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The paradox of assessing greenhouse gases from soils for nature-based solutions

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Abstract

Quantifying the role of soils in nature-based solutions require accurate estimates of soil greenhouse gas (GHG) fluxes. Technological advances allow to simultaneously measure multiple GHGs and now is possible to provide complete GHG budgets from soils (i.e., CO_2, CH_4 and N_2O fluxes). We propose that there is a conflict between the convenience of simultaneously measuring multiple soil GHG fluxes at fixed time intervals (e.g., once, or twice per month) and the intrinsic temporal variability and patterns of different GHG fluxes. Information derived from fixed time intervals -as is commonly done during manual field campaigns- had limitations to reproduce statistical properties, temporal dependence, annual budgets, and associated uncertainty, when compared with information derived from continuous measurements (i.e., automated hourly measurements) for all soil GHG fluxes. We present a novel approach (i.e., temporal univariate Latin Hypercube sampling) that can be applied to optimize monitoring efforts of GHG fluxes across time. We suggest that multiple GHG fluxes should not be simultaneously measured at few fixed time intervals (especially once a month), but an optimized sampling approach can be used to reduce bias and uncertainty. These results have implications for assessing GHG fluxes from soils and consequently reduce uncertainty on the role of soils in nature-based solutions.

Keywords: Carbon dioxide, methane, nitrous oxide, representativeness, uncertainty

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1. Introduction

Soils are important for nature-based solutions for their role in climate mitigation potential through the implementation of different natural pathways (Griscom et al., 2017; Bossio et al., 2020). The climate mitigation potential of soils is dependent on multiple factors such as weather variability (Kim et al., 2012), ecosystem type (Oertel et al., 2016), soil structure (Ball, 2013), management practices (Shakoor et al., 2021), or disturbances (Vargas, 2012), where soils can ultimately act as net sources or sinks of greenhouse gases (GHGs). Therefore, accurate quantification of the magnitudes and patterns of soil GHGs fluxes is needed to understand the potential of soils to mitigate or contribute to global warming across ecosystems and different scenarios.

Most of our understanding of soil GHGs has come from manual measurements performed throughout labor intensive field campaigns and experiments (Oertel et al., 2016). While most studies around the world have focused on soil CO_2 fluxes (Jian et al., 2020), there are early examples reporting coupled measurements of soil CO_2, CH_4 and N_2O fluxes across tropical forests (Keller et al., 1986) and savannas (Hao et al., 1988), temperate forests (Bowden et al., 1993) and peatlands (Freeman et al., 1993). These pioneer studies provided an early view of the importance of integrated measurements of multiple soil GHG fluxes to understand the net global warming potential of soils, but also demonstrate the technical limitations and challenges associated with these efforts. For example, it is known that manual measurements have the strength of providing good spatial coverage during field surveys but provide limited information about temporal variability (Yao et al., 2009; Barba et al., 2021).

Technological advances have opened the opportunity to simultaneously measure multiple soil GHG fluxes (i.e., CO_2, CH_4 and N_2O) at unprecedented temporal resolution (e.g., hourly). These efforts have demonstrated differences in diel patterns and pulse events (e.g., rewetting) due to wetting and drying cycles across tropical (Butterbach-Bahl et al.,

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2004; Werner et al., 2007), subtropical (Rowlings et al., 2012), and temperate (Savage et al., 2014; Petrakis et al., 2017) ecosystems. These approaches provide more accurate information to calculate net GHG budgets and the global warming potential of soils (Capooci et al., 2019). That said, performing automated measurements of multiple GHGs is expensive and this approach usually has lower representation of the spatial heterogeneity within ecosystems (Yao et al., 2009; Barba et al., 2021).

Ideally, we would like to measure everything, everywhere, and all the time, but this is not possible due to logistical, technological, physical, and economic constraints. Light weight and low powered laser-based spectrometers have reduced technical barriers for simultaneously measuring multiple GHGs fluxes from soils, and it is now easier and faster to perform discrete manual surveys across time. This opportunity creates a paradox concerning when to measure different GHG fluxes from soils when performing manual measurements. In general, researchers tend to perform simultaneous measurements of multiple GHGs during manual surveys, but this convenience could result in biased information. We propose that there is a conflict between the convenience of measuring multiple GHGs at few fixed time intervals and the intrinsic temporal variability of magnitudes and patterns of different GHG fluxes.

Here, we test how a subset of measurements derived from a fixed temporal stratification (FTS) for simultaneous measurements (i.e., stratified sampling schedule) or using an optimized sampling (i.e., temporal univariate Latin Hypercube sampling (*tuLHs*)), compared with automated measurements of soil CO_2 ($F_A CO_2$), CH_4 ($F_A CH_4$), and N_2O ($F_A N_2O$) fluxes in a temperate forest. We reveal that reporting measurements of GHG fluxes using a FTS for simultaneous measurements, results in biased information of temporal patterns and magnitudes. This study shows how a biased sampling schedule could influence our understanding of GHG fluxes and ultimately the climate mitigation potential of soils.

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2. Materials and Methods

2.1 Study site

The experiment was performed in a temperate forest located at the St Jones Estuarine Reserve (a component of the Delaware National Estuarine Research Reserve [DNERR] in Delaware, USA. The site has a mean annual temperature of 13.3 °C and mean annual precipitation of 1119 mm. Soils are classified as Othello silt loam with a texture of 40% sand, 48% silt, and 12% clay within the first 10 cm (Petrakis et al., 2018). The dominant plant species are bitternut hickory (*Carya cordiformis*), eastern red cedar (*Juniperus virginiana* L.), American holly (*Ilex opaca*), sweet gum (*Liquidambar styraciflua* L.), and black gum (*Nyssa sylvatica* (Marshall)). The site has a mean tree density of 678 stems ha^{-1} and diameter at breast height (DBH) of 25.7±13.9 cm (mean±SD) (Barba et al., 2021).

2.2 Automated measurements of soil GHG fluxes

We performed automated measurements (45 minutes time intervals) of soil emissions of three GHGs (i.e., CO_2, CH_4 and N_2O) between September 2014–September 2015. Continuous measurements of soil GHGs were taken by coupling a closed-path infrared gas analyzer (Li-COR LI-8100 A, Lincoln, Nebraska) and nine dynamic soil chambers (Li-COR 8100–104) controlled by a multiplexer (Li-COR 8100-104) with a cavity ring-down spectrometer (Picarro G2508, Santa Clara, California). Detailed description of experimental design, measurements protocol are described in previous studies (Petrakis et al., 2018; Barba et al., 2021, 2019). Briefly, for each flux observation, we measured CO_2, CH_4 and N_2O concentrations every second with the Picarro G2508 for 300 seconds and calculated fluxes (at 45 minutes time intervals) from the mole dry fraction of each gas (i.e., corrected for water vapor dilution) using the SoilFluxPro software (v4.0; Li-COR, Lincoln, Nebraska, USA).

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Fluxes were estimated using both linear and exponential fits and we kept the flux calculation with the highest R^2. We applied quality assurance and quality control protocols using information from all three GHGs as established in previous studies (Petrakis et al., 2018; Barba et al., 2021, 2019; Capooci et al., 2019; Petrakis et al., 2017). Using these time series, we extracted values to represent discrete temporal measurements based on FTS and using an optimization approach as described below.

2.3 Temporal subsampling of time series

Subsampling of time series was performed using FTS and a temporal optimization following a univariate Latin Hypercube (*tuLHs*) approach. The difference between FTS and temporal optimization is that the first approach is focused on a fixed schedule (e.g., sampling once per month), and the second is focused on reproducing the statistical properties and temporal dependence relationship of the original GHG time series with a subset of measurements. This means that optimized subsamples may not be spaced systematically (e.g., every 15 days) and selected dates may vary for each GHG flux due to their specific statistical properties and temporal variability.

FTS represents a traditional schedule for performing manual measurements of GHG fluxes from soils. The FTS is usually performed with manual measurements because they require extensive logistical coordination due to travel time and costs, availability of instrumentation (e.g., gas analyzers) and personnel to perform the measurements, and weather conditions. During these scheduled visits researchers usually collect fluxes from all three GHGs and analyze them in a systematic manner to calculate magnitudes and patterns throughout the length of the experiment. Usually, researchers perform manual samples during the early hours of the day (between 9 am and 12 pm) to avoid confounding effects due to large changes in temperature and moisture as demonstrated by information summarized by

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the soil respiration global database (Cueva et al., 2017; Jian et al., 2020). Consequently, we selected subsamples from each original GHG time series (derived from automated measurements) using flux measurements from 10 am at fixed intervals of once per month (n=12), twice per month (n=24), or four times per month (n=48) starting on the first week of available data from automated measurements.

We applied *tuLHs* as an alternative subsampling approach to obtain an optimized subsample with the same univariate statistical properties and temporal dependence relationship of the original GHG time series. Optimization was performed to select subsamples for each GHG flux using the same number of samples as for fix temporal stratification: twelve (*k*=12), twenty-four (*k*=24) or forty-eight (*k*=48) measurements throughout the year of available data from automated measurements.

2.4 Temporal Univariate Latin Hypercube Sampling (tuLHs)

Let $S = \{(x_1, y_1, z_1), (x_2, y_2, z_2), \ldots , (x_n, y_n, z_n)\}$ be observations of the variables *X, Y* and *Z* in a time series, where X, Y and Z are soil GHGs (i.e., CO_2, CH_4 and N_2O). Each variable of the time series is characterized by two functions: the univariate probability distribution function and the temporal dependency function. Once these two functions are known, then the behaviors of the variable can be reproduced (Le et al., 2020; Chilès and Delfiner, 2009; Trangmar et al., 1986; Pyrcz and Deutsch, 2014). The *tuLHs* consists of three steps: (1) modeling the univariate behavior of the variable using the empirical cumulative univariate probability distribution function; (2) modeling the temporal dependence using the empirical variogram function; and (3) optimizing a subsample applying a global optimization method, differential evolution, using the previously obtained variogram function as an objective function.

First, to model the univariate behavior of the variables from the observations of S, the empirical univariate cumulative distribution function F^*_n (x) of X is estimated by:

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$$F_n^*(x) = \frac{1}{n}\sum_{i=1}^{n} I\,\{x_i \leq x\} \qquad (1)$$

where *I* represents an indicator function equal to 1 when its argument is true, and 0 otherwise. Similarly, the empirical univariate distribution function of the variables *Y* and *Z* can be derived. Second, to model the temporal dependence of the variables from the observations of *S*, the empirical temporal correlation function (i.e., temporal variogram function) $\gamma^*(t)$ of X is estimated by:

$$\gamma^*(t) = \frac{1}{2N(t)}\sum_{i=1}^{N(t)} [X(t_i + t) - X(t_i)]^2 \qquad (2)$$

where *N(t)* is the number of pairs $X(t_i + t)$ *and* $X(t_i)$ are separated by a time *t*. The variogram functions of the variables Y and Z are analogous. Third, To optimize the subsample it is required to choose the "optimal" data points with the selected sample size (i.e., *k*=12, 24 or 48; where *k* << *n)* that will have the same behavior of the original observations of *S* (i.e., GHG fluxes derived from automated measurements). To achieve this objective we use the differential evolution, a global optimization method (Storn and Price, 1997), using the variogram function as an objective function. The procedure consists of dividing the univariate empirical probability distribution in Eq. (1) into *k* equiprobable strata, which is equivalent to k ordered data subsets. From each subset, only one value must be chosen to satisfy the condition of a univariate Latin hypercube. The differential evolution method is applied to find the optimal points that minimize the difference between the subsample variogram γ (t) and the data variogram γ * (t) in Eq. (3).

$$OF_1 = \sum_{i=1}^{N(t)} [\gamma(t) - \gamma^*(t)]^2 \qquad (3)$$

where *OF* is the objective function and the variograms γ (t) and γ * (t) are calculated using Eq. (2).

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2.5 Statistical analyses

The t-test was used to compare the means and the Kolmogorov-Smirnov test to compare the probability distribution of measurements derived from each different sampling protocol. All tests were done with the 95% confidence level. In addition, their statistical properties such as mean, median, standard deviation, first and third quartile are compared. The differences of the experimental semivariograms were calculated as a comparison measure for the temporal dependence of the samples and the original time series of GHG fluxes. For cumulative sums of GHG flux, their mean is calculated as the most likely value and their quantile difference between 97.5 and 2.5 is used to quantify the range of uncertainty.

3. Results

3.1 Relationships among GHG fluxes from soils

Justification in support of FTS for simultaneous measurements of GHG fluxes would require evidence of strong linear correlations between magnitudes and temporal dependence among soil GHG fluxes. First, we did not find strong linear relationships between any combination of GHG fluxes from soils derived from automated measurements (Fig. A1). Therefore, our data did not support the assumption that the magnitude of one GHG flux was associated with a linear increase or decrease of another GHG flux. Second, semivariogram models demonstrated differences in the temporal dependence for each GHG flux. Automated measurements of soil CO_2 fluxes ($F_A CO_2$) showed a temporal dependence following a Gaussian variogram model, with a nugget of 4, a sill plus nugget of 28, and a correlation range of 80 days (Fig. A2a). Automated measurements of soil CH_4 fluxes ($F_A CH_4$) also showed a temporal dependence but followed a spherical variogram model, with a nugget of 7×10^{-8}, a sill plus nugget of 1.5×10^{-7}, and a correlation range of 110 days (Fig. A2b). In

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contrast, automated measurements of soil N_2O fluxes (F_AN_2O) did not show a temporal dependence, where a pure nugget effect was present, and with a correlation range of 0 days (Fig. A2c). Consequently, the magnitudes and temporal patterns of these GHG fluxes were different and did not provide support in favor of FTS for simultaneous measurements.

3.2 Optimization of GHG sampling protocols

We applied a *tuLHs* approach to identify subsamples that had the same statistical properties and temporal dependence for each one of the original GHG time series from automated measurements. Subsamples were identified for twelve (*k*=12), twenty-four (*k*=24) or forty-eight (*k*=48) measurements throughout the year for each GHG time series. All subsamples represent measurements collected at 10 am. Our results show that the optimized measurement dates were different for each GHG flux (Fig. 1), and we provide explicit examples for *k*=24 (Fig. 1) and *k*=12, 48 (Fig. A3, A4).

The optimized CO_2 subsamples were well distributed throughout the year for all sampling scenarios (i.e., *k* from 12 to 48), because F_ACO_2 had a strong temporal dependence and a small nugget effect with respect to the sill (Fig. A2a). The optimized CH_4 subsamples were also relatively well distributed throughout the year, especially for scenarios of *k*=24 and *k*=48, as F_ACH_4 also had a temporal dependence but with a higher nugget effect with respect to the sill (Fig. A2b). Finally, the optimized N_2O subsamples were more difficult to define especially with a small sample size (i.e., *k*=12; Fig. A3c) because F_AN_2O did not have a temporal dependence (Fig. A2c).

3.3 Differences in statistical properties and temporal dependency of subsamples

Overall, there were no statistically significant differences among the mean values derived from automated measurements and those from FTS or the *tuLHs* approach (Fig. 2 for *k*=24; Fig. A5

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for *k*=12; Fig. A6 for *k*=48; Tables A1 and A2). Although this appears to be a promising result, the simple comparison of the means is not enough to fully evaluate the information derived from different sampling scenarios. Here, we present results based on comparing the means, standard deviation, probability distributions, and semivariograms derived from automated measurements and the different sampling scenarios for all GHG fluxes.

The mean of F_ACO_2 was 5.9, while the mean for FTS 5.5 μmol CO_2 m^{-2} s^{-1}, and 5.9 μmol CO_2 m^{-2} s^{-1} for the *tuLHs* approach with *k*=24 (Fig. 3a-c). These results were comparable with the means derived from FTS (5.4 and 5.4 μmol CO_2 m^{-2} s^{-1}), and from the *tuLHs* approach (6.2 and 5.9 μmol CO_2 m^{-2} s^{-1}) using *k*=12 and *k*=48, respectively (Figs. A5, A6; Table A1). The standard deviation of F_ACO_2 was 3.9 and 3.2 μmol CO_2 m^{-2} s^{-1} for FTS, and 3.9 μmol CO_2 m^{-2} s^{-1} for the *tuLHs* approach with *k*=24 (Figs. 3a-c). These results were comparable with the standard deviations derived from FTS (3.1 and 3.3 μmol CO_2 m^{-2} s^{-1}), and from the *tuLHs* approach (4.1 and 3.9 μmol CO_2 m^{-2} s^{-1}) using *k*=12 and *k*=48, respectively (Fig. A5, A6; Table A1). Our results show that the semivariograms of optimized samples using the *tuLHs* approach closely approximate the semivariograms of automated measurements for *k*=24 (Fig. 4a) and *k*=12 and 48 (Figs. A7a, A8a). These results are consistent with the sums of absolute differences between the semivariograms of the samples and the semivariogram of F_ACO_2 with differences of 69.31, 54.39, 49.42 for FTS, and 5.69, 1.99, 1.39 for the *tuLHs* approach for *k*=12, 24, 48, respectively (Table A2).

The mean of F_ACH_4 was -0.93, while -0.86 nmol CH_4 m^{-2} s^{-1} for FTS and -0.94 nmol CH_4 m^{-2} s^{-1} for the *tuLHs* approach with *k*=24 (Fig. 3d-f). These results were also comparable with the means derived from FTS (-0.83 and -0.88 nmol CH_4 m^{-2} s^{-1}), and from the *tuLHs* approach (-0.87 and -0.92 nmol CH_4 m^{-2} s^{-1}) using *k*=12 and 48, respectively (Figs. A5, A6; Table A1). The standard deviation of F_ACH_4 was 0.36 and 0.26 nmol CH_4 m^{-2} s^{-1} for FTS, and 0.34 nmol CH_4 m^{-2} s^{-1} for the *tuLHs* approach with *k*=24. These results were comparable with

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the standard deviations derived from FTS (0.27 and 0.29 nmol CH_4 m^{-2} s^{-1}), and from the *tuLHs* approach (0.33 and 0.35 nmol CH_4 m^{-2} s^{-1}) using k=12 and k=48, respectively (Figs. A5, A6; Table A1). The semivariograms of optimized samples using the *tuLHs* approach closely approximate the semivariogram of automated measurements for k=24 (Fig. 4b) and k=12 and 48 (Figs. A7b, A8b). Consequently, the sums of absolute differences between the semivariograms of the samples and the semivariogram of F_ACH_4 were 0.63, 0.48 ,0.49 for FTS, and 0.06, 0.04, 0.02 for the *tuLHs* approach with k=12, 24, 48, respectively (Table A2).

Finally, the mean of F_AN_2O was 0.45 and 0.61 nmol N_2O m^{-2} s^{-1} for FTS, and 0.51 nmol N_2O m^{-2} s^{-1} for the *tuLHs* approach with k=24 (Fig. 3g-i). These results were also comparable with the means derived from FTS (0.59 and 0.25 nmol N_2O m^{-2} s^{-1}), and from the *tuLHs* approach (0.58 and 0.49 nmol N_2O m^{-2} s^{-1}) using k=12 and 48, respectively (Figs. A5, A6; Table A1). The standard deviation of F_AN_2O was 1.62 and 1.97 nmol N_2O m^{-2} s^{-1} for FTS, and 1.54 nmol N_2O m^{-2} s^{-1} for the *tuLHs* approach with k=24. These results were comparable with the standard deviations derived from FTS (1.38 and 0.91 nmol N_2O m^{-2} s^{-1}), and from the *tuLHs* approach (1.58 and 1.54 nmol N_2O m^{-2} s^{-1}) using k=12 and k=48, respectively (Figs. A5, A6; Table A1). Our results show that there is no temporal dependence for N_2O fluxes, but the semivariograms of optimized samples using the *tuLHs* approach closely approximate the semivariogram of automated measurements for k=24 (Fig. 4c) and k=12 and 48 (Figs. A7c, A8c). Consistently, the sum of absolute differences between the semivariograms of the samples and the semivariogram of F_AN_2O were 10.01, 12.25, 16.75 for FTS, and 0.82, 1.13, 3.57 for the *tuLHs* approach with k=12, 24, 48, respectively (Table A2).

These results show that the *tuLHs* approach reproduced with greater precision the probability distribution and the temporal dependence of the time series derived from automated measurements than FTS for all GHGs. In the next section, we explore the implications of these differences for calculation of cumulative GHG fluxes.

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3.4 Calculation of cumulative GHG fluxes

We calculated the cumulative flux for all GHGs using available information from automated measurements (Fig. 2; Table A3). The cumulative sum for available measurements of F_ACO_2 was 5758.5 g CO_2 m^{-2} [893.9, 13860.8; 95% CI]; for F_ACH_4 was -0.47 g CH_4 m^{-2} [-0.81, -0.19; 95% CI]; and 0.63 g N_2O m^{-2} [-0.75, 5.19; 95% CI] for F_AN_2O.

We used the mean for each GHG flux derived from the *tuLHs* approach or the FTS to calculate the cumulative sum (Table A3). We found that the FTS underestimated the cumulative flux (-8.4, -6.2, -7.1%) and the uncertainty (-32.6, -21.6, -19.3%) of F_ACO_2 for k=12, 24, 48, respectively (Fig. 5a). In contrast, the *tuLHs* approach overestimated the cumulative flux (6.5, 1.1, 0.1%) and underestimated the uncertainty (-9.1, -4.4, -3.7%) for k=12, 24, 48, respectively (Fig. 5a).

The FTS underestimated the cumulative flux (-9.1, -6.1, -3.1%) and the uncertainty (-31.8, -27.3, -15.9%) of F_ACH_4 for k=12, 24, 48, respectively (Fig. 5b). In contrast, the *tuLHs* approach underestimated the cumulative flux (-6.1%) only for k=12, but underestimated the uncertainty (-15.9, -6.8, -4.5%) for k=12, 24, 48, respectively (Fig. 5b).

The FTS substantially underestimated the cumulative flux (-168, -170, -173%) of F_AN_2O for k=12, 24, 48, respectively. Uncertainty was overestimated for k=12 and 24 (3.6 and 26%) and underestimated for k=48 (-31%; Fig. 5c). In contrast, the *tuLHs* approach overestimated the cumulative flux (29.5, 13.4, 9.1%) for k=12, 24, 48, respectively (Fig. 5c). This approach underestimated the uncertainty for k=12 and 24 by -11.2 and -13.8%, but overestimated the uncertainty by 2.9% for k=48 (Fig. 5c). These results show that the *tuLHs* approach consistently provided closer estimates for cumulative sums and uncertainty ranges than a FTS for all GHG fluxes.

4. Discussion

Applied challenges, such as quantifying the role of soils in nature-based solutions, require accurate estimates of GHG fluxes. To do this, two fundamental questions exist for designing environmental monitoring protocols: where to measure and when to measure? Ultimately a monitoring protocol aims to quantify the attributes of an ecosystem, so it can be compared in time within that ecosystem or with other ecosystems. Because we cannot measure everything, everywhere, and all the time, we can argue that any monitoring protocol has assumptions that are based on physical, economic, social, and practical reasons to address a specific scientific question. These assumptions for designing monitoring protocols could result in misleading, biased or wrong conclusions and therefore is critical to assess the consequences of different monitoring efforts. As Hutchinson described in "The Concept of Pattern in Ecology", we do not always know if a given pattern is extraordinary or a simple expression of something which we may learn to expect all the time (Hutchinson, 1953).

Automated measurements of soil GHG fluxes have revolutionized our understanding of the temporal patterns and magnitudes of these fluxes in soils (Vargas et al., 2011; Savage et al., 2014; Bond-Lamberty et al., 2020; Tang et al., 2006). That said, these types of measurements have limitations to represent spatial variability and have higher equipment costs that limits their broad applicability across study sites (Vargas et al., 2011). Consequently, discrete manual measurements are a common approach to simultaneously measure multiple GHG fluxes and report patterns, budgets, and information to parameterize empirical and process based models (Phillips et al., 2017; Wang and Chen, 2012). In this study, we argue that the convenience of simultaneously measuring multiple GHGs using FTS may result in bias estimates; therefore, optimization of sampling protocols is needed when there is a limited number of measurements in time (i.e., k=12, 24, 48).

We show that the magnitude of one GHG flux is not associated with a linear increase or decrease of another GHG flux, and the temporal dependencies of each GHG flux are different from each other (Fig. A1). Therefore, it is not possible to infer the dynamics of one GHG flux based solely on information from another under the assumption that they share similar (or autocorrelated) biophysical drivers. Multiple studies have shown that the importance of different biophysical drivers (e.g., temperature, moisture, light) is different for soil CO_2, CH_4 or N_2O fluxes (Luo et al., 2013; Tang et al., 2006; Ojanen et al., 2010). Our results show that soil CO_2 fluxes have a strong temporal dependence (Fig. A2a), likely as a result of the strong relationship between these fluxes and soil temperature in temperate mesic ecosystems (Hill et al., 2021; Bahn et al., 2010). The temporal dependence decreased for soil CH_4 fluxes (Fig. A2b),where there is less evidence for such strong correlation with soil temperature (Bowden et al., 1998; Castro et al., 1995), and where multiple variables are usually needed to explain the variability of these fluxes (Luo et al., 2013; Castro et al., 1994). Soil N_2O fluxes had no temporal dependence (Fig. A2c), showing a strong decoupling from soil CO_2 and CH_4 fluxes (Wu et al., 2010), likely as a result of independent biophysical drivers regulating soil N_2O fluxes (Luo et al., 2013; Bowden et al., 1993; Ullah and Moore, 2011).

To address the limitations of a FTS protocol, we propose a novel optimization approach (i.e., *tuLHs*) to reproduce the probability distribution and the temporal dependence of each original time series of GHG fluxes. Traditional approaches usually optimize subsamples by either focusing on reproducing the probability distribution of the original information (Huntington and Lyrintzis, 1998), or by focusing on reproducing the temporal dependence of the original information (Gunawardana et al., 2011). The *tuLHs* is a simple approach that consists of using the univariate probability distribution function and the temporal correlation function (i.e., variogram) as objective functions for each GHG flux. Our

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results show that optimized subsamples do not coincide in time for the three GHGs, suggesting that information should be collected based on the specific statistical and temporal characteristics of each GHG flux (Fig. 1). This study provides a proof of concept for the application of the *tuLHs* and demonstrates how optimization can be performed to improve estimates of soil GHG fluxes.

The more temporal data we can collect, the better, but in many cases measurement protocols are limited to a few measurements per year (i.e., k=12 to 48). Our results demonstrate that for a small sample size (i.e., k=12) the optimized measurements for soil CO_2 fluxes are consistently spread across the year, for soil CH_4 fluxes are centered within the growing season, and for soil N_2O fluxes are concentrated within the fall season (Fig. 1a). Our optimization approach shows how measurements can be distributed across time as more samples are available (i.e., k=24 to 48; Fig. 1b-c) and demonstrates that optimization is critical when a limited number of measurements are available. In other words, a few measurements properly distributed across time provide better agreement with information derived from automated measurements. We highlight that this optimization approach should be tested across different ecosystems as it will result in site-specific recommendations. That said, a similar conclusion was proposed for the spatial distribution of environmental observatory networks, where a network of few sites properly distributed (e.g., across a country) improves our understanding of the target variable than a spatially biased network (Villarreal et al., 2019). Thus, the need for representativeness assessment of information collected across time and space is needed for accurate evaluation of environmental measurements and quantification of nature-based solutions.

An initial approach suggested no statistical differences among the mean flux values derived from different sampling protocols. Arguably, this simplistic approach is a false-negative due to biased information from the FTS that does not accurately represent the

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probability distribution and the temporal variability of soil GHG fluxes (e.g., Figs. 3-4). In contrast, the optimization approach resulted in closer probability distributions and temporal variabilities for all GHGs, providing additional evidence against the FTS approach.

There are several implications of biased monitoring protocols for the understanding of soil GHG fluxes and nature-based solutions. First, temporal patterns and temporal dependency may not be properly represented with the FTS approach. Soil GHG fluxes have complex temporal dynamics that vary from diurnal to seasonal and annual scales that FTS is not able to reproduce (Barba et al., 2019; Bréchet et al., 2021). Second, soil GHG fluxes could present hot-moments, which are transient events with disproportionately high values that are often missed with a FTS approach (Vargas et al., 2018; Butterbach-Bahl et al., 2004). Third, cumulative sums and uncertainty ranges are biased or misleading when derived using a FTS approach (Capooci and Vargas, 2022; Tallec et al., 2019; Lucas-Moffat et al., 2018). For this third point, our study demonstrates that an optimized approach consistently provided closer estimates for cumulative sums and uncertainty ranges when compared with automated measurements (Fig. 5). We postulate that representing the variability of soil N_2O fluxes is more sensitive to the FTS approach (>170% and >30% for cumulative sums and uncertainty ranges, respectively) than for soil CH_4 and CO_2 fluxes. Fourth, it is possible that if information derived from the FTS approach is biased, then functional relationships could also be different from those derived from automated measurements (Capooci and Vargas, 2022). It has been discussed that hypothesis testing and our capability for forecasting responses of soil GHG fluxes to changing climate conditions is also biased with information from the FTS approach (Vicca et al., 2014). Finally, because soils have a central role for nature-based solutions within countries and across the world (Griscom et al., 2017; Bossio et al., 2020), accurate measurements are required to properly assess management practices, environmental variability and the contribution of GHGs from soils (Anderegg, 2021).

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Conclusion

We highlight that we do not always know if a given pattern is extraordinary or a simple expression of something which we may learn to expect all the time (Hutchinson, 1953). Furthermore, the "Knowledge Paradox" has been recognized for soil science, where innovative knowledge has often not been accepted by or implemented in society (Bouma, 2010). Here, we postulate that with emergent technologies there is a convenience of measuring multiple GHGs from soils; however, few measurements collected at fixed time intervals results in biased estimates.

We recognize that potential bias in measurements is dependent on the magnitudes and temporal patterns of each GHG flux and could be site-specific. Nevertheless, evaluations are needed to quantify potential bias in estimates of GHG budgets and information used for model parameterization and environmental assessments. In this study, we propose a novel optimization approach (i.e., temporal univariate Latin Hypercube sampling) that can be applied with site-specific information of different ecosystems to improve monitoring efforts and reduce bias of GHG flux measurements across time. We highlight that constant biased environmental monitoring may provide confirmatory information which we have learned to expect, but modifications of monitoring protocols could shed light into extraordinary patterns. These unexpected patterns are the ones that will test paradigms and push science frontiers.

Data Availability. All data used for this analysis is available at: https://doi.org/10.6084/m9.figshare.19536004.v1

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Author Contributions. R.V. conceived this study and V.H.L. designed and performed the primary analysis with input from R.V in all phases. R.V. wrote the manuscript with input from V.H.L.

Competing Interest Statement. None

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FIGURES

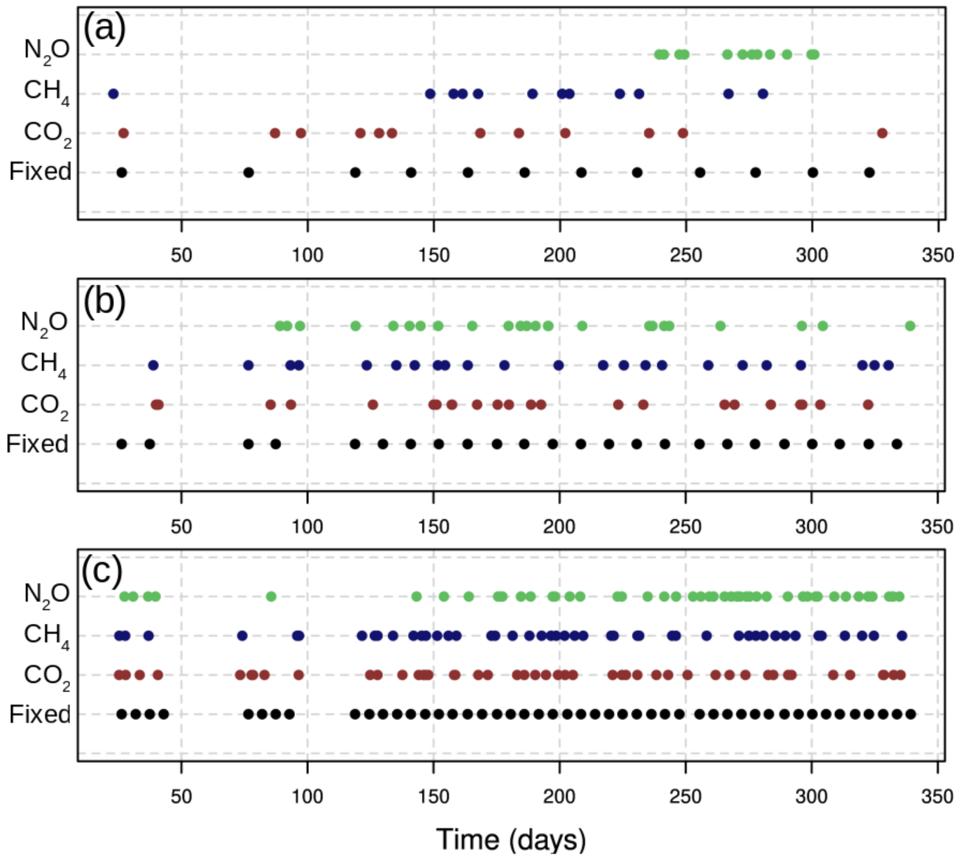

Figure 1. Temporal distribution of fixed temporal stratification (i.e., stratified manual sampling approach) and optimized sampling using a temporal univariate Latin Hypercube (*tuLHs*) approach for: *k*=12 (a), *k*=24 (b), and *k*=48 (c). Fixed temporal stratification is in black, soil CO_2 fluxes in red, soil CH_4 fluxes in blue, and soil N_2O fluxes in green.

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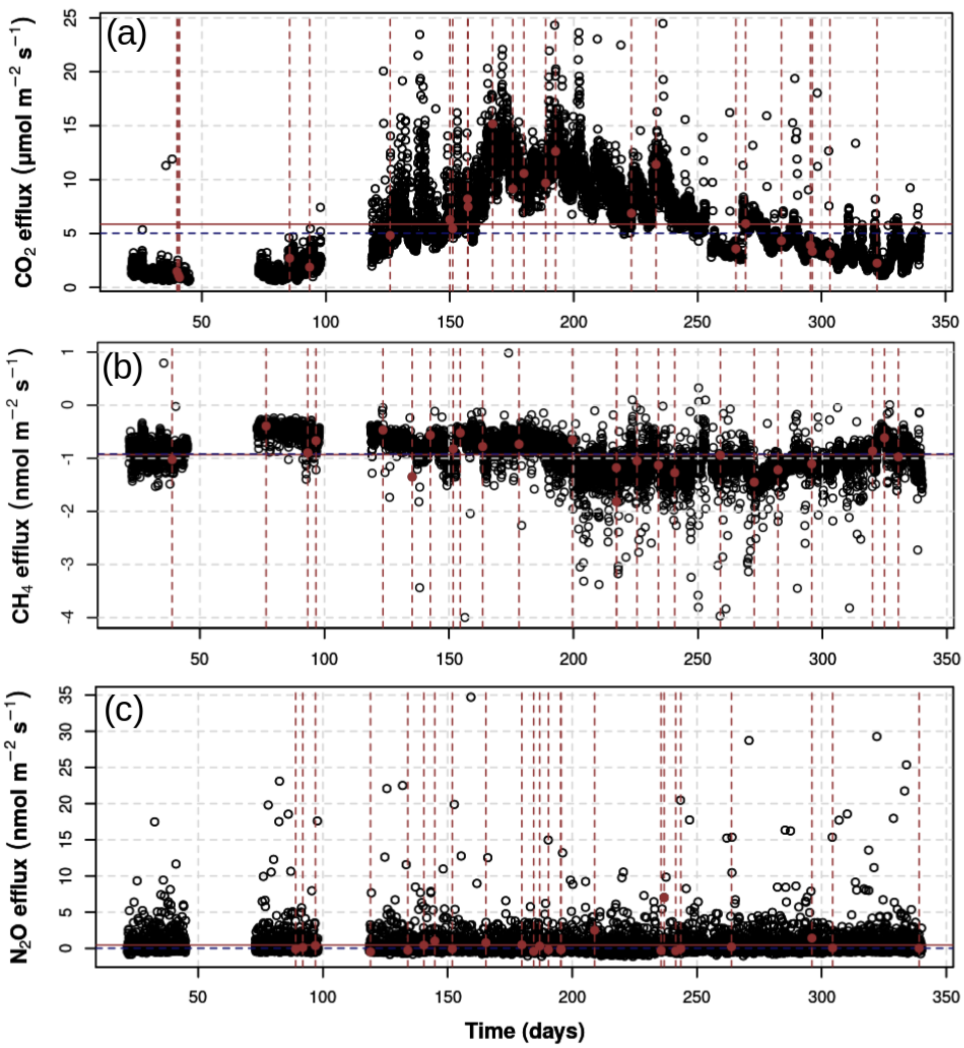

Figure 2. Time series of automated measurements (F_A) of soil greenhouse gas fluxes (black circles) and optimized samples (k=24) using a temporal univariate Latin Hypercube sampling (*tuLHs*) approach for soil CO_2 (a), soil CH_4 (b) and soil N_2O (c) fluxes. Horizontal red line represents the mean and horizontal blue line the median of each greenhouse gas flux derived from automated measurements. Selection of datapoints for k=12 and 48 are presented for each soil greenhouse gas time series in Figs. A3 and A4, respectively.

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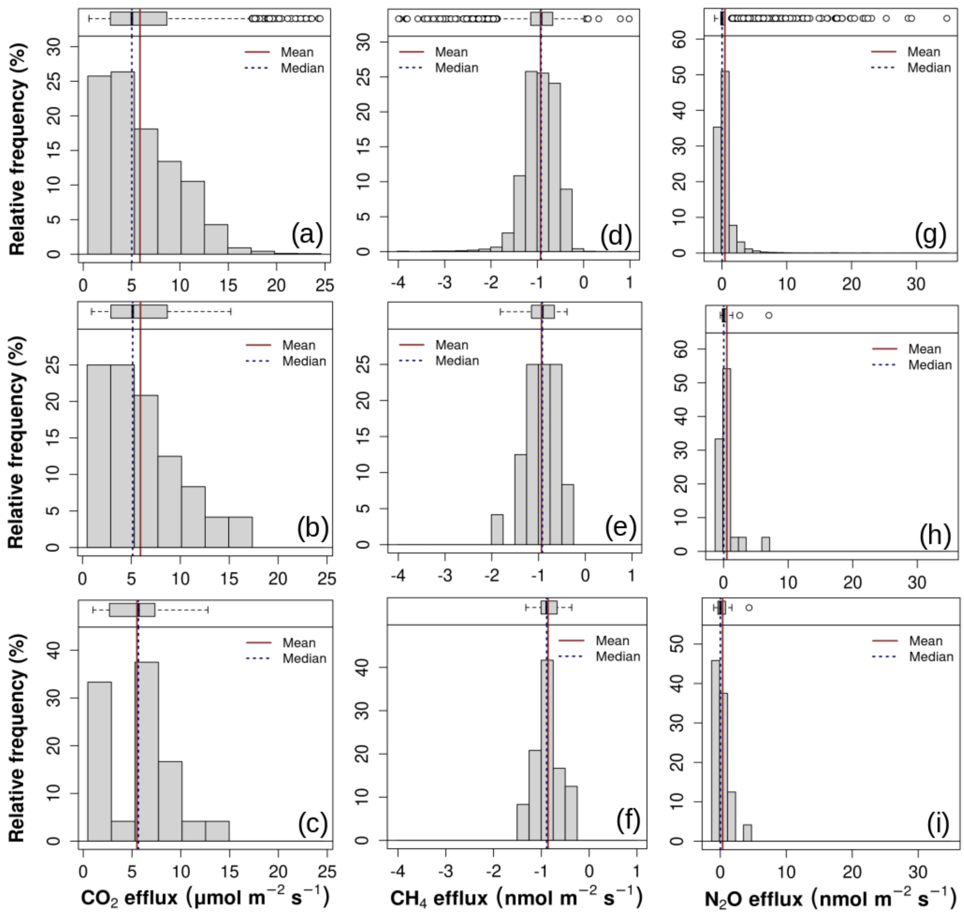

Figure 3. Histograms for automated measurements of soil CO_2 (F_A CO_2; a), soil CH_4 (F_A CH_4; d) and soil N_2O (F_A N_2O; g). Histograms for optimized samples (k=24) using a temporal univariate Latin Hypercube sampling (*tuLHs*) approach for soil CO_2 (b), soil CH_4 (e) and soil N_2O (h) fluxes. Histograms for fixed temporal stratification (i.e., stratified manual sampling schedule) (k=24) for soil CO_2 (c), soil CH_4 (f) and soil N_2O (i) fluxes. Appendix A includes results for measurements with k=12 (Fig. A5) and k=48 (Fig. A6).

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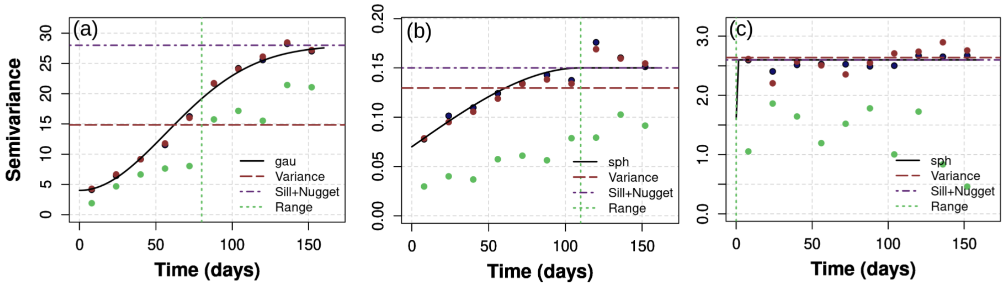

Figure 4. Comparison of semivariograms between automated measurements (F_A) of soil greenhouse gas fluxes (solid black line) and for optimized samples using a temporal univariate Latin Hypercube sampling (*tuLHs*) approach (red circles) or fixed temporal stratification (green circles) with k=24. Semivarograms are presented for soil CO_2 (a), CH_4 (d) and N_2O (c) fluxes. Semivariograms for measurements with k=12 and k=48 are presented in supplementary Figs. A7 and A8, respectively. Semivariogram fits were gaussian (Gau) or spherical (sph).

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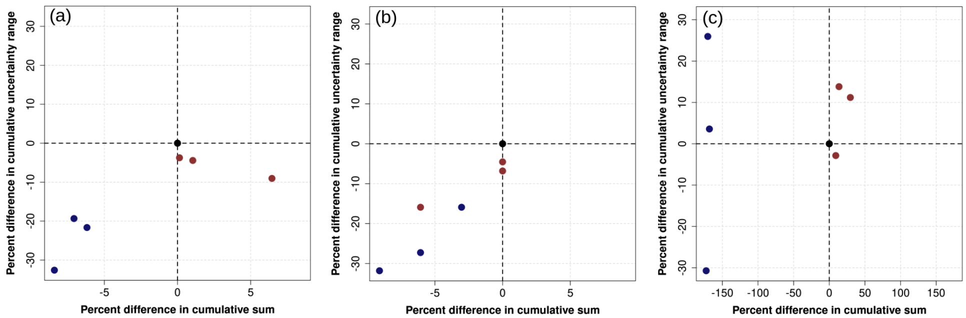

Figure 5. Comparison of percent differences from cumulative sums and associated uncertainty (95% CI) between greenhouse gas fluxes derived from automated measurements (F_A) and using an optimized sampling approach (*tuLHs*) or a fixed temporal stratification. Differences are represented for of soil CO_2 (a), soil CH_4 (b) and soil N_2O (c) fluxes. Black circle in the center (0,0) of a plot represents the values derived from automated measurements (F_A). Blue circles represent estimates from fixed temporal stratification, and red circles represent estimates from an optimized sampling approach (*tuLHs*). Estimates were calculated based on the 258 available automated measurements (Fig. 2) and numeric estimates are in Table A3.

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Appendix A – Supplementary Tables and Figures

Table A1. Statistical properties for automated measurements of soil CO_2 (F_A CO_2), soil CH_4 (F_A CH_4) and soil N_2O (F_A N_2O) fluxes, optimized samples (k=12, 28, 48) using a temporal univariate Latin Hypercube sampling (*tuLHs*), and fixed temporal stratification (k=12, 28, 48). Units for soil CO_2 fluxes are in µmol m^{-2} s^{-1}, and for soil CH_4 and N_2O fluxes in nmol m^{-2} s^{-1}.

	Number of measurements (k)	1st. Quartile	Median	Mean	3rd. Quartile	Standard Deviation
$F_A CO_2$	8259	2.81	5.03	5.87	8.65	3.85
tuLHs approach (**CO_2**)	12	3.19	5.30	6.25	8.88	4.06
	24	3.00	5.13	5.93	8.44	3.90
	48	2.84	4.97	5.88	8.54	3.87
Fixed temporal stratification (**CO_2**)	12	2.68	5.82	5.37	7.10	3.15
	24	2.69	5.66	5.50	7.07	3.24
	48	2.69	5.53	5.45	8.05	3.29
$F_A CH_4$	8259	-1.14	-0.92	-0.93	-0.67	0.36
tuLHs approach (**CH_4**)	12	-1.11	-0.89	-0.87	-0.66	0.33
	24	-1.14	-0.92	-0.94	-0.66	0.34
	48	-1.13	-0.91	-0.92	-0.66	0.35
Fixed temporal stratification (**CH_4**)	12	-1.01	-0.83	-0.83	-0.67	0.27
	24	-1.01	-0.89	-0.86	-0.68	0.26
	48	-1.10	-0.86	-0.88	-0.66	0.29
$F_A N_2O$	8259	-0.18	0.01	0.45	0.49	1.62
tuLHs approach (**N_2O**)	12	-0.18	-0.01	0.58	0.50	1.58
	24	-0.18	0.03	0.51	0.45	1.54
	48	-0.17	0.02	0.49	0.45	1.54
Fixed temporal stratification (**N_2O**)	12	-0.35	0.51	0.59	0.83	1.38
	24	-0.21	-0.08	0.61	0.36	1.97
	48	-0.31	0.00	0.25	0.53	0.91

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Table A2. Comparison of errors between experimental variogram for automated measurements of soil greenhouse gases (F_A; k=8259) and experimental variograms for data using temporal univariate Latin Hypercube sampling (*tuLHs*) and fixed temporal stratification.

	Approach	**Number of measurements (*k*)**	**Error (Sum of absolute differences)**
Soil CO_2 fluxes	Fixed	12 24 48	69.31 54.39 49.42
	tuLHs	12 24 48	5.69 1.99 1.39
Soil CH_4 fluxes	Fixed	12 24 48	0.63 0.68 0.49
	tuLHs	12 24 48	0.06 0.04 0.02
Soil N_2O fluxes	Fixed	12 24 48	10.01 12.25 16.75
	tuLHs	12 24 48	0.82 1.13 3.57

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Table A3. Cumulative sum and associated uncertainty of greenhouse gas (GHG) fluxes derived from automated measurements (F_A) and using an optimized sampling approach (*tuLHs*) or a fixed temporal stratification. Cumulative sum represents the total flux from available measurements derived from automated measurements for all GHG fluxes.

	Number of measurements (*k*)	**Cumulative Sum**	**Uncertainty 95% CI**		**Uncertainty Range**
F_ACO_2 ($g\ CO_2\ m^2$)	8259	5758	893	13860	12966
tuLHs approach ($g\ CO_2\ m^2$)	12	6130	1423	13218	11794
	24	5818	1046	13438	12391
	48	5766	946	13429	12482
Fixed temporal stratification ($g\ CO_2\ m^2$)	12	5273	1376	10117	8740
	24	5402	1196	11356	10160
	48	5351	1162	11621	10458
F_ACH_4 ($g\ CH_4\ m^2$)	8259	-0.33	-0.58	-0.14	0.44
tuLHs approach ($g\ CH_4\ m^2$)	12	-0.31	-0.49	-0.12	0.37
	24	-0.33	-0.57	-0.16	0.41
	48	-0.33	-0.56	-0.14	0.42
Fixed temporal stratification ($g\ CH_4\ m^2$)	12	-0.3	-0.45	-0.15	0.3
	24	-0.31	-0.46	-0.14	0.32
	48	-0.32	-0.51	-0.14	0.37
F_AN_2O ($g\ N_2O\ m^2$)	8259	0.44	-0.53	3.67	4.2
tuLHs approach ($g\ N_2O\ m^2$)	12	0.57	-0.48	4.19	4.67
	24	0.5	-0.43	4.35	4.78
	48	0.48	-0.5	3.58	4.08
	12	-0.3	-0.83	3.52	4.35
	24	-0.31	-0.43	4.86	5.29

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Fixed temporal stratification (g N_2O m^2)	48	-0.32	-0.7	2.21	2.91

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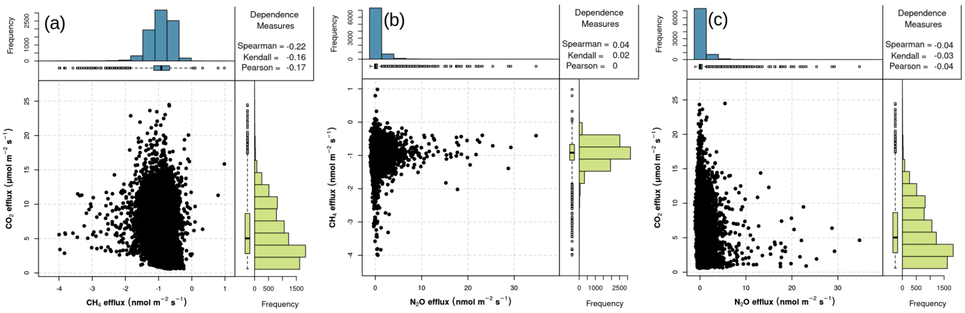

Figure A1. Relationships between soil CO_2 (F_A CO_2) with soil CH_4 (F_A CH_4) fluxes (a), soil CH_4 (F_A CH_4) with soil N_2O (F_A N_2O) fluxes (b), and soil CO_2 (F_A CO_2) with soil N_2O (F_A N_2O) fluxes. None of these relationships were significant at α=0.05. These relationships were derived using all available data from automated measurements (F_A) of soil greenhouse gas fluxes.

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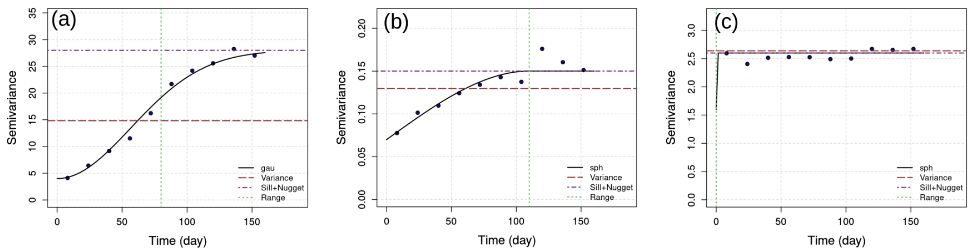

Figure A2. Semivariograms of soil CO_2 (F_A CO_2; a), soil CH_4 (F_A CH_4; b) and soil N_2O (F_A N_2O; c) fluxes. These semivariograms were derived using all available data from automated measurements (F_A) of soil greenhouse gas fluxes. Semivariogram fits were gaussian (Gau) or spherical (sph).

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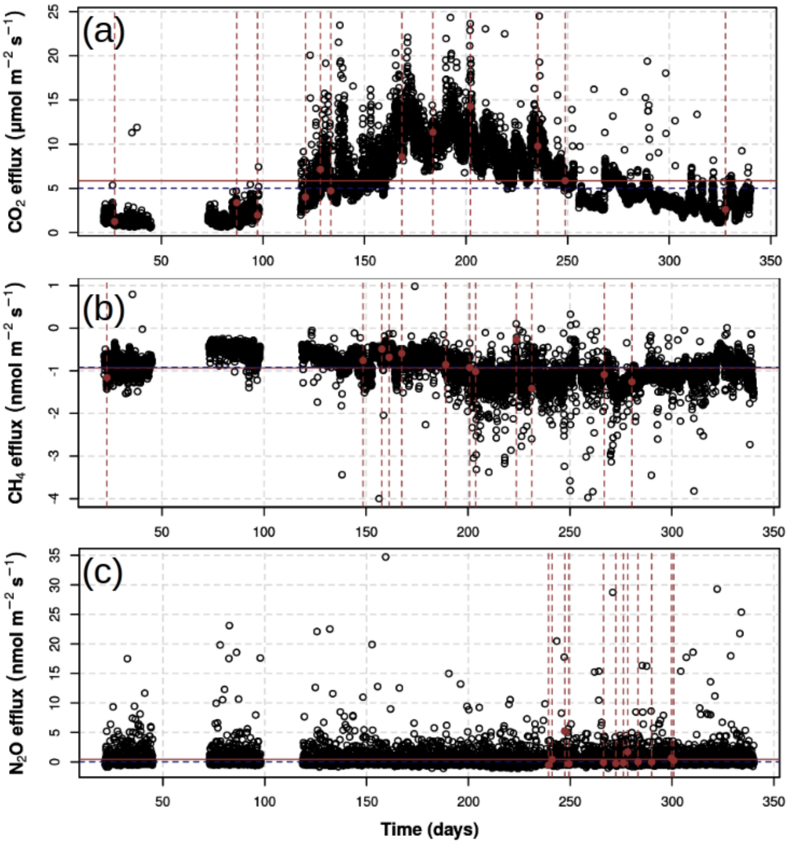

564
565
566 **Figure A3.** Time series of automated measurements (FA) of soil greenhouse gas fluxes
567 (black circles) and optimized samples (*k*=12) using a temporal univariate Latin Hypercube
568 sampling (*tuLHs*) approach for soil CO_2 (a), soil CH_4 (b) and soil N_2O (c) fluxes. Horizontal
569 red line represents the mean and horizontal blue line the median of each greenhouse gas flux
570 derived from automated measurements.
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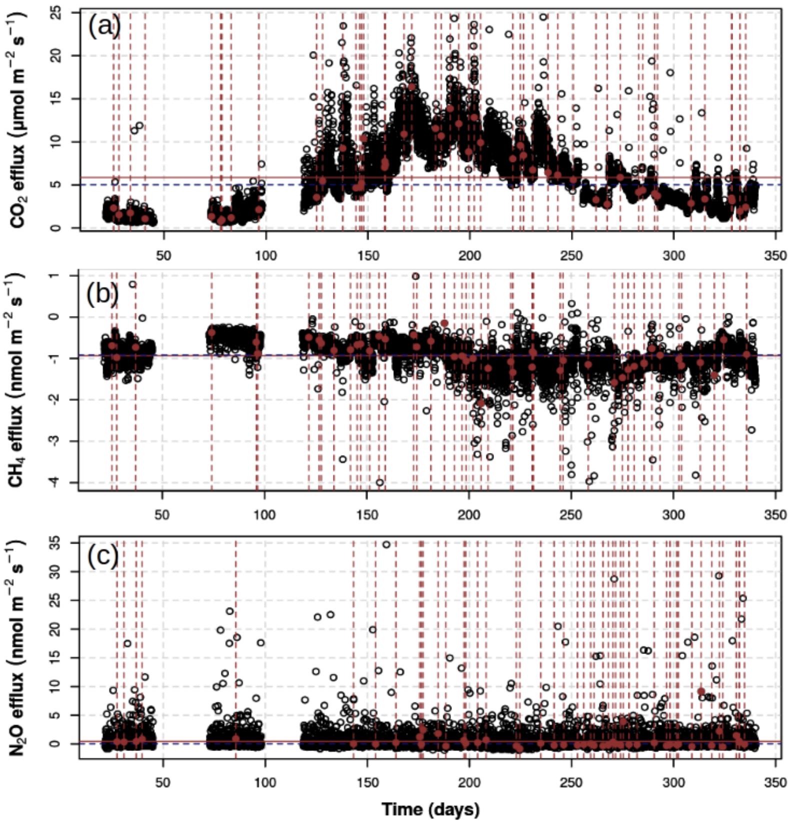

Figure A4. Time series of automated measurements (FA) of soil greenhouse gas fluxes (black circles) and optimized samples (*k*=48) using a temporal univariate Latin Hypercube sampling (*tuLHs*) approach for soil CO_2 (a), soil CH_4 (b) and soil N_2O (c) fluxes. Horizontal red line represents the mean and horizontal blue line the median of each greenhouse gas flux derived from automated measurements.

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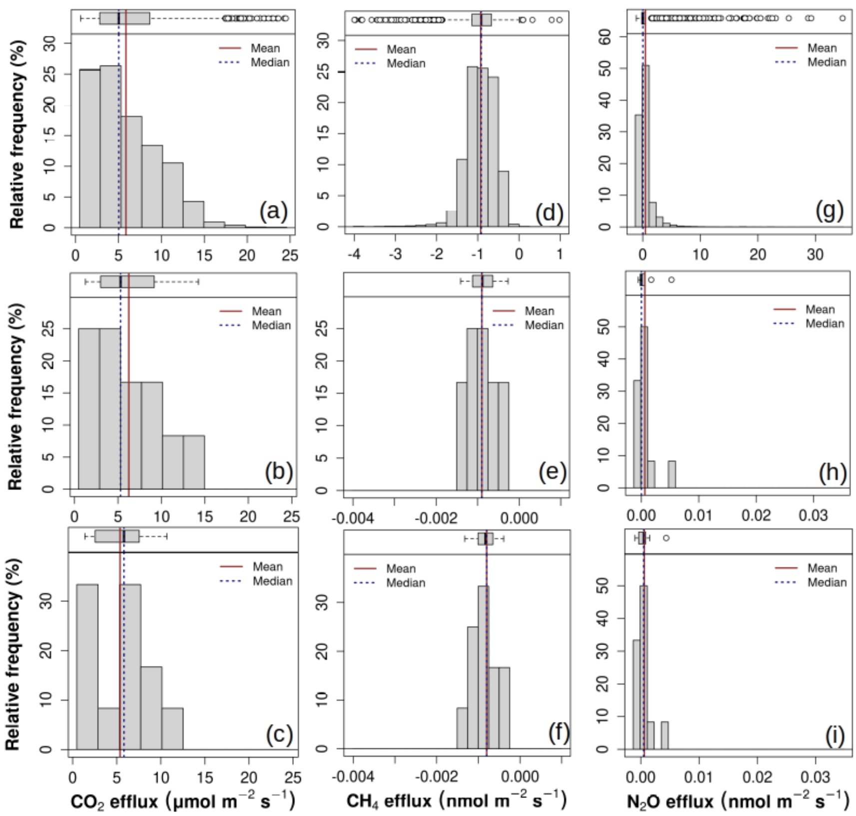

Figure A5. Histograms for automated measurements of soil CO_2 (F_A CO_2; a), soil CH_4 (F_A CH_4; d) and soil N_2O (F_A N_2O; g) fluxes. Histograms for optimized samples (k=12) using a temporal univariate Latin Hypercube sampling (*tuLHs*) approach for soil CO_2 (b), soil CH_4 (e) and soil N_2O (h) fluxes. Histograms for fixed temporal stratification (i.e., stratified manual sampling schedule; k=12) for soil CO_2 (c), soil CH_4 (f) and soil N_2O (i) fluxes.

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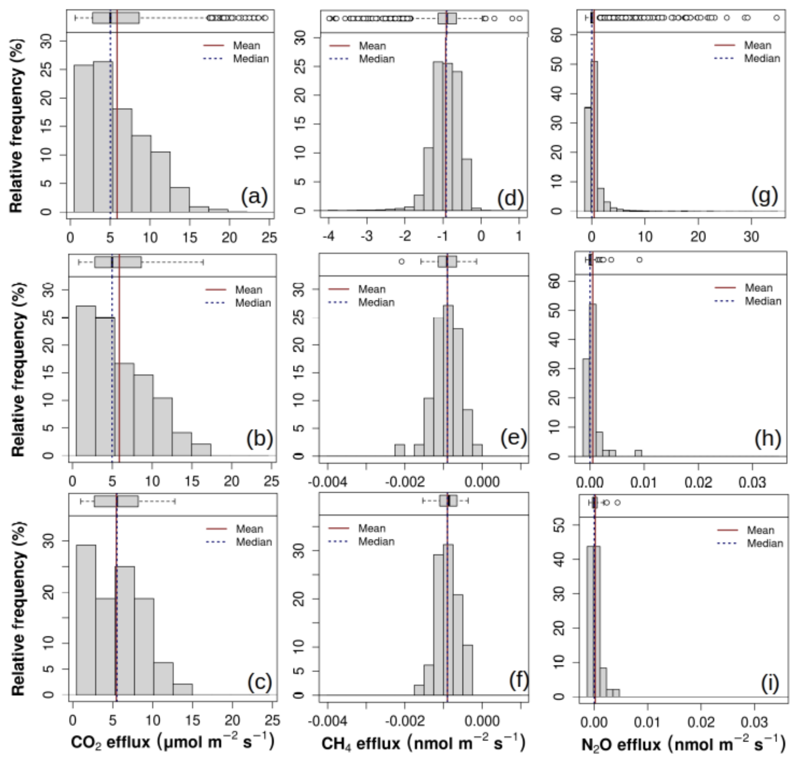

Figure A6. Histograms for automated measurements of soil CO_2 (F_A CO_2; a), soil CH_4 (F_A CH_4; d) and soil N_2O (F_A N_2O; g) fluxes. Histograms for optimized samples (k=48) using a temporal univariate Latin Hypercube sampling (*tuLHs*) approach for soil CO_2 (b), soil CH_4 (e) and soil N_2O (h) fluxes. Histograms for fixed temporal stratification (i.e., stratified manual sampling schedule; k=48) for soil CO_2 (c), soil CH_4 (f) and soil N_2O (i) fluxes.

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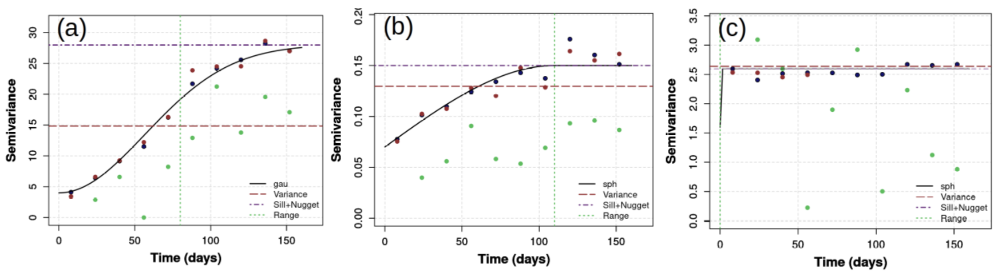

Figure A7. Comparison of semivariograms between automated measurements (F_A) of soil greenhouse gas fluxes (solid black line) and for optimized (red circles) or fixed temporal stratification (green circles) with k=12. Semivarograms are presented for soil CO_2 (a), CH_4 (d) and N_2O (c) fluxes. Semivariogram fits were gaussian (Gau) or spherical (sph).

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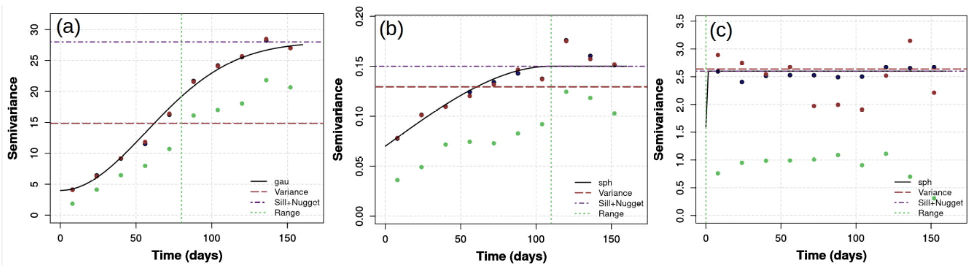

Figure A8. Comparison of semivarograms between automated measurements (F_A) of soil greenhouse gas fluxes (solid black line) and for optimized (red circles) or fixed temporal stratification (green circles) with k=48. Semivarograms are presented for soil CO_2 (a), CH_4 (d) and N_2O (c) fluxes. Semivariogram fits were gaussian (Gau) or spherical (sph).

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