# Use of Geochemistry Data Collected by the Mars Exploration Rover Spirit in Gusev Crater to Teach Geomorphic Zonation through Principal Components Analysis

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## ABSTRACT

This paper presents a laboratory exercise used to teach principal components analysis (PCA) as a means of surface zonation. The lab was built around abundance data for 16 oxides and elements collected by the Mars Exploration Rover Spirit in Gusev Crater between Sol 14 and Sol 470. Students used PCA to reduce 15 of these into 3 components, which, after quartimax rotation, very strikingly divided the surface traversed by Spirit's into three distinct zones. Students then used such concepts as the Bowen reaction series, typical minerals in Earth's basalts and andesitic arcs, the periodic table, and the Goldschmidt classification, together with Pancam images from Spirit and the Mars Orbiter Camera, to interpret the surfaces over which the rover moved. Students found this foray to Mars a challenging but enjoyable project, and it made PCA memorable to them long after the class had ended. Some variant on this lab could work for multivariate statistics courses in geology, geography, and environmental science, as well as advanced courses in the content of those disciplines, particularly those dealing with zonation. *© 2011 National Association of Geoscience Teachers*. [DOI: 10.5408/1.3604826]

## INTRODUCTION

This paper presents an exercise that uses Mars Exploration Rover geochemical data to teach principal components analysis (PCA) for geomorphic or geological zonation. The data come from the Spirit rover's Alpha Particle X-ray Spectrometer (APXS), which collected spectra from 93 rocks and soil samples (Gellert *et al.*, 2006) during its travel over three distinctive zones on the floor of Gusev Crater. These zones consisted of a cratered basaltic plain, the West Spur of the Columbia Hills with bedded materials and evaporites, and the northwest side of Husband Hill where very diverse aqueous and acid–aqueous altered rocks and soils were found. PCA is a data reduction technique that has increasingly been used in the geosciences since the early 1960s, making its acquaintance of value in the education of geoscience majors. The APXS data can make the technique memorable to such majors as it produces a coherent zonation from 15 different oxides and elements.

A classic task in the geosciences is zonation of complex surface patterns into areal units and demarcating transition zones or boundaries between them, often along a transect in the field. So, for example, a soil catena can be zoned by changes in soil particle size, underlying bedrock and regolith, topographic relief, drainage, erosion and deposition processes, weathering, organic matter, and geochemistry (Milne 1935; Bushnell, 1942; Webster, 1973; Raynolds *et al.*, 2006). Ground-penetrating radar can be used along a transect to infer subsurface stratigraphy for geological mapping (Baker and Jol, 2007). An environmental ecotone might be zoned by field sampling of soils and censusing of species presence and abundance along a transect. For example, a transect could be taken down a catena, across a wetland–upland interface, or through a seasonal surface water and groundwater boundary (Fortin *et al.*, 2000).

Zonation can be vertical and temporal in geological usage, not just horizontal and spatial in mapping usage. So, for example, fossils, grain size, bulk density, and geochemistry can be used for temporal zonation and sequencing of stratigraphic units (e.g., Patterson *et al.*, 2000; Brown and Pasternack, 2004; Peterson *et al.*, 2008).

Zonation, then, is a common task in the field and laboratory activities of geoscientists. The process can seem superficially straightforward, but the zoning schemes that result can color analytic results. Complications include scale, edge effects, spatial autocorrelation, and aggregation effects. These distortions and biases are collectively called the Modifiable Areal Unit Problem or MAUP (Dark and Bram, 2007) or the analogous Modifiable Temporal Unit Problem (MTUP). The MTUP is less commonly discussed, largely in criminology contexts (e.g., Taylor, 2010), but it is clearly relevant to geoscientists' work. Concern about zoning has driven development of statistical techniques to let image processing, GIS, and statistical software handle the kinds of remote sensing, field, and laboratory data generated and used by geoscientists.

One of the common statistical techniques used in zonation is principal components analysis or PCA, a member of the factor analytic (FA) family of techniques. PCA is primarily concerned with data reduction or grouping of many variables into fewer components. FA is mainly concerned with identifying or testing underlying factors that may not be directly measurable themselves but which are expressed in commonalities in measurements of empirical variables (Bryant and Yarnold, 1995; Rogerson, 2006; Davis, 2002). PCA is more empirical and inductive; FA is more theoretical and in some versions can test deductive hypotheses about expected underlying factor structure.

In the geosciences, PCA/FA is a common method underlying the unsupervised classification of remote

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sensing imagery. It can also be performed on large data sets collected in the field. These could include sampling down through a geological column, sediment core, or ice core, for example, or to process observations across space, as is the case in the laboratory exercise presented here. It can, thus, assist in both temporal and spatial zonation, making it a tool of increasing utility to a variety of geoscientists. For that reason, PCA/FA, particularly PCA, is increasingly encountered in the geoscience literature since its disciplinary début in the early 1960s (e.g., Reyment, 1961; Wong, 1963; Imbrie and Van Andel, 1964). For that reason, practice in its application would enhance the professional preparation of geoscience students, especially at the advanced undergraduate and beginning graduate levels.

For all its usefulness, PCA/FA is not the most "user friendly" approach for students. The mathematical complexities are now easily handled by the common statistical software packages. These include SPSS, Statistica, Minitab, Matlab, Scilab, R, the freeware programs PAST and WinIDAMS, and others, Their widespread availability makes PCA/FA accessible to undergraduate students. The underlying concepts, however, are difficult to convey, because PCA/FA represents the many variables in the analysis as dimensions and the data collected as occupying an n-dimensional data cloud. Trying to "visualize" this is a tough sell to students! The point of PCA, especially, is to reduce the dimensionality of the data cloud to a small number of usually orthogonal components. These can then be projected through the data cloud and aligned with most of the data points when "viewed" through various "rotations" of the emergent model. Each of the original variables will "load" highly along one of the components (some may load less dramatically on more than one component). That is, most of the original variables will show strong correlations with one of the artificial variables, or components. The result for geoscientists can be a meaningful zonation of time or space. PCA zonation is generated from the data themselves, rather than from a priori schemes that can give rise to the MAUP and MTUP. The only way to motivate students to acquire this tool is to show it in operation on a data set that otherwise would overwhelm them but, processed in PCA, becomes intelligible to them.

Anyone who has ever taught a statistics course knows that the worst part is finding or creating a data set that meets the requirements of a given technique, produces results that can enable teachable moments, and, ideally, has something to do with the discipline in which the statistics course is taught. This paper introduces a geoscience-related data set, discusses how it was shaped for classroom use, shows the results of a PCA taught through its use, and then evaluates student outcomes. The exercise vividly models the utility of PCA for geochemical data reduction and geomorphic zonation.

The database contains 16 oxide and element abundances collected from untouched, brushed, or abraded rocks, which were selected by the Mars Exploration Rover science team for APXS during Spirit's traverse in Gusev Crater. The lab exercise, using SPSS and Excel, is available at <http://www.csulb.edu/~rodrigue/geog400/project5.html>.

## DATA AND METHODS

The data were originally published in Gellert *et al.*, 2006, where they are presented in the second table of the article. This table can be saved as a tab-delimited file for import into a spreadsheet program. There, the data can be further edited to fit the needs of a statistical software program or an instructor's goals.

This table has as the record labels the "sol" or the martian day after landing, on which the sample record was taken. The table covers the first 470 sols of Spirit's activities. Martian sols are slightly longer than Earth days at 24 h, 37 min, and 23 s, and the date of landing for Spirit was 4 January 2004 on Earth. The second variable is the type of surface from which Spirit's APXS took spectra on a given sol. These include rock undisturbed by Spirit (RU), rock brushed off (RB), rock "RATted" or abraded by the rock abrasion tool (RAT), RAT fines or abrasion debris (RF), soil undisturbed (SU), soil disturbed (SD), and soil trenched (ST). The third variable is the sometimes whimsical nickname given to an individual rock or soil surface. Norm or geometric norm is a relative measure of the standoff distance between the APXS and the sample surface in millimeters. This distance affects how much background elemental noise is included in a reading. The variable normalizes the sum of all oxides to 100% to allow measurement of relative contributions by each oxide or element. T is the time in hours that the instrument took to integrate the spectrum. Following these three columns are two columns for each of the oxides and elements. The first gives the relative abundances of the 12 oxides (wt. %) and 4 elements (parts per million), and the other reports the statistical error bounds set at $\pm 2$ standard deviations. The table, then, has 37 columns and 93 rows of records.

The use of PCA on these data offers opportunities to encourage students' critical thinking about examples of PCA they encounter in the literature or their own future work. The data set presented here conforms to some but not all of the assumptions for the proper use of the technique, and students should be able to identify these departures and conclude that their results will be tentative. For example, the number of records is below the 100 usually recommended as a minimum sample size for PCA.

The variables used should, ideally, be roughly normal in the distribution of their values, though PCA does not depend on normality in all variables as a critical assumption. Students should get in the habit of assessing distributions, though. One way is to construct histograms of each of the 15 variables for visual inspection of their distributions. Alternatively, they can compare each variable's mean value to its median value and then calculate Pearson's skewness measure: $Sk = [3(Mn - Md)]/s$, where Sk is Pearson's Skew, Mn is the mean, Md is the median, and s is the standard deviation for the sample. $Sk > |0.2|$ can be considered skewed, the direction of the outliers given by the sign of the statistic. Alternatively, statistics packages commonly include tests for non-normality, such as the Shapiro–Wilk W, the Kolmogorov–Smirnov, or the D'Agostino–Pearson omnibus test. However students evaluate normality, some of the variables are approximately normal in distribution, but some will emerge as non-normal, and bromine is markedly right-skewed.

Other assumptions of PCA are fully met. The measurement level for all variables entered into PCA must be scalar, whether interval or ratio, and these are. Having students check on this will help reïnforce their sometimes shaky grip on the concept of measurement levels (nominal, ordinal, scalar). The subjects-to-variables ratio (SVR), or the ratio of records to columns, should be at least 5. With 93 records and 15 variables (the dropping of zinc is discussed below), this data set provides an SVR of 6.2 (leaving zinc in gives an SVR of 5.8).

Given that the purpose of doing the PCA here is for zonation of the crater floor surface by oxide and element composition, many of the columns may be dispensed with for the exercise. This leaves only those columns with identifiers and the oxide and element abundances. The result is a 93 record by 16 column (1 identifier and 15 oxides and elements) spreadsheet. The identifier should be sol.

Instructors can import the resulting spreadsheet into a statistical package at this point and run the PCA several times to become thoroughly familiar with the package's PCA defaults and options and the effects they have on the outcomes. The defaults on SPSS, for example, will produce four components that will be very difficult for students to interpret. The fourth component only has zinc as the single high loading variable on it. Some options at this point might be forcing the software to meet a higher cutoff value to retain a component or specifying that only three components are desired. This entails more lecture and demonstration work to get students to modify the PCAs and to understand the modifications, when they are struggling just to grasp the peculiar PCA hyperspace to begin with.

Alternatively, the zinc column can be omitted, which leads to a simple three component solution using the common PCA defaults. This is ideal for demonstration purposes and for the subsequent student work needed to interpret the outcome and, so, I recommend sacrificing the zinc data for the pedagogical goals of the lab. The discussion below uses the 15 oxides and elements version of the spreadsheet, which may be accessed at <http://www.csulb.edu/~rodrigue/geog400/gusevminimal.xls>.

## RESULTS

Students should be guided through the process that the statistics software uses to generate the components. It is important to have the software save the components as regression variables, which will be appended as new columns in the data display matrix. These three new columns should then be copied to the original spreadsheet for graphing (both Excel and OpenOffice/Libre Office Calc will work satisfactorily).

### Eigenvalues

An important part of the output is the total variance explained, showing the eigenvalues for each eigenvector or principal component. The sum of eigenvalues equals the number of original variables, but the percentage of total variation in the data cloud explained by each additional component declines sharply. This produces a progressively smaller gain in cumulative variance explained with each new component extracted. At some point, the marginal gain in cumulative explanation becomes insignificant. The eigenvalue for each component or the percentage of explained variance for each component can be graphed against component number in an X–Y plot. This graph is commonly referred to as a "scree plot," in a refreshingly geoscientific turn of phrase! The scree graph can identify the number of useful components visually by the nick point between the steeper part of the slope and the flatter part. The software package will default to an eigenvalue of 1.0, ceasing to extract new components with eigenvalues smaller than that, which accords well with visual examination of the scree plot.

### Component Matrix and Rotation

Another critical part of the output is the component matrix, which shows the loadings of each of the original variables onto each of the extracted artificial variables or components. The first component will show high positive or negative loadings for several variables, and only a very few will be close to 0. The second component will also show that pattern of high positive and negative loadings. The high loading variables, however, are typically variables that had very low loadings on the first component. There are often fewer high loaders on the second component than on the first, as there is less variance to account for after the first component "soaked" up a substantial amount of it. Also, the highest loadings on the second component may well be lower than the highest loadings on the first component, though this is not always the case. The pattern continues into the third component, with fewer and fewer high loading variables and often, though not always, lower maximum loadings.

The original raw component matrix will show this pattern as described, but it is very common for the range of loadings to be small enough to make it hard for students to judge which of the variables are "high" loading versus "low" loading. To make the picture crisper, it is possible to rotate the model or, more accurately, rotate the vantage point from which the model is "viewed." The goal here is to figure out the polarities represented by the components and, in some fields, it is common practice to come up with evocative names for these artificial variables, though this is less commonly done in the geosciences.

For PCA, the two most common rotations are varimax and quartimax. Varimax rotates the component matrix so as to drive some of the variable absolute loadings within a component column higher at the expense of driving other variable loadings closer to 0 on that component column. This exaggerates the range of absolute values down the column. Quartimax does the same sort of thing, but it exaggerates differences along the variable rows, helping assign variables more readily to components. This seems the more helpful with this particular data set, so I would encourage the reader to have students perform a quartimax rotation and concentrate on the resulting rotated component matrix. Varimax will work nicely enough, though. If that is the only rotation method provided by the software, an instructor can be confident that students will still be able to interpret their results well with that rotation system, too.

Something I have found which helps students (and myself) interpret a component matrix is to use a highlighter on the printout to mark the highest loading (on component 1, 2, or 3) for each variable. At this point, they can apply their geoscience background to figure out associations among variables loading highly positively on each component and among those other variables loading highly negatively on each component. Table I presents the Quartimax rotated component matrix generated by SPSS with these data, with high loadings bolded.

**TABLE I: Rotated component matrix.**

| | Component | | |
|---|---|---|---|
| **Variable** | **1** | **2** | **3** |
| $Na_2O$ | **0.772** | 0.221 | 0.362 |
| MgO | **-0.629** | -0.573 | 0.090 |
| $Al_2O_3$ | **0.769** | 0.306 | 0.493 |
| $SiO_2$ | 0.169 | -0.011 | **0.965** |
| $P_2O_5$ | **0.710** | 0.195 | -0.548 |
| $SO_3$ | -0.157 | -0.140 | -0.920 |
| Cl | 0.101 | **-0.870** | 0.019 |
| $K_2O$ | **0.751** | 0.029 | 0.013 |
| CaO | 0.196 | **0.885** | -0.073 |
| $TiO_2$ | **0.866** | 0.203 | -0.017 |
| $Cr_2O_3$ | **-0.830** | 0.385 | 0.121 |
| MnO | **-0.642** | 0.571 | -0.020 |
| FeO | **-0.850** | 0.162 | -0.179 |
| Br | 0.099 | **-0.648** | -0.232 |
| Ni | -0.313 | **-0.675** | -0.009 |

Note: Extraction Method: Principal component analysis, rotation method: Quartimax with Kaiser normalization highest component loading for each variable in bold

## Identifying and Understanding the Extracted Components

Why might potassium oxide and alumina cluster together with high positive loadings on component 1, for example (Table I)? Why, alternatively, might magnesium oxide and ferrous oxide also be packaged together on component 1, but with very high negative loadings? What is the dichotomy being picked up by component 1? Among the resources I gave students for sorting this out was the annotated rock composition chart at <http://www.csulb.edu/~rodrigue/geog400/rockcompositions.jpg>.

The two halogens come out with high negative loadings on component 2, while calcium oxide pops up with high positive loadings on that component (Table I). Resources to help students interpret that component would include the periodic table and, for the calcium issue, the rock composition chart. Nickel loads positively along with the halogens, which can be used for a side discussion about what might put the highly siderophilic nickel on the surface of a planet.

On the third component, only two variables load very highly, silica in the positive direction and sulfur trioxide in the negative direction (Table I). I point students back to the rock composition chart. Additionally, I have students look up the Goldschmidt classification of the periodic table into siderophilic, chalcophilic, lithophilic, and atmophilic elements. A discussion about sulfate chemistry in water might be helpful, too, as silica can be freed from mafic materials by small amounts of strongly sulphur–acidified cold water moving through them. Once liberated by acid–water alteration of basalt, the silica can then be precipitated by evaporation (McAdam *et al.*, 2008). That may be why silica and sulfur trioxide are linked on the third component.

This analysis of the polarities among variables loading onto each of the three components is the most challenging part of the lab for students. It requires them to excavate and apply their basic geoscience background to figure out the pattern in the statistics. On the first component, they should suggest the mantle–crust or mafic–felsic dichotomy or the Bowen reaction series. On the second component, they might come up with an aqueous versus nonaqueous or evaporite versus nonevaporite theme. On the third component, students might propose the chalcophilic–lithophilic dichotomy, mantle–crust division, or acidic alteration of basalt.

## Geovisualization and Zonation

Once students have some idea what the three components might mean, they can graph the departures of each component from neutral by sol, or across space. This is most easily accomplished in a spreadsheet, so have the students copy the three columns for PC1, PC2, and PC3 into their original spreadsheet.

I have students make a line chart of the abundance of each oxide or element by sol. This can be done 15 times or, to reduce tedium, a few line charts can be constructed with several variables on each chart. For example, two could be created from the variables with high positive scores and with high negative scores on PC1, while another two could show those with high loadings in either direction on PC2 and on PC3. Examination of these many line charts will prove intentionally frustrating to the students, as no real pattern readily emerges, and it can be hard to pick out similarities between any pair of oxides or elements. A spreadsheet containing the original data, the component scores, and several XY graphs are available in Excel 97/2000/XP format at <http://www.csulb.edu/~rodrigue/geog400/GusevChemJGE.xls>.

At this point, I have students make one chart with the three lines corresponding just to the component scores, instead of the variable values (Fig. 1). Students highlight the sol column and, holding down the control key, separately tap each of the three component columns in turn as well. The resulting line chart will be pretty messy, but students can clean it up by formatting the X axis sol labels to run vertically and the Y axis to have 0 or 1 decimal places in order to declutter it.

Have the students pay close attention to the first part of Spirit's traverse and identify which component is diverging the most strongly upward most of the time and which other component is diverging the most strongly downward. PC2 dominates in the positive direction and PC1 in the negative direction, while PC 3 stays fairly close to 0. As their eyes move to the right, they will notice that a different pair of components diverges most strongly. This time PC2 diverges very strongly below neutral and PC3, most of the time, diverges somewhat above neutral, while PC1, most of the time, stays closest to neutral. At the rightmost part of the graph, things change quite drastically, with PC3 diverging very unstably and often with extreme values below neutral. PC1 shows a similarly spiky positive dominance of most of this area, with PC2, mostly, clinging to neutral. Thus, three zones have been identified by PCA. Students can use the line–draw function (or just a pencil) to sink vertical lines marking the points on the graph where the components shift their positive and negative dominance patterns. They should note the sols on which these switches take place (roughly sol 158 and sol 315):

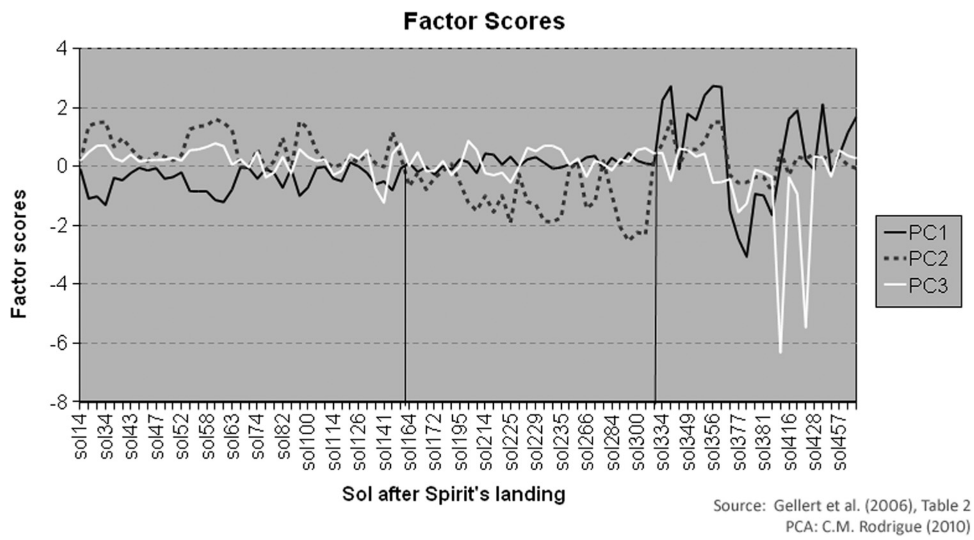


**FIGURE 1: PCA factor scores for MER Spirit APXS oxides and elements.**

These mark the boundaries among the three zones, or the sols on which Spirit crossed onto a different kind of terrain. Students are generally pretty impressed by how readily the landscape is zoned, especially if they had struggled to make heads or tails of the individual oxide and element line charts. Now, they can compare this zonation visually with the landscape of Gusev Crater.

Turning to a map of Spirit's traverse <http://marsrovers.jpl.nasa.gov/mission/tm-spirit/images/MERA_A1457_2_br2.jpg>, as well as a labeled Spirit Pancam image <http://marsrover.nasa.gov/mission/tm-spirit/images/sol_572_in_sol149Pan.jpg>, students should find the two dates marking the boundaries of the three zones. They will find that the first zone is spatially by far the most extensive, a long, almost straight shot across a cratered basaltic plain. The second zone is the short curving segment around the westernmost spur of the Columbia Hills, a territory featuring the bedded rocks that the MER team had originally hoped to find when selecting Gusev Crater for Spirit's landing. The third zone is the ascent into the Columbia Hills, where there proved to be a great diversity of rock and soil types and team interest sent the rover to explore this diversity, leading to the very spiky pattern in the third zone. This third zone, then, foregrounds the team's interests perhaps even more than the tenor of the terrain itself.

Depending on time available, faculty can have students pick out finer scale features, too. Students should note the sols at which components may switch "polarity" or magnitude of scores for brief spells within the three zones and then compare those sols on the traverse map with labeled features. In the first zone, for example, students easily spot the signals of Spirit crossing onto Bonneville Crater's ejecta blanket, then its movement about the rim, and then its descent down the blanket toward Missoula Crater. The ejecta blanket surface produces specially marked and persistent divergences in PC1 and PC2, where the impact excavated and ejected deeper basaltic materials.

In the following section, the surface characteristics of the three zones emerging from PCA are discussed. The first zone consists of cratered basaltic plains. The second one often features bedded materials evidencing evaporites. The third zone is a complex mix of diverse materials suggestive of acid–aqueous alteration. The discussion section also includes consideration of finer scale subzones in each of the three major zones and then finishes with a discussion of processes creating the three main zones.

## DISCUSSION OF THE ZONATION PRODUCED WITH PCA IN GUSEV CRATER

Statistical results and graphs need to be interpreted within the concepts of the disciplines generating them. These are challenging enough in this case to require a fair amount of unobtrusive faculty facilitation for students to understand. Faculty in geoscience disciplines, for the most part, work on Earth, and Mars is peripheral to their normal activities. There are many excellent books and other resources to become more comfortable with Mars, but a comprehensive work on the martian surface that includes the new data from the MER rovers is Carr (2006).

In terms of statistical misunderstandings, it is easy for students to interpret negative component scores as "low" scores and positive component scores as "high" scores, for example. It is important to get across that principal components are rather like see-saws, with, in this case, different oxides and elements "seated" on opposite ends of each component. When the positive side swings up strongly with highly positive component scores, so do the chemicals seated on that side (those with positive loadings on the component). Similarly, the negative side can also swing up into high (negative) component scores, lifting the chemicals with negative loadings into view. Understanding which oxides and elements are "lifted into the air" (diverge from the neutral 0 component score line in either direction) is important for figuring out the nature of the surface. With these precautions, Fig. 2 shows Spirit's transect divided into the three zones created by PCA.

### Zone 1: Cratered Basaltic Plain

So, in the first zone of Spirit's transect, PC 1 diverges strongly in the negative direction. This calls attention to the dominance of ferrous oxide, magnesium oxide, manganese oxide, and chromium sesquioxide. These oxides indicate

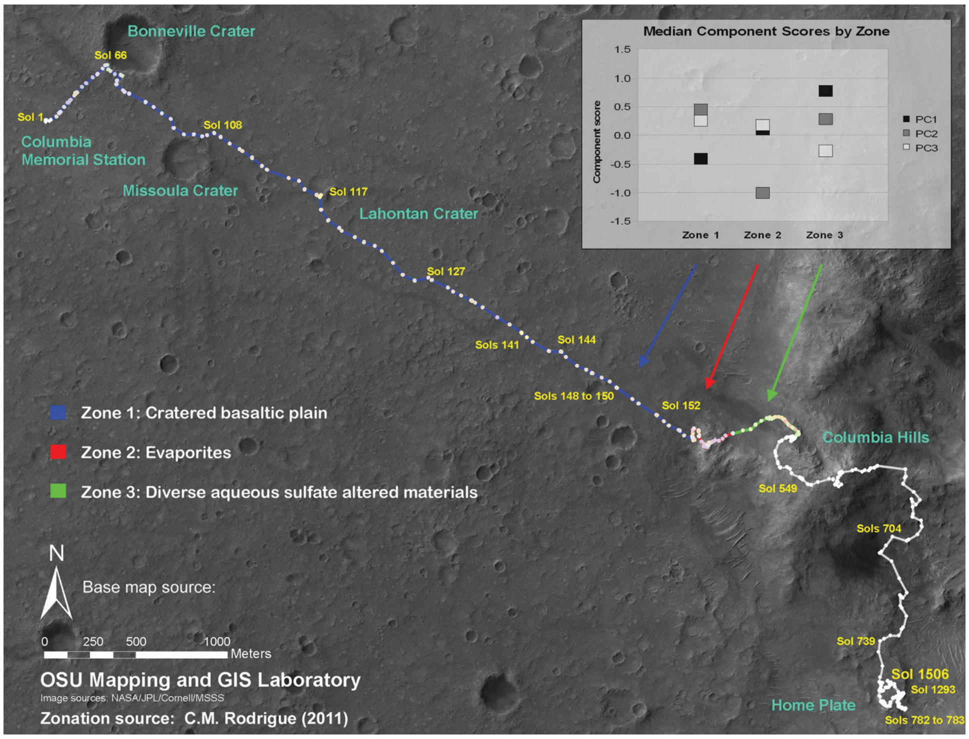


**FIGURE 2: Spirit traverse map showing median component scores and PCA-derived zonation of the traverse from sols 14 through 470.**

olivines and pyroxenes and other minerals associated with basalts and the highest temperatures along the reactive branch of the Bowen reaction series. This component, shifted so far negatively, hints at the lack of aqueous or acid–aqueous alteration along the olivine-to-feldspar join in A-CNK-FM compositional space (Nesbitt and Young, 1989). It also expresses the aeolian deposition of thin coatings of iron oxides on rock and regolith surfaces. These oxides were liberated from basalts by the action of atmospheric oxidants, such as hydrogen peroxide. Then, they have been carried around the planet by winds to the point of near homogeneity of global dust composition (Yen *et al.*, 2005).

PC2, meanwhile, diverges very strongly in the positive direction in this zone, carrying calcium oxide into prominence. Since calcium is common in basalts and calcium plagioclase dominates the highest temperatures in the nonreactive arm of the Bowen reaction series, the upward swing of PC2 is not surprising. It reïnforces the impression of a basalt and basaltic regolith landscape dominated by oxides of siderophilic and lithophilic elements. This is the same signal picked up by the negative swing in PC1.

## Zone 2: Evaporites

The second zone, crossed into by Spirit around sol 158 as it began its exploration of the West Spur of the Columbia Hills, sees PC2 swing strongly into the negative direction. This carries into prominence the three elements that loaded strongly onto the negative end of PC2: chlorine, bromine, and nickel. Nickel is associated with certain meteorites, so its presence on any martian surface is not surprising.

Chlorine and bromine, however, are markers of evaporative concentration. They were often found within cracks and voids in rocks analyzed by the APXS, starting in the latter part of zone 1 and then very prominently in zone 2 (Erickson *et al.*, 2005). These two halogens, then, constitute a hint of water or groundwater. This hint counters the impression of basalts highlighted in the lab's PCA trends back in zone 1. Mössbauer spectroscopy on the Spirit rover supports the PCA identification of a mafic surface there. This instrument detects minerals and identified an abundance of unaltered or very weakly altered olivine along Gusev's transect in zone 1 (Morris *et al.*, 2006). Olivine has a strong proclivity for rapid alteration in the presence of water, so its prevalence in the first zone suggests dryness after the basalt flow event. With the two halogens made prominent by the negative deviation of PC2, then, this second zone evidences the presence of small amounts of water in the older materials outcropping above the basalt surface. These were probably in the form of groundwater or frost deposition and subsequent aqueous alteration of regolith.

The component most frequently diverging in the positive direction, though not too strikingly, is PC3. The only chemical to load strongly positively on PC3 is silica. On Earth, silica can derive from magma fractionation in the crust or from alteration of basaltic materials through sulfate geochemistry. Mars had a great deal of sulfur pumped into its atmosphere by volcanic activity from ~4.2 billion years ago (Ga) to ~3.8 Ga. This was copious enough to produce geochemical cycles dominated by very acidic sulfate chemistry. So, these silicas may reflect the "Theiikian" or sulfate era (Bibring *et al.* 2006; McAdam *et al.*, 2008).

In this region, PC1 occasionally surpasses PC3 in positive deviation, carrying a signal of the oxides of aluminum, sodium, potassium, and titanium. These similarly concentrate by fractionation but in such minerals as orthoclase and sodium feldspar. The Spirit team noted that the rock materials in zone 2 were softer for the RAT to cut into (Erickson *et al.*, 2005). They commented on a trend of increasing detection of small amounts of water alteration in the cratered basaltic plains along the long straight trajectory occupying the rover until sol 158. They note that some of the rock appears layered after sol 158, comprising a mix of fine and massive beds, each of which shows relatively poor size sorting and includes some large grain sizes. This suggests deposition in a high energy environment, such as impact gardening, with subsequent alteration and softening by more water than is evidenced on the basaltic floor of Gusev. This, no doubt, accounts for the change in the polarity and magnitudes of the three principal components marking the transition from zone 1 to zone 2.

## Zone 3: Diversity in Aqueous Sulfate Geochemistry

As Spirit began to climb the northwestern slope of Husband Hill in the Columbia Hills after sol 315, the landscape took on a third character geochemically as well as topographically. In this zone, PC3 swings negatively, in a couple of cases quite spectacularly so. Sulfur trioxide is the chemical with a strong negative loading on PC3, bringing up sulfur chemistry again. Sulfate itself (SO4) is not part of the database derived from Gellert *et al*. (2006), but Erickson *et al*. (2005) comment that sulfate was abundant in the individual rocks and soils. This corresponds to the sharp negative deviation in PC3 seen in this lab. Along with the $SO_3$ highlighted by PC3's negative deviation, the sulfates mentioned by Erickson *et al*. suggest an aqueous chemistry, the kind associated with the acidic waters produced by sulfate geochemistry (McAdam *et al*., 2008). Reïnforcing the impression of sulfate chemistry in the third zone are the half dozen samples in which PC1 drops sharply into negative scores. Erickson *et al*. (2005) describe these as basaltic grains cemented by magnesium sulfate salts (the "Peace" and "Alligator" rocks).

It is PC1, however, that diverges strongly positively in most of the third zone, foregrounding the oxides of titanium, sodium, aluminum, potassium, and phosphorous. These are often seen in the granites and rhyolites (quartz and the potassium and sodium feldspars) that result from the final fractionation of magmas in the Bowen reaction series, but Mars is not noted for strong magma fractionation. Gellert *et al*.'s (2006) paper suggests instead that water acidified by sulfates and chlorine tends not to leach feldspars with any efficiency. This may account for their presence or persistence in this zone as seen by the felsic oxides detected by the APXS, which again underscores acidic aqueous action.

## Finer Scale Zonation

Instructors might opt to have students tackle finer-scale zonation as well. Each of the three zones shows subzones that depart somewhat from the overall component pattern in the zone.

In zone 1, for example, the most extreme divergence of PC1 and PC2 (roughly sols 18–63 and again sols 82–150a) coincides with the ejecta blankets around Bonneville and Missoula craters. Sols 65–81b show a convergence of all three components toward neutral, which coincides with Spirit's exploration of the rocks along Bonneville Crater's rim.

In zone 2, students could look for areas that are extremely rich in halogens and carry a suggestion of silica (sols 197–199, 228–235, 300–304). Another subzone type features halogen-rich areas with felsic oxides and the aqueous alteration they imply (sols 266–274, 291). Students can also spot areas close to neutral on all three components, suggesting aeolian homogenization (sols 172–178, 227, 240–259).

In zone 3, students can identify an area of marked alteration toward the oxides of elements common in felsic rocks, with PC1 scores predominantly strongly positive (sols 334–357). Another area adjacent to it has strongly negative PC1 scores. This indicates mafic oxides, and this area also shows a weak halogen and sulfate signal from somewhat negative PC2 and PC3 scores (sols 374–385b). Immediately adjacent is another area in which PC1 scores return to strongly positive scores but with two rocks showing extremely negative PC3 scores. Scores on these two rocks indicate a very strong sulfate signal (sols 401 and 427). Zone 3 shows the most internal variation of all three zones. This reflects both greater diversity of rocks and soils in the Columbia Hills and the Spirit team's interests in exploring the extremes of diversity there.

## From Zonation to Processual Analysis

In short, then, the 15 oxides and elements in this PCA lab exercise yield three principal components that produce a coarse but clear zonation of three different surface types by geochemistry. These are visually distinct on the Spirit traverse map. If an instructor desires, students can search for several finer-scaled subtypes within each zone. The three main zones can be turned into a meaningful geoscience narrative even by undergraduate students. To do so, they must apply their introductory general geology or physical geography coursework preparation, which will require some facilitation by their faculty. Students should have enough information from their previous coursework and the lab itself to posit a plausible history along the lines of Mars accreting and forming a crust, followed by a period of bombardment and impact cratering. During or after the bombardment, there was a possibility of fluvial deposition of sediments into Gusev Crater by Ma'adim Vallis. With or without such deposition, there clearly was aqueous (groundwater?) alteration of impact gardened regolith on the floor of Gusev. After these fluvial and/or aqueous alteration processes had left their marks, volcanic activity (perhaps from Apollinaris Patera to the north of Gusev Crater) covered some of these sediments with basaltic lava. This would have been at a time of continued strong bombardment, as the basalt is heavily cratered. Bombardment went on very heavily until ~3.7 Ga and continues at a drastically lower rate even today. The Columbia Hills were stranded as an outcrop of the older water-altered sediments above the younger lava fill. After the volcanic flow event and after the bombardment of Mars' surface dwindled, the long, slow desiccation, oxidation, and aeolian homogenization of "modern" Mars began, veneering rocks and soil with iron oxide dust.

A geological timeline must remain imprecise on Mars until the Mars Sample Return Lander and subsequent missions can return rock materials for radiometric dating. Dating of surfaces now depends on crater counting techniques (Hartmann, 2005) and geological reasoning from superposition relationships.

The martian timeline has been divided into three periods (Barlow, 2008), named for region types. The oldest is the Noachian, which lasted from planetary formation until

~3.7 Ga. This was a period characterized by severe bombardment and the collapse of Mars' planetary magnetic field. It also featured aqueous processes, possible precipitation-fed surface flow and standing water, and associated fluvial processes. Surfaces are badly cratered but, here and there, dendritic networks believed to be surface water channels are seen. The Hesperian, debatably ending ~3 Ga, was a time of high volcanic activity and extreme flood events represented by the largest outflow channels. These massive outflows were perhaps triggered by magma interaction with subsurface water and ice. The most recent period is the Amazonian, characterized by desiccation, oxidative geochemistry, loss of most of the atmosphere, and, ironically, the dominance of aeolian processes. Given the lack of radiometric dating and lingering controversies over crater-counting, the boundaries among the three periods are somewhat variable in the literature.

An alternative periodization (Bibring *et al.*, 2006) focuses on dominant geochemical weathering processes. The oldest era in this scheme is the Phyllosian, named for phyllosilicate clays associated with neutral to alkaline water. The Phyllosian concides with the early to middle Noachian. The second era is the Theiikian, extending from ~4.1 to 3.5 Ga, or from the late Noachian through much of the Hesperian. In this era, Mars switched into a sulfate-dominated acidic geochemistry, possibly due to the massive and pervasive volcanic activity of the late Noachian and Hesperian periods. The Siderikian era roughly concides with the Amazonian period and is characterized by oxidative weathering of the mafic rocks, which are so common on the martian surface. This is connected with decline (and spatial concentration) in volcanism, loss of atmospheric pressure, and nearly instantaneous evaporative loss of any liquid water exposed at the surface.

The zones identified by PCA in this lab can be linked tentatively to these timeframes. Zone 2 exposes the older rocks and soils evidencing acidic water, probably groundwater, and probably in small amounts. The prominence of the halogens implies evaporative concentration, a Mars already beginning to lose its surface waters. This suggests Theiikian processes going back to the later Noachian or early Hesperian. Zone 1 is covered by low viscosity basaltic flows. These flows are possibly a signal of the heightened volcanic activity of the latest Noachian and Hesperian, not so young to escape serious impact pummeling but young enough to show a nearly completely dry Mars. Zone 3 is in many ways an extension of the acidic alteration seen in zone 2. Sulfate and oxidative geochemistry is the keynote here, marking the acidic Theiikian processes and transition into the Siderikian ones. The hilly surface is probably approximately the same age as those of zone 2 but with a strong aeolian signal as the oxidized dust of Amazonian Mars concentrated in certain sites here.

The linkage of zones with specific periods and eras of martian geological time is not something that can be expected of students in a geoscience course in statistics. It could, however, be asked of advanced geoscience students in a planetary geoscience course that made use of this data set and PCA. Students in a statistics course in a geoscience department, however, can be expected to come up with a reasonable sequence of events shaping the surface of Gusev Crater, applying superposition relationships to the zones produced in the lab.

## STUDENT LEARNING OUTCOMES ASSESSMENT

I have utilized this laboratory exercise in two elective sections of multivariate statistics during the Spring of 2008 and the Spring of 2009, after having taught PCA with a different data set in two earlier sections taught in the Spring of 2001 and the Spring of 2006. The course focuses mainly on multiple regression, multivariate binary logistic regression, and PCA. A multivariate statistics course often does not generate a sufficient enrollment in the many departments that want to expose their majors to such techniques. As a result, the geography course on our campus has been promoted by advisors outside of the department. I, therefore, try to include exercises that accommodate the interests of the many different kinds of students in the class each semester. Originally, this exercise was designed to pique the interest of several geology, physical geography, and environmental science majors in the Spring 2008 section.

What follows is a description of three assessments of the outcomes of this lab exercise, organized by the timeframe of impact. The first describes the immediate grade performance of the "Mars-enhanced" sections in comparison with the others that learned PCA using a U.S. Census-derived human geographic database: the "Mars treated" group and the "control" group. A second phase of this assessment comprises a qualitative anecdote about the participation of a graduate student in a research team, in which I was involved, as she independently applied PCA to a major project stretching over a year past the end of the class. The third phase summarizes the responses to an e-mail survey I distributed to these two sections of the class long after the course had concluded, in order to evaluate the lab's long term effects.

### Student Grade Performance in Class

The Mars treated group consisted of 32 students, the "control" group of 29. To assess how the Mars treated group compared with the control group in terms of how well they had learned PCA, I conducted a basic pretest and post-test evaluation. This entailed using scores on an introductory lab given to both groups in order to establish whether the two student groups were statistically comparable. This was the pretest. The post-test compared their performance on the PCA lab as a diagnostic of their relative success in understanding PCA. Scores on both labs used a 100 point scale. Intergroup differences were evaluated with a t-test of the difference of means, with a probability of $<0.05$ deemed significant.

The first lab project in the course is a refresher on basic simple linear regression using variously transformed variables. The mean scores of the two groups of students were 89.7 and 87.5 out of 100, respectively, with standard deviations of 5.8 and 8.6, respectively. A t-test of the difference of means yielded a t score of 1.18 (prob=0.24), establishing that the two groups were not significantly different as the class began (the pretest). This finding, then, justified proceeding with the post-test. The fifth lab was the PCA exercise. The Mars treatment group averaged 88.0, with a standard deviation of 9.9, while the control group earned 82.9, with a standard deviation of 10.2. This yielded a t score of 2.0, which was significant (prob $< 0.05$). The Mars treatment group did significantly better than the control group in demonstrating their mastery of this complex technique.

### One Student's Use of PCA After Class

A geology master's student in the Spring 2008 course subsequently applied PCA for her course term project. She did her class final project and then a follow-on project using PCA to analyze marine cores taken in the Santa Barbara Channel off the Southern California coast, going back ~33,000 yr (calibrated). She used the deviations in the two components that emerged from six paleoclimate proxies to pick out the signals of several climate changes. These included the terminal Pleistocene glaciation, pre-Bølling warming, deglaciation, and the Holocene, as well as several smaller-scale events, such as the Younger Dryas, four Dansgaard-Oeschger events, the last glacial maximum, and three Heinrich events. She went on to present her work at the American Geophysical Union (Peterson *et al.*, 2008) and came back to my class a year later to discuss what she had done and inspire the next cohort of students. She is now in a Ph.D. program in earth science.

### Survey 1–2 Years after Class

In the Spring of 2010, I e-mailed the 32 students who had taken the two sections that used this lab exercise and asked them eight questions about the the lab and its data set:

(1) whether they felt they would be able to do a PCA again if they had access to appropriate software,
(2) whether they ever had had a chance to do another PCA,
(3) whether they have read about and been able to follow others' use of PCA,
(4) their ranking of the three multivariate techniques by personal interest in them,
(5) their ranking of the three by personal difficulty,
(6) their ranking of the four data sets I used to teach the three techniques (gun crime and socioeconomic data, archaeological site analysis, educational assessment, and martian geochemistry),
(7) their ranking of the personal difficulty of the databases, and
(8) an open-ended question on whether the martian data made PCA harder or easier, more or less interesting, or more or less memorable.

Eight students out of the 32 responded (25%). All eight expressed confidence that they could do PCA on their own using SPSS or other statistical software. Three stated that they had had to employ a PCA since taking the course: These three are graduate students, including the individual profiled above. They reported later using the technique in graduate seminars or in a conference presentation. Seven reported encountering PCA in an article they had had to read and said that their memory of the technique came back and gave them a better understanding of what they were reading.

In terms of ranking the techniques by degree of personal interest, PCA was the favorite technique of six of the students, with the other two listing it as least interesting. PCA was ranked the most difficult technique by four and the second most difficult by another four. No one selected it over multiple regression or logistic regression as easiest.

In terms of data sets, the martian data were overall rated the most interesting data set. This was in comparison with the two data sets used for multiple regression (gun crime data and an educational assessment) and for logistic regression (archaeological site prediction). These impressions are quite polarized, however: five rated it the most interesting data set, while three rated it the least interesting. There was no association with either the major or concentration of the students. In terms of the difficulty of working with the various data sets, though, the martian data were rated the hardest to handle, with three students rating them the hardest and another three rating it the second hardest. Again, this rating cut across all majors and concentrations.

The open-ended question generated a series of adjectives and phrases about the use of martian data. These fell into four clusters. Four students described them as *interesting* or *fun*. Three characterized the martian data as making it *harder* for them because of the amount of *information outside their training* they had to absorb to get through the lab. Three others said that these data made it *easier* for them to learn PCA because they were so interesting. Six of the eight said that the martian data made the technique much more *memorable* and gave them a better and longer-lasting understanding of the technique, whether or not they found it interesting or difficult.

## CONCLUSIONS

The triangulation of three different forms of evidence encourages wider use of these martian geochemical data in geoscience statistics courses. First, there was significant improvement in student grade performance in the PCA lab using the martian data over the performance level of those using a different data set. Second, a graduate student left the class immediately able to apply the technique to her own research. Third, despite different levels of student interest and difficulty, students reported an enduring ability to understand PCA-based research. Fourth, the martian data made the technique memorable long after the class ended.

These mutually reïnforcing lines of evidence may make this data set appealing to other geoscience faculty teaching multivariate statistics or geostatistics. It is always a challenge to find data that can be processed with the technique to be taught, which produce clear results readily linked back to the discipline. I highly recommend wider use of the data provided by the Gellert *et al*. team (2006) for any educator teaching statistics in a geosciences program, as well as efforts to evaluate the replicability of the results reported here.

Potential lines for further work include the following. First, other instructors who teach PCA in statistics or quantitative methods courses could try alternating the use of this martian geochemistry data set with whichever data set they currently use. The pretest/post-test methodology described here would be easily implemented and could allow multiple pairs of Mars treatment and non-Mars treatment groups to be evaluated for student mastery of the PCA technique. Second, geoscience instructors teaching geomorphic or geological zonation could utilize this lab to do a similar comparison of "PCA treated" and "non-PCA treated" student groups. They could evaluate whether exposure to PCA promotes a better understanding of zonation in comparison with other techniques, such as field observation, air photo interpretation, or software-mediated classification of remote sensing data. Construction of a shared assessment data clearinghouse on either of these topics could facilitate curricular development in geoscience departments. Such a clearinghouse could be made public through the Digital Library for Earth System Education (DLESE) or the Education Resources Information Center (ERIC).

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