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# Predicting nitrous oxide emissions with a random-effects model

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ABSTRACT

The main source of anthropogenic $N_2O$ emissions is the application of nitrogen fertilizer to agricultural soils. We present an approach for predicting $N_2O$ emissions based on a statistical random-effects model: the $N_2O$ emission response to applied nitrogen fertilizer is described by an exponential function, the parameters of which are assumed to vary randomly between locations. One of the advantages of this model is that its parameters are easily adjusted to one or several location-specific $N_2O$ measurements. The adjusted model can then be used to predict $N_2O$ emissions for nitrogen fertilizer doses other than those applied at the considered location. We evaluated the accuracy of model prediction, with real and simulated data. The use of location-specific rather than average predictions reduced prediction errors in most cases. Location-specific predictions could be used to estimate background emission in on-farm studies.



## 1. Introduction

$N_2O$ is a potent greenhouse gas with a lifetime in the atmosphere of 114 years and a global warming potential 298 times greater than that of $CO_2$ for a 100-year horizon (IPCC, 2007). Atmospheric $N_2O$ concentration has risen from 270 parts per billion (ppb) in the pre-industrial period to 319 ppb in 2005 (IPCC, 2007). $N_2O$ is emitted due to nitrification and denitrification processes. Thus, all factors modifying these physicochemical exchanges affect $N_2O$ emission. The main source of anthropogenic emissions is nitrogen (N) fertilizer application to agricultural soils (Davidson, 2009; Mosier et al., 1998; Snyder et al., 2009; Stehfest and Bouwman, 2006). Many other factors may also modify $N_2O$ emissions in cultivated areas. These factors are of three main types (Freibauer and Kaltschmitt, 2003): (i) soil characteristics (e.g. soil organic content, soil texture), (ii) climate characteristics (e.g. rainfall, freeze–thaw cycle (Freibauer and Kaltschmitt, 2003)) and (iii) management practices (e.g. N fertilization, tillage (Rochette, 2008)).

The amount of N applied and other management practices are often reported in $N_2O$ emission experiments, but information about soil and climate characteristics is often missing. For example, in the dataset of Stehfest and Bouwman (2006), the amount of applied N was systematically reported, but 29% of soil organic content data, 12% of soil texture data and 94% of annual precipitation data were missing. Datasets including $N_2O$ measurements have been used to develop simple statistical models relating $N_2O$ emissions to the amount of applied N through linear or exponential functions (Bouwman, 1996; Hoben et al., 2011; Philibert et al., 2012). Philibert et al. (2012) showed that statistical models based on an exponential function outperformed linear models. In their paper, Philibert et al. (2012) showed how their statistical models could be used to estimate the average response of $N_2O$ emission to the amount of N applied. This average response is useful for estimating $N_2O$ emissions in average over a large number of locations, but it cannot be used to derive reliable local estimates due to the strong between-location variability of $N_2O$ emissions. We show here how the models of Philibert et al. (2012) can be extended in order to derive location-specific $N_2O$ predictions using location-specific $N_2O$ measurements, when such measurements are available.

Several authors have suggested that $N_2O$ emission could be predicted from several input variables relating to soil characteristics, climate characteristics and management practices (Berdanier and Conant, 2012; Leip et al., 2011; Lesschen et al., 2011). However, as mentioned above, little information about soil and climate characteristics is generally given and it is often difficult to establish robust relationships between $N_2O$ emissions and environmental variables (Lesschen et al., 2011). Mechanistic models have been developed for the prediction of $N_2O$ emissions as a function of soil and climate characteristics and management practices (DNDC

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model; Li, 2000; Lugato et al., 2010). These models are highly attractive but require large numbers of input data that are not frequently available in practice, particularly for farmers' fields, and are often too costly in terms of computation time (Villa-Vialaneix et al., 2012). Numerous models with different degrees of complexity are available for predicting $N_2O$ emissions. Many of them have been presented in Heinen (2006).

We present here a new approach for predicting $N_2O$ emissions in experiment and farmers' fields. Our approach involves relating $N_2O$ emissions to the amount of applied N through an exponential function, the parameters of which are assumed to vary between locations. One of the major advantages of the proposed model (a statistical random-effects model) is that its parameters are easily adjusted to one or several location-specific $N_2O$ measurements, when such measurements are available. The adjusted model can then be used to predict $N_2O$ emissions for N fertilizer doses other than those applied at the considered location or in the farmer's field. This method does not require any information about soil and climate characteristics; these characteristics are taken into account through the single or small number of location-specific $N_2O$ measurements used to adjust the model.

The approach described here could be used in several applications. It could, for example, be applied to a farmer's field, to estimate background $N_2O$ emission (i.e., the emission occurring in the absence of N fertilizer application), or to estimate the consequences of decreasing or increasing the amount of N fertilizer applied by the farmer. Our approach can also be used at experimental sites at which a limited number of N doses are tested, to estimate $N_2O$ emission for other amounts of applied N, smaller or larger than those applied in the trial.

We aimed to assess the ability of two different random-effects models (one Bayesian, one frequentist) to predict $N_2O$ emissions from one or several location-specific $N_2O$ measurements for the locations for which $N_2O$ predictions were performed. We assessed the accuracy of model predictions and used the results to evaluate the benefits of adjusting random-effects models on the basis of location-specific measurements.

## 2. Material and methods

### 2.1. Data

We used the dataset of Stehfest and Bouwman (2006), discarding observations for amounts of applied N greater than 500 kg N $ha^{-1}$, because such high doses of fertilizer are not usually applied to farmers' fields (Roelandt et al., 2005; Spiertz, 2010; Tilman et al., 2002). The resulting dataset includes 985 $N_2O$ emission measurements, extracted from 203 publications. Each publication reported a set of $N_2O$ emission measurements for several N fertilizer treatments at a single location. Each paper corresponds to one specific site with two exceptions; Henault et al. (1998) and Lemke et al. (1998) where three sites in France and two sites in Alberta (Canada) were respectively considered. In all cases, all sites were located within the same climate category according to Stehfest and Bouwman (2006). $N_2O$ emission values ranged from 0.003 to 46.44 kg N $ha^{-1}$ $year^{-1}$, with a mean of 2.4 kg N $ha^{-1}$ $year^{-1}$ and a median of 1.07 kg N $ha^{-1}$ $year^{-1}$. These data were obtained for N fertilizer doses of 0–500 kg N $ha^{-1}$, with a mean of 124 kg N $ha^{-1}$ and a median of 100 kg N $ha^{-1}$. The number of doses tested at each location ranged from 1 to 13, with a mean of 2.54 and a median of 2. In total, 92 of the publications came from Europe, 57 from North America, 25 from Asia, 21 from Latin America and eight from Oceania.

### 2.2. Statistical models

Two random-effects models were considered (Philibert et al., 2012). Both used an exponential function to relate $N_2O$ to applied N and both assumed that the two parameters of this function varied randomly between locations. A nonlinear model based on an exponential function was proposed by Millar et al. (2010). Philibert et al. (2012) showed that models based on an exponential function outperformed linear models.

The two models used the same equation but differed in terms of the method used to estimate model parameters. One model was a frequentist method based on an approximate maximum likelihood method, whereas the parameters of the second model were estimated by a Bayesian method.

Both models are based on the following equations:

$$Y_{ijk} = \exp(\alpha_{0i} + \alpha_{1i}X_{ij}) + \varepsilon_{ijk} \quad (1)$$

with $\varepsilon_{ijk} \sim N(0,\tau^2)$, $\alpha_{0i} \sim N(\mu_0,\sigma_0^2)$ and $\alpha_{1i} \sim N(\mu_1,\sigma_1^2)$.

$Y_{ijk}$ is the $N_2O$ emission (kg N $ha^{-1}$ $yr^{-1}$) measured at the $i$th location ($i = 1, \ldots, 203$), for the $j$th applied N dose $X_{ij}$ ($j = 1, \ldots, N_i$), and the $k$th replicate ($k = 1, \ldots, K_{ij}$). $\mu_0$ is the log mean background emission, $\alpha_{0i}$ is the log location-specific background emission (random), $\mu_1$ is the log mean applied N effect, $\alpha_{1i}$ is the log location-specific applied N effect (random), and $\varepsilon_{ijk}$ is the residual error term. The random terms $\alpha_{0i}$, $\alpha_{1i}$ and $\varepsilon_{ijk}$ were assumed to be independent and normally distributed.

In the first model, the values of $\mu_0$, $\mu_1$, $\sigma_0$, and $\sigma_1$ were estimated by an approximate maximum likelihood method, with the nlme R statistical package (Pinheiro and Bates, 2000). The estimated values were $\mu_0 = 0.19$, $\sigma_0 = 0.72$, $\mu_1 = 0.0037$, $\sigma_1 = 0.0025$. In the second model, the parameters were estimated by a Bayesian method implemented with a Markov chain Monte Carlo algorithm (MCMC). In this second model, $\tau$, $\sigma_0$ and $\sigma_1$ had uniform and independent prior probability distributions—$\tau$, $\sigma_0$, $\sigma_1 \sim U(0.100)$—whereas $\mu_0$ and $\mu_1$ had normal and independent prior probability distributions: $\mu_0$, $\mu_1 \sim N(0,1000)$. The posterior distributions of the parameters were calculated with WinBUGS software (Lunn et al., 2000), with three chains of 100,000 MCMC iterations. The posterior means of $\mu_0$, $\sigma_0$, $\mu_1$ and $\sigma_1$ were equal to −0.21, 0.92, 0.0038, and 0.0032 respectively. Convergence was checked with the Gelman–Rubin method (Brooks and Gelman, 1998). Random-effects models were compared to fixed-effects models using AIC (Akaïke Information Criterion), BIC (Bayesian Information Criterion), and DIC (Deviation Information Criterion) (Bennett et al., 2013). All criteria were lower for the random-effects models and showed that the random-effects model performed better.

A comparison between fixed effect and random effect models has been presented in details in Philibert et al. (2012). Fixed-effect models are not considered in this study because it is not possible to fit the fixed effect models location by location; this type of model assumes that the parameter values do not vary across locations. No location-specific parameter estimate can thus be derived for this type of model. As the main purpose of this paper is to assess the value of deriving location-specific predictions, we focus here on random-effect models. Two types of $N_2O$ prediction can be performed with the considered random-effects models: average predictions and location-specific predictions. Average predictions are expressed as:

$$Y_{avg}(X) = exp(\hat{\mu}_0 + \hat{\mu}_1 X) \quad (2)$$

where $\hat{\mu}_0$ and $\hat{\mu}_1$ are the values of $\mu_0$ and $\mu_1$ estimated by frequentist or Bayesian methods (posterior means).

Location-specific predictions are calculated from one or several location-specific $N_2O$ measurements, as follows:

$$Y_{loc}(X) = exp(\hat{\alpha}_{0loc} + \hat{\alpha}_{1loc} X) \quad (3)$$

where $\hat{\alpha}_{0loc}$ and $\hat{\alpha}_{1loc}$ are the values of $\alpha_{0i}$ and $\alpha_{1i}$ estimated for the locations considered, from one or several $N_2O$ measurements obtained at the location concerned. In Eq. (3), $\hat{\alpha}_{0loc}$ and $\hat{\alpha}_{1loc}$ are equal to the best linear unbiased prediction (BLUP) of $\alpha_{0i}$ and $\alpha_{1i}$ (Pinheiro and Bates, 2000). In the second model, $\hat{\alpha}_{0loc}$ and $\hat{\alpha}_{1loc}$ are equal to the estimated expected values of the posterior distribution. Note that, in both cases, $\hat{\alpha}_{0loc}$ and $\hat{\alpha}_{1loc}$ can be calculated if at least one $N_2O$ value for one N fertilizer dose is available for the considered location.

### 2.3. Evaluation of model predictions with real data

Cross-validation was used to assess the prediction capacity of the frequentist random-effect model. Cross-validation was performed as follows:

- Step i: A location/dose combination was chosen and the corresponding data were removed from the dataset (i.e. all measurements of $N_2O$ emission corresponding to a given amount of applied N at a given location),
- Step ii: The parameters of equation (1) were estimated with nlme, excluding the data at step i,
- Step iii: The values of $\hat{\mu}_0$, $\hat{\mu}_1$, $\hat{\alpha}_{0loc}$ and $\hat{\alpha}_{1loc}$ obtained in step ii were used to calculate average and locations-specific predictions (Eqs. (2)–(3)) for the location/dose combination for which the data were removed in step i.

We did not consider locations for which data were available for only one N dose, because location-specific predictions could not be calculated for such locations by the cross-validation procedure described above.

Prediction accuracy was measured by calculating the root mean squared error of prediction (RMSEP) for both average and location-specific predictions. RMSEP was calculated separately, for four groups of locations differing in terms of the number of N fertilizer doses tested per location (Table 1). RMSEP values were also calculated for several ranges of N fertilizer doses used to predict $N_2O$ emission (Table 2).

The procedure described above was not used in the Bayesian model, due to the long computation times required (1200 s for each prediction). Predictions for a small number of location/dose combinations were calculated and evaluated, for