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Evaluating Raw Data And Factor Scores For Trend Surface Mapping With Special Reference To The Kutch-Kathiawar Geomorphotectonics

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Abstract
This research paper evaluates the distinctions between raw data and factor scores in trend surface mapping, with a specific focus on the geomorphotectonics of the Kutch-Kathiawar region in India. It emphasizes that raw data maps represent the spatial distribution of directly measured variables, capturing both signal and noise, while factor score maps present a more abstract spatial pattern derived from multivariate statistical analysis. Utilizing principal component analysis (PCA), the study identifies five significant factors related to geochemical variables in India's hot springs, explaining 84.037% of total variance. The trend surface analysis (TSA) enhances these findings by visually depicting the distribution of these geochemical variables, revealing notable geological implications. The paper challenges the prevailing notion that the Kutch-Kathiawar outlier is an extension of the Indian Peninsula, arguing instead for its distinction based on litho-tectonic patterns and other geological features, supporting its classification as a product of the Great Himalayan Orogeny. Ultimately, the study illustrates how raw data trend surfaces may appear more informative than factor score maps, yet each serves a unique purpose in geological analysis.

Keywords: *PCA analysis, Factor scores, Raw data, Trend surface analysis, geothermal geochemistry, Peninsular and Extra-Peninsular India, Kutchch-Kathiawar outlier, geomorphotectonics*

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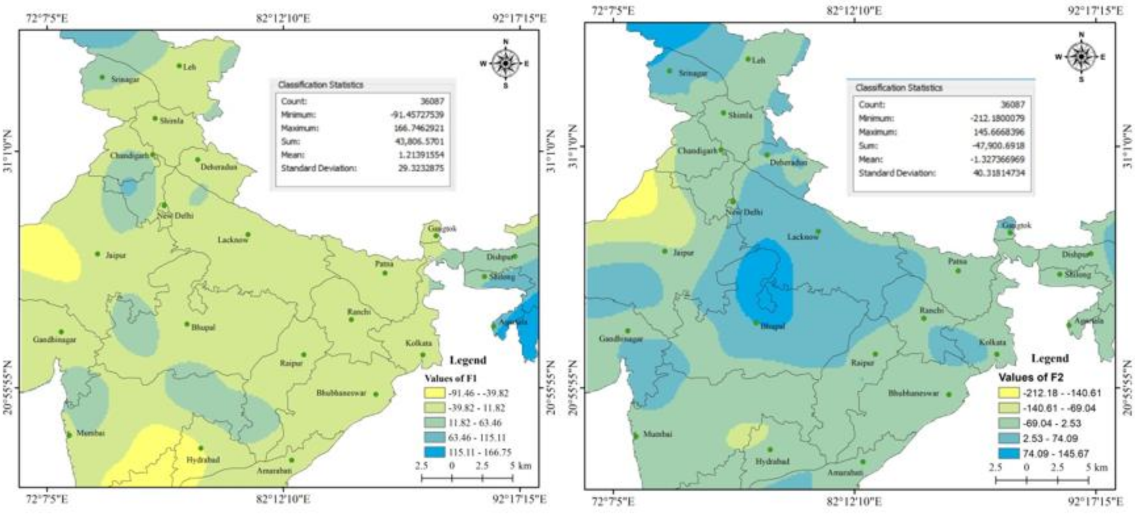
In trend surface mapping, the fundamental distinction between raw data and factor scores is that raw data maps represent the spatial distribution of a singular, directly measured variable, whereas factor score maps illustrate the spatial pattern of abstract, unobserved factors statistically derived from multiple original variables.

Fig. 1. Cubic Polynomial PCA Factor Scores Trend Surface Maps



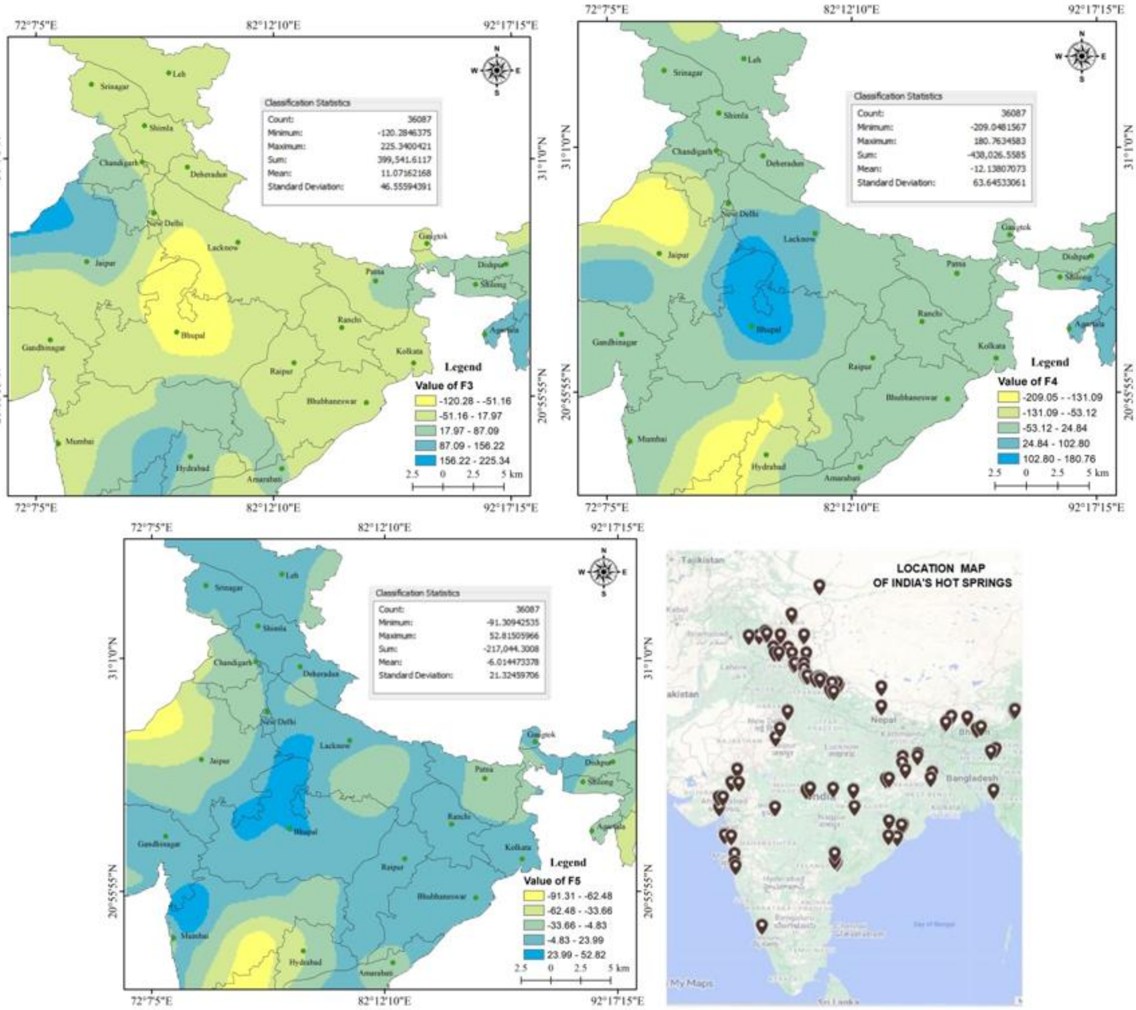
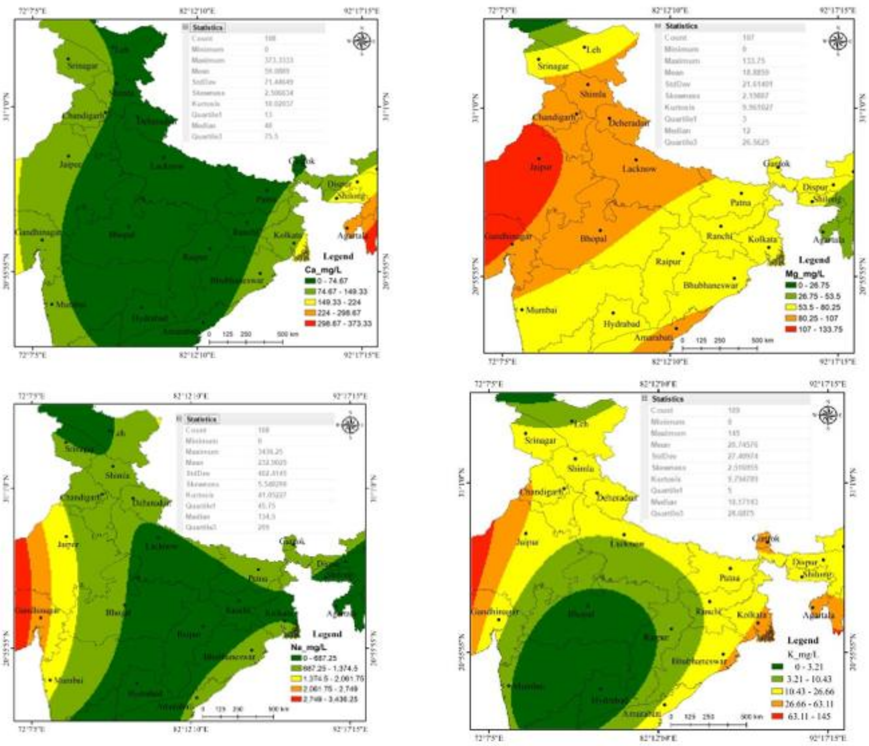
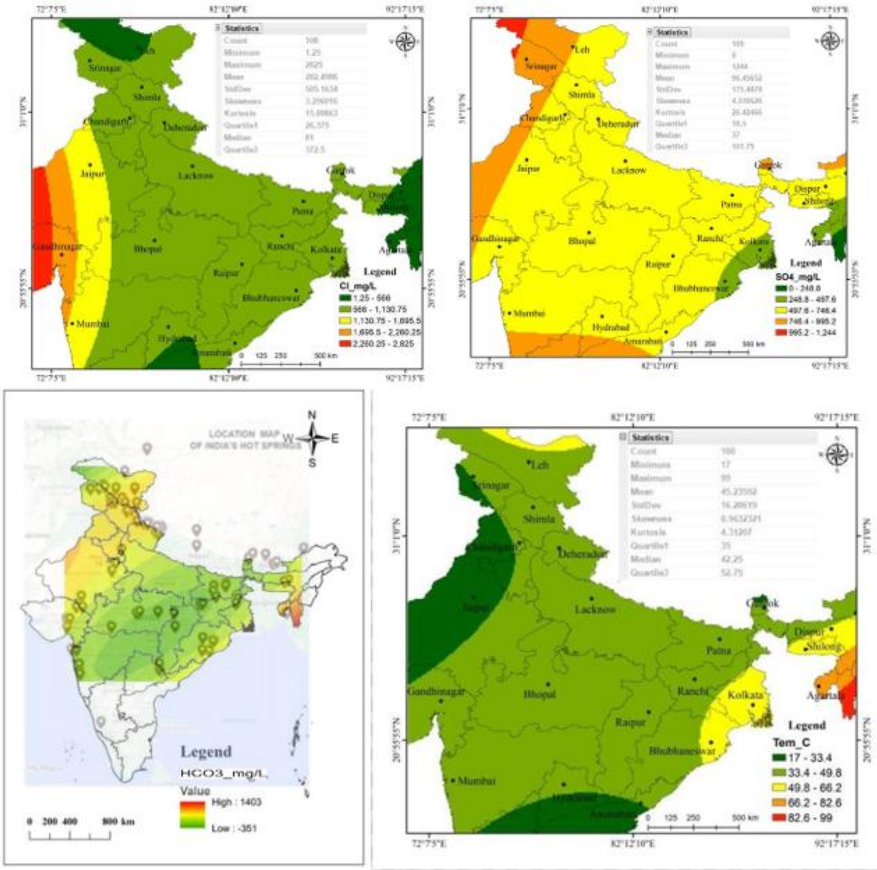


Fig. 2. Cubic Polynomial Raw data Trend Surface Maps





Here are the major causes behind the differences:

Raw data trend surface map

A raw data trend surface map is constructed by fitting a mathematical surface (often a low-order polynomial) to the original data points.

- **Shows both signal and noise**: This map shows the whole spatial pattern of the original data, including regional "signal" and local "noise" or residuals. The surface reflects the overall trend, and the remaining variances (the residuals) comprise the finer, local-scale changes.
- **More complex:** When higher-order polynomial fits or more advanced interpolation methods (such as Kriging) are used, the resulting map can appear more intricate and textured because they directly reflect the raw measurements' local fluctuations.

Factor score trend surface map

A factor score trend surface map is a spatial representation of a multivariate statistical construct. Factor analysis reduces a large number of correlated variables into a smaller set of underlying dimensions or "factors". The trend surface is then created by interpolating the scores for one of these abstract factors, not the original variables.

- **Filtering Effect:** Factor scores effectively "filter" the original data. They primarily capture the *common* variance shared among related variables, while potentially downplaying or removing the unique variance or noise associated with individual raw variables. This inherent smoothing or abstraction process means the resulting factor scores may show less local variation or "jaggedness" than the raw data, resulting in a less detailed or "different" looking surface.
- **Dimensionality Reduction:** By reducing the data into fewer factors, some information is inevitably lost. The trend surface of a factor score reflects only the spatial pattern of that specific underlying dimension, not the entire, complex spatial pattern of all the original, individual variables combined.

Interpretation and Scale

- **Raw Data Maps:** These maps are directly interpretable in terms of the original variable's units and values (e.g., elevation in meters, fluoride content in mg/l). They show the actual measured distribution across the surface.

- **Factor Score Maps:** These maps depict the spatial patterns of the *latent* factors, which are inferred constructs. Their interpretation relies on understanding which original variables load highly onto that factor. The surface shows the spatial expression of this abstract concept, which may not align visually with a single, concrete raw data map.

In summary, the raw data map might seem "better" because it is a more complete and direct representation of the original measurements. The factor score map is an analytical tool that presents a more abstract, generalized, and filtered view of the underlying structure of the data, which serves a different purpose in spatial analysis.

Why raw data may seem "better"

The "better" quality that one perceives in a map is most likely an instinctive reaction to viewing the map created from measured raw data. A map of factor scores is a step away from reality, indicating a theoretical dimension rather than a measurable variable. This abstraction is useful for statistical research, but it may feel less "right" or informative when viewed as a geographical surface. The sense that the raw data map is "better" is likely due to the fact that it displays full spatial detail and is easier to interpret. The raw data map is more similar to the "ground truth" of your field measurements. The factor score map takes a step back, expressing a statistical abstraction of underlying processes rather than direct observations.

Finally, the decision is based on the objective. If one wants to see the particular spatial patterns of a single, directly observed variable, a raw data map is appropriate. A factor score trend surface map is the appropriate tool for identifying and mapping the regional spatial patterns of underlying dimensions that influence a wide range of variables.

A case study with a focus on the Kutch-Kathiawar geomorphotectonic outlier

Factor score trend surface map

Two data types are essential for trend surface analysis: geographical location (data point coordinates) and continuous multivariate numeric variables that define each data point's measurements. The primary dataset used in this study, GTHREV.xlsx, contains 181 rows and 11 columns, with coordinates and multivariate data. A reduced subspace, TSA_FSCORES.xlsx, from PCA analysis, features two columns for coordinates and five for calculated factor scores (Amitabha Roy, 2024).

Outcomes from the principal component analysis (PCA) reveal significant insights into fluid geochemical variables within India's hot springs. Retaining five PCA factors—F1 (Ca, Mg, Na, K), F2 (HCO3), F3 (SO4), F4 (Temperature), and F5 (Cl)—these factors collectively account for 84.037% of the total variance, as indicated by the scree plot. The eigenvalues considered significant are greater than or equal to 0.6, underscoring the relevance of the variables for these factors.

Trend Surface Analysis (TSA) utilising GIS techniques enhances the PCA results by offering a visual depiction of the calculated scores, reflecting the actual distribution of geochemical variables (Fig. 1). Using polynomial trend surfaces with power 3 generates clearer patterns than the original data.

Notably, the basic/alkaline group F1 is moderately common in India's peninsular hot springs. Intensity variations of the acid-base group F2 (HCO3) exist across different locations, while F3 (SO4) shows lower concentrations in central highlands but increases towards western and southern India. An interesting inverse relationship between SO_4 concentrations and temperature in central highlands warrants further investigation.

Additionally, F5 (Cl) is consistently found across peninsular and extra-peninsular hot springs. The TSA contours, characterized by southeasterly convexity in the western region, especially for HCO3, SO4, Cl, and Temperature factors, resemble the geological formations of the Kirther-Sulaiman hills in Pakistan, illustrating the broader geological implications of the findings.

Raw data trend surface map

Fig. 3, Juxtaposition of Sulaiman-Kirther-Hindukush and Kutchch-Kathiawar arcate

Following the same statistical definition of an outlier—an outlier is an observation that differs significantly from other values in a random sample of a population—the author disputes the widely held belief that the Kutchch-Kathiawar outlier is an extension of the main Indian Peninsula, despite its distance from the unit under consideration. Kathiawar and Kutch terranes differ significantly in many ways, including litho-tectonic pattern, volcanism and magmatism (Girnar Hill granites), Girnar laccoliths, concordant body with a flat bottom and convex upward dome-shaped hills, mini-arcuate east-southeasterly convexity, and active seismicity resembling the western extension of smaller arcs of the Himalayan extension in central and south Asia (Karakorams-Hindukush and its southern extension, Sulaiman-Kirther hills in Pakistan), and Orthophragminids foraminifera from the Bartonian Fulra Limestone in Kutch, India, and the coeval or contemporary units in the Sulaiman Range in Pakistan (Ercan Özcan`et. Al, 2018), all of these distinguishing features of the Kuchch-Kathiawar outlier strongly support its outlier status and genesis as synonymous with the Great Himalayan Orogeny, as opposed to the widely held belief that it is an extension of the main Indian Peninsula, despite its remote location. Finally, the spatial statistical technique used in this study adds sophistication to the analysis, allowing for a better understanding of the geological dynamics at play in the Kathiawar (Saurashtra)-Kutchch anomaly.

Comparing Fig. 3 with Fig. 2, it is quite obvious that raw data trend surface maps give a "better" quality as compared to the factor score maps (Fig.1) that one perceives in a map of geomorphotectonics of the Kutchch-Kathiawar outlier and overall geotectonic settings of Peninsular and especially Extra-Peninsular (Himalayan) as synonymous with the Great Himalayan Orogeny, as opposed to the widely held belief that it is an extension of the main Indian Peninsula, despite its remote location. The most noticeable feature is that the trend surfaces reflect the overall trend, curvilinear east and southeasterly convexity, straight faults connecting Kutchch-Kathiawar all the way through the Karakoram-Hindukush hills in the northwest Himalayas, and the remaining variances (the residuals) represent finer, local-scale changes. This zone is particularly vulnerable to major earthquakes, and any development works would be suicidal.

I. Conclusions

In conclusion, while both raw data and factor score trend surface maps are valuable tools in geological analysis, they serve distinct purposes: raw data maps offer a direct representation of measured variables, capturing both signal and noise, and factor score maps present a more abstract, statistically filtered view of underlying dimensions. As exemplified by the Kutch-Kathiawar geomorphotectonics case study, raw data maps may subjectively appear "better" due to their detailed spatial representation, but factor score maps are crucial for identifying regional patterns influencing multiple variables, ultimately supporting the classification of the Kutch-Kathiawar outlier as a product of the Great Himalayan Orogeny, rather than an extension of the Indian Peninsula.

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