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# Trend Surface Mapping of Principal Component Factor Scores to Assess the Geothermal Geochemistry of India's Peninsular and Extra-Peninsular Hot Springs

Amitabha Roy[1], Ex-Senior Director, Geological Survey of India;
Sk Mafizul Haque[2], Assistant Professor, Cartography, RS, and GIS,
*Geography Department, University of Calcutta, India*

***Abstract***
*This research paper presents a comprehensive analysis of the geothermal geochemistry of hot springs in India, focusing on two distinct regions: the tectonically active Extra-Peninsular Himalayan region and the relatively stable Late-Precambrian mobile belts of Peninsular India. Utilizing multivariate statistical techniques, particularly Principal Component Analysis (PCA) and Trend Surface Analysis (TSA), the study investigates approximately 340 hot springs by examining their geochemical data. The PCA results identify five significant factors that account for 84.037% of the total variance in the geothermal data, facilitating the classification of geochemical components into distinct groups. The TSA further enhances the understanding of spatial patterns in the geothermal geochemistry by providing a graphical representation of the computed PCA factor scores, revealing the distribution of geochemical variables across the study area. The findings of this study contribute valuable insights into the geothermal potential of India, highlighting the interplay between geological settings and geothermal characteristics, and serve as a foundation for future geothermal energy development initiatives in the region.*

***Keywords:*** *PCA analysis, Factor scores, Trend surface analysis, geothermal geochemistry, Peninsular and Extra-Peninsular India*

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## I. Introduction

This study expands on previous research that examined spatially dependent multivariate geothermal hot spring data from two regions with diverse geologic-tectonic settings: a 2,400 km-long arc in the tectonically active Extra-Peninsular Himalayan region and the relatively stable Late-Precambrian or Proterozoic mobile belts in Peninsular India's Central Highlands. employing a variety of robust multivariate statistical techniques. to spatially dependent multivariate geothermal geochemistry data from hot springs in two regions with. There are around 340 hot springs located throughout India, including the Peninsular and Extra-Peninsular regions. Schlagintweit compiled the first list of hot springs in India in 1852. In 1991, the Geological Survey of India produced a 'Geothermal Atlas of India' (Ravi Shanker), and the Indian government established a 'Hot Spring Committee' to investigate the development of geothermal power plants. Projects in the Puga Valley and Parvati aim to harvest 5000 MWh of geothermal energy, which is enough to run a 20 MWe power plant (Jonathan Craig, 2013). GTHERMIS is a computerised geothermal database system developed by the GSI (A. Roy, 1994).

The current study explores the multivariate geospatial fluid geochemistry of geothermal hot spring data in two ways: statistically and graphically using the GIS approach.

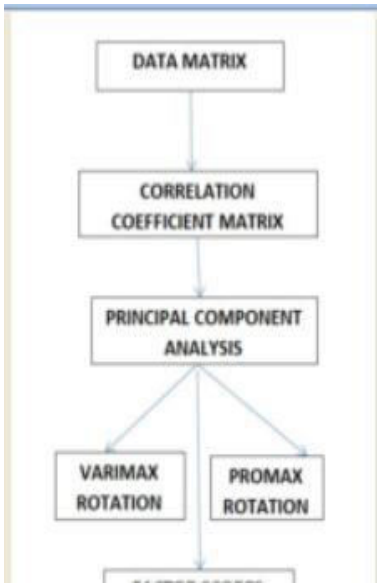
**Software choice**

Principal component analysis (PCA) was performed in Excel using the XLSTAT statistical software's 14-day trial add-on feature located under the Analyse Data menu. Dr Sk Maffizul Haque performed interpolation by polynomial trend surface analysis of statistically computed data using ArcGIS software in his Cartography, RS, GIS laboratory at Calcutta University's Geography Department.

## II. PCA Mathematics

Principal Component Analysis (PCA)
Observations/variables table: Workbook = GFACTREV.xlsx / 181 rows and 9 columns
PCA type: Pearson Correlation
Filter factors: Maximum number = 5
Standardisation: (n)

**Table I. Computational strategy / Flow chart of Principal Component (PCA)**




**Algorithm 1** Principal Component Analysis

1: **function** PCA($X$)
2: Compute the correlation matrix by:

$$r_{xy} = \frac{\sum(x_i - x)(y_i - y)}{\sqrt{\sum(x_i - \bar{x})^2 \sum(v_i - \bar{v})^2}}$$

3: Compute the eigenvalues and eigenvectors of $\Sigma_x$
4: Define the transformation matrix $T = [\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_d]$ with the d eigenvectors associated to the d largest eigenvalues.
5: Project the data $X$ into the PCA subspace:

$$\mathbf{y}_i = T\mathbf{x}_i \quad \text{for} \quad i = 1, 2, \ldots, n$$

6: **return** $Y$
7: **end function**

F

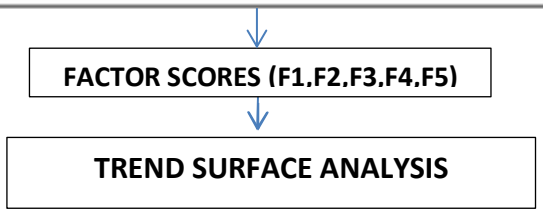
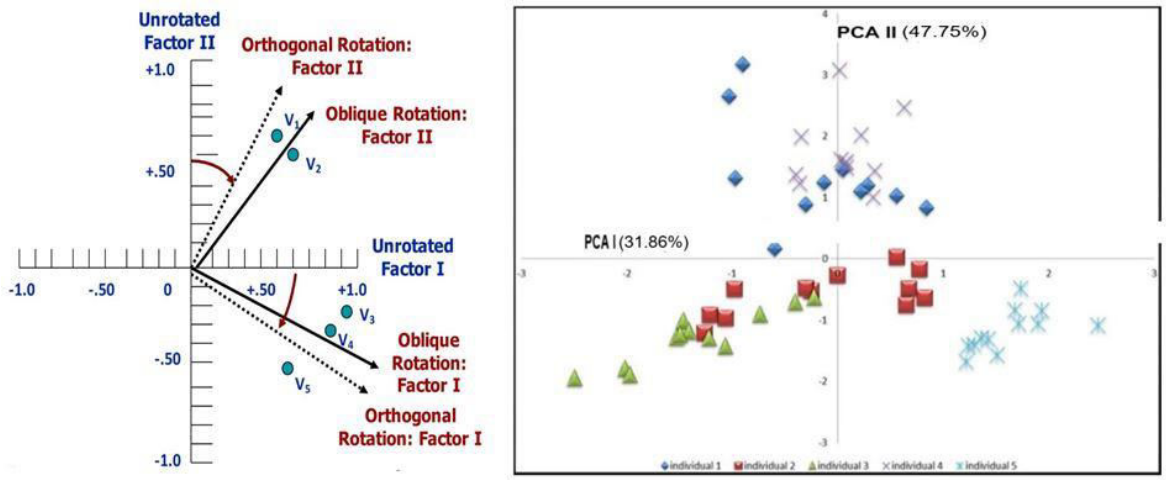


**Fig.1.Schematicdiagramof unrotated PCA in relation to rotated Varimax&Promax**




Principal component analysis (PCA) is the foundation of a statistical approach for data reduction, or 'dimension reduction' of a dataset with multiple variables as input. It generates a dataset in a lower subspace that is a new reduced orthogonal or uncorrelated variable known as principal components, which are obtained as linear combinations of the original variables, thereby extracting the principal components containing the most significant information and rejecting noise or insignificant data while preserving all critical details. Recomputing a set of factor scores involves assigning values to these new variables based on observations. The correlation coefficient matrix is the initial stage in PCA analysis (Tables 2-6).

Unrotated Principal Component Analysis (PCA) brings about a linear orthogonal transformation of m original variables, geochemical elements in the m-dimensional measurement space to m new statistically independent variables or principal components where each new variable is a linear combination of the old. The PC analysis extracts m-eigenvectors (principal component axes) and corresponding m-eigenvalues (the variance measured along the eigenvector) from m x m symmetrical matrix of correlation. The results of PC analysis is given in Table-4B.3, and 4B.4. The columns of this PCT matrix are all orthogonal and hence inter-column correlations are near Zero. These columns represent eigenvectors (directions) and eigenvalues (coefficients attached to eigenvectors) from the correlation coefficient matrix. The eigenvalues account for all of the original data variances in the decreasing order such that each has variance or eigenvalue less than previous ones. The principal components are then converted into factors scores by multiplying each element of the principal components or eigenvectors (V) by the square root of the corresponding eigenvalues (that is, $H=\lambda^{1/2} V$). These, besides the direction, also represent the variances.

In the Exploratory Factor Analysis the most baffling issue is to determine the number of factors to retain significant few from many insignificant ones. There are different criteria suggested by different researchers namely,

● The Eigenvalue > 1

● From the inflection point of scree or Elbow curve plot i.e. a graph of the eigenvalues (Y-axix) against the factors (X-axis) listed in the descending order (Fig. 4B.2).

● Communalities for each of the variables (somewhat like R2 from Regresion analysis) at least 0.5

● The factor loadings for each variable should be ≥0.6 (Awang, 2014).

In the present study, the scree plot was used for the selection of five factors which accounts for 84.037% of the total variance of the original varables "load"on a factor of Principal component is retained.

**Presenting the output results of PCA**

**Table 2. Correlation matrix (Pearson (n):**

| Variables | HCO3 mg/L | Cl mg/L | SO4 mg/L | Ca mg/L | Mg mg/L | Na mg/L | K mg/L | F mg/L | Temp_C |
|---|---|---|---|---|---|---|---|---|---|
| HCO3 mg/L | **1** | 0.047 | 0.143 | -0.033 | 0.113 | 0.065 | 0.542 | 0.021 | 0.057 |
| Cl mg/L | 0.047 | **1** | 0.188 | 0.344 | 0.168 | 0.429 | 0.311 | -0.159 | 0.066 |
| SO4 mg/L | 0.143 | 0.188 | **1** | 0.670 | 0.126 | 0.058 | 0.377 | -0.052 | 0.009 |
| Ca mg/L | -0.033 | 0.344 | 0.670 | **1** | 0.489 | 0.434 | 0.286 | -0.152 | -0.069 |
| Mg mg/L | 0.113 | 0.168 | 0.126 | 0.489 | **1** | 0.757 | 0.287 | -0.092 | -0.014 |
| Na mg/L | 0.065 | 0.429 | 0.058 | 0.434 | 0.757 | **1** | 0.292 | -0.098 | 0.010 |
| K mg/L | 0.542 | 0.311 | 0.377 | 0.286 | 0.287 | 0.292 | **1** | -0.011 | 0.020 |
| F mg/L | 0.021 | -0.159 | -0.052 | -0.152 | -0.092 | -0.098 | -0.011 | **1** | 0.216 |
| Temp_C | 0.057 | 0.066 | 0.009 | -0.069 | -0.014 | 0.010 | 0.020 | 0.216 | **1** |

**Principal Component Analysis:**

**Table 3. Eigenvalues:**

| | F1 | F2 | F3 | F4 | F5 | F6 | F7 | F8 | F9 |
|---|---|---|---|---|---|---|---|---|---|
| Eigenvalue | 2.867 | 1.430 | 1.239 | 1.111 | 0.917 | 0.707 | 0.359 | 0.201 | 0.170 |
| Variability (%) | 31.860 | 15.886 | 13.766 | 12.339 | 10.185 | 7.852 | 3.990 | 2.229 | 1.891 |
| Cumulative % | 31.860 | 47.747 | 61.513 | 73.852 | 84.037 | 91.890 | 95.880 | 98.109 | 100.000 |

**Fig. 2. Scree plot**

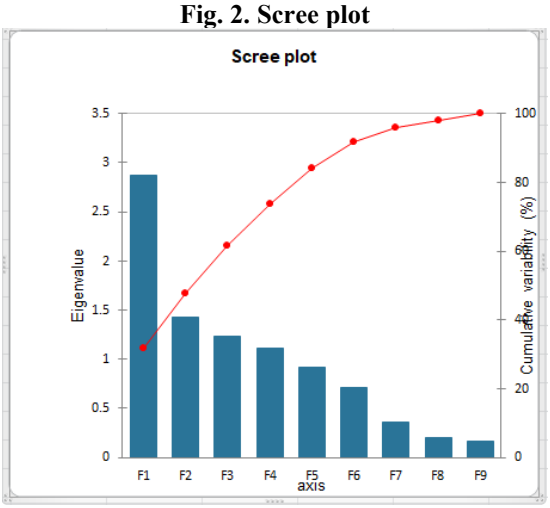



**Table 4. Eigenvectors:**

| | *F1* | F2 | F3 | F4 | F5 |
|---|---|---|---|---|---|
| *HCO3 mg/L* | *0.176* | 0.624 | -0.079 | -0.423 | -0.053 |

| | | | | | |
|---|---|---|---|---|---|
| *Cl mg/L* | *0.335* | -0.068 | -0.046 | 0.050 | 0.711 |
| *SO4 mg/L* | *0.335* | 0.193 | 0.566 | 0.349 | -0.118 |
| *Ca mg/L* | *0.461* | -0.169 | 0.308 | 0.305 | -0.153 |
| *Mg mg/L* | *0.426* | -0.224 | -0.370 | -0.061 | -0.366 |
| *Na mg/L* | *0.439* | -0.261 | -0.441 | -0.059 | -0.046 |
| *K mg/L* | *0.379* | 0.473 | 0.020 | -0.221 | 0.026 |
| *F mg/L* | *-0.121* | 0.335 | -0.315 | 0.485 | -0.416 |
| *Temp C* | *-0.009* | 0.294 | -0.381 | 0.559 | 0.380 |

**Table 5. Factor loadings:**

| | *F1* | F2 | F3 | F4 | F5 |
|---|---|---|---|---|---|
| *HCO3 mg/L* | *0.297* | 0.746* | -0.088 | -0.446 | -0.051 |
| *Cl mg/L* | *0.568* | -0.081 | -0.052 | 0.053 | 0.681* |
| *SO4 mg/L* | *0.567* | 0.230 | 0.630* | 0.367 | -0.113 |
| *Ca mg/L* | *0.780** | -0.203 | 0.343 | 0.321 | -0.146 |
| *Mg mg/L* | *0.721** | -0.267 | -0.412 | -0.064 | -0.351 |
| *Na mg/L* | *0.743** | -0.312 | -0.491 | -0.062 | -0.044 |
| *K mg/L* | *0.642** | 0.566 | 0.023 | -0.233 | 0.025 |
| *F mg/L* | *-0.204* | 0.401 | -0.351 | 0.511 | -0.398 |
| *Temp C* | *-0.015* | 0.352 | -0.424 | 0.589* | 0.363 |

**Note:** * ≥ 0.6

**Table 6. Factor scores:**

| X_LONG | Y_LAT | F1 | F2 | F3 | F4 | F5 |
|---|---|---|---|---|---|---|
| 87.25 | 23.52 | -1.119 | -0.560 | 0.051 | -0.062 | 0.469 |
| 87.25 | 23.52 | -0.870 | -0.107 | -0.182 | 0.032 | 0.326 |
| 84.862 | 19.2647 | -0.117 | 1.206 | -1.322 | 1.228 | -0.930 |
| 842350 | 19.2905 | -1.452 | 0.679 | -1.050 | 1.483 | -0.395 |
| 84.0212 | 23.4515 | -0.931 | -0.473 | 0.245 | 0.000 | 0.645 |
| 84.294 | 23.492 | -0.789 | -0.497 | 0.037 | -0.168 | 0.354 |
| 85.25 | 25.01 | -1.391 | -0.787 | 0.083 | 0.008 | 0.608 |
| 85.41 | 24.09 | -1.038 | -0.611 | 0.183 | 0.030 | 0.669 |
| 93.15 | 28.2 | -0.618 | 0.100 | -0.055 | -0.552 | 0.370 |
| 93.26 | 28.25 | 0.609 | 0.038 | 1.176 | 0.177 | -0.218 |
| 93.25 | 28.273 | -0.626 | -0.236 | 0.382 | -0.617 | 0.227 |
| 77.1502 | 32.3295 | -0.605 | -0.750 | 0.913 | -1.639 | -0.239 |
| 77.3473 | 32.0278 | -1.143 | 0.938 | -0.896 | 1.369 | -2.812 |
| 78.37 | 32.0345 | 5.859 | 1.859 | 2.681 | 1.704 | -0.916 |
| 77.47 | 31.314 | -0.467 | -0.267 | 0.243 | -0.384 | 0.115 |
| 77.582 | 31.342 | -0.538 | -0.147 | 0.201 | -0.758 | 0.535 |
| 78.105 | 31.3 | 0.640 | 0.372 | 1.326 | -0.412 | -1.205 |
| 78.223 | 31.35 | -1.439 | 0.802 | -1.123 | 1.683 | -0.650 |
| 78.23 | 31 | -0.291 | 0.696 | -0.803 | 0.920 | 1.240 |
| 78.25 | 30.572 | -0.884 | -0.077 | -0.312 | 0.682 | 0.132 |
| 78.3336 | 30.5502 | -1.413 | -1.051 | 0.444 | -0.474 | 0.015 |
| 78.4012 | 30.5325 | -1.247 | 0.750 | -0.888 | 1.253 | -0.467 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 78.433 | 30.5325 | -0.758 | 0.037 | -0.455 | 0.431 | -0.587 |
| 79.0135 | 30.3905 | -0.356 | 0.721 | -1.364 | 0.741 | -1.255 |
| 79.293 | 30.4445 | 0.649 | 0.344 | -1.126 | 1.323 | 2.282 |
| 79.352 | 30.4158 | -0.384 | -0.416 | -0.719 | 0.646 | 0.303 |
| 79.313 | 36.325 | -1.012 | -0.523 | 0.156 | 0.067 | 0.526 |
| 79.481 | 30.36 | 1.150 | 1.357 | -1.793 | -0.996 | -1.217 |
| 79.373 | 30.293 | -0.547 | -0.251 | -0.197 | -0.104 | 0.248 |
| 80.5313 | 30.0527 | -1.300 | -0.630 | -0.147 | 0.252 | 0.462 |
| 80.0856 | 29.58 | 0.977 | 2.455 | -0.923 | -1.731 | -0.024 |
| 80.2023 | 30.0853 | 0.102 | 0.845 | 0.310 | -1.667 | -0.209 |
| 80.3384 | 29.515 | -0.362 | 0.634 | -0.871 | 0.420 | 0.603 |
| 773240 | 34.465 | -0.995 | 0.258 | -0.221 | 0.535 | 0.377 |
| 77.333 | 34.4525 | -0.646 | 0.100 | -0.058 | -0.018 | 0.481 |
| 77.2825 | 34.564 | 0.742 | 2.962 | -0.207 | -2.953 | 0.010 |
| 75.0345 | 33.162 | 3.965 | -0.289 | 5.407 | 3.080 | -1.600 |
| 75.443 | 33.431 | 0.493 | -0.066 | 0.743 | 1.530 | -0.079 |
| 75.523 | 33.303 | -1.493 | -0.328 | -0.334 | 0.721 | 0.248 |
| 76.562 | 33.204 | -1.491 | 0.995 | -1.292 | 2.358 | -0.429 |
| 78.195 | 33.13 | -1.565 | -0.185 | -0.349 | 0.864 | -0.972 |
| 78.21 | 33.22 | -1.525 | 0.266 | -1.021 | 1.866 | -0.349 |
| 76.0425 | 32.421 | 0.198 | 0.256 | -0.364 | -0.574 | 0.415 |
| 76.105 | 32.0755 | -0.624 | -0.806 | 0.632 | -1.234 | -0.373 |
| 76.431 | 32.071 | -1.195 | -1.203 | 0.694 | -0.938 | -0.009 |
| 77.04 | 28.15 | 2.322 | -0.583 | -1.087 | 1.824 | 0.204 |
| 77.04 | 28.15 | -0.348 | -0.777 | 0.711 | -1.122 | -0.423 |
| 76.193 | 26.353 | -0.016 | -0.444 | 0.834 | -1.007 | -0.190 |
| 76.53 | 27 | -0.017 | -0.299 | -0.186 | -0.304 | -0.482 |
| 73.411 | 24.11 | -0.063 | -0.329 | -0.196 | -0.736 | -0.113 |
| 73.424 | 24.13 | -0.848 | -0.022 | -0.371 | 0.351 | -0.779 |
| 72.1544 | 21.4053 | 9.517 | -4.682 | -5.473 | -0.689 | -2.277 |
| 72.1544 | 21.4053 | -0.589 | -0.197 | 0.035 | -0.494 | 0.252 |
| 72.12 | 22.15 | 2.686 | -1.547 | -1.170 | -0.335 | 2.630 |
| 72.41 | 22.14 | 4.631 | 4.078 | 1.452 | -3.438 | 1.704 |
| 71.4331 | 23.4329 | 1.129 | -1.320 | -0.410 | -0.568 | 1.003 |
| 73.56 | 23.2 | -0.699 | -0.797 | 0.221 | -0.419 | 0.051 |
| 72.51 | 19.423 | 3.115 | -1.792 | 0.340 | 0.827 | 5.059 |
| 72.543 | 19.4105 | 0.391 | -1.774 | 1.588 | -0.517 | 0.303 |
| 73.05 | 19.293 | 1.488 | -1.494 | 1.395 | 1.238 | 1.125 |
| 73.27 | 18.04 | -0.508 | -0.130 | -0.286 | 1.732 | 1.179 |
| 73.24 | 17.43 | -0.530 | -0.903 | 0.362 | -0.076 | 0.702 |
| 73.35 | 17.15 | -0.511 | -0.928 | 0.545 | 0.002 | 0.658 |
| 76.1666 | 21.4196 | 0.074 | -0.985 | -0.068 | 0.361 | 0.262 |
| 74.25 | 23.1435 | -1.077 | 0.505 | -0.827 | 1.295 | 0.976 |
| 80.4315 | 17.55 | -0.925 | 0.948 | -0.825 | 0.842 | -0.086 |
| 80.563 | 17.383 | -0.301 | -0.415 | 0.325 | 0.040 | 0.384 |
| 80.4425 | 17.5545 | 0.655 | -0.554 | -0.298 | -0.503 | -0.593 |
| 80.43 | 17.56 | -0.740 | 0.095 | -0.163 | 0.895 | 0.139 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 80.4 | 18.06 | -0.511 | -1.222 | 1.170 | -1.119 | -0.397 |
| 83.6839 | 23.6988 | -0.152 | 2.609 | -1.334 | -0.258 | 1.463 |
| 90.43 | 27.51 | 2.776 | -0.082 | 2.713 | -0.419 | -0.418 |
| 85.23 | 27.67 | 0.370 | -0.957 | 0.760 | -1.424 | -0.082 |
| 81.8661 | 21.2787 | -0.020 | 1.121 | 0.502 | -2.968 | 0.204 |
| 75.5 | 33.291 | -1.299 | -0.523 | 0.017 | 0.063 | -0.076 |
| 84.4881 | 20.8453 | 0.357 | 0.831 | -0.040 | -0.574 | -0.719 |
| 85.2066 | 20.9573 | 1.636 | 0.971 | 1.402 | -2.196 | -0.658 |
| 85.5625 | 20 | -0.778 | -0.968 | 1.173 | -1.421 | -0.420 |
| 84.294 | 23.492 | -1.014 | -0.726 | 0.529 | -0.186 | 0.185 |
| 85.19 | 24.55 | -1.364 | -1.461 | 0.949 | -1.278 | -0.267 |
| 85.294 | 25.0015 | -1.370 | -1.458 | 0.964 | -1.270 | -0.254 |
| 73.8413 | 18.4916 | -0.553 | -0.974 | 1.063 | -1.448 | -0.574 |
| 78.37 | 32.0345 | 5.806 | 2.093 | 2.427 | 2.085 | -0.967 |
| 77.47 | 31.314 | 1.620 | 0.635 | -0.457 | 0.385 | 0.586 |
| 78.002 | 31.322 | -0.283 | 0.775 | -0.330 | 0.229 | -0.195 |
| 78.0525 | 31.312 | -0.750 | 1.444 | -1.110 | 1.782 | -0.266 |
| 78.105 | 31.3 | 0.631 | 0.990 | 0.559 | 0.756 | -0.458 |
| 78.1945 | 31.363 | -1.340 | 0.482 | -0.646 | 1.289 | -0.626 |
| 78.203 | 313615 | -0.947 | -0.780 | 0.618 | -0.536 | -0.187 |
| 78.223 | 313500 | -1.368 | 0.494 | -0.791 | 1.183 | -0.576 |
| 78.23 | 31 | -0.350 | 0.813 | -0.903 | 1.061 | 0.880 |
| 78.263 | 30.584 | 6.171 | 1.713 | 2.608 | 0.341 | -1.394 |
| 78.25 | 30.572 | -0.803 | -0.130 | -0.329 | 0.691 | 0.676 |
| 78.1415 | 30.53 | 0.248 | -0.162 | 0.222 | -0.867 | -0.016 |
| 78.2855 | 30.504 | -0.185 | -0.302 | 0.157 | -1.132 | -0.739 |
| 78.41 | 30.56 | -0.339 | 2.279 | -1.249 | 0.610 | -0.339 |
| 78.41 | 30.542 | -0.420 | 1.735 | -0.853 | 0.019 | -0.446 |
| 78.4012 | 30.5325 | -1.077 | 0.204 | -0.345 | 0.426 | 0.006 |
| 78.3912 | 30.5145 | -0.661 | 1.005 | -0.579 | -0.189 | -0.216 |
| 78.3505 | 33.453 | 0.394 | 0.458 | -0.510 | -1.145 | -0.643 |
| 78.43 | 30.5325 | -0.575 | -0.336 | -0.157 | -0.041 | 0.251 |
| 78.5412 | 30.4447 | -0.161 | 0.922 | -0.510 | -0.568 | -0.480 |
| 79.0135 | 30.3905 | -0.049 | -0.052 | -0.675 | -0.344 | -0.181 |
| 79.293 | 30.4445 | 0.710 | -0.259 | -0.392 | 0.237 | 1.835 |
| 79.352 | 30.4158 | -0.354 | -1.092 | 0.146 | -0.625 | -0.497 |
| 79.313 | 36.325 | -1.071 | -0.001 | -0.473 | 0.999 | 0.869 |
| 79.2902 | 30.2902 | 0.439 | 0.514 | -0.684 | -0.645 | -0.430 |
| 80.013 | 30.434 | 1.447 | 2.557 | 0.015 | -2.317 | 0.066 |
| 79.481 | 30.36 | -0.005 | 1.838 | -0.592 | -1.039 | 0.099 |
| 80.5313 | 30.0527 | -1.264 | -1.001 | 0.307 | -0.419 | 0.171 |
| 79.5556 | 29.593 | 0.037 | -0.608 | -0.363 | -1.394 | -0.840 |
| 80.0752 | 29.5832 | -0.885 | -0.088 | 0.478 | -1.226 | -0.024 |
| 80.1509 | 30.0806 | -0.553 | 1.493 | -0.854 | 0.139 | -0.177 |
| 80.173 | 30.0308 | 0.830 | 0.317 | -0.464 | -0.607 | -1.097 |
| 80.404 | 30.034 | -0.869 | -0.610 | 0.520 | -0.478 | 0.031 |
| 80.414 | 29.5825 | -0.231 | -0.800 | 0.578 | -0.870 | -0.505 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 80.3384 | 29.515 | -0.392 | 0.506 | -0.618 | 0.128 | -0.122 |
| 77.324 | 34.465 | -1.319 | 1.332 | -1.297 | 2.174 | -0.476 |
| 77.333 | 34.4525 | -0.952 | 0.566 | -0.348 | 0.467 | -1.155 |
| 77.2825 | 34.564 | 0.406 | 4.315 | -1.642 | -0.789 | -0.507 |
| 74.243 | 33.143 | -0.360 | 0.423 | -0.410 | -0.051 | 0.059 |
| 742940 | 33.123 | -0.726 | -0.538 | -0.142 | -0.084 | -0.154 |
| 74.294 | 33.123 | -0.699 | -0.881 | 0.588 | -0.876 | -0.254 |
| 74.48 | 33.11 | 0.655 | 1.287 | -0.471 | -0.611 | 0.099 |
| 75.0345 | 33.162 | 3.878 | 0.051 | 5.049 | 3.622 | -1.750 |
| 75.0345 | 33.162 | -0.427 | -1.014 | 1.437 | -0.556 | -0.404 |
| 75.072 | 33.17 | 1.127 | 1.395 | -0.407 | -0.079 | 0.809 |
| 75.443 | 33.431 | 0.577 | -0.988 | 1.879 | -0.148 | -0.845 |
| 75.5 | 33.291 | -1.177 | -1.114 | 0.683 | -0.833 | -0.100 |
| 75.523 | 33.303 | -1.354 | -1.256 | 0.750 | -0.892 | -0.102 |
| 76.562 | 33.204 | -1.265 | 0.174 | -0.441 | 1.073 | 0.043 |
| 76.0425 | 32.421 | 0.184 | 0.221 | -0.303 | -0.661 | 0.253 |
| 76.105 | 32.0755 | -0.639 | -0.420 | 0.134 | -0.503 | 0.102 |
| 76.431 | 32.071 | -1.425 | -0.278 | -0.286 | 0.541 | -0.371 |
| 76.193 | 26.353 | -0.018 | -0.166 | 0.467 | -0.470 | 0.215 |
| 76.52 | 27 | 0.098 | -1.037 | 0.670 | -1.580 | -0.727 |
| 73.4118 | 24.11 | -0.080 | -0.453 | -0.012 | -1.000 | -0.438 |
| 73.424 | 24.13 | -0.624 | -0.639 | 0.207 | -0.539 | 0.003 |
| 72.1544 | 21.4053 | -0.646 | -0.869 | 0.254 | -0.466 | 0.101 |
| 72.1544 | 21.4053 | 9.537 | -4.639 | -5.552 | -0.578 | -2.057 |
| 71.05 | 21 | -0.098 | 0.171 | -0.289 | 0.785 | 0.493 |
| 72.41 | 22.14 | 4.590 | 5.413 | -0.278 | -0.901 | 3.426 |
| 72.1553 | 22.4818 | -0.282 | -0.431 | -0.048 | -0.654 | 0.952 |
| 72.2157 | 23.495 | -0.404 | -0.281 | 0.104 | -0.638 | 0.309 |
| 71.4331 | 23.4329 | 1.157 | -1.225 | -0.567 | -0.344 | 1.362 |
| 73.56 | 23.2 | -0.691 | -0.771 | 0.178 | -0.356 | 0.156 |
| 72.51 | 19.423 | 3.109 | -1.603 | 0.095 | 1.186 | 5.303 |
| 72.543 | 19.4105 | 0.306 | -1.008 | 0.662 | 0.855 | 0.820 |
| 73.05 | 19.293 | 1.210 | -0.686 | 0.572 | 2.424 | 0.512 |
| 73.23 | 18.05 | -0.167 | -0.538 | 0.612 | 0.819 | 0.328 |
| 73.27 | 18.04 | -0.565 | -0.760 | 0.613 | 0.428 | -0.223 |
| 73.113 | 17.564 | 0.218 | -0.828 | 0.279 | 0.987 | 1.103 |
| 73.24 | 17.43 | -0.578 | -0.830 | 0.318 | -0.002 | 0.442 |
| 73.24 | 17.35 | 0.637 | -0.866 | -0.020 | 1.625 | 1.366 |
| 73.38 | 16.38 | -0.823 | -0.179 | 0.143 | -0.639 | 0.358 |
| 80.4315 | 17.55 | -0.667 | -0.558 | 0.898 | -1.728 | -0.402 |
| 80.563 | 17.383 | -0.219 | -1.073 | 1.112 | -1.127 | 0.007 |
| 80.53 | 17.51 | -0.694 | -0.112 | 0.199 | 0.499 | -0.170 |
| 80.53 | 17.51 | -0.720 | -0.088 | -0.071 | 0.432 | -0.408 |
| 80.4425 | 17.5545 | -0.793 | 0.095 | 0.219 | 0.385 | -0.262 |
| 80.4 | 17.58 | -0.723 | -0.445 | -0.289 | -0.030 | -0.672 |
| 80.4 | 18.06 | -0.693 | -0.373 | 0.239 | 0.286 | -0.454 |
| 80.4 | 17.554 | -0.466 | 0.157 | -0.026 | -0.484 | -0.446 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 80.4 | 18.03 | -1.027 | -0.554 | 0.361 | 0.169 | -0.401 |
| 81.2 | 29.6 | -1.133 | -0.078 | -0.222 | 0.327 | -0.574 |
| 85.3 | 28.3 | -0.754 | 0.386 | -0.601 | 1.105 | -0.276 |
| 80.6 | 29.9 | -1.318 | -0.448 | 0.004 | 0.127 | -0.273 |
| 80.6 | 29.7 | -1.419 | -0.429 | -0.316 | 0.688 | 0.889 |
| 83.7 | 29.8 | 0.293 | -0.061 | 0.071 | 0.697 | -1.816 |
| 82.3 | 29.3 | -1.207 | -0.096 | 0.221 | 0.053 | -0.542 |
| 82.1 | 29.2 | -1.249 | -0.472 | 0.187 | 0.580 | -0.028 |
| 83.3 | 28.22 | -0.003 | 1.381 | -1.132 | 0.540 | -0.187 |
| 83.57 | 27.56 | -0.381 | 0.159 | -0.436 | 0.865 | -0.760 |
| 82.2 | 27.55 | -0.231 | -0.525 | -0.645 | 0.262 | -0.077 |
| 84.2 | 28.4 | -0.628 | -0.260 | 0.276 | 0.397 | 0.314 |
| 82.15 | 27.47 | -0.681 | 0.409 | -0.855 | 0.366 | -1.466 |
| 83.7 | 28.5 | 1.412 | 2.073 | -0.444 | 0.618 | -1.062 |
| 77.524 | 34.798 | -0.926 | -0.015 | 0.093 | 0.122 | 0.293 |
| 74.45 | 24.7 | -1.514 | -0.520 | -0.101 | 0.301 | -0.386 |
| 89.363 | 27.41 | -0.874 | 0.113 | -0.142 | -0.333 | -0.041 |
| 90.5 | 27.6 | -0.229 | 2.009 | -0.684 | -0.596 | -0.305 |

## III. Trend Surface Analysis

More recent studies furnish a geostatistical explanation of spatially dependent multivariate geothermal data representing two spatially distinctive regions of diverse geologic-tectonic settings: one from a 2400 km long arcuate belt of the tectonically active Extra-Peninsular Himalayan region and the other from Late-Precambrian or Proterozoic mobile belts in the Central Highland in an otherwise stable landmass or shield of Penininsular India. Geothermal hot springs spread over these areas, conspicuously coinciding with the respective tectonic zones of different degrees of severity. Peninsular India's hot springs are restricted to the Proterozoic mobile belts of the Central Highlands, leaving the more stable southern Deccan plateau nearly devoid of any hot springs. In the present study, the two sets of data representing Peninsular and Extra-Peninsular India in entirety were considered for trend surface analysis or trend surface mapping. While mapping, polynomial power was set at 3 or cubic, which gives a better recognisable pattern than the original raw data.

**Mathematical consideration**

A trend surface model is a particular case of a bivariate regression model with two independent variables, the coordinates X and Y, and a dependent variable, the thematic variable Z, to be modelled. In other words, the principle of a trend surface model is a regression function that estimates the variable value Zi at any location based on the Xi and Yi coordinates of this location. The general function is:

$$Z_i = f(Y_i, X_i)$$

Where:

$Z_i$ = variable value at location i

$Y_i, X_i$ = geographic coordinate values at location i

f = regression function

One can select a linear regression function (first order) or, if the spatial distribution is more complex, a polynomial function (2nd, 3rd,..., or nth order). The modelled surface will correspond to a flat, oriented plane or a curved surface with an increasing number of polynomial order.The trend surface analysis technique is applied to separate the raw data into two components: the regional or background trend (regression) and the local anomalous values or residuals (deviations). It is in reality a mathematical curve fitting technique that accomplishes "best-fitting' a series of polynomial surfaces by the least squares criterion of multiple regression and determines a value about which the variance is a minimum. The goodness-of-fit of the appropriateness of trend surface curves to the data can be tested by the analysis of variance. A progressive higher-order trend surface fit to the data can be represented by the polynomial equation of arbitrary degree n:

$$Y_i = \sum_{r=0}^{n} a^r X_i^r$$

Where $Y_i$ represents the calculated value in the i-th observation, $a^r$ (r = 0,1,2,...n) indicates arbitrary complex coefficients, and $X_i$ indicates the independent variable in the i-th observation. The 'best' is obtained when the sums of squares of differences between the observed values ($y_i$) for a particular application (in the present case, factor scores derived from PCA analysis) and the corresponding calculated values ($Y_i$) are as small as possible. That is

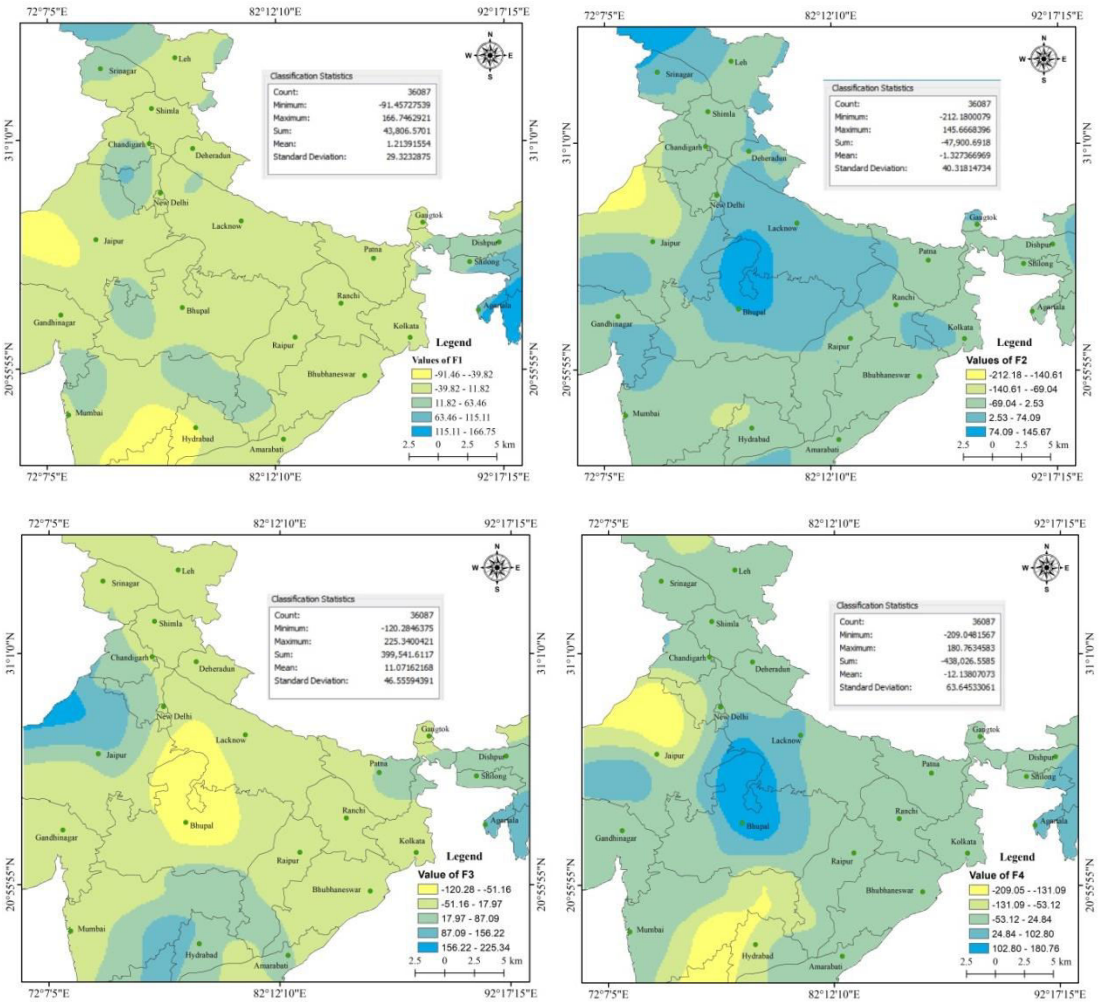
$$\sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} (Y_i - y_i)^2 = \text{minimum}$$

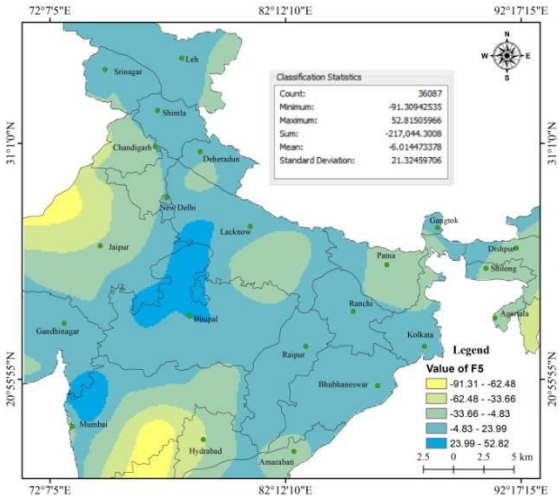
The differences ($d_i$) are called residuals. Moreover, in the case of two-dimensional trend surface mapping, ($X_i$) is defined as a function of the independent variables, such as mutually perpendicular geographic coordinates $X_i$ (the easting) and $Y_i$ (the northing). The trend is therefore a linear function of the geographic coordinates of a set of observations, minimising squared deviations from the trend.

## IV. Data selection

Two types of data are required for trend surface analysis: geographical location, such as data point coordinates (latitude and longitude), and continuous multivariate numeric variables, which characterise each data point's value and variable measurements. The original dataset, or observations/variables table, or workbook = GTHREV.xlsx, used in this study comprises 181 rows and 11 columns, including two for LAT_LONG and seven for multivariate data. The reduced subspace, TSA_FSCORES.xlsx, obtained from PCA analysis of multivariate geothermal geochemical variables, has two columns for LAT_LONG and five for calculated factor scores data (Table- 6).

**Fig. 3. Cubic Polynomial Trend Surface Mapping of PCA Factor Scores**





## V. Interpretation of results

**Outcomes of principal component analysis (pca) and graphical visualization of calculated component scores applying trend surface analysis**

**PCA Analysis**

Based on the scree plot (Fig. 2), we retain five factors that account for 84.037% of the total variance in the original variables "load on a factor of principal component". PCA factors are orthogonal, thus they are uncorrelated; nonetheless, correlation occurs between the variables inside each factor. We regard eigenvalues ≥ 0.6 as significant, indicating the relevance of variables for factors (Table- 5).

F1 (Ca, Mg, Na, K) = Basic/alkaline
F2 (HCO3) = Both acidic and basic (Amitabha Roy, 2024)
F3 (SO4) = Acidic
F4 (Temp▫C)
F5 (Cl) = Acidic

**Trend Surface Analysis (TSA)**

Figures (Fig. 3) show the real distribution of fluid geochemical variable values within a research region. Outside of the measured region, trend surface estimates become unrealistic. This is referred to as "edge effects." These are the places to avoid. In the current investigation, the polynomial of power 3, i.e., cube, trend surfaces from computed PCA factor scores F1, F2, F3, F4, and F5 (Table-6) provide a more recognisable pattern than the original raw data.

The basic/alkaline group F1 = Ca, Mg, Na, and K appears to be common, although not intense, in India's peninsular hot springs. Hot springs in India's peninsular and extra-peninsular locations have the acid-base group F2 = HCO3 in various degrees of intensity. The intensity of the group F3 = SO4 is rather low in the middle of the central highlands, but it climbs to relatively high levels in western and southern India. The group F4 = Temp▫C displays a 'high' that corresponds to exceptionally low $SO_4$ concentrations in the central highlands. Further study is needed to understand the inverse relationship between $SO_4$ and temperature in the central highlands region. The group F5 = Cl is equally prevalent across India's extra-peninsular and peninsular hot springs. Arcuate TSA contours with southeasterly convexity in the western region, particularly for factor scores attributed with HCO3, SO4, Cl, and TEMP, represent a conspicuous resemblance of arcate hills in the Kirther-Sulaiman hills of Pakistan.

## VI. Conclusions

In conclusion, the trend surface analysis and principal component analysis (PCA) of the geothermal geochemistry data from India's Peninsular and Extra-peninsular hot springs revealed significant spatial patterns and geochemical relationships.The PCA identified five significant factors, each associated with specific geochemical elements, while the trend surface analysis provided a graphical representation of the spatial distribution of fluid geochemical variables. The findings not only enhance our understanding of the interplay between geological settings and geothermal characteristics but also lay a crucial foundation for advancing sustainable energy initiatives in India.

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