

## USING MULTIVARIATE ANALYSIS IN THE SEARCH FOR LIFE ON MARS

The Unscrambler<sup>®</sup> X was used to develop models to analyze Martian soil data from NASA's most sophisticated Mars rover.



**CAMO**

Bring data to life

On the 26<sup>th</sup> November 2011, NASA launched its largest and most sophisticated Mars ever. Officially named the Mars Science Laboratory (MSL), the 'Curiosity' rover will explore the mineral-rich Gale Crater region of Mars in an attempt to find traces of water that may have supported life on the red planet.

To analyze the data collected by Curiosity, advanced multivariate data analysis models will be used, developed using The Unscrambler® X software.

Weighing one tonne and measuring 3 metres long, 2.7 metres wide and 2.1 metres tall at its mast, the nuclear powered Curiosity is much larger than the two previous Mars rovers, Spirit and Opportunity, which landed in 2004. Using a drill combined with a powerful laser and other equipment, the Curiosity will try to understand the chemical composition of the rocks and soil and search for signs of water.

One of the keys to analyzing the chemical composition of the rocks and soil is the use of laser-induced breakdown spectroscopy (LIBS), a powerful analytical technique used in extraterrestrial applications for the first time on Curiosity.

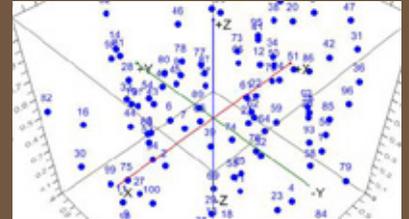
Because the LIBS approach collects an enormous amount of data, equally powerful statistical software was required to analyze the data. The Unscrambler® X was chosen to develop the analysis methodology for its leading multivariate capabilities which are ideally suited to analyzing large or complex data sets.

Dr Frank Westad, Chief Scientific Officer at CAMO Software, says "It's very exciting that multivariate analysis will be used for such a high-profile mission. It demonstrates the power of multivariate analysis for getting a deeper understanding of the important patterns and make predictions from large data sets, whether that is Martian soil, biotech products, petrochemical processes or machinery performance."

Curiosity is due to land in August 2012 and will explore Mars for at least two years, during which time it will cover approximately 20 kilometers.

**For more details please see our Scientific Note overleaf**

## WHAT IS MULTIVARIATE DATA ANALYSIS?



Multivariate Analysis is the investigation of many variables, simultaneously, in order to understand the relationships that may exist between them. This can be as simple as analyzing two variables right up to millions.

While traditional (univariate) statistical approaches such as mean, median, standard deviation etc serve their purposes for investigating and understanding simple systems, when the relationships between variables become more complex, a single variable cannot adequately describe the system. This is the case for most large data sets or processes in industries such as manufacturing, life sciences, energy, agriculture, finance, retail and technology.

To find out more, download our free introductory guide to Multivariate Data Analysis.

 [What is Multivariate Analysis?](#) 

Curiosity rover Image: NASA  
Front cover image: NASA

## SCIENTIFIC NOTE

### Using Laser-induced breakdown spectroscopy (LIBS) for classification of carbonate minerals on Mars

The first laser-induced breakdown spectroscopy (LIBS) instrument for extraterrestrial applications will be used onboard the NASA Mars Science Laboratory (MSL) Rover 'Curiosity,' which launched on 26th November 2011.

Researchers at Los Alamos National Labs and the University of New Mexico are using LIBS to understand the chemical composition of rocks, determine if they can classify the rocks and deduce information about the presence and amount of water on Mars. LIBS data will be collected by the Rover at a distance of up to 7 meters from the Martian samples and multivariate data analysis models developed using The Unscrambler® X will be used to classify the rocks based on their composition.

#### Applying multivariate analysis to LIBS data

LIBS data, with over 6000 variables per sample, are highly multivariate. The use of Principal Component Analysis (PCA), a powerful multivariate analytical tool, allows for a rapid visualization of sample groupings, and from this analysis, classification models can be developed to identify Mars rocks in situ during exploration.

LIBS is a powerful technique for determining the elemental composition of samples. A laser is focused onto a sample (solid, liquid or gas) to create a plasma. Emissions from the plasma are then collected and analyzed spectroscopically and the atomic spectral lines are used to determine elemental composition. Multivariate analysis is applied to the LIBS data to classify samples based on their compositional differences. This work is being done to enable measurement by LIBS of samples of materials on the surface of Mars to determine if water is or has been present on Mars.

#### Materials and methods

The ChemCam is an instrument designed to be mounted on the MSL rover mast, and is comprised of a LIBS instrument and a remote micro imager (RMI). A LIBS database of several carbonate materials is being developed in the laboratory with a system similar to the ChemCam LIBS. Samples include natural rocks collected from various locations, as well as some reference standard samples. The LIBS spectra of calcite ( $\text{CaCO}_3$ ), dolomite ( $\text{CaMg}(\text{CO}_3)_2$ ), siderite ( $\text{FeCO}_3$ ), and rhodochrosite ( $\text{MnCO}_3$ ), have been measured under martian atmospheric conditions (~7 Torr  $\text{CO}_2$ ).

The region of the LIBS spectrum with the most elemental information of the samples was used in the analysis. The multivariate analysis tool of PCA is used which provides a map of samples and variables, helping to identify the variables that relate to the sample and their differences.

By using PCA, a new coordinate system is computed (the principal components) which define the variance in the data. The data is reduced as there are typically fewer Principal Components needed to explain the variance in the data than there are variables in the data set. The PCA scores plot, a projection of samples plotted in the new coordinate system, gives a map of the samples. Similar samples lie closer together than dissimilar samples. Analysis will be done using methodologies developed with The Unscrambler® X software.

#### Results and discussion

A PCA analysis of the LIBS Spectra over the range 460-820 nm was run and samples can be seen to be separated into four groups in the scores plot. From this it can be seen that classification of different carbonate materials is possible based on their LIBS spectra. By adding more samples of the expected classes of materials that may be found on Mars, a model that can identify these materials will be developed. Likewise regression models can be developed to measure the concentration of major elements in the samples. This will allow for rapid identification of unknown samples during the Mars Rover experiments in 2012.

For complete details of this work please see Nina L. Lanza, Roger C. Wiens, Samuel M. Clegg, Ann M. Ollila, Seth D. Humphries, Horton E. Newsom, and James E. Barefield, "Calibrating the ChemCam laser-induced breakdown spectroscopy instrument for carbonate minerals on Mars," Appl. Opt. 49, C211-C217 (2010)

## ABOUT CAMO SOFTWARE

Founded in 1984, CAMO Software is a recognized leader in Multivariate Data Analysis and Design of Experiments software. Our flagship product, The Unscrambler® X, is known for its ease of use, world-leading analytical tools and data visualization. More than 25,000 people in 3,000 organizations use our solutions to analyze large or complex data sets, improve process or equipment monitoring and build better predictive models. We help our clients make better decisions through deeper insights from their data, reduce R&D costs, improve production processes and product quality.

**Software:** The Unscrambler® X

**Methods:** Principal Component Analysis (PCA), Soft Independent Modeling of Class Analogy (SIMCA)

**Data type:** Laser-Induced Breakdown Spectroscopy (LIBS)

**Industry:** Geology, space exploration

**Purpose:** During an upcoming exploration of Mars, surface rocks will be measured by LIBS with the intent to classify them and look for evidence that Mars might once have supported life

**Benefits of The Unscrambler® X:** Selected The Unscrambler® X for its powerful multivariate analysis tools

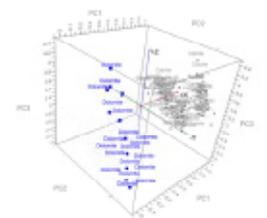


Figure: 3-D Scores plot showing separation of the classes of different carbonate materials.

# CAMO SOFTWARE

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Leading multivariate analysis software used by thousands of data analysts around the world every day. Includes powerful regression, classification and exploratory data analysis tools.

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### Unscrambler® X Prediction Engine & Classification Engine

Software integrated directly into analytical or scientific instruments for real-time predictions and classifications directly from the instruments using multivariate models from The Unscrambler® X.

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