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HAL Authorization

1 **Analysis of extreme values of soil ecosystem services predicted from associated soil**
2 **properties and weather conditions**

3 Short running title: *Extreme value analysis of soil ecosystem services*

4 Tristan Senga Kiessé^{1,*}, Blandine Lemerrier¹, Michael S. Corson¹, Yosra Ellili-Bargaoui²,
5 Christian Walter¹

6 ¹UMR SAS, INRAE, Institut Agro, F-35000 Rennes, France

7 ²Interact, UniLaSalle, F-60000 Beauvais, France

8 *corresponding author: tristan.senga-kiesse@inrae.fr. ORCID iD: [0000-0003-2710-5825](https://orcid.org/0000-0003-2710-5825)

9 **Abstract**

10 Soils provide services that can increase food security and mitigate global warming. Simulation
11 modeling of biophysical processes is one approach used to estimate values of soil ecosystem
12 services (SES) based on soil properties and climate conditions. The SES are usually investigated
13 using statistical approaches that assume that values of SES are normally distributed. This
14 assumption, however, ignores atypical values of SES, which deviate strongly from average
15 values. Classic approaches have therefore failed to identify such atypical values of SES. To
16 address this issue, we applied extreme value theory (EVT) as a statistical tool to identify
17 thresholds above which SES can be considered as “extreme”. EVT was applied to a dataset of
18 four SES – climate regulation, groundwater recharge, water-to-plant provision and plant
19 biomass provision – estimated by biophysical soil and crop modeling based on a dataset of 64
20 cultivated soils located in northwestern France under a single climate observed over 30 years
21 (1988-2018) and a single crop management of a maize and wheat rotation. Extreme values of
22 the SES considered in our study were identified, and soil properties associated with these values
23 were characterized. For instance, soils with extreme minimum values of climate regulation
24 service had the highest pH, clay and organic carbon contents and maximum rooting depth.
25 Applying EVT also enabled identification of the “return period”, which is the amount of time
26 after which an extreme value of SES is likely to occur again. For instance, under the maize and
27 wheat rotation simulated and weather conditions equivalent to those from 1988-2018, storage
28 of organic carbon in the soil of 1000 kg C ha⁻¹ year⁻¹ is expected to be exceeded by at least one
29 of the 64 of soils once every 2 years. This approach can thus be useful for decision making in

30 natural resource management by identifying atypical values of SES and predicting how
31 frequently they may occur.

32 **Keywords:** biophysical process, crop model, extreme ecosystem services, return period

33 **Highlights**

- 34 • Extreme value theory identified soils with extreme values of ecosystem services (SES)
- 35 • Some soil properties differed significantly among samples of extreme values of SES
- 36 • Soils in extreme samples of SES were identified as a function of their parent material
- 37 • The mean extreme maxima of the SES were expected to be exceeded every 2 years

38

39 **1. Introduction**

40 Ecosystem services (ES) represent the contribution of ecosystem structure and function to
41 human wellbeing (Burkhard et al., 2012). ES are also a tool for policy and decision making at
42 global, national, regional and local levels about sustainable management of natural resources,
43 environmental protection, nature conservation and restoration, territorial and landscape
44 planning, nature-based solutions, climate-change mitigation, disaster risk reduction, education
45 and research (Braat and De Groot, 2012; Fossey et al., 2020).

46 In general, ES are quantified biophysically using indicators (Hauck et al., 2016). Soil ecosystem
47 services (SES) are assessed from soil properties and climate data as a function of soil cover
48 (e.g., crops, pastures, forests) and/or soil management (e.g., fertilization, tillage). Regardless of
49 the approach considered (e.g., dynamic soil-plant modeling, proxies), nearly all existing ES
50 assessment studies consider only means and standard deviations of input data, and also assume
51 that estimated values of SES are normally distributed. Examples include specific studies from
52 national/international programs of SES mapping, such as the EnviroAtlas in the United States,
53 (Cochran et al., 2020), MAES in Europe (Maes et al., 2018) and EFES-EA in France (Therond
54 et al., 2017).

55 Combinations of certain soil properties and weather conditions may result in atypical values of
56 SES depending on the soil cover and/or soil management. Modeling soil processes is generally
57 useful to estimate biophysical indicators of SES, particularly those that are difficult to measure
58 in the field, in order to predict how their values may vary over time. Atypical or extreme
59 conditions are rarely considered when assessing SES, or more generally in soil science, unlike

60 in disciplines such as hydrology, in which extreme data (e.g., floods) are a focus of study
61 because of the associated risks (Ramesh and Davison, 2002). One reason for this lack of
62 research could be the perception of soil as a buffered medium that evolves only slowly. Another
63 reason may be the lack of appropriate methods to identify thresholds above which SES and the
64 associated soil properties may be considered as atypical.

65 Extreme value theory (EVT) was initially developed to study flood levels and is now applied
66 to other fields, such as finance, meteorological events and environmental sciences. For instance,
67 EVT was applied to examine trends in hydrological extremes due to the anticipated
68 intensification in the hydrological cycle caused by climate change (Katz et al., 2002). Likewise,
69 EVT was applied in medical research to model hospitalization and death peaks due to
70 cardiovascular disease in Canada (Chiu et al., 2018) and to analyze atypical forage-related
71 characteristics of dairy farms (Senga Kiessé et al., 2020). EVT provides a framework to
72 rigorously test and identify extreme values and suitable probability distribution functions (pdfs)
73 to model the tails of distributions. EVT has rarely been applied to soil data, except to analyze
74 the influence of soil water content on extreme temperatures (Whan et al., 2015) or droughts
75 (Burke et al., 2010). To our knowledge, it has not been used to assess SES.

76 The aims of the present study were to (1) investigate uncommon, atypical levels (i.e. extreme
77 values) of SES and their return periods and (2) identify soil properties (i.e. pH, soil organic
78 carbon (SOC) content, clay content, maximum rooting depth) associated with them, based on a
79 dataset of soils in eastern Brittany (northwestern France). Soils identified in samples of extreme
80 values of SES were also compared to each other according to other characteristics, such as their
81 parent material and natural drainage class.

82 **2. Materials and Methods**

83 The soil dataset was previously studied by Ellili-Bargaoui et al. (2019) and used as input data
84 in the STICS soil-crop model to predict values of six SES (Ellili-Bargaoui et al., 2021), four of
85 which were used in the present study. We briefly describe the dataset, model and SES assessed
86 (see the studies of Ellili-Bargaoui et al. for more details).

87 **2.1. Dataset**

88 The soil dataset contained data from 64 sites of cultivated land extracted from a larger dataset
89 of 135 sites throughout the department of Ille-et-Vilaine, which is located in eastern Brittany
90 (northwestern France) and covers 6775 km². The 135 sites were selected in a two-step approach.

91 First, 45 locations were identified following a random sampling design stratified according to
 92 soil parent material (Table S1), which was derived from an existing 1:250,000 soil map (Le
 93 Bris et al., 2013). Second, for each of the 45 locations, the corresponding topographic transect
 94 was defined, and a sampling location was positioned in upslope, mid-slope and downslope
 95 sections. Values of SES were predicted for the 64 cultivated sites.

96 Soil samples were collected at all sites at 6 depth intervals within the limit of total soil depth
 97 according to *GlobalSoilMap* specifications (Arrouays et al., 2014): 0-5, 5-15, 15-30, 30-60, 60-
 98 100 and 100-200 cm. Physico-chemical analyses of the 5-15, 30-60 and 100-200 cm samples
 99 were performed to measure properties such as SOC content by dry combustion, pH 1:5 H₂O
 100 (soil pH in water with 1:5 soil-to-water ratio, NF ISO 10390), soil total N content (NF ISO
 101 13878), cation exchange capacity (NF X 31-130), total carbonate content (NF ISO 10693) and
 102 particle size distribution in five classes (NF X 31-107). For the present study, we focused on
 103 the influence of 4 soil properties – pH, clay content and SOC content in the 5-15 cm layer and
 104 maximum rooting depth – of the 64 soil profiles on SES (Table 1). By considering physical
 105 obstacles to root penetration, maximum rooting depth was shallower than total soil depth.

106 Table 1. Descriptive statistics of pH, clay content and organic carbon content in the 5-15 cm
 107 layer and maximum rooting depth of the 64 cultivated soil profiles (Ellili-Bargaoui et al., 2019).

Property	Minimum	Mean	Maximum	Standard deviation
Soil pH	4.1	6.6	8.8	0.9
Clay content (%)	11.8	21.3	55.9	9.0
Organic carbon content (g kg ⁻¹)	9.8	19.1	45.4	7.0
Maximum rooting depth (cm)	30.0	74.6	100.0	25.0

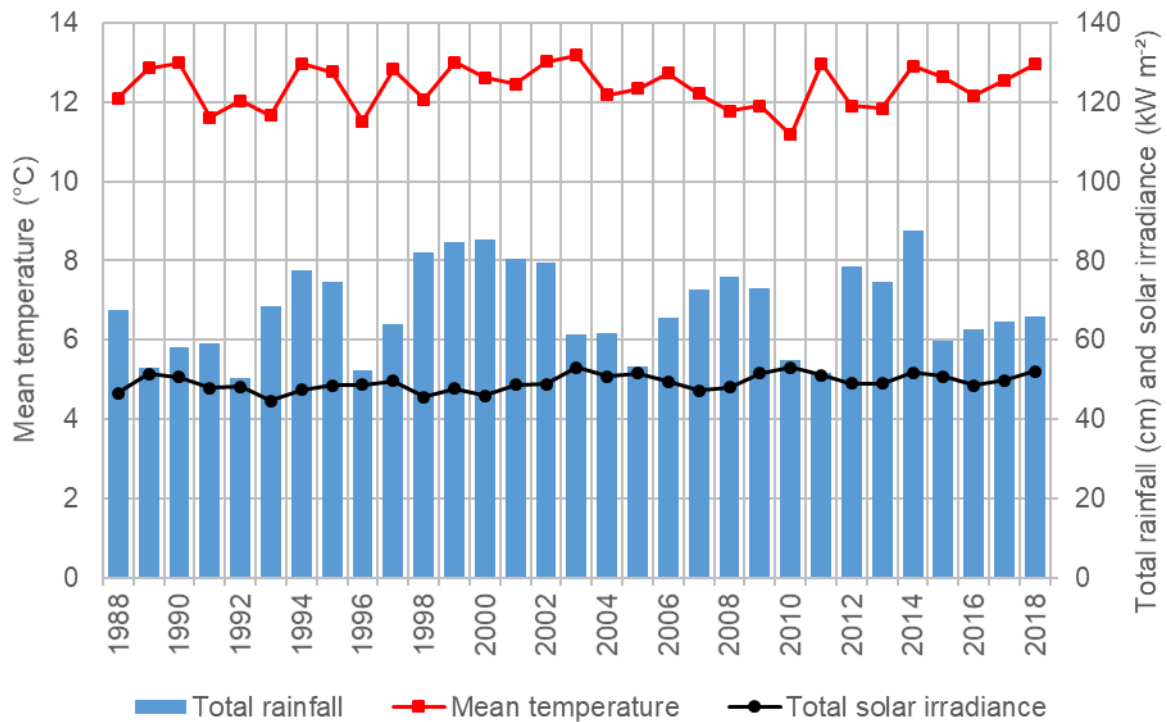
108

109 Soil characteristics (i.e. depth, type, natural drainage class and parent material) were defined
 110 according to the French soil classification (Baize and Girard, 2009). For instance, drainage class
 111 was classified as well drained (0), moderately drained (1) or poorly drained (2). Likewise, the
 112 soil parent material was gneiss (1 of 64 soil profiles), alluvial deposits (1), medium schist (3),
 113 continental alluvium (3), granite (4), sandstone (4), gritty schist (5), alluvial terrace (7), aeolian
 114 loam (9), alluvial marsh (11), soft schist (16).

115 The climate of the department of Ille-et-Vilaine is temperate oceanic. Weather
 116 conditions were assumed to be the same throughout the study area and at all sites. Weather data
 117 came from the weather station of Rennes-St Jacques, located near the center of the study area.
 118 Data such as daily rainfall (mm), air temperature (°C) and solar radiation (kW m⁻²) were

119 collected (Figure 1). The crop-management dataset reflected the main conventional crop
120 rotation used by farmers in the study area: a 2-year rotation of silage maize, wheat and a catch
121 crop.

122



123

124 Figure 1. Total annual rainfall (mm), mean annual temperature (°C) and total annual solar
125 irradiance (kW m⁻²) near the center of the study area from 1988-2018 (adapted from Ellili-
126 Bargaoui et al. (2021))

127

128 2.2. STICS soil crop-model

129 The STICS soil-crop model (version 9.0) (Brisson et al., 2009) was used to simulate crop
130 development and soil processes that connect water, N and carbon (C) dynamics in the soil-
131 plant-atmosphere continuum. STICS is a one-dimensional mechanistic model with a daily time
132 step that can run multi-year simulations. The soil is considered as a succession of up to five
133 horizontal layers that form interdependent compartments. Input parameters came from the crop
134 management, soil and weather databases.

135 During the simulated study period, all soil characteristics remained static except SOC, N and
136 water content, since they were influenced by crop development and weather conditions. The
137 three crops in the rotation were simulated sequentially: maize (10 Apr-30 Oct), wheat (1 Nov-
138 31 Jul), and a catch crop of white mustard (5 Sep-3 Mar). STICS was used to simulate the 64
139 sites for 30 agricultural years (1988-2018) with the aid of a Java package developed to automate
140 simulations.

141 STICS provided more than 200 outputs, from which 4 outputs were selected to calculate the 4
142 SES indicators: crop transpiration, crop yield, water drainage and SOC in humified organic
143 matter. Previous studies (e.g., Brisson et al. (2002); Schnebelen et al. (2004); Constantin et al.
144 (2012); Constantin et al. (2015)) have evaluated the accuracy with which STICS predicted some
145 of these outputs (including atypical values) for a variety of field and cover crops. A review of
146 studies that used STICS to simulate 15 field crops at a total of 76 sites in France (Coucheney et
147 al., 2015) found that its accuracy was “very good” for whole-profile soil water content (mean
148 relative root mean square error (rRMSE) = 10%) and “good” for plant fruit biomass at harvest
149 (i.e. yield) (mean rRMSE = 33%). They concluded that STICS had sufficient accuracy and
150 robustness for large-scale use under the soil and climate conditions in France. In addition, SOC
151 predictions for seven long-term field experiments in Europe using the AMG model (Andriulo
152 et al., 1999), on which STICS bases its simulation of C dynamics, were considered sufficiently
153 accurate (rRMSE = 28%) (Levavasseur et al., 2020). We expected that by simulating the same
154 crop rotation and weather for all 64 soil profiles, STICS would be able to predict relative
155 differences among the profiles with high accuracy for each of the 4 SES studied.

156 Since a succession of field interventions was simulated every year on the same dates over the
157 study period and for each soil profile, sources of variation when predicting SES corresponded
158 to differences in weather conditions among years and to soil properties among sites. Overall,
159 the soil-property/SES dataset contained 256 variables for soil properties (4 properties (pH, clay
160 content and organic carbon content in the 5-15 cm layer and maximum rooting depth) \times 64
161 profiles) and 7680 variables for SES (4 SES \times 64 profiles \times 30 years of simulation).

162

163 2.3. Soil ecosystem services

164 Four SES were studied: the regulating SES of climate regulation and groundwater recharge,
165 and the provisioning SES of water-to-plant provision and plant biomass provision. Using
166 STICS outputs, the value of each SES was estimated for each calendar year simulated.

167 a. *Climate regulation* was estimated through C sequestration (CS), which represented the
168 amount of organic C that the soil was able to store at a given site. CS was quantified as the
169 annual change in the stock of SOC in the topsoil (0-30 cm deep):

$$CS_j = CStock_j - CStock_{j-1} \quad \text{Equation 1}$$

170 where $CStock_j$ is the SOC stock in the topsoil in year j . $CStock_j$ was calculated from the
171 soil organic nitrogen (N) content (N_{org} , %), the C:N ratio of organic matter (CN, unitless),
172 bulk density (BD, $g\ cm^{-3}$) and coarse-fragment content (CF, % by volume):

$$CStock = N_{org} \times CN \times BD \times \left(1 - \frac{CF}{100}\right) \times 100 \quad \text{Equation 2}$$

173 $CStock$ at the beginning of the simulation was initialized from the field data measured at each
174 site, and its dynamics were predicted by STICS, based on equations of the AMG model, in
175 which the total SOC stock equals the sum of an active and an inert compartment of SOC.

176

177 b. *Groundwater recharge* (GW) corresponds to the amount of water that infiltrates into the
178 soil and percolates into the groundwater. GW was quantified as the annual sum of the water
179 drained daily through the soil, which was assumed to reach the groundwater:

$$GW_j = \sum_{i=1}^{365} D_i \quad \text{Equation 3}$$

180 where i is the day of year (1-365) and D_i is the amount of water drained daily from the soil
181 (mm).

182 c. *Water-to-plant provision* (WP) describes the amount of water that the soil can retain and
183 deliver to plants for their growth without irrigation. WP depends mainly on the soil's
184 available water capacity estimated up to the maximum rooting depth, total rainfall and crop
185 phenological stage. The indicator chosen was developed by (Therond et al., 2017) as

186 transpiration of a cash crop from planting to harvest. Thus, to calculate total transpiration
 187 per calendar year, daily transpiration of maize and/or wheat in the rotation was summed for
 188 the first (Equation 4) or second (Equation 5) year of each 2-year rotation.

$$WP_j = \sum_{i=100}^{303 \text{ (maize harvest)}} E_i + \sum_{k=305}^{365 \text{ (wheat sowing)}} E_k \quad \text{Equation 4}$$

$$WP_j = \sum_{k=1}^{212 \text{ (wheat harvest)}} E_k \quad \text{Equation 5}$$

189 where i and k are the day of year, and E_i and E_k are daily maize and wheat transpiration,
 190 respectively.

191 d. *Plant biomass provision* (YE) represents the soil's ability to produce plant biomass by
 192 photosynthesis. YE equals the annual yields of cash crops expressed as a unit of energy (GJ
 193 $\text{ha}^{-1} \text{ year}^{-1}$):

$$YE_j = \frac{1}{n} \sum_{i=1}^n B_i * k \quad \text{Equation 6}$$

194 where B_i is the dry matter of harvested biomass, and k is the energy content of biomass: 13.984
 195 and 13.356 kJ g^{-1} for maize and wheat, respectively (Roy et al., 2005).

196

197 **2.4. Extreme value theory**

198 EVT enables identification of pdfs of a sequence of independent and identically distributed (iid)
 199 random variables (rv) X_1, X_2, \dots, X_n that are characterized by extreme variation (Embrechts et
 200 al., 1996). The fundamental result of EVT is that limit laws for the (normalized and centered)
 201 maximum Z_n of the iid inputs X_1, X_2, \dots, X_n belong to asymptotic pdfs of type Fréchet, Weibull
 202 or Gumbel. A maximum sequence of inputs can be extracted by applying EVT to a dataset, and
 203 then appropriate pdfs (such as the generalized Pareto distribution (GPD)) can be used to fit this
 204 sequence (Coles, 2001). Likewise, EVT also enable one to extract a minimum sequence and
 205 then fit it using extreme value distributions.

206 **2.4.1. Generalized Pareto distribution and threshold selection**

207 The distribution function $P(X \leq x|X > \mu)$ of excesses above a threshold μ , extracted from
208 observations x of the rv X , can be approximated by a GPD function defined by the empirical
209 distribution function

$$G(x|\mu, \sigma, \varepsilon) = 1 - \left[1 + \varepsilon \left(\frac{x - \mu}{\sigma}\right)\right]^{-1/\varepsilon} := G_{\mu, \theta}(x) \quad \text{Equation 7}$$

210 for parameter $\theta=(\sigma, \varepsilon)$ such that $\varepsilon \neq 0$ and $1 + \varepsilon \left(\frac{x - \mu}{\sigma}\right) > 0$. The parameters $\sigma > 0$ and ε are
211 the scale and shape, respectively (Beirlant et al., 2004). GPD also enables one to approximate
212 distribution functions of values below another fixed threshold μ extracted from observations x
213 of the rv X .

214 To select the threshold μ , several minimum and maximum extreme quantiles were tested and
215 then used to calculate the corresponding values of μ (Senga Kiessé et al., 2020). A compromise
216 is required between selecting too-small values of μ , which increases the sample size of extremes
217 and the bias of estimated parameters, and too-large values of μ , which decreases the sample
218 size of extremes and increase the variance in estimated parameters. Finally, μ must be
219 sufficiently large to ensure that the GPD is a reliable model (Scarrott and MacDonald, 2012).

220 In the present study, five quantiles of the soil-property/SES dataset were tested to extract
221 minimum extreme samples (1.0%, 2.5%, 5.0%, 7.5% and 10.0%) of each SES over time (30
222 years) and five were tested to extract maximum extreme samples (90.0%, 92.5%, 95.0%, 97.5%
223 and 99.0%) of each SES over time.

224 **2.4.2. Statistical tests and root mean squared error**

225 The adequacy with which the GPD represented the distribution of each extracted sample was
226 tested using the Kolmogorov-Smirnov (K-S) test (null hypothesis H_0 : “the extracted sample
227 followed the GPD”). Likewise, stationarity and independence of each extracted sample were
228 tested using Mann-Kendall (M-K) and Wald-Wolfowitz (W-W) tests, respectively, to verify
229 whether the sample had no trend (i.e. constant mean and variance) and was independent,
230 respectively (three H_0). Differences in mean soil properties between the minimum and
231 maximum samples of SES were also tested by performing the Mann-Whitney (M-W) U test
232 (H_0 : “soil properties in the minimum and maximum samples of SES followed the same
233 distribution”). For all statistical tests, H_0 was rejected at $p < 0.05$. For each quantile tested, the

234 extracted sample was also compared to the fitted GPD using the root mean squared error
235 (RMSE). We used the “evd” (Stephenson, 2002) and “extremefit” (Durrieu et al., 2017)
236 packages of R software (R Core Team, 2020) to apply EVT.

237 **2.4.3. Return period**

238 EVT also enabled calculation of “return periods” of extracted extremes. A “return period” T is
239 the mean time after which a value is expected to exceed a threshold μ again (Salvadori et al.,
240 2011) such that

$$T(p) = \frac{1}{1-p} \geq 1 \quad \text{Equation 7}$$

241 which is related to the quantile $p = G_{\mu,\theta}(x)$ of the GPD (Equation 7). The return period T is
242 associated with a “return level” (i.e. the threshold that is expected to be exceeded), which is
243 obtained by inverting equation $p = G_{\mu,\theta}(x)$. Return levels were plotted as a function of return
244 periods (in years) by plotting the points $[T(p), G_{\mu,\theta}^{-1}(p)]$. The threshold μ represents the return
245 level that is expected to be exceeded on average once a year, which corresponds to points with
246 coordinates $(\mu, 1)$. For each SES, a return period was estimated for exceeding a return level
247 equal to the mean of the maximum sample (for GW and YE) or to the mean rounded down to a
248 whole number (for CS and WP), assuming stationarity and independence of the sample and
249 weather conditions equivalent to those from 1988-2018. The uncertainty in both return periods
250 and return levels was estimated by calculating their 95% confidence intervals, and was also
251 studied by increasing the return level set for each SES by 5% and recalculating the return period
252 for exceeding it.

253

254 **3. Results**

255 **3.1. Identification of extreme values of SES**

256 We present results from applying EVT to the 1920 values for each SES (64 profiles \times 30 years)
257 in the soil-property/SES dataset to identify thresholds above or under which the SES could be
258 considered as extremely high or low, respectively.

259 **3.1.1. Climate regulation**

260 When applying EVT to CS data, the K-S test did not reject the H_0 of the adequacy of the GPD
261 for any of the extracted samples considered. However, M-K and W-W did sometimes reject the

262 H_0 of no trend and of independence, respectively, of the extracted samples, depending on the
 263 quantiles tested. For the minimum sample (CS_{MIN}), the 2.5% quantile (Min_{CS} threshold = -664
 264 kg C ha⁻¹ year⁻¹, n = 49) was selected (Table 2, Figure 2 and Supplementary Figure S1). This
 265 quantile did not have the smallest RMSE, but its K-S and W-W tests did not reject H_0 , and the
 266 p-value of its M-K test was 0.03, close to the non-rejection threshold of 0.05. For the maximum
 267 sample (CS_{MAX}), several thresholds could have been chosen. The 99.0% quantile selected
 268 (Max_{CS} threshold = 864 kg C ha⁻¹ year⁻¹, n = 24) did not reject the H_0 of the three tests (although
 269 it did not have the largest p-values) and had the smallest RMSE. Minimum, mean and maximum
 270 values of CS were -1828, 126 and 1279 kg C ha⁻¹ year⁻¹, respectively, compared to the mean
 271 and maximum of CS_{MIN} (-937 and -665 kg C ha⁻¹ year⁻¹, respectively) and the minimum and
 272 mean of CS_{MAX} (870 and 1032 kg C ha⁻¹ year⁻¹, respectively) (Table S2).

273

274 Table 2. Results of applying extreme value theory to extract minimum (MIN) and maximum
 275 (MAX) samples of the indicator of climate regulation (CS) (kg C ha⁻¹ year⁻¹) as a function of
 276 six of the quantiles tested of the entire dataset of soil ecosystem services in Brittany (France).
 277 Bold values are associated with the quantiles retained as thresholds. RMSE = root mean squared
 278 error, K-S = Kolmogorov-Smirnov, M-K=Mann-Kendall, W-W=Wald-Wolfowitz.

Sample	Quantile	Threshold CS	Sample size	Estimated shape $\hat{\epsilon}$	Estimated scale $\hat{\sigma}$	RMSE	Statistical test (p-value)		
							K-S	M-K	W-W
MIN	1.0%	-935	19	-0.12	292	375	0.75	0.007	0.01
	2.5%	-664	49	-0.006	277	391	0.99	0.03	0.31
	5.0%	-495	99	0.040	252	374	0.87	<0.001	0.10
MAX	95.0%	611	95	-0.07	180	235	0.68	0.16	<0.001
	97.5%	709	49	-0.41	263	241	0.22	0.55	<0.001
	99.0%	864	24	-0.41	196	194	0.23	0.22	0.73

279

280 3.1.2. Groundwater recharge

281 The 2.5% quantile (Min_{GW} threshold = 8 mm year⁻¹, n = 49) and 97.5% quantile (Max_{GW}
 282 threshold = 403 mm year⁻¹, n = 24) of GW data were selected (Table 3, Figure 2 and Figure
 283 S1). The former had the smallest RMSE among GW_{MIN} samples, and the latter did not reject
 284 the H_0 of K-S, M-K or W-W tests among the GW_{MAX} samples. However, the quantiles selected
 285 did not have the largest p-values of the three statistical tests. Other choices of thresholds were
 286 also possible, such as the 95.0% and 97.5% quantiles for the GW_{MAX} sample, which did not

287 reject the H_0 of the three statistical tests. Minimum, mean and maximum values of GW were 0,
 288 182 and 451 mm year⁻¹, respectively, compared to the mean and maximum of GW_{MIN} (2 and 8
 289 mm year⁻¹, respectively) and the minimum and mean of GW_{MAX} (404 and 420 mm year⁻¹,
 290 respectively) (Table S2).

291

292 Table 3. Results of applying extreme value theory to extract minimum (MIN) and maximum
 293 (MAX) samples of indicator of groundwater recharge (GW) (mm year⁻¹) as a function of six of
 294 the quantiles tested of the entire dataset of soil ecosystem services in Brittany (France). Bold
 295 values are associated with the quantiles retained as thresholds. RMSE = root mean squared
 296 error, K-S = Kolmogorov-Smirnov, M-K=Mann-Kendall, W-W=Wald-Wolfowitz.

Sample	Quantile	Threshold GW (mm year ⁻¹)	Sample size	Estimated shape $\hat{\epsilon}$	Estimated scale $\hat{\sigma}$	RMSE	Statistical test (p-value)		
							K-S	M-K	W-W
MIN	1.0%	0	28	--	--	--	--	--	--
	2.5%	8	49	-1.03	8	7	0.25	0.90	0.19
	5.0%	20	99	-1.30	26	13	<0.001	0.59	0.65
MAX	95.0%	352	95	-0.49	51	42	0.58	0.90	0.35
	97.5%	384	49	-0.36	29	28	0.88	0.67	0.87
	99.0%	403	24	-0.43	24	21	0.86	0.50	0.47

297

298 3.1.3. Water-to-plant provision

299 The 1.0% quantile (Min_{WP} threshold = 81 mm year⁻¹, n = 19) and 99.0% quantile (Max_{WP}
 300 threshold = 396 mm year⁻¹, n = 50) of WP data were selected (Table 4, Figure 2 and Figure S1).
 301 For the WP_{MAX} sample, the statistical tests did not reject the H_0 for the 92.5%, 95.0% and 97.5%
 302 quantiles tested, but the 99.0% quantile selected had the smallest RMSE. For the WP_{MIN} sample,
 303 the 1.0% quantile selected had the largest p-value for the three statistical tests, but the p-value
 304 of 0.02 of its W-W test rejected the H_0 of independence, while the RMSE of the other quantiles
 305 tested were similar. Minimum, mean and maximum values of WP were 7, 212 and 464 mm
 306 year⁻¹, respectively, compared to the mean and maximum of WP_{MIN} (59 and 81 mm year⁻¹,
 307 respectively) and the minimum and mean of WP_{MAX} (398 and 424 mm year⁻¹, respectively)
 308 (Table S2).

309 Table 4. Results of applying extreme value theory to extract minimum (MIN) and maximum
 310 (MAX) samples of indicator of water-to-plant provision (WP) (mm year⁻¹) as a function of six
 311 of the quantiles tested of the entire dataset of soil ecosystem services in Brittany (France). Bold
 312 values are associated with the quantiles retained as thresholds. RMSE = root mean squared
 313 error, K-S = Kolmogorov-Smirnov, M-K=Mann-Kendall, W-W=Wald-Wolfowitz.

Sample	Quantile	Threshold WP (mm year ⁻¹)	Sample size	Estimated shape $\hat{\epsilon}$	Estimated scale $\hat{\sigma}$	RMSE	Statistical test (p-value)		
							K-S	M-K	W-W
MIN	1.0%	81	19	0.37	14	32	0.70	0.20	0.02
	2.5%	93	49	0.26	12	26	0.58	0.04	<0.001
	5.0%	105	99	0.04	17	25	0.23	<0.001	<0.001
MAX	95.0%	342	99	-0.24	43	45	0.28	0.28	0.33
	97.5%	369	50	-0.34	41	39	0.54	0.88	0.27
	99.0%	396	22	-0.63	45	33	0.97	0.65	0.97

314

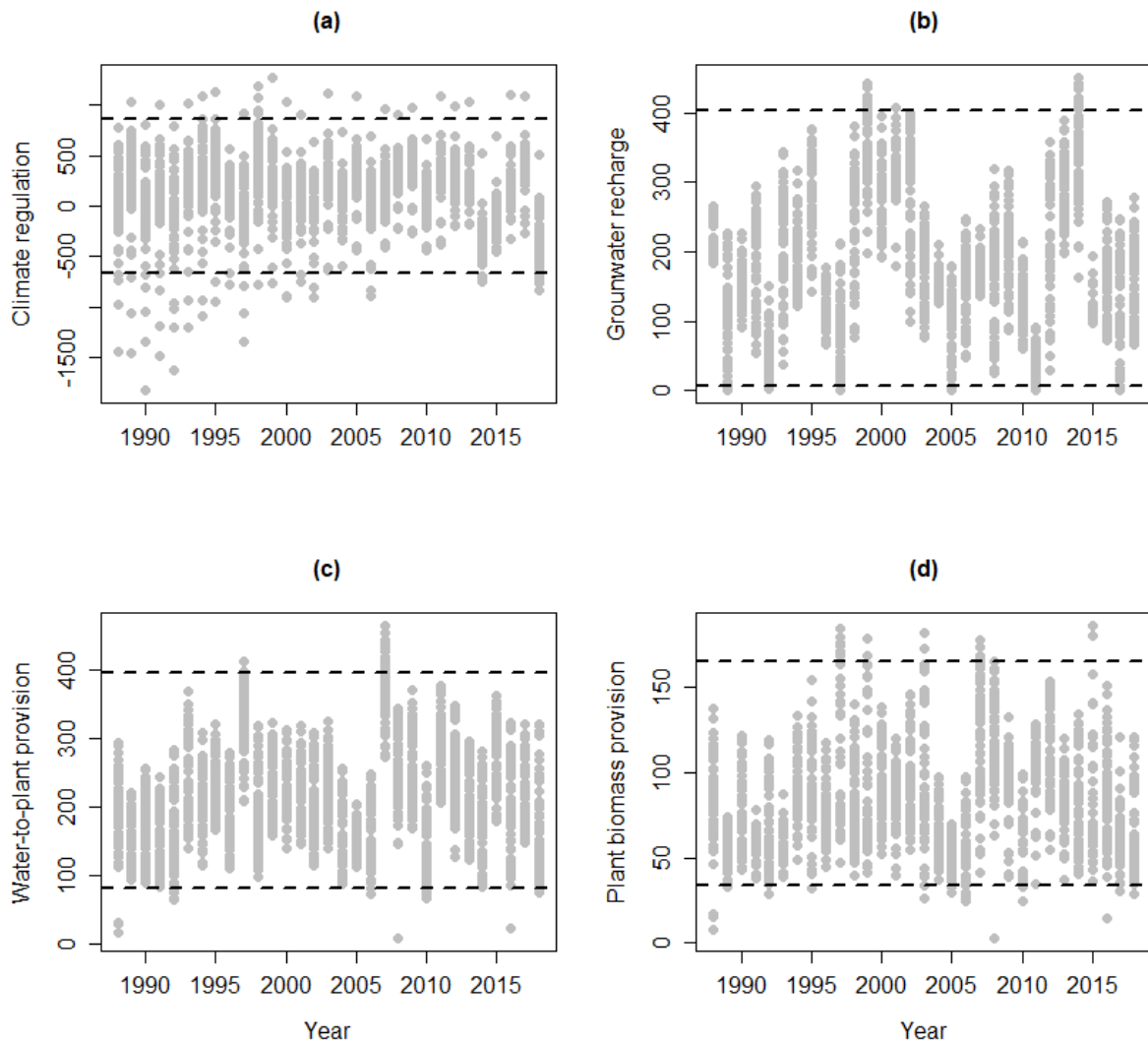
315 3.1.4. Plant biomass provision

316 The 1.0% quantile (Min_{YE} threshold = 34 GJ ha⁻¹ year⁻¹, n = 19) and 99.0% quantile (Max_{YE}
 317 threshold = 166 GJ ha⁻¹ year⁻¹, n = 21) of YE data were selected (Table 5, Figure 2 and Figure
 318 S1). Both quantiles selected did not reject the H₀ of the three statistical tests. The 99.0% quantile
 319 selected for the Max_{YE} sample had the smallest RMSE. Minimum, mean and maximum values
 320 of YE were 2, 82 and 187 GJ ha⁻¹ year⁻¹, respectively, compared to the mean and maximum of
 321 YE_{MIN} (25 and 34 GJ ha⁻¹ year⁻¹, respectively) and the minimum and mean of YE_{MAX} (166 and
 322 175 GJ ha⁻¹ year⁻¹, respectively) (Table S2).

323 Table 5. Results of applying extreme value theory to extract minimum (MIN) and maximum
 324 (MAX) samples of indicator of plant biomass provision (YE) ($\text{GJ ha}^{-1} \text{ year}^{-1}$) as a function of
 325 six of the quantiles tested of the entire dataset of soil ecosystem services in Brittany (France).
 326 Bold values are associated with the quantiles retained as thresholds. RMSE = root mean squared
 327 error, K-S = Kolmogorov-Smirnov M-K=Mann-Kendall, W-W=Wald-Wolfowitz.

Sample	Quantile	Threshold YE $\text{GJ ha}^{-1} \text{ year}^{-1}$	Sample size	Estimated shape $\hat{\epsilon}$	Estimated scale $\hat{\sigma}$	RMSE	Statistical test (p-value)		
							K-S	M-K	W-W
MIN	1.0%	34	19	-0.002	21	13	0.80	0.23	0.05
	2.5%	34	23	0.08	19	12	0.25	0.08	0.03
	5.0%	37	99	0.07	11	7	0.86	0.01	<0.001
MAX	95.0%	141	97	-0.17	37	19	<0.001	0.97	0.81
	97.5%	153	47	-0.25	32	16	0.02	0.97	0.54
	99.0%	166	21	-0.30	22	11	0.20	0.19	0.20

328



330
 331 Figure 2. Indicators of the soil ecosystem services (a) climate regulation ($\text{kg C ha}^{-1} \text{ year}^{-1}$), (b)
 332 groundwater recharge (mm year^{-1}), (c) water-to-plant provision (mm year^{-1}) and (d) plant
 333 biomass provision ($\text{GJ ha}^{-1} \text{ year}^{-1}$) estimated from soil profiles in the dataset of 64 observation
 334 sites in Brittany (France) from 1988-2018 (dashed lines indicate the minimum and maximum
 335 thresholds selected)

336

337 3.2. Differences in soil properties between minimum and maximum extreme samples 338 of SES

339 3.2.1. Extreme samples of climate regulation

340 Soils in the maximum sample of CS (CS_{MAX}) had lower mean pH (-46%) than those in the
 341 minimum sample (CS_{MIN}). This difference in pH was significant according to the M-W test

342 (Table 6 and Figure 3). Likewise, soils in CS_{MAX} had mean clay content, SOC content and
343 maximum rooting depth significantly lower (-61%, -52% and -21%, respectively) than soils in
344 CS_{MIN}. The parent material of soils in CS_{MAX} (i.e. soft schists) also differed from that in CS_{MIN}
345 (i.e. marsh) (Figure S2). Based on the 30 years of simulated weather conditions, soils in CS_{MAX}
346 were moderately drained during the study period, while those in CS_{MIN} were poorly drained.
347 The CS value of at least one soil exceeded the maximum threshold frequently (i.e., every 1-2
348 years) from 1988-2018, while it fell below the minimum threshold as frequently, but for more
349 soils, and only until 2002 (Figure 2a).

350 **3.2.2. Extreme samples of groundwater recharge**

351 All soil properties differed significantly between maximum (GW_{MAX}) and minimum (GW_{MIN})
352 samples of GW (M-W test) (Table 6). Soils in GW_{MAX} had significantly lower mean pH (-14%)
353 and maximum rooting depth (-61%), but significantly higher mean clay content (+11%) and
354 SOC content (+42%), than those in GW_{MIN}. Soils in GW_{MAX} had developed from a variety of
355 parent materials (e.g., granite; soft, medium and gritty schists; alluvial terraces) and are well
356 drained, while soils in GW_{MIN} had developed from aeolian loam, soft schist and marsh and
357 belonged to all three hydromorphic classes (Figure S3). Based on the 30 years of simulated
358 weather conditions, the GW value of at least one soil exceeded the maximum threshold in 1999,
359 2001 and 2014, while it fell below the minimum threshold in 1989, 1992, 1997, 2005, 2011 and
360 2017 (Figure 2b).

361 **3.2.3. Extreme samples of water-to-plant provision**

362 In contrast to extreme samples of GW, soils in WP_{MAX} had significantly higher mean pH
363 (+14%) and maximum rooting depth (+114%), but significantly lower mean clay content
364 (-30%) and SOC content (-34%), than those in WP_{MIN} (Table 6). Soils in WP_{MAX} had developed
365 mainly from granite, aeolian loam, soft and gritty schists and marsh and belonged to all three
366 hydromorphic classes, while those in WP_{MIN} had developed from granite, gneisses and soft and
367 gritty schists and were well or poorly drained (Figure S4). Based on the 30 years of simulated
368 weather conditions, the WP value of at least one soil exceeded the maximum threshold in 1997
369 and 2007, while it fell below the minimum threshold in 1988, 1992, 2006, 2008, 2010, 2016
370 and 2018 (Figure 2c).

371 **3.2.4. Extreme samples of plant biomass provision**

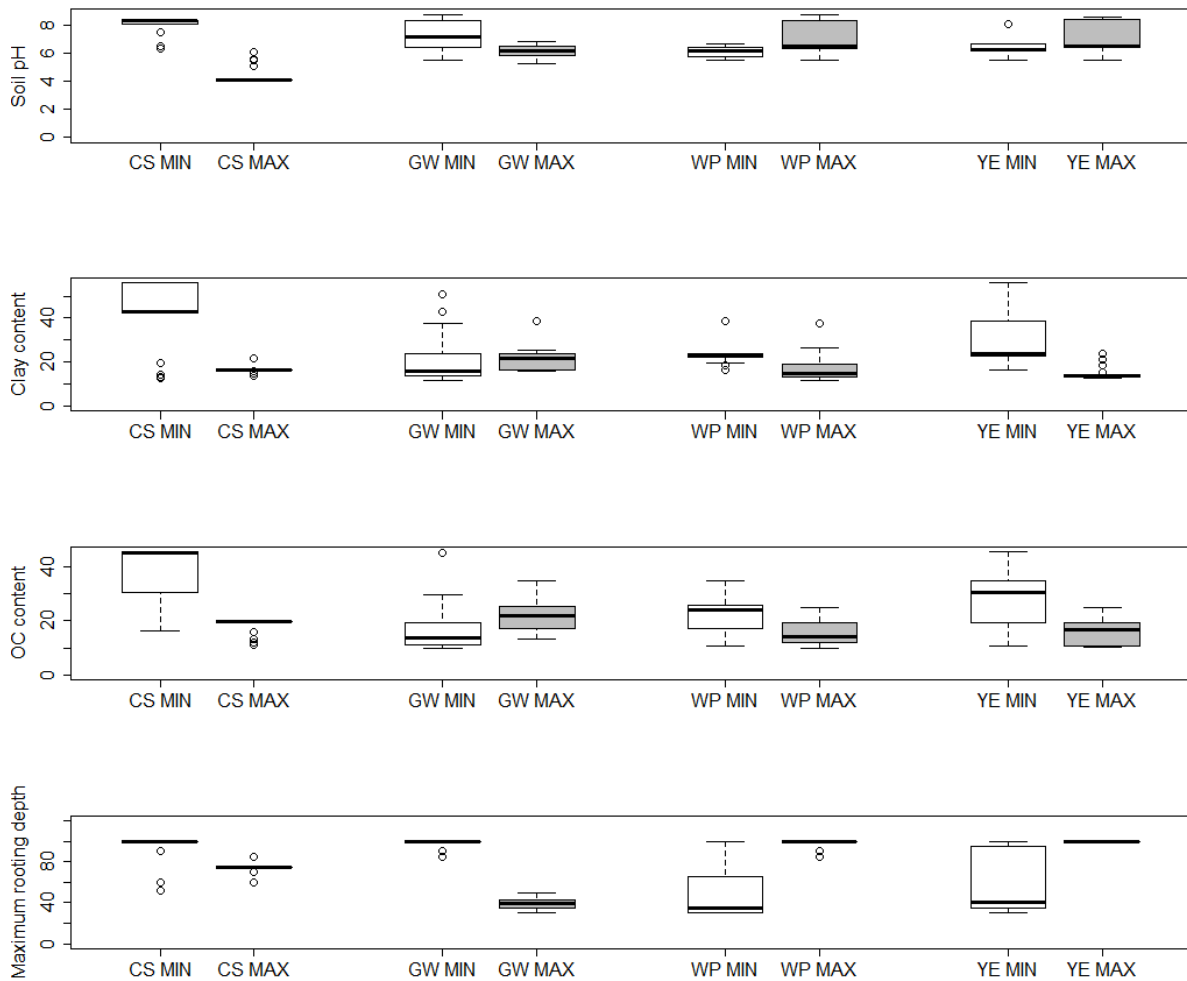
372 Soils in YE_{MAX} had significantly lower mean clay content (-50%) and SOC content (-46%), but
 373 significantly higher maximum rooting depth (+67%), than those in YE_{MIN} (Table 6). The pH
 374 also differed significantly between soils in YE_{MAX} and YE_{MIN}, although this difference was
 375 smaller than those for the three other soil properties. Soils in YE_{MAX} had developed mainly from
 376 aeolian loam, soft schists and marsh, while those in YE_{MIN} had developed from granite, gneisses,
 377 soft and gritty schists and marsh. Soils in YE_{MAX} belonged to all three hydromorphic classes,
 378 while those in YE_{MIN} were well or poorly drained (Figure S5). Based on the 30 years of
 379 simulated weather conditions, the YE value of at least one soil exceeded the maximum
 380 threshold in 1997, 1999, 2003, 2007, 2008 and 2015, while it fell below the minimum threshold
 381 in 1988, 1989, 1992, 1995, 2003, 2005, 2006, 2008, 2010, 2017 and 2018 (Figure 2d).

382

383 Table 6. Mean and coefficient of variation (CV) of soil properties (pH, clay and organic carbon
 384 (OC) contents in the 5-15 cm layer, and maximum rooting depth) for the entire dataset and for
 385 soils in minimum (MIN) and maximum (MAX) samples of ecosystem services. % diff. =
 386 percentage difference from the minimum to maximum sample.

Data	Sample/Metric	pH		Clay content		OC content		Max. rooting depth	
		Mean	CV	Mean	CV	Mean	CV	Mean	CV
Unit		none	%	%	%	g kg ⁻¹	%	cm	%
Entire dataset		6.6	14%	21.3	42%	19	38%	75	33%
Climate regulation	MIN sample	8.0	7%	42.6	31%	39	24%	94	15%
	MAX sample	4.4	13%	16.4	8%	19	14%	74	5%
	% diff.	-46%		-61%		-52%		-21%	
Groundwater recharge	MIN sample	7.2	15%	20	48%	15	40%	99	3%
	MAX sample	6.2	7%	22	26%	22	28%	39	17%
	% diff.	-14%		11%		42%		-61%	
Water-to-plant provision	MIN sample	6.1	5%	24.1	23%	23	35%	46	47%
	MAX sample	7.0	15%	17	35%	15	26%	98	4%
	% diff.	14%		-30%		-34%		114%	
Plant biomass provision	MIN sample	6.5	13%	30.3	46%	29	42%	60	48%
	MAX sample	7.0	16%	14.9	20%	16	29%	100	2%
	% diff.	7%		-50%		-46%		67%	

387



389

390 Figure 3. Boxplots of pH, clay content (%) and organic carbon (OC) content (g kg⁻¹) in the 5-
 391 15 cm layer, and maximum rooting depth (cm) of soils in minimum (MIN) and maximum
 392 (MAX) samples of soil ecosystem services: climate regulation (CS), groundwater recharge
 393 (GW), water-to-plant provision (WP) and plant biomass provision (YE)

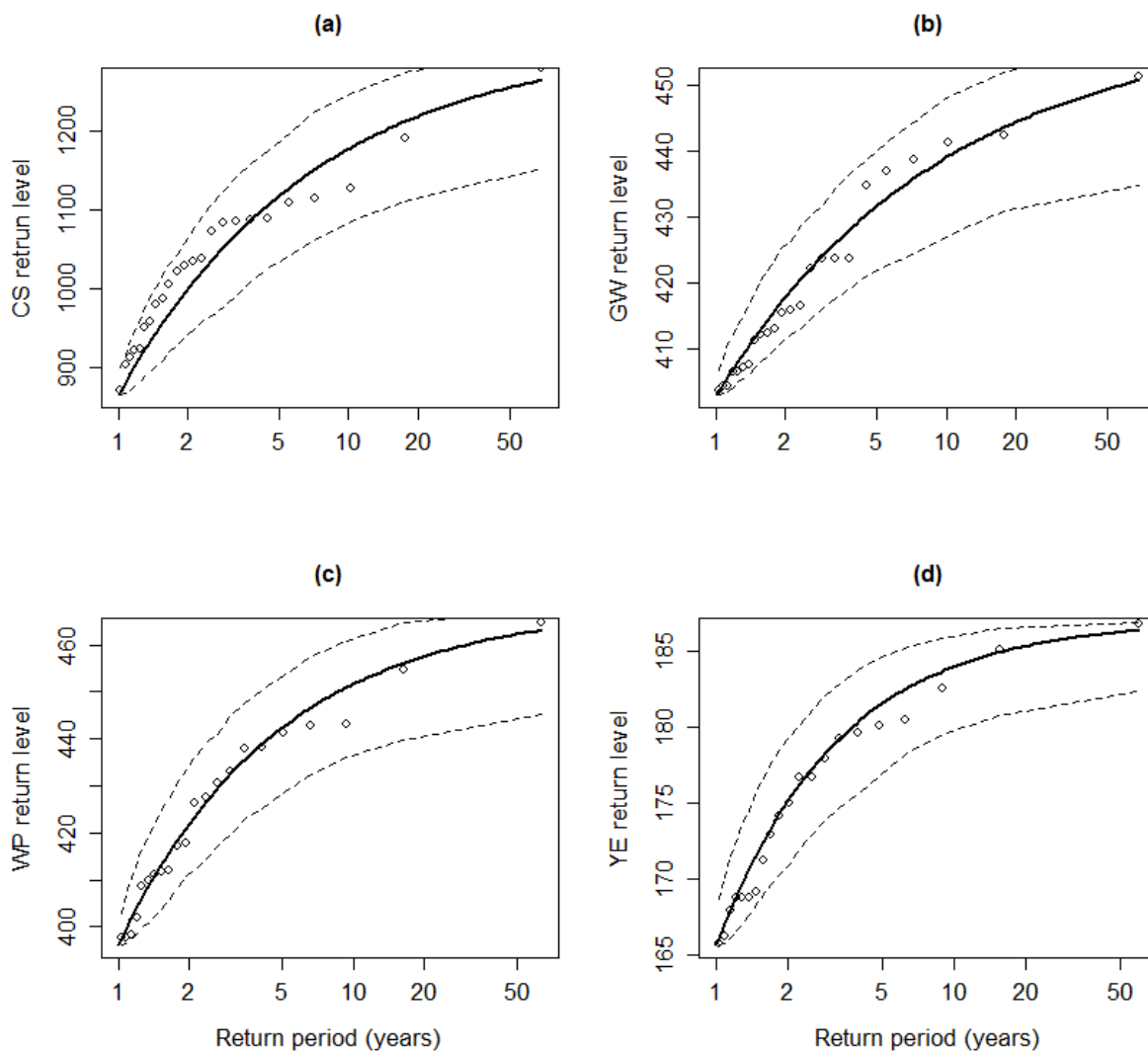
394

395 3.3. Return periods as a function of return levels of extreme maximum SES

396 For all four SES, return levels were set equal or close to the mean of the extreme maximum
 397 sample: 1000 kg C ha⁻¹ year⁻¹ for CS, 420 mm year⁻¹ for GW and WP, and 175 GJ ha⁻¹ year⁻¹
 398 for YE; Table S2). These return levels were expected to be exceeded by at least one soil profile
 399 an average of once every 2 years (i.e. the return period) (Figure 4). When the return level for
 400 CS, GW, WP and YE was increased by 5% to assess uncertainty (i.e. 1050 kg C ha⁻¹ year⁻¹, 440

401 mm year⁻¹, 440 mm year⁻¹ and 184 GJ ha⁻¹ year⁻¹, respectively), the mean return period
 402 increased to once every 3, 12, 5 and 15 years, respectively (Figure 4). When the return level
 403 increased, the number of soil profiles that exceeded it decreased, which increased uncertainty
 404 in the return periods (i.e. 95% confidence intervals (c.i.)). For instance, increasing the return
 405 level for CS by 5% (from 1000 to 1050 kg C ha⁻¹ year⁻¹) increased the 95% c.i. of the return
 406 period from once every 1.5-5 years to once every 2-10 years (Figure 4).

407



408

409 Figure 4. Semi-log plots of return levels as a function of return periods of extreme maximum
 410 of (a) climate regulation (CS, kg C ha⁻¹ year⁻¹), (b) groundwater recharge (GW, mm year⁻¹), (c)
 411 water-to-plant provision (WP, mm year⁻¹) and (d) plant biomass provision (YE, GJ ha⁻¹ year⁻¹)
 412 estimated from soil profiles in the dataset of 64 observation sites in Brittany (France) from
 413 1988-2018. Points are observed values from extreme samples, black lines are theoretical fitted

414 values from a generalized Pareto distribution model and dashed lines are 95% confidence
415 intervals of return periods and levels.

416 **4. Discussion**

417 **4.1. Accuracy of STICS predictions**

418 In the most relevant subset of the studies reviewed by Coucheney et al. (2015), Brisson et al.
419 (2002) evaluated STICS's accuracy at predicting a wide range of yields of wheat (2.6-11.4 t
420 ha⁻¹) and maize (0.2-13.8 t ha⁻¹) in France (rRMSE = 18% and 21%, respectively). They also
421 evaluated predictions of final soil water content in the rooting zone for both crops combined
422 (rRMSE = 11%). A later study that used STICS to simulate a rotation of wheat, rapeseed,
423 maize and peas in central France (Schnebelen et al., 2004), evaluated STICS's accuracy at
424 predicting a range of mean annual water drainage (51-189 mm) and soil water content at
425 harvest (273-433 mm) (mean rRMSE = 29% and 9%, respectively). A study that used STICS
426 to simulate cover crops at three sites in France (Constantin et al., 2012) evaluated the accuracy
427 of its predictions of water drainage and soil water content at harvest (mean rRMSE = 43% and
428 17%, respectively). Another recent study that used STICS to simulate cover crops in France
429 (Constantin et al., 2015) evaluated the accuracy of its predictions of final soil water content
430 (rRMSE ≤ 8%). The results of these studies, like those of the review of STICS (Coucheney et
431 al., 2015), indicated that STICS predictions of soil water content were most accurate (rRMSE
432 = 8-17%), followed by those of plant variables (rRMSE = 15-21%) and water drainage
433 (rRMSE = 29-43%). As mentioned, since STICS appears relevant for a variety of soil and
434 weather contexts in France, its predictions of relative differences among soil profiles were
435 expected to be robust.

436 **4.2. Characteristics of soils that provide extreme values of SES**

437 Our results identified combinations of soil properties that provided extreme values of SES.
438 Maximum CS was provided by soils that had lower pH, clay and SOC contents and maximum
439 rooting depth. These results agree with negative correlation coefficients calculated between CS
440 and the four soil properties considered in this study (Supplementary Table S3). Soils in extreme
441 samples of CS differed significantly in pH, a property that strongly influences the microbial C
442 cycle. For instance, increasing soil pH had a negative influence on SOC stocks in the United
443 Kingdom (Malik et al., 2018). Because lower SOC content was associated with maximum CS
444 in the present study, the soils studied are able to store additional organic C (Chen et al., 2019);
445 like most cropland soils in France, they are not saturated in SOC (Chen et al., 2018). Maximum

446 GW was provided by soils with both lower soil pH and maximum rooting depth or both higher
447 clay and SOC contents. Soils in extreme samples of GW differed particularly in maximum
448 rooting depth. Soil depth, texture and structure influence groundwater recharge (Dominati et
449 al., 2014) because they have a strong influence on the soil's available water capacity and thus
450 on the distribution of rainfall between evapotranspiration and deep drainage. In contrast to
451 maximum GW, maximum WP was provided by higher soil pH and maximum rooting depth
452 and lower clay and SOC contents. GW and WP were thus negatively correlated (since the water
453 taken up by plants is no longer available for groundwater recharge), which indicated a trade-off
454 relation between these SES (Supplementary Table S3).

455 Maximum values of GW or WP did not occur in the same years as minimum values, which
456 highlighted the influence of annual weather conditions on these SES. This result was the same
457 for extreme values of YE, except for 2003 and 2008; while France experienced heatwaves and
458 droughts in 2003, the weather of 2008 was relatively normal. Conversely, until 2002, extreme
459 minimum and maximum values of CS often occurred in the same years.

460 The results also identified soils in samples of extreme values of SES as a function of their parent
461 material. For instance, Fluvisols developed from marsh material were included in samples of
462 minimum CS and GW, as well as maximum WP and YE; these calcareous polder soils had high
463 pH (> 8) and differed in this respect from all other sites, which had an acidic pH. Other soils
464 from marsh material, classified as Gleysols, were also included in the sample of minimum YE;
465 these soils had high SOC content linked to high clay content and soil waterlogging. These
466 results agree with those obtained in the previous study of the properties of these soils as a
467 function of parent materials (Ellili-Bargaoui et al., 2019). In that study, soils from marsh
468 material had significantly higher SOC content (at higher depths) and pH than those from other
469 materials, but other soil properties did not differ significantly as a function of parent material.

470 **4.3. Relation between soil properties and extreme values of SES**

471 Using STICS to estimate SES values considered soil functions by explicitly representing
472 dynamics of soil processes based on soil properties, weather conditions, technical interventions
473 and the soil's initial state. For instance, estimating WP required assessing the function of soil
474 water provision over time by simulating actual water needs of the crop. Thus, assessing soil
475 functions was an intermediate step in STICS modeling, although only the fraction of this
476 function that was useful for the crop was used to estimate WP. Despite this approach, how soil
477 properties (and other factors) combine to influence soil functions and produce extreme values

478 of SES can be difficult to identify. While effects of some properties were simpler to explain
479 (e.g., lower maximum rooting depth decreases WP), indirect effects of other properties (e.g.,
480 soil pH) were less intuitive. Further investigations are therefore needed into the use of statistical
481 methods to identify relations that have not been revealed by soil processes.

482

483 **4.4. Return periods and return levels of extreme values of SES**

484 The return period provides useful information about the frequency of exceeding or falling below
485 certain extreme values of SES (i.e. return levels). While our examples focused on exceeding
486 return levels, decisions can also be based on the frequency of falling below one (e.g., “How
487 often will crops produce less than 30 GJ ha⁻¹ year⁻¹?”). They could also consider a specific
488 return period (“What level of water provision to crops should occur only once every 100
489 years?”). In an agricultural context, predicted return periods and return levels could help
490 decision makers attempt to manage natural resources in a more resilient manner.

491 However, the return period is estimated from a given set of management practices and period
492 of weather conditions. Estimating the return period requires assuming that extracted extreme
493 values of SES are independent, especially when extracting values every year (i.e. the value of
494 an SES in a given year is not influenced by the weather, soil or crop conditions of the previous
495 year). Independence cannot be not assumed for crops whose cycle length covers two years or
496 for ecosystem services that are sensitive to initial conditions: for instance, groundwater recharge
497 during the end of winter can be influenced by soil rewetting conditions during the autumn of
498 the previous year.

499 Moreover, the return period, as a mean estimate of the time after which a given return level may
500 be exceeded, has a degree of uncertainty. Potential changes in climate, soil properties and
501 management practices should be investigated to better understand their influence on predicted
502 return periods of extreme values of SES.

503 **4.5. EVT**

504 Applying EVT enables to identify soils with extremely low or high ecosystem service. EVT is
505 not limited by assumptions about normal distribution of underlying data, contrary to parametric
506 approaches usually used to explore data (e.g., linear regression). The presence of extreme
507 values may be also detected by using a principal component analysis, although this approach
508 did not provide a complete analysis (identification of threshold, modeling distribution of

509 extreme sample, predicting return period) of extreme sample like EVT does. To pursue the
510 present study, a bivariate EVT should be investigated to analyze the simultaneous occurrence
511 of extreme values of two SES.

512 **4.6. Spatial dimensions**

513 Our study focused particularly on the temporal dimension of extreme values of SES, but the
514 spatial dimension should be also considered, since soil data were collected from many locations.
515 However, although the soil-property/SES dataset was designed to represent the study area's
516 range of soil diversity, not all pedological situations were modeled. Thus, in the study's context,
517 spatially explicit probabilities of the occurrence of extreme values of SES were not estimated,
518 but they could help highlight the influence of soil conditions on SES and the importance of
519 preserving certain sites. The use of extreme value theory in spatial statistics should be
520 investigated to assess the dependence between locations of sampling sites and high values of
521 SES. Results of these analyses may help identify both when and where soils have extreme
522 values of SES. The spatial dimension of the results may be of particular interest to a regional
523 manager whose region contains a variety of soil types.

524 **4.7. Conclusion**

525 The present study identified thresholds above which values of SES can be considered as
526 extreme and soil properties associated with them. Combinations of certain soil properties and
527 weather conditions may result in extreme values of SES, which modeling of soil processes can
528 help to estimate, since they can be difficult to measure in the field. Moreover, return periods of
529 SES values that fall below minimum return levels should be also investigated to analyze the
530 risk of experiencing low SES, such as plant biomass provision. Nevertheless, the mechanisms
531 by which the combination of soil properties and weather conditions generate extreme values of
532 SES remain complex and require further research. Statistical methods could be used along with
533 mechanistic modeling of soil processes and functions to explain relations among them. Finally,
534 this approach could be useful at a regional level, with a variety of soils, but could be also applied
535 to a given location to help guide farmer decisions.

536 **CRedit authorship contribution statement**

537 **Tristan Senga Kiessé:** Writing – original draft, Visualization, Methodology,
538 Conceptualization, Formal analysis. **Blandine Lemercier:** Writing – review & editing,
539 Methodology, Funding acquisition, Data curation, Conceptualization. **Michael S. Corson:**

540 Writing – review & editing, Visualization, Methodology, Conceptualization. **Yosra Ellili-**
541 **Bargaoui:** Writing – review & editing, Methodology, Funding acquisition, Data curation,
542 Conceptualization. **Christian Walter:** Writing – review & editing, Methodology, Funding
543 acquisition, Data curation, Conceptualization

544 **Conflict of Interest**

545 This manuscript has not been published and is not under consideration by another journal. The
546 authors have approved the manuscript and agree with submission to your esteemed journal.
547 There are no conflicts of interest to declare.

548 **Data Availability Statement**

549 Data sharing is not applicable to this article since no new data were created in this study.

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