
Nisyros island (Greece). Photographer: Orlando Vaselli.

GEOCHEM NEWSLETTER

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IN THIS ISSUE

So.Ge.I. – ITALIAN GEOCHEMICAL SOCIETY

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Letter from the President

Orlando Vaselli

Dear Friends and Colleagues,

Happy 2025. This is the third issue our GeochemNewsletter that refers to the past year.

It is a relatively short issue since the contributions we had were very few. Once again, I do invite to be more active for populating this newsletter. I know that all of us are very busy with deadlines, classes, projects, calls for proposal, national and international fieldworks and congresses. By the way, I think that it is very important that the most relevant activities are to be known by the members of the Italian Society of Geochemistry. It is not a matter of writing pages and pages. A couple of pages accompanied by a couple of photos are more than OK. According to the publications of our members in the third quarterly of 2024, the list appears to be very long (116 papers! Jacopo Cabassi, who is warmly thanked, assembled this long list). This suggests that all of us are very active and preparing a few sentences to let our members know what you are dealing with should not be a big deal.

Having said this, I would like to thank Caterina Gozzi and Antonella Buccianti for their contributions to this newsletter. Caterina Gozzi has prepared a new episode of "R", titled: Principal Component Analysis: R Package Factoextra where "*an easy-to-use package created to extract and visualize the output of different exploratory multivariate data analyses, including PCA*" is described. This is the 10th contribution on "R" applications by Caterina Gozzi.

What Antonella Buccianti has written is something different. A few years ago, she participated to a public call to be part of the Ministerial Technical Committee for the Evaluation of the Environmental Impact by mining activity, hydrocarbons exploitation, geological storage, geothermics, *decomissioning* of nuclear plants and so forth. Thus, from 2020 to 2024 she has been an important member of this committee, and her position was renewed for the next four-year period (2025-2028). Her contribution to this newsletter is aimed at illustrating her duties within this committee and a couple of examples of the topics she has to deal with are described. In agreement with Antonella Buccianti, we decided to have this pages in Italian. We wanted to avoid that the English translation would have affected the meaning of this message since the policy behind this committee mostly concerns the Italian legislation. I would like to congratulate Antonella Buccianti for this important appointment on behalf of the Italian Society of Geochemistry.

Another important achievement is that by Elisa Sacchi. For the next two years she will be the President of the International Association of Geochemistry (https://www.iagc-society.org/) and she was also appointed as Co-Editor in Chief of Applied Geochemistry. On behalf of the Italian Society of Geochemistry, I wish all the best to Elisa Sacchi for these two new scientific adventures.

What's up in 2025? We are expected to have at least three events. In chronologically order, from the 9th to the 14th of June, 2025 a lot of Msc, PhD and post-doc students will be joining the "International Vulcano Summer School on in situ measurements and sampling of volcanic gases" that will be held in the beautiful atmosphere of the Vulcano Island. A perfect laboratory to learn how geochemistry works. The Organizing Committee is composed by Rebecca Biagi, Sergio Calabrese, Lorenza Li Vigni, Giovannella Pecoraino, Antonio Randazzo, Franco Tassi, Francesco Tripodi and Stefania Venturi, but a lot researchers from national and international universities and research centers will be present in the island ready to teach what it is possible to do in an active volcanic system. If interested, please, visit our website for more information (https://www.societageochimica.it). The School is free-of-charge. The participants have to arrange travel and accommodation on their own.

From the 1st to the 4th of July, 2025, at the Department of Earth Sciences of Naples it will be held the 5th School of CAMGEO (Sampling and Analysis of Geological Matrices). This School will be dedicated to geochemistry in contaminated sites. PhD students, young researchers, professional and technicians are welcome to participate to this School. By the end of January 2025, the first circular of this School will be coming out. Stefano Albanese is in charge of the organization and I wish to thank Stefano for being available to organize this biennial appointment.

Finally, a two-days meeting (2nd and 3rd September, 2025) is expected to be held at Abbadia San Salvatore (Mt. Amiata). The main target will obviously be Mercury and the title of this meeting will be: *Il mercurio da elemento "ricercato" a elemento "bandito"* (the English translation sounds "Mercury from "wanted" element to "banned" element"). More details will be provided in the forthcoming weeks.

I do conclude this short letter to thank Stefania Venturi for handling this newsletter issue and, as already mentioned, Jacopo Cabassi for assembling the list of publication of our members.

I do take this opportunity to remind to those who have not renewed the annual fee to the Italian Society of Geochemistry to do it as quick as possible. All the info related to the payment can be found at https://www.societageochimica.it/iscriviti

R-Corner

Caterina Gozzi

Download and install R and R Studio

R is completely free software that can be used on Linux, Windows and Mac operating systems. Visit https://www.r-project.org and follow the instructions to download the version of R compatible with your system.

R Studio provides an integrated environment for R with numerous features to improve the user experience and make using R easier. After installing R, you can download and install R Studio for free from http://www.rstudio.com/.

Principal Component Analysis: R Package Factoextra

Introduction

When analyzing geochemical data, Principal Component Analysis (PCA) is one of the most powerful and widely used techniques for gaining a deeper understanding of the dataset. PCA is a statistical method used for dimensionality reduction. In essence, it transforms the n-dimensional space (i.e., variables) of the geochemical data into a new coordinate system, capturing the essential structure of the data with fewer dimensions, while retaining as much as possible the original variance. Preserving as much variability as possible can be translated into finding new variables that are linear functions of those in the original dataset, that successively maximize variance and that are uncorrelated with each other (Jolliffe & Cadima., 2016). The benefits of performing PCA are numerous. For example, it simplifies data visualization and analysis, helps to identify patterns through multi-element trends, and provides an initial method for detecting element associations and potential exploration indices within the dataset.

PCA Visualization with Factoextra

In this *R Corner*, we will present briefly the R package Factoextra (Kassambara, A., 2023), an easy-to-use package created to extract and visualize the output of different exploratory multivariate data analyses, including PCA. As example of application, here we consider a subset of geochemical data from the Eastern Siberian River Chemistry database (Liu et al., 2022). The code examples are reported in the flowcharts from n. (1) to (7), and we refer to the data frame to be analyzed as "data," which should be imported into R beforehand. The first step is to install and then load the “FactoMineR” (Husson et al., 2020) and “factoextra" packages (1). The first package contains the actual function to perform PCA() while `res.pca` is typically the object that stores the results of this function (2). It is possible to extract the results of the analysis using the functions `get_eig`, `get_pca_var`, and `get_pca_ind` which allow to obtain the eigenvalues/variances, the variable loadings, and the individual scores, respectively, as shown in panel (3) of the flowchart. For a quick visualization of the results, the `fviz_screeplot` function can be used to create a scree plot, which visually represents the proportion of variance explained by each principal component (4). This can help to easily identify how many components are necessary to capture most of the data variability. In the reported example of Siberian River chemistry, the first two components account for approximately 78% of the data variability.

Furthermore, the Factoextra package provides several functions for creating customizable PCA plots, making it easy to visualize individual observations with the command `fviz_pca_ind` (5), variables with `fviz_pca_var` (6) or both in a biplot using `fviz_pca_biplot` (7). The `repel = TRUE` parameter helps to prevent text labels from overlapping. It is very useful to enhance the readability of the plot, although it may slow down the plotting process when dealing with many points. Similarly, the `label = TRUE` parameter avoids text label overlapping. The argument `col.ind` controls the coloring of the individuals. It is possible to assign a single color (see code 5) or color the points based on a specific variable or factor to visually distinguish groups or highlight patterns in the data. This is demonstrated in code (7), where the points are colored according to the Total Dissolved Solids (TDS) of the corresponding sample. In a similar way, the parameter `col.var` controls the coloring of the variables (arrows) in the plot, also allowing to assign colors to the variables based on their contribution to the principal components (`col.var = "contrib"`, code 6).

Key Remarks: The Effect of Compositional Data on PCA Results

From the previous example (6-7), it is important to note that, on the first dimension, the arrows point in the same direction, indicating positive loadings on PC1 for all variables. This alignment presents challenges for geochemical interpretation of the component, since most of the chemical species strongly contribute to PC1. Such alignment suggests that these variables are positively correlated and tend to vary together, meaning that the proportions of these components likely increase or decrease simultaneously across the samples.

Although this might seem surprising, it demonstrates a key characteristic of compositional data. Geochemical data are inherently compositional because they represent proportions of a whole (e.g., percentages), and the sum of their components is constrained to a constant (e.g., 100%) (Aitchison, J.,1986). This closure constraint induces, in a multivariate framework, a dependence between the components and, in the context of PCA, this interdependence often leads to the phenomenon where the arrows representing all the variables point in the same direction. This occurs because the variance-covariance structure of the data is biased, as demonstrated by Chayes F., (1960).

To conclude, the R package Factoextra represents a very flexible tool for exploring and visualizing the results of a PCA. It can also be used with different PCA functions, rather than the one from the FactoMineR package. For example, a function for computing robust compositional PCA, such as that from the robCompositions package (Templ et al., 2011) can be used instead (e.g., see Gozzi et al., 2021). Given the critical importance of the properties of compositional data in the analysis of geochemical data, in the next R Corner we will explore in greater detail the theory of Compositional Data Analysis (CoDA).

(1) Loading packages

```
library(FactoMineR)
library(factoextra)
```

(2) Performing Principal Component Analysis

```
res.pca <- PCA(data, graph = FALSE)
```

(3) Extract and visualize results

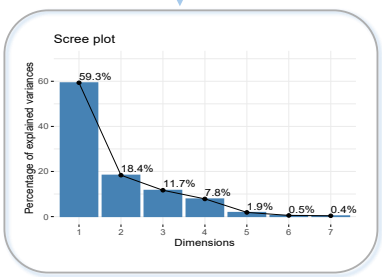
```
get_eig(res.pca)              # Extract eigenvalues/variances

var <- get_pca_var(res.pca) # Extract the results for variables
head(var$coord)             # Coordinates of variables
head(var$contrib)           # Contribution of variables

ind <- get_pca_ind(res.pca) # Extract the results for individuals
head(ind$coord)             # Coordinates of individuals
```

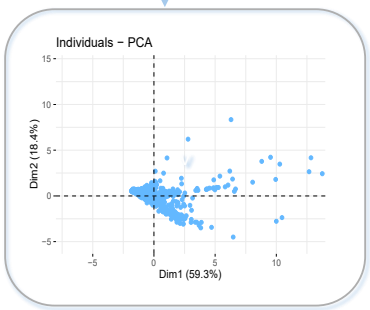
(4) Visualize explained variances - Scree plot

```
fviz_screeplot(res.pca,
addlabels = TRUE, ylim = c(0, 70))
```



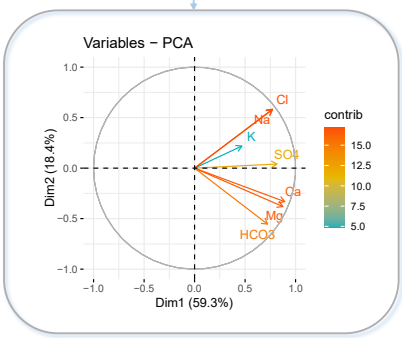
(5) Graph of individuals

```
fviz_pca_ind(res.pca,
repel = FALSE,# Use repel = TRUE to avoid overplotting
col.ind ="steelblue1",  # Control the color
label = FALSE) # Use label = TRUE  to plot labels
```



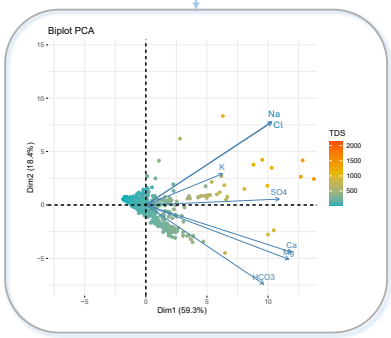
(6) Graph of variables

```
fviz_pca_var(res.pca,
col.var="contrib",
gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
repel = TRUE) # Avoid text overlapping
```



(7) Biplot (individuals and variables)

```
fviz_pca_biplot(res.pca,
axes = c(1, 2),
geom = "point",
col.ind = data$TDS,
addEllipses = FALSE,
legend.title = "TDS",
title = "Biplot PCA",
gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"))
```



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Members' Activities

Il ruolo della Geochimica nella Valutazione di Impatto Ambientale

Antonella Buccianti

La Valutazione d'Impatto Ambientale (VIA) nasce negli Stati Uniti nel 1969 con il National Environment Policy Act (NEPA) ed è stata introdotta in Europa dalla Direttiva Comunitaria 85/337/CEE (Direttiva del Consiglio del 27 giugno 1985, valutazione dell'impatto ambientale di determinati progetti pubblici e privati) quale strumento fondamentale di politica ambientale e sostenibilità.

La valutazione ambientale ha come obiettivo quello di verificare e, quindi, permettere, che l'attività antropica sia compatibile con la capacità rigenerativa degli ecosistemi e delle risorse, con la salvaguardia della biodiversità e che vi sia un'equa distribuzione dei vantaggi connessi all'attività economica. La procedura di VIA si basa dunque sul così detto principio dell'azione preventiva, in base al quale la migliore politica ambientale consiste nel cercare di "prevenire" gli effetti negativi legati alla realizzazione dei progetti anziché combatterne successivamente gli effetti.

La VIA è stata recepita in Italia con la Legge n. 349 dell'8 luglio 1986 e s.m.i., legge che istituiva il Ministero dell'Ambiente e le norme in materia di danno ambientale. Con il D.P.C.M. 27 dicembre 1988 e s.m.i sono state pubblicate poi le Norme Tecniche per la redazione degli Studi di Impatto Ambientale e la formulazione del giudizio di compatibilità. La direttiva VIA del 1985 è stata modificata cinque volte, nel 1997, nel 2003, nel 2009, nel 2011 e nel 2014.

Nel contesto generale della valutazione ambientale la commissione nazionale nella sua configurazione "plenaria" prevede anche la VAS – Valutazione Ambientale Strategica cioè la valutazione degli effetti di determinati piani e programmi sull'ambiente naturale proposti da enti (ministeri, autorità di bacino etc.), così come stabilito nell'art. 4 del D. Lgs. 152/2006.

Nel periodo 2020-2024 ho avuto l'onore di far parte della Commissione Tecnica di Valutazione dell'Impatto Ambientale partecipando ad un bando di selezione pubblica. Nel corso di questi 4 anni sono stata referente del Gruppo Istruttore che si è occupato di miniere, idrocarburi, stoccaggio geologico, geotermia e *decomissioning* degli impianti nucleari. Il lavoro è stato ampio e diversificato, nonché intenso, e mi ha permesso non solo di verificare l'importanza della geologia nella valutazione ambientale ma il ruolo preminente della geochimica. In tutti i progetti che vengono valutati, indipendentemente dalla scala, vi sono da studiare le importanti interrelazioni tra acqua, aria, suolo e sottosuolo, tutte matrici che il progetto potrebbe influenzare, così determinando modifiche al ciclo degli elementi chimici, anche di quelli potenzialmente pericolosi. Un esempio interessante è quello delle piattaforme marine presenti in Adriatico per la coltivazione di idrocarburi (*Fig. 1*).

Molte di queste piattaforme hanno pozzi dove si è prelevato, e tuttora si preleva, gas metano. Le acque di produzione che accompagnano l'estrazione del gas dopo essere trattate su piattaforma, vengono rilasciate in mare, seguendo apposita normativa. Questo comporta la necessita di effettuare nel tempo dettagliati monitoraggi rispetto ad un areale di "bianco" predeterminato al fine di verificare il comportamento della parte biotica e le variazioni geochimiche delle acque marine sia considerando elementi classici ma anche presenti nei composti antropici utilizzati per mantenere il pozzo integro (biocidi, Ba presente nei fanghi di perforazione, idrocarburi, etc.).

Un altro esempio interessante riguarda il Regolamento Europeo sulle materie prime critiche adottato dal Consiglio lo scorso marzo. A partire dalle 34 materie prime critiche individuate, è stato stilato un elenco specifico di materie prime strategiche (*Fig. 2*) cioè le materie prime di cui si prevede una

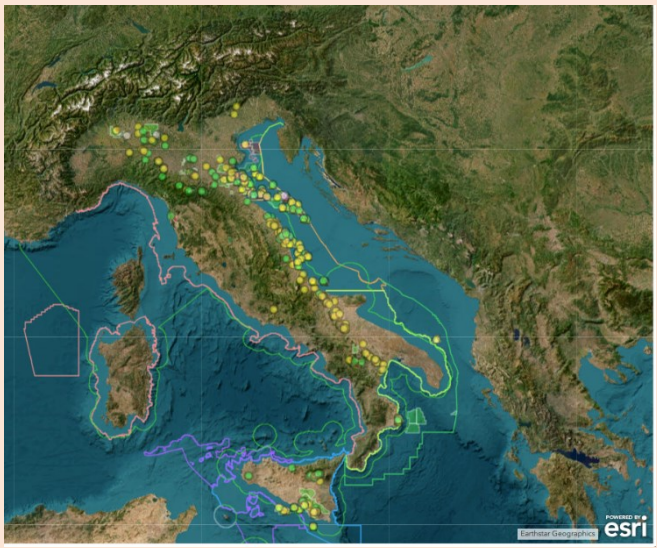

Fig. 1 Localizzazione delle piattaforme/pozzi per la ricerca e coltivazione di idrocarburi (i diversi colori corrispondo al diverso stato di vita delle piattaforme/pozzi, le linee colorate alla delimitazione delle zone marine e al limite delle 12 miglia dalla linea di costa e dalle aree marine protette; da WebGIS UNMIG-MASE).

crescita esponenziale in termini di approvvigionamento, che hanno esigenze di produzione complesse e sono quindi esposte a un rischio più elevato di problemi di approvvigionamento. Come Referente del Gruppo Istruttore dove era incluso anche il minerario nello scorso quadrienno abbiamo valutato diversi progetti di esplorazione mineraria tutti localizzati in ambienti estremamente fragili dal punto di vista ecosistemico e spesso ricchi di acque. Anche qui ho potuto verificare il ruolo fondamentale della geochimica e lo sguardo "olistico" sul sistema ambientale che da questa ne deriva.

La mia posizione nella commissione come Referente di Gruppo Istruttore è stata rinnovata per il prossimo quadriennio, 2024-2028 e le sfide da affrontare sono tante, tra queste c'è anche la definizione della mappa nazionale dei siti idonei in cui conferire scorie radioattive a media-bassa intensità. In particolare, la Commissione di Valutazione Ambientale Strategica dovrà valutare il piano proposto dal Ministero dell'Ambiente e della Sicurezza Energetica. Anche qui, come è ben comprensibile la geochimica avrà un ruolo fondamentale.

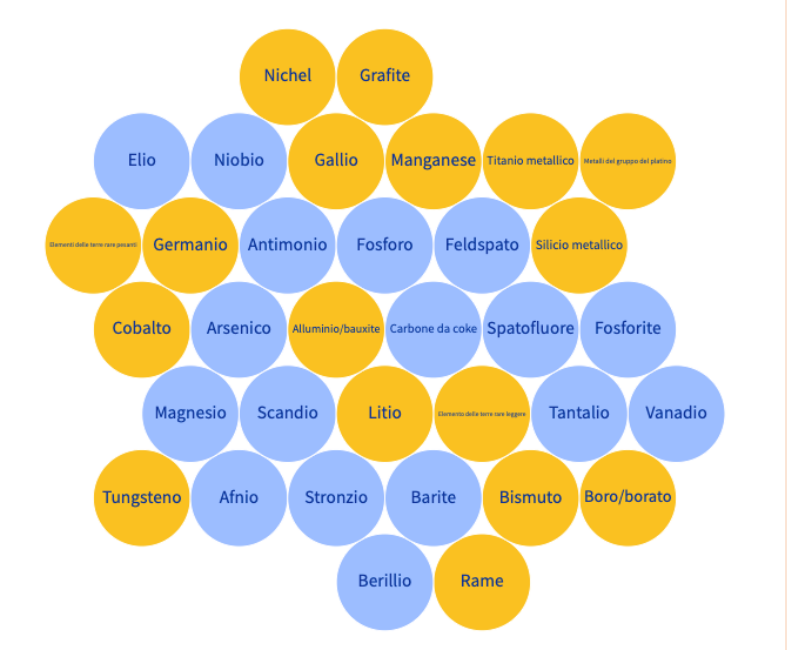

Fig. 2 Materie prime strategiche in Europa (giallo), incluso elementi delle terre rare leggere, metalli del gruppo del Pt, elementi delle terre rare pesanti.

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Members' Publications

List of Members' Publications

referred to the period September 05, 2024 – December 31, 2024

Anselmi, M., Slabaugh, G., Crespo-Otero, R. & **di Tommaso, D.** (2024). Molecular graph transformer: stepping beyond ALIGNN into long-range interactions. *Digital Discovery*, *3*(5), 1048–1057. https://doi.org/10.1039/d4dd00014e

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