

1 **Technical Note: A bootstrapped Loess regression**
2 **approach for comparing soil depth profiles**

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9 **Abstract**

10 Understanding the consequences of different land uses for the soil system is important to better
11 inform decisions based on sustainability. The ability to assess change in soil properties,
12 throughout the soil profile, is a critical step in this process. We present an approach to examine
13 differences in soil depth profiles between land uses using bootstrapped Loess regressions
14 (BLR). This non-parametric approach is data-driven, unconstrained by distributional model
15 parameters and provides the ability to determine significant effects of land use at specific
16 locations down a soil profile. We demonstrate an example of the BLR approach using data
17 from a study examining the impacts of bioenergy land use change on soil organic carbon
18 (SOC). While this straightforward non-parametric approach may be most useful in comparing
19 SOC profiles between land uses, it can be applied to any soil property which has been measured
20 at satisfactory resolution down the soil profile. It is hoped that further studies of land use and
21 land management, based on new or existing data, can make use of this approach to examine
22 differences in soil profiles.

23

24 **1 Introduction**

25 Understanding the consequences of different land uses for the soil system is important to better
26 inform decisions based on sustainability (Foley et al., 2005; Haygarth and Ritz, 2009). The
27 ability to assess change in soil properties effected by altered land use or management is
28 therefore a critical step in this process. Greatest change is likely in the surface layers with
29 factors such as tillage and plant inputs impacting the physical, chemical and biological
30 properties of the soil. Many soil properties, however, will also be modified below this depth,
31 particularly as time since land use change (LUC) increases (Popelau et al., 2011). It is therefore
32 important that changes can be assessed below the topsoil and throughout the soil profile.

33 As a prime example, a number of studies, including global meta-analyses, have summarised
34 the impacts of LUC on soil organic carbon (SOC) concentration and stocks (e.g. Guo and
35 Gifford, 2002; Maquere et al., 2008; Laganière et al., 2010; Poeplau et al., 2011). SOC (*sensu*
36 organic matter) is generally concentrated in the top 30 cm of the soil and so LUC is generally
37 expected to have the greatest impact on SOC in these upper layers (Lorenz and Lal, 2005;
38 Laganière et al., 2010). Even within this surface soil, however, the magnitude and sometimes
39 direction of the effects of LUC on SOC can depend on the depth that is being considered (Guo
40 and Gifford, 2002; Popelau et al., 2011). It is also becoming more evident that, in addition to

41 there being a large proportion of total SOC stocks resident in the subsoil, important C dynamics
42 may also occur deeper in the soil (Jobbágy and Jackson, 2000; Lorenz and Lal, 2005).

43 The turnover time of SOC generally increases with depth and hence the stabilisation of C
44 may take place in deeper soil. Stabilisation pathways are likely through biochemical
45 stabilisation driving reduced decomposition, by the inherent recalcitrance of root litter (e.g.
46 lignins) and by physicochemical stabilisation (e.g. complexing with minerals and clay in
47 subsoils)(Lorenz and Lal, 2005). Conversely, priming of the decomposition of older SOC may
48 occur following LUC, especially with woody species (see Fontaine et al., 2007). This is
49 particularly relevant for LUC to perennial vegetation or forest where deeper rooting plants are
50 involved. For example, the root systems of perennial or tree species are likely to be more
51 permanent and extensive in the subsoil, with a greater contribution of recalcitrant litter and
52 potential priming down the soil profile (Fontaine et al., 2007). Altered land use or management
53 may also impact the translocation of particulate and dissolved organic C likely to occur down
54 the soil profile via effects on leaching. Such mechanisms may produce more complex
55 relationships between soil depth and soil characteristics, and even discontinuous horizonation,
56 rather than linear gradients.

57

58 **2. Existing approaches to model soil depth profiles**

59 Differences in SOC across transitions and soil depth profiles can be tested with both land use
60 and depth included as fixed factors in an interaction model, and appropriate random terms to
61 account for non-independence of depth increments within the same core and/or plots. There
62 are, however, various potential modelling approaches that have been used to examine soil depth
63 profiles including, for example, modified exponential decay (Maquere et al., 2008), depth
64 distribution functions which utilise multiple regression (Indorante et al., 2013) and spline
65 functions (Bishop et al., 1999; Malone et al., 2009; Wendt and Hauser, 2013). Another common
66 method for non-linear modelling is the use of Generalised Additive Models (Hastie and
67 Tibshirani, 1990).

68 Recent work modelling depth profiles has focussed on deriving parametric non-linear
69 relationships between soil depth and the response of interest. Maquere et al. (2008) adopt a
70 parametric form with modified exponential decay, whereas Myers et al. (2011) use an approach
71 based on asymmetric peak functions. Whilst capturing the non-linear form of the soil depth
72 profile, neither exponential decay nor polynomial methods adequately handles the associated
73 uncertainty and hence confidence intervals, with the method in Maquere et al. (2011) assuming

74 a *t*-distribution and the method in Myers et al. (2008) failing to produce confidence envelopes
75 at all. Regression-based approaches similar to the popular GAM method have also been
76 adopted using multiple covariates to account for any non-linearity (Indorante et al., 2013) and
77 fitting cubic splines directly (Wendt and Hauser, 2013). However, the multiple regression
78 approach assumed a normal distribution of the response variables, which is often not realised,
79 and the cubic spline method presented by Wendt and Hauser does not provide any measure of
80 uncertainty.

81 Non-linear relationships between SOC and soil depth across LUC transitions can also be
82 incorporated by the inclusion of flexible splines (Bishop et al. 1999; Wood, 2003; Malone et
83 al. 2009). In particular, the use of equal-area smoothing splines has long been considered as a
84 beneficial approach to alleviate issues of modelling continuous soil depth functions using
85 increment or horizon data (Bishop et al. 1999) and recent work has utilised the approach in the
86 large-scale mapping of soil properties (Malone et al. 2009; Odgers et al. 2012; Adhikari et al.
87 2014). Equal-area spline functions consist of locally fitted quadratic functions tied together
88 with knots at horizon boundaries (Malone et al. 2009), and the areas under/over the fitted curve
89 optimised for equality in each horizon (Bishop et al. 1999). Confidence intervals and
90 significance tests are, however, based upon the assumption that the response variable is drawn
91 from the exponential family of distributions and inference is very sensitive to this assumption.
92 Malone et al. (2009), in their study mapping continuous depth functions of SOC and water
93 storage, highlighted the need for better estimation of uncertainty in such model outputs,
94 suggesting the use of simulation and re-sampling approaches.

95 Simulation and re-sampling techniques avoid the necessity to assume a distributional form
96 for the response variable in order to obtain confidence intervals and test hypotheses. Such
97 approaches are rarely used to investigate soil depth relationships despite the often flawed
98 assumptions made by the more commonly applied methods. Clifford et al. (2014) adopted a
99 simulation routine from a master database to impute missing values and this clearly
100 demonstrated another strength of the simulation approach, though they did not apply the
101 method directly to test specific hypotheses relating to changes along the soil profile.

102 We sought to develop an approach which 1) would be able to compare and test for
103 significant differences between potentially non-linear depth profiles of land uses (or across
104 land use transitions), 2) did not need to meet any parametric distribution assumptions given
105 that individual datapoints in soil datasets are typically non-independent (i.e. vertically or
106 horizontally nested measurements) and 3) would be generally applicable regardless of specific

107 contexts of land use and soil type. Below, we describe the resulting non-parametric approach
108 and provide an example comparing SOC depth profiles across a land use transition.

109

110 **3. A bootstrapped Loess regression (BLR) approach**

111 The developed approach combines bootstrapped resampling of data with local least squares-
112 based polynomial smoothing (Loess) regression. Consequently, this non-parametric method
113 benefits from being data-driven and unconstrained by distributional form or rigid model
114 parameterisation. Like spline approaches (Malone et al. 2009; Wendt and Hauser, 2013), it
115 doesn't assume constant values for soil layers or horizons. Such a non-parametric approach is
116 highly suitable where data are non-independent. This is particularly applicable in soil profiles
117 where measurements made in depth increments down a soil profile may be correlated and even
118 more relevant where data are cumulative (e.g. cumulative C stocks). It is also appropriate where
119 soil cores have been sampled using a nested spatial design with multiple cores taken from
120 within plots.

121 The BLR approach is intended to make use of soil data which has been measured at fixed-
122 depth intervals down the soil profile at a generally high resolution, or at least at a resolution
123 satisfactory for the purposes of an assessment. The vertical sampling resolution is not limited
124 to any specific depth interval (e.g. 10 cm increments) but clearly a greater, and regular,
125 resolution provides more detailed information on potential differences and their specific
126 location in the soil profile. Low sample sizes will affect the amount of smoothing that can be
127 done by the Loess algorithm. As the algorithm fits polynomial regressions within local
128 neighbourhoods, the definition and size of the neighbourhood determines the smoothness and
129 sensitivity of the fitted regression line. Typically a minimum of 3 observations per
130 neighbourhood would be required.

131 The initial dataset comprises all data for the soil variable of interest from the two land uses
132 ($LU_1 \cup LU_2 = LU_{ALL}$) which are to be compared, with the associated depth and/or soil mass as
133 reference. A subset is then created containing only data from the 'second' land use (LU_2). In
134 theory, it doesn't matter which of the land uses are subsetted for LU_2 but one may be more
135 intuitive given the direction of a specific land use transition. It is also useful to plot the data to
136 determine whether the datasets contain outliers that may need to be excluded before
137 bootstrapping to prevent skewing the Loess regression. For cumulative mass-based data, if
138 datapoints from the bottom depths of either LU_1 or LU_2 are at distinctly greater cumulative
139 masses than others, these could also be trimmed so that the comparison is made to the same

140 approximate lower bounds of the reference. Using a large number of bootstrap samples,
141 however, should negate the need for extensive data cleansing prior to analysis.

142 The combined data (LU_{ALL}) is re-sampled by bootstrap with replacement, with the number
143 of data-points resampled equal to the number of data-points in LU_2 . This is repeated $n=1000$
144 times. Each bootstrapped set of data are then modelled using Loess regression and these
145 regressions are used to generate 95% confidence intervals around a modelled soil depth profile
146 by taking pointwise percentiles at each depth. As each sub-sample is taken from the union of
147 the two land uses, this confidence interval (or confidence envelope) represents the null
148 hypothesis that there is no difference between the LU_1 and LU_2 . The data from only LU_2 is then
149 modelled using Loess regression; if the modelled line for the LU_2 profile sits outside the
150 confidence envelope of the null hypothesis it can be inferred that the soil variable is
151 significantly different between LU_1 and LU_2 at that particular point in the profile. Overall P
152 values for the difference between depth profiles can be obtained by taking normalised test
153 statistics across the full set of bootstrap samples and taking the percentile of these values
154 corresponding to the same statistic obtained from the LU_2 data. This is a similar approach to
155 that adopted in the spatial statistics literature when analysing K functions under resampling as
156 demonstrated in Diggle et al. (2008) and Henrys and Brown (2009) for example.

157 This relatively straightforward non-parametric method may be most useful in comparing
158 SOC profiles between land uses, but it can be applied to any soil property which has been
159 measured at satisfactory resolution down the soil profile. Many of these other properties
160 measured in soil (e.g. bulk density, pH, root biomass) can vary in a non-linear fashion down
161 the soil profile, with potential horizonation. The effects of land use change are typically
162 examined using either a paired-site or chronosequence approach. These assume that each
163 paired or chronosequence site only differs in their age or, for example, time since disturbance
164 and have comparable biotic and abiotic histories (Laganière et al., 2010). While this BLR
165 method benefits from being unconstrained by assumptions of parametric methods, it must
166 still satisfy the assumptions of the paired-site and chronosequence approaches, particularly if
167 space-for-time substitution is used (Indorante et al., 2013). Here, we provide an example
168 comparing SOC depth profiles between land uses. The approach is, however, not limited to
169 comparing soil depth profiles between land uses. It could also be usefully adopted to
170 examine, for example, depth functions in lake systems or to compare temporal trajectories in
171 soil metrics between experimental treatments.

172

173 **4. Applying a BLR approach - an example of bioenergy land use change**

174 The bootstrap re-sampling and Loess regression used to test differences between soil profiles
175 was conducted using the R statistical programming language (R Core Team, 2015). Example
176 code to demonstrate the BLR approach using real data are available via
177 <http://doi.org/10/f3jp5d> (Keith et al., 2015). These data are from a study examining the
178 impacts of bioenergy LUC on SOC in the UK (Rowe et al., 2016). A LUC transition from
179 arable to Short-Rotation Coppice (SRC) willow was selected and the data were separated into
180 subsets of those from each component of the transition (i.e. arable and SRC willow samples)
181 before analysis. Data on SOC concentration (expressed as a percentage), cumulative SOC
182 stock and cumulative dry soil mass were derived at 10 cm increments to 1 m depth in order to
183 construct fixed-depth profiles of SOC concentration (Figure 1a) and mass-based depth
184 profiles of SOC stocks (i.e. the relationship between soil mass and SOC *sensu* Gifford and
185 Roderick, 2003) (Figure 1a). Cumulative soil mass was used because measured SOC stock in
186 small fixed-depth increments (as was required in this study) may not be directly comparable
187 across LUC transitions, due to potential variation in bulk densities and any compression or
188 expansion introduced through sampling (e.g. Gál et al., 2007). An approach using soil mass
189 as the independent variable overcomes this issue more generally because profiles can be
190 directly compared at a particular reference soil mass (Gifford and Roderick, 2003; Wendt and
191 Hauser, 2013). Gifford and Roderick (2003) suggest a reference dry soil mass of 4000 t ha⁻¹
192 and 12000 t ha⁻¹ may be used to approximate sampling to 30 cm and 1 m depth in agricultural
193 systems, respectively. This is not an issue when examining SOC concentration, as these data
194 are not directly influenced by core volume and apparent bulk density.

195 There was generally a good fit between observed and modelled data, with all modelled
196 means well within a standard deviation of the observed means in each depth increment, and
197 the majority very close to the actual observed mean (Supplementary Figure 1). The poorest
198 fits appeared to be for SOC concentration around the plough layer of the arable land use (20-
199 40 cm; Supplementary Figure 1a) and in the upper layers of the SRC willow land use (0-20
200 cm; Supplementary Figure 1c). The RMSE values for the depth profiles were 0.037, 0.487,
201 0.028 and 0.929 for arable SOC concentration, arable SOC stock, SRC willow SOC
202 concentration and SRC willow SOC stock, respectively.

203 Individual datapoints for each land use, the confidence envelope of the null hypothesis and
204 the modelled profile for the SRC willow were plotted following BLR (Figure 1). Where the
205 modelled line sits outside the confidence envelope it can be inferred whether there are
206 significant effects of land use in the soil profile, at either a particular depth or references soil
207 mass. In Figure 1a, the SOC concentration is significantly greater under SRC willow

208 compared with arable at 10 cm and 20 cm, where the modelled line sits to the right of the
209 confidence envelope. The modelled line sits within the confidence envelope between 40 cm –
210 100 cm and so there is no significant difference (Figure 1a). Nevertheless, the two depth
211 profiles are significantly different overall ($P < 0.01$). The depth profile of SOC concentration
212 is reflected in the cumulative SOC stock profile, with the modelled line for SRC willow
213 moving further from the confidence envelope up to approximately 5000 t ha^{-1} (Figure 1b).
214 The difference in cumulative SOC stock between arable and SRC willow is maintained to
215 100 cm and, consequently, is significantly different down the whole soil profile ($P < 0.01$;
216 Figure 1b).

217

218 **5. Conclusions**

219 We modelled soil profiles and tested differences in soil characteristics between land use or land
220 management using a non-parametric approach combining bootstrap sampling and Loess
221 regression. The development of this approach was driven by a need for a flexible method which
222 could compare potential non-linear relationships between land uses (or across land use
223 transitions) and would not be constrained to specific contexts. While there are several other
224 methods which can be used to model non-linear relationships in soil depth profiles, the BLR
225 approach is flexible because it is data-driven and does not need to meet any distributional
226 assumptions. The confidence envelopes obtained are robust to miss-specification of the error
227 distribution and provide clear inspection of significant differences across the full depth profile.
228 There can be issues of model fit when profiles are discontinuous or change abruptly. This is
229 not exclusive to the BLR approach though and it also affects equal-area spline models (see
230 Odgers et al., 2012). It has been proposed that the use of pseudo-horizons may help towards
231 overcoming this challenge (Malone et al. 2009; Odgers et al., 2012). We acknowledge that in
232 some circumstances the equal area spline functions are a viable alternative to Loess regression
233 for producing a fitted profile. This could, however, easily be incorporated into the non-
234 parametric estimation and bootstrapping framework that we present here.

235 Sampling to depth and increasing the resolution of depth increments can provide useful
236 profiles or ‘fingerprints’ of soil properties under different land uses and soil types. In particular,
237 assessment of SOC to depth, and determining the response of SOC to land use change (LUC)
238 or land management change is essential to understand the sustainability of different soil use
239 options. This may be particularly important for land-use transitions to perennial crops, which
240 have deeper and more permanent rooting systems that may influence the C balance deeper in

241 the subsoil via priming of decomposition, C stabilisation or translocation. The BLR approach
242 can be, however, applied to any soil property of interest giving the ability to assess land use
243 effects at any point down the soil profile. Being data-driven and flexible, it is hoped that further
244 studies of land use and land management, based on new or existing data, can make use of this
245 approach to examine differences in soil profiles.

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248 *Author contributions.* A. M. Keith and R. L. Rowe conducted sampling and created the data.
249 A. M. Keith and P. Henrys developed the statistical approach. All authors contributed to
250 preparation of the manuscript.

251 *Acknowledgement.* This work was supported by the ELUM (Ecosystem Land Use Modelling
252 & Soil Carbon GHG Flux Trial) project, which was commissioned and funded by the Energy
253 Technologies Institute (ETI).

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Figure

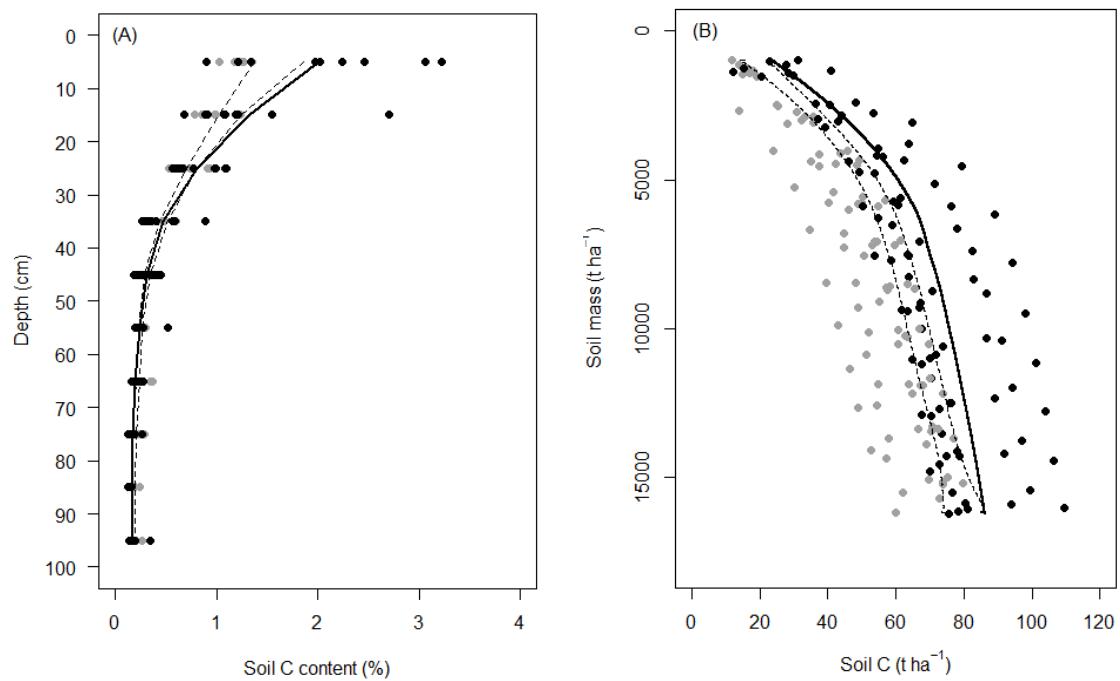


Figure 1. Depth profiles of (A) Soil C concentration as a function of sampling depth and (B) Cumulative soil C stock as a function of soil mass. Depth represents values of samples from 10 cm increments. Grey and black symbols represent SRC willow and arable data-points, respectively. Dashed lines represent upper and lower bounds of 95% confidence intervals from bootstrapped ($n = 1000$) Loess regressions of combined arable and SRC willow data; solid lines represents Loess regression of percent C and cumulative soil C in SRC willow only, if this line sits outside the confidence interval it can be inferred that arable and SRC willow are significantly different.