Reply to Referee #2

Dear reviewer,

We strongly appreciate your positive feedback and constructive comments that help to substantially improve our study. Our detailed responses to each of your suggestions were attached and we hope these would be helpful to solve your concerns. All comments are given in black and responses are shown in blue text.

Author and Co-authors

COMMENTS FROM REVIEWER #2

With great interest, I have read and reviewed the manuscript by Wang et al. This manuscript explores the joint evolution and causal interactions within eco-hydrological systems by introducing a comprehensive framework that integrates correlation relationships, causality analysis, together with satellite data and in-situ observations. Eight subregions of the Yellow River Basin (YRB) that I am interested in are used as cases for study. Correlations between ecological and hydrological subsystems are found to be decoupled in downstream areas, with the underlying causes investigated through causality analysis and attributed to various human activities. In addition, factors such as climatic forcing are found to create spurious relationships between eco-hydrological variables.

To my opinion, the study presents a promising framework and provides some interesting insights on eco-hydrological interactions in the YRB. The topic of the paper is timely and relevant to the readership of this journal. My recommendation is to be accepted after the following points are revised.

Reply: Thank you again for your time and effort in reviewing our manuscript, as well as for your valuable suggestions for improvement.

Major comments:

(1) One critical issue is that the description of some technical terms is difficult to understand, such as modularity and the degree of synchronization (Section 2.2.2). An explanation in the form of a diagram would make the terms clearer. A schematic diagram of the causal discovery process (Section 2.3) is also suggested to improve the readability of the corresponding texts.

Reply: Thank you for pointing this out. Some terms and the methodology regarding causal discovery were not clearly illustrated. **In the revised manuscript, we have added the schematic diagrams describing the network metrics (i.e., modularity and degree of synchronization)** to the flowchart. The improved Figure 1 is shown below:

Figure 1. (a) Conceptual diagram of eco-hydrological processes in a basin. (b) Flowchart of the study. Blue circles represent variables of hydrological subsystem and green circles represent variables of ecological subsystem. Blue lines stand for connections between hydrological variables, green lines are connections between ecological variables, and the red lines indicate connections between hydrological and ecological variables.

In addition, to better illustrate the causal discovery process in Section 2.3, we have added more information to Figure 2. The detailed information is shown below:

Figure 2. Overview of the causality analysis. (a) An example to illustrate causality, where a lagged variable X^4 ^{*t-1*} (the brown square) is said to be a cause of X^1 ^t (the brown circle) if X^4 ^{t-1} has a significant dependence or predictive power over X^I , while removing the effect of all other potential variables influencing X^4 _{t-1} or X^1 , except X^4 _{t-1} (the yellow squares). (b) Four types of assumptions can be used to construct physically possible and plausible links. τ_{max} means the maximum lag time. (c) Physically possible and plausible links between the included eco-hydrological variables in PCMCI. PCMCI will test shown links for significant causality and yield the final causal network as a subset of this. SMSA=soil moisture storage anomalies; GWSA=groundwater storage anomalies; R=regional runoff; SL= regional sediment loads; SCA= snow cover area; NDVI=normalized difference vegetation index; GPP=gross primary productivity; WUE=ecosystem water use efficiency; ET=actual evapotranspiration; P=precipitation; T=temperature; RSC=reservoir storage change; WW=water withdrawals.

(2) Further analysis and discussion of the results would be good (especially in Sections 5.1.1 and 5.1.2). There are many studies focusing on the ecohydrological processes in the YRB, more comparisons with these studies are suggested to increase the reliability of the results. In addition, are there any other cases that illustrate such confounding issues in Section 5.1.1?

Reply: Thank you for your comments. As suggested, we have added more comparisons with other studies in Sections 5.1.1 and 5.1.2 to make the discussion more thorough. **Section 5.1.1 focuses on the discussion of common drivers such as climatic forcing, and other cases illustrating such confounding issues have been complemented. The revised texts are as follows:**

"Similarly, Bonotto et al. (2022) found that streamflow and groundwater were forced by rainfall and potential evapotranspiration, and hence the identified causal links might be the result of a third (or more) strong common forcing when identifying causal links by using CCM. A synthetic study showed that streamflow and subsurface flow could always exhibit CCM convergence due to the common meteorological forcing (Delforge et al., 2022).

Our study also presented a good example to illustrate this. The source region of the YRB (Region I) experienced a warmer and wetter climate in the past decades (Wang et al., 2018b), and most ecohydrological variables (except GWSA and WUE) exhibited a joint increase. Results showed that the increasing T had minor influences on the hydrological subsystem. This is due to the relatively small proportion of snow and glaciers (about 6% of the area; Table S2) and the insignificant contribution of the frozen-ground thawing process to soil moisture and runoff during the growing season (Qin et al., 2017; Yang et al., 2023). However, T was important for maintaining vegetation growth and physiological activity, and similar results can also be found in Bo et al. (2022). P dominated the evolution of hydrological components and Li et al. (2024) also reported that P exerted the greatest impact on terrestrial water storage, soil moisture, and snowmelt water in the source region."

In Section 5.1.2, we focus on discussing the potential impacts of human activities on asynchronous evolution trends in hydrological and ecological subsystems. The revised texts are as follows:

"The increase in regional P may also lead to increased SMSA, largely due to enhanced landatmosphere interactions that accelerate local moisture recycling following revegetation (Zhang et al., 2022b). In Regions III and IV (mainly grassland), we found positive GPP (NDVI)→SMSA effects with a delay of 1 month. That is to say, although revegetation leads to water consumption from the soil (Lv et al., 2019; Ge et al., 2020; Li et al., 2020; Zhao et al., 2022), it is potentially beneficial to soil water storage in turn. Wang et al. (2024) also concluded that revegetation had a notably positive impact on root zone soil moisture and terrestrial water storage in the upstream grasslands. In this case, the overall evolution trends of SMSA and GPP/NDVI showed similar upward trends in these regions.

On the other hand, revegetation was found to have significant adverse impacts on SMSA in Regions V-VII (Figure 6), which was consistent with Cao et al. (2022). This was evidenced by the negative GPP/NDVI→SMSA links with a lag of 3 months, which were more significant than the positive lagged links from GPP to SMSA. These regions are mainly croplands and forests, having a greater impact on water consumption than grasses due to higher canopy covers and more developed rooting systems (Zhang et al., 2022b)."

(3) Although the authors have stated the importance of proposed approaches, more discussion on this is suggested. Eco-hydrological/hydrological models also analyze eco-hydrological interactions, so what are the advantages of your methods over physically-based models? It is promising that "such findings are important to understand the general watershed functioning and could further guide the development of more accurate and region-specific eco-hydrological models (lines 534-535)", and I think it would be better to give more explanations.

Reply: Thank you for raising this important point. We fully agree that eco-hydrological models also play a fundamental role in understanding relevant processes of the system or subsystem.

Models are based partly on differential equations representing known processes and partly on semiempirical relationships representing unknown processes or approximating known processes (Runge et al., 2019). However, models have uncertainties when simulating internal fluxes/states (Kelleher et al., 2017). Sometimes a model may fit the descriptive statistics of the observational data (e.g., GPP) well. Still, the model may not simulate the physical mechanisms affecting GPP well due to multiple model formulations and parameterizations, even if incorrect, may fit the observations equally well. In addition, many models cannot account for human activities, and how to parameterize various human activities in a model is a problem (Tursun et al., 2024).

Hence, compared to the physically-based models, the advantages of our approach are summarized as follows. (1) Inferring causal relationships based on observations is more directly linked to physical processes, avoiding the large uncertainties in physical mechanisms raised from model structure deficiencies and equifinality in parameterizations. (2) According to different research objectives and available data, our approach is more convenient and more flexible in selecting variables and time scales to study. (3) Our approach better incorporates processes that are difficult to consider in eco-hydrological models (e.g. human activities).

We see causality analysis through our approach as a tool to understand the overall functioning of the watershed and provide complementary information to guide the establishment of ecohydrological models. Models contain several formulations based on "causal assumptions" by developers, and the models that are causally similar to observations (i.e., our causality results) may yield more reliable future projections (Runge et al., 2019). For example, in the area where snowmelt contributes significantly to runoff, a snowmelt module considering the accurate influencing time is required in the model. In places where groundwater contributes greatly to the upper soil layers and the water uptake by roots, modules regarding groundwater and soil water movement should be considered carefully. On the other hand, we have to acknowledge that we cannot observe everything, everywhere, or all the time. Therefore, we promote the use of observations and models together in the future to more formally address the perceptions of causality in hydrology. This will allow us to test our assumptions about eco-hydrological interactions and better prepare for a wide range of possible futures. As suggested, the relevant content will be added in the Discussion section in the revised manuscript.

(4) Occasional grammatical errors should be checked and corrected.

Reply: Thank you! We will carefully check the text and correct the errors.

Minor comments:

(1) Lines 24-27 - It would be better to expand the introduction of eco-hydrological systems and internal interactions with more information.

Reply: As suggested, we have added more introduction to this and rephrased the first paragraph. The detailed information is as follows:

"The hydrosphere and biosphere are intrinsically coupled subsystems of the Earth. Hydrological conditions shape the distribution, structure, and function of terrestrial ecosystems, which, in turn, affect the hydrological components via modulations of land-atmosphere water and energy fluxes (Pappas et al., 2017). Hence, eco-hydrological systems are complex with time-dependent interactions occurring between and within the atmosphere, vegetation, soil, and water bodies (Yan et al., 2023). These interactions contain intensifying and mitigating mechanisms, e.g., vegetation coverage can be enhanced by warmer temperatures, increased water availability, and afforestation, and can be further reduced by the decrease of water storage through root uptake. Together, these interactions among multiple components dictate a collective behavior of the eco-hydrological system (Goodwell et al., 2018). In the context of climate change and increasing human activities, eco-hydrological processes have undergone substantial changes. Therefore, it is a pressing need for a comprehensive understanding of how the system behaves (phenomenon) and unravelling the multivariate interactions (mechanisms) that drive such behaviors at the system level."

(2) Lines 85-87 - More emphasis should be placed on the reason for using the YRB as the study area. **Reply:** Thanks for your comment. We use the Yellow River basin (YRB) in China due to the following reasons: (1) The YRB is an important ecological corridor, hosting more than 12% of population and creates about 14% of GDP of China. (2) The YRB has a vast area with different climatic conditions, land use types, and human disturbances, providing various types of eco-hydrological regimes for investigation. (3) The YRB has undergone significant changes in eco-hydrological processes due to climate change and intensive human activities. Hence, there is a need to investigate the exhibited evolution trends and the internal mechanisms in such eco-hydrological systems.

As suggested, we will explain the reasons in a brief way in the revised manuscript.

(3) Line 88 - A short presentation of the structure of the paper would be good here.

Reply: Thanks for the suggestion. A short presentation of the structure of the paper will be added in the last paragraph of Introduction. The detailed information is as follows:

"The study is structured as follows. Section 2 describes the framework developed. Section 3 introduces the study area and the data used. Section 4 presents the results for each subregion of the YRB, followed by a discussion of the findings in Section 5, including the significance of the study, comparisons with previous studies, and limitations. Finally, some conclusions are drawn in Section 6."

(4) Lines 125-126 - I think the threshold has a significant influence on the construction of the network.

How would the network and clustered modules change if you used a different threshold?

Reply: Yes, we fully agree with your comment that the threshold could influence the construction of the network. For comparison, Pearson's correlation coefficient (PCC)>0.4 and PCC>0.5 are also used as thresholds here. Although the existence of some links changes when different thresholds are used, the conclusions of the study remain unchanged. Overall, from the upper to the lower reaches, the modularity (M value) of the synchronous relationships increases (except for the downstream area) and the synchronization between the ecological and hydrological subsystems generally (S value) decreases.

Figure R1. Synchronous networks and corresponding clustered modules (when PCC>0.4).

Figure R2. Synchronous networks and corresponding clustered modules (when PCC>0.5).

(5) Figure 2 - In terms of physically possible and plausible links, there is a connection between soil water storage (SMSA) and gross primary productivity (GPP), but not between soil water storage (SMSA) and normalized difference vegetation index (NDVI). Why is this?

Reply: In this study, NDVI represents vegetation coverage (i.e., the land surface condition) and GPP represents the physiological activity of vegetation. We assume the physically possible and plausible links based on Poppe Terán et al. (2023), i.e., enhanced photosynthesis (GPP) is directly supported by water supply from soil (SMSA) and contributes to the active growth of plants (NDVI). However, increased vegetation coverage (NDVI) in turn consumes water (SMSA) through physiological activity (GPP). Therefore, it is assumed that the relationship between NDVI and SMSA is mediated by the variable GPP and is considered to be a spurious causal relationship. In the revised manuscript, we will make an explanation for this.

(6) Lines 201-202 - "PCMCI tests possible links and provides the final results as a subset of the total possible network……" However, in Figure 6, there are lines between SMSA and NDVI, as well as between GWSA and GPP (although you have defined them as spurious ones). It seems that the links beyond your hypothesis are also tested. Please check if the expression here is correct.

Reply: Thank you for making us notice. Our previous expression was inappropriate.

In this study, we mainly use three types of link assumptions, they are: (1) the link from variable X^i to X^{j} at some time lags (or contemporaneous) may exist, and its direction is specified; (2) the link from variable X^i to X^j at some time lags may exist, but its direction is not specified (the direction is then given by the time order); and (3) the link that is "physically impossible" to have direct causality and is removed from the test.

As stated in the reply to Question (5), we assume the link between SMSA and NDVI to be spurious due to GPP. Similarly, soil moisture affects the physiological activities of vegetation directly, and we think that groundwater usually affects vegetation by supplying water to the upper soil layers, so here the relationships between GWSA and GPP are assumed to be spurious too. However, we did not remove them from the causality test as "physically impossible" links, but left them in default status as we found such "spurious links" sometimes could be helpful in illustrating eco-hydrological mechanisms. We will revise the description of this in the revised manuscript as suggested.

(7) Section 4.1 - The ecohydrological conditions of eight subregions are not clear enough to me. This may hinder the understanding of the underlying mechanisms in the following sections. Apart from trends, I would recommend describing the average conditions of the subregions in brief.

Reply: Thanks for your suggestions. We will clarify the average eco-hydrological conditions of each subregion before describing the trends of eco-hydrological variables. Some sentences will be reorganized to make this section more reader-friendly.

(8) Figure 4 - "A gray box denotes no data ……" However, grey and blue are difficult to distinguish

in Figures 4(d) and 4(h). In addition, Figure 4(h) lacks a ")", and the symbol "*" in Figure 4(i) is difficult to recognize.

Reply: Thank you for bringing the point to our attention. We have revised this Figure in the revised manuscript.

(9) Figures 5 and 6 - The resolution needs to be enhanced.

Reply: We have enhanced the resolution of these figures.

(10) Figure 6 - This figure is interesting and contains a large amount of information. To my best knowledge, the source region (subregion I) has frozen soil, yet temperature does not appear to significantly affect soil moisture. Could you explain this further?

Reply: Thank you for your comments. Seasonally frozen ground, sporadic permafrost, and predominantly continuous permafrost coexist in the source area of the YRB, and the spatial distribution of the frozen ground is diverse and complex (Song et al., 2024). However, it is difficult for us to obtain reliable frozen ground data, so the variable directly describing the frozen ground is not included in this study. The relationship between air temperature (T) and soil water storage (SMSA) may partially reflect the degradation of permafrost due to warmer climate and its potential impact on runoff. However, no significant causality between T and SMSA is captured in our case study, meaning that the increase in SMSA during the growing season (i.e. the thaw period) is mainly due to the contribution of precipitation (P). Similar results are found in Li et al. (2024). Meanwhile, previous studies have indicated that the effects of frozen ground degradation on soil moisture and runoff generally occur in winter in the source area of the YRB (Yang et al., 2023). The reduction in frozen ground depth has only a small positive effect on soil moisture in the growing season (Qin et al., 2017), because the soil ice content decreases and the soil liquid water content increases with increasing temperature, but this water can be quickly consumed by the evapotranspiration process.

As suggested, some explanations will be added in the Discussion of the revised manuscript.

(11) Lines 355-359 - "Instead, increased T (Figure S3) was the dominant factor stimulating GPP……" "Meanwhile, increased P (Figure S3) was the crucial driver of the increases in the hydrological subsystem……" To interpret the mechanisms clearer, I prefer to present the temperature and precipitation time series (or trends) in the main body of the manuscript.

Reply: Thank you! In the main body of the revised manuscript, we will include the figures on trends in P and T as suggested.

(12) Lines 375-377 - I think "essentially" here is strange. The sentence needs to be rephrased. **Reply:** Thank you! We have rewritten this sentence in the revised manuscript.

(13) Line 420 - I think "modest" here is not appropriate. The sentence needs to be rephrased. **Reply:** Thank you for the comment. We have rewritten this sentence in the revised manuscript.

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