GEOLOGICAL INFORMATICS

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MODELLING SOIL WATER REPELLENCY IN AN ABANDONED AGRICULTURAL FIELD

(Reviewed by the editorial board member O. Menshov)

Soil Water Repellency (SWR) is a natural property of soils with impacts on soil erosion, water infiltration, superficial and subsurface hydrology, nutrients leaching and plant growth.

Purpose: Study the spatial distribution and identify the most accurate interpolation method to estimate SWR in an abandoned agricultural field.

Methodology: A plot with 21 m^2 (07x03 m) was designed. Inside this plot SWR was measured in the field every 50 cm. In order to identify the most reliable map, we tested several interpolation methods, as Ordinary Kriging (KRG), Inverse Distance to a Weight (IDW) with the power of 1, 2, 3, 4 and 5, Radial Basis Function (RBF) (Inverse, Multiquadratic, Multilog, Multiquadratic, Natural Cubic Spline and Thin Plate, Spline) and, Local Polynomial, with the power of 1 and 2.

Findings: The results show that SWR was very heterogeneous, even in small distances, showing that soil hydrological properties can change very quickly in space. The spherical model was the best predictor of SWR and the most accurate interpolation method was the Multilog and the more biased the Natural Cubic Spline.

Originality: The test of several interpolation methods in SWR spatial distribution were not explored in detail, and this study represents an advance in this field.

Practical value: A better interpolation of SWR and other variables will help to have a better understanding of small scale processes in larger areas. Mapping with a better accuracy will improve models and contribute to a better prediction.

Introduction

Soil water hydrophobicity (SWR) is a natural property of soils. Among other factors, SWR depends on soil moisture, mineralogy, texture, pH, organic matter, aggregate stability, fungal and microbiological activity and plant cover. It has implications for plant growth, soil water infiltration, superficial and subsurface hydrology, soil erosion and nutrients leaching [5]. Depending on the level, SWR can also have positive impacts on soil structure and aggregate stability, carbon sequestration and protects soil from crusting [17, 1, 11].

Soil water repellency has been widely studied around the world in the most diverse climate regions [13] and environments, including forests [7, 14] grasslands, pastures [20], heathlands [35], steppes [8], sand dunes [5], golf fields [22], fire affected areas [4, 17, 21, 27] and agriculture fields [30, 32, 11, 10]. Previous studies showed that soil management in agricultural areas have important implications concerning the persistence, intensity and spatial distribution of SWR. Blanco-Canqui and Lal [2] and Roper et al. [31] observed that no-tillage soils have a higher SWR than tilled soils. The authors attributed this to the presence of soil organic matter that normally increases SWR [35].

Soil water repellency is highly variable in space and time [11, 29], even in small distances [16], imposing a challenge in mapping this small distance variation. Small scale variation modelling is important to understand large scale processes [3, 24]. Mapping small scale variations is complex due to the heterogeneous data distribution, and normally it is recommended to test several interpolation methods in order to know the less biased spatial predictor [26]. The objective of this work is testing the best interpolation method to estimate SWR in an abandoned agricultural field.

Materials and Methods

The studied area is located in an abandoned agricultural field located near Vilnius city (54 49' N, 25 22', 104 masl), Lithuania. The mean annual rainfall is 735 mm and temperature is 8.8°C. In a flat area an experimental plot with 21 m^2 (07x03 m) was designed and SWR repelency was assessed. Inside this plot, we measured SWR in the field every 50 cm, collecting a total of 105 sample points. Measurements were carried out on 28 May, 2012, after a period of 15 days without rainfall. Soil water repellency was assessed placing 5 droplets (±0.05 ml) in soil surface and measuring the water drop penetration time (WDPT) in seconds (s) [33].

Some statistical analyses were carried out: Mean (m), Standard Deviation (SD), Coefficient of Variation (CV%) Minimum (Min), 1^{st} quantile (Q1), median (M), 3^{rd} quantile, Maximum (Max), Skewness (SK) and Kurtosis. The spatial autocorrelation of SWR was assessed with the Moran's *I* Index, a measure similar to Pearson correlation coefficient. A value near 0 represents a random pattern, +1 a strong positive autocorrelation (clustered) and -1 a strong negative autocorrelation (dispersion) [23].

Previous to data modelling, normal distribution was tested with the Kolmogorov-Smirnov (K-S). Data normal distribution was considered at a $p>0.05$. This method, SK and Kur evaluate the data distribution and asymmetry that affect the interpolation methods accuracy. Previous studies show that it is desirable that data be as close as possible to normal distribution. If data is highly skewed, it may have negative impacts on the variogram modelling and interpretation [19, 23]. In this study we used the transformations, currently used in previous studies, Neperian logarithm (ln), Square root (SQR) and Box-Cox (BC), which were not powerful enough to normalize data distribution [23. 24].

The spatial patterns of SWR were analysed with an experimental omnidirectional variogram (it is assumed that SWR variability is equal in all directions) that observes the spatial continuity of SWR. The nugget effect, range, sill and nugget/sill ratio were measured. For the interested readers, details of variogram modelling can be consulted in Fu et al. [9] and Pereira et al. [24] [23]. Data interpolation tests were carried out using the most common methods, such as Ordinary Kriging (KRG), Inverse Distance to a Weight (IDW) with the power of 1, 2, 3, 4 and 5, Radial Basis Function (RBF) (Inverse, Multiquadratic, Multilog, Multiquadratic, Natural Cubic Spline and Thin Plate, Spline) and, Local Polynomial, with the power of 1 and 2. For detailed information about these methods Pereira and Ubeda [25] can be consulted. The best interpolation method was assessed with the cross validation method that compares the observed and estimated values of SWR. The cross validation was obtained by taking the value of a determinate sample point and estimating it from the remaining ones. The residuals produced were used to evaluate the accuracy of each method. The Mean Error (ME) and the Root Square Mean Error (RMSE), calculated from the residuals, were used to assess interpolation methods performance. The method with the lower RMSE was considered the best estimator. More information about these indices can be found in Pereira and Ubeda [25]. Pearson correlation coefficient was calculated between the observed and estimated values. Significant differences were considered at a $p<0.05$. Statistical analyses were carried out with Statistica 7.0 and interpolation methods assessment with Surfer 9.0 for windows.

Results and Discussion

Soil water repellency varied from 1 to 772 s, and had an average of 25.73. The CV% was 361.09%, showing that in this small plot SWR was extremely high variable. The results of SK show that the majority of the values were concentrated in lower values of the distribution (Positive SK) that is evidence of the presence of extreme positive outliers. Data also showed an extremely high KUR, which means that data have a peaked distribution (Table 1). The result of the Moran's *I* index was 0.026, $p<0.513$, suggesting that the distribution of SWR was random and no specific pattern was observed. According to the results of the K-S test, the original and transformed distributions were considered not normally distributed ($p<0.05$). To model the spatial distribution of SWR, we used the Ln transformed data since they were closer to normal distribution and presented the lower SK and KUR values (Table 1). This criterion was used in previous works [14, 36, 34, 23). In this case we did not remove the outliers because it would mean loss of important information.

Table 1

Descriptive statistics of SWR and results of K-S test. Original data in seconds (s)

	m	SD	CV%	Min	Q1	M	Q3	Max	SK	KUR	K-S *p*
Original data	25.73	92.93	361.09	1	1.66	2.66	7	772	6.13	43.10	0.01
Ln	1.49	1.46	98.16	0	0.51	0.98	1.94	6.64	1.50	2.02	0.01
SQR	3.06	4.06	132.72	1	1.29	3.06	2.64	27.78	3.85	17.02	0.01
BC	4.95	3.51	71.06	2.48	3.03	4.95	5.09	22.48	2.77	8.69	0.01

Among all the tested models, the spherical was the best fitted to explain SWR spatial variability (Figure 1), as observed in previous studies [28]. The nugget effect was 1.2, the range 101 cm, the Sill, 2.22 and Nugget/Sill ratio 54.05%. The nugget effect is normally attributed to the small number of samples, small distance variance and presence of outliers [18]. In this case the nugget effect may be due to the small scale variance of SWR and to the presence of outliers, since the data that we used was not normally distributed. The spatial correlation of SWR increased with the distance until the distance of 101 cm. This suggests that spatial correlation range was higher than the sample density (50 cm), showing that the sample design was good to measure SWR variability. It is important to mention that the spatial correlation was short in the space, which confirms the random pattern identified with the Moran's *I* index. The nugget/sill ratio result suggested that the SWR has a moderate spatial dependency. According to Chien et al. (1997), ratios less than 25% show that the variable has a strong spatial dependence, between 25 and 75%, the variable has a moderate spatial dependence, and when higher than 75, the variable has a weak spatial dependence.

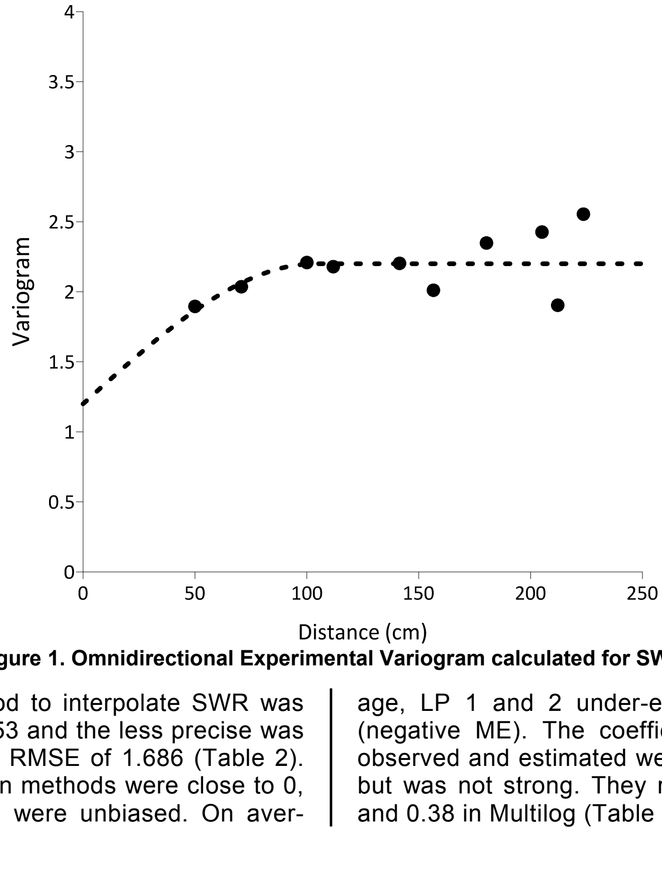

Figure 1. Omnidirectional Experimental Variogram calculated for SWR

The most accurate method to interpolate SWR was Multilog, with a RMSE of 1.353 and the less precise was Natural Cubic Spline with an RMSE of 1.686 (Table 2). The ME of all the interpolation methods were close to 0, showing that the predictions were unbiased. On average, LP 1 and 2 under-estimated the original values (negative ME). The coefficient of correlation between observed and estimated were significant in all the cases but was not strong. They range between 0.25 in IDW1 and 0.38 in Multilog (Table 2).

Table 2

Summary statistics of the accuracy of interpolation methods. Numbers in bold indicate the most accurate method and underlined, the least accurate. Correlations between observed and estimated values significant at **p<0.01 and ***p<0.001

	Type	Min	Max	ME	RMSE	Obs *vs* Est
KRG	Ordinary (Point)	-4.844	2.461	0.003	1.406	0.37***
IDW	Power (1)	-4.997	1.587	0.011	1.425	0.25**
	Power (2)	-4.702	1.733	0.013	1.377	0.32***
	Power (3)	-4.646	1.873	0.013	1.369	0.34***
	Power (4)	-4.726	2.060	0.012	1.378	0.35***
	Power (5)	-4.772	2.135	0.011	1.386	0.35***
RBF	Inverse multiquadratic	-4.685	1.871	0.001	1.379	0.37***
	Multilog	-4.798	2.188	0.003	1.353	0.38***
	Multiquadratic	-4.814	2.736	0.004	1.447	0.37***
	Natural cubic spline	-4.558	4.612	0.013	1.686	0.36***
	Thin Plate Spline	-4.738	3.754	0.007	1.552	0.36***
LP	1	-4.911	2.136	-0.026	1.392	0.28**
	2	-4.695	2.437	-0.016	1.382	0.32***

The interpolation methods tested allowed us to identify the best spatial predictor and the most precise SWR spatial distribution. The map interpolated with the best method showed that SWR was low in the northeast part of the plot, and high at northwest and in the south of the area of interest (Figure 2a). The interpolation with the less biased method showed that the distribution is more heterogeneous and no clear pattern was identified (Figure 2b). This suggests that previously to mapping any variables, it is essential to test several methods in order to have the best data interpolation, as observed in previous studies [24, 23]. The maps of the residuals produced are in the figures 2c and 2d. The interpolated map with the most accurate method residuals showed that the major errors were identified in the areas where SWR was high. This correlates the observed with the results from the SK which suggest that data were mostly concentrated in the lower values (positive SK) and few samples had high values. The cross-validation procedure, estimated them substantially lower than the original ones. The errors were high and heterogeneous in the less accurate method than in the best one, suggesting that the Natural Cubic Spline interpolation has produced high positive and negative errors. In comparison to Multilog, the values predicted by Natural Cubic Spline were very distant from the original values.

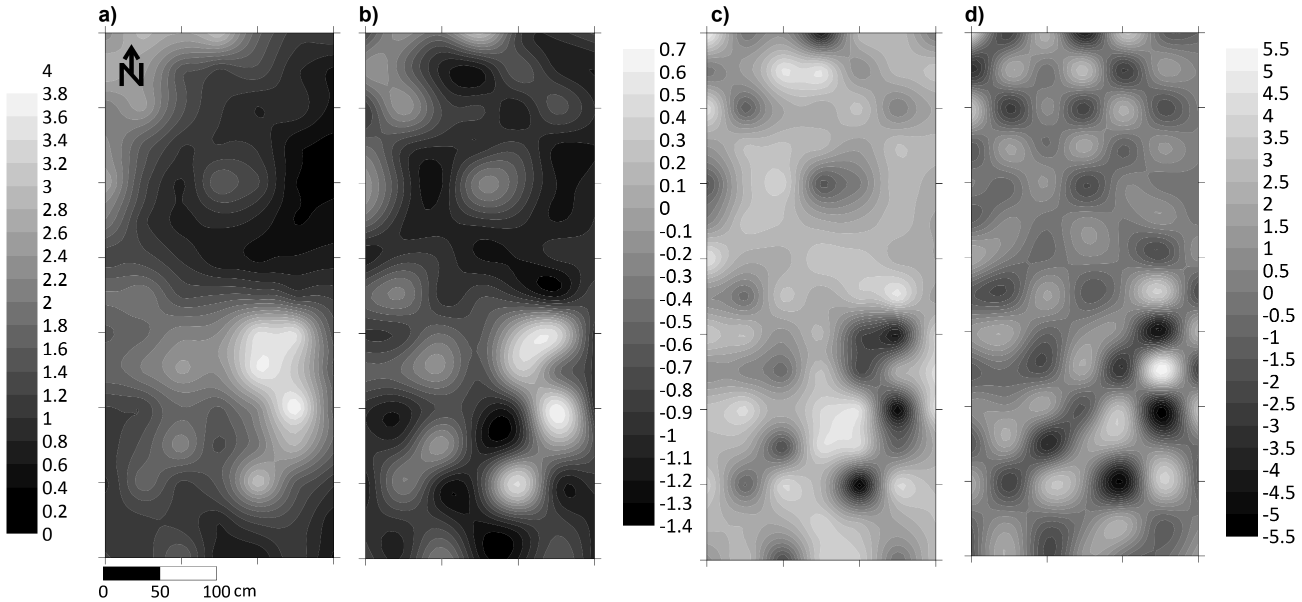

Figure 2. Soil water repellency interpolation according to the most a), less b) accurate method and the residuals obtaned from the best c) and worst d) interpolation technique

Conclusions

1. Soil water repellency was highly variable in the studied plot and had a random pattern distribution, suggesting that soil hydrological properties can be very heterogeneous at short distances.
2. The spherical was the best model to explain SWR variability. The SWR range was short, but the sample density was adequate to measure SWR spatial variability.
3. The best SWR interpolator was Multilog and the less accurate was Natural Cubic Spline. The lowest SWR was identified in the northeast and south of the plot, while highest values were observed in the south and northwest.
4. The interpolated maps with the most and least accurate method showed different spatial configurations, highlighting the need for testing several interpolation methods, previous to mapping any variables.

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МОДЕЛЮВАННЯ ГІДРОФОБНИХ ВЛАСТИВОСТЕЙ ГРУНТІВ В УМОВАХ НЕОБРОБЛЮВАНИХ СІЛЬСЬКОГОСПОДАРСЬКИХ УГІДЬ

Гідрофобність грунтів є природною властивістю, яка пов'язана з впливом ерозійних процесів, інфільтрації води, поверхневих і підземних гідрогеологічних процесів, поживних речовин, вилуговування і росту рослин.

Мета: Дослідження просторового розподілу і визначення найбільш точних методів інтерполяції для оцінки гідрофобності грунтів у межах необроблюваних сільськогосподарських угідь.

Методика: Було обрано ділянку площею 21 м^2 (7х3 м). Усередині цієї ділянки гідрофобність грунтів визначалася з кроком 50 см. З метою визначення найбільш надійної карти було протестовано кілька методів інтерполяції – звичайний крігінг, зворотня відстань до ваги з силою 1, 2, 3, 4 і 5, Радіальна базисна функція (Зворотня, мультиквадратична, мультилогарифмічна, натуральний кубічний сплайн і тонкої пластини, сплайн), Локальна поліномна з силою 1 і 2.

Результати: Отримані результати показують, що гідрофобність грунтів дуже неоднорідна, навіть на невеликих відстанях. Останнє свідчить, що гідрологічні властивості грунтів можуть змінюватися дуже швидко в просторі. Сферична модель стала найкращим передвісником гідрофобності грунтів. Крім того, найбільш точним методом інтерполяції виявлено Мультилогарифмічний метод, а найбільш обгрунтований метод кубічного сплайну.

Новизна: Дослідження декількох методів інтерполяції просторового розподілу гідрофобності грунтів не вивчалися раніше, а отже наведені матеріали несуть нову інформацію у даній сфері досліджень.

Практичне значення: Більш точна інтерполяція гідрофобності грунтів та інших показників допоможе глибше зрозуміти тонкі процеси у межах великих площ. Картування з вищою точністю поліпшить моделі та зробить вагомий внесок у прогнозування ерозії грунтів.

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МОДЕЛИРОВАНИЕ ГИДРОФОБНЫХ СВОЙСТВ ПОЧВ В УСЛОВИЯХ НЕОБРАБАТЫВАЕМЫХ СЕЛЬСКОХОЗЯЙСТВЕННЫХ ЗЕМЕЛЬ

Гидрофобность почв является естественным свойством, которое связано с влиянием эрозионных процессов, инфильтрации воды, поверхностных и подземных гидрогеологических процессов, питательных веществ, выщелачивание и роста растений.

Цель: Исследование пространственного распределения и определение наиболее точных методов интерполяции для оценки гидрофобности почв в пределах необрабатываемых сельскохозяйственных земель.

Методика: Был избран участок площадью 21 м^2 (7х3 м). Внутри этого участка гидрофобность почв определялась с шагом 50 см. С целью определения наиболее надежной карты были протестированы несколько методов интерполяции – обычный кригинг, обратное расстояние к весу с силой 1, 2, 3, 4 и 5, Радиальная: базисная функция (Обратная, мультиквадратическая, мультилогарифмическая, натуральный кубический сплайн и тонкой пластины, сплайн), Локальный полином с силой 1 и 2.

Результаты: Полученные результаты показывают, что гидрофобность почв очень неоднородна, даже на небольших расстояниях. Последнее свидетельствует, что гидрологические свойства почвы могут меняться очень быстро в пространстве. Сферическая модель стала лучшим предвестником гидрофобности почв. Кроме того, наиболее точным методом интерполяции стал Мультилогарифмический метод, а наиболее обоснованный метод – кубического сплайна .

Новизна: Исследование нескольких методов интерполяции пространственного распределения гидрофобности почв изучалось ранее, а следовательно приведенные материалы несут новую информацию в данной сфере исследований.

Практическое значение: Более точная интерполяция гидрофобности почв и других показателей поможет глубже понять тонкие процессы в рамках больших площадей. Картирование с высокой точностью улучшит модели и сделает весомый вклад в прогнозирование эрозии почв.

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MODELLING OF STRESS-STRAIN STATE OF CRUSTAL SYSTEMS IN CONTEXT OF SPACE PROBLEM DURING THE GRANITE FORMATION

(Reviewed by the editorial board member V. Shevchuk)

The problem of granites holds a special place in geology. Research of the granite formation problem leads to a number of partial problems, among those the question of depth of the granite generation and mechanisms of provision of space for large granitoid solids are distinguished. In the problem of space the geomechanical constituent is of primary importance. The major factors forming the stress-strain state in the system of the granite formation are permanently acting mass gravitation forces, tectonic forces of inter-slabs interaction, pseudo-mass forces, forces of volumetric thermoelastic effects, phase transitions in processes of metamorphism, metasomatism, partial and complete fusion. In existing investigations of stress-strain state of crust systems the geological mediums are supposed to be quasi-homogeneous. The objective of this work is to develop the general approach to computer modeling of the behavior of geological and mechanical systems of mega-blocks range, in context of space problem during the granite formation, taking into account structure anisotropy of the system.

While the possibilities of full-size modeling of complex multifactorial magmatogene systems are limited, the possibilities of mathematical modeling are more appropriate, especially in view of the mechanical systems modeling. Verification of geological hypotheses and empirical data by constructing simple models with its further complication by means of transition to more and more complex combinations of force factors, rheological states, boundary conditions, and other factors is the most optimal. In the article the problem of stress-strain assessment of geological and mechanical system of mega-blocks range is analyzed. Assuming that the temperature of medium is known, there were obtained governing relations describing the behavior of geological and mechanical system at combined action of the gravity, non-homogeneous temperature field and power and kinematic influences imposed on the boundaries of considered system. The algorithm for solving of elastic problem is developed by means of the modified boundary element method.

The governing relations of the considered problem are obtained as well as the numerical and analytical algorithm of stress-strain assessment of the considered geological and mechanical system is developed.

Mathematical model and corresponding algorithm of the numerical calculation of stress-strain state of the considered system allow analyzing the stress-strain state of geological and mechanical system at combined action of gravity, non-homogeneous temperature field and imposed on the boundaries of considered system power and kinematic influences, taking into account structure anisotropy of the system.

Thus the method proposed herein allows investigating the nature of stresses fields, and hence to forecast geometry of potential zones of relative decompression and tension, which are the most auspicious for granite formation.

The problem of granites holds a special place in geology. From question of origin of rock of certain composition it transformed into complex problem wherein the petrological aspect is connected with structural and tectonic (dynamic and kinematic, geomechanical) and other aspects [1, 3].

Research of the granite formation problem leads to a number of partial problems, among those the question of depth of the granite formation and mechanisms of provision of space for large granitoid solids are distinguished. The question of space, occupied by the large granitoid rocks, in its turn, is connected with the tectonic position of granitoid complexes and geodynamic conditions of mass granite formation [5, 12].

In the problem of space the geomechanical constituent is of primary importance. Dimensional parameters of large granitoid solids, direct connection of the granite formation with orogeny of crystallization and deformation processes, as well as the character of structural anisotropy of granitoids indicate the complex hierarchical pattern of stress-strain state and the influence of many power factors of different origin on the cumulative stress-strain states.

Modeling of magmatogene processes and structures is a powerful tool of studies. While the possibilities of full-size modeling of complex multifactorial magmatogene systems are limited, the possibilities of mathematical modeling are