Geographic Information Technology Training Alliance (GITTA) presents:

Continuous spatial variables

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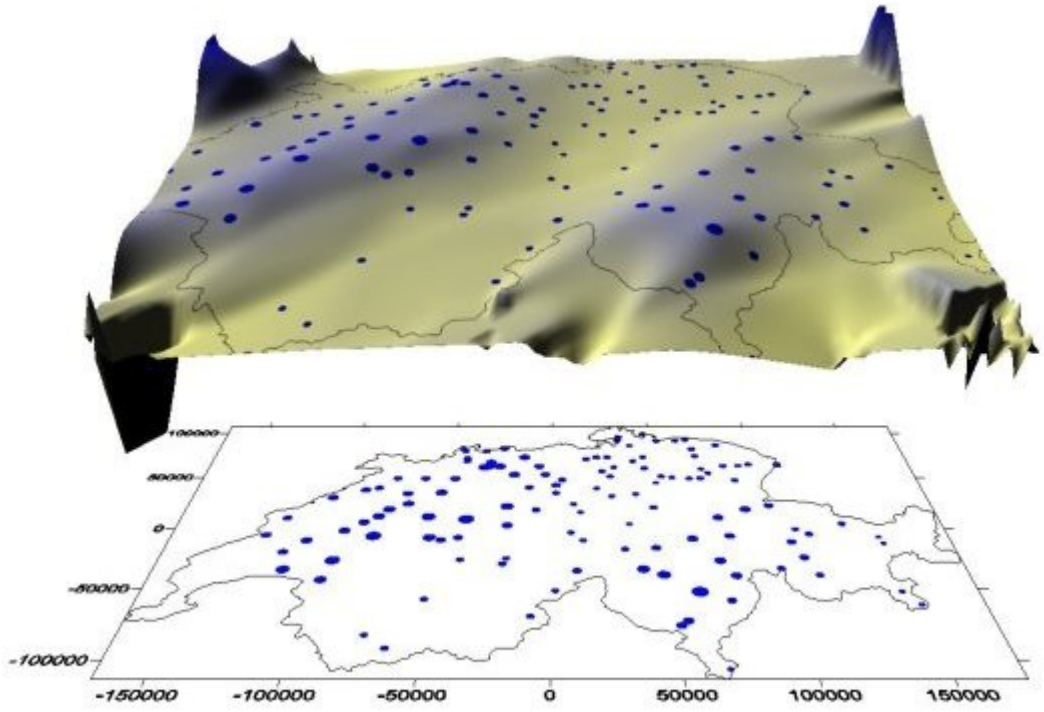
1. Continuous spatial variables



Precipitation surface of Switzerland - Niederschlagsoberfläche der Schweiz (oben), Karte der Messstationen (unten)

The figure shows a precipitation surface of Switzerland: the blue dots represent monitoring stations; their size corresponds to the amount of rainfall at that station. The different heights of the surface and their color are associated with rainfall as well. The issues addressed in this lesson are:

- How can we construct a continuous surface from approx. 100 monitoring stations?
- Which tool can help us do this?
- What knowledge is necessary and which methods exist?

What do we mean by ''continuous spatial variables''?
In our example, rainfall is the variable. Let's perform a thought experiment: Imagine you could measure rainfall on any position along a route. You would have a spatially continuous measurement. Adjacent measurements would be either identical or vary only slightly (according to your definition of "neighborhood"). You may argue that precipitation often shows very well defined boundaries – and you're right. The "continuum of precipitation" is not mathematically perfect. Another example of a spatially continuous variable is sea level. However, virtually every natural spatially continuous phenomenon is subject to certain random fluctuations. Therefore, they can hardly be described in a mathematically perfect way (e.g. a function that exactly describes the rise of a slope, the distribution of different soil pH levels, or rainfall, etc.).

Random Function

From statistics we know deterministic (i.e. exactly predictable and mathematically recordable) and stochastic (i.e. purely random, unpredictable) phenomena. An example for a deterministic phenomenon is the fall of an object: we can calculate in advance the position of the object along the slope line at any point in time. In contrast, rolling dice is a purely stochastic phenomenon. In spatial analysis, we find phenomena that fall between deterministic and stochastic. They are referred to as random functions. Let's do another thought experiment: take a look at the flash-animation below. The points represent measurements of height. The actual heights between the measurement points follow a function that we do not know. However, we will assume that the heights of the unknown profile are not just random but are similar to the known adjacent points. Let's create a profile along the blue dashed line. In other words, we define a linear function between the measurement points. The red solid line shows the actual height profile. In the last image you can see a comparison of both profile lines. The height in this example is a random function – it is neither exactly mathematically recordable nor purely coincidental!

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Please note: although the grid spacing is actually using discrete spatial units, continuous spatial variables are generally better suited to a raster model.

Learning Objectives

- You can describe the main types of spatial sampling.
- You can provide information about the reasonable size of spatial samples.
- You have mastered the basics of explorative variography.
- You can explain why knowledge of spatial dependencies is important for the analysis of continuous variables.
- You know the fundamentals of spatial estimation methods (interpolation).
- You can reasonably name applications for interpolations.

1.1. Spatial sampling

How do we begin the analysis of continuous variables?

The first step is to create a spatial sample. For the example in the beginning (rainfall in Switzerland), this would be the meteorological measurement stations. Their positions are fixed and are not freely selectable (unless you use just a subset of all existing stations). However, if you want to analyze e.g. the distribution of contaminants in the soil you first need to define the measuring points. You must be aware of the following characteristics of the sample:

- Representativeness
- Homogeneity
- Spatial distribution of measurements
- Size (i.e. number of measurements)

Representativeness, homogeneity, spatial distribution, and size are related. A size of 5 monitoring stations for an estimation of the total Swiss rainfall would hardly make sense and is neither representative. Nor would the selection of all the Swiss-german monitoring stations be representative for the overall estimation of Swiss rainfall. The size could be sufficient but not the spatial distribution. Selecting all stations below 750 masl the sample could be sufficient according to size and distribution but the phenomenon is not homogeneously represented in the sample. A subsequent estimate would be significantly distorted mainly in the areas above 750 masl.

1.1.1. Characteristics

Representativeness
The phenomenon being analyzed should be represented in all forms in the sample. Minima and maxima are of particular importance. For the precipitation example this means that stations with peak values should be present in the sample. However, if we are planning our own sampling scheme we usually do not know whether or not we have recorded the locations of minima and maxima.

Homogeneity
As mentioned earlier, the spatial dependence of data among themselves is a very important prerequisite for a meaningful analysis. This relationship should be homogenous over the entire study area! Take the example of the precipitation monitoring stations: two stations at a distance of 2 km, for example should both have similar values in Ticino as well as in Jura, Fribourg, or Grison etc. This prerequisite is also called "stationarity".

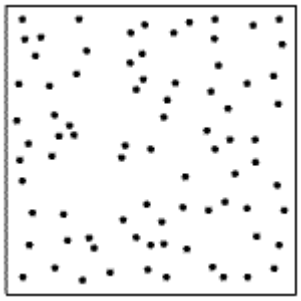
Spatial distribution
Spatial distribution is of great importance. It can be completely random, regular, or clustered. You can see examples of these distributions below in the "Typology" section. An indication about the spatial distribution of a sample can be statistically obtained by using the "nearest neighbor" method, for example. It is one of the "point pattern analysis" techniques, i.e. methods that can help statistically characterize and analyze the spatial distribution of points.

Size
The size, i.e. the number of samples, depends on the phenomenon and the surface area. In some cases, practical limitations constrain the sample size. Think of measurements in difficult terrain, or technically complex and expensive measurements. It is impossible to provide an ideal sample size for any task.

1.1.2. Typology

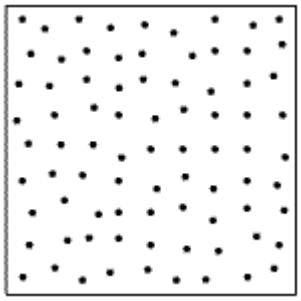
Different types of design can be used in spatial sampling. The choice of the sampling design depends on the phenomenon investigated or may also be influenced by the methods of measurement.

Random sample
Note the ranges without samples – the phenomenon to be analyzed is underrepresented there.



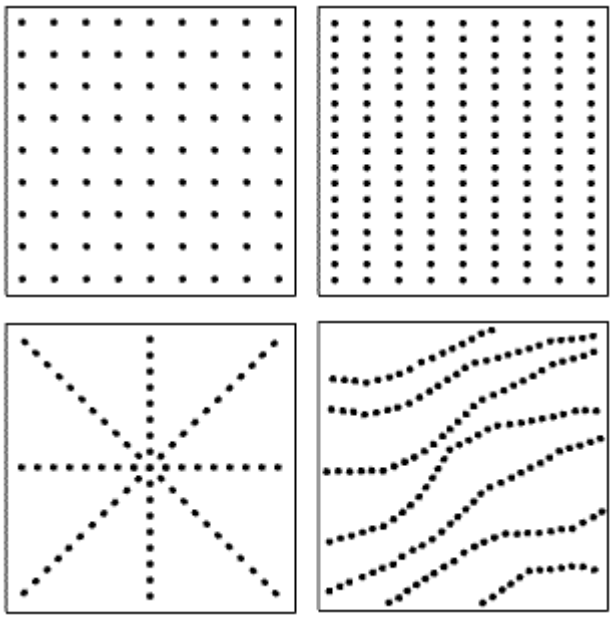
Random sample

Uniform random sample (with a minimum distance between points)



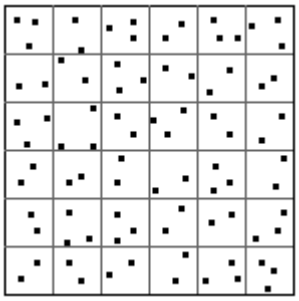
Uniform random sample

Systematic random sample
The selection shown below is by no means complete. However, it shows that "systematic" does not necessarily mean, "square"!



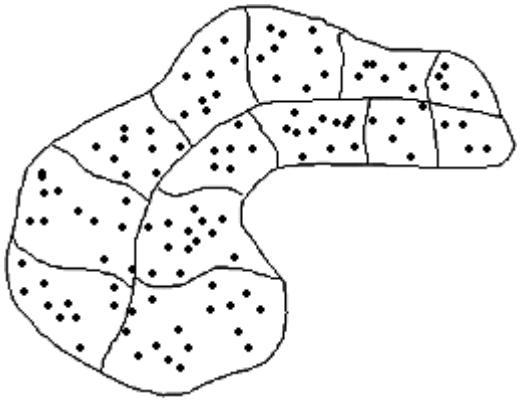
Examples of systematic samples

Stratified random sample with a regular grid (here at least two points per grid box)
Do you recognize the similarity of this type with the uniform sampling? The criterion here is not a minimum distance, but the division of the area into uniform subsets (strata).



Stratified random sample with a regular grid

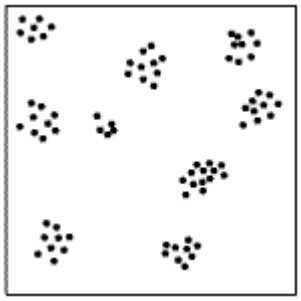
Stratified random sample with an irregular grid (hierarchical or authoritative sample)
The idea of a stratified random sample is applied here to an irregular grid. For example, this could represent administrative districts.



Stratified random sample with an irregular grid

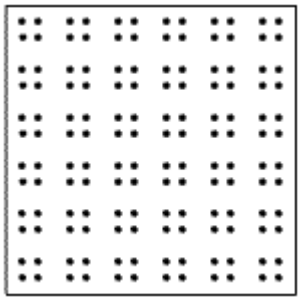
Clustered random sample

You should have good reasons for selecting this sampling design. This design could also be a primary stage for values to be averaged within the cluster.



Clustered random sample

Clustered systematic sample



Clustered systematic sample

Examples of different types of sampling

Have a look at the following Flash animation showing examples of different types of sampling applied to Switzerland. The digital elevation model is shown as background information.

Only pictures can be viewed in this version! For Flash, animations, movies etc. see online version. Only screenshots of animations will be displayed. [link]

1.2. Analysis of spatial dependence

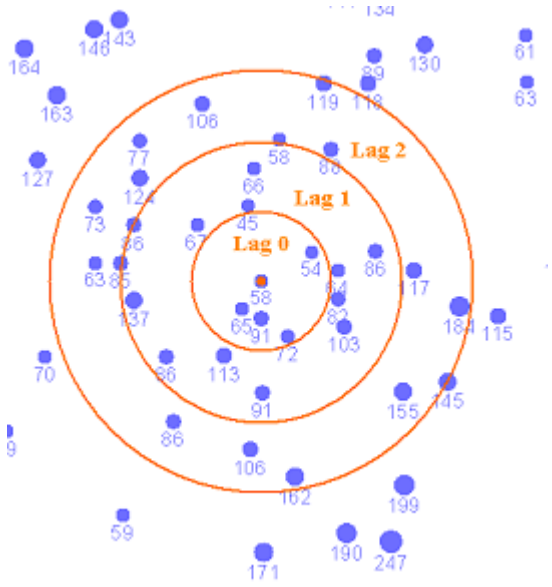
After the appropriate spatial sample has been chosen, the next step is to determine whether spatial dependencies exist between the data, and to which extent. There are several methods to do this. The two which will be presented in the following section are:

- The variogram, or explorative variography, respectively
- "Moving window" statistics

Why do we have to worry about spatial dependencies at all? Is it not enough to have an accurate sample? No! Without spatial relationships between our samples we cannot make a statement about the points where no samples were taken. This goes back to a statement by Waldo Tobler, which is known as the "1st law of geography":
"*(...) the first law of geography: everything is related to everything else, but near things are more related than distant things.*" (Tobler 1970)
In most cases, this legality is indeed true. However, we should not rely on it blindly, especially not while standing on the edge of a cliff...

1.2.1. Variogram

Let us first get acquainted with the problem by looking at an example: Imagine a digital terrain model and take samples. The value of a sample is the height above sea level. Adjacent samples may have been randomly taken along a valley floor of the same altitude. Another pair of samples with approximately the same distance between them may have been taken on a ridge. If you compare the values of the two pairs you will notice a match or at least a similarity of the values. Let's compare samples with a greater distance between them. It is possible that they have similar values but it is more likely that their values (i.e. the sea level) are dissimilar.
Variography is a method that performs this pairwise comparison for all of our samples: every point is compared to every other point. This can add up to a lot of pairs of points depending on the number of samples. To be exact, it adds up to *= n*(n-1)/2 (n ... number of samples)*. You might ask, "Where does the distance come into play?" While each point is compared to every other point, the distance (and direction) of the pairs is determined as well!



Precipitation

3 lags (Lag 0, Lag1, Lag2) for a data point (value 58) are shown. The numbers are values of Swiss precipitation monitoring stations.

Pairs of values:
for Lag0
58,65
58,91
58,54
58,72
for Lag1
58,45
58,64
58,82
etc.

From these numerous pairs of values the so-called "semivariance" is calculated as a measure of similarity (and we can also interpret it as "dependency").

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i,j=1}^{N(h)} (v_i - v_j)^2$$

Formula for semivariance

... Semivariance for the distance *h*
... Number of pairs within distance *h*
... Values at position *i* and *j*

In simple words, the difference between the value pairs is squared and halved. This parameter is calculated for each distance interval h – only the value pairs within this distance are included in the calculation. This distance h is called a "lag". Enter all value pairs within one lag on a scatter plot and you will get the so-called h-scatterplot. From the semivariances per lag, the empirical (or experimental) semivariogram is created as a line graph. Move the mouse over the lag points to display the corresponding h-scatterplot for the first 8 lags):

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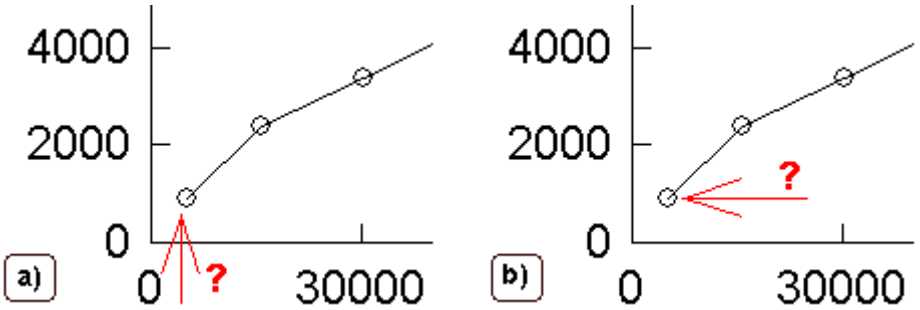
Can you imagine why there are clearly fewer points in the h-scatterplots of low distances than in those of the higher lags?

Because in the lower lags, fewer pairs of points are in a smaller overall area.

The x-axis shows the increasing distance between pairs of points; the y-axis shows the semivariance per lag. The circular symbols on the curve mark the individual lags. In this example, the lag interval is 15'000. How do we interpret a curve like that? The more similar the pairs of values are per lag, the lower the semivariance for this lag; the more dissimilar, the higher the semivariance and thus the curve rises. This curve confirms: the values of our data are more similar at low distance. There is a direct connection between the distance between the data points and their similarity in value! There are two key figures to keep in mind to help you describe this curve:

- Range – the distance h, where the curve flattens
- Sill – the value of semivariance where the curve reaches its range

If the lag interval in the example above is 15'000 then why is the first lag (= lag 0 or h0) not in the coordinate origin? Simply because the pairs of points in lag 0 are at a certain distance from one another. Their average distance is now the position for lag 0 on the x-axis. But why does the curve not start at semivariance 0, i.e. on the x-axis? Because the data in lag 0 are not all identical (this is often the case). That is the reason why the origin of the semivariogram curve usually lies just above the x-axis. This is called the nugget effect. This term comes from the use of this method in geological exploration. In samples of gold, nuggets can occur selectively, i.e. the values of immediately adjacent samples may differ considerably.



a) Lag 0 includes all pairs of points within the first lag. The average distance between the points marks the lag on the x-axis; b) The pairs of points in lag 0 show different values; therefore, the semivariance is not equal to 0 but slightly above the x-axis (=nugget effect)

In the simplest form, the pairs of values of each point in every direction are formed and an isotropic semivariogram is created. As an extension and refinement to this method, variogram programs can create pairs of points in specific directions. By doing this, you can examine if values in your dataset have higher spatial dependencies in certain directions. Think about the example above with sea level: if – in your data – there is a valley running in N-S-direction, points in this direction will show higher similarities than in E-W-direction. The result is now an anisotropic semivariogram. If you have lost sight of the overall goal: all this information about spatial dependencies and its structure can be used to estimate the unknown values.

Use the following interactive semivariance calculator and enter pairs of values. First, choose similar values (up to 99), then vary the values and let them be more dissimilar. Observe how the semivariance changes! Note how easily the semivariance formula is implemented.

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What happens if you enter the same value for every point? Is it of any importance, in what order you enter the pairs of values?

- If all points have the same value, i.e. are identical, there is a perfect spatial dependency and the semivariance will be 0.
- The order of the pairs of values does not matter since negative values become positive by squaring them.

1.2.2. Moving Windows

Variography allows us to detect spatial dependencies. What it does not detect is whether or not these dependencies are uniform throughout the whole study area. There could be large regional differences and in that case, our variogram would not be representative for the entire area! It only provides information about the spatial variability of our data.
The simple technique of the "moving windows"-statistics can help. A "window" of defined size and shape is moved over the data, the moving distance is equal to the width of the window. All data located within the window section are statistically summarized: the number and average of all points inside the window, the minimum / maximum values, the standard deviation, the coefficient of variation (= standard deviation / mean), etc. The results are again points – the centers of the moving windows and as their attributes the statistical indicators of these windows. In the case of sparse data, the window is only moved by one half of the window width to obtain more data to calculate (= moving window with overlap). The principle is shown in this animation:

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Both window size and form may be varied with this method. In practice, it is used in an explorative way accordingly: an analysis is performed with windows of varying dimensions and the statistics are compared. In particular, the coefficient of variation is a significant parameter – if its values are > 1, this indicates a high variation (= high spatial variability) in this window pane.
Consider the following example of a "moving window"-statistic for the Swiss precipitation data. Regions with higher rainfall are relatively easy to spot; two of them form a kind of NE-SW axis. The size of 30x30 km and the option of overlap are chosen for the window. The size of such a window is shown as a gray square. There is also the possibility to omit windows with less than a defined number of points, e.g. 4, since with such few points no meaningful statistics can be calculated. That is why there are a few "holes". The mean values reflect the precipitation totals. However, the coefficient of variation is of particular interest because it indicates regions with larger value fluctuations. In this situation, the two highest values are located at the southern tip of Ticino.

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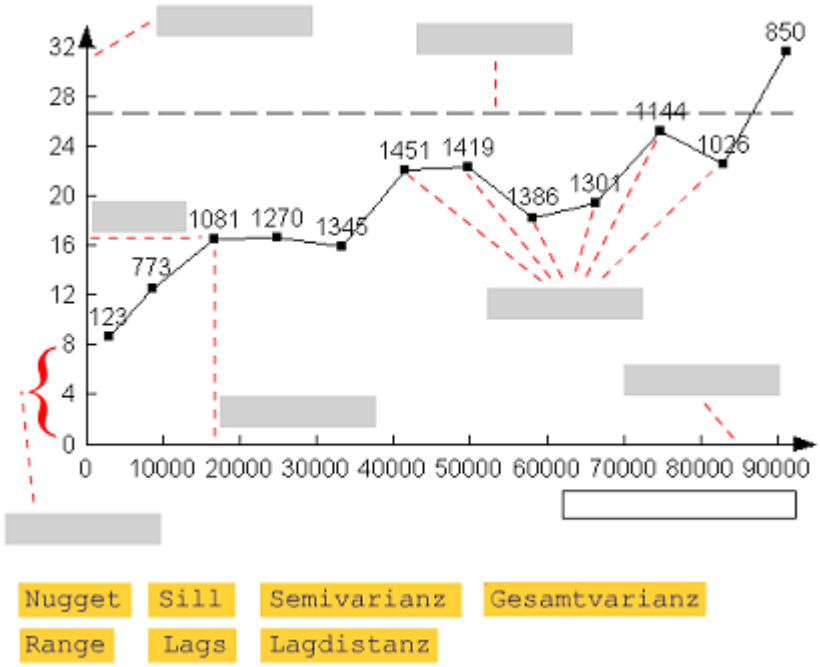
In which of the eight windows from the first example will you find the highest coefficient of variation and what value does it have?

Window 4 – the coefficient of variation has a value of 4.8 / 44 = 0.109

1.2.3. Correctly assigning semivariogram-parameters

Drag the terms to the correct position in the semivariogram figure. Don't worry – after several failed attempts you will get help.

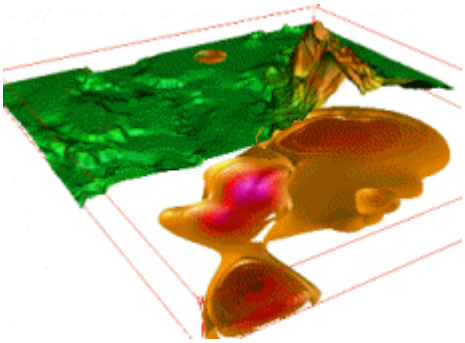


Correctly assigning semivariogramm-parameters

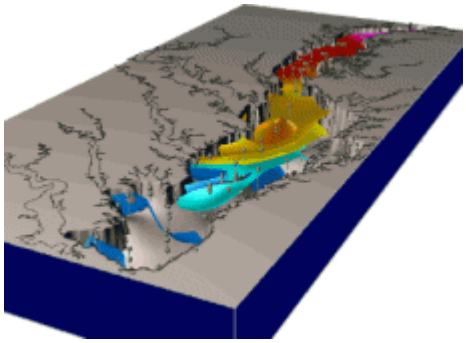
1.3. Spatial Interpolation

Examples of interpolation results

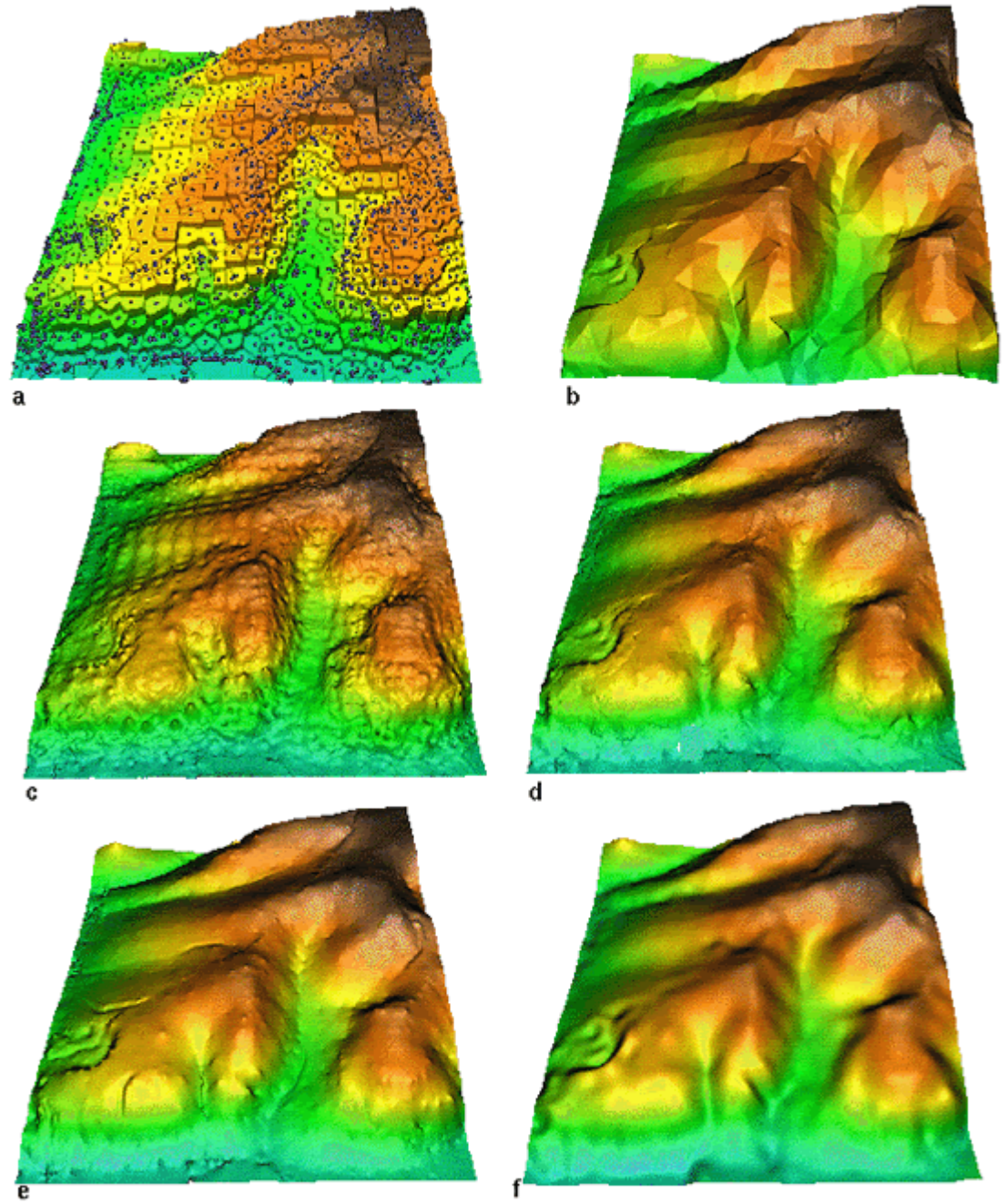
Click on the two pictures below to see a simulation of the changing chemical concentration.



Concentration of chemicals in the soil (Mitas et al. 1998)



Chemical concentration in a water (Mitas et al. 1998)



Interpolation of a DEM from scattered point data using methods available in GIS: a) given data and Voronoi polygons, b)TIN based linear interpolation, c) inverse distance weighting d) kriging, e) spline with tension and stream enforcement, f) regularized spline with tension and smoothing.

Comparison of different interpolation methods (Mitas et al. 1999)

The examples shown above are the result of careful and sophisticated interpolations from a wide range of potential applications.

After looking into sampling and the analysis of spatial dependencies in the previous chapter, we now proceed to the "heart" of this lesson – spatial interpolations. Many of these techniques do not count to the easiest application in spatial analysis. That is why we deliberately restrict ourselves to a brief overview of the methods. The following techniques of interpolation are discussed:

- Distance-based interpolation

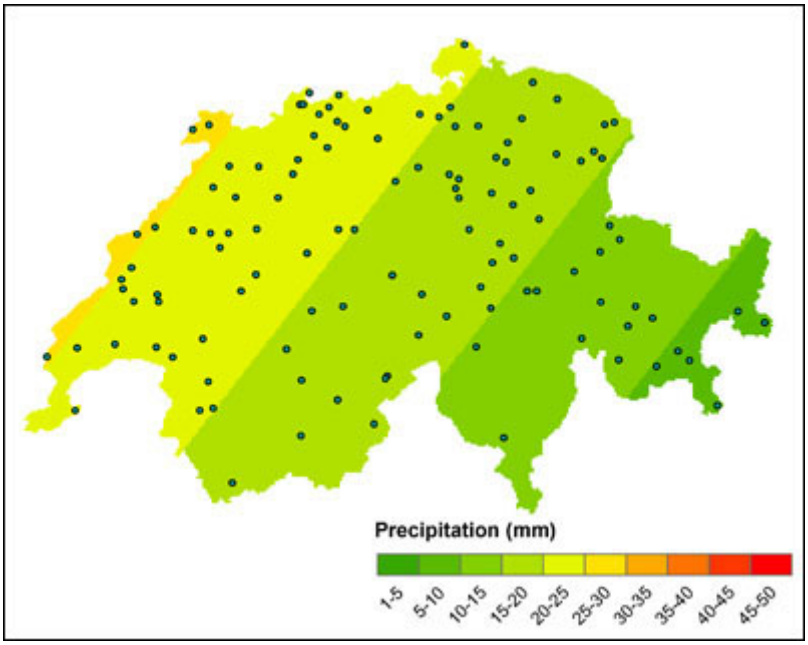
- Geostatistic methods

The latter being the subject of advanced courses and is not discussed in detail. What actually are spatial "interpolations"? This refers to the computation of unknown values based on neighboring known values.

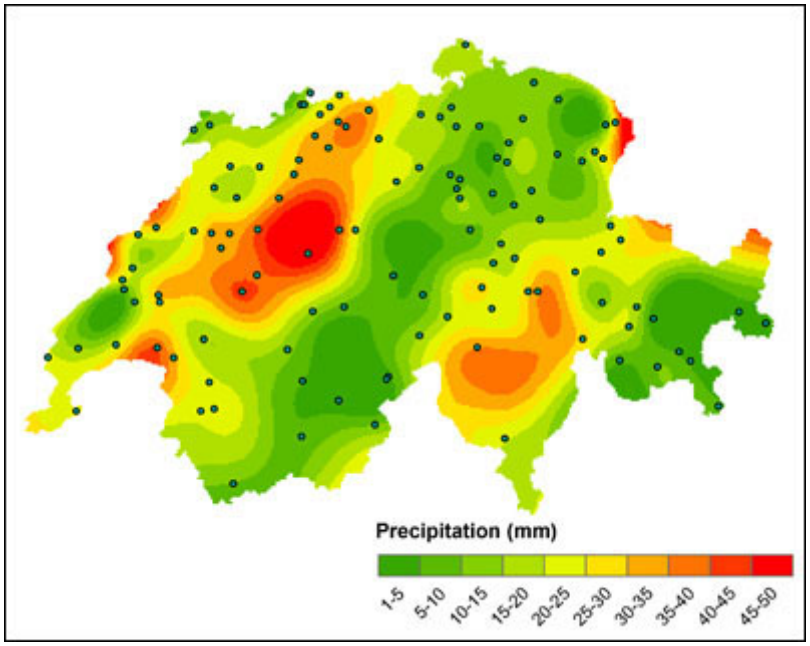
1.3.1. Typology

"Inverse distance" weighting, "radial basis" functions, "splines", "ordinary kriging", "natural neighbor", "polynomial regression" methods, "universal kriging", etc. These are just some interpolation methods found in commercial software. The diversity of methods and their parameterizations can be confusing. Therefore, we will first try to classify the methods into schemes. In the following table, different approaches can be seen:

Local vs. global interpolation
Global methods are applied to ALL data in the study area; local methods on the other hand, are only applied to spatially defined subsets. Global interpolation is therefore not suited for the determination of exact values but to assess global spatial structures.
As examples, you can see a linear trend surface which was determined by regression from Swiss rainfall data and shows a trend toward increased precipitation totals from SE to NW, and a local interpolation using a radial basis interpolation:



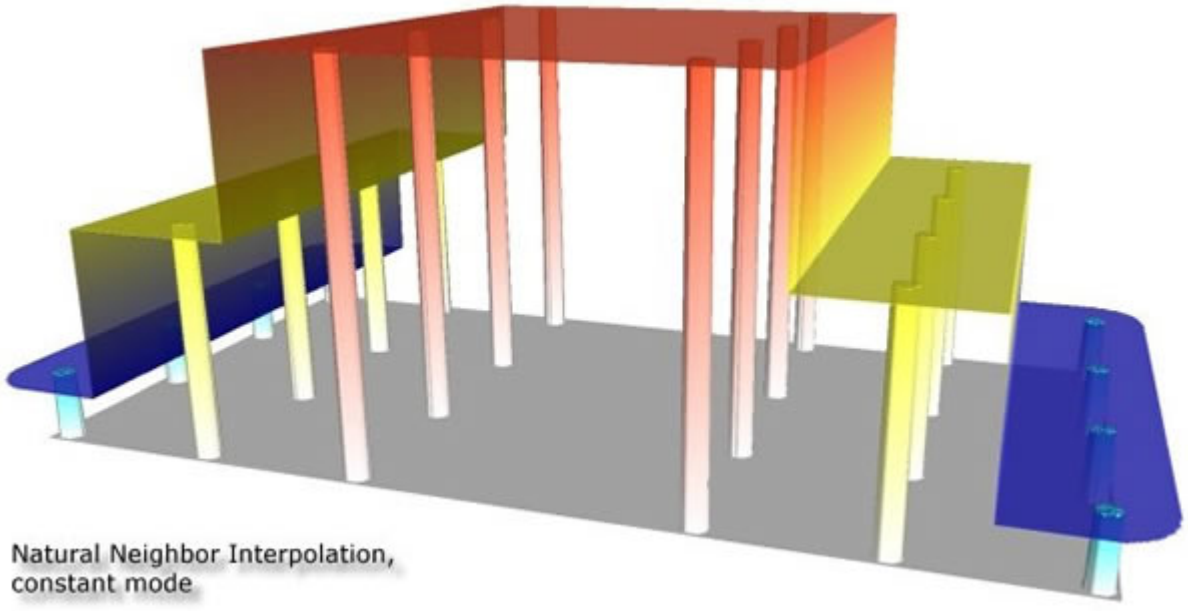
Example of a global interpolation – linear trend surface for Swiss rainfall data. (Provided by Ross Purves)



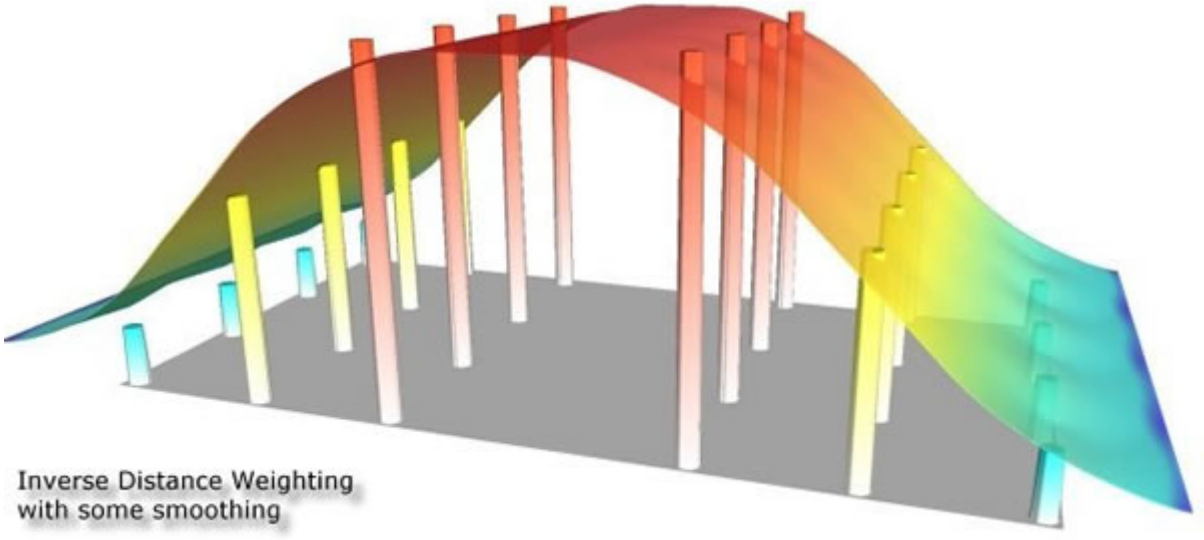
Example of a local interpolation – spline interpolation for Swiss rainfall data. (Provided by Ross Purves)

Exact vs. approximate interpolation

Exact interpolation means: the estimated surface passes through all points whose values are known. In approximate interpolation, the estimates of known points can vary from known values. The latter method can be usefully applied when the known data is already somewhat fuzzy.



Exact Interpolation: the estimated surface passes exactly through the known points (here schematically shown as columns) (Wyatt 2000)



Approximate Interpolation: the estimated surface does NOT pass through the known points (here schematically shown as columns) (Wyatt 2000)

Gradual vs. abrupt interpolation
This distinction mainly refers to the resulting estimation surface. Were there breaklines (naturally abrupt changes in values such as in cliffs or lakefronts) included in the interpolation or not?

Deterministic vs. stochastic interpolation
Techniques of deterministic interpolation are based on exactly predetermined (= deterministic) spatial contexts; in stochastic approaches on the other hand, random elements have an impact as well. Deterministic methods show clear disadvantages in interpolating natural spatial phenomena, since a given degree of uncertainty always exists.

1.3.2. Distance-based interpolation

In the simplest case, we can proceed with distance-based methods the same way as with the **"moving windows" method**: we define a certain "neighborhood" of known data points around the unknown position to be estimated each time; the arithmetic mean of these known measurement values is our estimate (= moving average). The neighborhood can be defined in different ways:

- A spatially fixed shape (rectangle, circle, etc.)
- A certain number of nearest neighboring points

However, this method is quite fuzzy because of the different distances between the position to be estimated and the poor integration of known points in the interpolation. The actual distance-based methods use exactly these distances between the estimation points and the known measurement points to weigh their influence in the calculation of the estimated value. By the way, they require a linear spatial correlation between the phenomena. Using the so-called "Inverse Distance Weighting" method or IDW, the weight of any known point is set inversely proportional to its distance from the estimated point. It is calculated as follows:

$\hat{v} = \frac{\sum_{i=1}^{n} \frac{1}{d_i} v_i}{\sum_{i=1}^{n} \frac{1}{d_i}}$ *Inverse Distance Weighting IDW – basic formula*	= value to be estimated = known value d_i..., d_n= distances from the *n* data points to the point estimated *n*

In most cases, you will find the following variation, in which the influence of the distance can be additionally controlled by an exponent (which is preset to 2 in most programs).

$\hat{v}_1 = \frac{\sum_{i=1}^{n} \frac{1}{d^p{}_i} v_i}{\sum_{i=1}^{n} \frac{1}{d^p{}_i}}$ *Most common form of IDW formula with added distance weighting exponent*	= value to be estimated = known value $d^p{}_i$..., $d^p{}_n$ = distances from the *n* data points to the power of *p* of the point estimated

The lower the exponent, the more uniformly all neighbors are incorporated into the calculation (regardless of their distance), and therefore, the "smoother" the estimated surface. The higher the exponent, the more accentuated and "unsettled" is the surface because only the weight of the nearest neighbors is integrated in the interpolation (see the following interactive animation).

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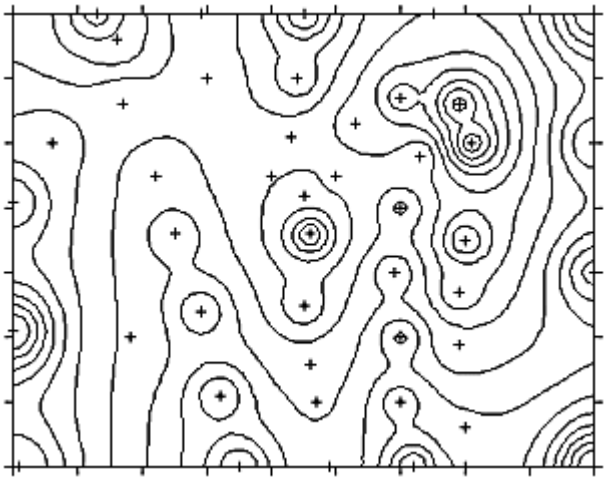
Advantages of the IDW interpolation:

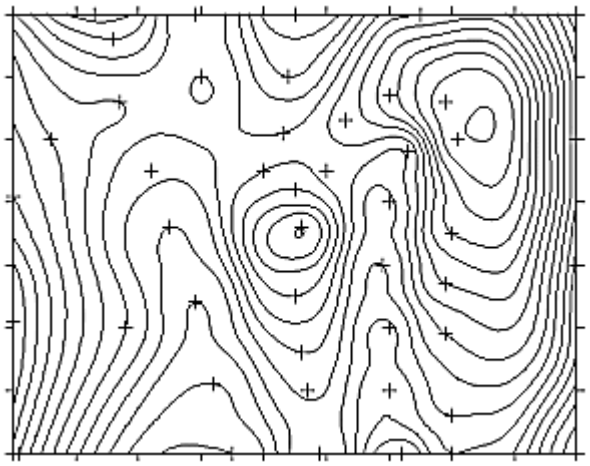
- It allows for very fast calculations
- Different distances are integrated in the estimation
- The distance-weighting exponent is able to precisely control the influence of the distances

Disadvantages of the IDW interpolation:

- It is not possible to do a direction-dependent weighting. That means that spatially oriented relationships are ignored (e.g. elevation points along a ridge).
- Unsightly artefacts are the so-called "Bulls-eyes" – these are circular areas of equal values around the known data points. However, applying a variation of the IDW-Interpolation developed by Shepard (1968) can reduce the Bulls-eyes:



IDW "Bulls eye" effect: concentric areas of the same value around the known points – an unwanted artefact of the IDW interpolation.



IDW modified after Shepard: the Bulls-eyes are definitely reduced.

Inverse Distance Weighting (IDW) – interactive animation

The following interactive animation shows 10 data points (blue) with known measurement values (numbers next to the points) and one point, which value is to be calculated (red). At the start of the animation, this value is calculated from the given values and distances. To get to know the principles of IDW interpolation better, you can now experiment with this animation:

- Change the position of one or all points with your mouse.
- Modify the default values for the known points (allowing a total of max. 4 digits).
- Set the distance-weighting exponent to a value other than 2 (total max. 4 digits allowed).

Only pictures can be viewed in this version! For Flash, animations, movies etc. see online version. Only screenshots of animations will be displayed. [link]

Answer the following questions keeping the experiment in mind:

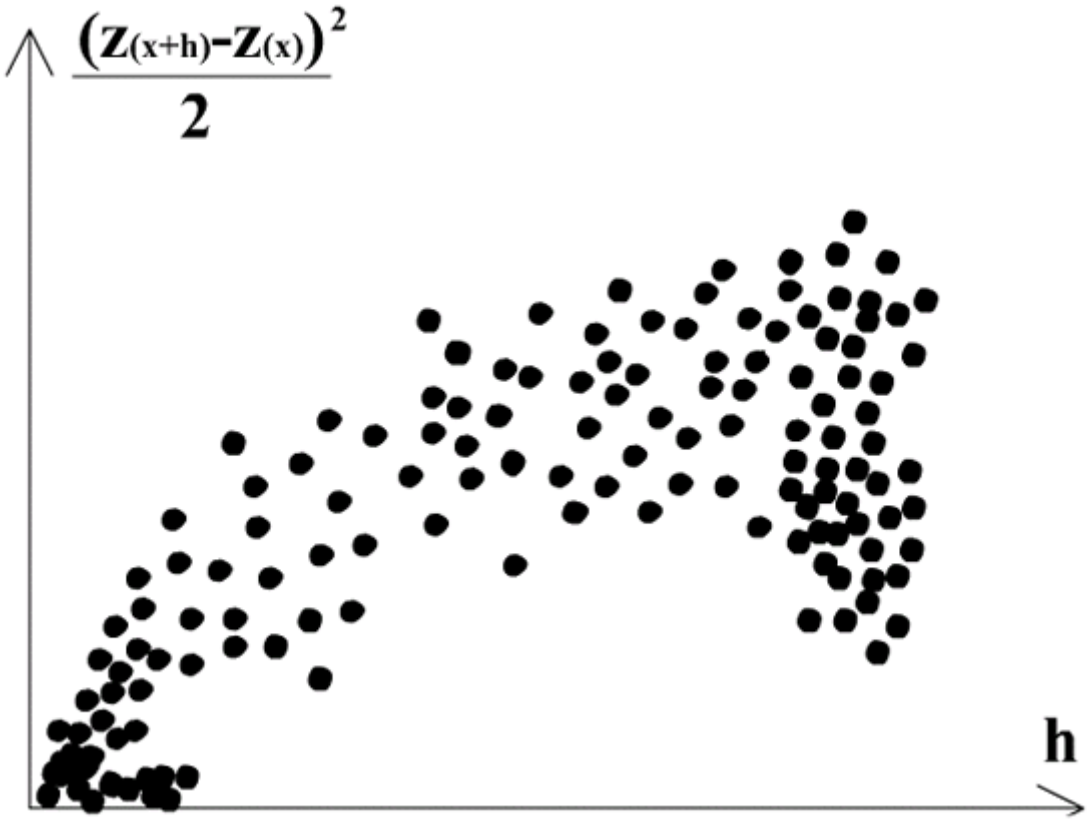
1. Which measurement values influence the result even more when exponent is set higher?
2. If the exponent is set to 0, how do different distances influence the estimation, or what does the result solely depend on in this case?

1. The higher the distance exponent is set, the more influence **the values of the nearest neighbors have on the result.**
2. Is the distance exponent set to 0 (zero), a weight of 1 is assigned to any distance, i.e. all distances are absolutely equal. **The result depends only on the measured values themselves and not on the distance.** The interpolation no longer has a spatial component.

1.3.3. Geostatistical Interpolation

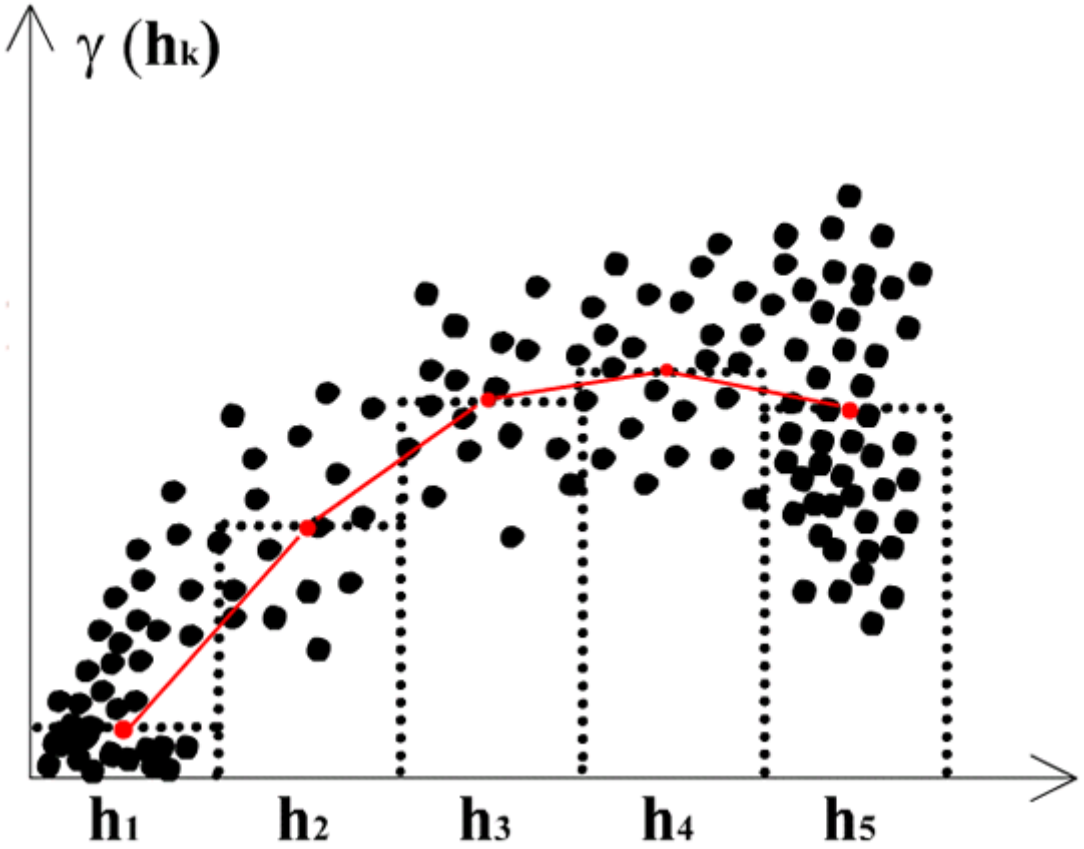
One of the disadvantages of the IDW interpolation is the lack of direction-specific (anisotropic) information. Therefore, spatial correlations are ignored and are not integrated into the result of the estimation. This disadvantage is leveled out by geostatistical interpolations.
The name "geo" already points to the most important feature of these methods: spatial-statistical parameters constitute the main basis for these interpolation methods.
The variogram or the variography (i.e. the method to derive it from spatial point data) is the basis for a successful geostatistical interpolation.
Geostatistical interpolations are advanced and to some extent complicate methods. Their sensible application requires a large amount of knowledge and experience. At this point, a few keywords about their implementation will be sufficient.
The main procedures are the Kriging methods. They are named after a South African engineer, D.G. Krige. In his diploma thesis in 1951, he laid the foundations for kriging. However, the main developments come from the work of G. Matheron in the 1960s.
Using variography, we get indications of how similar or dissimilar the measurement values of adjacent data points are as a function of their distance from each other.

Variography
a) First, we constitute pairs of all the data points and compare their two values. Of each data pair we know the difference (semivariance) and the distance (h):



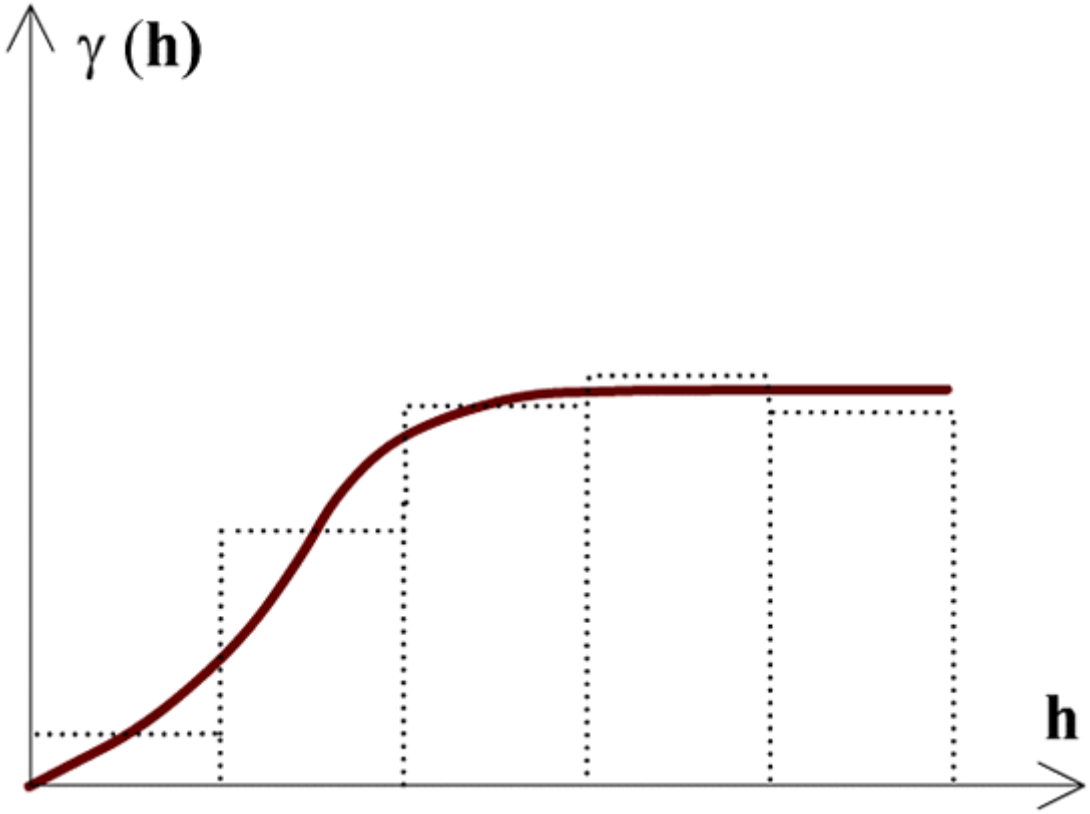
Variogram cloud, differences between data points vs. spatial distance between these points

b) Second, we divide the distances (x-axis) into intervals (so-called lags) and we take the mean of the semivariances of the data pairs within (red dots). By connecting these red points of every lag, we get the experimental variogram. This curve describes how similar the values of two adjacent positions are as a function of their distance from each other.



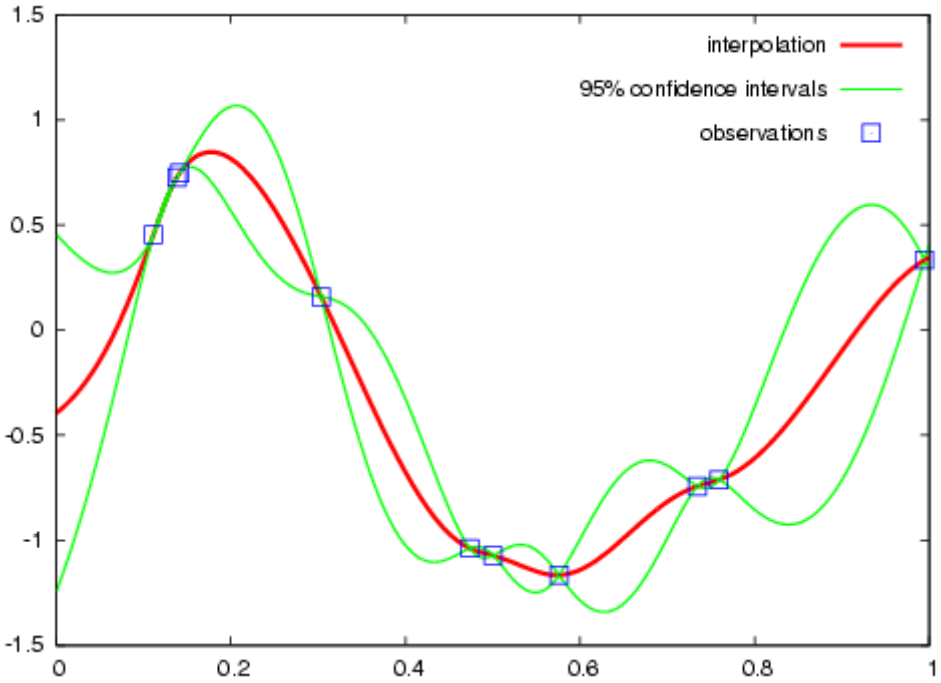
Experimental variogram, the differences are averaged per defined class (h1…h5 = lag intervals)

c) To better handle this representation of spatial (dis-)similarity, we can construct simple curve functions onto the experimental variogram to match it as well as possible. This curve is called the theoretical variogram.



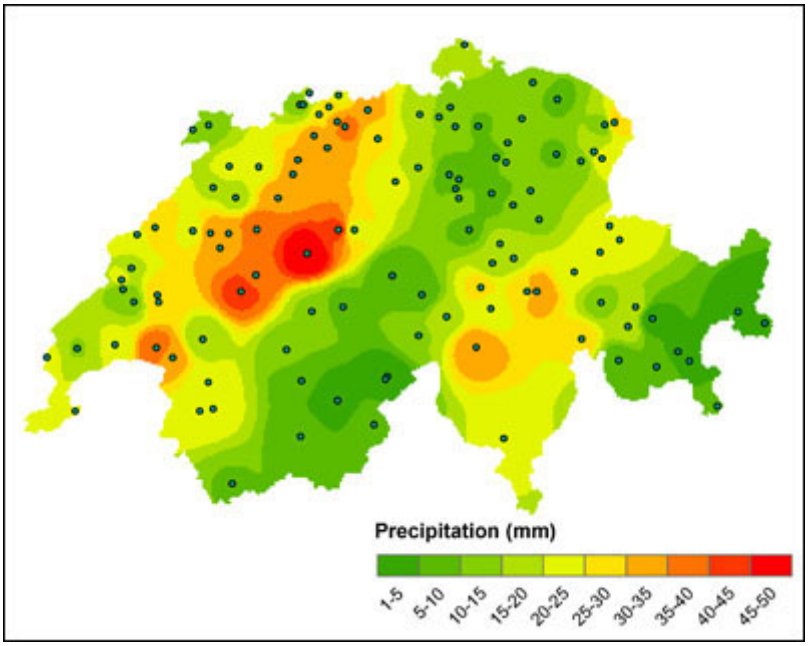
Theoretical variogram, a theoretical variogram function is matched onto the sequence of the averaged differences per class (= per lag).

Now, we attempt Kriging by incorporating our data into this model of spatial continuity – the model that we have developed or found in the section about variogram modeling. Based on such a model we can calculate error variance for our estimations and seek their minimum.
Interpolation with Kriging is a kind of curve fitting: from our known data points we have derived a model of how the spatial relationships might be designed. Based on that model we now estimate the unknown points. If we consider it in two dimensions only (for simplicity), we work with a regression technique: a curve fitting.

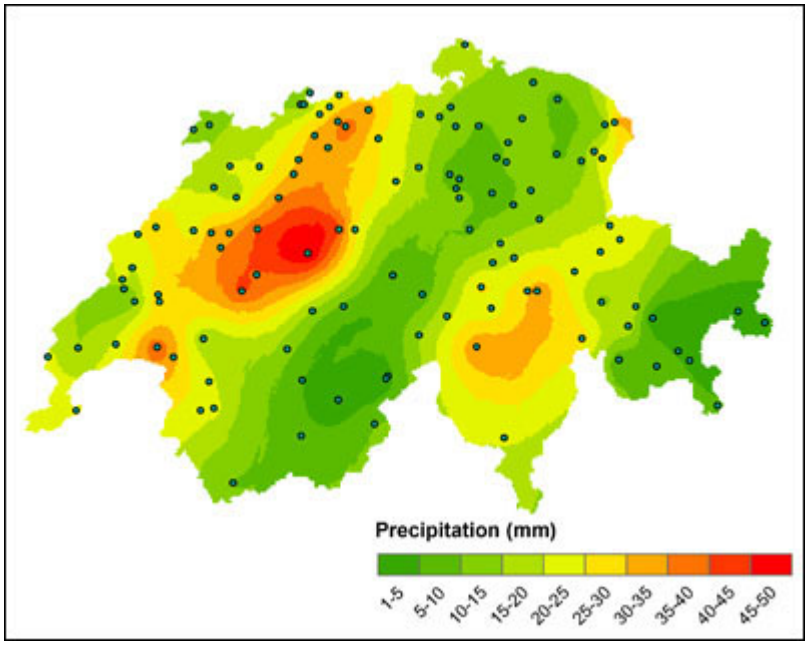


Kriging in zwei Dimensionen: Die blau umrandeten Quadrate sind unsere bekannten Datenpunkte, die rote Linie ist der geschätzte Verlauf, und die grünen Linien repräsentieren die statistischen Rahmenparameter aus unserem Modell (Wikipedia)

You often hear the term "exact interpolator" in connection with Kriging, just like IDW and some other estimation methods. This means that a surface estimated with one of these methods is intersecting the known data points. If we perform the Kriging calculation at a position of a known value, Kriging will typically give us exactly that value in return.
In comparison, see below for the result of an inverse distance weighting compared to that of a Kriging interpolation:



Estimation surface by using inverse distance weighting; Swiss rainfall data; Note that there are some „corona“ (regions of the same values) around known data points. (Provided by Ross Purves).



Result of a Kriging interpolation with Swiss rainfall data; here, no corona are to observe because the Kriging method „knows“ spatial relationships. It obtains this information from the variogram. (Provided by Ross Purves).

Other important parameters for interpolations: Search neighborhood

All interpolation methods can additionally be controlled by the definition of a search neighborhood, i.e. how many or which known data points are used to calculate an unknown position. If we ignore this neighborhood, all available known data are used for the estimation of every point. In the case of the Swiss rainfall data, this would mean that for the calculation of a precipitation value in Ticino, the values of observation stations in Jura are included as well. This just does not make any sense.

1.4. Summary

Spatially continuous phenomena such as rainfall or sea level cannot simply be described by a mathematical function. To analyze these variables, a spatial sample, i.e. a certain number of measurement points, is set up. To visualize a continuous spatial variable, the values between the measurement points need to be interpolated. First, the spatial sample or the set-up of the measurement points must be defined according to these characteristics: representativeness, homogeneity, a spatially optimal distribution, and sufficient number of points. Depending on the phenomenon and the measurement method, the design type of the spatial sample can vary (e.g. random sample, systematic sample, stratified sample, or clustered sample). Before the interpolation, we need to check if there is a dependency between the spatial data. Two methods are suited for this purpose: variography or the “moving windows”-method. Variography shows spatial dependency of the samples but not whether or not this dependency is equally distributed over the whole study area. For this, the “moving window”-method is applied. For the interpolation itself, several approaches with different consequences exist. Two ways to interpolate are presented here: the distance-based interpolation IDW (inverse distance weighting), and the geostatistical interpolation. With IDW, different distances are incorporated differently into the estimation. The influence of the distance weighting can be controlled by choosing the distance-weighting exponent. The higher the exponent, the more influence the measurement values of the adjacent points have on the result. However, it is not possible to have a direction-dependent weighting. With the geostatistic interpolation, the variography as the basis is derived from statistically distributed parameters. From the variography, the similarity of adjacent data points as a function of their distance from each other is indicated. The most important geostatistic interpolation methods are the Kriging methods.

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