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A Markov chain method for simulating bulk density profiles in boreal peatlands

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ABSTRACT

Bulk density is a key determinant of numerous physical characteristics in peat including hydraulic conductivity, smouldering combustion vulnerability, and water retention in the unsaturated zone. A Markov chain model based on peat type (primarily Sphagnum, sedge, and sylvic peats) was applied to the depth-wise structure of boreal peatlands using 143 cores from western Canada as source data. Bulk density and peat type were modelled in 2160 simulated peat profiles by driving Markov chains associated with bulk density distributions by peat type and depth. The model closely reproduced the expected change in bulk density between vertically adjacent peat horizons. Markov-derived peat profiles showed somewhat greater variance in organic matter load in the upper 135 cm compared to observed cores due to the lack of whole-profile bias or trends in density. The method and derived Markov chains shown here have utility in hydrological modelling, regional carbon estimates, and in the modelling of disturbances such as wildfire.

1. Introduction

Northern peatlands store 500 ± 100 Pg of carbon (Yu, 2012); in Canada, these peatlands can be 2 m or more in depth, and typically store over 75 kg C m^{-2} (Beilman et al., 2008). The vulnerability of the carbon stored in these northern peat reserves to decomposition or wildfire combustion is dependent in a large part on key hydrological feedbacks that maintain a high water table position and high water content of the near-surface peat (Waddington et al., 2014). For many of these feedbacks, such as the water table-peat deformation feedback where the compression of peat during declining water tables imposes a concomitant decrease in hydraulic conductivity, the density and vegetative origin of the peat are key factors in determining the strength of the feedback (Whittington and Price, 2006). Peat bulk density has also been shown to influence key hydrological and carbon cycling processes such as unsaturated water retention (Weiss et al., 1998), specific yield (Boelter, 1968), smouldering combustion propagation (Benscoter et al., 2011), peat compression (Price et al., 2005), methane bubble storage (Kettridge and Binley, 2011), and methane bubble ebullition (Coulthard et al., 2009).

Current models of peatland biophysical processes (e.g. Kettridge et al., 2012a) are able to utilize detailed information on the vertical patterns of peat attributes such as unsaturated water retention or hydraulic conductivity which are determined in a large part by bulk density. However, there is currently no reliable method of producing such vertical patterns of peat density and other attributes beyond peat cores, which are limited in number and costly to acquire. Existing methods of simulating depth-wise peat density for use in models rely on linear trends (e.g., Bauer et al., 2006) and do not reproduce the often abrupt changes in peat properties that are the result of changes between previous ecosystem states (Kuhry, 1994). In organic soil combustion, such large density contrasts have recently been shown to limit the extent of smouldering (Benscoter et al., 2011). Moreover, existing datasets on the spatial patterns of peat bulk density and their associated properties therein are limited, resulting in an overly simplistic, and potentially incorrect, representation of peat stratigraphy in land surface models (e.g. Letts et al., 2000).

Stochastic simulations may provide a useful alternative to simple linear modelling of peat properties, and have the advantage of allowing for abrupt or non-linear patterns similar to those observed in the peat core record. We suggest that the first step towards to the ultimate simulation of a 3-D peat density structure is the use of the Markov chains for creating 1-D vertical simulated peat profiles of density and peat type. Markov chains have been widely used as a statistical technique to develop 1-D vertical profiles in the study of geological stratigraphy (e.g. Krumbein and Dacey, 1969). In an ecological context, Markov chains have been used in a variety of areas such as ecological transition modelling (Baltzer, 2000) and more recently in simulating the horizontal distribution of soil catenas (Li and Zhang, 2007).

Here we present a Markov chain model to describe vertical transitions in peat properties using a high resolution dataset of peat cores from a Canadian wetland database (Zoltai et al., 2000). Most existing

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databases for peat cores are coarse in vertical resolution, and often emphasize an economic peat resources component (e.g. Riley, 1987). Such databases often encompass only 3–4 peat samples per core, necessitating a linear extrapolation between samples that can approach 1 m in thickness. While high-resolution datasets of peat cores exist for carbon accumulation studies (e.g. Yu et al., 2003), such studies are focused primarily on carbon dating and thus largely exclude peat type, decomposition state, or other properties that influence physical processes such as hydraulic conductivity (Päivänen, 1973). Given the strong relationships between peat type and density (Päivänen, 1973; Thompson and Waddington, 2013; Fig. 1; Table 1), as well as the abundance of data on peat type peat macrofossil studies (Kuhry, 1994), a Markov chain framework driven by peat type is well-suited for driving simulations of vertical density and other peat properties.

Through the novel analysis of the Zoltai et al. (2000) data of boreal peat cores the objectives of this study were to: (1) determine the depth-wise distribution of peat types and density across differing peat types; (2) create a series of depth-stratified Markov chains of peat type for the creation of simulated peat profiles; and (3) to attribute physical properties (primarily density) to peat profiles simulated using Markov chains.

2. Methods

2.1. Source data

This model relies entirely on a set of selected data from the database (Zoltai et al., 2000) that we refer to as the Zoltai dataset. The database contains 626 vertical peat cores containing 6443 peat samples (sections of cores). In a majority of cases, only one peat core was taken from each site, so the Markov chains presented here are limited to vertical patterns and do not take into account any horizontal variation. Of the 626 sites in the database, all bogs and poor fens in the provinces of Manitoba, Saskatchewan, and Alberta were selected for a total of 143 peat cores. Of the cores used, 76 came from the Boreal Plain or Taiga Plain ecozones (Fig. 2), while 56 were taken from the Boreal Shield ecozone (Ecological Stratification Working Group, 1995). The remaining 11 cores were taken from the aspen parkland–Boreal Plain transition at the southern edge of the Boreal Plain. The subset of the larger database was selected because the sites share a similar continental climate and are generally forested and *Sphagnum*-dominated. The majority of peat samples were sectioned at 15 cm increments, though a small number of cores featured smaller or larger sampling intervals. While a large number of chemical parameters such as metal or nutrient concentration were measured for each peat sample, here we only examine a few key physical parameters: peat type, bulk density, and von Post's humification (von Post and Granlund, 1926). More detail on the additional parameters measured as well as collection and analysis techniques can be found in Zoltai et al. (2000).

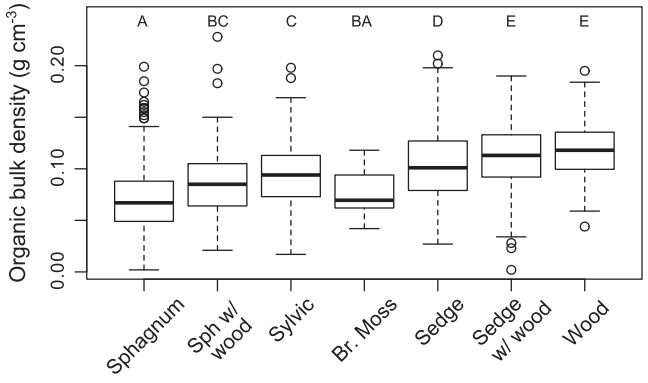

Fig. 1. Organic bulk density across all depths as a function of peat type. Letters above boxes indicated statistically significant differences in group mean via Tukey's Honest Significant Difference test.

Table 1
Analysis of variance of peat organic bulk density from Zoltai et al. (2000) as a function of peat type and depth interval.

	DF	*F*	*p*
Peat type	6	152.1	<0.001
Depth interval	8	51.1	<0.001
Type:depth	41	2.33	<0.001

2.2. Markov chains

A total of 72 cores within the Zoltai dataset (one half of the dataset) were randomly selected for the construction of Markov chains, while the remaining 50% was set aside as a control group. For each 15 cm depth interval, the change in peat type at the between-sample interface occurring in that depth interval was logged, and the count of each peat type transition (e.g. sedge to *Sphagnum*) was summed and divided by the total number of sample interfaces at that depth interval to calculate a probability of transition between the two peat types within a specific depth interval. Taken together, an empirically-derived Markov chain of peat type transition per depth interval was produced. Only Markov chains from the upper 135 cm (9 depth intervals) were constructed, as it limits samples to those distant to the basal peat where high inorganic content can modify physical properties.

Organic bulk density (subtracting the density due to inorganic content) was calculated using the equation:

$$\rho_o = \rho_b(1-f_{ash}) \quad (1)$$

where ρ_o is the organic bulk density (g cm^{-3}), ρ_b is the bulk density (g cm^{-3}), and f_{ash} is the ash proportion by weight (-). For each combination of peat type and depth with greater than 10 observations (37 combinations in total), the observed distribution of sample organic density found therein was fit to the Johnson distribution (Johnson, 1949) in the R programming language (R Core Team, 2012) using the SuppDists package (Wheeler, 2009) which is an implementation of fitting the Johnson distribution by quantile estimators (Wheeler, 1980). The Johnson distribution was fit to one of the three variants: (i) log normal; (ii) bounded; or (iii) unbounded; alternatively, a normal distribution was used where the fit exceeded that of any of the Johnson distribution variants. The three forms of the Johnson distribution are given by Hill et al. (1976) as:

(i) log normal: $z = \gamma + \delta \ln(x - \xi);\ \xi < x$
(ii) unbounded: $z = \gamma + \delta \sinh^{(-1)}\frac{x-\xi}{\lambda}$
(iii) bounded: $z = \gamma + \delta \ln\left(\frac{x-\xi}{\xi+\lambda-x}\right);\ \xi<x<\delta$

where z is a standardized normal variable and δ, γ, λ, and ξ are the four fitted parameters. The advantage of using the Johnson distribution is the ability to fit a range of distribution forms from normal to right-skewed and log-normal distributions within a single distribution under four unified parameters and a single computational step. For each combination of type and depth with insufficient sample size for a fit to the Johnson distribution (a total of 24 combinations), only a median was calculated. Despite being 40% of the total possible combinations of peat type and depth, these combinations only represent 7% of the entire population of samples in the portion of the Zoltai dataset used for model construction.

The Markov chain was initiated at the lowermost horizon (depth 120–135 cm) using a randomly selected peat type weighted according to the observed distribution of peat type at the 120–135 cm depth interval. The subsequent peat type for the layer above was selected following the probabilistic transition matrix (i.e. Markov chain; Table 2). For transitions into a different peat type the bulk density was independently sampled from the corresponding Johnson distribution for the peat type at the depth interval, or median bulk density if a sample size less than 10 was present. Changes in bulk density between adjacent samples of the same peat type was modelled not as an independent realization of