

The Isoscape Approach in Ecological Studies

Use of Stable Isotopes in Environmental Investigations

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Mission 4 "Education and Research" - Component 2: "From research to business" - Investment
3.1: "Fund for the realisation of an integrated system of research and innovation infrastructures"



Isoscapes: What?



Isoscapes: What?

J B West, G J Bowen, T E Dawson, K P Tu

Isoscapes

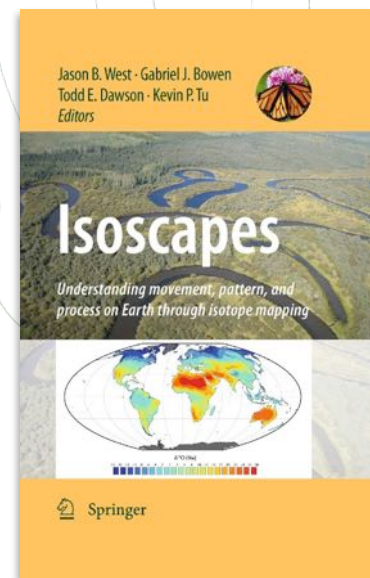
Understanding Movement, Pattern,
and Process on Earth Through
Isotope Mapping

Springer (2010)

DOI 10.1007/978-90-481-3354-3

Gathering and Using Spatially Explicit Isotope Data

Published 2010



DOI 10.1007/978-90-481-3354-3

Isoscapes: For what?

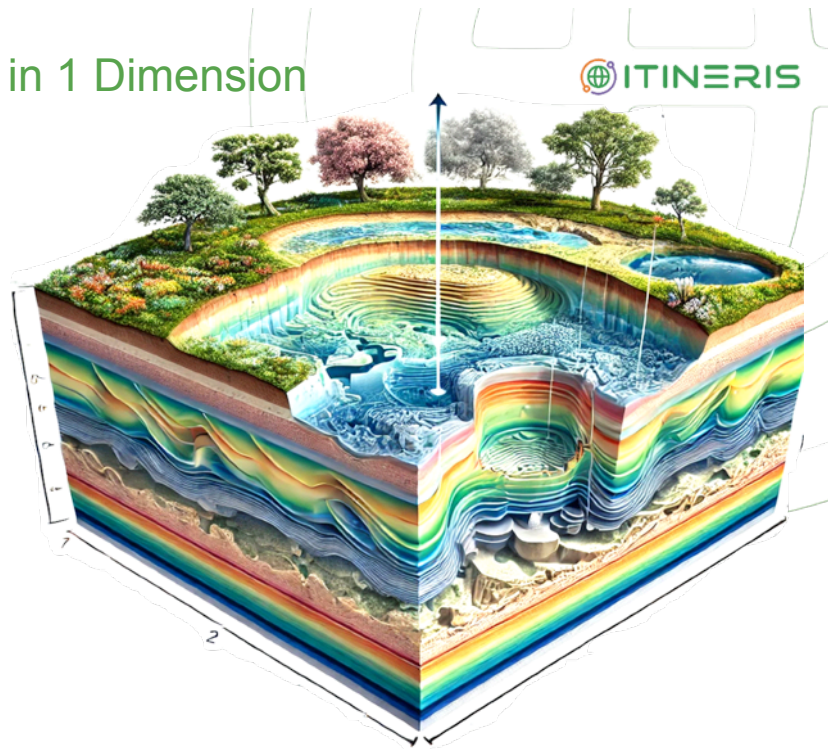
Gathering and Using Spatially Explicit Isotope Data. For what?

- 🌐 Assessing global change patterns (air $\delta^{13}\text{C}$, precipitation $\delta^2\text{H}$ and $\delta^{18}\text{O}$)
- 🌐 Tracking animal migration (e.g. migratory birds feathers, $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ from food, $\delta^2\text{H}$ and $\delta^{18}\text{O}$ from water intake)
- 🌐 Hydrology and meteorology (i.e. ground and atmosphere water, $\delta^2\text{H}$ and $\delta^{18}\text{O}$)
- 🌐 Plant ecosystem dynamics, organisms symbiosis ($\delta^{13}\text{C}$, $\delta^{15}\text{N}$, and $\delta^{18}\text{O}$)
- 🌐 Trophic chain analysis ($\delta^{13}\text{C}$ and $\delta^{15}\text{N}$)
- 🌐 Mineral formation, weathering, and fluid movements ($\delta^{13}\text{C}$, $\delta^{34}\text{S}$, and $^{87}\text{Sr}/^{86}\text{Sr}$)
- 🌐 Forensics, food and commodities geographical origin ($\delta^n\text{X}$ but not alone)

Isoscapes: Finding Patterns in 1 Dimension

A **1D isoscape** represents isotopic variation along a linear path, such as a river, elevation gradient, or migration route.

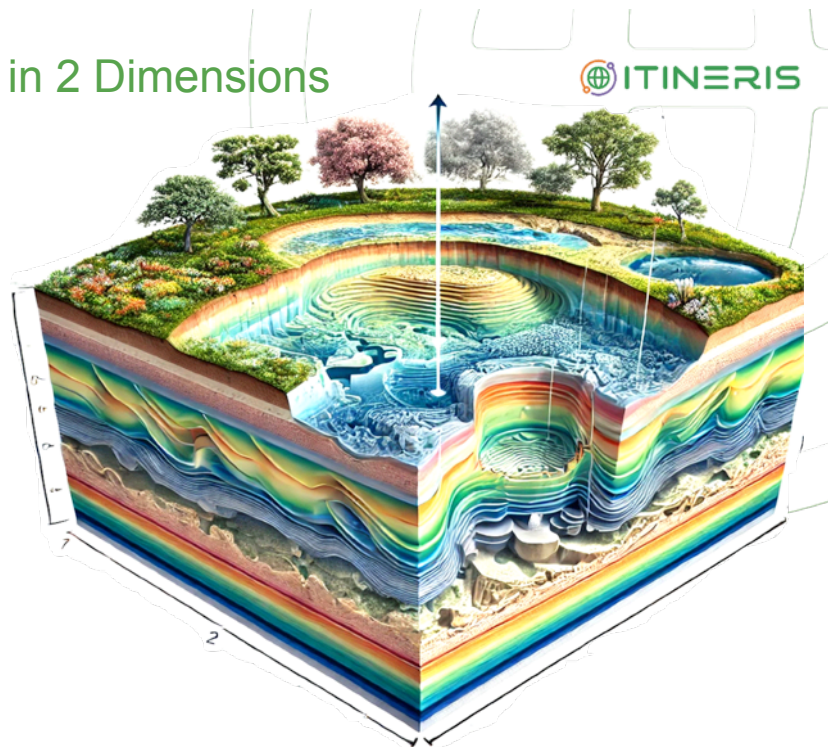
These transects help analyze how isotopic signatures change with distance or altitude, providing insights into hydrological cycles, biological movements, or geological transitions.



Isoscapes: Finding Patterns in 2 Dimensions

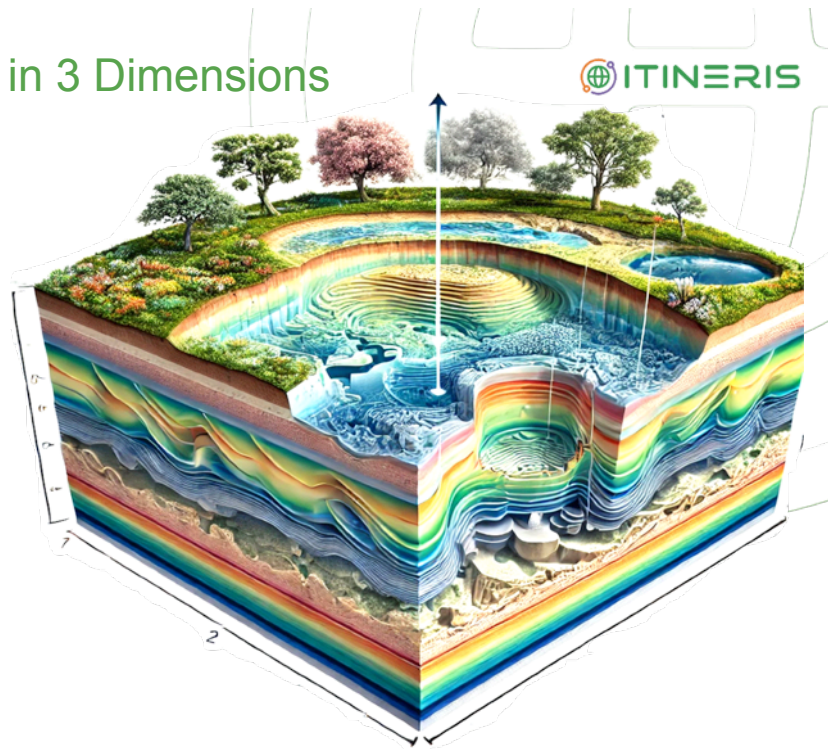
A **2D isoscape** is a spatial representation of isotopic variation over a geographic area. It is often visualized as a contour or heatmap, where color gradients indicate different isotopic values.

These maps are widely used in ecology, climatology, and forensic science to track water sources, animal migration, and environmental changes.



Isoscapes: Finding Patterns in 3 Dimensions

A **3D isoscape** extends isotopic mapping into depth, incorporating variations in the subsurface, soil layers, and atmosphere. This approach is essential in **critical zone science**, where isotopic signals reveal interactions between rock, water, air, and living organisms. By capturing isotopic gradients through depth, 3D isoscapes provide a holistic view of Earth's biogeochemical processes.

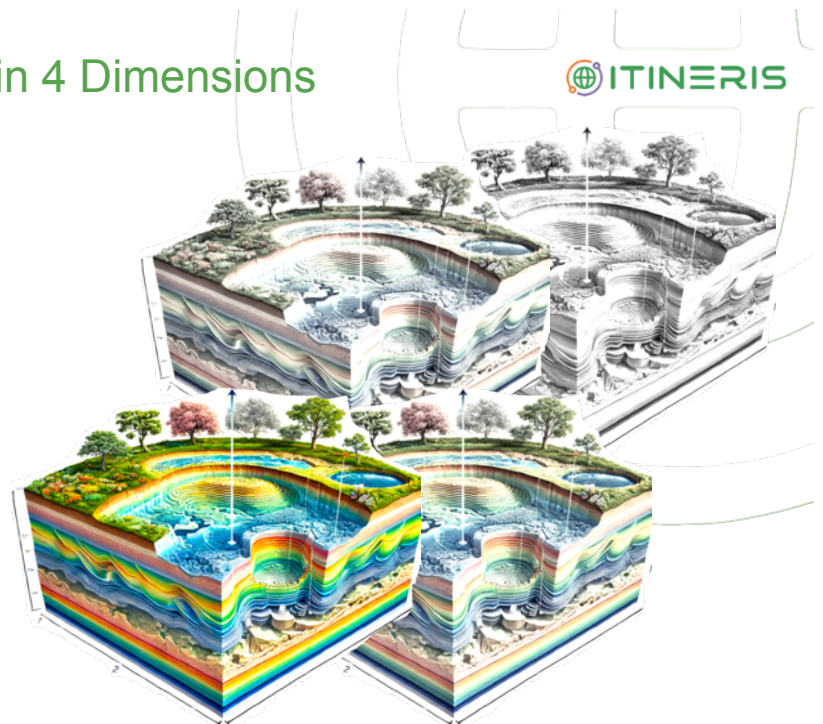


Isoscapes: Finding Patterns in 4 Dimensions

An isoscape typically captures conditions at a specific moment in time. However, in principle, all phenomena are time-dependent.

Isoscapes can be made time-dependent in various ways, making it a dynamic and innovative field within geostatistics.

Time is not merely another coordinate. It adds a lot of complexity.

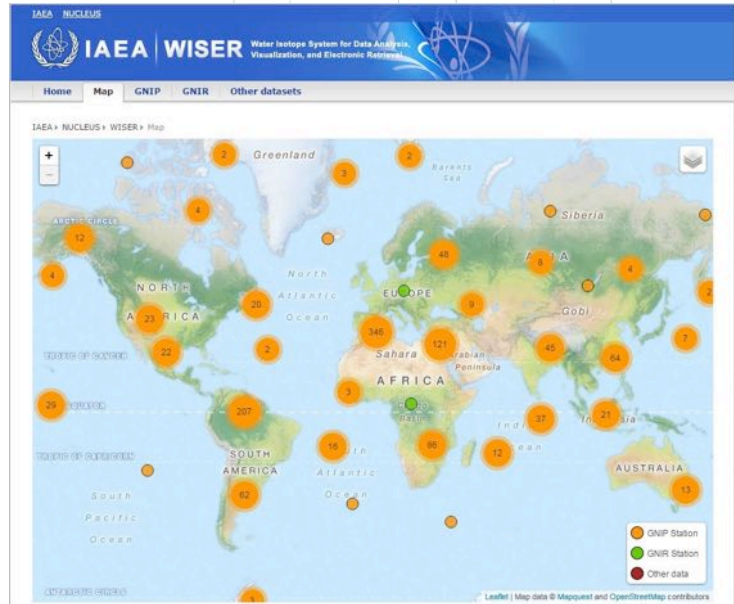


Examples: Precipitations Water

The **Global Network of Isotopes in Precipitation (GNIP)** was established in **1961** by the International Atomic Energy Agency and the World Meteorological Organization.

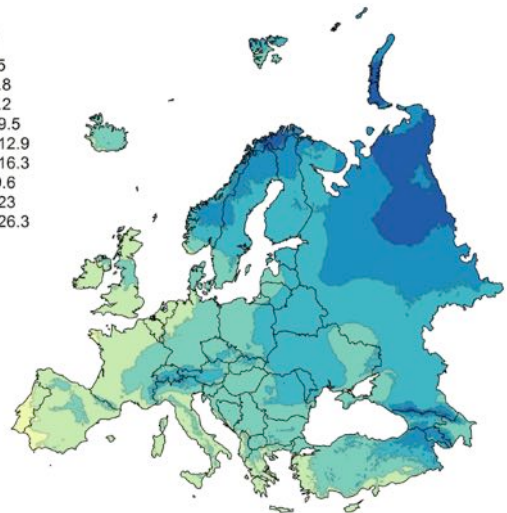
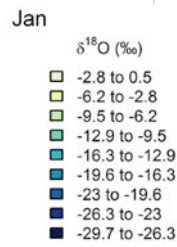
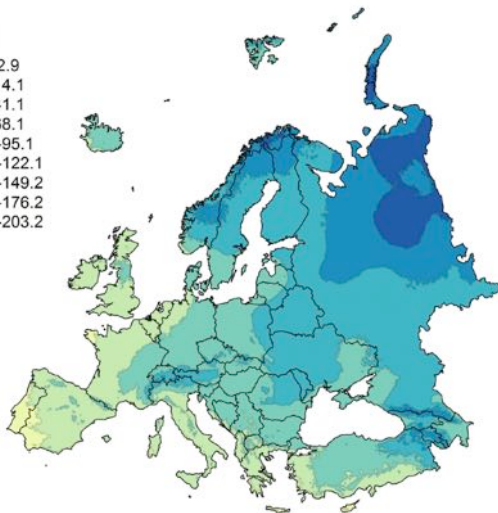
Not yet maps.

The most widely used base ingredients for isoscapes.



© <https://www.iaea.org/services/networks/gnip>

Examples: Rain Water Cartoons



© <http://waterisotopes.org>

Precipitation water $\delta^2\text{H}$ and $\delta^{18}\text{O}$ — From GNIP data and other sources

examples: Rain Water $\delta^{18}\text{O}$ Isoscape - Italy 2003

Even though the term *isoscape* does not yet appear, there are earlier examples before 2010, e.g.

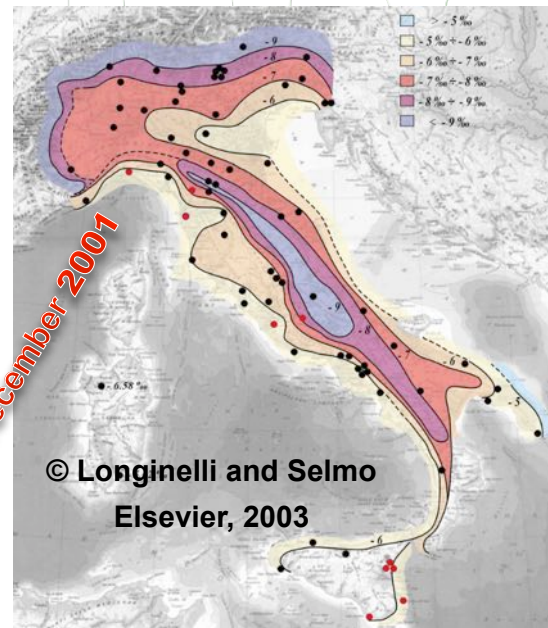
A. Longinelli and E. Selmo

Isotopic composition of precipitation in Italy: a first overall map

Journal of Hydrology 270 (1-2) 2003

[https://doi.org/10.1016/S0022-1694\(02\)00281-0](https://doi.org/10.1016/S0022-1694(02)00281-0)

Received 6 December 2007



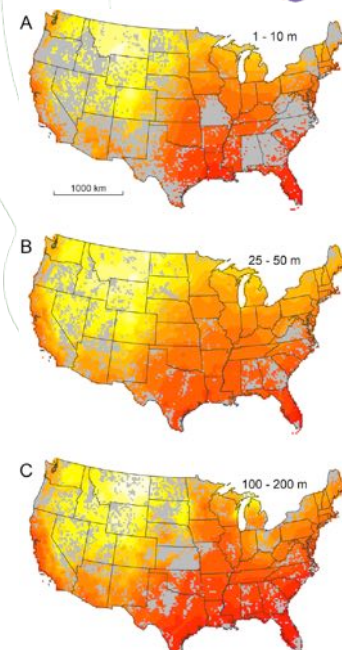
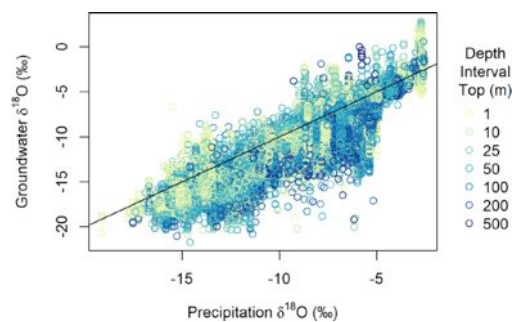
DOI: 10.1016/S0022-1694(02)00281-0

Examples: Groundwater $\delta^{18}\text{O}$

Bowen et al. (2022)

A 3-D groundwater isoscape of the contiguous USA for forensic and water resource science.

PLoS ONE 17(1): e0261651.



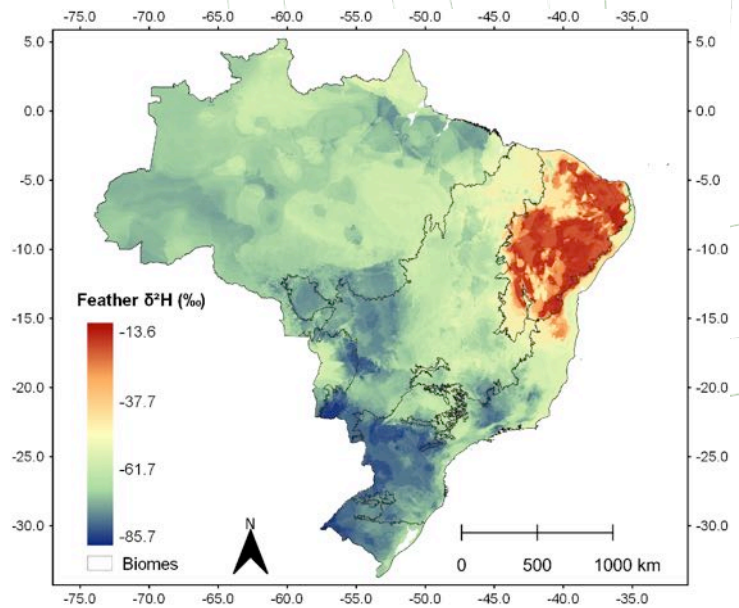
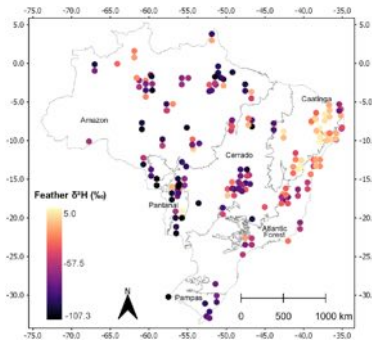
DOI 10.1371/journal.pone.0261651

Examples: Bird Feather $\delta^2\text{H}$

Alquezar et al. (2022)

A feather hydrogen ($\delta^2\text{H}$) isoscape for Brazil.

PLoS ONE 17(8): e0271573.



DOI 10.1371/journal.pone.0271573

Examples: Food and Commodities

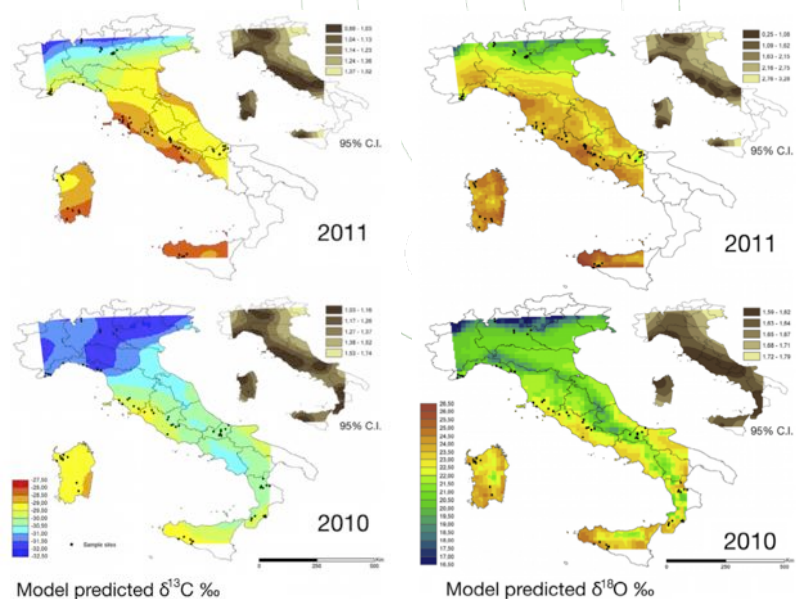
Extra virgin olive oil isoscapes for geographical origin assessment.

Maps obtained by Kriging each years' samples values.

Inset maps show the accuracy of the estimate.

EVOO $\delta^{13}\text{C}$

EVOO $\delta^{18}\text{O}$

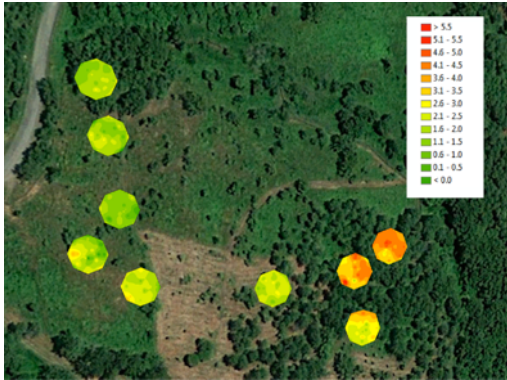


DOI: 10.1016/j.foodchem.2016-04-146

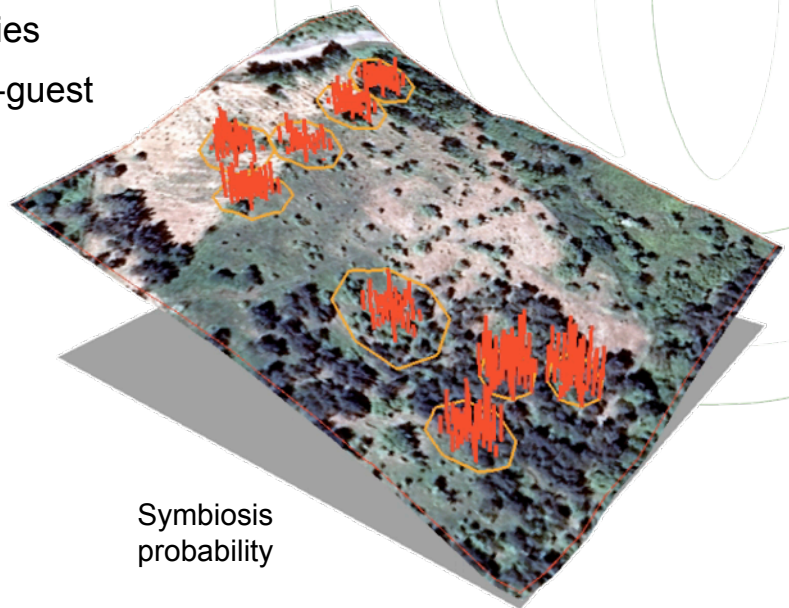
Examples: Tree-Fungi Symbiosis (1)

Tuber aestivum survival strategies

Symbiosis probability from host-guest $\Delta^{13}\text{C}$ and $\Delta^{15}\text{N}$ modeling.



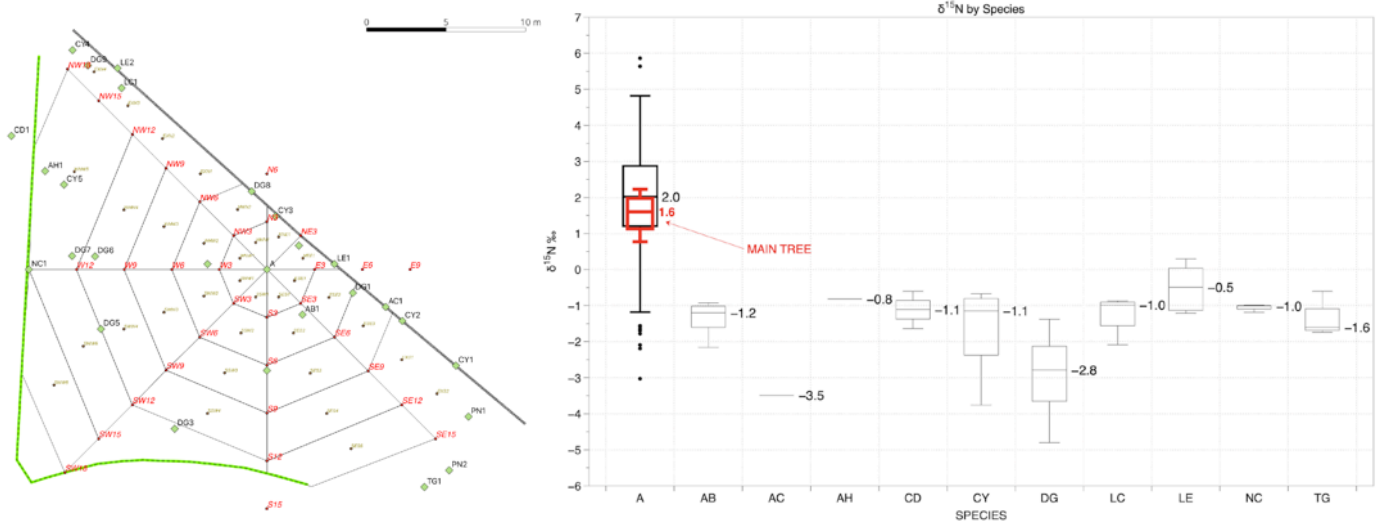
Multiple soil $\delta^{15}\text{N}$ isoscapes



ISBN 978-88-7843-046-4

Examples: Spatial Sampling & Non-spatial Analysis

Ailanthus altissima vs autochthonous species leaf $\delta^{15}\text{N}$





Spatial data is not just samples with coordinates.

No maps can be generated when sampling is done only along transects, as spatial continuity is lost.

3D isoscapes can be generated, but they require a vast number of cells, significant computational resources, and an extensive amount of input data, making the process highly complex.

The spatial reference must be carefully chosen, in order to minimize computing needs and have a smooth GIS workflow.

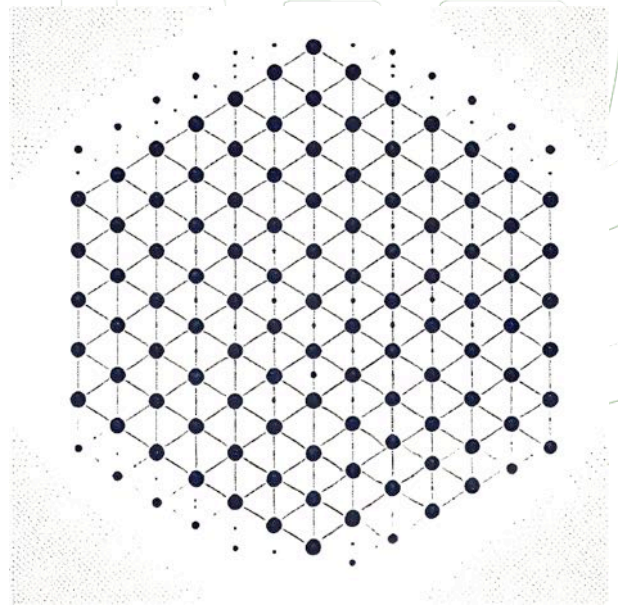
Sampling - Regular Lattices

Lattice arrangements of sample points are commonly used in isoscapes to ensure systematic and uniform spatial coverage.

The choice of lattice depends on the spatial structure of the variable being mapped.

Regular grids in Cartesian coordinates provide ease of interpolation but may not account for natural anisotropies.

Packed hex grids are geometrically robust, but hard to implement on the field.



Sampling - Global Spherical Coordinates

Longitude and Latitude must be reserved only to datasets spanning the whole Earth.

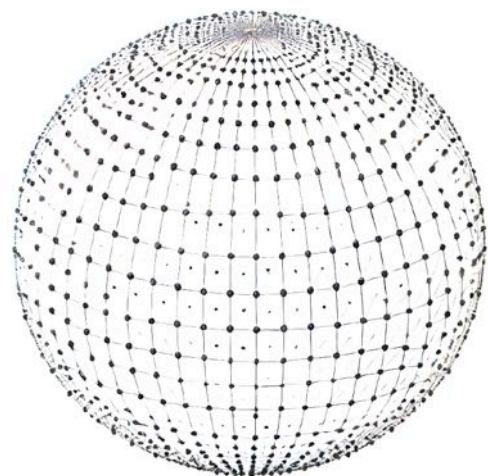
The distances have to be calculated along geodesics: intensive, time consuming maths.

Even whole continents can be effectively projected on a plane.

Use decimal degrees, or better yet radians.

Tip:

Never use degrees° minutes' seconds”.

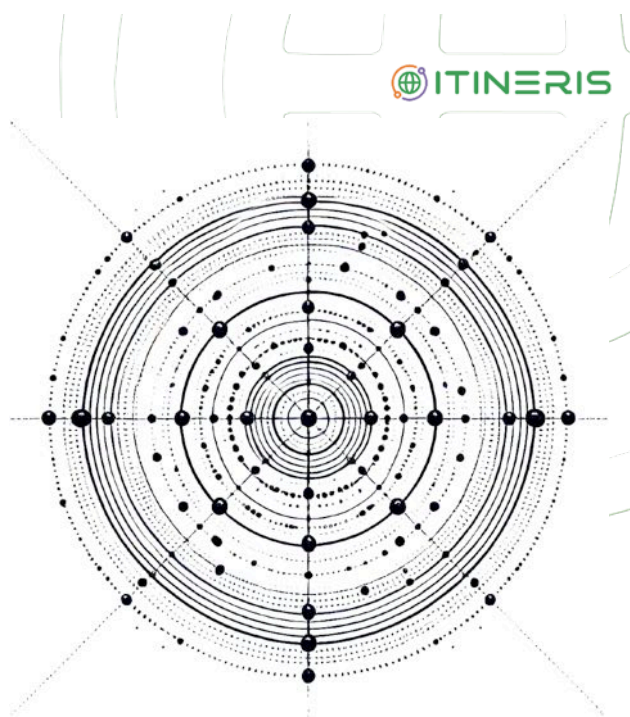


Sampling - Polar Coordinates

Polar coordinates are particularly useful when there is a central point of interest, as they naturally describe positions relative to a fixed origin.

In polar coordinates, only the central reference point needs to be GPS-located with high accuracy, while other positions can be determined relative to it.

This system is especially effective for analyzing anisotropies.

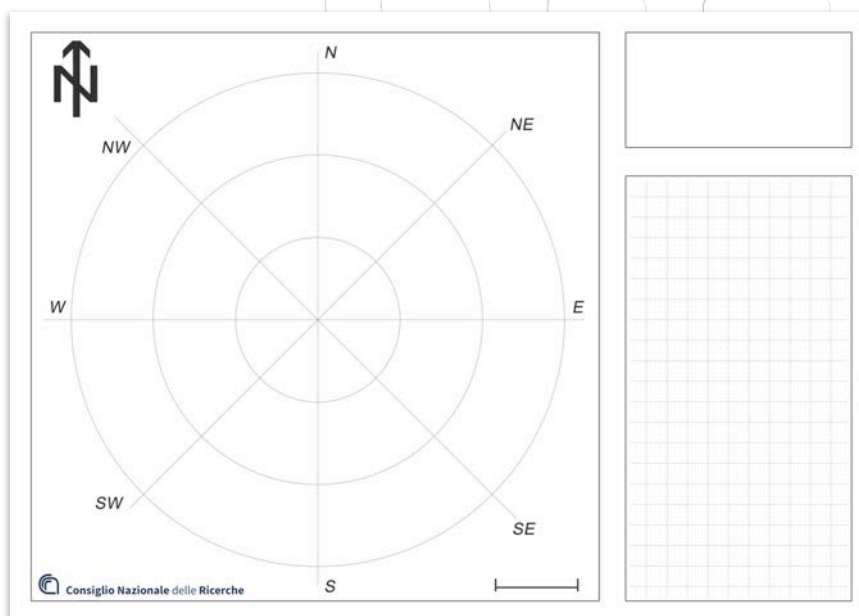


Isoscapes: Field Sampling

Tip:

Prepare in advance your polar coordinates sketch sheets.

25 sampling points (a center and three sites per eight direction arms) is a fair sampling scheme.

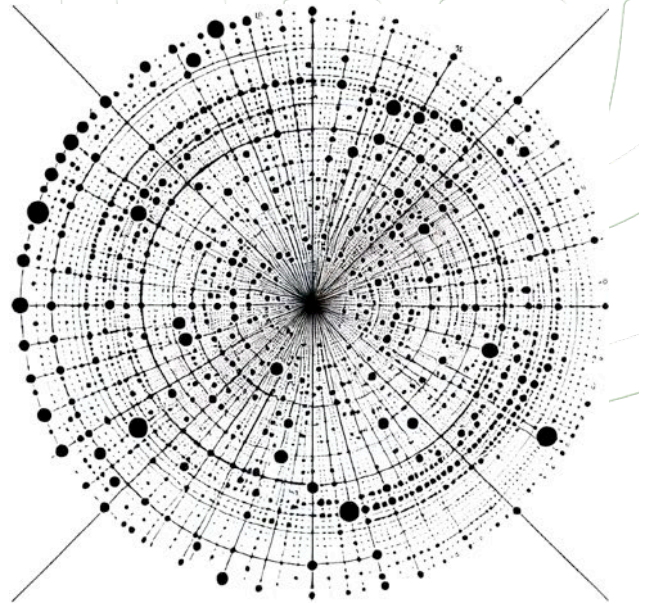


Sampling - Be Flexible!

Tip:

Whatever your sampling strategy, be prepared for any changes on the field.

On even terrain, a Monte Carlo arrangement of sampling points can be considered, as it provides a randomized yet statistically representative distribution, helping to capture spatial variability without systematic bias.



Isoscapes: Mapping






Isoscapes: Mapping - Coordinates

All coordinates are equivalent, but not all coordinates are equal.

There are the spherical geographical coordinates. Only for global models - to be avoided unless there is no projection that can accommodate all the input data.

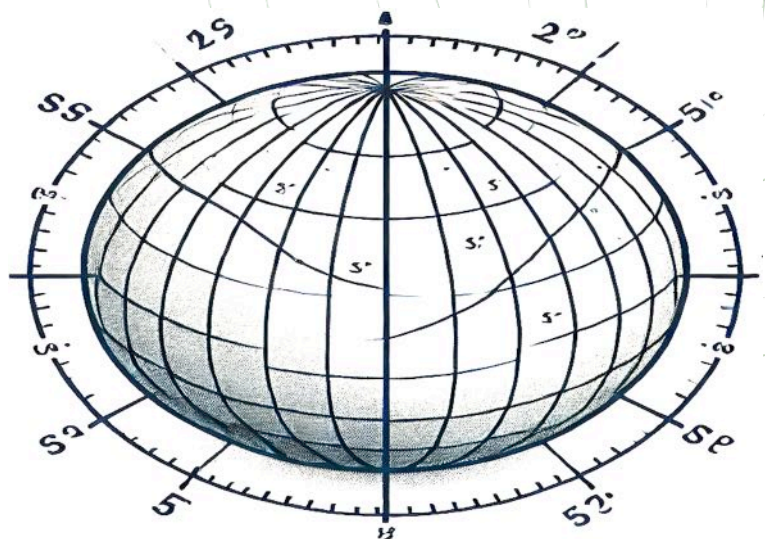
There are three kinds of projected coordinates:

-  Equivalent , i.e. area-preserving
-  Equidistant, i.e. distance-preserving
-  Conformal, i.e. angle-preserving

Isoscapes: Mapping - Datum

A **datum** is a reference system used in geodesy and cartography to define the shape of the Earth and establish coordinate locations. It consists of a mathematical model of the Earth's surface as an **ellipsoid**.

Datums can be **geocentric** (i.e. Earth-centered, like WGS84) or **local**, fit to a specific region, like the ETRS89 in Europe.



Isoscapes: Mapping - Projected Coordinates

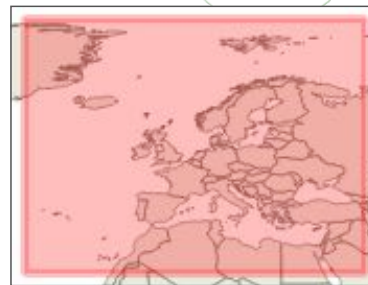
Traditionally, the most used coordinates are **UTM** - Universal Transverse Mercator, a **conformal** projection.

In **Europe**, use **Lambert** projections, e.g. EPSG:3035 Lambert Azimuthal Equal Area, an equivalent projection.

Tip:

EPSG:3035 is used in all Copernicus products covering EU27 and beyond.

Universal
Transverse
Mercator



Lambert
EPSG:3035

Isoscapes: Mapping - Set up your GIS

Prepare your GIS environment.

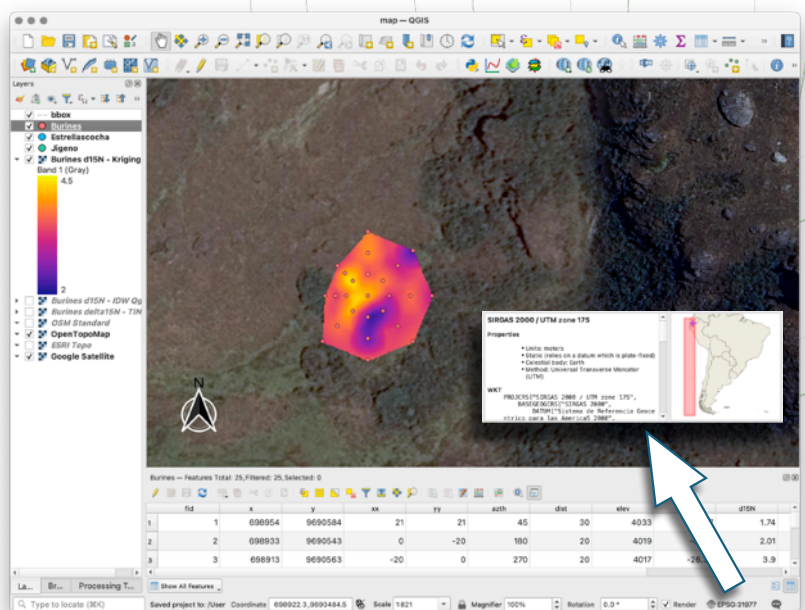
Possible choices: QGIS, R.

Tip:

Use the same projection for all the layers to prevent isoscapes inconsistencies.

Double check projections!

Alternative: ESRI ArcGIS - MS Windows only.





Isoscapes: The Maths Behind the Models

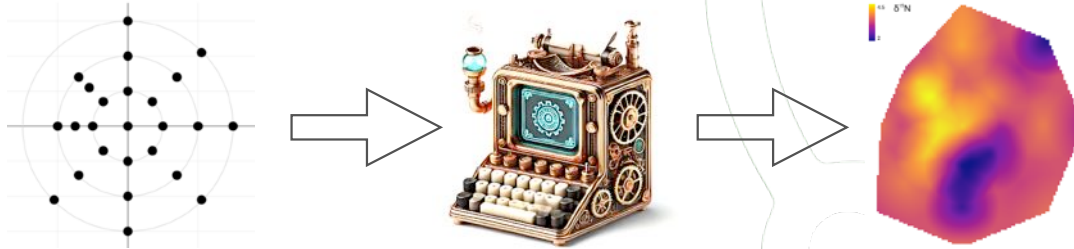
An **isoscape** is a **scalar field** that represents spatial or spatiotemporal variations in isotopic compositions across a landscape. It is typically modeled as a continuous surface where each point is assigned a scalar value corresponding to an isotopic ratio (δ -isoscape) or, more rarely, an isotopic fractionation (Δ -isoscape).

In a purely spatial isoscape, the field describes isotopic variation across geographic space, often used in ecology, hydrology, and forensic science.

In a spatiotemporal isoscape, the field evolves over time, capturing seasonal or long-term changes in isotopic distributions, such as shifts in precipitation patterns or migration pathways.

From a data science perspective, **an isoscape is simply a georeferenced dataset**, usually easily handled by the computing power of modern PCs and laptops.

Isoscapes: The Maths Behind the Models



An nX **isoscape** is a **raster image** generated from the spatial distribution of isotopic abundances of element X taken at **discrete sampling points**.

Using **interpolation** algorithms such as Kriging or inverse distance weighting, **the values** at these points **are extended to** create a continuous **surface** representing spatial variation of δ^nX — or even Δ^nX .

The **accuracy** of the isoscape depends on the **density** and **distribution** of the sampling points, as well as the chosen interpolation method.

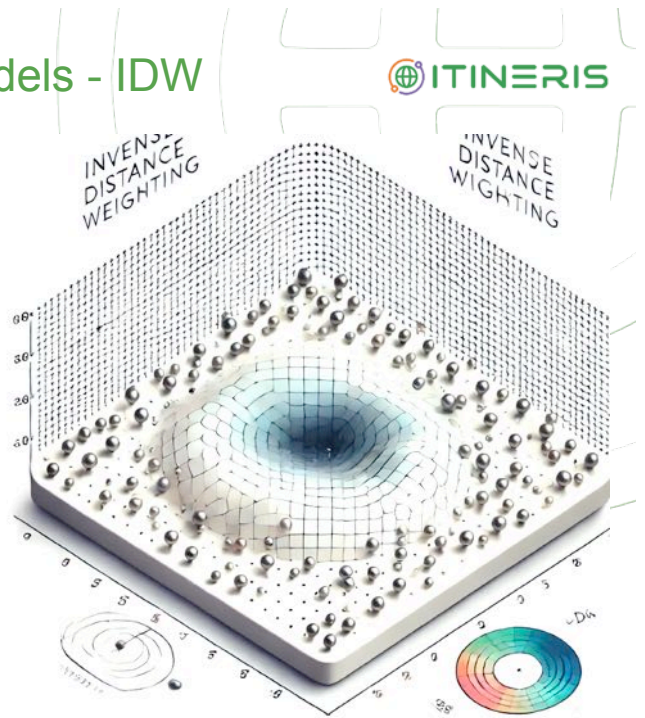
Isoscapes: The Maths Behind the Models

- 🌐 **Inverse Distance Weighting** — Fast and easy to implement, but may not capture complex trends well. Excellent for generating a quick first-impression map.
- 🌐 **Kriging** — Geostatistical method based on spatial autocorrelation. Smooth and reliable estimates but computationally intensive. Estimates model uncertainty.
- 🌐 **Triangulated Irregular Network** — Great for terrain modeling, preserves sharp changes but may introduce artifacts. Not much used for isoscapes.
- 🌐 **Spline Interpolation** — Produces smooth results by minimizing curvature.
- 🌐 **Polynomial Regression** — Captures broad trends but ignores local variation.
- 🌐 **Bayesian Interpolation** — Bayesian statistics applied to spatial interpolation, e.g. Bayesian Kriging models initial distribution as a Gaussian process.
- 🌐 **Moving average, Voronoi tessellation, Radial basis interpolation...**

Isoscapes: The Maths Behind the Models - IDW

Inverse Distance Weighting is a deterministic spatial interpolation method that estimates values at unknown locations based on the weighted average of nearby known points. The influence of each known point is inversely proportional to its distance from the unknown location: closer points have a greater impact, while farther points contribute less.

IDW often produces a bulls-eye pattern around data points and does not account for spatial autocorrelation.

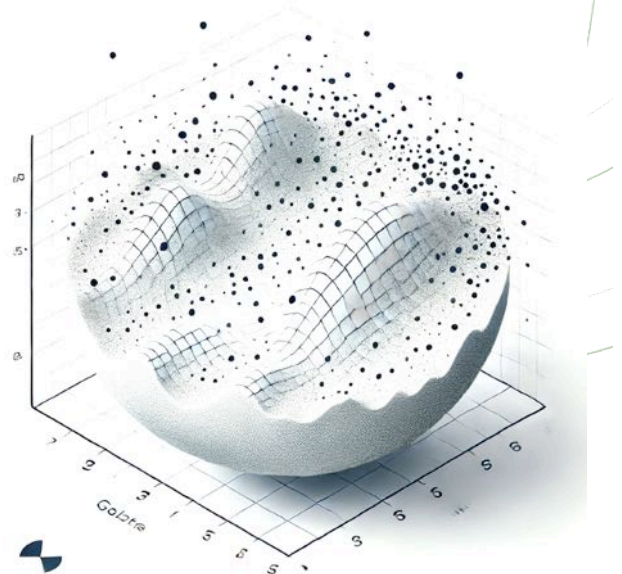


Isoscapes: The Maths Behind the Models - Kriging

Kriging is a geostatistical interpolation method that estimates values at unknown locations based on both distance and spatial autocorrelation, it uses a variogram model to quantify how data points relate over space.

There are different *flavors* of Kriging, each suited to specific data spatial patterns:

- 🌐 Ordinary Kriging assumes a constant but unknown mean.
- 🌐 Simple Kriging assumes a known global mean.
- 🌐 Universal Kriging models a spatial trend along with local variations. Often the first choice.
- 🌐 Bayesian Kriging extends traditional Kriging by incorporating prior probability distributions.

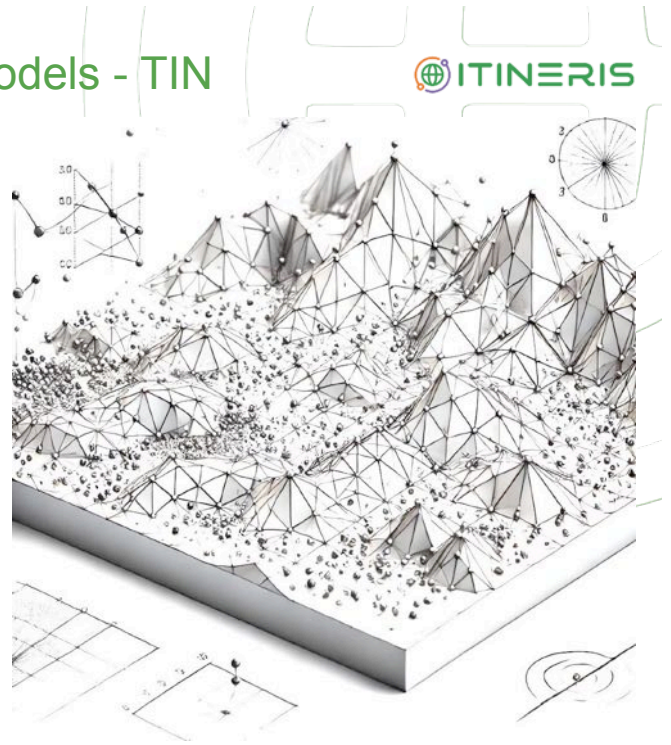


Isoscapes: The Maths Behind the Models - TIN

Triangulated Irregular Network represents a surface using non-overlapping triangles formed from irregularly spaced data points. It is particularly useful for terrain modeling, as it preserves sharp features like ridges and valleys better than grid-based methods.

TIN adapts to data density, using more triangles in areas with high variability and fewer in flatter regions.

TINs are rarely employed for isoscapes, but they should be considered when dealing with high value differences for very close points.

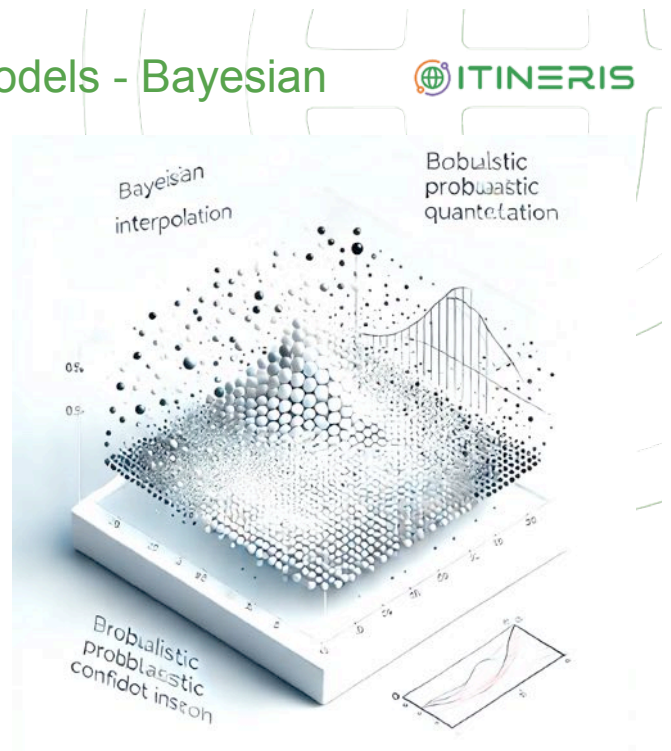


Isoscapes: The Maths Behind the Models - Bayesian

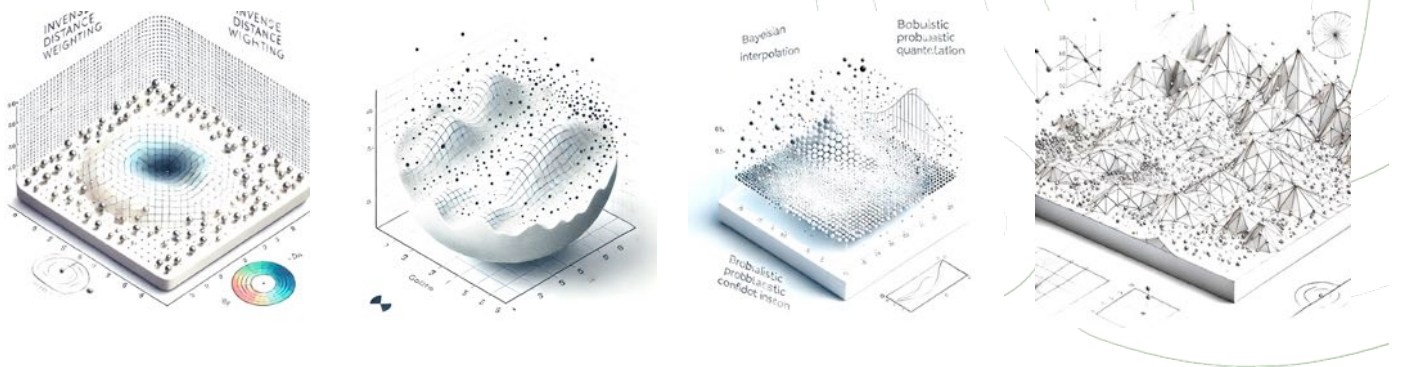
Bayesian interpolation is a probabilistic approach to spatial estimation that incorporates prior information and updates predictions as new data become available. Unlike deterministic methods, it provides a full probability distribution for each predicted value, allowing for uncertainty quantification rather than just a single estimate.

A common application is Bayesian Kriging, integrating prior knowledge about spatial relationships, making it particularly useful in data-scarce environments.

It is computationally intensive.



Isoscapes: The Maths Behind the Models



Tip:

Do not to dive headfirst into Kriging while neglecting other interpolation algorithms. Furthermore, Kriging requires a thorough analysis of input distribution, based on variogram.

Spatiotemporal Modeling

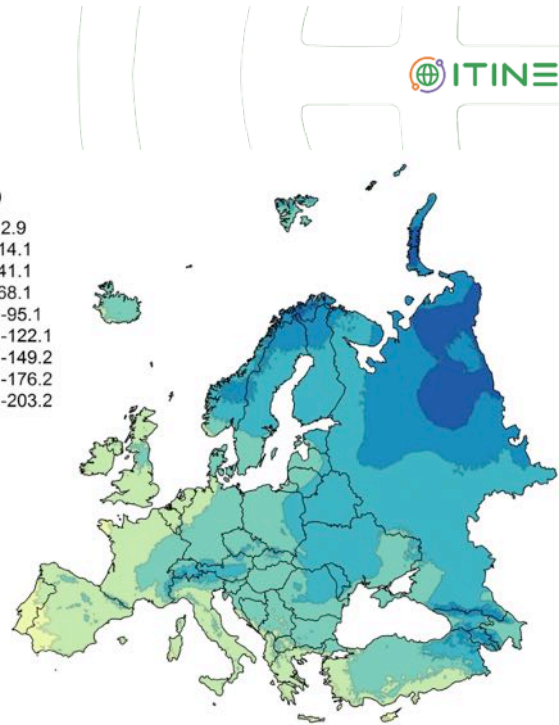
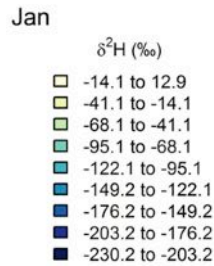


Not a Spatiotemporal Model

Precipitation Water $\delta^2\text{H}$

Each model is obtained with values medians from 1961 to 2024.

Not a spatiotemporal model but a collection of monthly averaged data: it is a stack of purely spatial isoscapes.



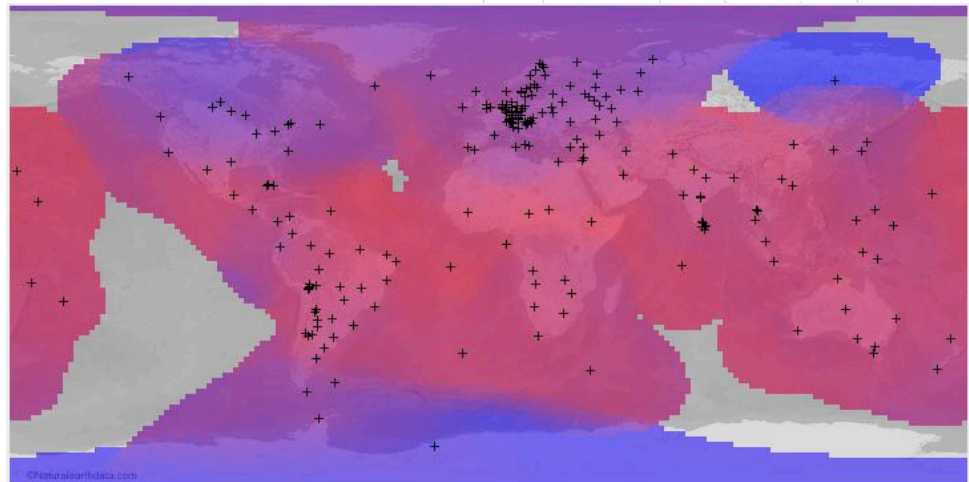
© <http://waterisotopes.org>

Global Water Spatiotemporal Model - $\delta^{18}\text{O}$

An actual spatiotemporal isoscape.

Measurements from 1975 to 1985.

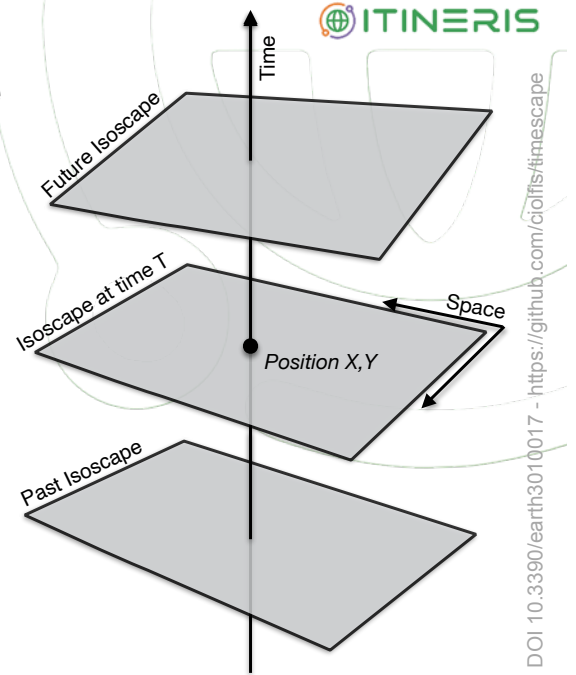
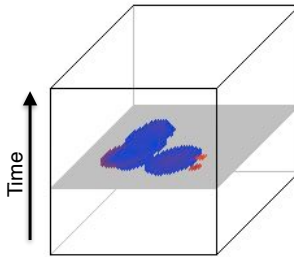
The *knowledge*, i.e. the covered areas, grow with time.



<https://sourceforge.net/projects/timescapeglobal/>

Spatiotemporal Modeling in a Nutshell

- Time is treated as a further pseudo-coordinate
- Memory demanding & computationally stressing
- Not so standard GIS and geostatistical procedures require programming skills
- Spatiotemporal versions of Kriging exist
- The notion of distance must be generalized
- Data fusion from multiple sources is a delicate process
- Non-standard data formats

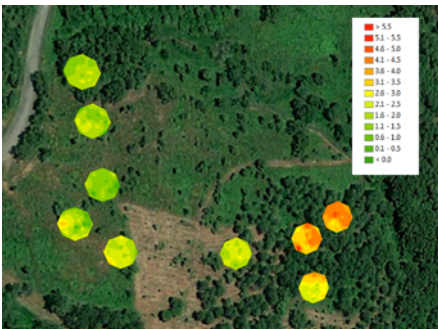


DOI 10.3390/earth3010017 - <https://github.com/ciolfi/timescape>

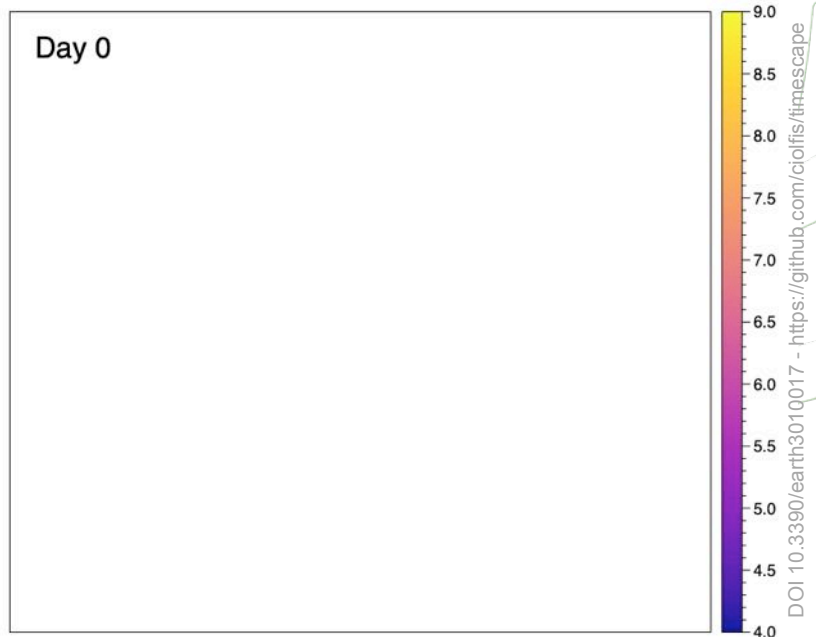
Examples: Tree-Fungi Symbiosis (2)

A **timescape** is needed when the $\delta^{15}\text{N}$ spatial and temporal patterns cannot be treated as purely spatial models or as time series: **entangled variability**.

Multiple soil $\delta^{15}\text{N}$ isoscapes



Fungi $\delta^{15}\text{N}$ timescape — 64 samples collection days



DOI 10.3390/earth3010017 - <https://github.com/ciolfi/timescape>

Spatiotemporal Modeling Toolbox

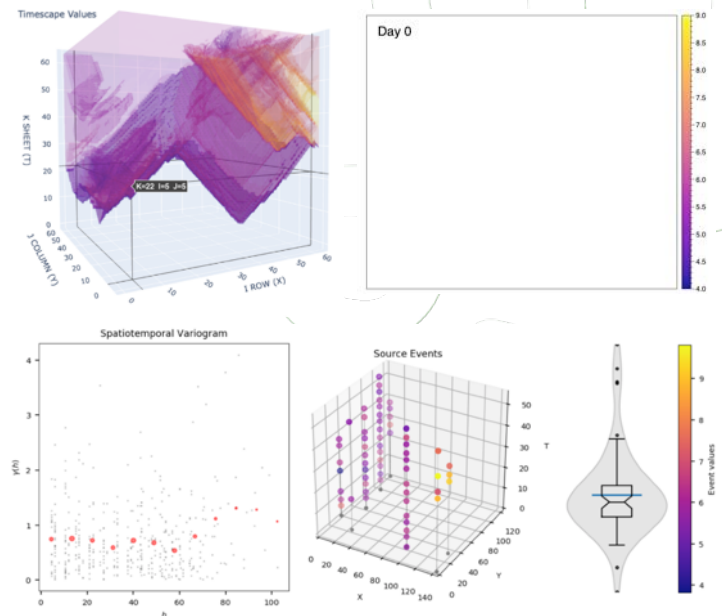
Spatiotemporal analysis integrates time series and geostatistics techniques.

Some R packages can help: stat, spTimer, RandomFields, spacetime...

There is no established toolbox - some computational improvisation is always required.

Tip:

Consider NetCDF, HDF5, GRIB... data formats



DOI 10.3390/earth3010017 - <https://github.com/ciolfi/timescape>

Isoscapes: A Working Example

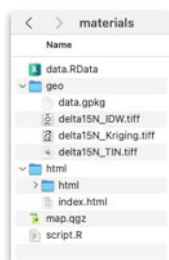


Exercise - Soil $\delta^{15}\text{N}$ - A Minimal Working Example

A complete dataset from three similar sampling sites.

Soil C%, $\delta^{13}\text{C}$, N%, and $\delta^{15}\text{N}$.

A full QGIS - R procedure for a $\delta^{15}\text{N}$ isoscape.



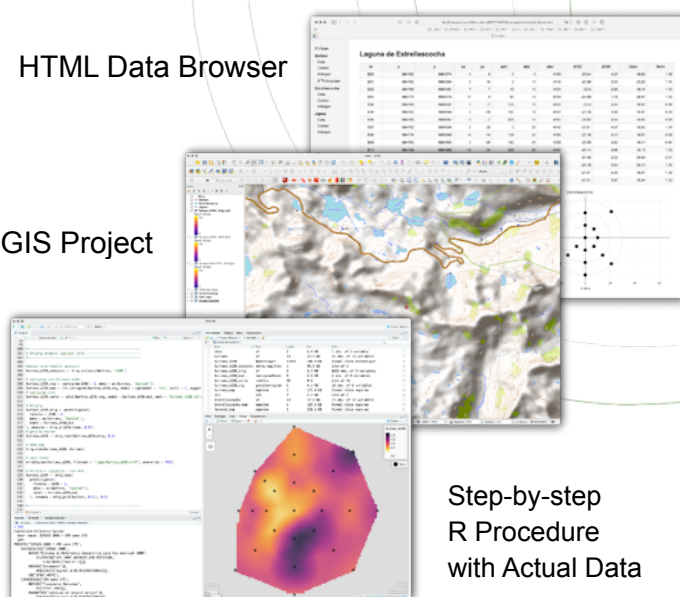
Files:

- html.gz
- qgis.gz
- r.gz

[Resource – Itineris Training Platform](#)

HTML Data Browser

QGIS Project



Step-by-step R Procedure with Actual Data

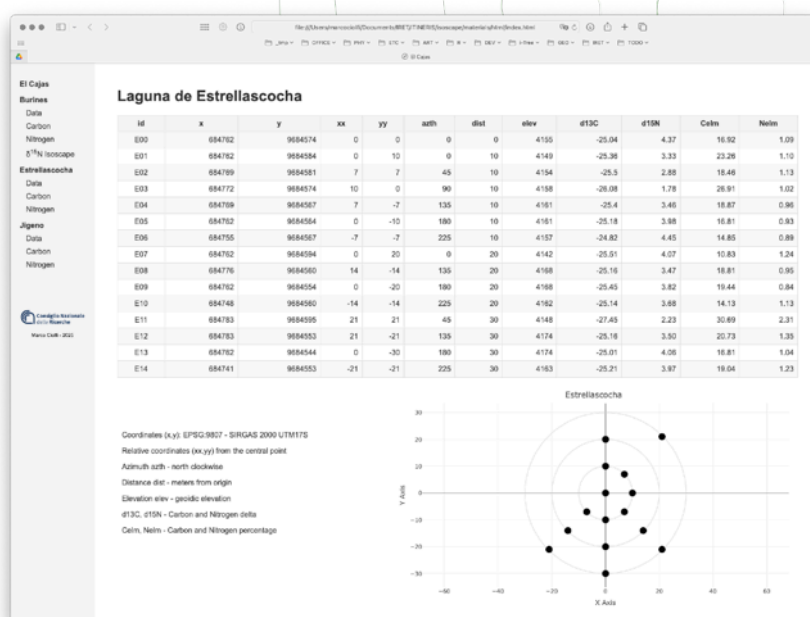
Exercise - Soil $\delta^{15}\text{N}$ - Materials: Data Viewer

HTML Data Browser

For each sampling site there is a table of data, including coordinates, elevation and the measured soil C%, $\delta^{13}\text{C}$, N%, and $\delta^{15}\text{N}$.

Includes interactive maps, variograms, etc.

The quantity and quality of samples differs from site to site.

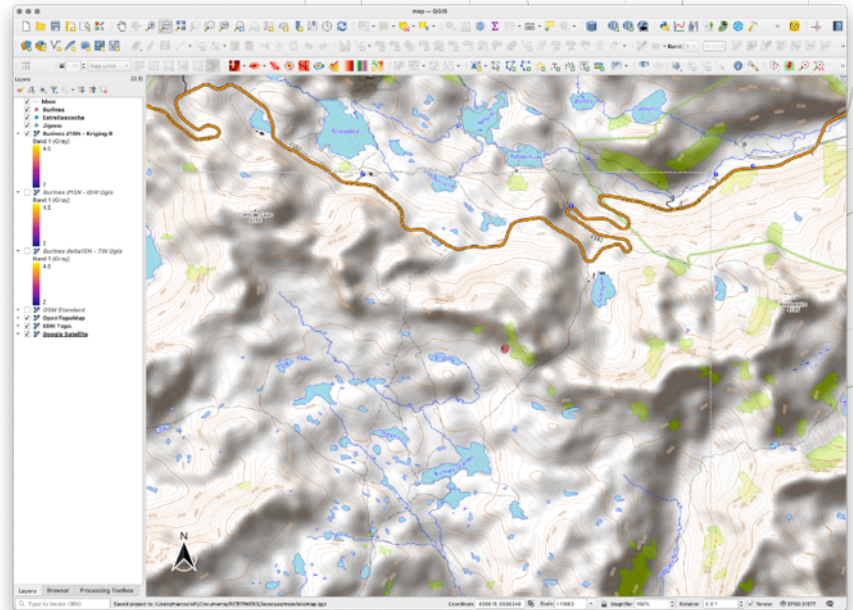


Exercise - Soil $\delta^{15}\text{N}$ - Materials: QGIS Mapping

QGIS Project

A GIS project including all the samples and three different $\delta^{15}\text{N}$ isoscapes (IDW, Kriging and TIN) build from the same dataset.

Uses projected coordinates.

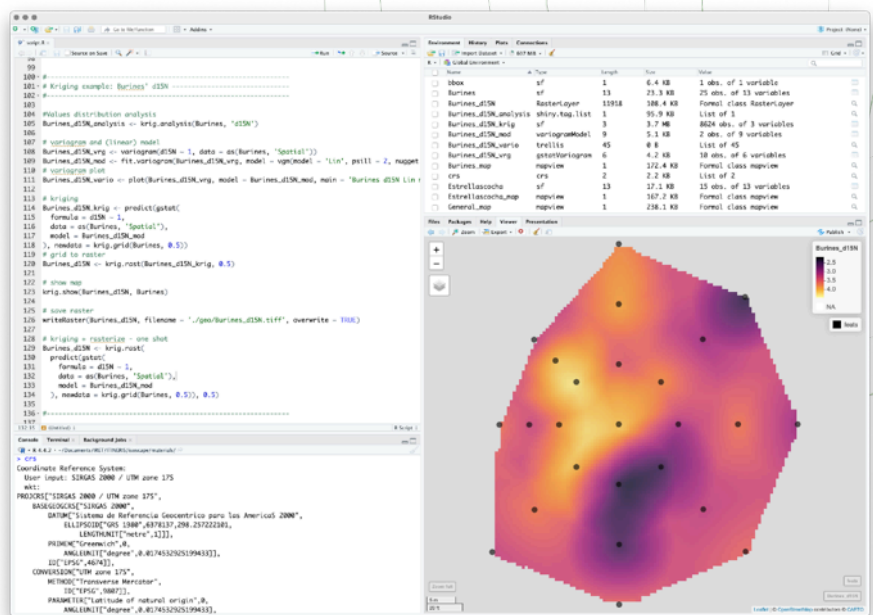


Exercise - Soil $\delta^{15}\text{N}$ - Materials: R Procedure

Step-by-step R Procedure

A fully-functional working example in R showing all the steps for evaluating a $\delta^{15}\text{N}$ Kriging isoscape.

Includes some custom developed functions based on the **sf**, **sp** and **gstat** packages for Kriging evaluation and maps visualisation.



Exercise - Soil $\delta^{15}\text{N}$ - Setup - Sampling Area



Exercise - Soil $\delta^{15}\text{N}$ - Setup - Samples Collection

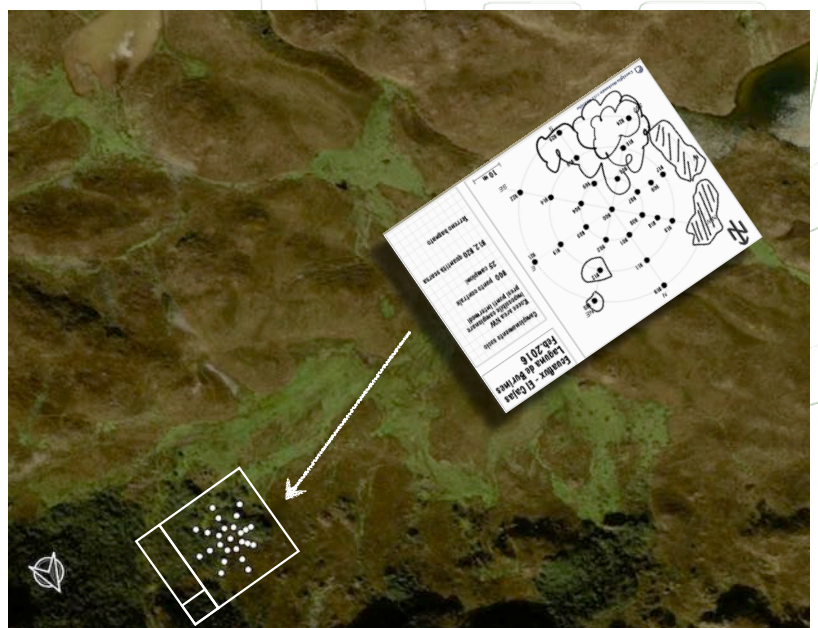
Isotopic data from the **Ecuaflex** project. Carbon fluxes in the Ecuadorian Andes, 2015-2016.

Soil samples dataset.

Shallow soil, small woods and grassland, intricate local hydrography: lakes, catchments, streams.

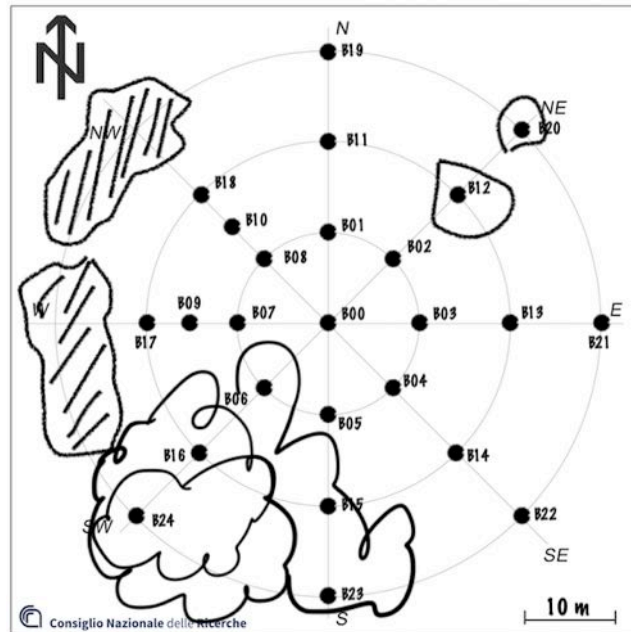
Example: **Laguna de Burines**.

Youtube [Projecto Ecuaflex](#)



Exercise - Soil $\delta^{15}\text{N}$ - Field notes

- Samples collection:
- 25 soil samples
- Polar coordinates
- Almost completely symmetrical
- 60 m diameter circle
- Woods / grassland interface
- A few rocks in the NW section



**Ecuaflex - El Cajas
Laguna de Burines
Feb.2016**

Campionamento suolo

Rocce area NW
impossibile campionare
presi punti intermedi

B00 punto centrale
25 campioni

B12, B20 quantità scarsa

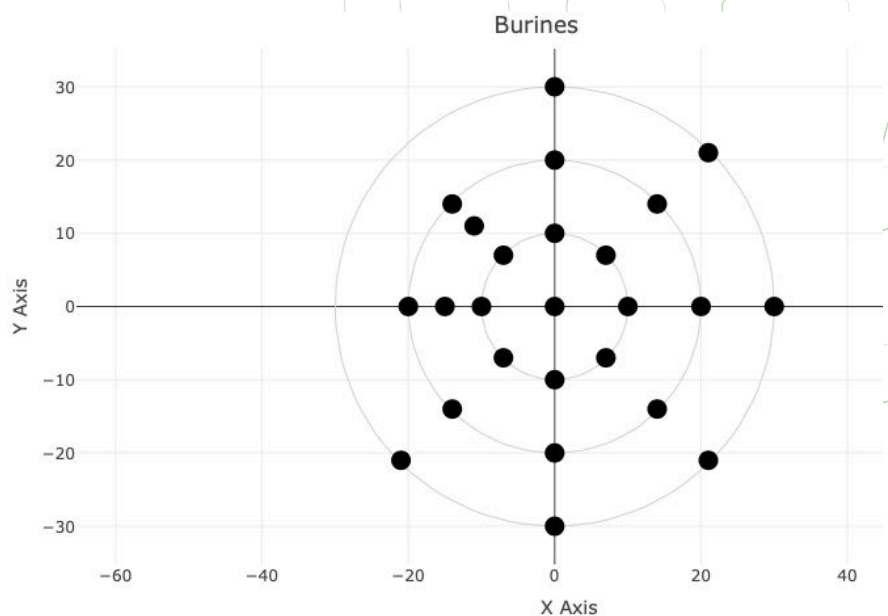
Terreno bagnato

Exercise - Soil $\delta^{15}\text{N}$ - Sampling Points Spatial Distribution

HTML Data Browser

Samples distribution.

EPSG:9807 and local coordinates emanating from the central point.



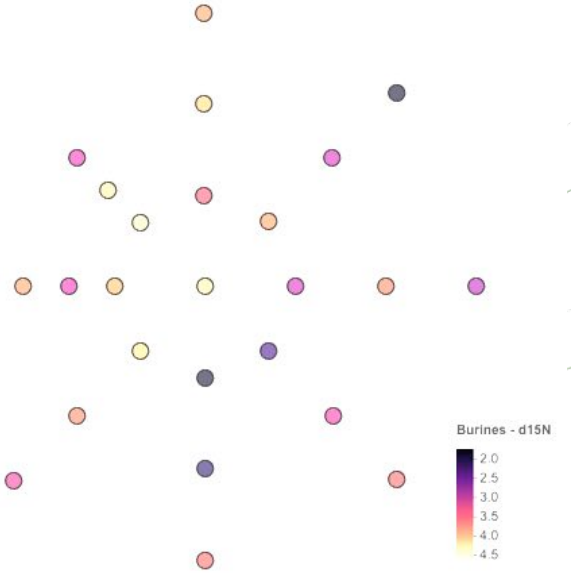
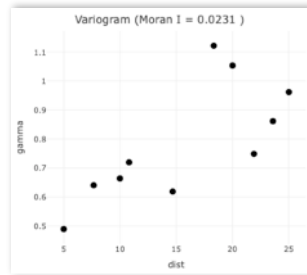
Exercise - Soil $\delta^{15}\text{N}$ - 2D Values Distribution

HTML Data Browser

$\delta^{15}\text{N}$ values distribution.

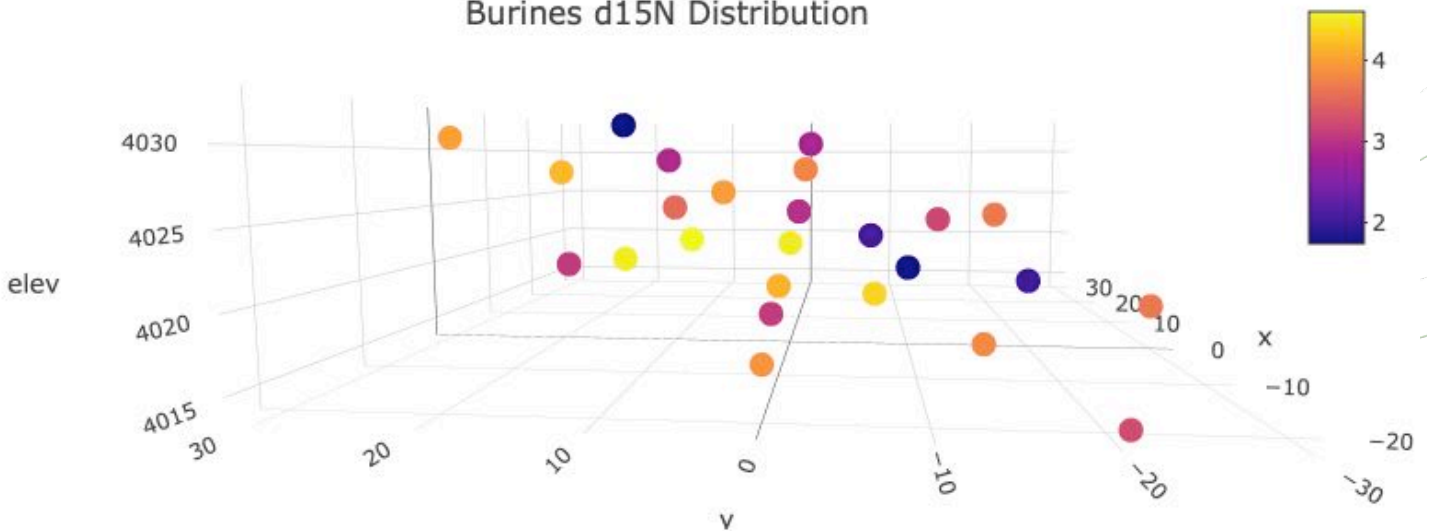
Variogram etc.

Elevation corrected spatial distribution (next slide).



Exercise - Soil $\delta^{15}\text{N}$ - 3D Values Distribution

Burines d15N Distribution



Exercise - Soil $\delta^{15}\text{N}$ - Variogram

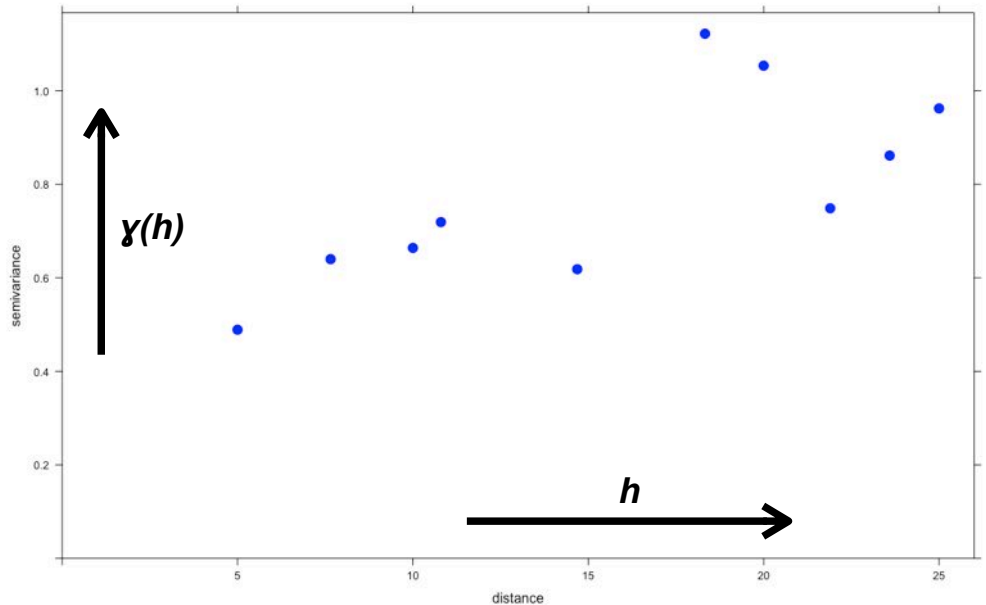
A variogram is a cumulative averaged

$\gamma(h)$ vs h

plot, where

h is the pairwise distance between samples

$\gamma(h)$ is the absolute value of the difference of said samples' values

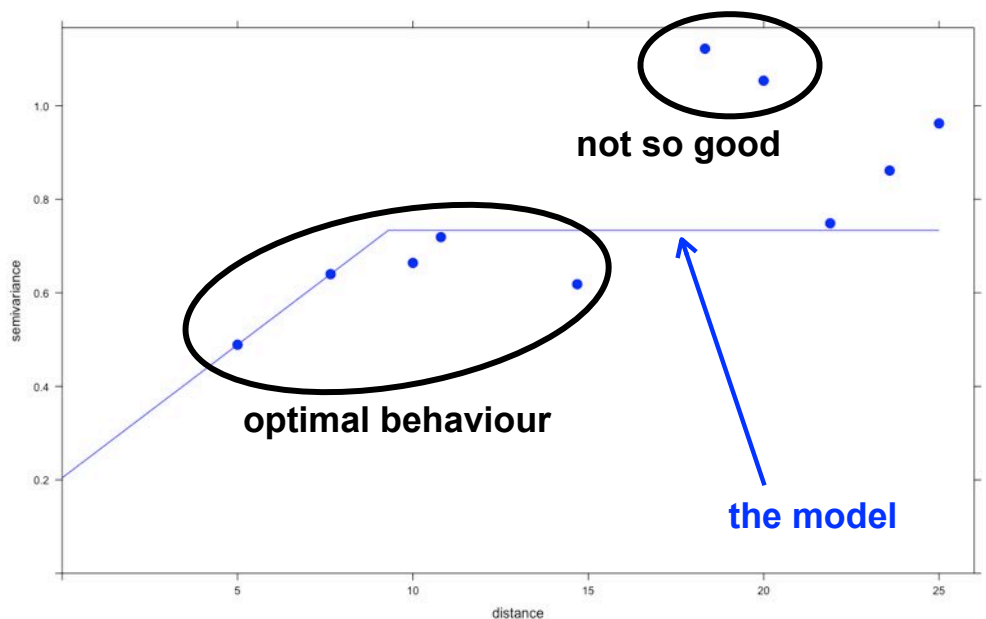


Exercise - Soil $\delta^{15}\text{N}$ - Variogram Model

From the variogram we infer a **model** that mimics the behaviour of the samples' values differences. We have:

- spherical
- exponential
- linear
- gaussian...

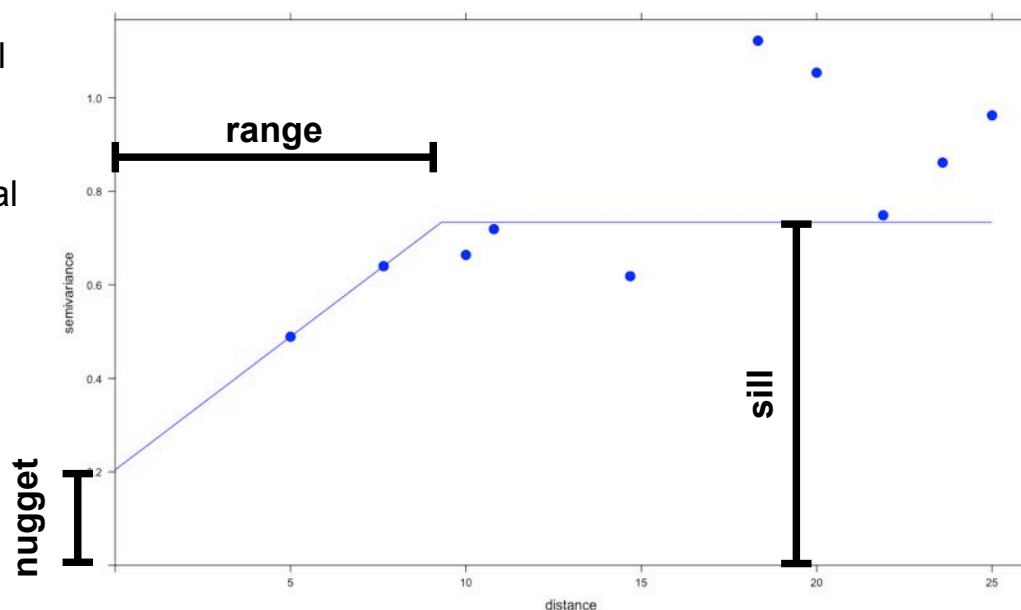
models



Exercise - Soil $\delta^{15}\text{N}$ - Model Elements

The **spherical** model is generally the first choice. Cannot be used with non-optimal variograms.

This one is a **(piecewise) linear** model.

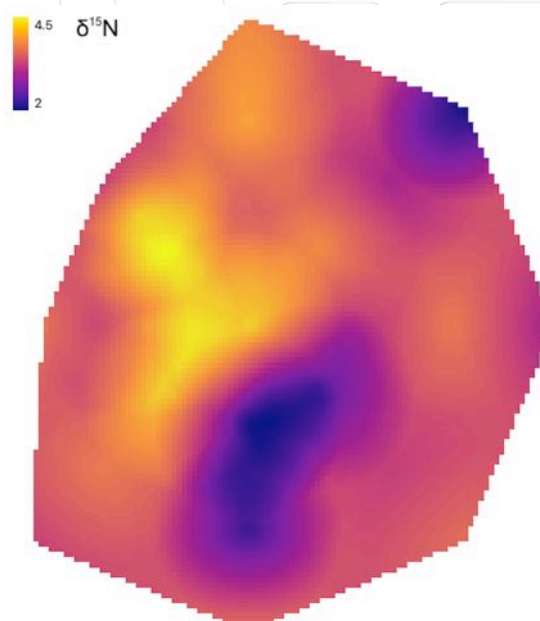


Exercise - Soil $\delta^{15}\text{N}$ - Kriging Isoscape

The variogram is the starting point for **Kriging**, a geostatistical interpolation method based on spatial autocorrelation. It provides an estimate of the reliability of the interpolated values too.

Kriging can be performed in R (sp and gstat packages), QGIS (Saga or GDAL tools), etc.

Alternative: ESRI ArcGIS - MS Windows only.



Exercise - IDW Algorithm

The **Inverse Distance Weighting** interpolation techniques are based on the hypothesis of a decreasing influence of the samples' values.

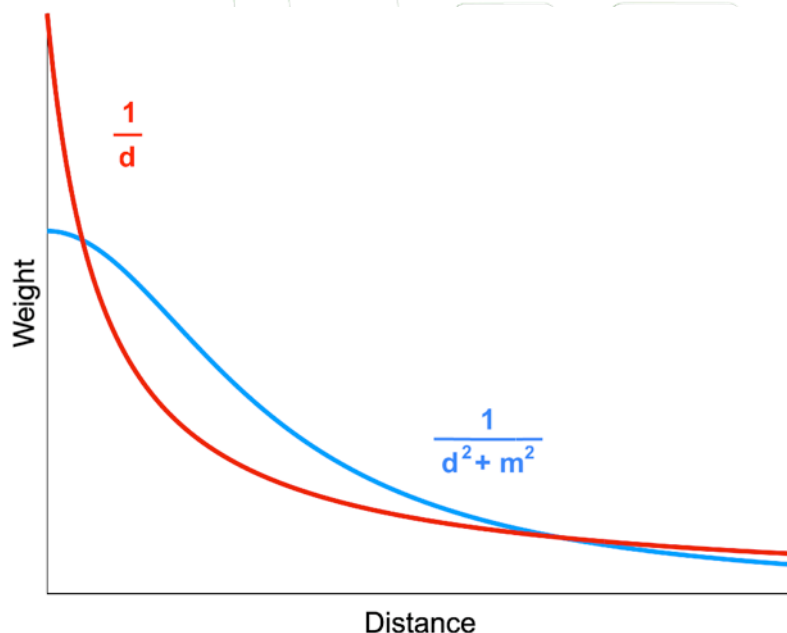
IDW is very easy to evaluate.

The values are weighted according to the distance, i.e.

$w = 1 / d$ the simplest

$w = 1 / (d^2 + m^2)$ smoother

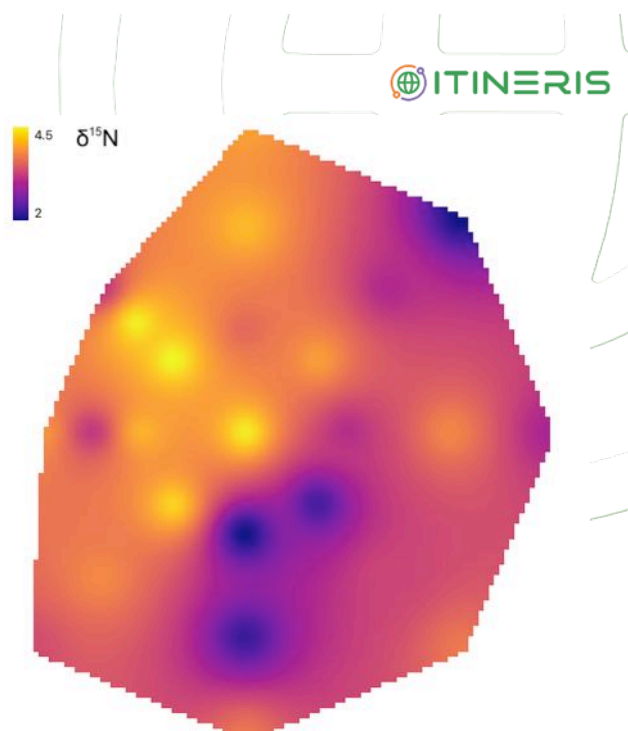
where m is an inertial parameter.



Exercise - Soil $\delta^{15}\text{N}$ - IDW Isoscape

The Inverse Distance Weighting interpolations exhibit a distinctive bulls-eye pattern, resulting in localized peaks and gradients, highlighting one of the key limitations of IDW compared to more sophisticated geostatistical techniques like Kriging.

Example evaluated in QGIS.



Exercise - TIN Algorithm

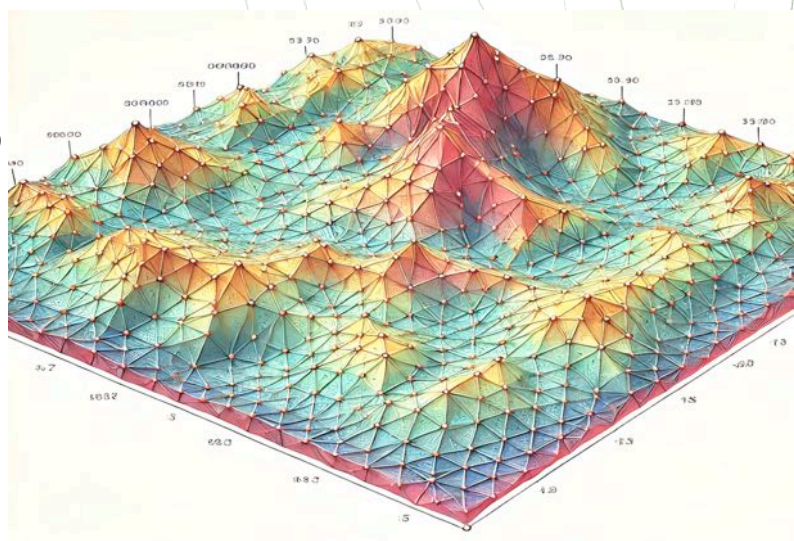
A **Triangulated Irregular Network** is a method of representing continuous surfaces using a network of triangles.

Widely used in spatial interpolation to model terrain elevation.

TIN adapts to variations in data spatial distribution and density (not our case).

TIN easily accommodates sharp variation of values.

Not the best for isoscapes, but it is worth knowing.



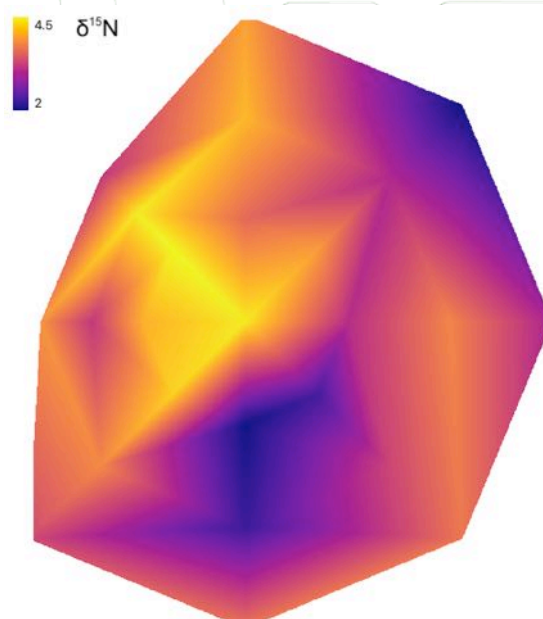
Exercise - Soil $\delta^{15}\text{N}$ - TIN Isoscape

A TIN isoscape is easily evaluated from any spatial distribution of data.

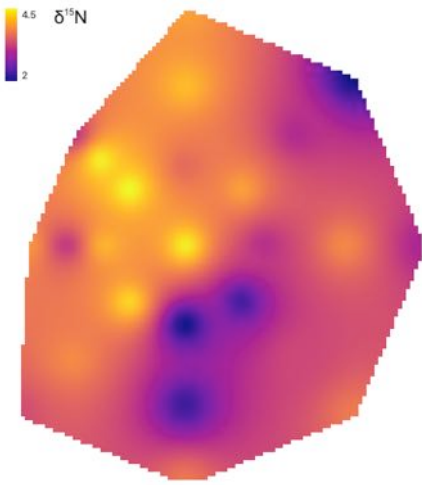
There is no smoothing of the interpolated values.

Aesthetically not much attractive, but the actual numbers are not so different from other interpolation techniques.

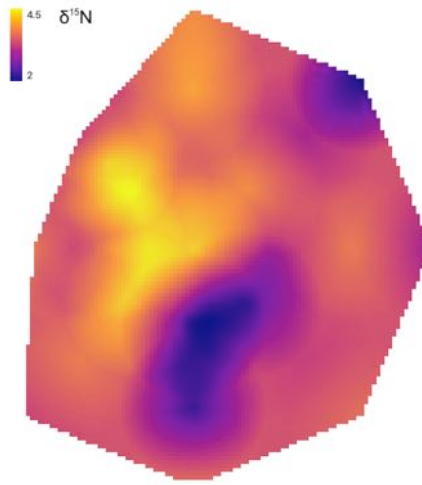
Example evaluated in QGIS.



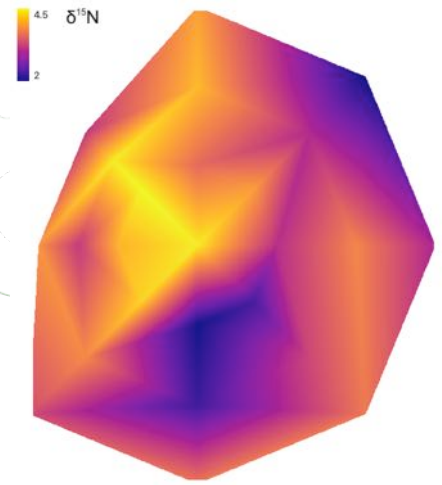
Exercise - Soil $\delta^{15}\text{N}$ - Isoscapes Comparison



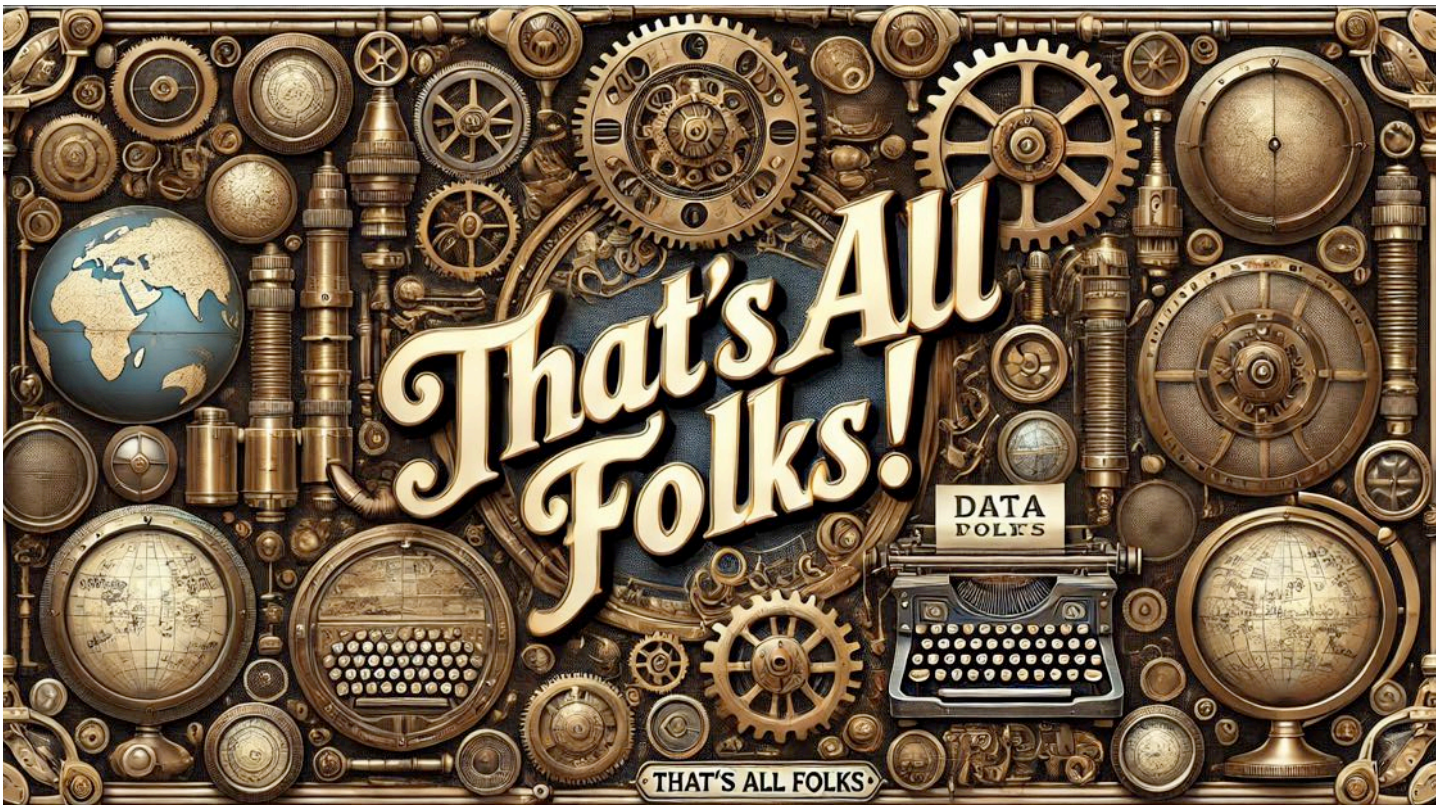
IDW



Kriging



TIN





THANKS!

IR0000032 – ITINERIS, Italian Integrated Environmental Research Infrastructures System
(D.D. n. 130/2022 - CUP B53C22002150006) Funded by EU - Next Generation EU PNRR-
Mission 4 "Education and Research" - Component 2: "From research to business" - Investment
3.1: "Fund for the realisation of an integrated system of research and innovation infrastructures"

