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Explainable AI for water, energy and carbon cycle understanding

Presenter: Wei Shangguan
PhD. student: Feini Huang
Master student: Yongkun Zhang

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Water, energy, Carbon & Machine Learning

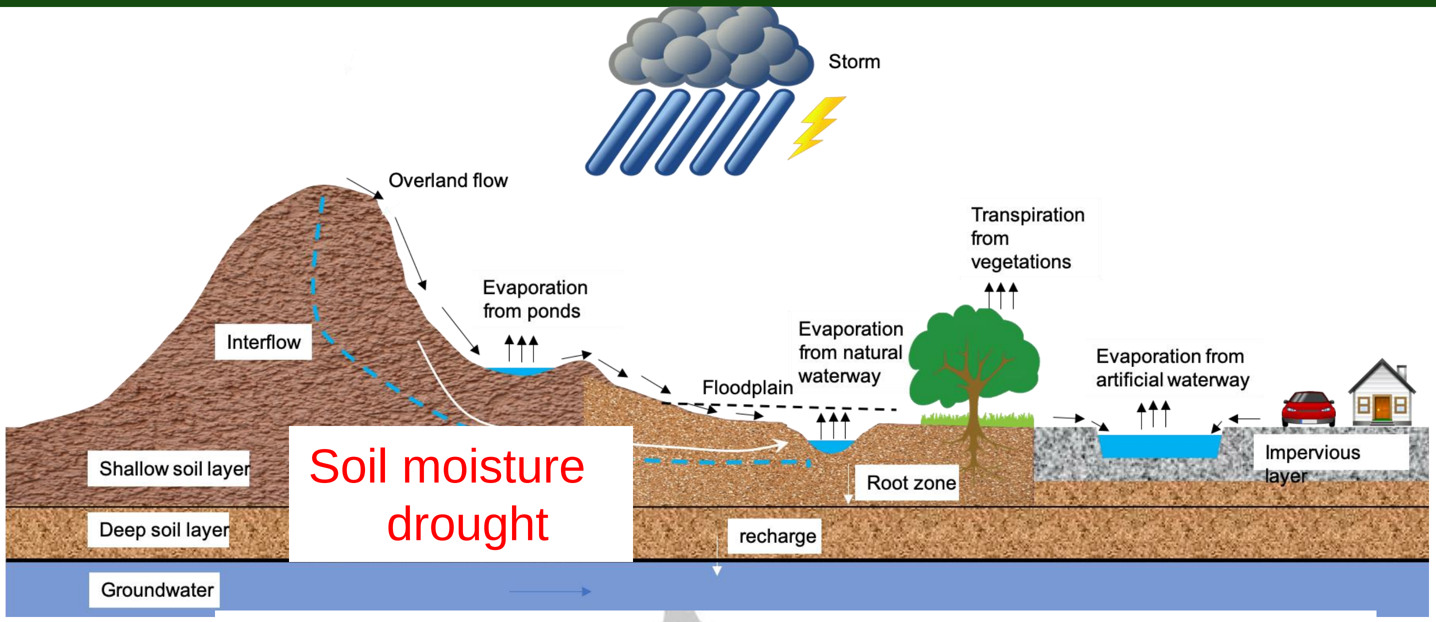
Machine learning has been widely applied to water, energy and carbon cycle.

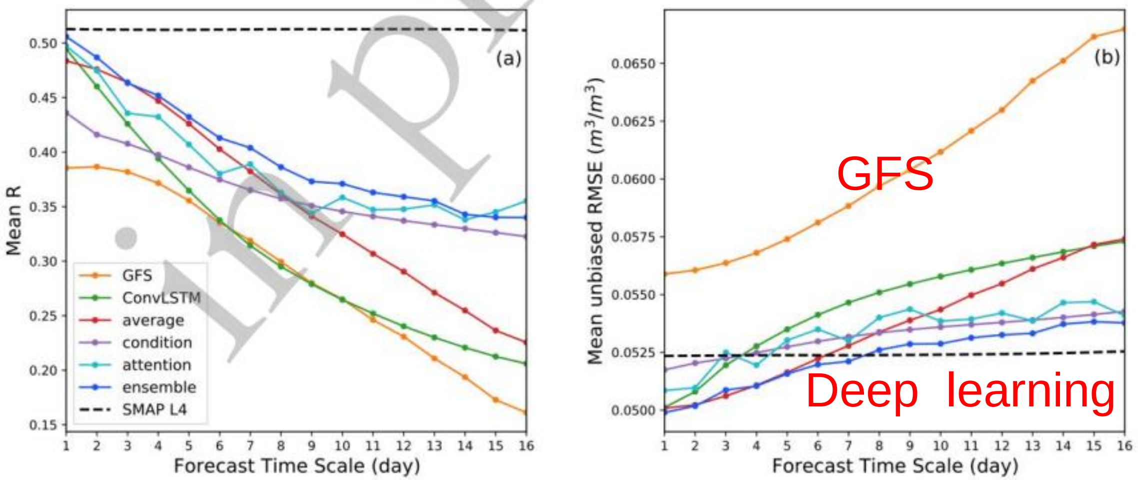
Soil water is an important component of the water cycle of the Earth System

Machine learning (ML., deep learning, DL) a powerful tool to predict water cycle.

In predicting soil moisture, machine learning has achieved an RMSE below 4%, according to various studies (1.4%~4%)[1-3].

Process-based model
Zhuo et al (2019) evaluate three land surface models: WRF-Noah, Noah-MP, CLM4
RMSE ranges from 6%~14%[4]





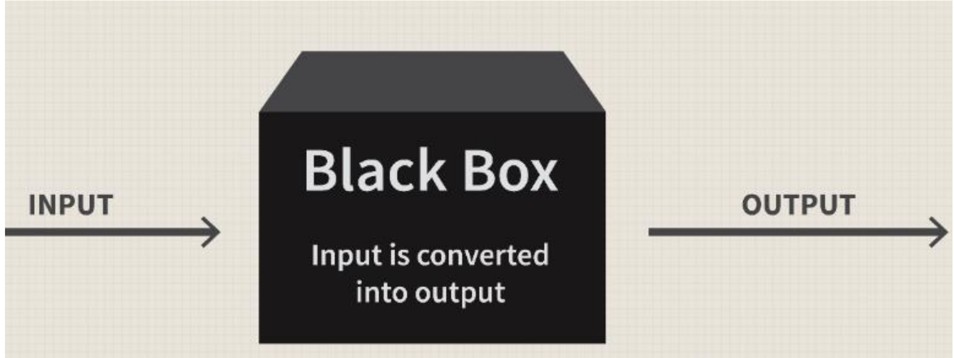
Li et al., 2023

[1] Fang, Kuai; Shen, Chaopeng; et al., 2017. Geophysical Research Letters, 44(21), 11,030–11,039.
[2] Zhang et al., 2023. Remote Sensing 15(2):366
[3] Li et al., 2023. Advances in Atmospheric Sciences, in press
[4] Zhuo, L, et al. 2019, Hydrol. Earth Syst. Sci., 23, 4199–4218

Blackbox Nature of Machine learning

We understand the algorithms, but we do not understand how the model arrives at a particular decision or prediction

Lack of Transparency



Effect

Users

- Difficulty in Trust and Adoption
  - •Users hesitate to trust and adopt ML models
- Challenges in Model Validation
  - •uncertainties about the model's generalizability and robustness

ML Modelers

- Model Troubleshooting and Improvement
- Potential for Bias and Unfairness
  - •difficult to identify and correct biases in training data

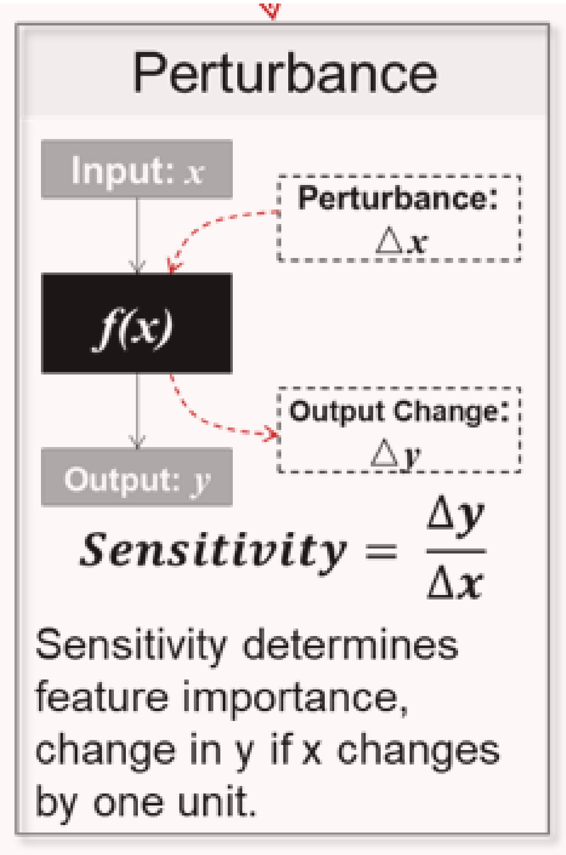
Domain Experts

- Communication with Domain Experts
  - •limit the model's utility and the integration of expert knowledge

Solution: Explainable AI (XAI)

- More transparent ML model
  - •e.g. Decision tree; White-box Transformer (Ma et al., 2023): Physical informed machine learning
- Methods to explain the decisions of ML
  - •e.g. Feature importance, SHapley Additive exPlanations (SHAP)

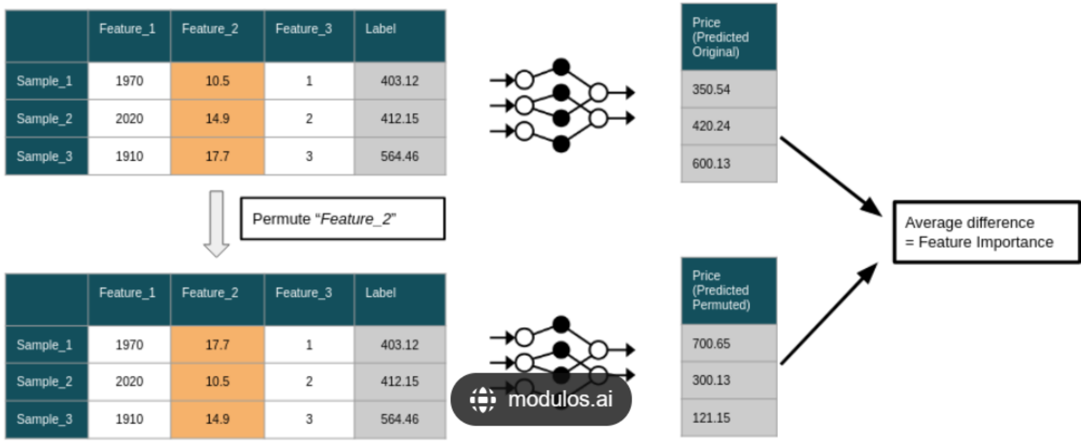
XAI- Perturbation-based method



Model-agnostic: any model

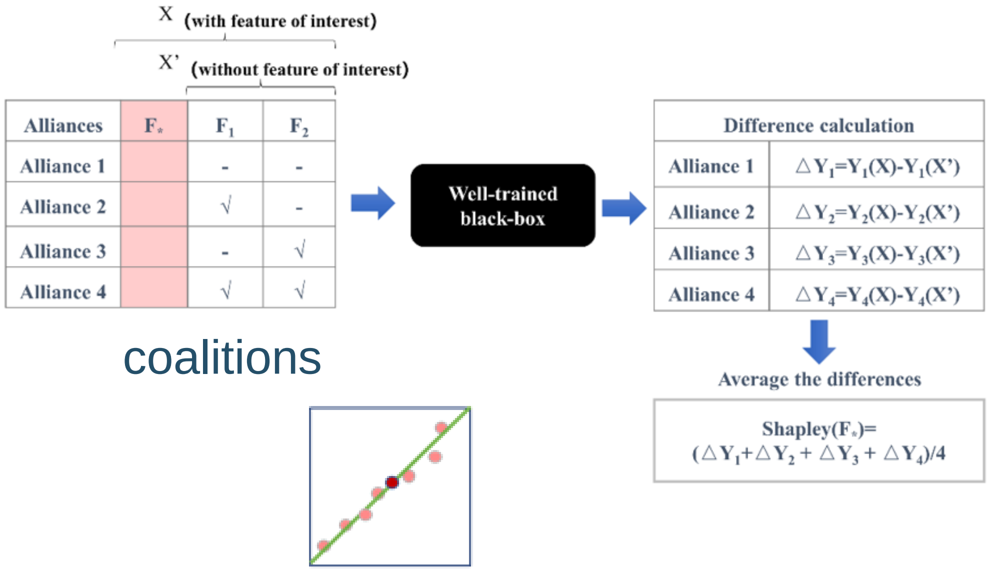
Permutation feature importance (PI)

Basic idea:
assess the impact of each feature on model performance by randomly altering the feature values across the dataset and observing the resultant changes in accuracy or performance.



SHapley Additive exPlanations (SHAP)

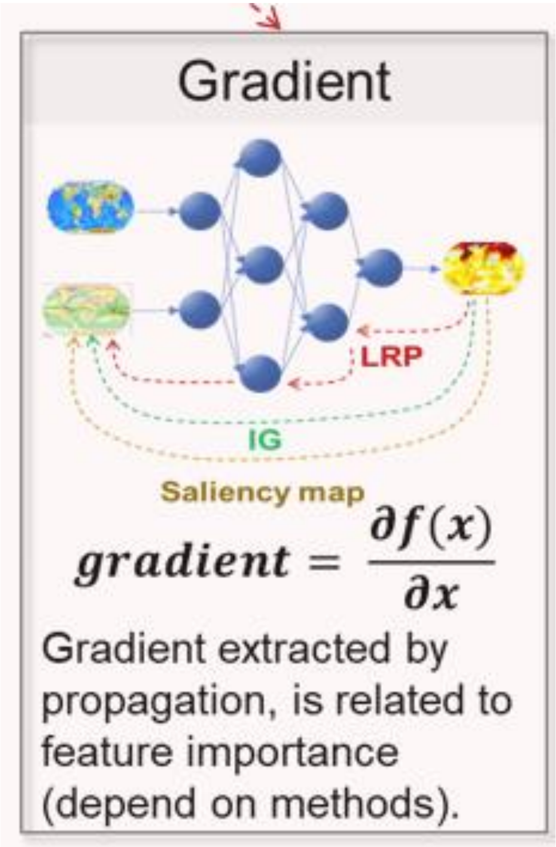
Basic idea: It connects optimal credit allocation with local explanations using the classic Shapley values from game theory and their related extensions



local linear regression

XAI-Gradient-based methods

Model-specific: neural networks



The smooth gradient (SG) method works as follows: first, some random noise is added to the input image, second, the pixel attribution is obtained by a saliency map of the noisy image, and third, the heatmap is averaged over multiple noisy images.

$$SG(x) = \frac{1}{n}\sum_{1}^{n} \frac{\partial F(x + \chi(0, \sigma^2))}{\partial x}$$

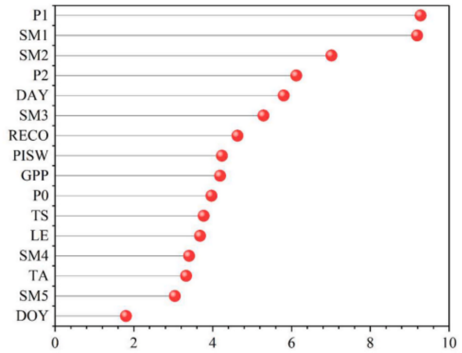
where x is the input in a neighborhood, n is the number of samples, χ is Gaussian noise with a standard deviation

Synergistic application of XAI methods

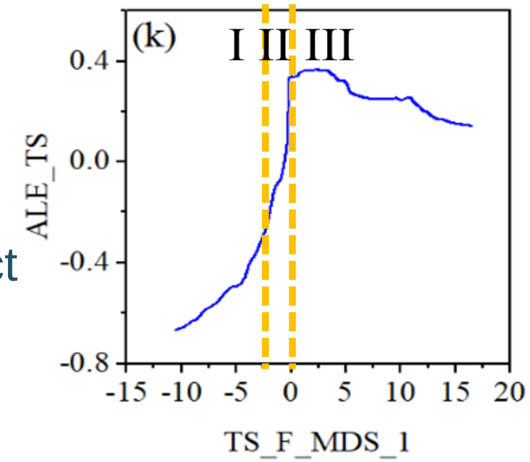
- XAI
  - Feature importance
    - global perturbation
      - Permutation importance
      - Tree-based importance
    - local perturbation
      - SHapley Additive exPlanations (SHAP)
      - Local Interpretable Model-Agnostic explanation (LIME)
  - Feature effect
    - Individual Conditional Expectation (ICE)
    - Partial Dependence Plot(ICE)
    - Accumulated Local Effect (ALE)
  - Pixel importance
    - Smooth Gradient (SG)

Three forms of interpretation

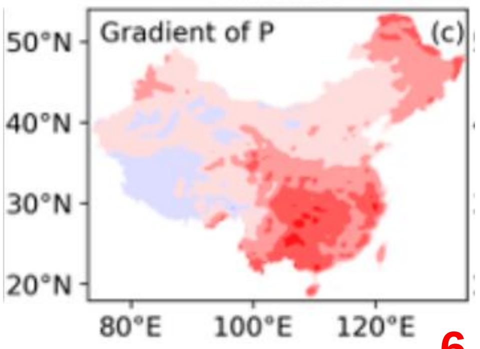
Importance plot



feature vs Its effect



Heat map



Synergistic application of XAI methods

Why use multiply XAI methods

1. Complementary Insights:

   --- diverse forms of interpretation provide a more comprehensive understanding

2. Validation of Explanations

   ---consistent explanations across different XAI methods increase confidence

3. Robustness to Method-Specific Assumptions

   ---reduce the risk of depending on a single method that may harbor biases or blind spots

Purpose of our studies

1. Understand the relationship and key drivers
2. Model validation and trust

   ---physical consistency. Or even improve model

3. Assess XAI methods

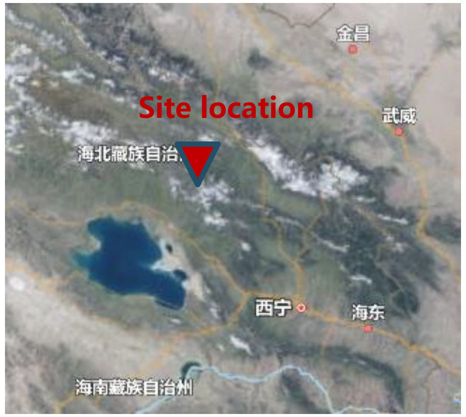
   --- which XAI method is better or more suitable for a specific case

1. Interpretations by XAI at a site

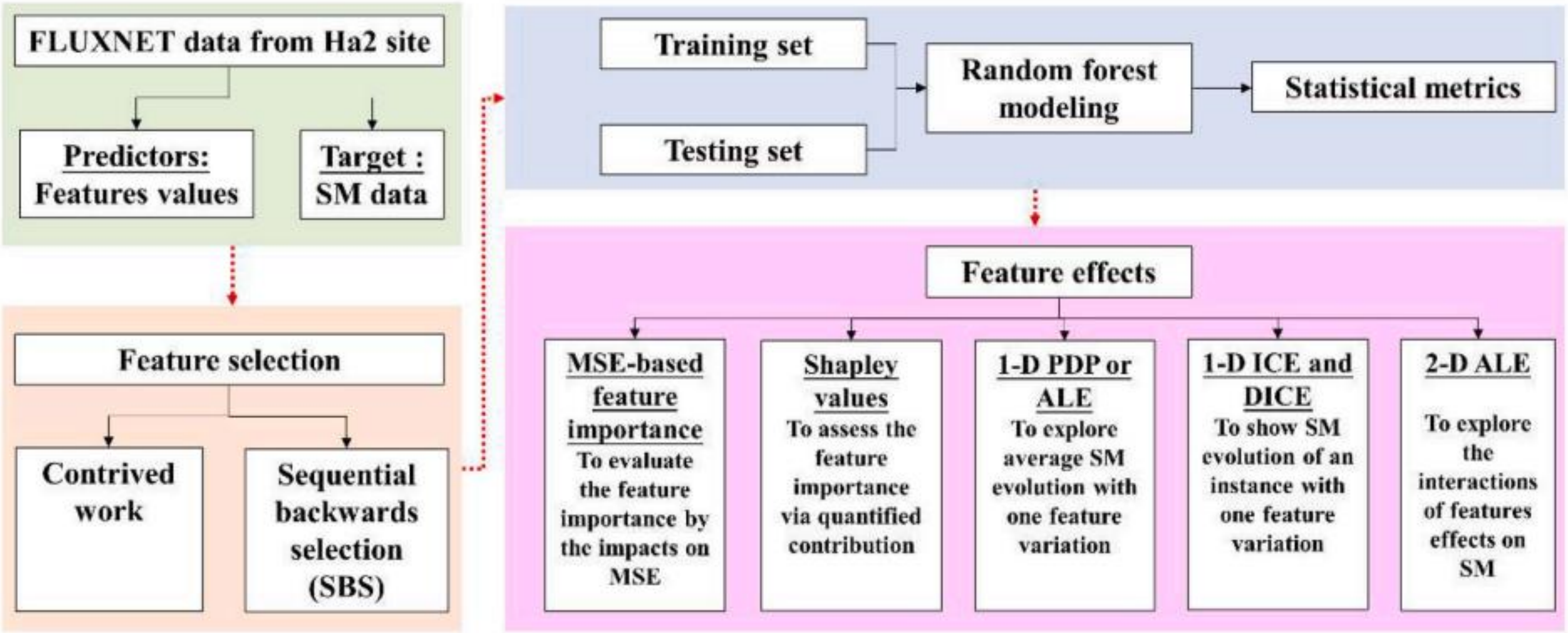
Contents lists available at ScienceDirect
Environmental Modelling and Software
journal homepage: www.elsevier.com/locate/envsoft

Beyond prediction: An integrated post-hoc approach to interpret complex model in hydrometeorology

Feini Huang [a], Wei Shangguan [a,*], Qingliang Li [b], Lu Li [a], Ye Zhang [a]

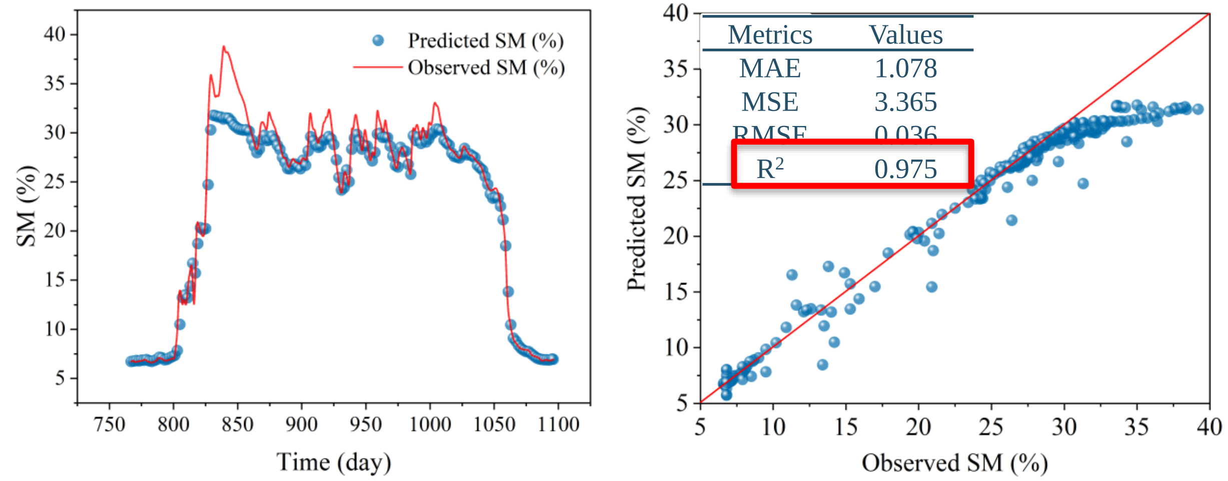


A toolbox named ExplainAI in python is provided with examples of hydrometeorology.



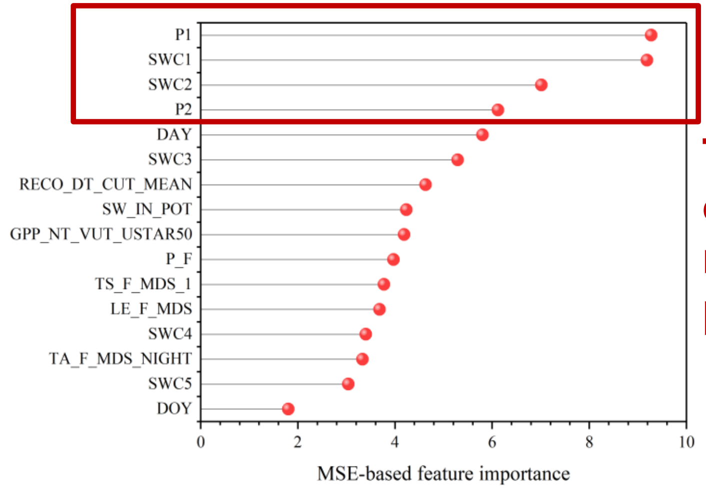
1. Interpretations by XAI at a site

Model performance



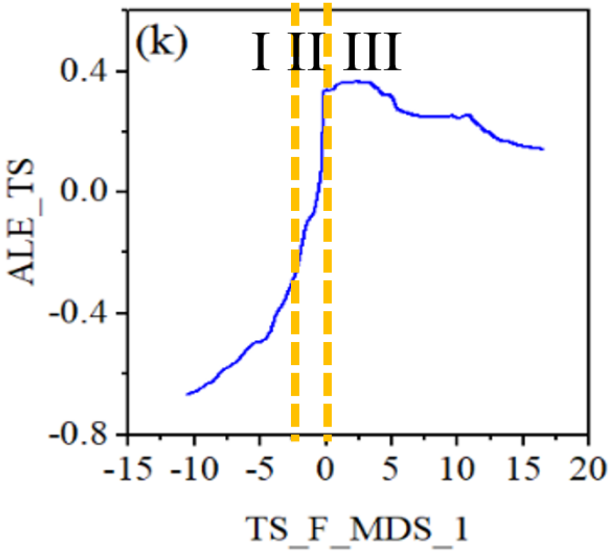
Predicted and observed soil moisture (2003-2005)

Feature Importance



The most important ones are lagged soil moisture and lagged precipitation

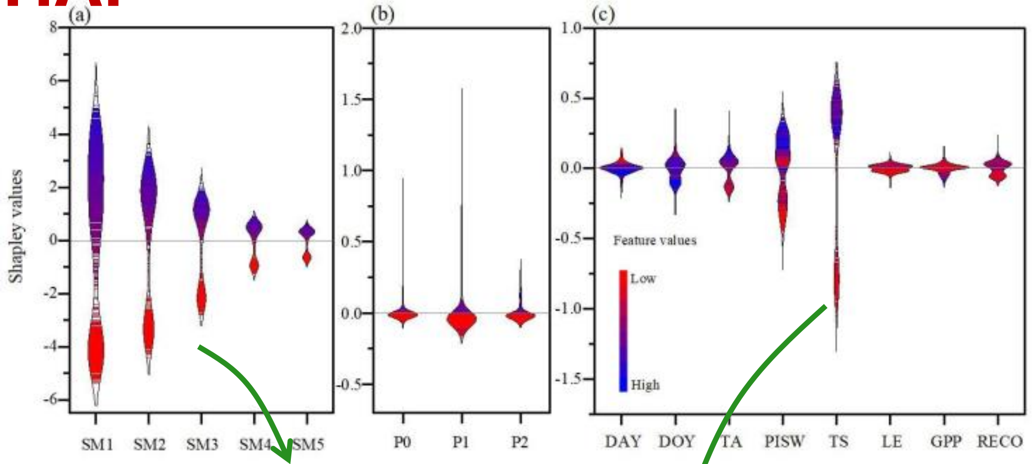
ALE



Three stages of the effect of soil temperature on SM:

- I: below -2℃, snow begins to melt
- II: around 0℃, with ongoing melting
- III: above 0℃, where postmelting, the soil dries out

SHAP



recent lagged soil moisture exerts a more substantial effect

When soil temperature is high, it has negative effect

2. Interpretations of soil moisture drought by XAI

ENVIRONMENTAL RESEARCH
LETTERS

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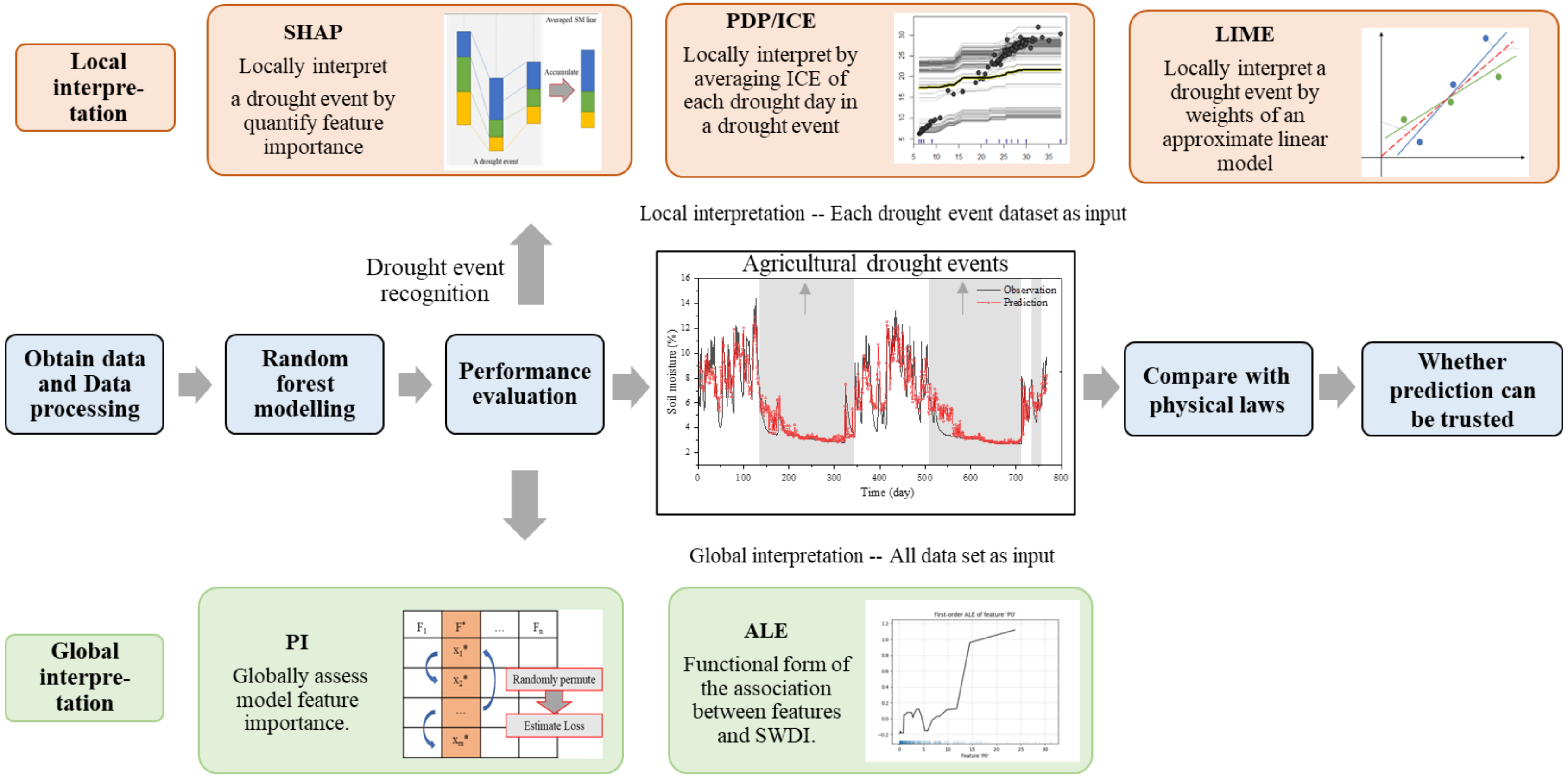
Towards interpreting machine learning models for predicting soil moisture droughts

Feini Huang[1], Yongkun Zhang[2], Ye Zhang[1], Wei Shangguan[1], Vahid Nourani[3], Qingliang Li[4] and Lu Li[5]

30 FLUXNET sites
for forest and grassland



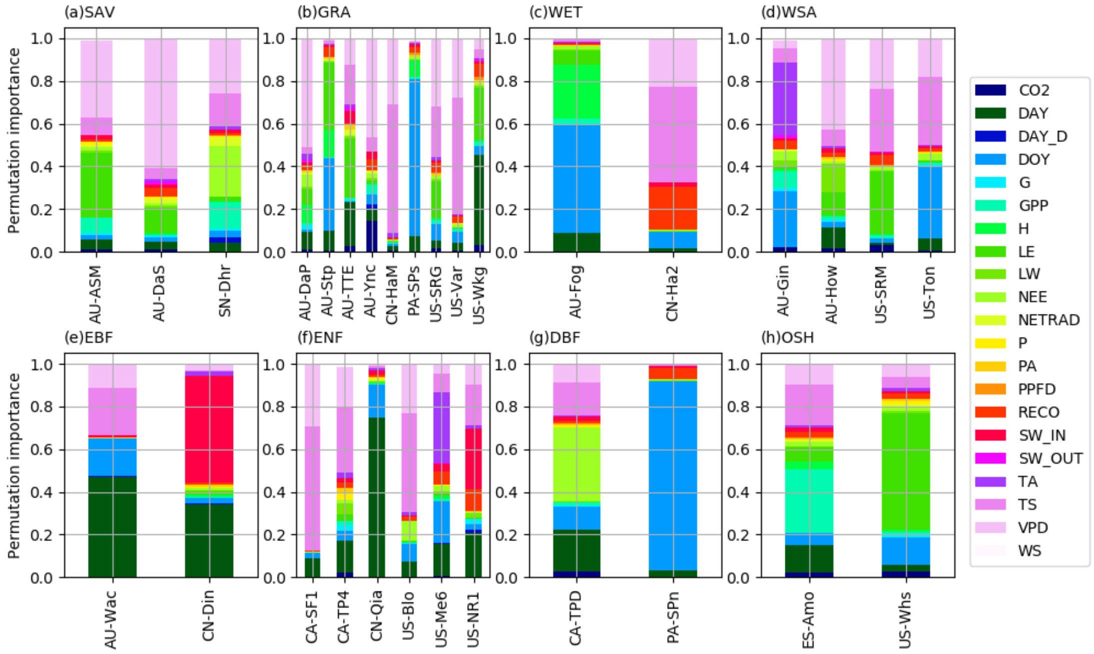
2. Interpretations of soil moisture drought by XAI

Model performance

RF model with R^2 0.6~0.95

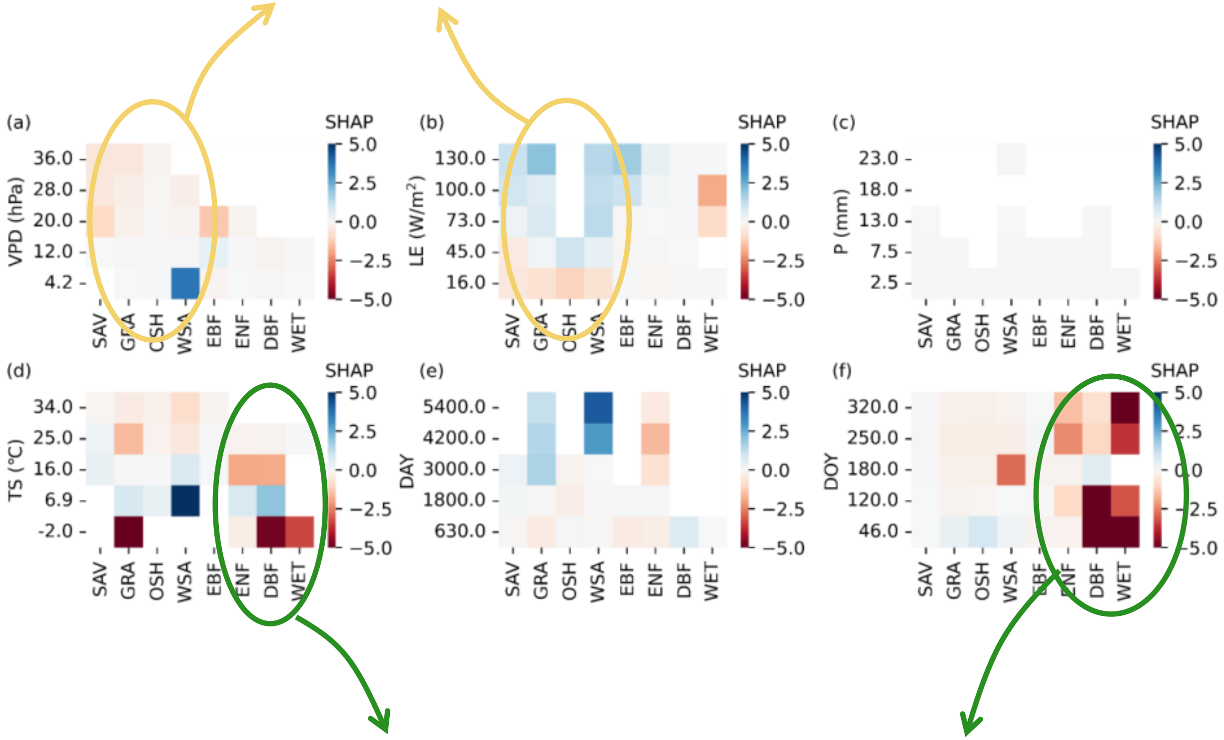
Permutation importance

VPD>TS(soil T)>DAY (Day of all years)>DOY



SHAP for extreme droughts

Grassland: Latent heat and VPD has lager effect



Forest: soil temperature and DOY has lager effect

3. Interpretations of spatial-temporal predictions by XAI

agriculture MDPI

Article

Interpreting Conv-LSTM for Spatio-Temporal Soil Moisture Prediction in China

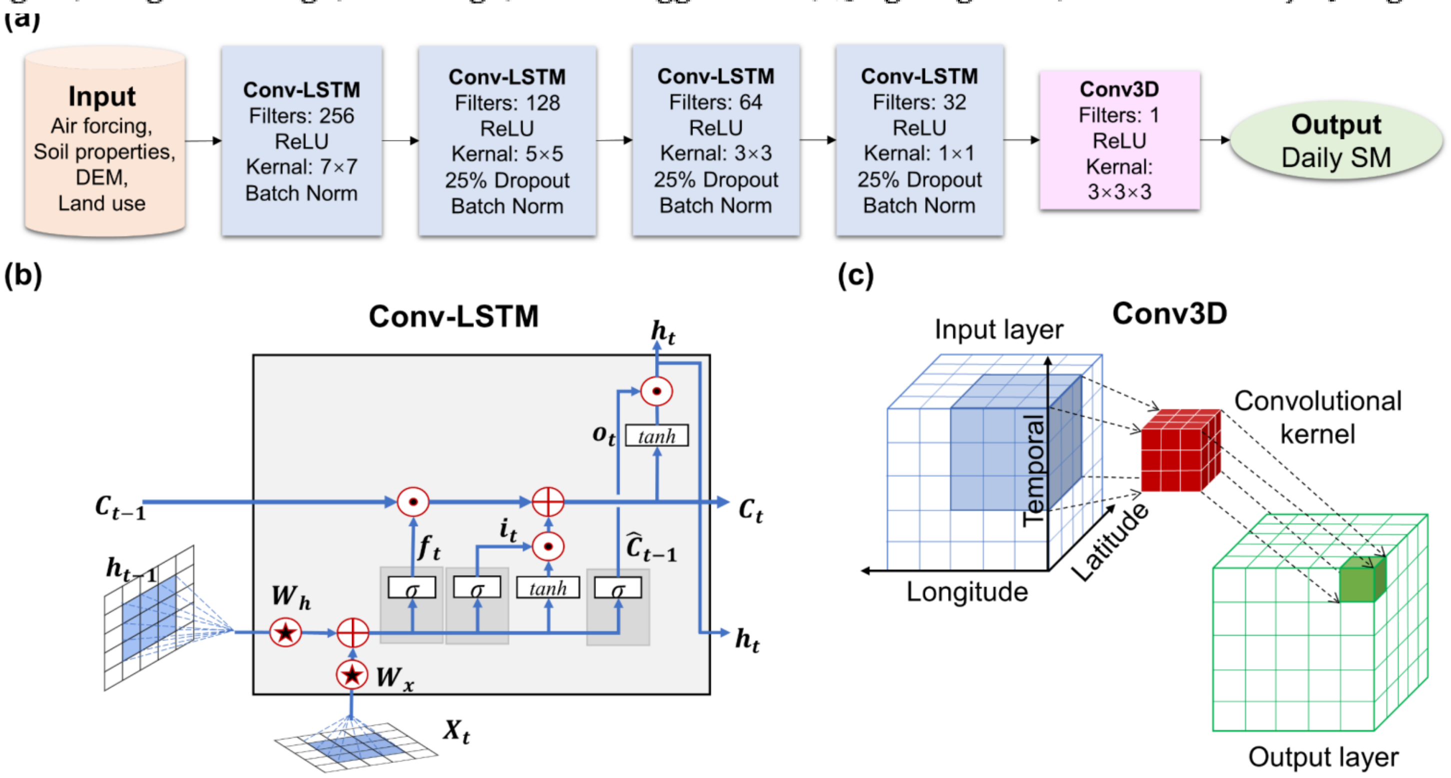
Feini Huang [1], Yongkun Zhang [2], Ye Zhang [1], Wei Shangguan [1,*], Qingliang Li [2], Lu Li [1] and Shijie Jiang [3]

Region: China

Data: ERA5-Land

Model: Conv-LSTM

XAI: PI, SG(smooth gradient)

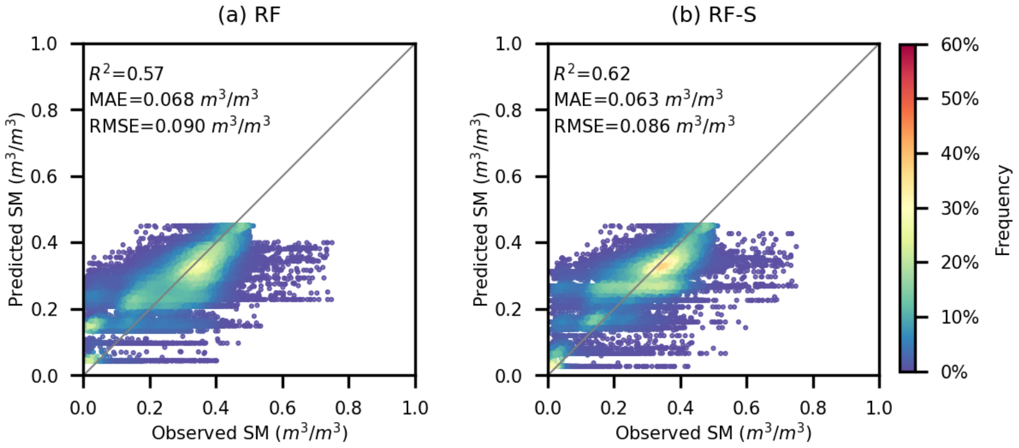


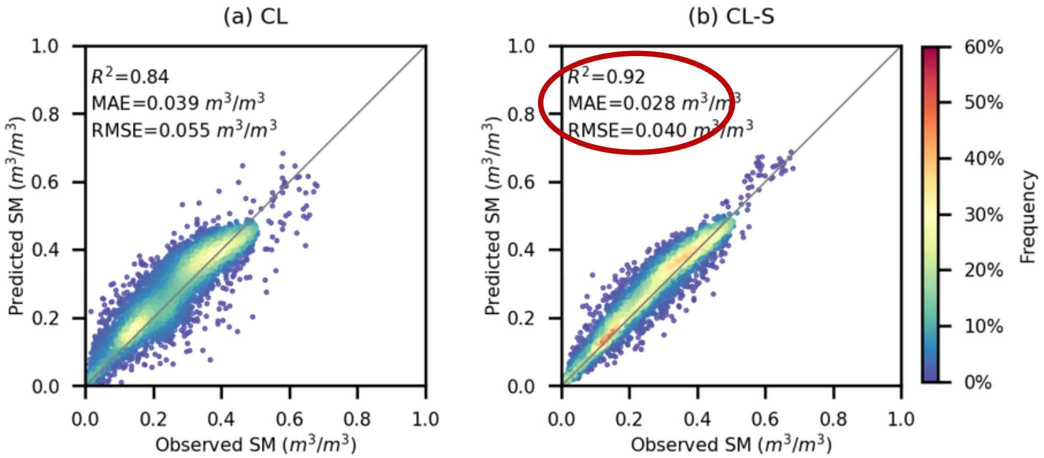
SG is the best XAI in correctly reflecting the relationships among the six:

SG, Saliency map (SA), square gradient (SqG), VarGrad (VG), integrated gradients (GI), gradient input (GI)

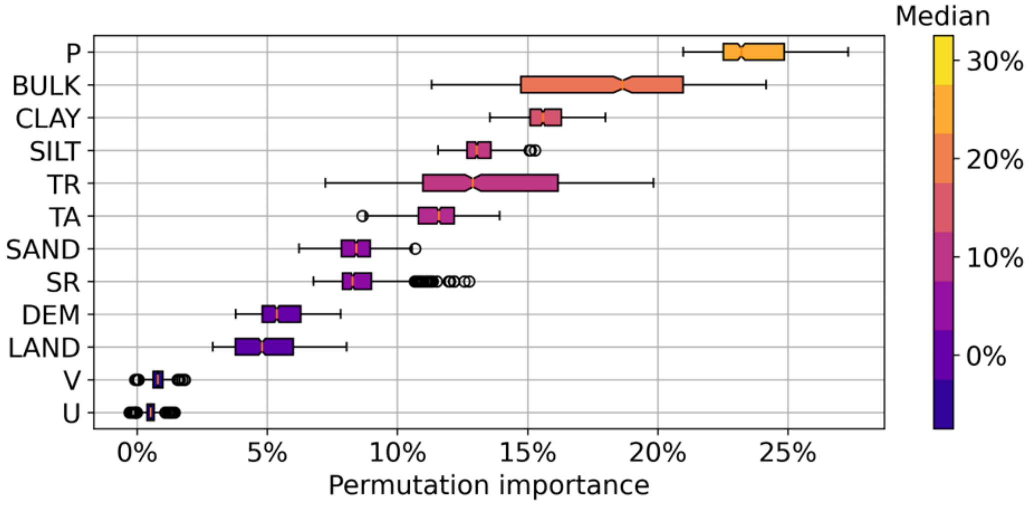
3. Interpretations of spatial-temporal predictions by XAI

Model performance

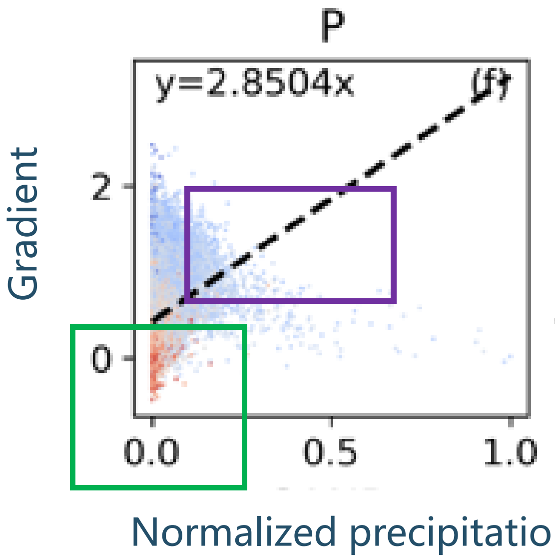




Permutation importance



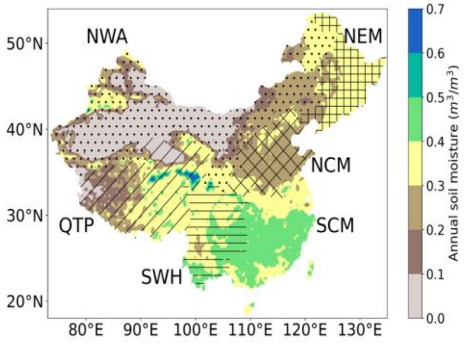
Gradient vs P

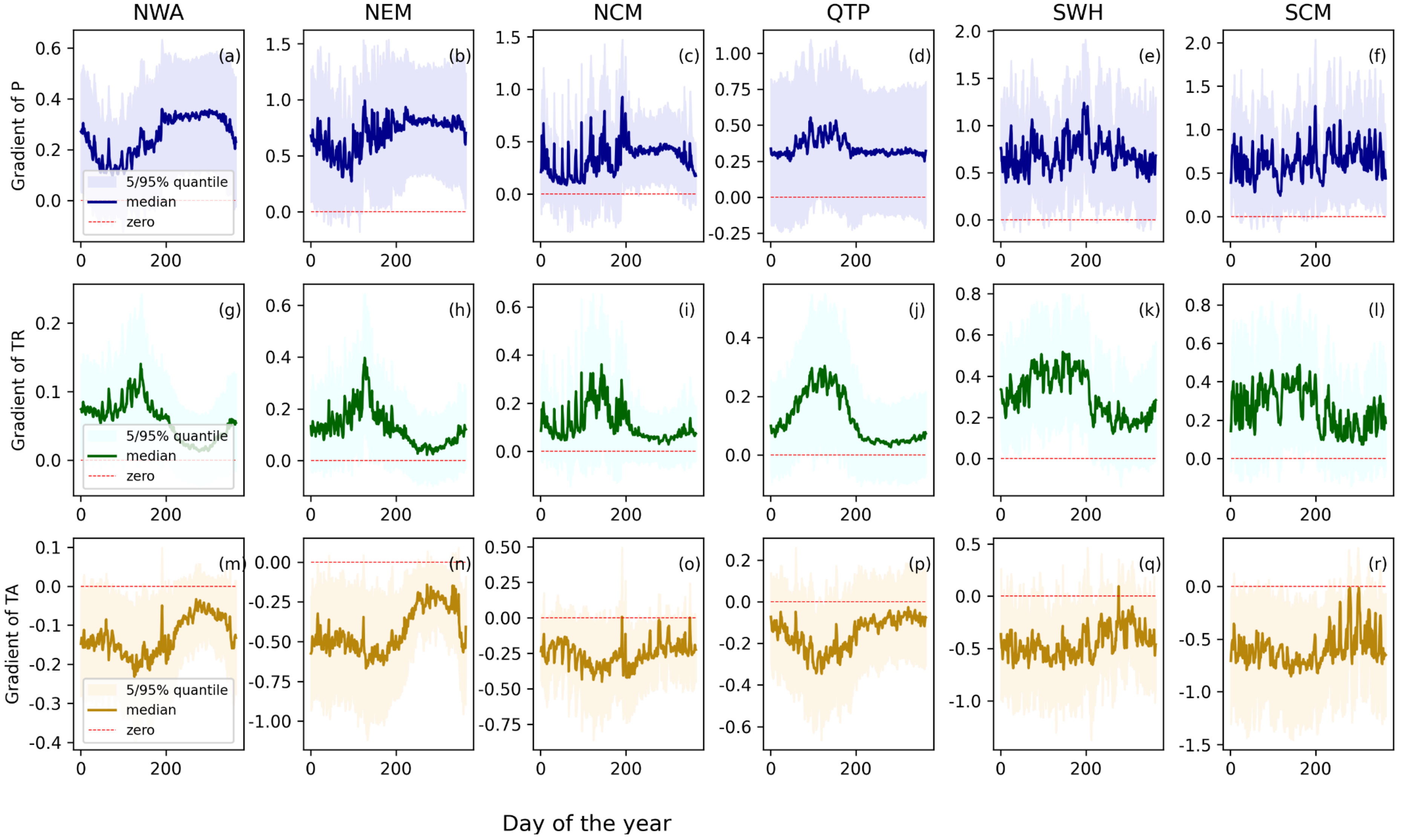


Precipitation (P)

- higher values correspo nded to a more substa ntial gradient effect, ali gning with physical exp ectations
- drier soils exhibited a l esser influence

Gradients of six regions





- drier regions exhibit more pronounced seasonality in gradient patterns
- wetter regions displayed higher gradient values

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XAI for Soil Organic Carbon: The Role of Carbon Fluxes

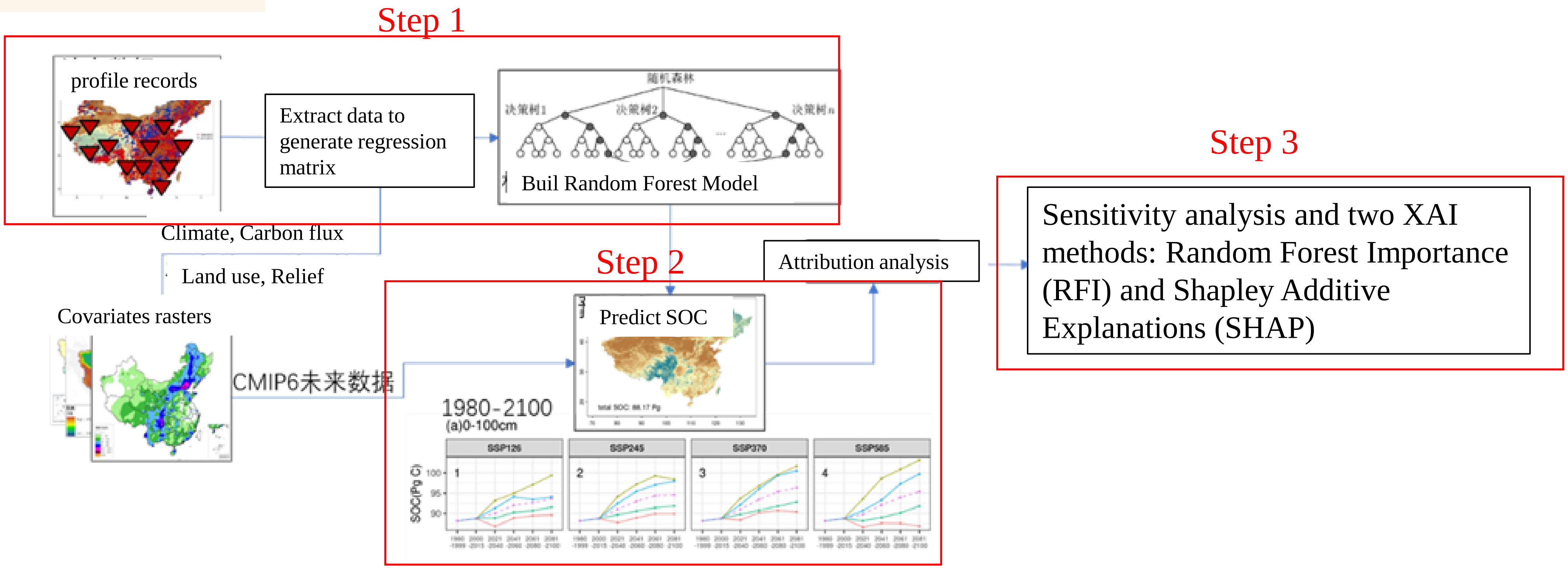
Scientific questions

(1)What degree of variation in SOC levels can be expected in China from 2021 to 2100 under multiple Shared Socioeconomic Pathways (SSPs)?

(2) What is the relative contribution of carbon fluxes to changes in SOC compared to the effect of climate change and land use change?

(3) How will carbon fluxes shape the trajectory of SOC in the future?

Methods



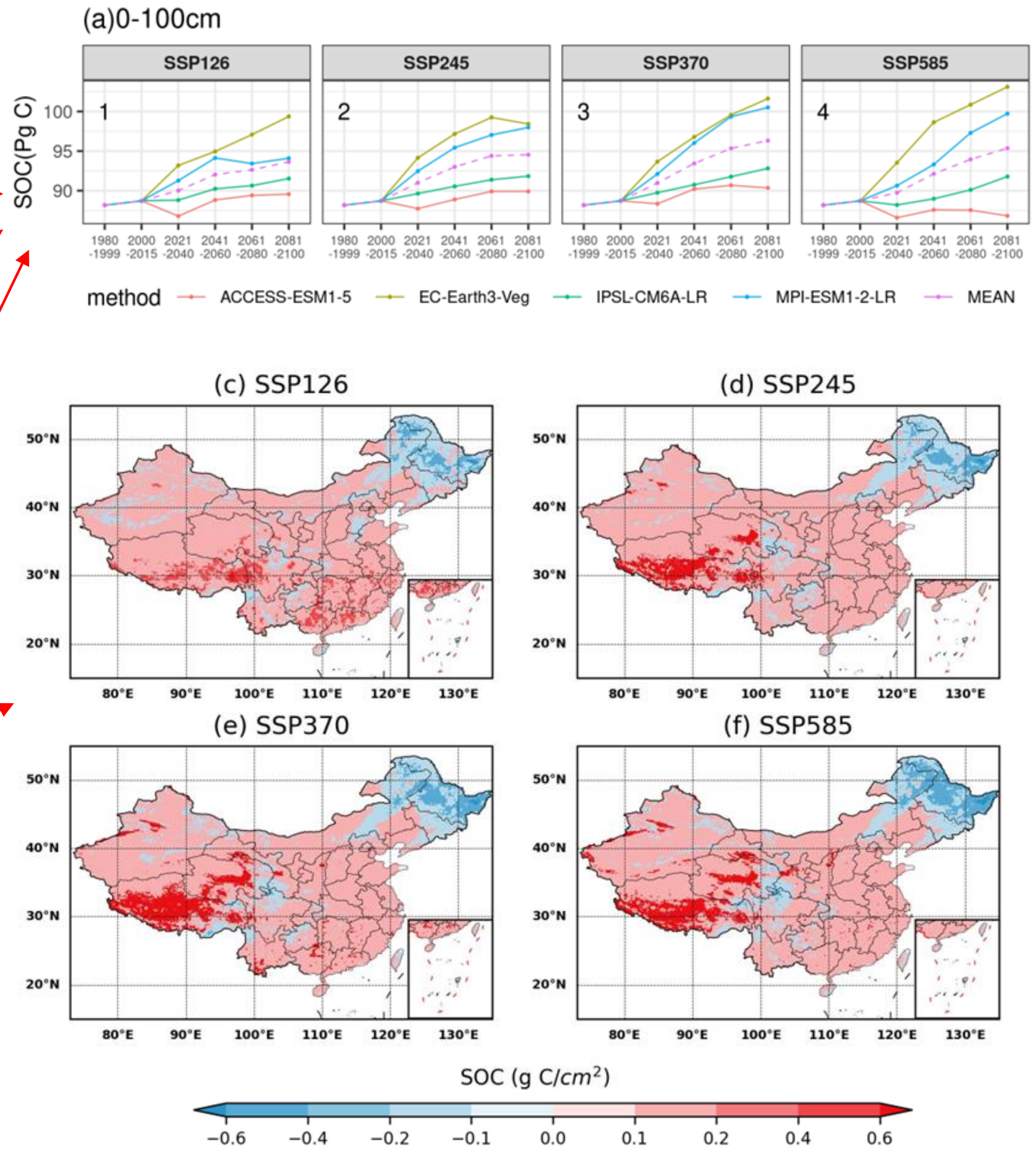
Step 1: A Random Forest model for SOC for spatial-temporal prediction is established using DSM.

Step 2: covariates for different periods are introduced to predict the SOC distributions at different times.

Step 3: An attribution analysis is conducted to explore how these variables influence the changes in SOC.

Results-Changes of SOC in future

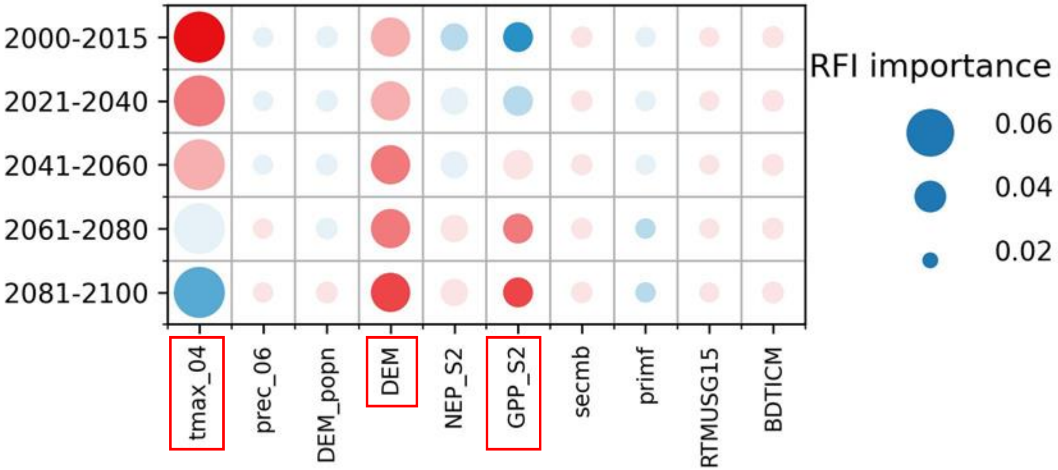
- In terms of total quantity, SOC shows an upward trend in the future.
- The differences between different ESMs data are quite obvious.
- In SSP370, the total amount of SOC rises more significantly.
- Most part of China increase, but Northwest decrease



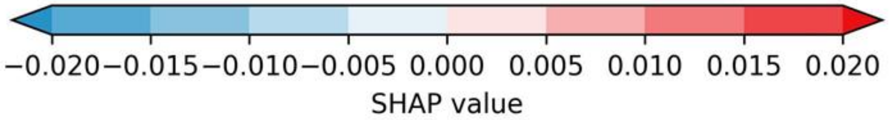
Analysis by XAI

GPP of summer (GPP_S2)

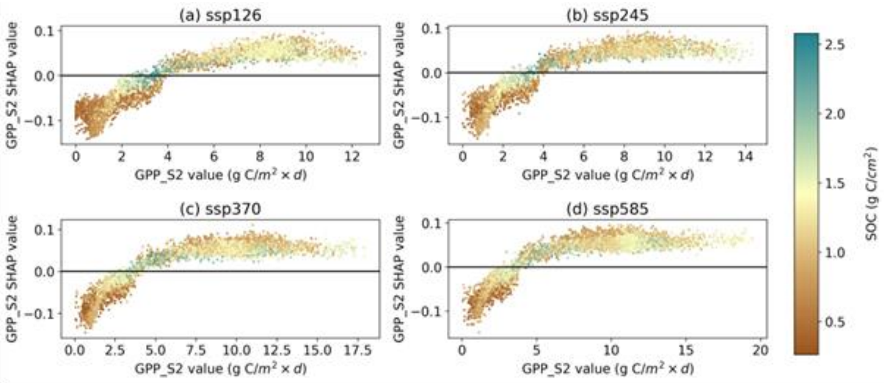
Shapley value



Temperature, DEM and GPP are the most important



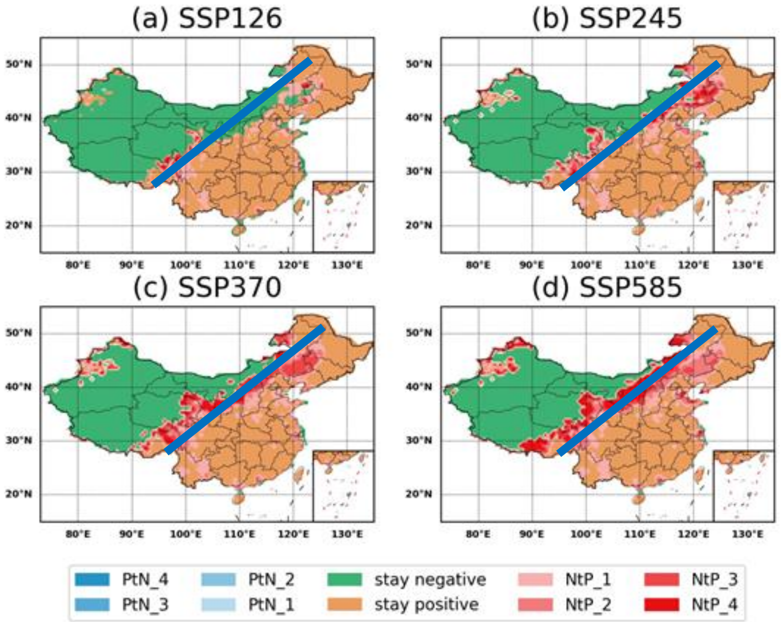
As time changes, temperature and GPP have shown a reversal in contribution.



Two Thresholds

Reversal: 3 gC $m^{-2}d^{-1}$

Plateaus: 7 gC $m^{-2}d^{-1}$



A critical zone for the reversal effect

located around 400 mm annual precipitation line

Published papers

XAI:

Huang, F., Shangguan, W.#, Li, Q., Li, L., & Zhang, Y. (2023). Beyond prediction: An integrated post-hoc approach to interpret complex model in hydrometeorology. Environmental Modelling & Software, 167: 105762. https://doi.org/10.1016/j.envsoft.2023.105762

Huang, F., Zhang, Y., Zhang, Y., Shangguan, W.#, Nourani, V., Li, Q., & Li, L. (2023). Towards interpreting machine learning models for predicting soil moisture droughts. Environmental Research Letters， 18: 074002. https://doi.org/10.1088/1748-9326/acdbe0

Huang, F., Zhang, Y., Zhang, Y., Shangguan, W.#, Li, Q., Li, L., Jiang, S. Interpreting Conv-LSTM for Spatio-Temporal Soil Moisture Prediction in China. Agriculture. 2023; 13(5):971. https://doi.org/10.3390/agriculture13050971

Machine learning in geoscience：

Shangguan W#, Xiong Z, Nourani V, Li Q, Lu X, Li L, Huang F, Zhang Y, Sun W, Dai Y. A 1 km Global Carbon Flux Dataset Using In Situ Measurements and Deep Learning. Forests. 2023; 14(5):913. https://doi.org/10.3390/f14050913

Zhang, Y.; Huang, F.; Li, L.; Li, Q.; Zhang, Y.; Shangguan, W#. Real-Time Forecast of SMAP L3 Soil Moisture Using Spatial–Temporal Deep Learning Model with Data Integration. Remote Sens. 2023, 15, 366. https://doi.org/10.3390/rs15020366

Li, Q., Shi, G., Shangguan, W.#, Li, J., Li, L., Huang, F., Zhang, Y., Wang, C., Wang, D., Qiu, J., Lu, X., and Dai, Y. 2022. A 1 km daily soil moisture dataset over China using in situ measurement and machine learning, Earth Syst. Sci. Data, 14, 5267–5286, https://doi.org/10.5194/essd-14-5267-2022

Li, Q., Zhu, Y., Shangguan, W.#, Wang, X., Li, L., Yu, F., 2022. An attention-aware LSTM model for soil moisture and soil temperature prediction. Geoderma, 409: 115651. https://doi.org/10.1016/j.geoderma.2021.115651

Li, Q., Li, Z., Shangguan, W.#, Wang, X., Li, L., Yu, F., 2022. Improving soil moisture prediction using a novel encoder-decoder model with residual learning. Computers and Electronics in Agriculture, 195: 106816. https://doi.org/10.1016/j.compag.2022.106816

Mao T, Shangguan W#, Li Q, Li L, Zhang Y, Huang F, Li J, Liu W, Zhang R. A Spatial Downscaling Method for Remote Sensing Soil Moisture Based on Random Forest Considering Soil Moisture Memory and Mass Conservation. Remote Sensing. 2022; 14(16):3858. https://doi.org/10.3390/rs14163858

Submitted papers

Zhang, Y., Shangguan, W., et al., Projections of Soil Organic Carbon in China: The Role of Carbon Fluxes Revealed by Explainable Artificial Intelligence, in preparation.

Huang, F., Shangguan, W., Jiang, S. et al., Explainable artificial intelligence technology in Earth system science: methods, achievements, future prospectives. Earth-Science Reviews. In review.

https://arxiv.org/abs/2406.11882

THANK YOU

Wei Shangguan 上官微
shgwei@mail.sysu.edu.cn
School of Atmosphere, Sun Yat-sen University

Researchgate:
https://www.researchgate.net/profile/Wei-Shangguan-2

Website:
https://atmos.sysu.edu.cn/teacher/372

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