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Functional linear models to test for differences in prairie wetland hydraulic gradients

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Abstract: Functional data analysis provides a framework for analyzing multiple time series measured frequently in time, treating each series as a continuous function of time. Functional linear models are used to test for effects on hydraulic gradient functional responses collected from three types of land use in Northeastern Montana at fourteen locations. Penalized regression-splines are used to estimate the underlying continuous functions based on the discretely recorded (over time) gradient measurements. Permutation methods are used to assess the statistical significance of effects. A method for accommodating missing observations in each time series is described. Hydraulic gradients may be an initial and fundamental ecosystem process that responds to climate change. We suggest other potential uses of these methods for detecting evidence of climate change.

Keywords*: Wetland hydrology, prairie potholes, functional linear model, climate change.*

1. BACKGROUND

Data are increasingly being collected with automated data loggers such that the process of interest is measured nearly continuously in time. Standard statistical methods are not designed to account for this sampling resolution, but functional data techniques (Ramsay and Silverman, 2005) have been developed to model the differences in the (nearly) continuously measured processes in time. Functional linear models (FLMs) build on typical linear model structures but attempt to explain variability in functional responses, with functional regression and functional ANOVA (analysis of variance) being special cases. We describe these methods and motivate their use to explain differences in vertical hydraulic gradients across a set of fourteen locations in Northeastern Montana, USA.

1.1 Introduction

Our wetland study was motivated by wildlife and agricultural interests in the Prairie Pothole Region (Figure 1) on behalf of the U.S. Department of Agriculture's Natural Resources Conservation Service (NRCS). Resource managers recognize the importance of these wetlands to nesting and migrating birds, especially waterfowl. We explored the role that land use has on wetland hydrology in small, seasonal wetlands. Specifically, can we explain wetland hydrologic patterns based on certain factors: land use, soils, hydraulic conductivities, and landscape topography? Farming, grazing, and grassland restoration are known to affect wetlands (van der Kamp et al. 2002). Geologic processes from Pleistocene continental glaciations have generated extensive areas of pothole wetlands in Northcentral North America (Fullerton et al. 2004). The geomorphology of the landscape in the study area is dominated by processes typical of stagnation and recessional moraines, characterized by interrupted drainage (Winter 1989; Winter and Rosenberry 1995), hummocky terrain, and thousands of shallow wetlands. These landscapes have till, outwash, and lacustrine deposits, and other glacial features, and the mixture allows for subterranean hydraulic conduits affecting the movement of groundwater between wetlands. We are aware of no similar work in or near Montana, although van der Kamp and Hyashi (1998) and van der Kamp et al. (2002) in the Canadian prairies collected similar field data but they were not able to statistically test any hypotheses related to hydraulic gradients or water levels such as those proposed here. We propose a new analysis method to be able to test for effects on multivariate hydrologic time series with missing observations. Our study area receives about 70% of the precipitation of Winter's Cottonwood Lake study area, about 400km Southeast of ours, and we have observed that salt tolerant plants are more common in seasonal wetlands than farther East. The hydrology in semi-arid regions tends to be depression-recharge (Lissey 1971; van der Kamp and Hayashi 1998). We surmised that small changes in temperature and precipitation related to climate variability and change might result in near-term changes in wetland hydrologic processes.

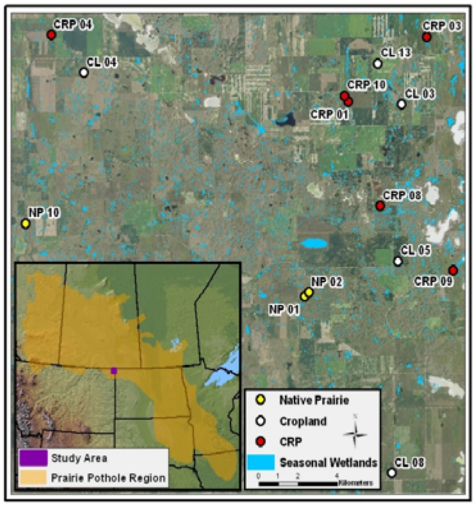

Figure 1. The inset shows the location of our study area within the Prairie Pothole Region. The photo shows study sites organized by land use type and all seasonal wetlands.

Study Site Selection Process:

The three land use types of interest were cropland (dryland wheat), native prairie, and lands retired from agricultural production under the Conservation Reserve Program (CRP). Uplands in this last category are planted to a mixture of grasses and legumes and are only grazed or hayed occasionally. We selected wetlands that were entirely surrounded by one of these types. Field sizes are smaller than catchments in this area, so we were not able to select wetlands with a single land use in the entire catchment. We applied the following nine criteria when selecting wetlands: (1)classified on the National Wetland Inventory as palustrine-emergent-seasonal (PEMC); (2)undrained; (3)soil series mapping units were either Dimmick, McKenzie, or Williams-Zahill; (4)agricultural landscapes were dryland spring wheat, cultivated at least 25 years; (5)CRP landscapes were planted between 1985-2001; (6)wetlands were 0.5-2.5 hectares; (7)wetland geometry was depressional and generally simple and round/oblong. Linear wetlands were not considered. (8) >100m from a road; (9)access was made available through NRCS, the Conservation District, or the USDI-Fish and Wildlife Service. We included two wetlands in native prairie on a Waterfowl Production Area (WPA) previously instrumented by Montana State University for a similar (but abandoned) study. Although that WPA, itself, had not been selected at random, wetlands within it had been and comply with all criteria.

Spatial data were secured from the Montana Geographic Information Clearinghouse (http://www.nris.state.mt.us/gis/). There were 821 PEMC wetlands in the Missouri Coteau of Sheridan County; and 567 met the selection criteria (other than access). We then instrumented selected wetlands, in priority provided by random numbers, with a maximum of ten (the number we could physically instrument with augered wells) in each land use. Equipment failure (e.g., destruction by cattle, flooding, etc.) or other logistical problems, resulted in there being data from 14 wetlands, 5 cropland, 3 native prairie, and 6 CRP, and a total of over 53,000 observations obtained during the 2009 field season.

1.2 Measuring Vertical Hydraulic Gradient

A key interest was whether a site was dominated by groundwater discharge (i.e., greater hydraulic head with increasing depth in the subsurface, causing water to move from the shallow aquifer towards the wetland) or by groundwater recharge (i.e., decreasing hydraulic head with depth in the subsurface, causing water to move into the shallow aquifer from the wetland). A groundwater well and a piezometer were installed less than a meter apart at each site. Groundwater wells were screened for their entire length and provided a measurement of the top of the saturated portion of the aquifer, or height of standing water if present. Piezometers were screened along a short interval at their base, providing the hydraulic head of the aquifer at the depth of the screen midpoint. The calculation of vertical hydraulic gradient depends on whether there is standing water in the wetland. In both cases, the difference in water levels between the groundwater well and piezometer is determined. When there is standing water, this difference is divided by the distance from the piezometer screen midpoint to the sediment-water interface. When no standing water is present, this difference is divided by the distance from the piezometer screen midpoint to the water level in the groundwater well (Figure 2). Hydraulic gradients vary over time and space and are related to the 3-D distribution of hydraulic conductivity of the sediment, precipitation, and evapotranspiration. Well pairs were constructed using polyvinyl chloride pipe with a diameter of 3.81 cm (piezometer) or 5.08 cm (groundwater well). Each was equipped with a capacitance rod data logger recording water height, in mm, every half hour. Due to the close spacing of the well pairs, differences in water heights is assumed to represent vertical gradients, calculated with no horizontal component.

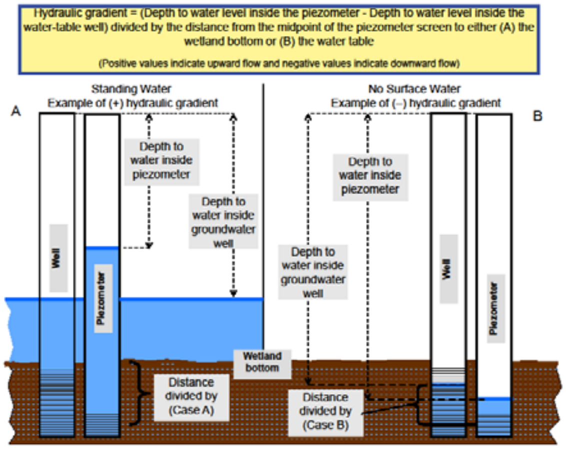

Figure 2. Schematic of how vertical hydraulic gradients were measured.

1.3 Explanatory Variables

Four explanatory variables were thought to directly affect groundwater-surface water interactions, based on either the ability of material to transmit water or the amount of water and its associated head. These are surrounding land use type, horizontal hydraulic conductivity (K), area of surrounding wetlands, and soil properties. To determine the hydraulic conductivity of the sediments beneath and adjacent to the wetlands, slug tests were performed on both the groundwater and piezometer wells (Bouwer and Rice 1976). Both falling and rising head tests were conducted on the piezometers, however, due to low water levels in the groundwater wells, only rising head slug tests were performed on them. The average of all available K measurements for each site was used. The area of wetlands was calculated by delineating a buffer of one kilometer around each study wetland. The lowest point of all wetlands with any portion of their area in that buffer was determined and the area of all wetlands topographically above the site was calculated. A final variable was based on the textual and chemical properties of the soil. Soil samples were collected from each wetland and analyzed by the USDA for particle size using the hydrometer method (Gee and Bauder, 1996). Of particular interest was the percent of clay minerals at depths of 0-15 cm and 35-50 cm because it may restrict flow. We also sampled Sodium, Calcium, and Magnesium at a depth of 35-50 cm because groundwater discharge in wetlands can concentrate such cations (Richardson et al. 2001; Knuteson et al. 1989) at these depths (Richardson and Hanson 1977). These five soil characteristic variables (Sodium was log-transformed because of skew) were combined using a principal components analysis with the first PC, which was most highly (negatively) correlated with log10-Sodium, Calcium, and Magnesium, used in the analysis (further exploration of each variable used in the PCA yielded similar results as those for the first PC discussed below).

The fourteen vertical hydraulic gradients that were analyzed from the 2009 field season are presented in Figure 3. We note that not all piezometers were started at the same times due to slug tests being performed, instrument failure, and water levels outside the measurement ranges. Diurnal patterns are present in some locations and not in others; e.g., NP02 and CRP08 show similar trends, but CRP08 contains high frequency variation that NP02 does not. In other locations, diurnal variation seems to be present at various times and absent in others. On average, 62 days of measurements are available for the fourteen locations (minimum=13, maximum=109), with measurements were taken every 30 minutes. The functional data approach converts this large volume of time series measurements into continuous functional representations for each location with a total sample size of 14.

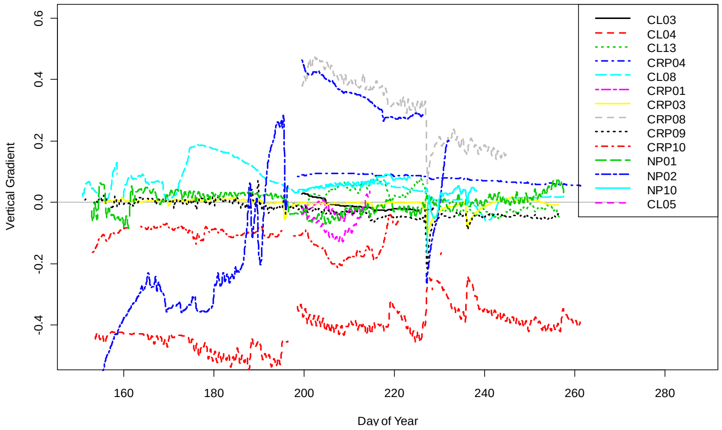

Figure 3. Plot of estimated vertical gradient functions. Note their position relative to the zero reference line. Values over zero indicate discharge, below zero recharge.

2.1 Functional Data and Functional Linear Models

Functional data analysis begins with converting each time series, y_t, into a functional representation, $y(t)$, using the model $y_t = y(t) + e_t$, where the subscript t is used to indicate the measurement is discrete in time, (t) indicates a continuous function of time, and e_t the random error at time t. Smoothing or penalized regression spline techniques with cubic B-spline basis functions are typically used to estimate $y(t)$. The choice of knots, locations where the piecewise polynomials are joined, is the first step in determining the flexibility of the estimated continuous function when estimated by penalized regression splines. Generalized cross-validation (GCV) is recommended to select an optimal amount of smoothing given the initial choice of knot locations. This can be performed using a generalized additive model as in `mgcv` (Wood, 2006) in R (R Development Core Team, 2009). The function `gam` was used to estimate the continuous functions using an adaptive smoothing algorithm, which allows the function to be rougher or smoother depending on local features in t. We used four knots per day and GCV to select the optimal estimate for each series, augmenting the effective degrees of freedom, a measure of complexity of the estimated spline function, by a multiplier of 1.4 as suggested by Kim and Gu (2004) in the GCV formula.

The FLM (Ramsay and Silverman, 2005) is defined as $\mathbf{Y}(t)=\mathbf{X}\boldsymbol{\beta}(t)+\boldsymbol{\varepsilon}(t)$. The components of the model are: $\mathbf{Y}(t)$ of dimension $nx1$ with n functional observations defined continuously over t; $\mathbf{X}$ is an nxp design matrix (see, e.g., Kutner et al., 2004); $\boldsymbol{\beta}(t)$ is a $px1$ vector of slope coefficients, usually including an intercept coefficient; and $\boldsymbol{\varepsilon}(t)$ is an $nx1$ vector of continuous residual error functions. Functional linear models are estimated using the `fRegress` function from the R package `fda` (Ramsay et al., 2010). Nonparametric techniques are typically used for hypothesis testing in these models since distributional assumptions for $\boldsymbol{\varepsilon}(t)$ are difficult to assess and to validate. Permutation testing methods make the less restrictive assumption of exchangeability of observations under the null hypothesis of interest.

Shen and Faraway (2004) suggest a test statistic for FLMs based on the sum of integrated squared residuals, e_i^2, $SSE_I = \sum_{i=1}^{n} \int e_i^2(t)dt$ and the total sums of squares, $SST_I =$

$\sum_{i=1}^{n}\int(y_i(t)-\hat{\mu}(t))^2dt$, where $\hat{\mu}(t)$ is the overall mean. Using these sums of squares and the typical ANOVA degrees of freedom, they define $F_I=MST_I/MSE_I$ and provide an approximate parametric distribution for hypothesis testing with F_I. Delicado (2007) suggests a permutation approach to finding the sampling distribution for F_I. Ramsay and Silverman (2005) define an alternative continuous F-statistic, $F(t)$, which is the point-wise application of the typical F-statistic and built on functional versions of the sums of squares for treatment, $SST(t)$, and error, $SSE(t)$. Ramsay et al. (2009) suggest using the maximum of $F(t)$ over t in a permutation test statistic. In simulations, Greenwood (submitted) found that F_I significantly outperforms $max(F(t))$, so we focus on F_I.

Delicado (2007) shows that the integrated sums of squares in F_I can be calculated by defining the distance, D_{ij}, between functions i and j as $D_{ij}^2=\int\left(y_i(t)-y_j(t)\right)^2dt$. This is the same definition used generally in calculating the *pseudo-F* statistic from permutational MANOVA (perMANOVA, Anderson, 2001). PerMANOVA is similar to standard MANOVA, but the test statistic is calculated directly from the distances between the responses. It has a decade of application in Ecology, partially because it is legitimate whether the dissimilarity measure is a full distance metric or not. To use perMANOVA for FLMs, the first step is to calculate the distance matrix, D_{ij}^2, between the responses. We integrate the squared difference of the two functions using a trapezoidal rule numerical integration. A function for performing perMANOVA, called `adonis`, is available in the R package `vegan` (Oksanen et al., 2010). It is also possible to perform perMANOVA tests in PC-ORD (McCune and Grace, 2002) and PRIMER-E (Clarke and Gorley, 2006). In perMANOVA, constraining the permutations within a blocking variable, such as our stratifying site type, is recommended where the design warrants it.

Vertical gradient data have missing observations in each series, as well as different starting and end points for each location. We want to maximize information used, so truncating the data set to only consider times with complete records leads to a short window of time to compare the locations. Using pairwise comparisons, we can compare each pair of locations using all common times of observation, estimating the difference based on all times of co-observation. The pairwise differences are standardized to account for differences in length of records compared. We accomplish this by estimating a function using a first order (constant) B-spline function, $I(t)$, that is 0 if y_t is missing at t and 1 if y_t is obtained at t. For any pair of locations, we can find the total time of common measurement as $\lambda=\int I_i(t)I_j(t)dt$. A new distance measure is defined to “standardize” the distance based on the time of common observation, $D_{ij}^2=\int\left(y_i(t)-y_j(t)\right)^2 I_i(t)I_j(t)dt/\lambda^2$, providing the difference per day between functions i and j, D_{ij}. This is a new extension for the distance-based approach to testing in FLMs. Our methods would reduce to the standard pairwise distance if the series were all observed over the same time. Due to the different times of comparison, it is possible for this measure to fail to meet all the properties of a distance metric. This is not problematic for applying the perMANOVA methods, but does represent an extension of the typical F_I. Calculating this augmented distance requires two numerical integrations with the numerator incorporating a weight function based on $I_i(t)I_j(t)$ to provide a weight of one where both functions are observed and zero otherwise. With this distance matrix in hand, we can test for effects of our explanatory variables on the observed vertical hydraulic gradients using our modified version of F_I.

3.1 Results

Little is known in the literature about the variables related to vertical hydraulic gradients measured at the resolution we considered. We chose to investigate whether land use affects hydraulic patterns, but other variables are thought to either (1)explain recharge versus discharge behaviour at locations, or (2)change as a function of long term recharge or discharge patterns. Winter (1989), Winter and Rosenberry (1995), and van der Kamp and Hayashi (1998) showed that wetlands topographically higher than a given wetland often contributed groundwater via discharge to that wetland. Thus, we hypothesized that the amount of wetland area topographically higher than the wetland of interest could be related to differences in the gradients, with greater amount of topographically high wetlands related to increased groundwater discharge. Gradients could be related to characteristics of the local soils such as hydraulic conductivity, percent clay, or Calcium, Magnesium, and Sodium concentrations. These cation concentrations can serve as proxies for term local groundwater discharge. To help control the number of tests, a principal component analysis of soil characteristics was used to reduce the dimension of these characteristics; the first principal component score was used as an explanatory variable. Horizontal hydraulic conductivity (K) values were thought to influence local vertical hydraulic gradients, but were skewed so were $\log_{10}$ transformed.

Four different hypothesis tests were considered to look for effects that significantly explain variation in the fourteen hydraulic gradients. Due to the small sample size, models including interactions were not considered, although future studies with larger sample sizes should explore reasonable interaction effects. For tests of quantitative explanatory variables, the permutations are constrained within land use type to reflect the stratified random sampling of sites. Testing for a land use effect is performed with unconstrained permutations. Of these tests, only $\log_{10}$-transformed K-values were significant in explaining differences in the hydraulic gradients with a *pseudo-F* of 6.0 and p-value of 0.0356. This test was based on 10,000 randomly sampled permutations, constrained within site type. With no constraints, the p-value was estimated to be 0.0161, but the constrained estimate is a more accurate and robust estimate of the p-value. None of the other tests were significant. PC1 of the soil data (p-value=0.41) and wetland area above each site (p-value=0.46) were not significant based on permutations constrained within land use type. For the land use effect, evaluated with unconstrained permutations, the p-value was 0.45.

3.2 Conclusions and Recommendations

By exploring gradients between wetlands over time, we found a significant difference in vertical hydraulic gradient based on horizontal hydraulic conductivity. Smaller conductivities (i.e., less permeable material) were associated with greater vertical gradients (i.e., more prominent discharge). At first, this might seem counterintuitive from the perspective of water moving towards the wetland (laterally or vertically) being less restricted when coarse-grained materials exist. But, the opposite is also true: the probability of water leaving the wetland to recharge the aquifer is also greater with coarse-grained materials. If groundwater recharge is impeded by tight materials, then the opportunity exists for evapotranspiration to drive the system, essentially pulling water towards the surface from those tight materials. Generally, wetland soils in the Coteau are dominated by clay rich tills. However, till can also have preferential flow paths within itself due to vertical fracturing (Grisak and Cherry 1974), or can be underlain by fluvially reworked glacial sediments such as outwash that are typically dominated by coarse-grained materials.

No differences were detected based on land use, textural and chemical soil properties, or the acreage of surrounding wetlands. While the sample size was small, land use does not appear to explain the differences in hydraulic gradients. However, our subjective observations allow us to perceive differences in wetland vegetation, which is thought to respond strongly to hydrologic parameters over relatively short time frames (Cronk and Fennessey, 2001; Kantrud et al., 1987). It is thought that agricultural production results in less surface water in prairie wetlands when compared to wetlands in native prairie catchments (van der Kamp et al., 2002). We were unable to demonstrate these effects on vertical hydraulic gradient in this study, possibly due to working near the end of a drought period when soil moisture may not have equilibrated towards wetter conditions. Richardson et al. (2001) has indicated that layers with increased carbonate levels may occur at depths (e.g., development of a K horizon) in wetland soils due to groundwater discharge over time periods required for soil formation. Our short term vertical gradient measurements did not show a relationship with soil properties measured. Lastly, wetland acreage topographically higher or lower than the study wetland did not exhibit a relationship with hydraulic gradients. This, too, may stem from soil moisture levels in the catchments still reflecting a relatively dry prior time period.

This analysis does not directly address climate change, except as it pertains to understanding variables that were associated (or not) with variability in vertical hydraulic gradients. However, similar FLMs could be used to assess evidence for change over time in data collected at "high" time frequency, where natural breaks in long time series exist. Specifically, temperature, streamflow, and snow pack are often delineated by "water year" or calendar year and are measured on at least a daily basis and are fraught with missing observations, making them prime candidates for this adaptation of functional linear models. For a single location, a trend test can be constructed using year to explain the changes in, for example, a yearly temperature function. We applied the same functional linear models to an analysis of daily temperature from 1911 to 2008 from the Medicine Lake, MT weather station, the weather station that was closest to our study area in the U.S. Historical Climatology Network (Easterling et al., 1996, http://cdiac.ornl.gov/epubs/ndp/ushcn/ushcn.html). A linear trend test provides evidence of a significant linear change in the yearly minimum temperature profiles (p-value=0.0002) but less evidence for a trend in the daily maximum temperatures (p-value=0.0504). The result for this location is not inconsistent with other studies documenting evidence of temperature change in Montana over the same time frame; Pederson et al. (2010) found evidence of linear trends in Montana temperatures after averaging temporally and spatially. The significant trend in minimum temperature curves could be due to a variety of types of change, from an overall shift to a change in the shape of the "average" minimum temperature curve, modifying the timing of the warmest or coolest parts of the year. These methods can detect nearly any type of consistent change in the functions over time, which is both their strength and weakness; finding a significant result is just the first step in understanding how the system is changing over time. Prior to the development of methods that can tolerate missing observations in functional data, we could not have addressed the first fundamental research question: Is there evidence of changing temperatures in this area?

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