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Session HS3.1: Hydroinformatics: data analytics, machine learning, systems analysis, optimization

Feature-based clustering of hydroclimatic time series

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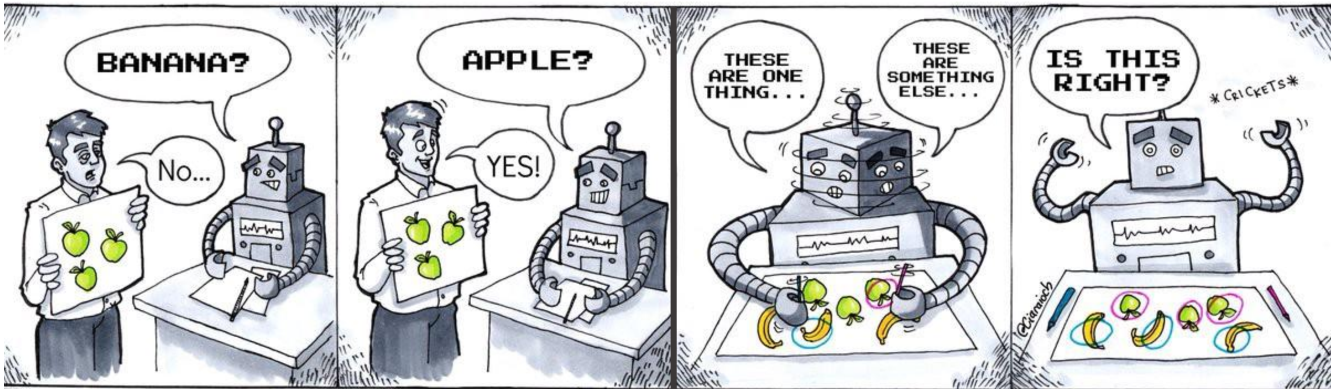
Machine learning basics with emphasis on clustering

Figure source: https://medium.com/data-solstice/wait-machines-can-learn-part-2-25e5d642652f

Definition



Supervised Learning

Unsupervised Learning

Task example

Probabilistic forecasting

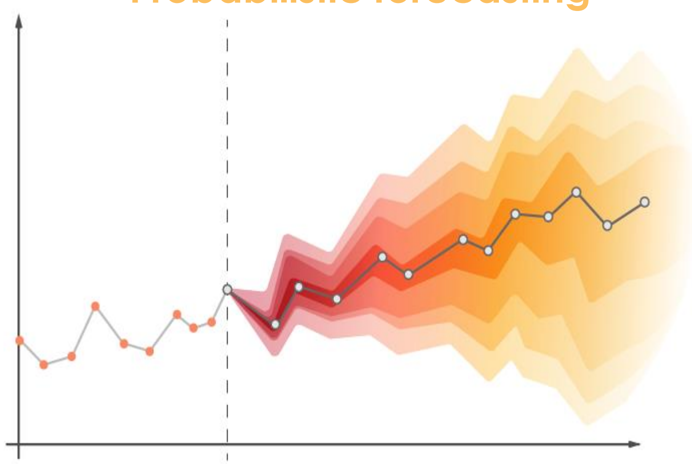


Figure source: https://medium.com/analytics-vidhya/time-series-forecasting-c73dec0b7533

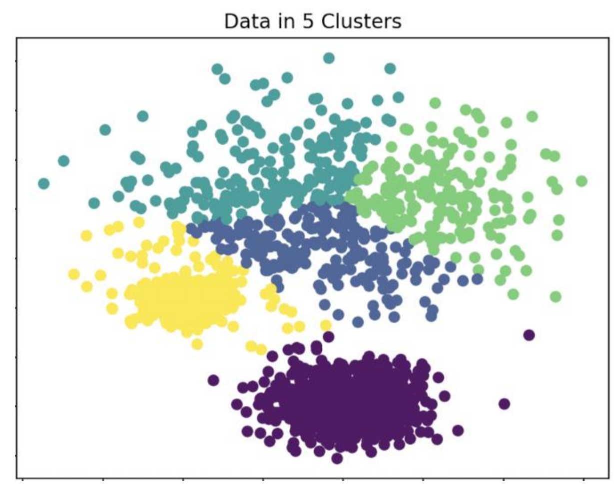


Figure source: https://www.ml-science.com/k-means-clustering

Cluster analysis

The importance and usefulness of cluster analyses

- A **clustering method** formulates and automates similarity guided groupings.
- Such groupings can support **technical and operational applications**.
- They can also support explorations by revealing **structures and patterns** in the data.
- Among others, they usually reveal interesting **spatial patterns**.
- The right above holds because real-world features are correlated in space.

Feature autocorrelation in space

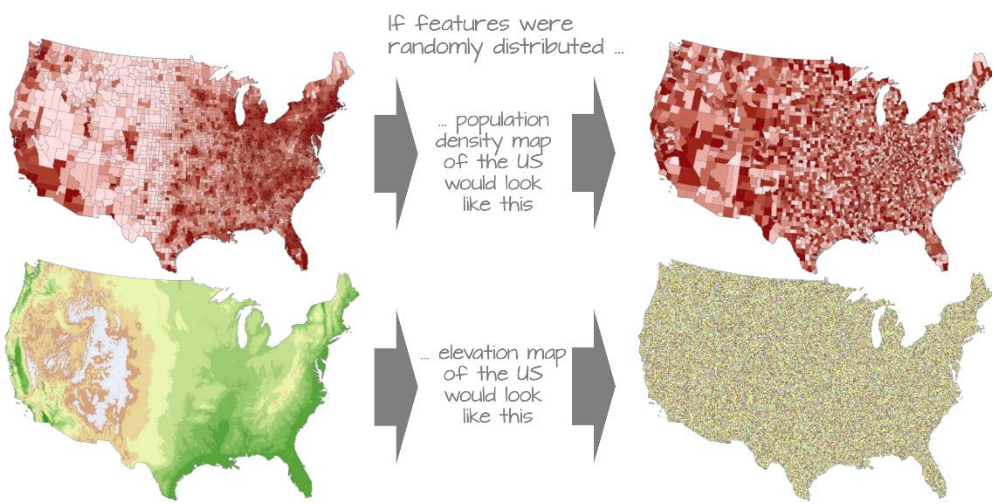


Figure source: https://mgimond.github.io/Spatial

Spatial patterns revealed through clustering

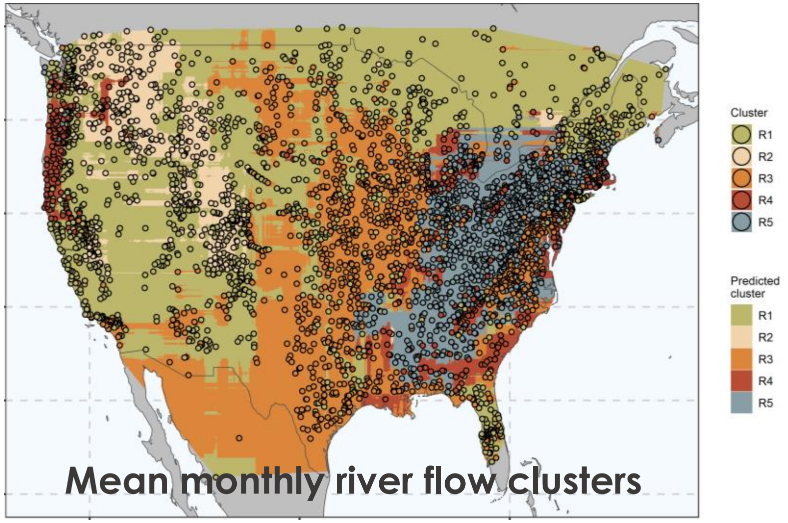
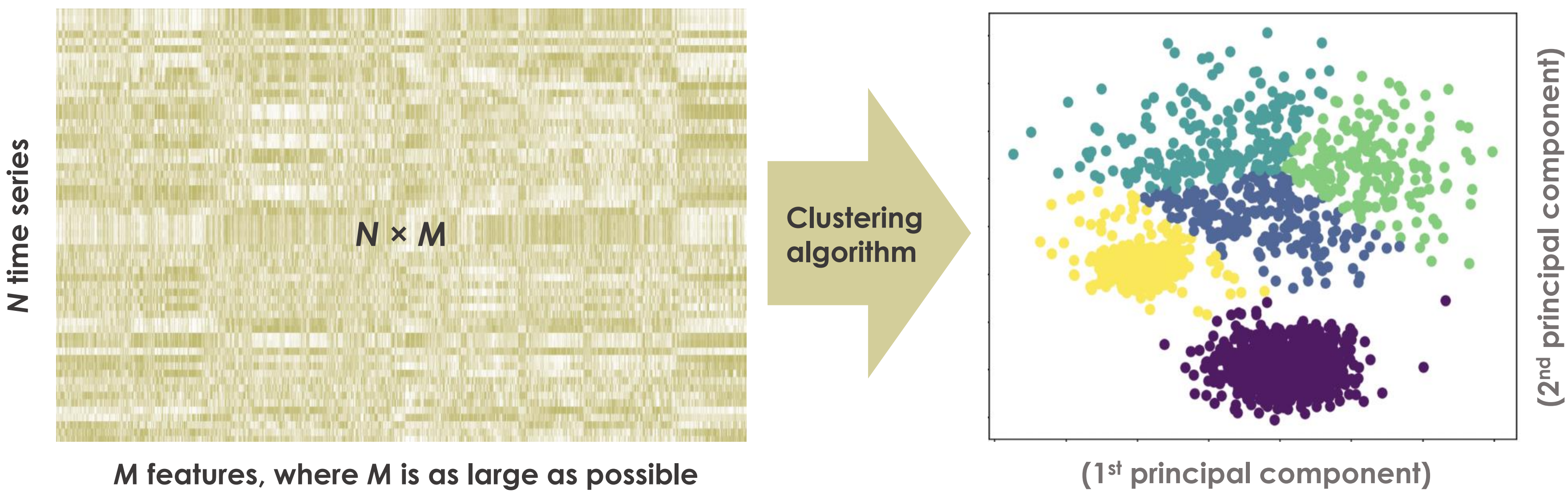


Figure source: Papacharalampous et al. (2021)

Massive feature extraction for hydroclimatic clustering

- There are two ways for improving clustering performance:
  - ✓ Improving the **clustering algorithm**;
  - ✓ Finding new informative **features** to cluster upon.
- Therefore, **massive feature extraction** (Fulcher and Jones 2014; Fulcher 2018) was proposed for clustering hydroclimatic time series by Papacharalampous et al. (2021).
- Indeed, this concept can lead to performance improvements, as it considerably increases the amount of information exploited by the clustering algorithm.



Examples of time series features and their compilations

- The existing general-purpose time series features and time series feature categories include **autocorrelation**, **partial autocorrelation**, **long-range dependence**, **entropy**, **temporal variation**, **seasonality**, **trend**, **lumpiness**, **stability**, **nonlinearity**, **linearity**, **spikiness**, **curvature** and **many more features**.
- Time series features are of fundamental interest in **stochastic (statistical) hydrology**.
- Examples of compilations of time series features for data science applications can be found in Wang et al. (2006), Fulcher et al. (2013), Hyndman et al. (2015), Kang et al. (2017, 2020) and Hyndman et al. (2020).
- Massive (or extensive) time series feature compilations introduced and successfully computed in stochastic hydrology can be found in Papacharalampous et al. (2021, 2022a,b).

Time series decomposition for feature extraction

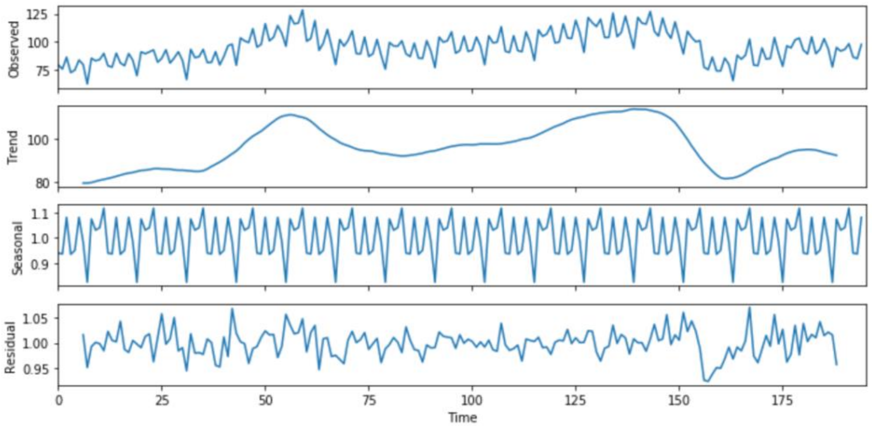


Figure source: https://datasciencebeginners.com/2020/11/25/time-series-forecast-and-decomposition-101-guide-python

Random forests for clustering upon numerous features

- **Random forests** (Breiman 2001) can be applied in unsupervised mode for **clustering** as detailed in Liaw and Wiener (2002).
- Their following **properties** (Tyralis et al., 2019, Section 2.8.1) make them appealing for clustering in general, and clustering upon numerous time series features in particular:
  - ✓ They demonstrate high performance compared to other algorithms.
  - ✓ They can handle highly correlated features.
  - ✓ They can operate successfully when interactions are present.
  - ✓ They are invariant to monotone transformations of the features.
- Lastly, they support the application of **explainable machine learning** through feature importance metrics.

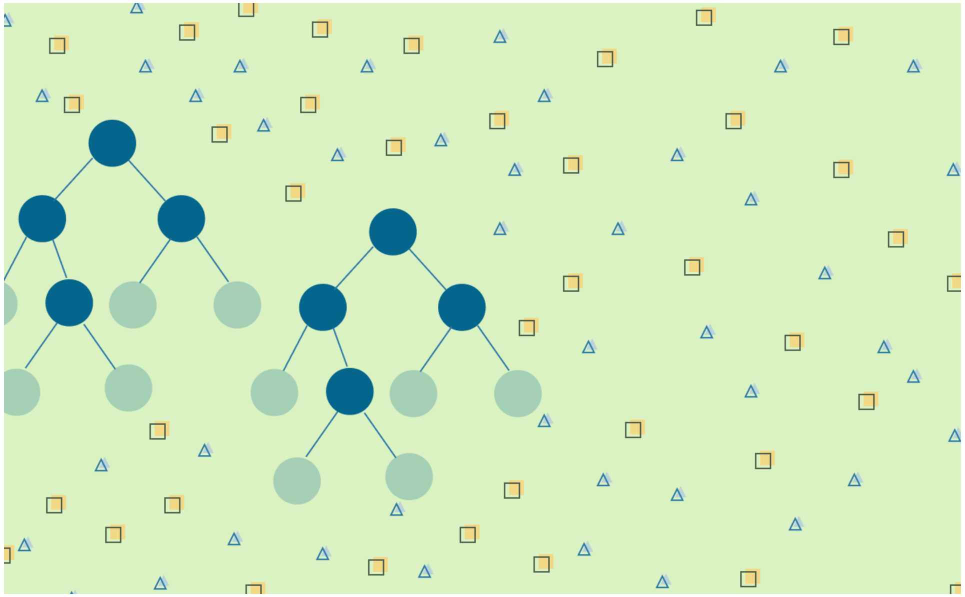


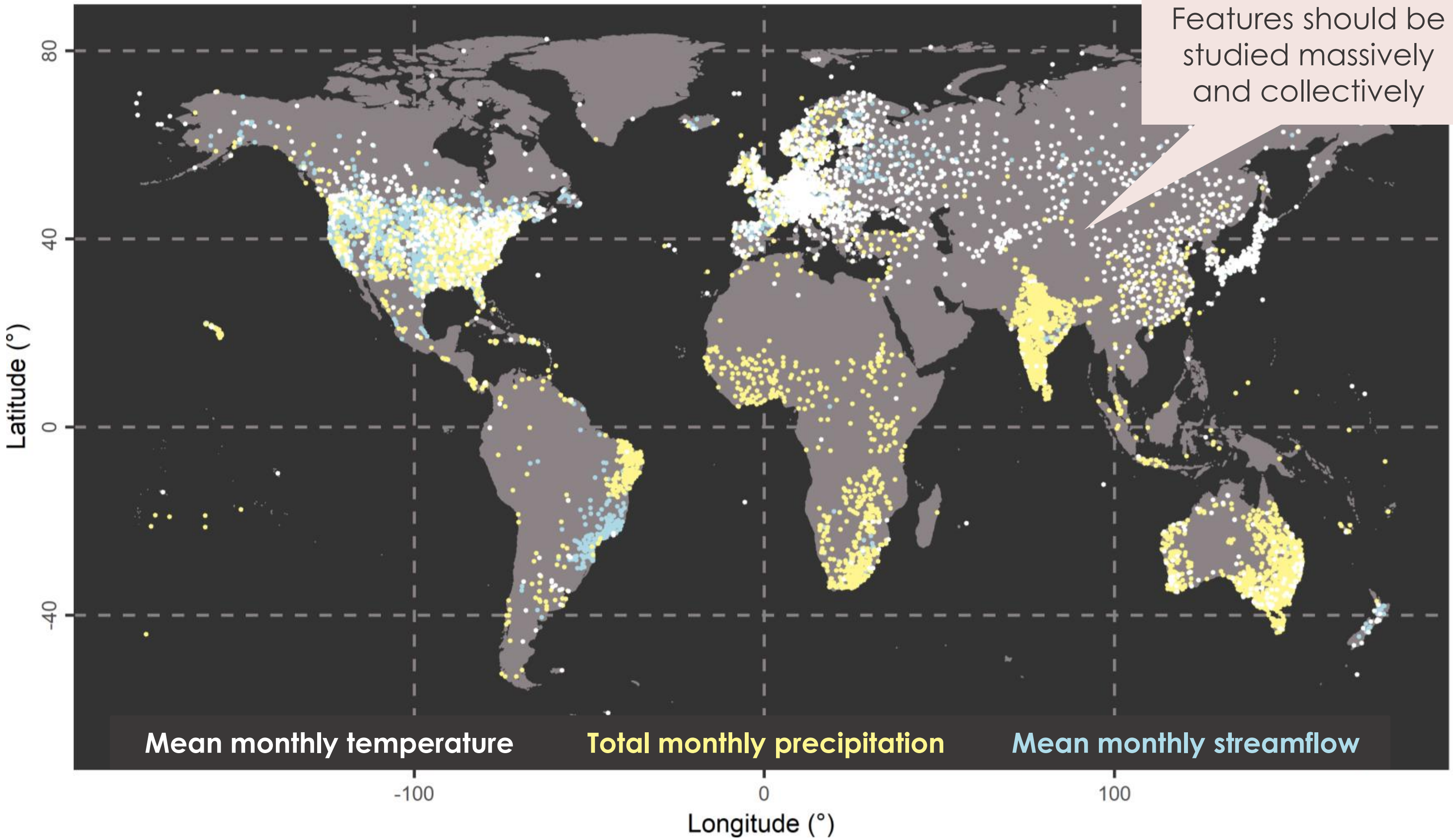
Figure source: https://towardsdatascience.com/random-forests-algorithm-explained-with-a-real-life-example-and-some-python-code-affbfa5a942c

Massive feature extraction for hydroclimatic clustering

Benefitting from 59 largely diverse time series features

Further reading: Papacharalampous et al. (2021)

Features should be studied massively and collectively

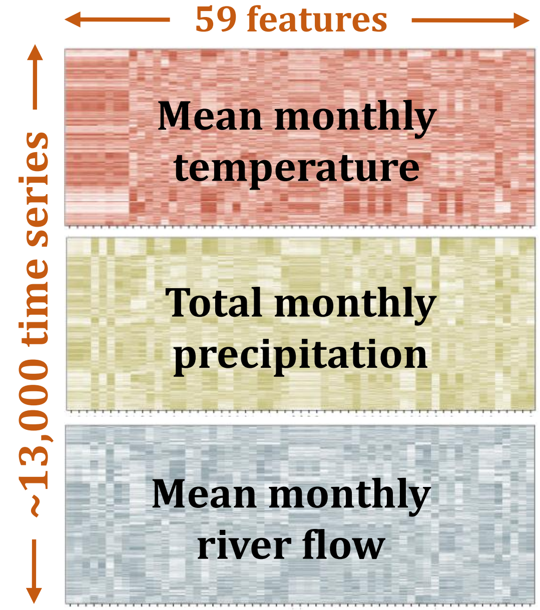


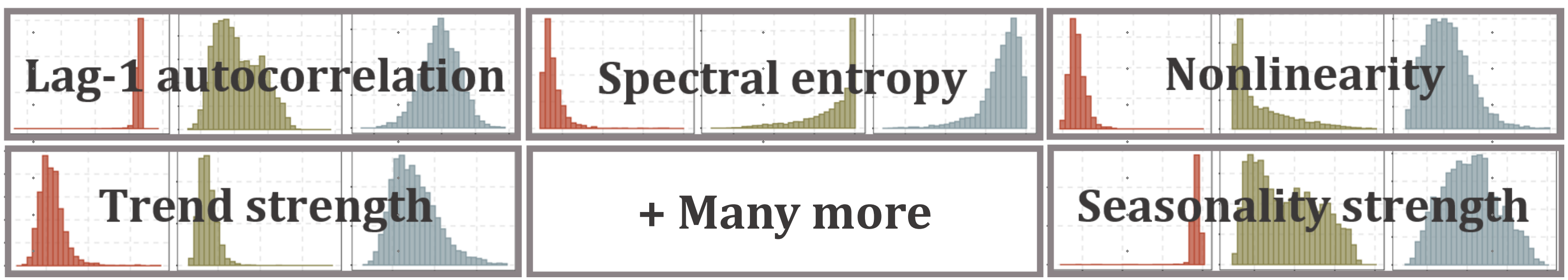
Massive feature extraction for hydroclimatic clustering

A compilation of 59 largely diverse features

x_acf1, ac_9, x_acf10, diff1_acf1, diff1_acf10, diff2_acf1, diff2_acf10, seas_acf1, firstzero_ac, firstmin_ac, embed2_incircle_1, embed2_incircle_2, trev_num, motiftwo_entro3, walker_propcross, x_pacf5, diff1x_pacf5, diff2x_pacf5, seas_pacf, localsimple_mean1, localsimple_lfitac, sampen_first, std1st_der, spreadrandomlocal_meantaul_50, spreadrandomlocal_meantaul_ac2, histogram_mode_10, outlierinclude_mdrmd, fluctanal_prop_r1, crossing_points, entropy, flat_spots, arch_acf, garch_acf, arch_r2, garch_r2, alpha, beta, gamma, lumpiness, stability, max_level_shift, time_level_shift, max_var_shift, time_var_shift, max_kl_shift, time_kl_shift, ARCH.LM, nonlinearity, unitroot_kpss, hurst, trend, spike, linearity, curvature, e_acf1, e_acf10, seasonal_strength, peak, trough

Massive feature extraction

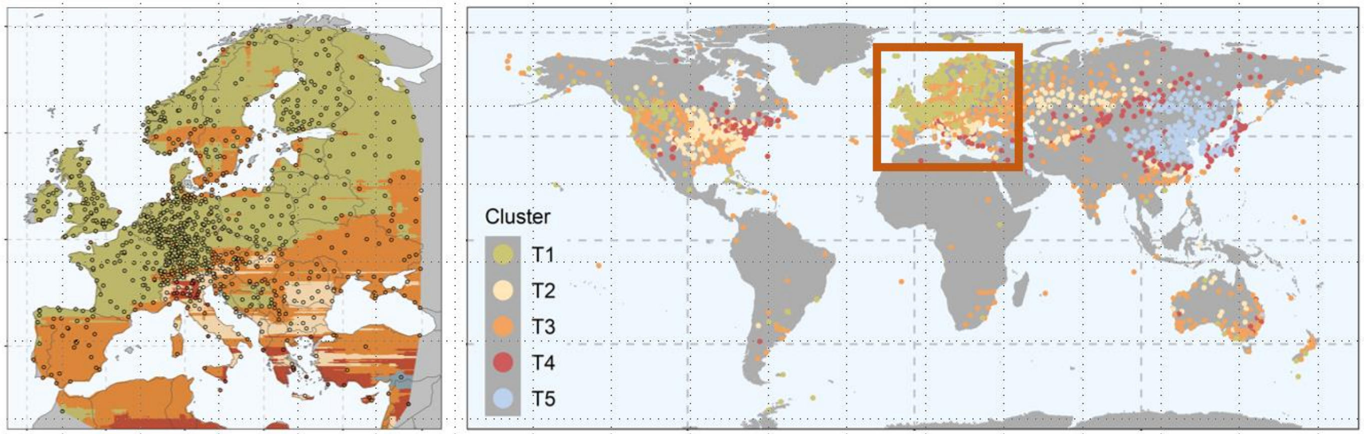




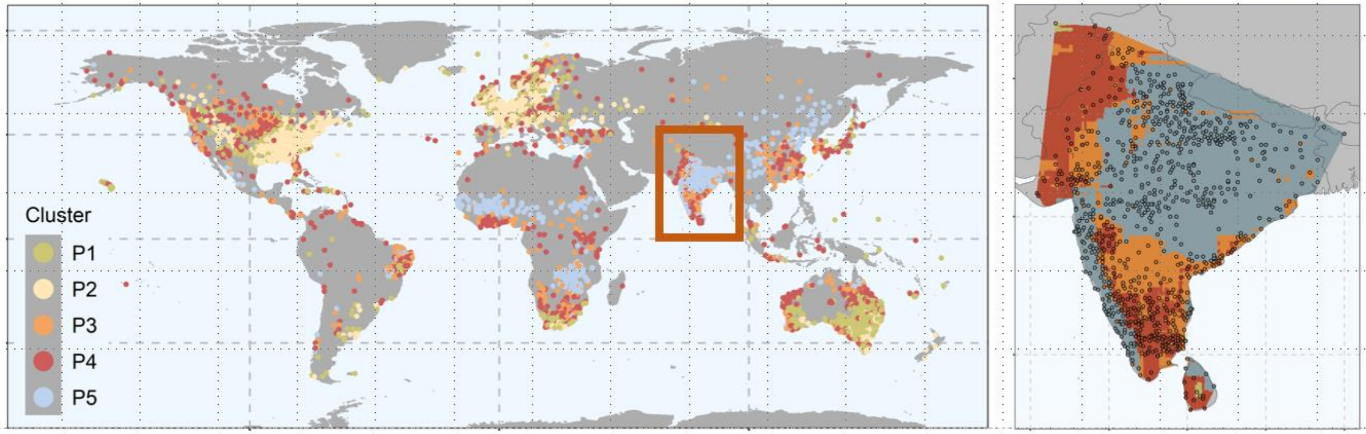
Further reading: Papacharalampous et al. (2021)

Hydroclimatic clusters based on 59 time series features

Mean monthly temperature

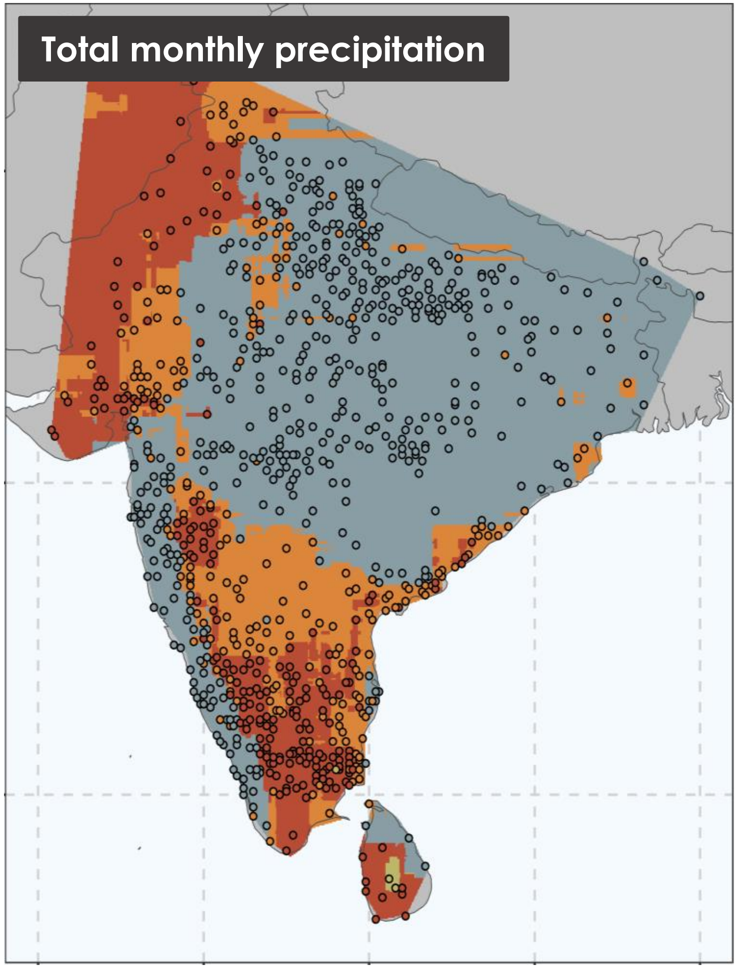


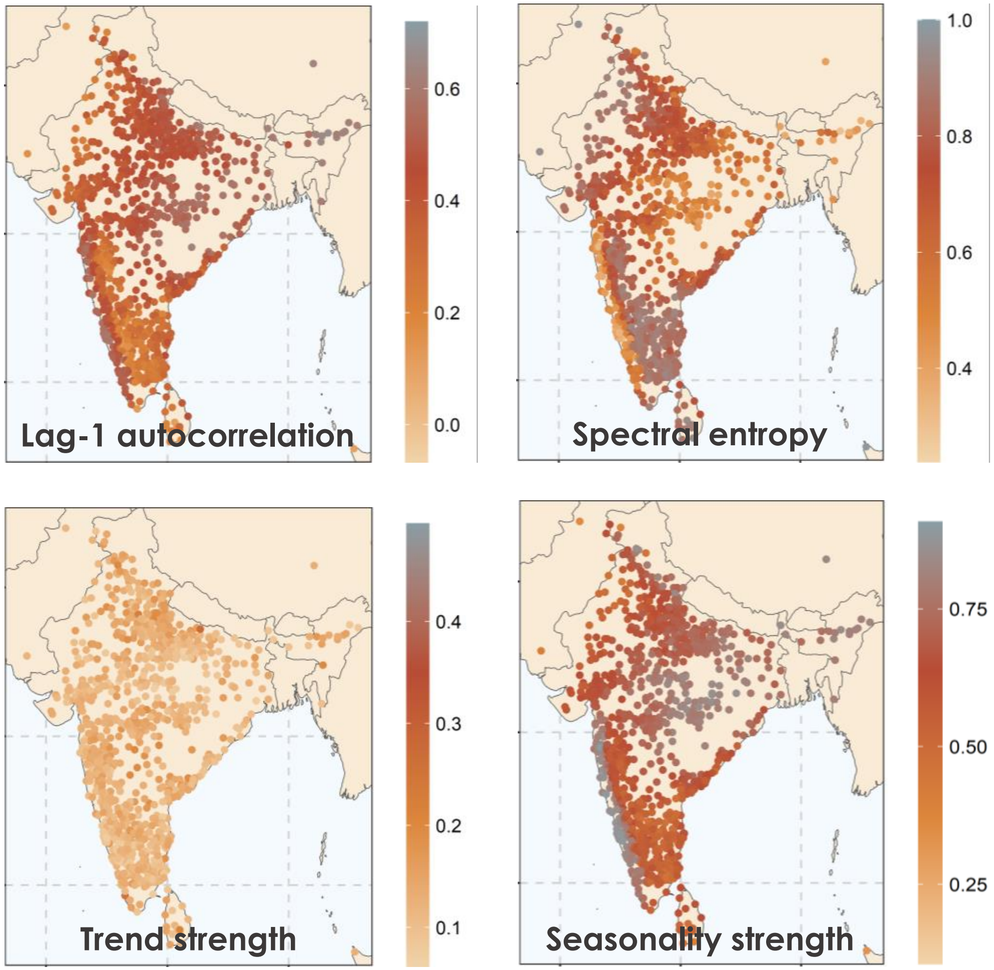
Total monthly precipitation



Further reading: Papacharalampous et al. (2021)

Hydroclimatic clusters based on 59 time series features



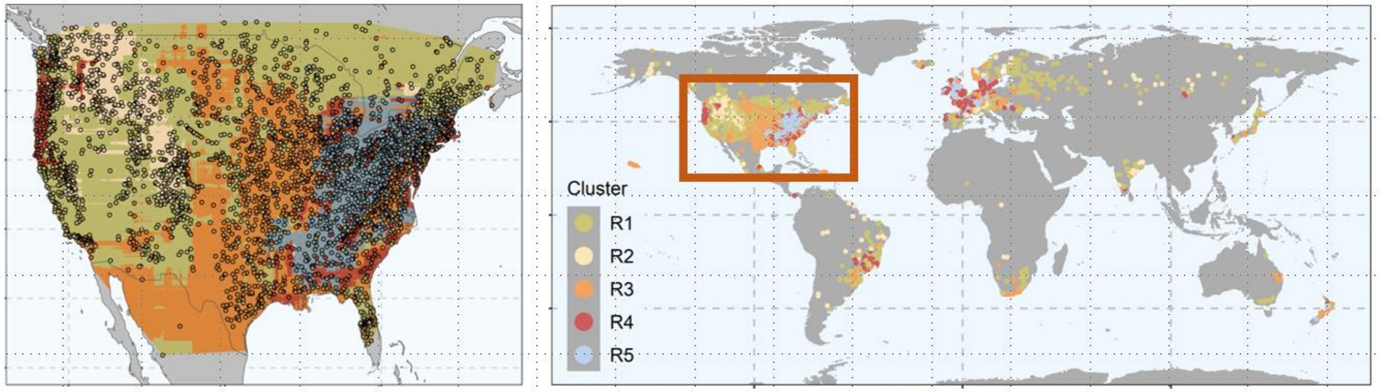


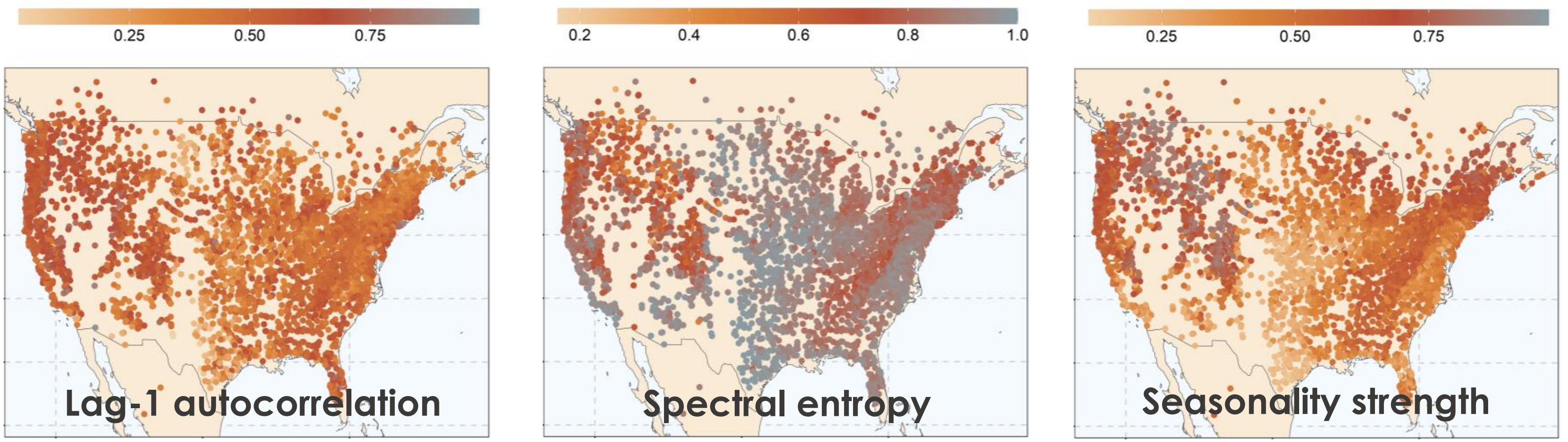
The legends present the global ranges of the feature values.

Further reading: Papacharalampous et al. (2021)

Hydroclimatic clusters based on 59 time series features

Mean monthly river flow



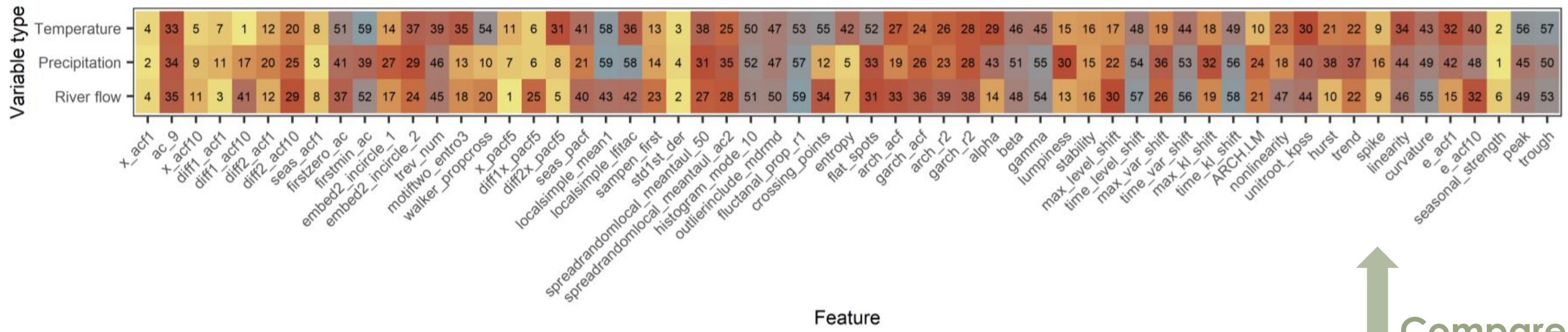


The legends present the global ranges of the feature values.

Further reading: Papacharalampous et al. (2021)

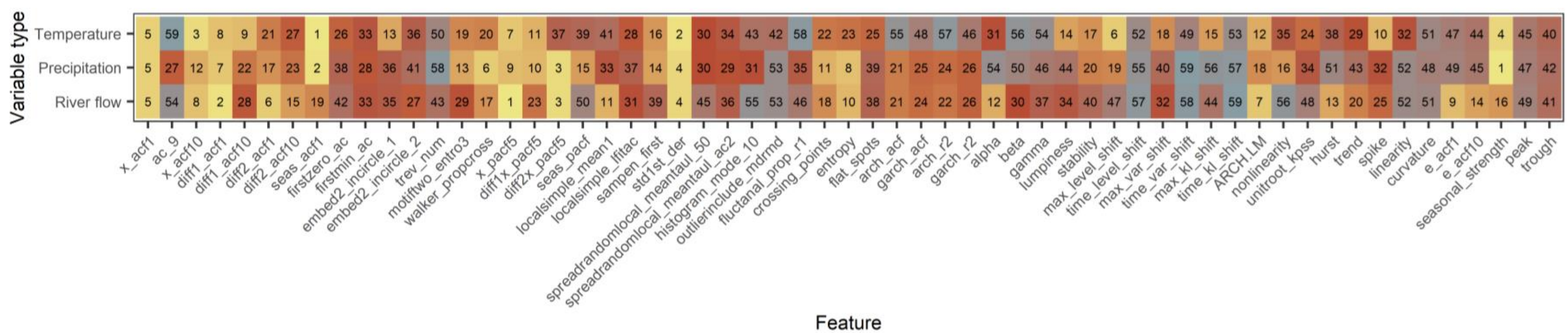
Feature importance in clustering different variable types

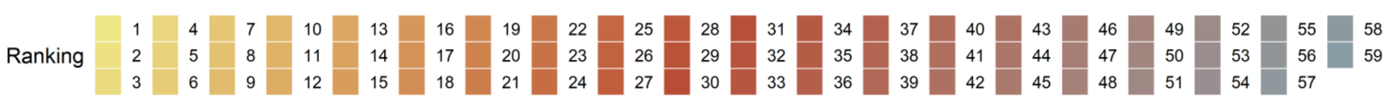
Rankings of the features from the most (1st) to the least (59th) important ones in clustering



Compare

Rankings of the features from the most (1st) to the least (59th) contributing ones to the 1st principal component

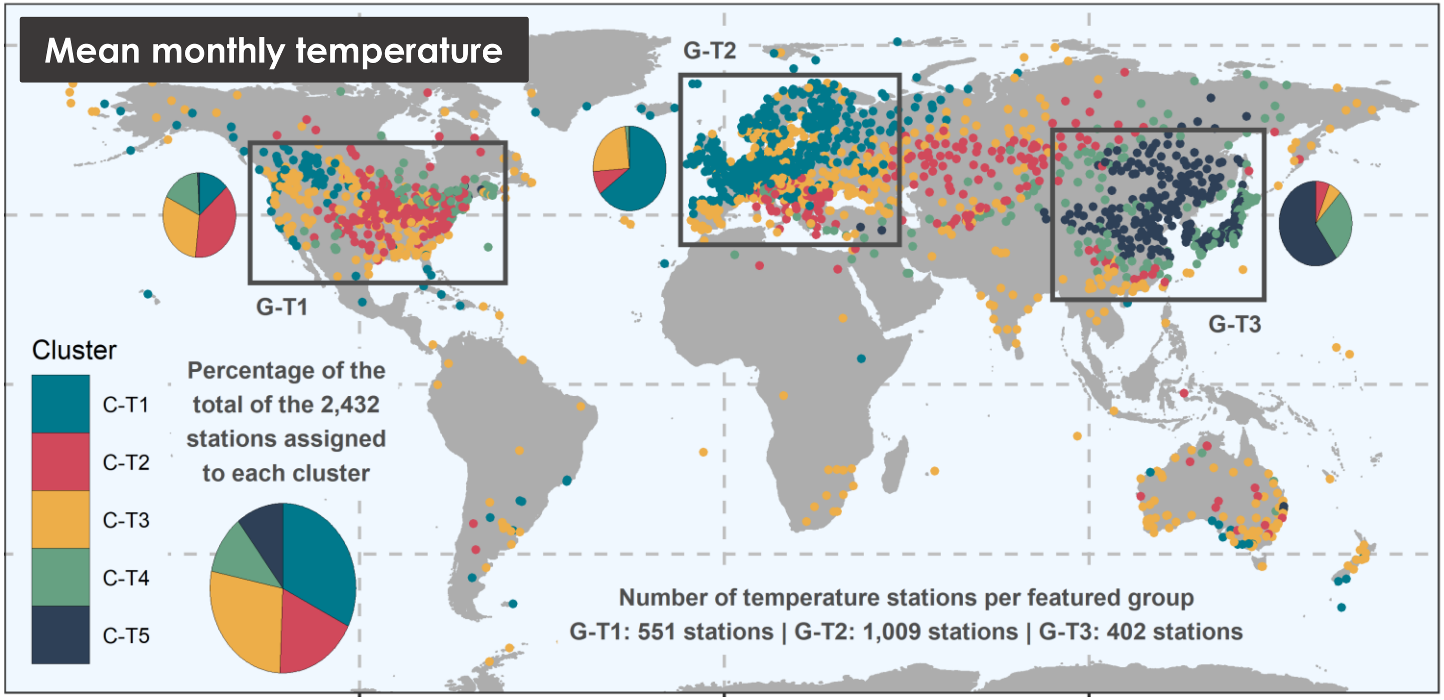




Further reading: Papacharalampous et al. (2021)

Forecastability comparisons across hydroclimatic clusters

Temperature time series forecastability in terms of Nash-Sutcliffe efficiency in the different clusters

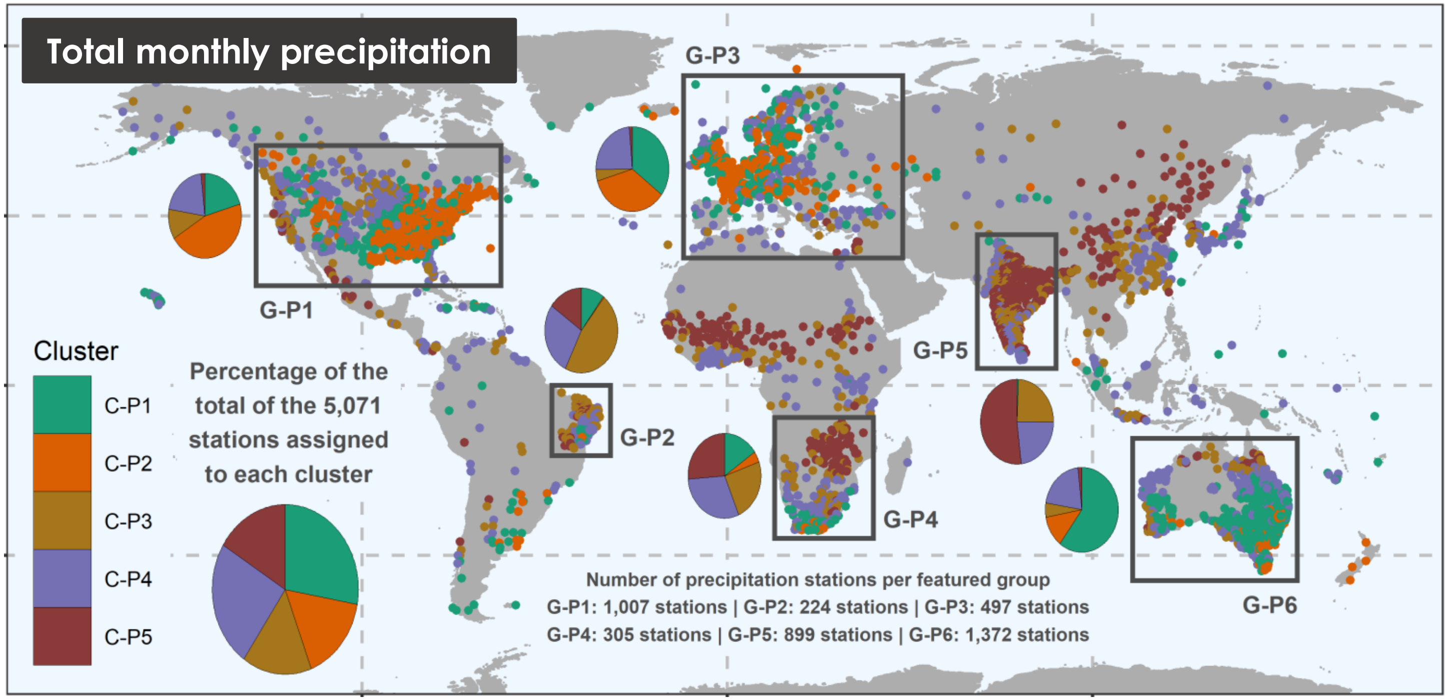


The clusters have been obtained by implementing a close variant of the method by Papacharalampous et al. (2021).

Further reading: Papacharalampous et al. (2022b)

Forecastability comparisons across hydroclimatic clusters

Precipitation time series forecastability in terms of Nash-Sutcliffe efficiency in the different clusters

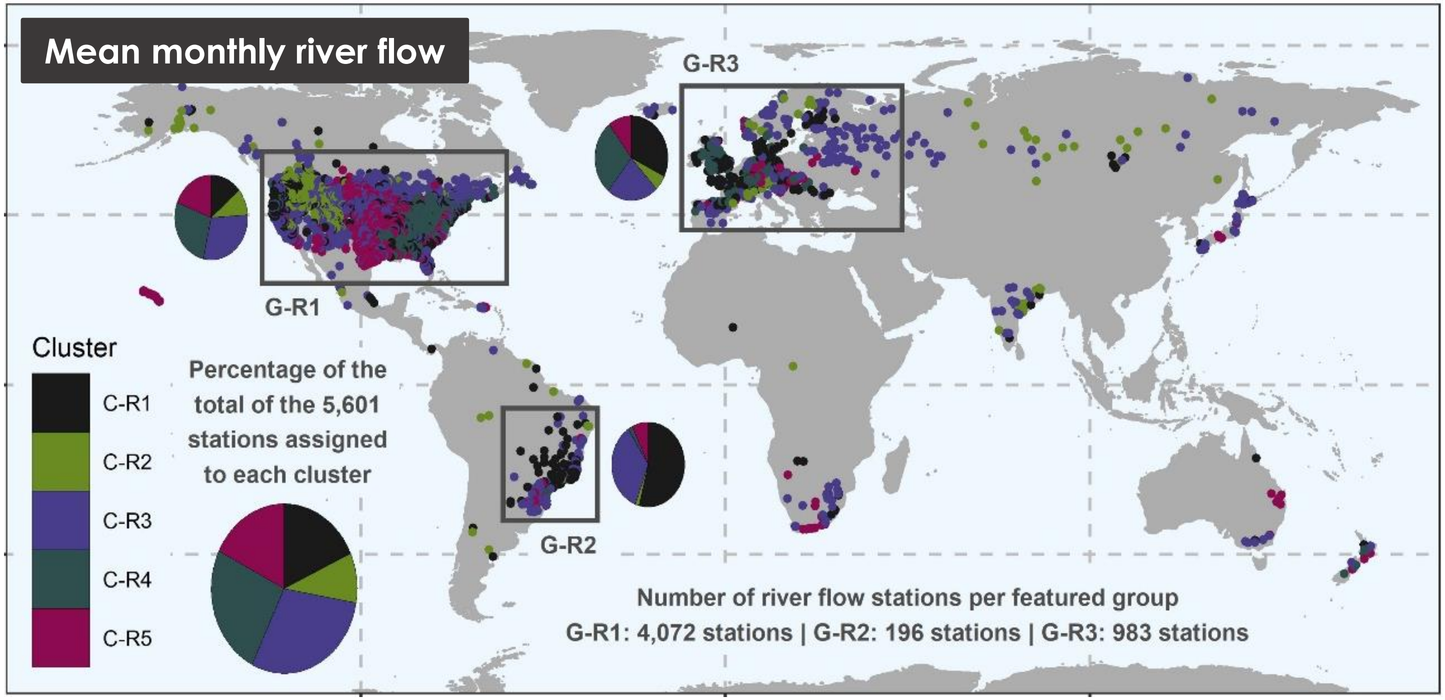


The clusters have been obtained by implementing a close variant of the method by Papacharalampous et al. (2021).

Further reading: Papacharalampous et al. (2022b)

Forecastability comparisons across hydroclimatic clusters

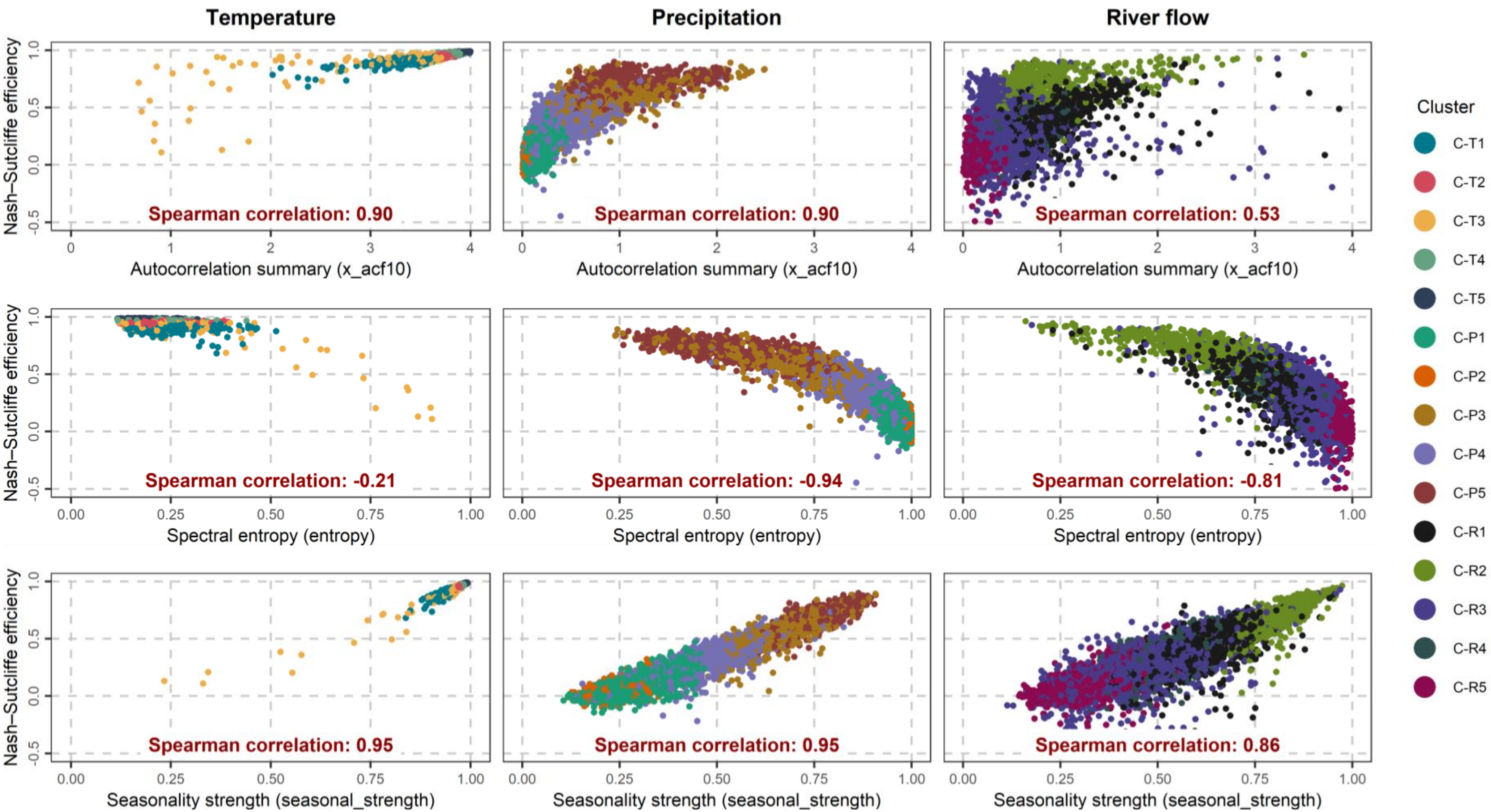
River flow time series forecastability in terms of Nash-Sutcliffe efficiency in the different clusters



The clusters have been obtained by implementing a close variant of the method by Papacharalampous et al. (2021).

Further reading: Papacharalampous et al. (2022b)

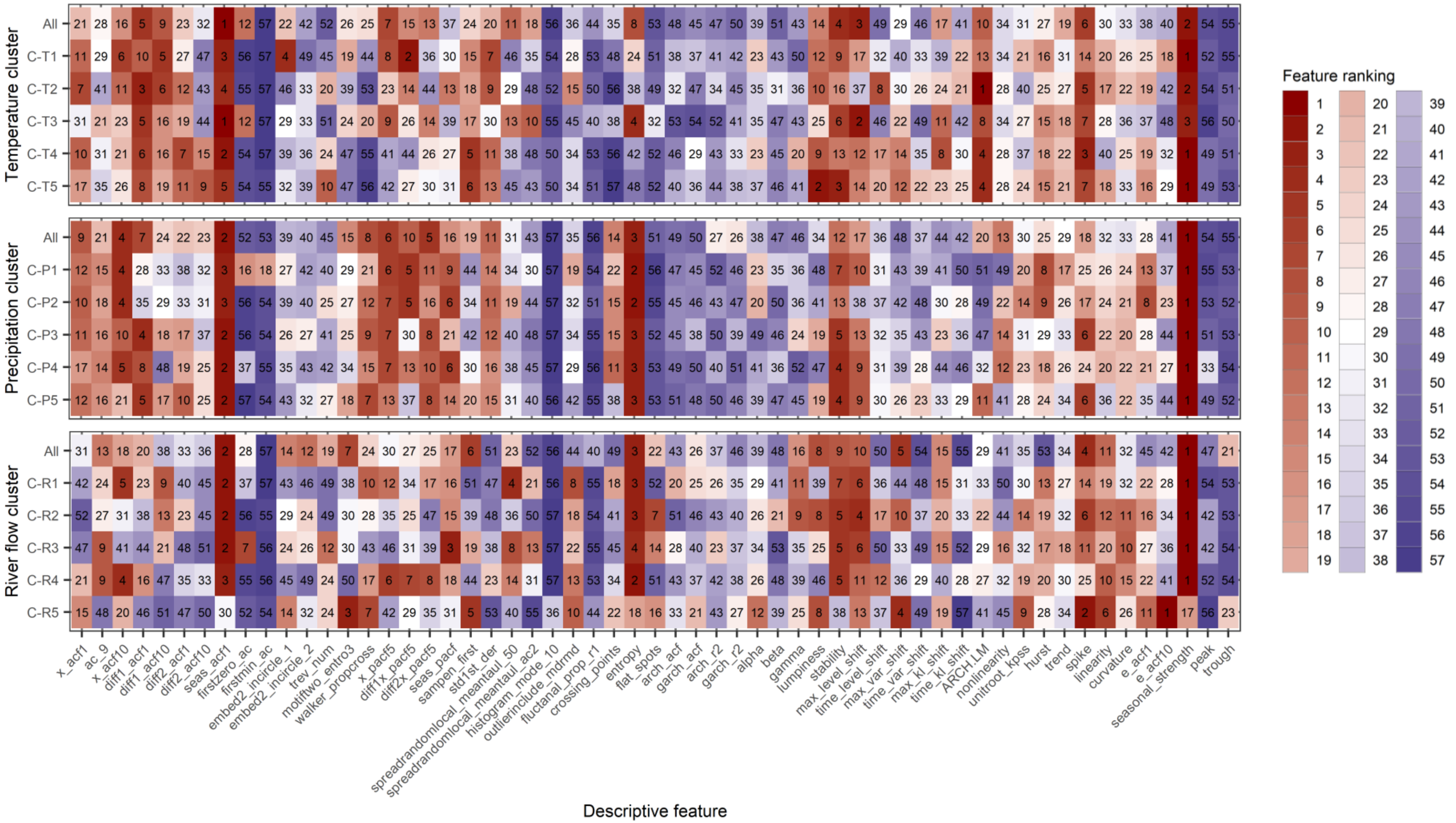
Forecastability comparisons across hydroclimatic clusters



The clusters have been obtained by implementing a close variant of the method by Papacharalampous et al. (2021).

Further reading: Papacharalampous et al. (2022b)

Forecastability comparisons across hydroclimatic clusters



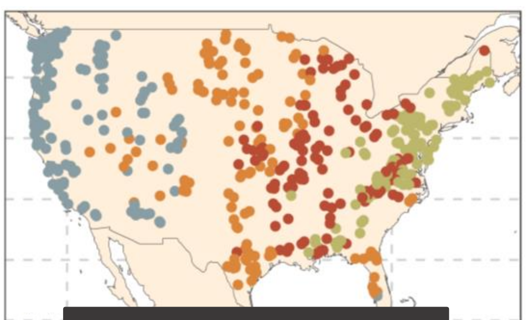
The clusters have been obtained by implementing a close variant of the method by Papacharalampous et al. (2021).

Further reading: Papacharalampous et al. (2022b)

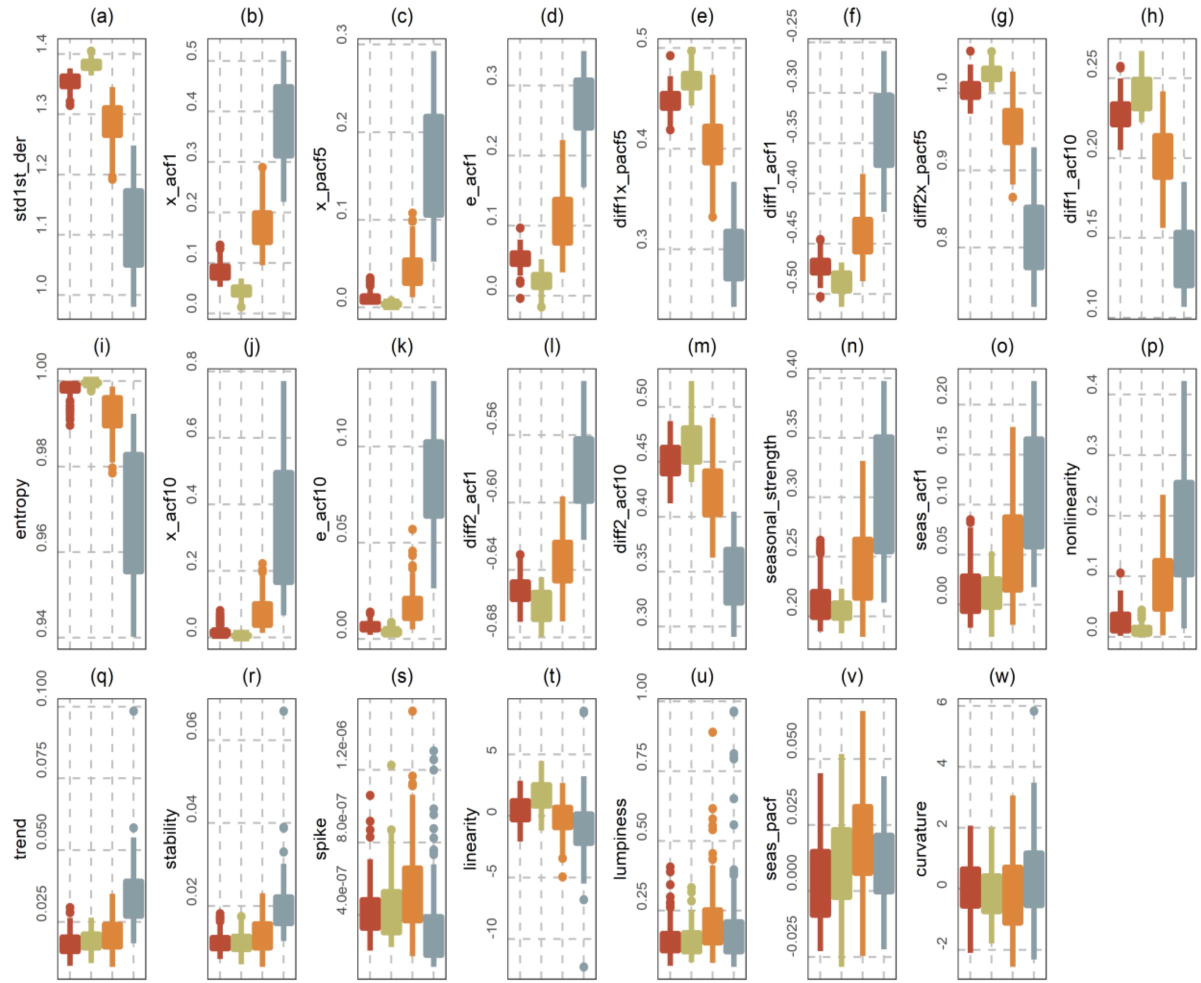
Hydroclimatic clusters based on 23 time series features

A compilation of 23 features for hydroclimatic time series analysis at multiple time scales

`x_acf1, x_acf10, diff1_acf1, diff1_acf10, diff2_acf1, diff2_acf10, seas_acf1, x_pacf5, diff1x_pacf5, diff2x_pacf5, seas_pacf, std1st_der, entropy, lumpiness, stability, nonlinearity, trend, spike, linearity, curvature, e_acf1, e_acf10, seasonal_strength`



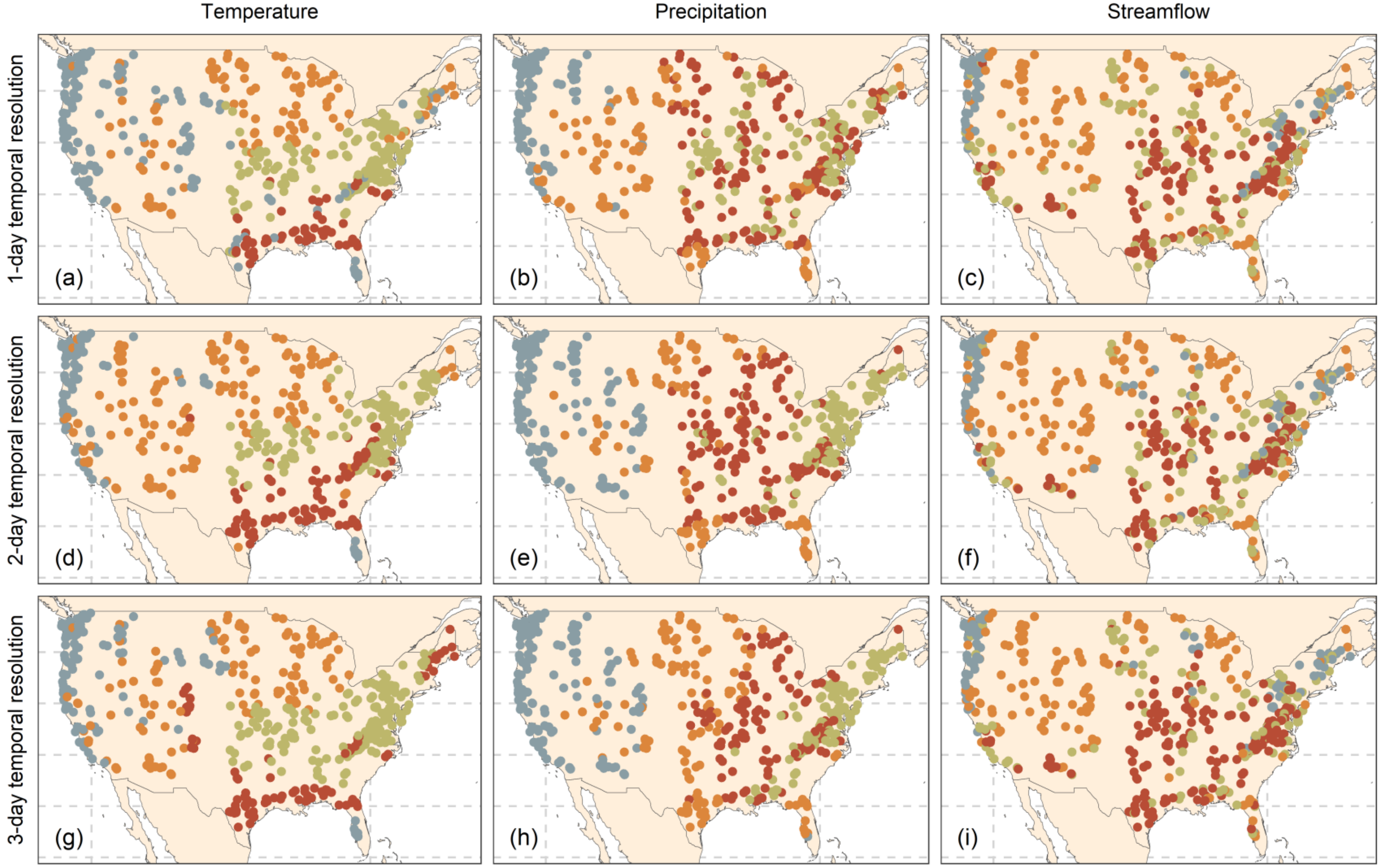
3-day temporal resolution



The feature importance in clustering decreases as we move from (a) to (w).

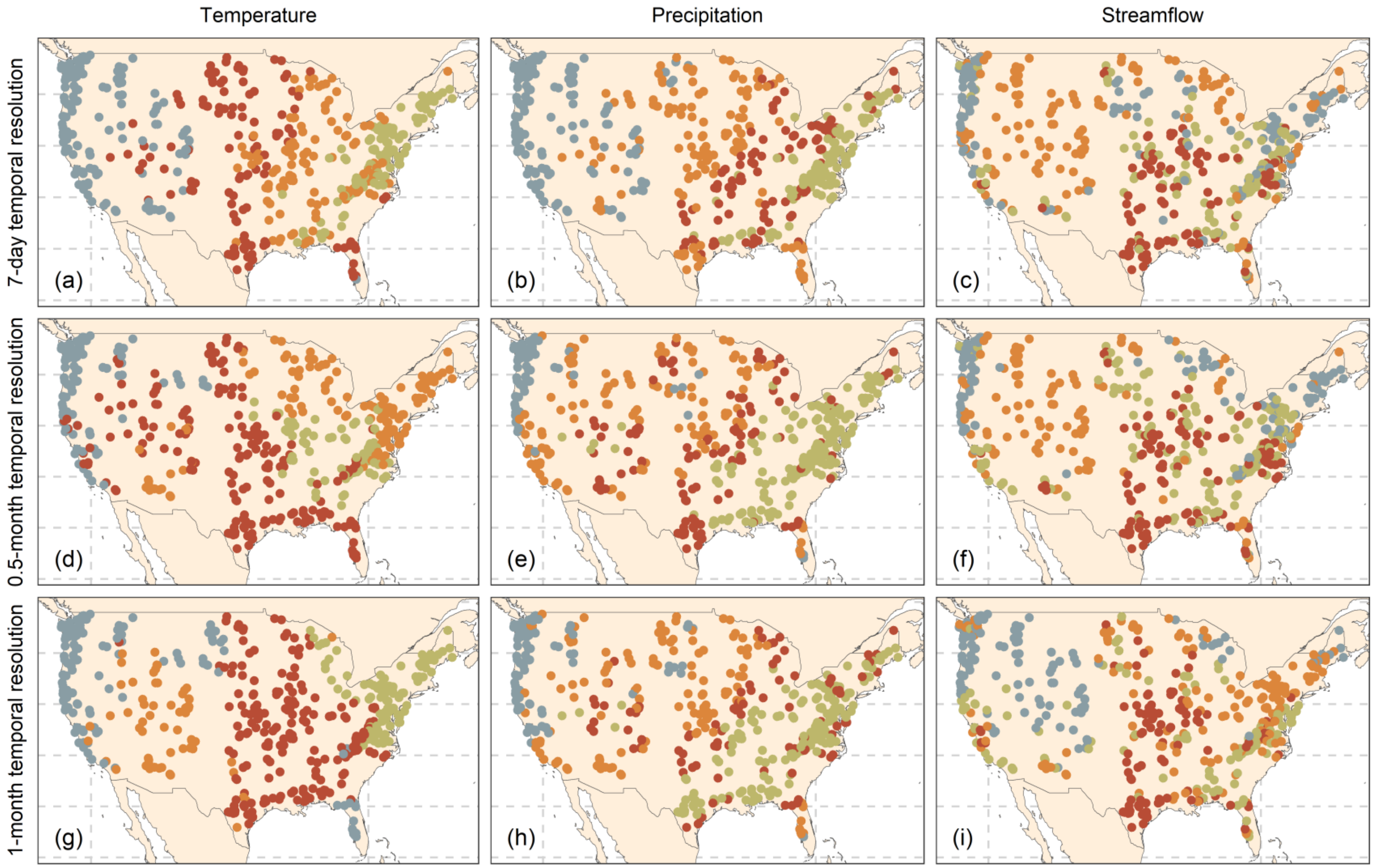
Further reading: Papacharalampous et al. (2022a)

Hydroclimatic clusters at multiple time scales



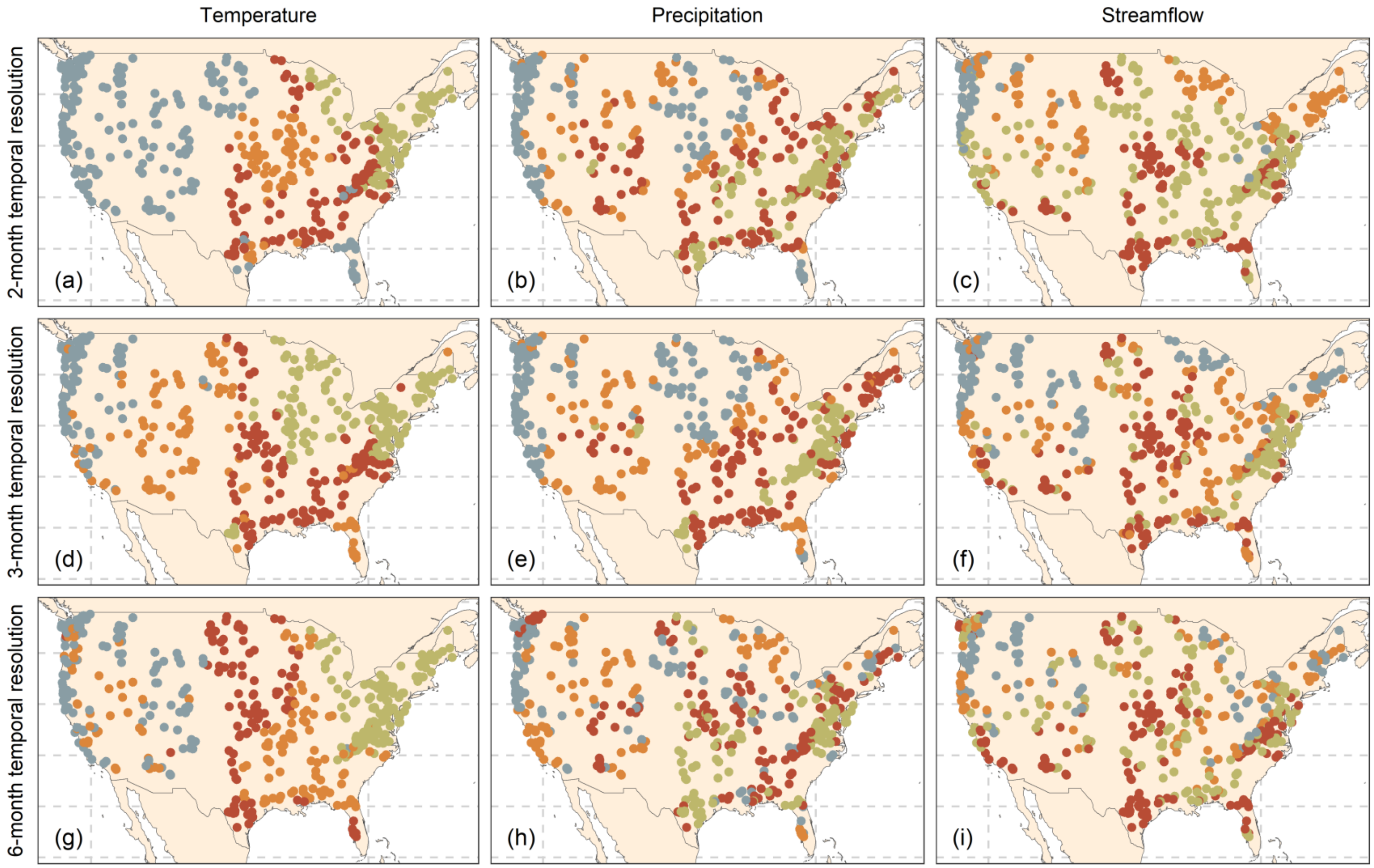
Further reading: Papacharalampous et al. (2022a)

Hydroclimatic clusters at multiple time scales



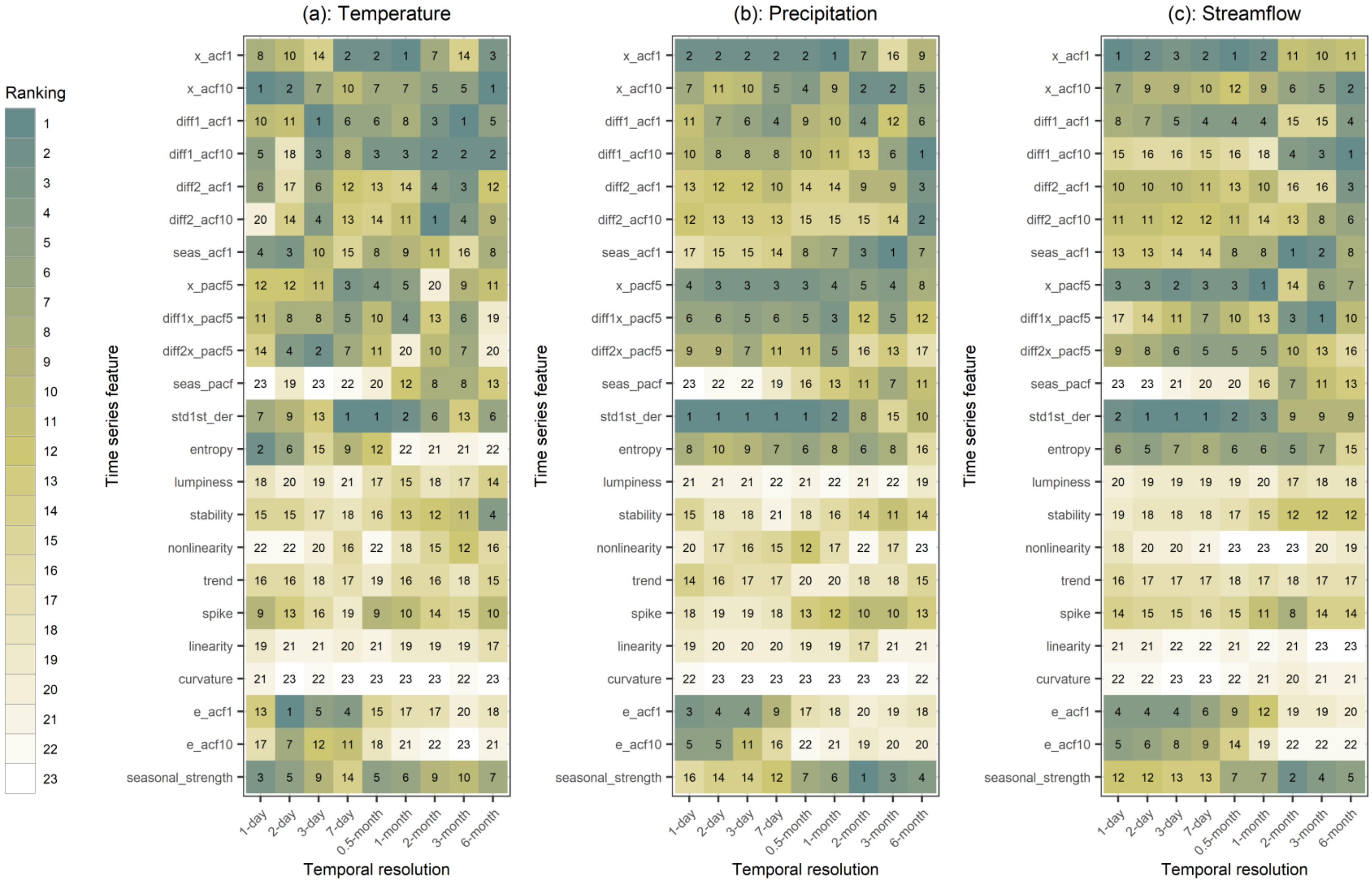
Further reading: Papacharalampous et al. (2022a)

Hydroclimatic clusters at multiple time scales



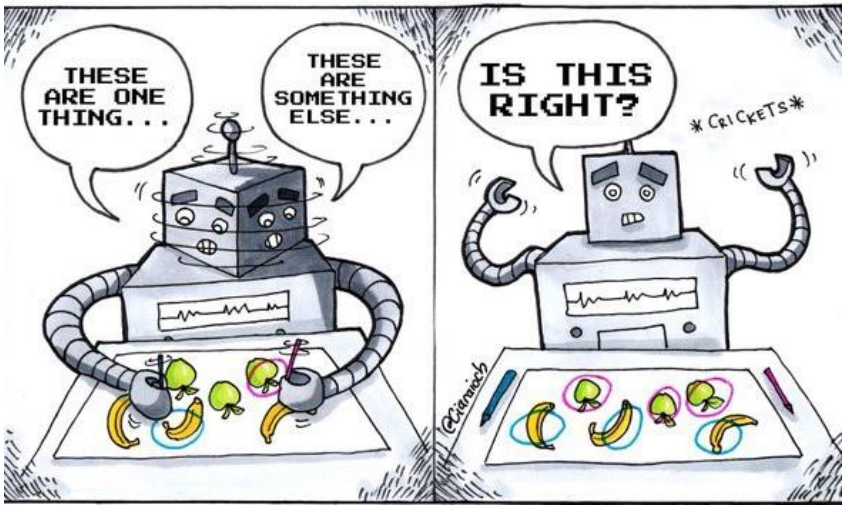
Further reading: Papacharalampous et al. (2022a)

Feature importance in clustering at multiple time scales



Further reading: Papacharalampous et al. (2022a)

Summary, discussion and take-home messages



- One way for improving clustering performance is finding **new informative features** to cluster upon.
- Therefore, Papacharalampous et al. (2021) proposed to cluster hydroclimatic time series by exploiting the concept of **massive feature extraction**.
- This concept is new in the field, although time series features are of fundamental and practical interest in stochastic (statistical) hydrology (see, e.g., the central themes, concepts and directions provided by Montanari et al. 2013).
- The usefulness of the new approach in hydroclimatic time series clustering was demonstrated through a variety of **global-scale** and other **large-scale investigations** (Papacharalampous et al. 2021, 2022a,b).
- These investigations were conducted for **temperature**, **precipitation** and **streamflow** variables at **several temporal scales**.

Summary, discussion and take-home messages

- Indeed, there are numerous **time series features** whose computation is meaningful for various hydroclimatic variables and at various temporal scales with **minimal adaptations** (e.g., the time series features in Papacharalampous et al. 2021, 22022a,b).
- The general purpose character of the proposed clustering methods differentiates them notably from signature-based clustering methods (e.g., from Jehn et al. 2020).
- An even more substantial difference with other clustering methods in hydrology (e.g., with the methods by Hall and Blöschl 2018; Jehn et al. 2020; Fischer and Schumann 2021) is the consideration of **both interpretable and less interpretable features** in the clustering under the proposed central concept.
- In fact, the application of **explainable machine learning** showed that features from either of the above categories can be important in hydroclimatic time series clustering (Papacharalampous et al. 2021, 22022a,b).

Explainable machine learning

Figure source: https://www.analyticsinsight.net/a-beginners-guide-to-four-principles-of-explainable-artificial-intelligence

Summary, discussion and take-home messages

- More generally, a **massive** and collective examination of **hydroclimatic features** is necessary for understanding **hydroclimatic variability**, **change** and **predictability**.
- Particular focus on a single feature or a single feature category (e.g., on trends) could be misleading in hydroclimatic time series analysis contexts.
- A few **limitations** characterize the to-date applications of the proposed approach to hydroclimatic time series clustering and suggest open themes for **future research**.
- Indeed, this approach could be coupled with external methods for identifying an **optimal number of clusters**.
- It could also be applied with other **algorithms** (e.g., with **boosting**; for its theoretical properties, see Tyralis and Papacharalampous 2021, Section 3).
- Lastly, it could exploit information from **additional time series features**.

The main concept behind boosting

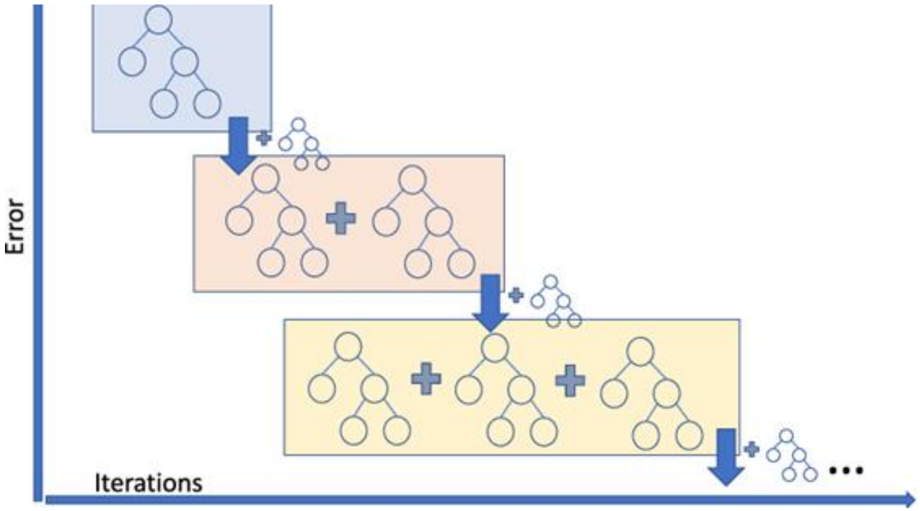


Figure source: https://medium.com/analytics-vidhya/what-is-gradient-boosting-how-is-it-different-from-ada-boost-2d5ff5767cb2

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