^{-1}}]$ the total amount of carbon respired by the ecosystem, includes autotrophic and heterotropic respiration (Tramontana et al., 2016). This dataset is derived from upscaling eddy covariance tower observations to a global scale using machine learning methods.

Net Ecosystem Exchange (NEE) $[\mathrm{gCm^{-2}day^{-1}}]$ The total exchange of carbon of the ecosystem with the atmosphere $\mathrm{NEE} = \mathrm{GPP} - \mathrm{TER}$ (Tramontana et al., 2016). This dataset is derived from upscaling eddy covariance tower observations to a global scale using machine learning methods.

Latent energy (LE) $[\mathrm{Wm^{-2}}]$ the amount of energy lost by the surface due to evaporation (Tramontana et al., 2016). This dataset is derived from upscaling eddy covariance tower observations to a global scale using machine learning methods.

Sensible Heat (H) $[\mathrm{Wm^{-2}}]$ the amount of energy lost by the surface due to radiation (Tramontana et al., 2016). This dataset is derived from upscaling eddy covariance tower observations to a global scale using machine learning methods.

Root-Zone Soil Moisture $[\mathrm{m^3m^{-3}}]$ the moisture content of the root zone~~, estimated by the GLEAM model (Martens et al., 2017)~~. This dataset is based on the GLEAMv3 model (Martens et al., 2017), using satellite data from ESA CCI and SMOS to derive a number of variables.

Surface Soil Moisture $[\mathrm{mm^3mm^{-3}}]$ the soil moisture content at the soil surface~~(Martens et al., 2017)~~. This dataset is based on the GLEAMv3 model (Martens et al., 2017), using satellite data from ESA CCI and SMOS to derive a number of variables.

Appendix B: Time–Space patterns of Components 1–3

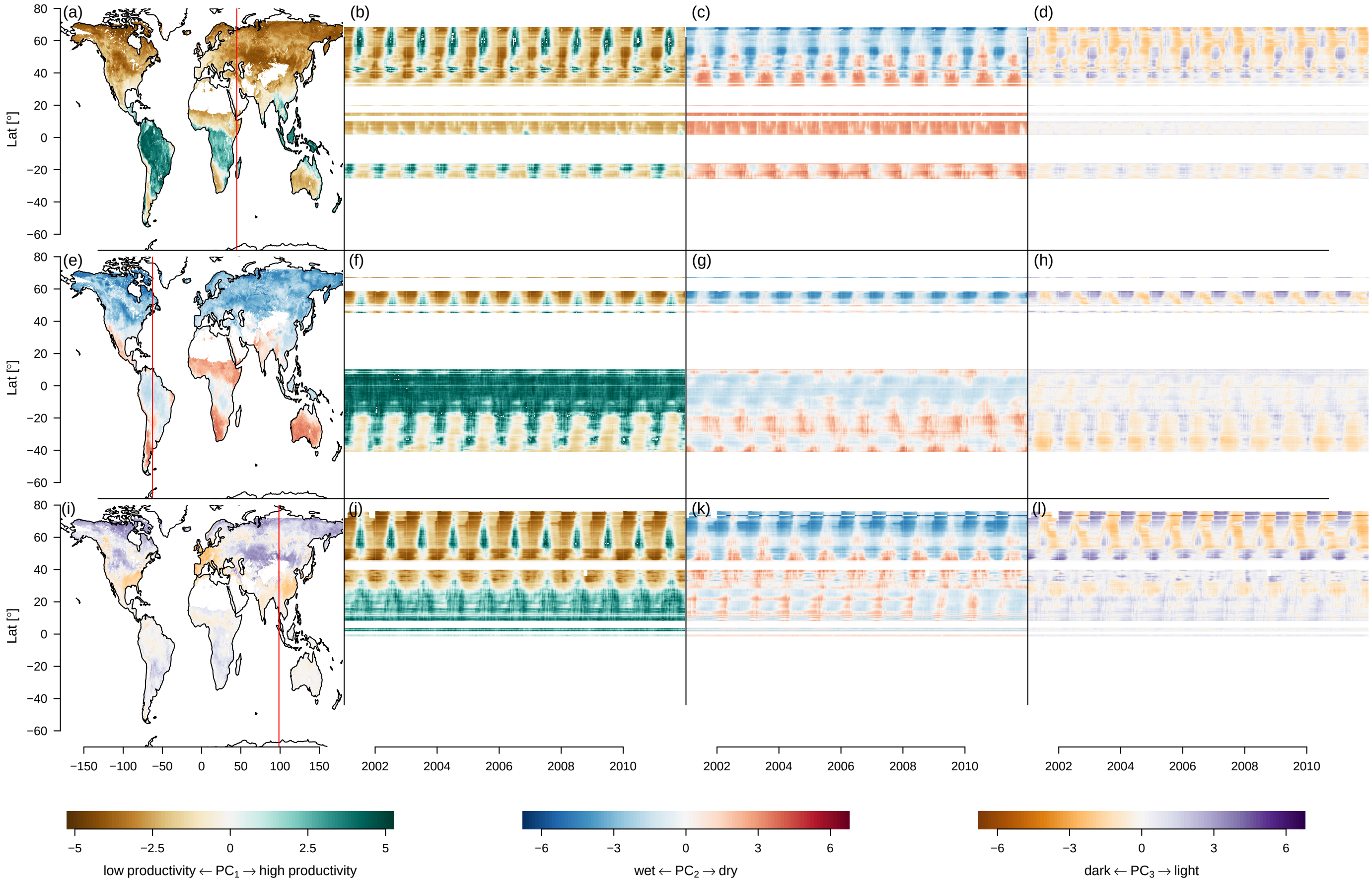

Figure B1. Time and space patterns of PC_1–PC_3, the cutpoints are the same as in fig. 8. Brown–green contrast shows the state of PC_1, from low to high productivity. Blue–red contrast shows the state of PC_2, from cold to dry. Brown–purple contrast shows the state of PC_3, from dark to light. (a), (e), and (i) are map showing the state of PC_1–PC_3 on the 1/1/2001 respectively. (b), (c), and (d) show longitudinal cuts of PC_1–PC_3 at the red vertical line in sub-figure (a) respectively. (f), (g), and (h) show longitudinal cuts of PC_1–PC_3 at the red vertical line in sub-figure (e) respectively. (j), (k), and (l) show longitudinal cuts of PC_1–PC_3 at the red vertical line in sub-figure (i) respectively.

Appendix C: Mean Seasonal Cycle Extrema

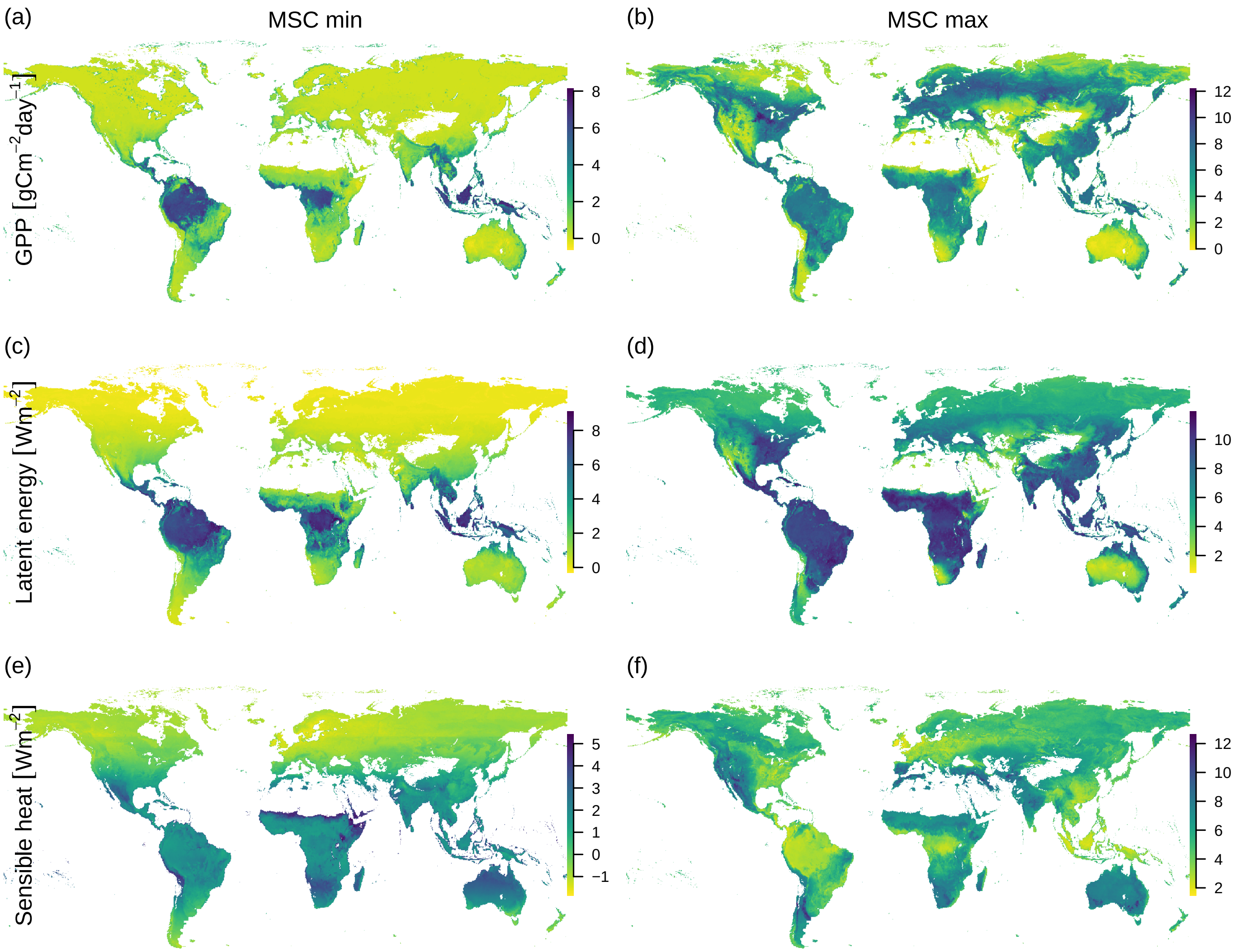

Figure C1. Shows the minimum (left column) and maximum (right column) mean seasonal cycles of GPP (upper row), Latent Heat (middle row), and Sensible heat (lower row). This illustrates the similarity of possibly very different ecosystems in terms of productivity and limitations. During peak growing season, many mid latitude areas have a similar productivity and latent energy release as tropical rainforests (subfigure b and d). The highest maximum seasonal sensible heat loss can be found in dry areas around the world and is lowest in areas with a wet climate such as tropical rainforests and maritime climates (subfigure f).

Appendix D: Spatial covariances of the components

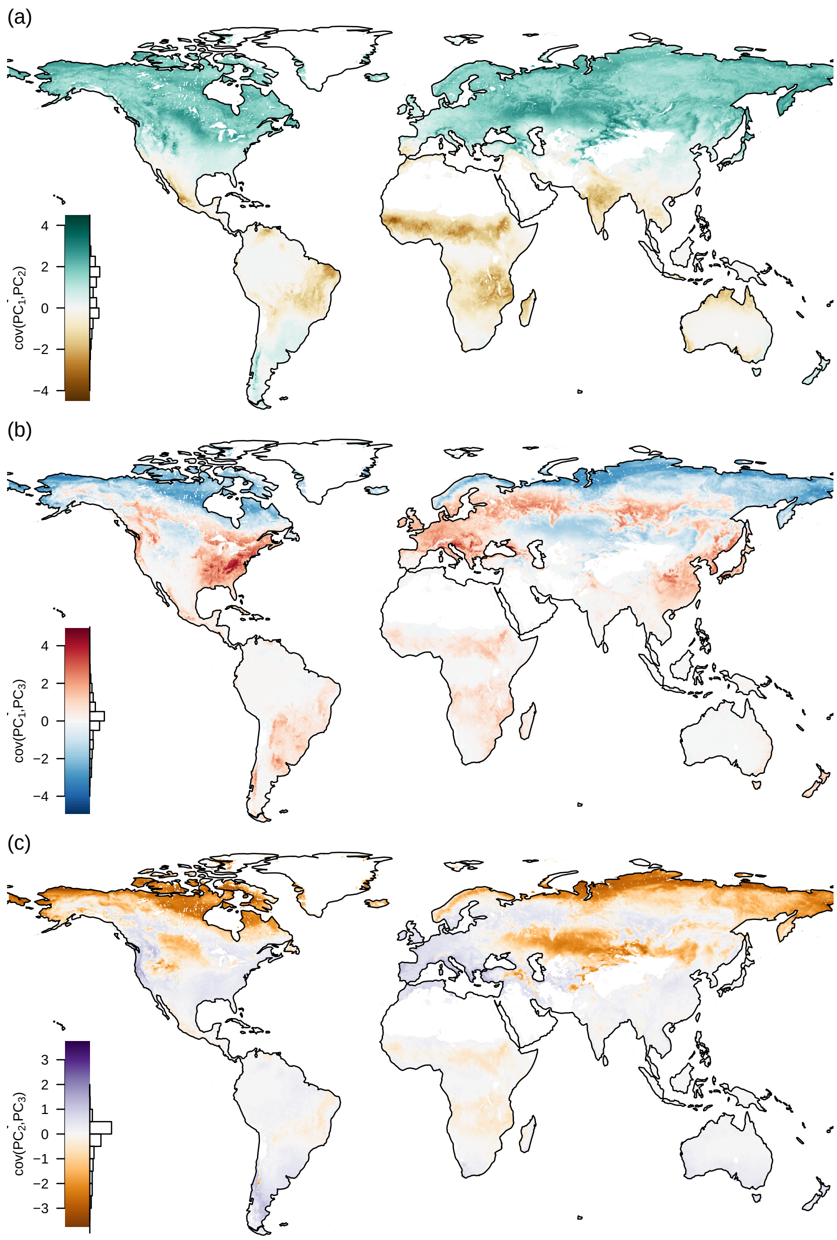

Figure D1. Pairwise covariances of the first three principal components mean seasonal cycles by space. (a) $\text{cov}(\text{PC}_1,\text{PC}_2)$, (b) $\text{cov}(\text{PC}_1,\text{PC}_3)$, and (c) $\text{cov}(\text{PC}_2,\text{PC}_3)$. The bar charts show the distribution of the covariances. It can be seen that although two principal components are globally uncorrelated by their way of construction, they covary locally.

Appendix E: Changes in the Seasonal Amplitude

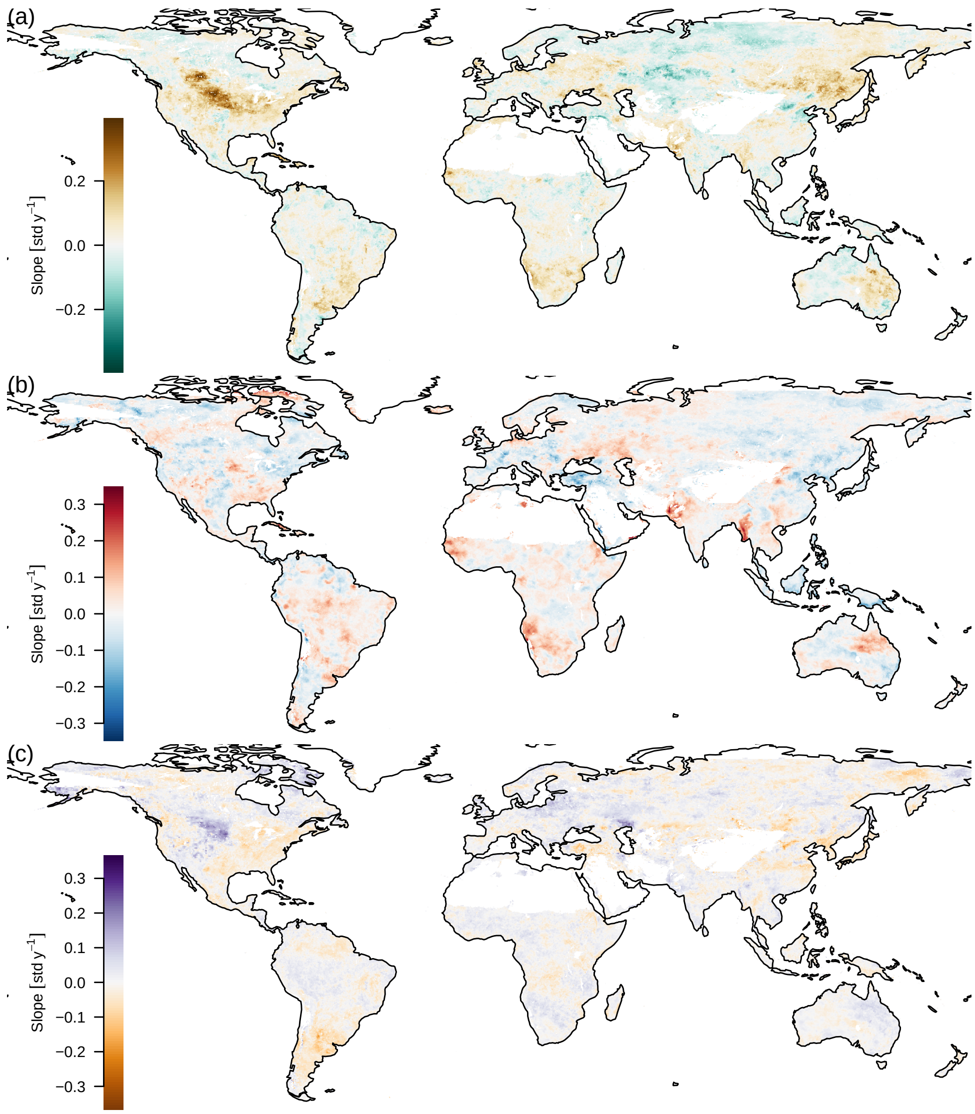

Figure E1. Trends in the amplitude of the yearly cycle, 2001–2011, Theil–Sen estimators only significant slopes ($p < 0.05$, *unadjusted*) are shown. Because there is only a single amplitude per year and therefore only 11 data points per time series, the Benjamini–Hochberg adjusted p-values are not significant.

Appendix F: Breakpoints in Trajectories

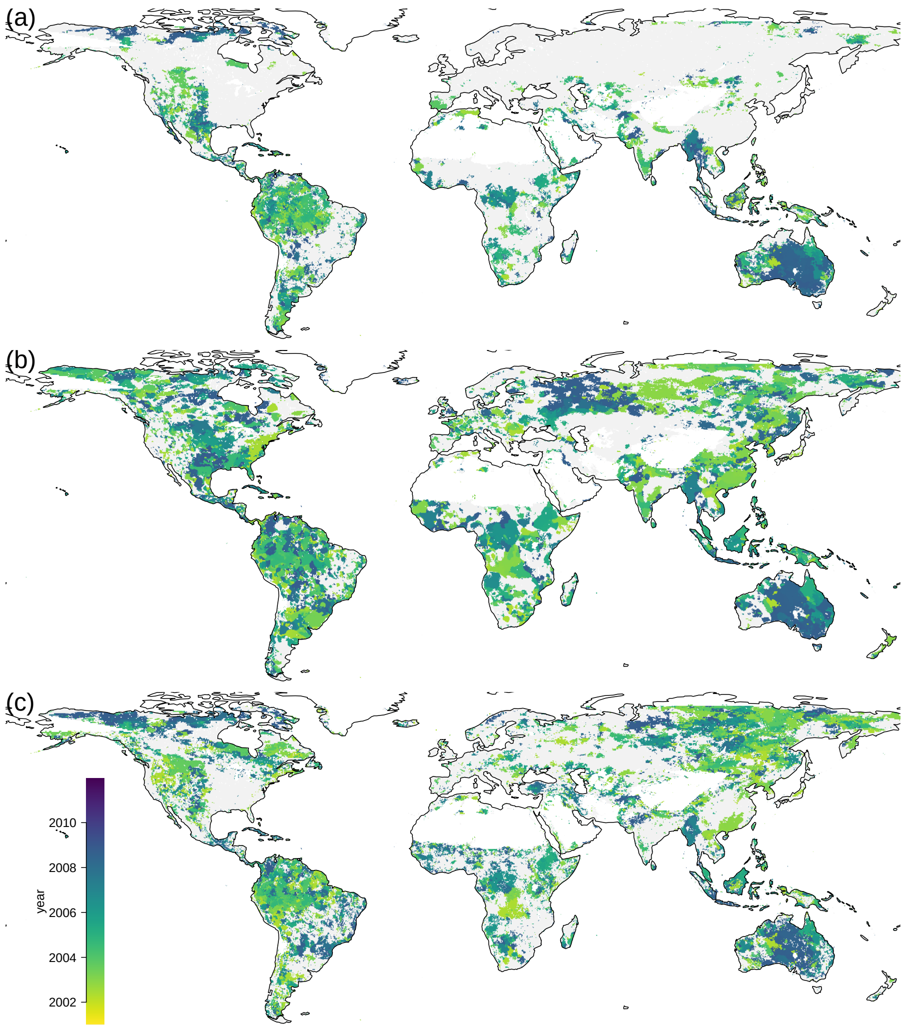

Figure F1. Breakpoint detection, (a) on PC_1, (b) on PC_2, and (c) on PC_3, the color indicates the year of the biggest breakpoint if a significant breakpoint was found, grey if there was no significant breakpoint found.

As the environmental conditions change, due to climate change and human intervention, the local ecosystems may change gradually or abruptly. Detecting these changes is very important for monitoring the impact of climate change and land use change onto the ecosystems. We applied breakpoint detection on the trajectories (fig. F1).

Breakpoints on the first component were found in the entire Amazon and the largest breakpoint is dated in the year 2005 during the large drought event. The entire eastern part of Australia shows its largest breakpoint towards the end of the time series because of a La Niña event, which caused lower temperatures and higher rainfall than usual during the years 2010 and 2011.

Author contributions. GK and MDM designed the study in collaboration with MR and GCV. GK conducted the analysis and wrote the manuscript with contributions from all co-authors.

Competing interests. The authors declare that they have no conflict of interest.

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