

Appendix:

A.1 Proposed figures to better explain the workflow for using SOM in hysteresis analysis

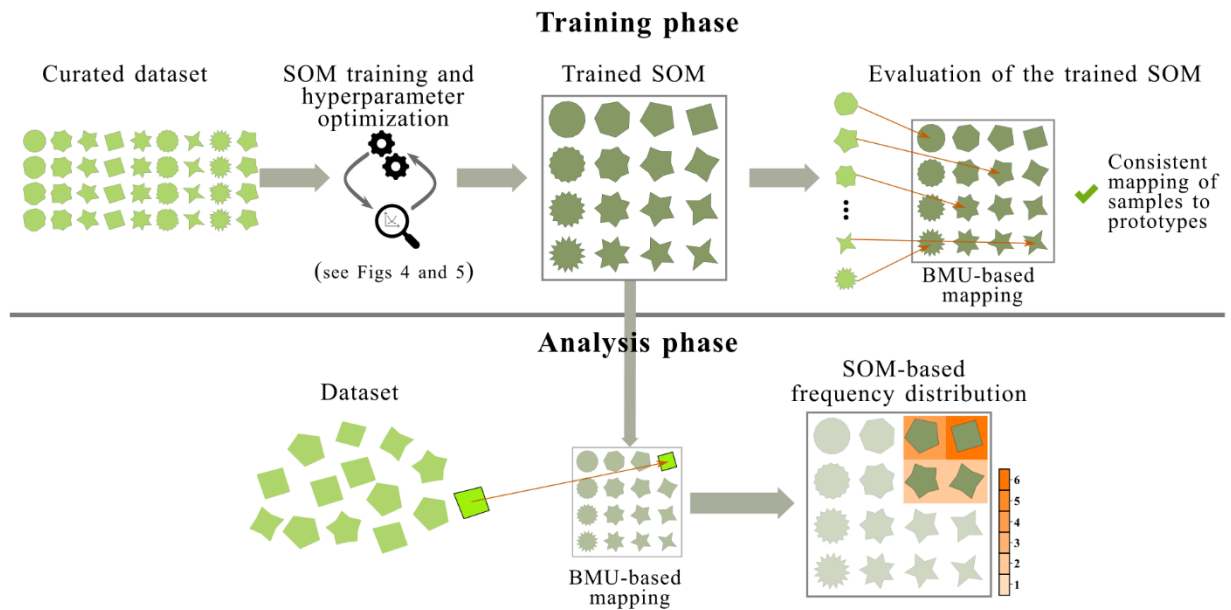


Figure 3. Workflow to generate an SOM for C-Q hysteresis loops (training phase) and apply the SOM for C-Q hysteresis analyses in watersheds (analysis phase). Here, we illustrate the generation of the SOM using different shapes, which are analogous to the hysteresis loop types that might be found for a dissolved or particulate constituent in a watershed. In the bottom panel (analysis phase), we demonstrate how hysteresis loops from a new dataset get mapped to the trained SOM, where the shade of orange represents the frequency with which the shape occurs in the dataset. The *HySOM* python package (see section 7) allows users to implement this workflow.

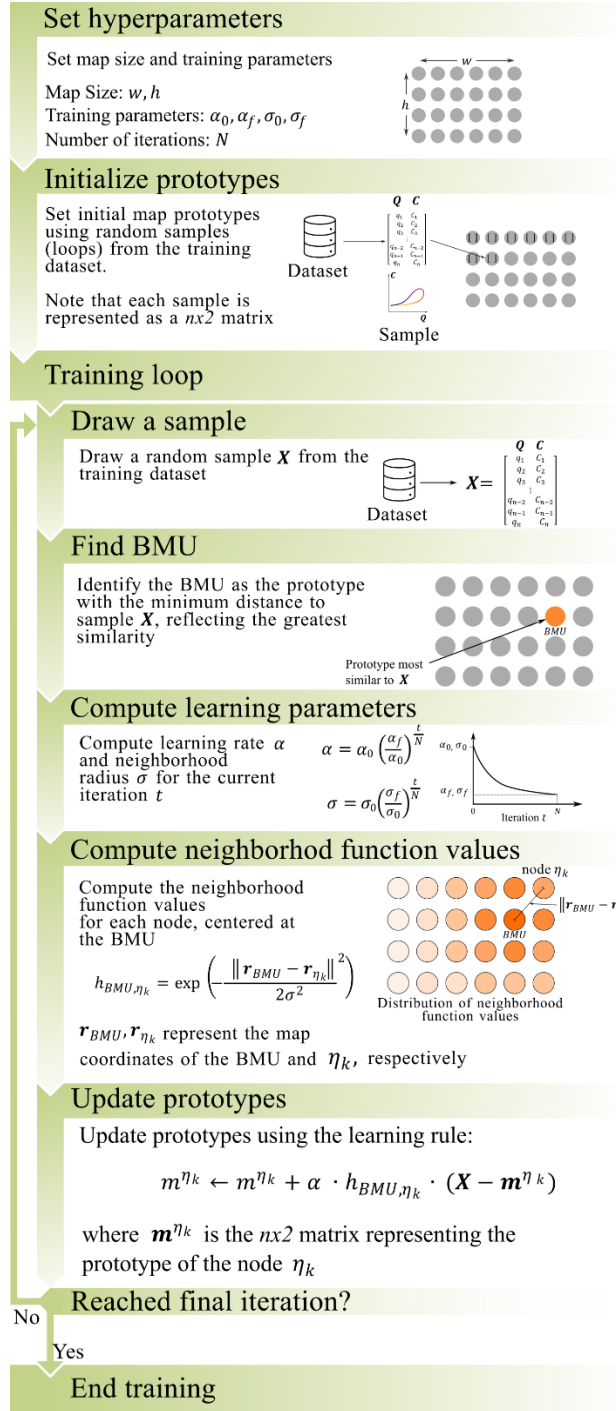


Figure 4. Workflow for training an SOM. α : learning rate, σ : neighborhood radius, subscripts 0, f indicate initial (first iteration) and final (last iteration) values, respectively. Q : Discharge, C : Concentration, n : length of the sequence of (Q, C) data pairs representing a loop (section 2.3). Other symbols are defined in the figure.

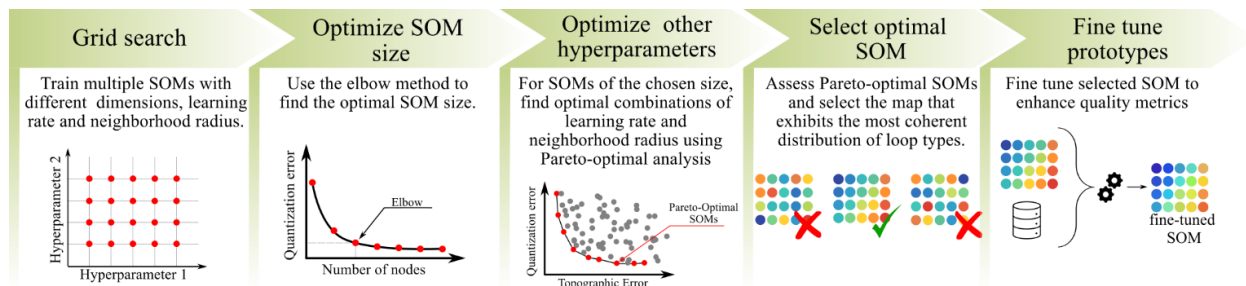


Figure 5. Workflow for fine-tuning SOM hyperparameters using a combination of quantitative metrics and qualitative assessment. The process begins with training multiple SOMs across a grid of map sizes, learning rates, and neighborhood radii. Quantization error is evaluated to identify the optimal map size using the elbow method. A subset of high-quality maps—selected from the Pareto frontier of topographic and quantization errors—is then examined in detail. SOM selection is based on visual inspection, prioritizing maps that exhibit coherent transitions between similar loop types and clear separation between contrasting ones. Finally, retraining of the selected SOM may enhance quantization accuracy.

A.2 Proposed new section S in the SI to better explain the DTW algorithm

S1. Dynamic Time Warping

Figure S1 illustrates the difference between Euclidean distance and dynamic time warping (DTW) for one-dimensional sequences. Euclidean distance compares time series by matching values at the same time index, resulting in larger distances if sequences are misaligned. In contrast, Dynamic Time Warping (DTW) flexibly matches points across time to minimize overall distance. For example, x_3 in the first sequence is matched with y_5 in the second sequence.

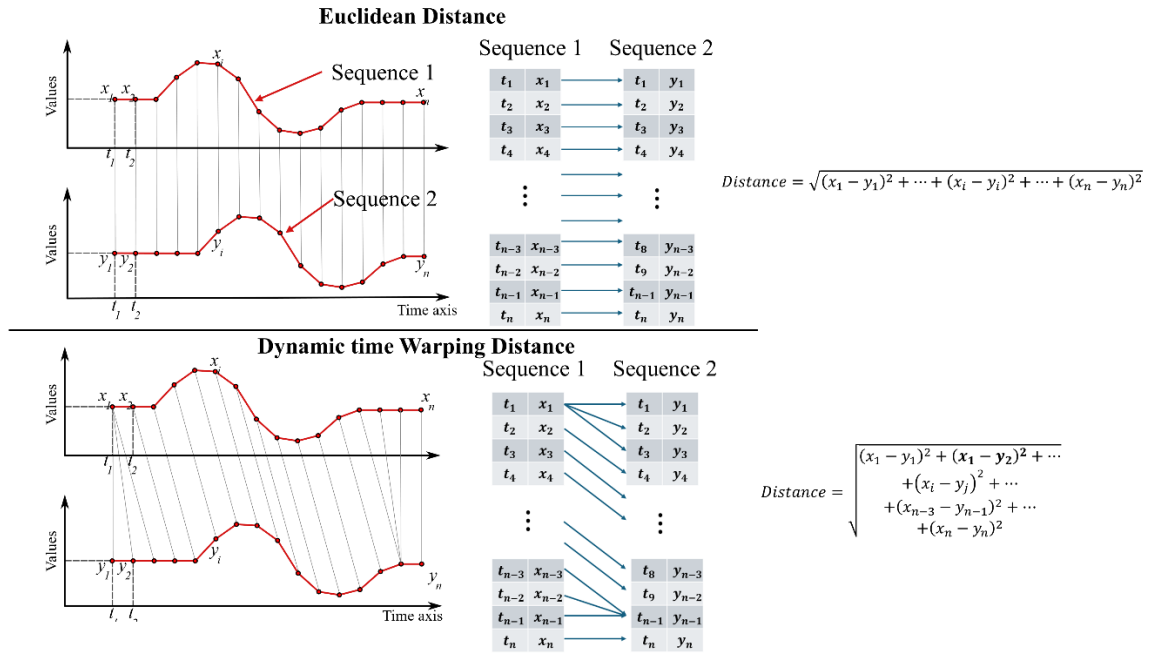


Figure S1. Comparison between Euclidean distance and Dynamic Time Warping distance for one-dimensional sequences

The same principle applies to two-dimensional sequences, as illustrated by the two hysteresis loops in Fig. S2. DTW flexibly matches nearby points along the trajectory on the Q-T plane, resulting in lower distances when the loops follow similar paths. In contrast, Euclidean distance is sensitive to time misalignments and compares points at fixed positions—leading to larger distances even when the overall loop shapes are similar.

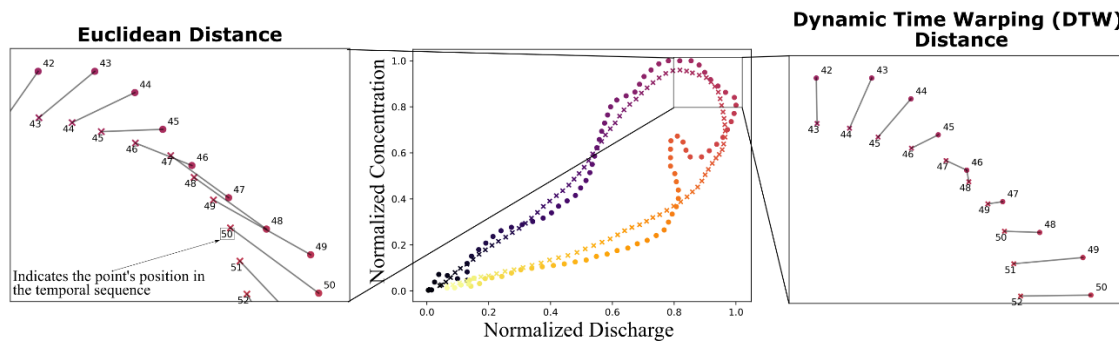


Figure S2. Comparison between Euclidean distance and Dynamic Time Warping distance for two-dimensional sequences