Comparing the Thiessen's Method against simpler alternatives using Monte Carlo Simulation*

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Abstract

Estimating the expected value of a function over geographic areas is problem with a long history. In the beginning of the XX-th century the most common method was just the arithmetic mean of the field measurements ignoring data location. In 1911, Thiessen introduced a new weighting procedure measuring influence through an area and thus indirectly considering closeness between them. In another context, Quenouville created in 1949 the jackknife method which is used to estimate the bias and the standard deviation. In 1979 Efron invented the bootstrap method which, among other things, is useful to estimate the expected value and the confidence interval (CI) from a population. Although the Thiessen's method has been used for more than 100 years, we were unable to find systematic analysis comparing its efficiency against the simple mean, or even to more recent methods like jackknife or boostrap. In this work we compared four methods to estimate de expected value. Sample mean, Thiessen, the so called here jackknifed Thiessen and bootstrap. All of them are feasible for routine use in a network of fixed locations. The comparison was made using the Friedman's Test after a Monte Carlo simulation. Two cases were taken for study: one analytic with three arbitrary functions and the other using experimental data from daily rain measured with a satellite. The results show that Thiessen's method is the best estimator in almost all the cases with a 95% of confidence interval. Unlike the others, the last two considered methods supply a suitable

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CI, but the one obtained through jackknifed Thiessen was even more accurate, opening the door for future work.

Key words: *Thiessen, Monte Carlo, bootstrap, jackknife.*

Resumen

La estimación del valor esperado de una función sobre áreas geográficas es un problema que data de tiempo atrás. Hasta principios del siglo XX el método más común solía ser calcular la media aritmética de las medidas obtenidas en el campo ignorando su posición geométrica. En 1911 Thiessen introdujo una nueva forma de cálculo que asignaba a cada punto de medición un peso relativo al área de influencia, que tenía en cuenta indirectamente la proximidad entre datos. En 1949 Quenouville crea, en otro contexto, el método de *jackknife* que se utiliza para estimar el valor esperado y la desviación estándar. En 1979 Efron inventa el método de *bootstrap* que, entre otras cosas, es apropiado para estimar el valor esperado de una población así como su intervalo de confianza (IC). Si bien el método de Thiessen lleva usándose hace más de un siglo, no se han encontrado estudios sistemáticos que comparen su eficacia frente al método anterior ni frente a variantes posteriores como *jackknife* o *bootstrap*. Este trabajo consiste en comparar cuatro métodos para la estimación del valor esperado: el de la media aritmética, el de Thiessen, el aquí denominado *jackknifed* Thiessen y el de *bootstrap*. Todos ellos son aptos para aplicaciones repetitivas en una red de observación fija. La comparación se realizó mediante el Test de Friedman tras una simulación de Monte Carlo. Para los datos se consideran dos casos: uno analítico mediante el estudio de tres funciones arbitrarias, y otro experimental con datos de lluvia diaria medidos por satélite. Los resultados obtenidos muestran que el método de Thiessen es el mejor estimador en prácticamente todos los casos con el 95% de nivel de confianza. Las últimas dos variantes tienen la virtud de suministrar un IC que se mostró adecuado, aunque *jackknifed* Thiessen resultó mucho más ajustado, abriendo así la puerta para futuras investigaciones.

Palabras clave: *Thiessen, Monte Carlo, bootstrap, jackknife.*

Resumo

A estimação do valor esperado de uma função sobre áreas geográficas é um problema que data de tempos atrás. Até o início do século XX o método mais comum consistia em calcular a média aritmética das medidas obtidas em campo, ignorando sua posição geométrica. Em 1911, Thiessen introduziu uma nova fórmula de cálculo que associava cada ponto de medição a um peso relativo a sua área de influência, que levava em conta indiretamente a proximidade entre dados. Em 1949, Quenouville cria, em outro contexto, o método jackknife que é usado para estimar o desvio padrão e a inclinação. Em 1979, Efron inventou o método do bootstrap que, entre outras coisas, é apropriado para estimar o valor esperado de uma população assim como seu intervalo de confiança (IC). Enquanto o método de Thiessen vem sendo usado por mais de um século, não são encontrados estudos sistemáticos que comparem sua eficácia comparado ao método anterior, nem com suas variantes posteriores como jackknife ou bootstrap. Este trabalho consiste na comparação dos quatro métodos de estimação do valor esperado: o do média aritmética, o de Thiessen, o aquí chamado de jackknifed Thiessen e o do bootstrap. Todos eles são adequados para aplicações repetitivas em uma rede de observação fixa. A comparação foi realizada através do Teste de Friedman feita em uma simulação de Monte Carlo. Para os dados são considerados dois casos: um analítico através do estudos de três funções arbitrárias e outro experimental com dados de chuva diária medidos por satélite. Os resultados obtidos mostram que o método Thiessen é o melhor estimador em praticamente todos os casos com nível de confiança de 95%. As últimas duas variantes tem a virtude de fornecer um IC que se mostrou adequado, embora o jackknifed Thiessen tenha resultados mais precisos, abrindo assim a porta para futuras investigações.

Palavras chave: *Thiessen, Monte Carlo, bootstrap, jackknife.*

Introduction

Either in the Geosciences as well as other areas it is sometimes necessary to estimate a representative value of a variable over a certain domain. As an example, we can mention the population density, the average rainfall over a catchment, etc. It is common in Geosciences that:

- The data to be observed is only known at selected locations (points)
- It is costly (or even impossible) to add points in arbitrary locations
- The mean areal value is more important than the individual readings

This and also other circumstances are valid for meteorological data. The network of measuring stations has been traditionally static, and thus the dataset is a collection of time series measured at fixed locations. One very popular variable is the daily rain; it is used in hydrological, climate or even agricultural calculations and is regularly published in statistical yearbooks in order to characterize the climate of a particular region. The motivation for this work is related with the expected areal value of the daily rain. There exist, of course, other applications even indirect. For example, the National Standard for Spatial Data Accuracy (FGDC, 1998) describes the procedure to calculate a number which is representative of the positional error of a given cartography. Its expression is:

$$Accuracy = 2.4477 * 0.5 * \left(RMSE_x + RMSE_y \right) \quad (1)$$

Each one of the last two terms comes, in turn, from a generic expression like

$$\left(RMSE_x\right)^2 = \frac{\sum_{i=1}^{N}\left(x_i - x_{exact,i}\right)^2}{N} \qquad (2)$$

which can be interpreted as the average of the squared difference between the coordinate of a control point and a value deemed to be exact for such point. The coordinates of the control point do not participate in the calculation except through the abovementioned difference. This formula for the average is exactly the same which was common before the work of Thiessen (1911) for meteorological variables like the daily rain. Can we do better? It will be shown below that the Thiessen's method was created to improve the crude estimate for the mean areal value given by expressions like this.

Since the deployment of the first meteorological networks it has been attempted to characterize the spatial variability of the measurements. The networks were designed considering such aspects (mutual distance, estimated values of spatial correlation, etc.) as well as practical considerations (easy access, energy availability, etc.). At the beginning of the XX century the computation capabilities were very limited, so the estimates of a "representative value" of the rain were simply an average of the available data, irrespective of the location and its mutual distance. As early as 1911, Thiessen (Thiessen, 1911) recognized that such numerical procedure suffers from bias, especially when the density of the data points varies in the region. If there is a group of stations close to each other, the average on the region was biased by the local value which was indeed a local phenomenon. That was the motivation to propose the method that is now known as the Thiessen's polygons. It adds weights to the average operation. The weight for a given point is proportional to the area of its neighborhood, defined as the region of points closer to it rather than other in the network. It is easy to show that such neighborhood is a convex polygon, bounded by segments of perpendicular bisectors defined between pairs of measuring points. A simple case is sketched in Figure 1.

It can be argued that the Thiessen criteria is somewhat related with the First Tobler's Law (Tobler, 1970) which can be summarized as "…"everything is related to everything else, but near things are more related than distant things…". Thiessen uses as proximity criteria the geometric distance, in a literal interpretation of what Tobler will formalize sixty years later.

Despite its simple formulation, the calculation of Thiessen's polygons is a very active topic, either in the geoscience community as well as mathematics and computer science ones. Outside the meteorological applications the problem is known as Voronoi Diagram, and even there exist a tradition of specific congress devoted to the topic <http://bioinf.spbau.ru/isvd2013/home> considering problems like new calculation methods, parallel computer implementations, new applications, etc.

The motivation for such sustained interest in the topic is related to the non-trivial nature of the computations, which for large number of points and/or large dimensions require special care. Taking this into consideration, it is fit to ask if it is worth the calculation effort considering the quality of the resulting estimate. Unlike what one might think, we were unable to locate any basic paper that compares the performance of other alternatives to compute the mean areal average. That was the motivation of this work, trying to confirm (or deny) that the Thiessen's method is superior to other alternatives, and that its higher computation complexity is justified by its better accuracy. In order to perform a fair comparison we should resort to a controlled experiment (to be described later) and to the application of statistical test to give confidence to the results. We will use the Friedman's Test (Friedman, 1937; 1939). The test assumes that a number of methods were applied to a particular problem (called event), and a ranking among them can be defined for each event. For other event the ranking might vary, and we assume that we collect all the rankings. Given a confidence level (usually 95%) the Friedman's Test analyzes the set of rankings and can prove or disprove that there exist a difference between the methods. In the case under analysis, the methods will be objectively ranked according to the proximity of the areal estimate and its true value.

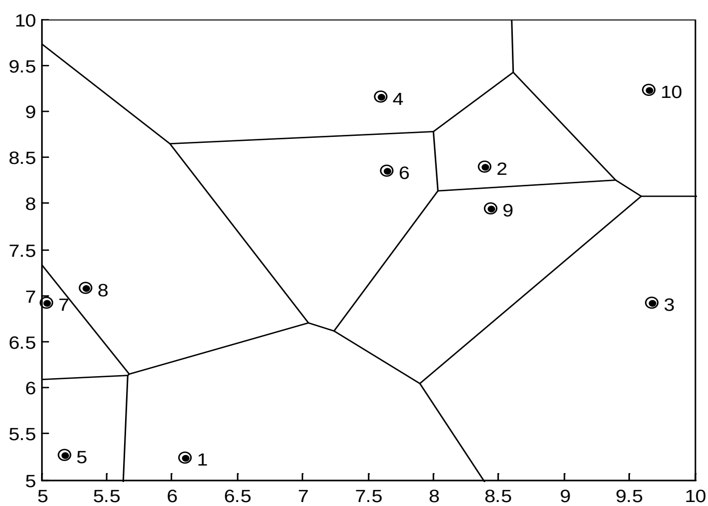

Figure 1. An example of the Thiessen's polygons for N=10.

Source: Own elaboration.

The Friedman's test requires some minimum number of methods and events. In order to fulfill such requirements we have considered the following methods: 1) simple average of all the available data 2) resampled mean (*bootstrap)* 3) standard Thiessen's method and 4) *jackknifed* Thiessen. They will be described below. The number of events will be decided as part of the Monte Carlo simulation. This paper is organized as follows: after the Introduction, we will expose the Methods used in the analysis. Afterwards we will describe the Data and finally we will present the Conclusions.

Methods

Thiessen's Method

In 1911 Alfred Thiessen proposed an alternative procedure for estimating the mean daily rain average over large areas. Given the study region and the location of the weather stations, he calculated the neighborhood area and used it as a weight in the computations. The process was later known as Thiessen's Tesselation, or Voronoi Diagram. The method has been used for over a century using rain as the variable of interest, but also for other meteorological variables and having a number of applications in other disciplines as well.

Despite Thiessen not used such concept, what is intended to estimate is directly linked to the integral of the rain in the domain. In numerical analysis for the estimation of integrals is standard that we first substitute the true function by an interpolant, and afterwards we perform the exact integral of the latter. The reason is very practical: the interpolant is designed to be simpler than the original function, and thus the computations will be cheaper. In the practical problem under study the function itself is not known (just its values at selected points), so we only have the interpolant (which in turn is not unique). The Thiessen estimate is the exact integral of one of them, named Nearest Neighbor. Such interpolant is discontinuous in the borders of the Thiessen's polygons and constant within them, taking the numerical value of its interior data point. Since the polygons are themselves the result of intersecting semi planes, it can be proved that the Thiessen polygons are convex.

Jackknifed Thiessen

This method is proposed in this paper. The *Jackknife* was described for the first time by Quenouille (1949) in the context of time series processing and quickly become popular. García-Guzmán and Calatrava-Requena (1978) summarized in general the procedure discussing advantages and disadvantages. The method consist in a sampling *without replacement* of the available population, producing N values of the desired estimate after processing N dataset each one holding N-1 elements, with the i-th missing. The standard Thiessen estimate is built for each configuration, and a resulting value is computed and stored. After that (and in this work) we calculated the median value of such N values and denote the resulting value as the *jackknifed Thiessen*. The maximum and the minimum values of the set will be considered to define a confidence interval (CI) calculated as (min+max)/2+2*(max-min)*[-1,1]. The "max" and "min" terms are the maximum and minimum value of the estimate in the set obtained after the N resampled cases. In many applications the number N is low (a few dozens) or mild (less than a hundred), so the computing time required by the *jackknifed* Thiessen is modest. This new method can easily be implemented if the Thiessen one is available, not needing a substantial extra programming effort.

Bootstrap

Efron (1979) presented this method as an alternative to the traditional Jackknife. Unlike it, he proposed to perform a sampling *with replacement*, and afterwards build the estimate as the average of the values of each sampling. Confidence intervals can be inferred as well. Sampling *with replacement* means that an individual point might be considered more than once in each sample. From the computational point of view this procedure is more demanding than the simple average but substantially less than the traditional Thiessen or the jackknifed Thiessen. The computer code is very simple, and just requires access to a library for pseudo-random number generation.

Data and methods

Problem description for the analytical case

For the analytical case we have a known function, so it is possible to have an exact value of the integral. Through a Monte Carlo Simulation we performed M events, consisting on the selection of N data points at random within the domain. In such locations we evaluated the function value and afterwards the arithmetic mean, the *bootstrap*, Thiessen and finally the *jackknifed* Thiessen are calculated independently. The result can be organized as a table with M rows and four columns which might be easily compared against the exact value. Thus, a ranking per row among methods can be objectively inferred.

For the analytical case we considered the following three functions:

$$\begin{gathered} f(x,y) = x^2 y \\ f(x,y) = \sin(x).\sin(3y) \\ f(x,y) = morrisonIII(1000x, 1000y) \end{gathered} \tag{3}$$

The first two are somewhat arbitrary. The third is due to Morrison (1971) and it is composed of a trigonometric series of 48 terms truncated to the third harmonic.

Its coefficients have been obtained after adjusting the expression to experimental data of a real topography. In all three cases we restricted the integration domain to the square [0 1]x[0 1]. Despite the exact analytical value of the integral is accessible, for simplicity we have calculated it through a standard quadrature routine requesting a relative error of 10^{-6}.

Problem description for the experimental case

In this second part we start using a satellite image with estimates of the daily rain, downloaded from <http://disc.sci.gsfc.nasa.gov/precipitation/tovas>. In the context of this work, the image can be considered as a table of values with P>>N points (pixels) observed in the field. As before, and to make a fair comparison, we simulate M times the selection of N points. Unlike the analytical case now we have no exact value of the integral to compare with. As an alternative we considered the Thiessen estimate using all the available pixels.

We have used the image covering the region between [-34.3 -30.5] latitude and [-52.5 -48] longitude from june 20th, 2014. The area includes all the catchment area of the Rincón del Bonete dam (Uruguay). The delineation of the catchment and the location of the center of the pixels are shown in Figure 2. After applying the Thiessen estimate using all the 270 pixels available, the mean rain average for such day was nearly 10.8 mm/day, which hereinafter was considered the exact value. For the Monte Carlo Simulation we just have an universe of 97 pixels which lie inside the catchment area (in blue in Figure 2).

How we organize the computation

Let N be the number of points with known values. We considered different values of N just to see the evolution of the accuracy of the estimate when N grows. We selected the cases of N equal to 5, 10, 20, 40 and 50. For each function and N, we performed a Monte Carlo Simulation. In each one and for the analytical case, the coordinates of the N data points were generated with the pseudo-random number generator, using a specific seed in order to make repeatable the computations. With such coordinates we evaluated the analytical functions, producing N functional values. With them, and for each event, we produced an estimate of the expected value using all four available methods. For the experimental case we selected also at random the N available points, thus keeping its value and coordinates.

We used the Friedman's Test (Friedman, 1937; 1939) to compare among methods. Its ultimate goal is to validate the hypothesis that the methods do not differ in performance. The input is a table holding a ranking among methods in each row, with as many rows as events. Each entry of the table is an ordinal number (1, 2, 3, etc.) which ranks the methods against its peers. The test considers the case of ties, both in the input and in the output. In this particular case there is no practical possibility of ties in the input, because we used as criteria for the ranking the absolute difference between the estimate and the reference value. The method with number 1 at the k-th event (row) would be the one with the smallest difference w.r.t. the reference value, and the one with 4 will have the largest difference. The Friedman's Test was applied to the 95% confidence level.

Initially we specified M=2000. We generate two disjoint simulations and compared the result of the Friedman's Test in each. Since there was no agreement, we extended the simulation for 2000 more events and repeated the Test. The process continues until we reached an agreement at 10000 events, which was deemed enough for assuming convergence in the process. All the remaining calculations used jointly the 20000 events. The computer used for the computations has an Intel i7 4770K processor (4 cores 3.5GHz) and the overall simulation required 96 hours.

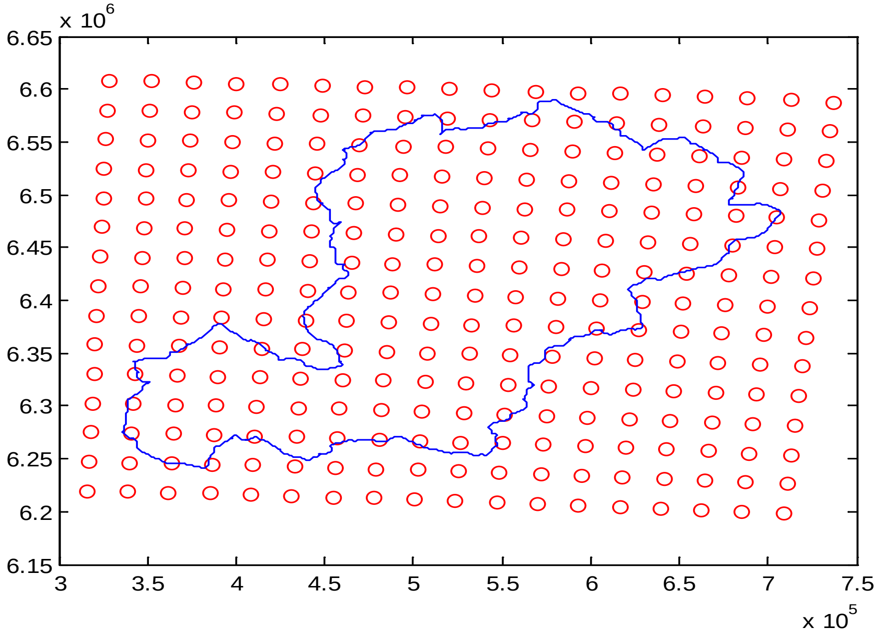

Figure 2. Sketch of the catchment area of the Rincón del Bonete dam and placement of the center of data pixels. Coordinates in UTM 21S. Source: Own elaboration.

Results

The following figures and results are organized according to the analytical function. In each figure the rows (from top to bottom) stands for different N cases, namely 5, 10, 20, 40, and 50. The columns (from left to right) are for each considered method: sample mean, bootstrap, Thiessen and jackknifed Thiessen.

From Fig. 3 describing the case of the function x^2*y it should be noticed the significant dispersion of the arithmetic mean (irrespective of N) while the opposite happens with the jackknifed Thiessen. Also the estimate are somewhat biased when N grows. The CI is, as expected, progressively narrower and the experimental distributions do not look as normal. In Fig. 4 and for the function sin(x)*cos(3y) the dispersion pattern is repeated, but the bias is less noticeable. For this example (maybe more realistic than the one before) the distributions seems to be more symmetric. In the case of the Morrison III function (Morrison, 1971) presented in Fig. 5 we show that the methods related with Thiessen are somewhat unbiased, and our proposed jackknifed Thiessen confirms its preference for narrower CI intervals. Never (for any function and for any N) the exact value of the integral was outside the 90% CI, but for the narrower ones it was closer to the maximum value. For the experimental case, reported in Fig. 6, the behavior of the four methods was similar to those of the analytical cases, providing again jackknifed Thiessen a better estimate with a decreasing bias when N grows. The dispersion plot shows a symmetric distribution closer to a normal one.

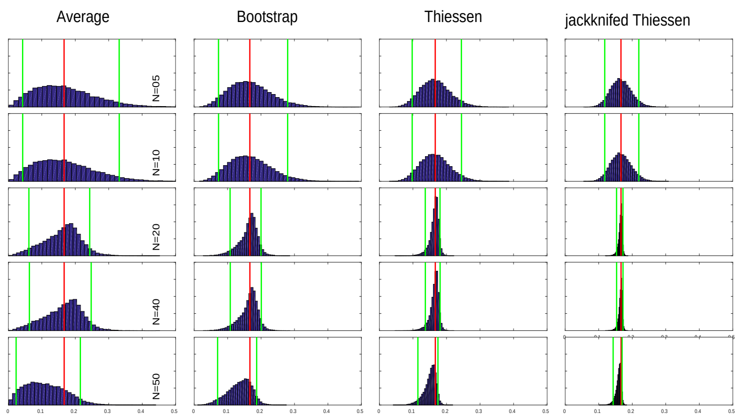

Figure 3: Results of the Monte Carlo Simulation for the x^2*y function. In red we denote the true value (identical for all the plots) and in green the experimental percentiles at 5 and 95%. The x-axes range is the same for all the plots. Source: Own elaboration.

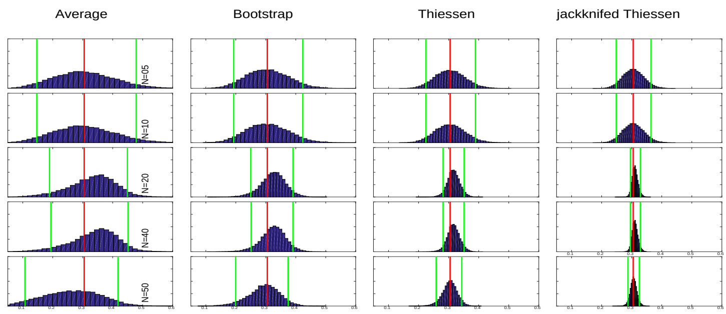

Figure 4. Results of the Monte Carlo Simulation for the sin(x)*cos(3y)function. In red we denote the true value (identical for all the plots) and in green the experimental percentiles at 5 and 95%. The x-axes range is the same for all the plots. Source: Own elaboration.

It is clear that the methods are already ordered, from left to right, according to the length of its CI. However, it should be stressed that the result should not be taken as definitive because what it is shown is the result of a simulation. In a practical case (a single event) it should be positively considered that both the *bootstrap* and *jackknifed* Thiessen generate themselves a CI for such event. In other computations (not presented here) we were able to notice that more than 90% of the cases the CI defined as [average-2*(sample deviation), average+2*(sample deviation)] computed after the *boostrap* indeed includes the exact value for the case N=10, 20, 40 or 50, while for the case of N=5 the same interval was adequate in 84% of the cases. The *jackknifed* Thiessen in turn includes the exact value in more than 92% of the events, irrespective of N.

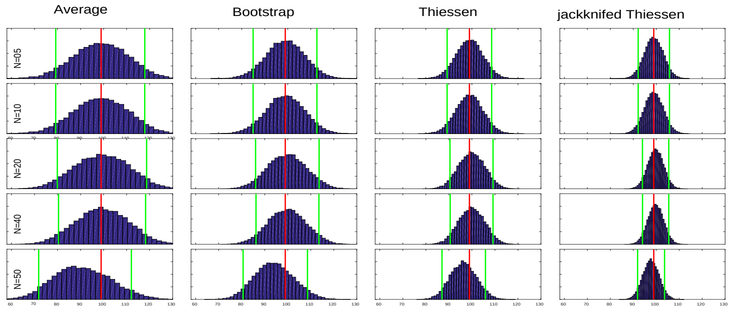

Figure 5. Results of the Monte Carlo Simulation for the Morrison III function. In red we denote the true value (identical for all the plots) and in green the experimental percentiles at 5 and 95%. The x-axes range is the same for all the plots.
Source: Own elaboration.

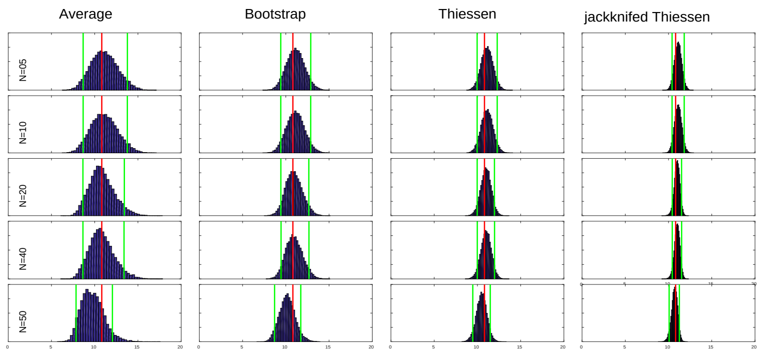

Figure 6. Results of the Monte Carlo Simulation for mean areal rain value of the region described at Figure 2. In red we denote the true value (identical for all the plots) and in green the experimental percentiles at 5 and 95%. The x-axes range is the same for all the plots. Source: Own elaboration.

Despite the results, the already presented figures were not conclusive to answer the question "*it is worth the effort to code Thiessen or any of its flavors instead of simpler alternatives?*" because we have used histograms thus loosing information within each event. For this purpose it is fit to use the Friedman's Test. In Table we can compare the ranking among the four methods for the three analytical cases and as a function of N. The value of "1" denotes the best while the value of "4" denotes the worst. If statistically we were unable to discern that one method is better than other it is denoted as a tie; see for example the case of the Morrison III function for the case of N=40, which has a tie between the third and fourth method. If, as the research question states, the comparison was between the simple average and the Thiessen methods, the conclusion is that for all the considered functions (except for Morrison III) the Thiessen alternative is always better. For the Morrison III function such precedence fails for low N (N=5, 10 o 20), while for larger N the Thiessen over performs the simple average.

The performance of the *jackknifed* Thiessen was completely unexpected. It was almost always the best option, except when N was too low, and was the second option for the rain case and just for N=10. In such case it is likely that the result has weak statistical consequences because of the small problem size. The *bootstrap* was no better but comparable to the simple average. However, its main advantage w.r.t. the simple average is that it is capable of producing a CI, even in practical situations, thus making highly recommendable as an alternative. The estimate of a CI is an advantage also offered by the *jackknifed* Thiessen.

Table 1
Results of the Friedman's Test for the three analytic functions considered. The ranking was built after considering all 20000 events, and the test was applied with a 95% confidence level

N	x^2y				*sen(x)*sen(3y)*				*Morrison III*				*Rain*			
5	3	4	1	2	3	4	1	2	2	3	4	1	3	4	2	1
10	3	4	1	2	3	4	2	1	2	3	4	1	3	4	1	2
20	3	4	2	1	3	4	2	1	2	2	4	1	3	3	1	2
40	3	4	2	1	3	4	2	1	3	3	2	1	3	4	1	2
50	3	4	2	1	3	4	2	1	3	4	2	1	3	4	1	2

Source: Own elaboration.

Conclusions

From the analysis of the Monte Carlo Simulation based upon the histograms and the Friedman's Test results it can be concluded that for all the studied functions (with the exception of the Morrison III for small N) the standard Thiessen's method offers systematically a better estimate than the arithmetic mean and its variant the *bootstrap*. After the simulations performed, such results might be stated with a confidence level of 95%, and according to the literature review such conclusion is an original one. The Morrison III function follows the same rule but only if N is larger than 40. An explanation for such behavior is the large variability of the surface in the interval. With a small N value simply the Thiessen method cannot catch such fluctuations.

In turn, the newly proposed *jackknifed* Thiessen was even better than the standard Thiessen for the analytical cases. Such improvement comes at the price of extra computing time, which is more significative when N grows. For the analytical cases the computing time was 1.3x for N=5, 2.8x for N=10 and 4x with N=20. Considering the increased computing time it is worth to ask if it can be justified in practice. One advantage of the *jackknifed* Thiessen procedure is that it also produced a CI. Due to the inherent parallel nature of the simulations it might be explored to perform this computation in a parallel environment like the GPU.

For the analyzed functions the *bootstrap* is in many cases comparable to the mere average. But, as in the case of the *jackknifed* Thiessen, this method offers a CI. Beyond our own results, *bootstrap* is a known and widely tested method for its accuracy, performance, and simplicity to code, and thus is a very practical alternative if a CI is required.

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