Modelling diffusion of innovation curves using radiocarbon data

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ABSTRACT

Archaeological data provide a potential to investigate the diffusion of technological and cultural traits. However, much of this research agenda currently needs more formal quantitative methods to address small sample sizes and chronological uncertainty. This paper introduces a novel Bayesian framework for inferring the shape of diffusion curves using radiocarbon data associated with the presence/absence of a particular innovation. We developed two distinct approaches: 1) a hierarchical model that enables the fitting of an s-shaped diffusion curve whilst accounting for inter-site variations in the probability of sampling the innovation itself, and 2) a non-parametric model that can estimate the changing proportion of the innovation across user-defined time-blocks. The robustness of the two approaches was first tested against simulated datasets and then applied to investigate three case studies, the first pair on the diffusion of farming in prehistoric Japan and Britain and the third on cycles of changes in the burial practices of later prehistoric Britain.

1. Introduction

The investigation of how and why a particular idea or technology spreads among a population is undoubtedly one of the most interdisciplinary research themes within the social sciences, with methodological and theoretical contributions spanning fields such as economics, ecology, sociology, and cultural evolutionary science (Bass, 1969; Henrich, 2001; Hoppitt et al., 2010; Lengyel et al., 2020; Manzo et al., 2018; Reader, 2004; Rogers, 2003; Steele, 2009). Much of the theoretical basis of the diffusion of innovation (DOI) literature shares some common ideas and concepts, most notably how the rate of diffusion of a particular product is the cumulative consequence of individual attitudes and propensity towards the innovation itself.

The seminal work by Rogers (1962;2003), has highlighted how time-series graphs portraying the proportion of adopters over time (known as diffusion curves) show surprising regularity, forming a characteristic s-shaped curve indicative of similar underlying processes across a wide range of technological adoption. Features of diffusion curves have subsequently been investigated through formal models and empirical studies to infer individual-level processes of cultural transmission from population-level data. For example, several studies have theorised and observed that s-shaped curves result from social learning, but when the

spread of the innovation is the result of independent individual learning processes, diffusion curves can take an r-shape, without a slow growth stage during the early stages of a spread (Henrich, 2001; Hoppitt et al., 2010; Reader, 2004). More sophisticated cultural transmission models have also incorporated the impact of different modes of cultural transmission (Henrich, 2001), task structure (Hoppitt et al., 2010), outgroup aversion (Smaldino et al., 2017), and geography (Lengyel et al., 2020).

Empirical studies of diffusion curves have often benefited from large datasets, in some cases sufficiently large to let scholars fit mathematical models to proportions or abundance data over time bins (e.g. Grasman and Kornelis, 2019), rather than directly to individual binary observations (i.e. whether a particular individual has or does not have the innovation). The range of mathematical models fitted to these empirical datasets has grown considerably since Rogers' work, especially in economics where these models are routinely used for forecasting or to evaluate the success of particular marketing strategies (Meade and Islam, 2006).

Archaeological contribution to this rich literature is somewhat more limited despite the opportunity to investigate a wider range of dynamics, such as slow adoption occurring over multiple generations or diffusion events driven primarily by a higher growth rate of migrant populations carrying the novel trait rather than its adoption by an incumbent

population. More generally, the archaeological record offers a wider range of case studies involving different products and populations. One can speculate that this lack of interest is at least partly derived from the limitations of the archaeological record itself, which hinders the direct application and borrowing of specific techniques from sister disciplines. While in most social sciences reliable time series of the proportion of adopters are readily available, most archaeological data are represented by indirect proxy variables in small samples, and often characterised by a substantial degree of chronological uncertainty. Indeed, in rare instances where these issues are less prominent and historical data are available, archaeological research does provide relevant contributions to the DOI literature (e.g. Amati et al., 2019; Scholnick, 2012).

The primary objective of DOI research is to estimate how changes in the proportion or abundance of a particular cultural innovation changes as a function of time, and possibly other factors. More formally we have

$$p_\theta = f(\theta) \qquad [1]$$

where the p_θ is the observed proportion of the innovation at time θ, and $f(\theta)$ is some function of time defining the shape of the diffusion curve. When dealing with small sample sizes, empirically observed values of p_θ are however going to fluctuate randomly due to sampling error. Thus, a better approach would be to estimate the probability that a given *observation* of a particular calendar age is associated with the old or new cultural variant. Thus, a more appropriate objective is to calculate the probability $P(x = 1|\theta = t)$, where x is the state of the observation ($x = 0$ old variant, $x = 1$ new variant) and θ is its calendar date. Using a probabilistic annotation, we have now:

$$x_i \sim \text{Bernoulli}(p_i) \qquad [2]$$

$$p_i = f(\theta_i) \qquad [3]$$

where the probability p_i of the sample i being in state 1 is given by some function of time $f(\theta_i)$. While DOI research has predominantly dealt with equation [1], we argue that equations [2] and [3] are better suited to account for the small sample sizes that characterise most archaeological datasets.

At its worst, archaeological data provides information about only the abundance of a given technology. In other words all samples have state $x = 1$, and hence changes in the frequencies can be assumed to be proportional to p only under a constant denominator i.e. stable population sizes and rates of production (e.g. Eerkens and Lipo, 2014). In some cases, it is possible to obtain sample proportions (e.g. ,the relative proportion of hand-built vs wheel-made ceramic; de Groot and Bloxam, 2022) which are more direct proxies of p. However, proportion estimates will inevitably be affected by sampling error unless a large number of observations are available. Both abundance and proportion data are also subject to the inevitable restrictions imposed by chronology. Archaeological assemblages could be time-averaged, and individual artefacts are rarely associated with precise and accurate time stamps. The consequence of these limitations is that modelling or even graphically displaying diffusion curves from archaeological data represents a considerable challenge.

While issues pertaining to the type of data (abundance vs. proportion) or the representativeness of the proxy variable is contingent on the specific context being investigated, the limitations dictated by chronology are universal for the majority of the archaeological record. However, recent interest in the collation of large datasets of radiocarbon dates (e.g. ,Bird et al., 2022), often with sample sizes over four and five digits, provides a possible avenue for pursuing DOI research in archaeology, with a comparatively reliable chronology (e.g. ,Bevan et al., 2017; Bloxam and Parker Pearson, 2022; Buchanan et al., 2022; de Groot and Bloxam, 2022; Schmid, 2020; Stevens and Fuller, 2012).

Initial exploration of this area of research has benefited from methodological developments designed to analyse large collections of radiocarbon dates, most typically to infer past population changes

through the so-called *dates as data* approach (Crema, 2022a; Rick, 1987). In their simplest form, DOI curves have been approached by visualising abundance or proportion data via summed probability distribution of radiocarbon dates (de Groot and Bloxam, 2022; Stevens and Fuller, 2012) and OxCal's Kernel Density Estimate Models (Capuzzo et al., 2020). Neither approach is ideal.

SPDs are easy to generate and can visually represent changes in both abundance and proportion. However, in its most common form, the visual interpretation of SPDs can be problematic, as observed changes can be simply the result of sampling error and in the case of abundance data, the result of the calibration process (Carleton and Groucutt, 2020; Crema, 2022a). More sophisticated techniques have been proposed in order to attempt to address some of these issues, for example by generating a confidence interval using bootstrapping or examining whether and when the relative proportion of an innovation changed via permutations tests (Bevan et al., 2017; Bloxam and Parker Pearson, 2022; Stevens et al., 2022). In the case of abundance data, OxCal's KDE (Bronk Ramsey, 2017) offers substantial improvement over visual inspections of SPDs, providing more robust solutions for visualising the uncertainty of sampling error and calibration effects. Nevertheless, its application is limited to smaller datasets due to its heavy computational requirements, and it currently does not allow for the visualisation of proportion data.

This paper introduces a new set of Bayesian inferential tools which are designed to analyse DOI using radiocarbon data, but which are not based on SPDs The approach we propose can be broadly applied and extended to any proportion data based on ^{14}C dates, but here we focus on two challenges: 1) heterogeneity in sampling practices across archaeological sites; and 2) diffusion dynamics that do not follow s-shaped curves. We test the robustness of our approach via simulated datasets and two sets of case studies: 1) the diffusion of agriculture in Britain and Japan (case studies 1a and 1b) and 2) cyclical changes in burial practices in later prehistoric Britain (case study 2). Section 2 will introduce the statistical framework we propose; section 3 will summarise contextual details of the three case studies; section 4 will provide details of material and the implementation of the methods; section 5 will briefly summarise the results; and section 6 will provide a discussion on the methodological and contextual relevance of our analyses.

2. Modelling diffusion curves from radiocarbon dates

As noted in the previous section, our key inferential goal is to model changes in the probability p of a sample i being associated with an innovation as a function of calendar time θ_i (see equation [3]). In the case that our sample is a radiocarbon date, we need to account for the fact that θ_i is associated with some random and systematic measurement error, and as such, can be modelled as follows:

$$y_i \sim \text{Normal}(c(\theta_i), \sigma_i) \qquad [4]$$

Where y_i is the radiocarbon age of the sample i, $c(\theta_i)$ is the radiocarbon age of the θ_i, and σ_i is the square root of the sum of the squares of the sample ^{14}C age error and the corresponding error in the calibration curve.

The combination of equations [2] to [4] provides the basic framework of the method proposed here. While a number of diffusion curve models have been suggested in the literature, here we take $f(\theta_i)$ to be simple sigmoid function:

$$p_i = \frac{1}{1 + e^{-(\beta_0 + \beta_1\theta)}} \qquad [5]$$

In this case, equation [5] is effectively just a logistic regression with an independent variable θ_i and coefficients β_0 and β_1.

2.1. Hierarchical model

Equation [5] describes the change over time of the probability *p* as a sigmoid function, with the steepness of the diffusion captured by the parameter β₁. More importantly, the model assumes that the rate of change of *p* increases as it approaches *p* = 0.5, and decreases as *p* gets closer to 1, capturing the frequency dependence characteristic of diffusion curves (Rogers, 2003). While this is a desirable feature in many situations, the two examples from our first case study will illustrate a typical situation where equation [5] might not be appropriate.

In the case of the diffusion of farming (see section 3.1 below), $x = 0$ implies that the sample is not associated with the cultivation of a particular crop, whilst $x = 1$ indicates the opposite. Establishing the clear presence (or absence) of farming is, however, not always trivial, particularly during its early stages of diffusion. The problem is further exacerbated by the fact that, ideally, we would like to have a direct link between our dated sample and the new subsistence practice rather than an indirect link based on stratigraphic association. A practical solution to this is to consider only direct dates from seeds, where $x = 1$ indicates that the sample is the domesticate (i.e. rice for Japan and wheat or barley for Britain, see below), and $x = 0$ indicates that the sample is *not* the domesticate of interest (e.g. wild nuts). In other words, *p* becomes the relative proportion of the domesticates to the combination of domesticates and non-domesticates.

This solution, however, raises two issues. Firstly, there is no reason to believe that crops fully replace wild plants. Indeed, most typically, we should expect to observe wild plants even after the introduction of farming, particularly during its early stages (Stevens et al., 2022). Secondly, a number of factors associated with different combinations of taphonomy and sampling design might lead to a situation where the radiocarbon date from a farming context might be from a wild plant. There are numerical consequences arising from these potential issues. Even if genuinely random samples are available, the proportion *p* of domesticates might plateau to values lower than 1 after the full diffusion of agriculture. For convenience, we will refer to the equilibrium value reached by *p* as *k*, with $0 < k < 1$. Furthermore, the probability of dating a sample from a domesticate when this is present in an archaeological assemblage is likely to be lower than 1 and *different* between archaeological sites. The net implication is that for given calendar time θ, we are likely going to have greater variability in the character state of *x* due to overdispersion.

A possible resolution to both these problems can be achieved by using the following hierarchical model:

$$p_{i,j} = \frac{k_j}{1 + e^{r(\theta_{i,j} - m)}} \qquad [6]$$

$$k_j \sim \text{Beta}(\gamma_1, \gamma_2) \qquad [7]$$

$$\gamma_1 = \mu\varphi + 1 \qquad [8]$$

$$\gamma_2 = (1 - \mu)\varphi + 1 \qquad [9]$$

Equation [6] is also a sigmoid function, but with a range between 0 and k_j instead of 0 and 1. Furthermore, each site *j* has its own upper bound k_j, with the intersite variability of this parameter modelled using a Beta distribution with shape parameters γ_1 and γ_2. These are, in turn, defined by a mode μ and a concentration parameter φ. In particular, equations [8] and [9] ensure that when φ = 0, k_j is uniformly distributed between 0 and 1. The parameters *r* and *m* are just a reparameterisation of β₀ and β₁ from equation [5], and indicate respectively the rate of diffusion and the time (in years BP) at which $p_{i,j}$ is equal to $k_j/2$.

The hierarchical model described above effectively accounts for any inter-site variation in the probability of dating a domesticate rather than a non-domesticate, while simultaneously modelling the general rate of diffusion of agriculture. The model does not distinguish whether this source variation is related to taphonomy, sampling practices, or genuine differences in the proportion of domesticates across sites. It is worth noting, however, that putative covariates that might explain this variation can be included in equation [6] with their own set of parameters.

2.2. Accounting for fluctuations in the diffusion curve

Equations [5] and [6] describe an s-shaped monotonic diffusion process. The spread of a particular cultural or technological trait might, however, be characterised by temporary episodes of reversion, or even repeated cycles where the relationship between *p* and θ can take a wide range of shapes (see section 3.2 below).

There are two possible ways to approach any deviations from an s-shape diffusion curve. The first consists of fitting equation [6] to the empirical data, and then to evaluate the goodness of fit to the observed data through posterior predictive checks. In the case of radiocarbon data, this effectively

Consists of first creating an empirical proportion SPD. This can be generated by calculating, for each calendar year, the ratio between the summed probability of samples with $x = 1$ and the summed probability of all samples. The same calculation can then be carried out for the fitted model. In this case we first randomly re-assign a new value to $x_{i,j}$ for each radiocarbon date *i* at site *j* with probabilities 1-$p_{i,j}$ (for $x_{i,j} = 0$) and $p_{i,j}$ (for $x_{i,j} = 1$) derived from the posterior samples of the fitted model, and then generate a fitted proportion SPD. This step is executed multiple times using different values of $p_{i,j}$ obtained from the posterior. The resulting distribution of fitted proportion SPD is then summarised for each calendar year by taking, for example, a 90% quantile range, to generate a simulation envelope. Finally, the observed empirical proportion SPD can be visually compared to the simulated envelope to detect any abnormally high or low proportion values. Because the underlying radiocarbon dates remain the same, the empirical proportion SPD and the simulation envelope will be both equally affected by sampling error and calibration effects, effectively bypassing the problems encountered with SPDs. The simulation envelope will effectively account for small sample sizes and minor fluctuations, and because equation [6] accounts for overdispersion, a marked deviation from the fitted model would occur only when the observed proportion at a particular time interval is greater or lesser than the overall variability we expect to observe across the archaeological sites. This approach makes the posterior predictive check a reasonably robust, if not conservative, solution in detecting deviations from an s-shaped diffusion curve.

In some circumstances, however, the expected deviation from an s-shape curve is so significant that the entire premise of trying to estimate its parameters can be regarded as flawed. Our third case study represents a typical instance where an innovation (cremation in this case) is not necessarily expected to reach a stable equilibrium in the population. While one could attempt to develop a complex model that accounts for possible cyclicity (e.g. using a sinusoidal model), a simpler solution is to model the diffusion as a random walk process using a intrinsic Gaussian conditional autoregressive (ICAR) model (Besag, 1974; Rue and Held, 2004). This approach consists of dividing our chronological window of analyses into a series of *n* time-blocks and estimating the associated vector of probabilities $p_{t=1}, p_{t=2}, ..., p_{t=n}$. The ICAR model effectively defines the conditional distribution of p_t as a Gaussian, with a mean equal to the average of adjacent time-blocks, and a variance τ that decreases as the number of neighbouring blocks increases. In practice, this means that when estimating p_t, we are partially informed by the estimates of p_{t+1} and p_{t-1}.

3. Case studies

3.1. Case study 1a and 1b: diffusion of agriculture in Japan and Britain

The diffusion of agriculture in Japan (case study 1a) and Britain (case study 1b) shares a number of similarities. The two regions are islands

located at opposite edges of the Eurasian continent and effectively represent the final phase of two separate major episodes of demic and cultural diffusion. While the specific crops introduced in the two islands are different (primarily wheat and barley for Britain, de Vareilles et al., 2023; rice, broomcorn millet and foxtail millet for Japan, Fujio, 2021) both islands were occupied by an incumbent population of hunter-gatherers whose subsistence practices relied on the consumption of a significant proportion of nuts (hazelnut in Britain; chestnut, buckeye, and acorns for Japan, Bishop et al., 2014; Sakaguchi, 2009). The large latitudinal span of the two islands entailed different environments and suitability for the diffusion of the new agricultural practices, and archaeobotanical evidence suggests in both islands episodes of reversion as well as a prolonged coexistence of wild resources during the early stages of transition to farming (Stevens et al., 2022). The two regions also benefit from the presence of large radiocarbon datasets, which include reasonably large samples of direct dates on seeds, that has already enabled statistical analyses on the fluctuations in the relative frequencies of different crops and wild foods (Bevan et al., 2017; Stevens and Fuller, 2012) as well as inferences on dispersal rates and regional arrival times of farming practices (Crema et al., 2022; Whittle et al., 2011).

For the British Isles the initial diffusion of agriculture (emmer wheat and barley, with cattle, goats, sheep and pig, with limited evidence for tetraploid free-threshing wheat and flax), has largely been dated to the last century of the 5th and the first three centuries of the 4th millennium BCE. These farming populations, associated with the Chasséen, Castellic, and Michelsberg cultures (Ray and Thomas, 2018; Sheridan, 2010), were present in regions of Belgium, northern France and Western Germany some 500–1000 years before agriculture dispersed north across the channel. Studies of ancient genomes supports that these agriculturalists largely descended from peoples originating within Anatolia/the Aegean, with low inputs from Western hunter-gatherers (Brace et al., 2019; Patterson et al., 2022). This, along with other lines of evidence, can be used to reject the hypothesis that once favoured adoption of agriculture by indigenous hunter-gatherer groups (Stevens et al., 2022). Rather, the input of hunter-gatherer lineages likely accumulated as these first agriculturalists dispersed across Europe through the introgression of pre-existing hunter-gatherer peoples into farming societies.

While some evidence of small-scale cultivation (e.g. barnyard millet, azuki, and soybeans) in Japan exists for the latter half of the Late and Final Jomon periods (mid-3rd millennium BCE ~ end of 2nd millennium BCE; Crawford, 2011), a more prominent transition of the subsistence economy occurred during the 1st millennium BCE, when migrant farmers from the Korean peninsula brought a cultural package which included rice and millet (broomcorn and foxtail) agriculture (Fujio, 2021). Unfortunately, a systematic analysis of the dispersal of millet farming is currently not possible due to the comparatively small number of direct dates from seeds (see Endo and Leipe, 2022 for indirect evidence from seed impression on pottery; see also Obata and Kunikita, 2022). In contrast, the relatively large number of dates on charred rice has recently allowed for the application of Bayesian analyses to estimate regional variations in its rates of dispersal (Crema et al., 2022; Leipe et al., 2020). The results of these analyses revealed multiple episodes of slow-down, and in some cases a hiatus in dispersal spanning several centuries before agriculturalists moved into the next region.

Statistical analyses of diffusion rates of farming in Japan and Britain (and most likely in other regions of the world) have a number of shared challenges. For example, the direct dating of seeds can overcome some of the problems associated with chronological and contextual uncertainty but also drastically reduces sample sizes, even in comparatively ^{14}C data rich regions such as Japan and Britain. Furthermore, although we would expect the relative proportion of ^{14}C dates associated with domesticated crops to increase over time, we have no reason to believe that this would reach 100% even when we observe a complete diffusion of farming practices (i.e. $k \neq 1$). Instead, we expect that diffusion curves would reach a plateau with a stable proportion, whose values would be conditioned by the extent of the persistence of wild plant resources and the baseline probability of dating each taxon. The latter is a complex issue, as it is dictated by how likely a particular taxon will be preserved and recovered from any given archaeological context, how easily the taxon can be identified, and what is the rationale of the excavator for choosing to date a specimen of this taxon rather than that of another species. These factors all contribute to the relative proportion of radiocarbon dates on domesticated crops, and there is no reason to believe that these would be identical or consistent across different sites. Simply put, two contemporary contexts associated with a full adoption of farming can have different probabilities of dating a seed of a domesticated crop.

3.2. Case study 2: burial practices in prehistoric Britain

Funerary practices vary substantially across the later prehistory of Britain and Europe. Some rites may emerge *de novo* in a region and remain geographically and chronologically restricted; other practices diffuse rapidly across long distances, creating the superficial appearance of supra-regional groups with shared cultural traits (Vander Linden, 2016). Even in cases where one set of cultural traits and practices is predominant, local variability in burial practices is common throughout prehistory (Bloxam and Parker Pearson, 2022; Caswell and Roberts, 2018; Furholt, 2014). A coexistence of multiple burial practices may point to diverse cultural origins and influences, but conversely can reflect within-group differential treatment on the basis of age, sex, or other personal characteristics (e.g. Fernández-Crespo et al., 2020; Haughton, 2021; Mittnik et al., 2019). As such, and contrary to the case of the diffusion of agriculture, there is no expectation that the balance between contemporaneous funerary practices should ever reach an equilibrium, or that any particular rite should become dominant over others.

Here, we focus on the changing importance of cremation in comparison to other modes of disposal of the dead (e.g. collective or individual inhumation burial) as a means of isolating the trajectory of one readily-identifiable and distinct set of funerary practices over time. Cremation can largely be considered as a binary — incomplete cremation is rare (Rebay-Salisbury, 2015) — but this does not mean it is a uniform practice wherever it appears. In Britain, cremation is sporadically recorded for the Mesolithic and earlier parts of the Neolithic, although inhumation burial practices appear to be by far the more prevalent in each period (Jay and Scarre, 2017). Although burial evidence is relatively sparse overall in the later part of the Neolithic, cremation seems to become the dominant rite for several centuries in the first half of the 3rd millennium BCE; here it is frequently unaccompanied by grave goods but is often associated with highly-visible circular monument forms (Willis, 2021). This is followed, from c.2450 BCE, by an episode dominated by inhumation associated with the arrival of the Beaker phenomenon from continental Europe (Parker Pearson et al., 2016). Cremation gradually increases in prevalence once again across Britain during the 2nd millennium BCE (e.g. (Bloxam and Parker Pearson, 2022; Caswell and Roberts, 2018). Within this later resurgence there is an initial period where inhumation and cremation practices can be found in correspondingly large numbers, are located at the same monument types, particularly round barrows, and are accompanied by similar Early Bronze Age artefact types including funerary ceramic urns (Garrow et al., 2014). This practice gradually gives way to a preference for a more homogenous form of unaccompanied cremation burial, located in large open cemetery sites, as it becomes the dominant rite by the Middle Bronze Age (Bloxam and Parker Pearson, 2022; Caswell and Roberts, 2018).

Because cremation destroys the organic component of bone, cremated remains have largely been excluded from recent studies investigating or critiquing the genetic evidence for the role of demic diffusion in the transmission of later prehistoric burial rites across Europe (Furholt, 2019; Olalde et al., 2018). In the absence of genetic

data, and with stable isotope analysis being a very recent development for this material (Snoeck et al., 2015), the diffusion and regional onset of cremation has to date been estimated either through qualitative assessment burial evidence, or through more formal (e.g. Bayesian) approaches to local site series (Garrow et al., 2014).

Statistical assessment of the fluctuating relationship between cremation and inhumation presents different kinds of challenges compared to the adoption of farming. On the one hand, radiocarbon dates provide in this case direct evidence of a particular innovation (at least compared to seeds, which remains a proxy variable), and as such, they provide a less-biased estimator of the proportion of individuals adopting different burial practices. On the other hand, we have no reason to expect a typical s-shaped diffusion curve; rates of diffusion are expected to vary over time and eventually even produce long-term fashion cycles (Manning et al., 2014). It follows that, in contrast to the diffusion of agriculture, fitting a sigmoidal function to the empirical data would be inappropriate, and the goal should instead be a reliable, "non-parametric" estimator of changes in the relative frequency of different burial customs over time.

4. Materials and methods

4.1. Materials

4.1.1. Simulated data

We first examined the robustness of the two statistical approaches we developed by examining whether they can accurately recover parameter values when dealing with sample sizes comparable to those observed in the case studies. While these simulated datasets represent ideal conditions where the data-generating process is equivalent to the statistical model, they nonetheless provide an experimental basis to establish a baseline on the level of precision and accuracy that our approach could achieve in recovering model parameters.

We simulated three datasets with sample sizes and time-windows equivalent to each observed dataset (see sections 4.1.2 and 4.1.3 below). Calendar dates were uniformly generated within the time window of analyses, back-calibrated in ^{14}C age, and associated with an arbitrary error of 20 years. For simulations 1a and 1b we randomly clustered the dates into groups (corresponding to the archaeological sites in the observed data) and randomly assigned to each a binary value using equations (5)–(8) with the following settings: $r = 0.01$, $m = 2900$ BP, $\mu = 0.65$, $\varphi = 50$ (simulation 1a); and $r = 0.008$, $m = 4500$ BP, $\mu = 0.8$, $\varphi = 40$ (simulation 1b). For simulation 2, we first created a 7th-order polynomial curve spanning the time window of analyses and normalised it to 0–1 via logistic transformation. This enabled the creation of a vector of probabilities p for each calendar year, which was then used to randomly generate a binary value for each simulated sample.

4.1.2. Case study 1a and 1b

We examined a total of 1479 ^{14}C dates on seed remains from Japan ($n = 551$, from 215 sites, Fig. 1a) and Britain ($n = 928$, from 314 sites, Fig. 1b). Japanese dates were collated from the radiocarbon database of Japan (Kudo et al., 2023) and the rice radiocarbon database used in (Crema et al., 2022). We considered dates with a cumulative calibrated probability mass equal to or larger than 0.5 for the interval 4000–1700 cal BP (approximately corresponding to Final Jomon and Yayoi periods) and excluded the island of Hokkaido and the Ryukyuan islands from our analyses due to their late historical adoption of rice agriculture. The resulting sample consisted of ^{14}C dates on rice ($n = 203$) and on various edible wild nuts consumed from the Jomon period onwards ($n = 348$), including chestnut, horse chestnut, walnut, and acorns.

Radiocarbon dates from Britain were obtained from Bevan et al. (2017). We filtered the initial dataset considering dates with a cumulative calibrated probability mass equal to or larger than 0.5 for the interval 7000–3000 cal BP (corresponding approximately to Late Mesolithic to Late Bronze Age). We used dates on wheat ($n = 261$) and barley ($n = 130$) as proxies of agriculture and dates on hazelnut ($n = 537$) as representative of wild plant consumption.

4.1.3. Case study 2

Radiocarbon dates associated with burial from the British Isles (Fig. 1c) were collated from different published sources and databases (Bevan et al., 2017; Bloxam, 2020; Bloxam and Parker Pearson, 2022; Healy, 2012; Mallick and Reich, 2023; Olalde et al., 2018; Wilkin, 2013; Willis et al., 2016). We chronologically filtered dates with a cumulative calibrated probability mass equal to or larger than 0.99 for the interval 5500–2000 cal BP. We used a higher probability threshold (0.99 instead of 0.5) to avoid any edge effects caused by the ICAR model. We examined the source material to distinguish dates associated with cremation ($n = 1417$) and inhumation ($n = 1119$).

4.2. Methods

Both the hierarchical model described in equations [5–6] and the random walk ICAR model were implemented using the NIMBLE (de Valpine et al., 2017, 2020) probabilistic programming language in R (R
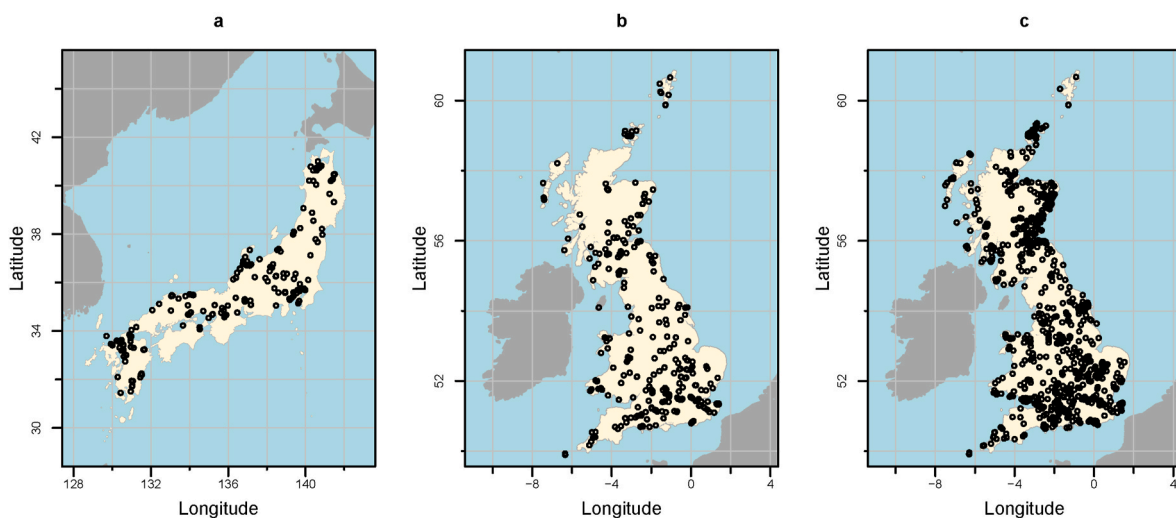

Fig. 1. Distribution of sampling sites for the radiocarbon dates in case studies 1a (panel a; rice agriculture in Japan), 1b (panel b; wheat and barley agriculture in Britain) and 2 (panel c; burial customs in Britain).

Core Team, 2020) and the *nimbleCarbon* R package (Crema, 2022b; Crema and Shoda, 2021).

For the simulated datasets 1a & 1b and case studies 1a & 1b we fitted our hierarchical models using equations [6–9] and the following weakly informative priors:

$$r \sim \text{Exponential}(100) \qquad\qquad [10]$$

$$\mu \sim \text{Beta}(2,2) \qquad\qquad [11]$$

$$\varphi \sim \text{Gamma}(5,0.1) \qquad\qquad [12]$$

Priors for the parameter *m* were modelled using a normal distribution truncated within with the time-window of analyses and a mean of 2500 and standard deviation of 500 years for simulation #1 and the Japanese dataset, and a mean of 5500 and standard deviation of 1000 years for simulation #2 and the British dataset. We fitted all four models with the same MCMC settings, using four chains, each with 1 million iterations (half discarded as burn-in) and with thinning set to 50. We evaluated the mixing of our model using the Gelman-Rubin statistic (Gelman and Rubin, 1992), except for the posterior of the individual dates (θ), which were examined using agreement indices (Bronk Ramsey 1995) given the target distribution does not necessarily follow a normal distribution. We also carried out posterior predictive checks for the two empirical case studies by visually comparing observed SPDs of the proportion of domesticated crops to an envelope of predictions generated using 1000 randomly selected parameters from the joint posterior distributions.

The ICAR model for case study 2 and the simulation dataset 2 was fitted using 36 time-blocks of 100 years (with mid-points at 5500, 5400, 5300 … 2000 cal BP), with the variance modelled as the reciprocal of the square of an exponential distribution with a rate of 1. To obtain our vector of posterior estimates, we used four chains, each with 100,000 iterations (20,000 of which were discarded for burn-in), with parameters collected every four steps. As for the hierarchical model, we evaluated the mixing of our model using the Gelman-Rubin statistic and the reliability of the estimated values of θ using agreement indices.
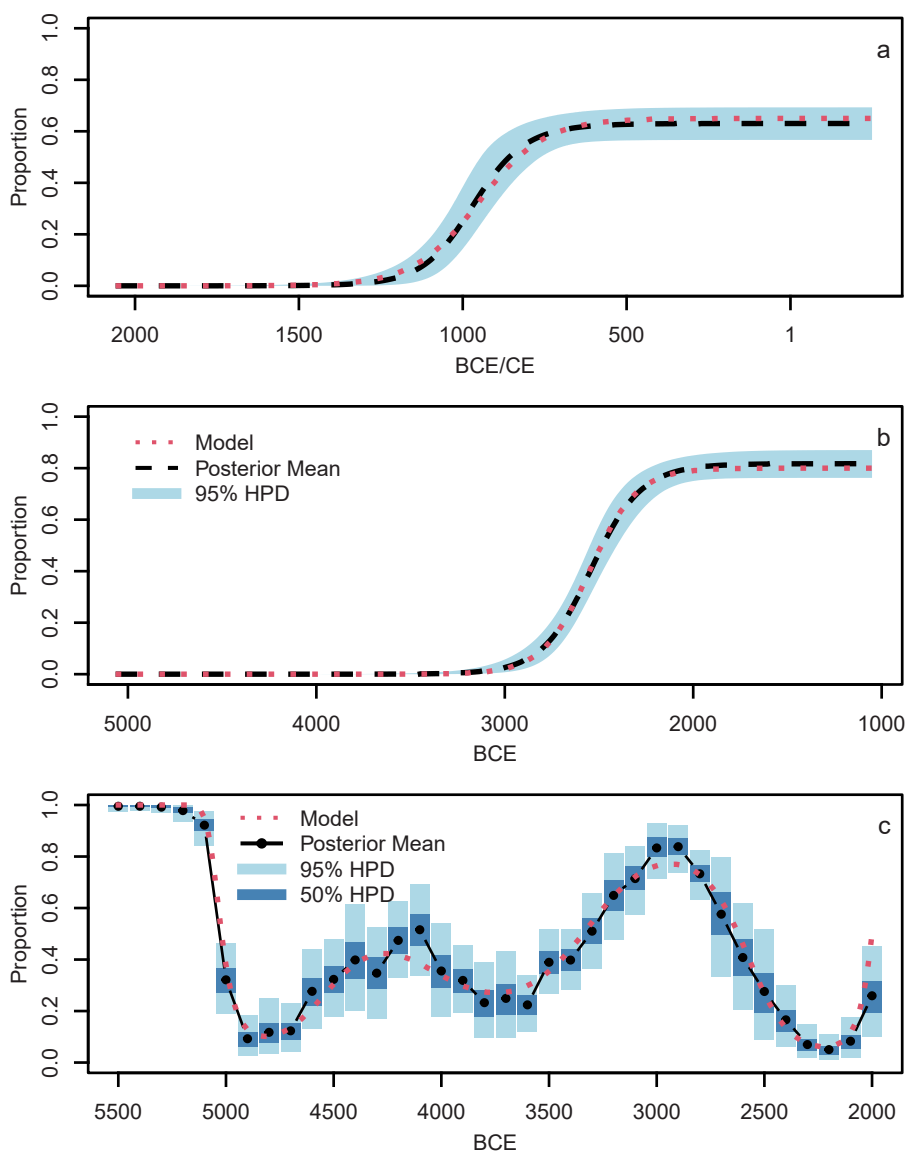

Fig. 2. Performance of the hierarchical (*a and b, simulations 1a and 1b*) and the ICAR model (c, simulation 2) on recovering changes in *p* as a function of time on simulated datasets. Model values (red dotted lines) are based on average values of *p* across all sites (i.e. $k_j = \mu$). Data structure (e.g. number of dates and sites) equivalent to the case studies (a: rice vs wild nut dates in Japan; b: wheat & barley vs hazelnut in Britain; c: cremation vs inhumation in Britain). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

We used the IntCal20 curve for all models (Reimer et al., 2020) using the calibration process defined in equation [3]. All data and R scripts are available on https://github.com/ercrema/diffusionCurve and permanently archived on https://doi.org/10.5281/zenodo.10782942.

5. Results

5.1. Case study 1a & 1b and simulated datasets 1a & 1b (hierarchical model)

Our hierarchical approach was able to accurately recover the shape of the diffusion curve in both simulated datasets, with the 'true' curve within the 95% posterior fitted range (Fig. 2a and b). Posteriors of all parameters were also recovered accurately with fairly narrow highest posterior density intervals (HPDI), suggesting that good precision can potentially be achieved for all parameter estimates with the sample sizes available (Fig. S1 - Fig. S2).

Results of the posterior predictive checks of the Japanese and British datasets (Figs. 3 and 4) have, instead, revealed a poor fit between the model and the empirically observed proportion SPDs, suggesting in both cases that the diffusion processes cannot be described by a sigmoid curve. In the case of Japan, the fitted model suggests that a stable and relatively high but extremely variable proportion of rice radiocarbon dates is reached quickly after a few centuries from the introduction of the crop (see Table 1). Posterior predictive checks show (Fig. 3), however, that the model overestimated the proportion of rice dates between c. 800 and 500 BCE and the observed proportion SPD was higher than the model prediction from 200 BCE onwards.

The fit between the model and empirical SPD was worse in the case of the British dataset. Model posteriors for the British Isles show low values for μ, a high inter-site variation in k_j (i.e. low φ) and a diffusion rate that was an order of magnitude smaller than Japan. The posterior predictive checks (Fig. 4) show both negative and positive deviations; the former primarily between ca. 3700 to 2300 BCE and the latter observed from 1600 BCE onwards.

5.2. Case study 2 & simulated dataset 2 (ICAR model)

The non-parametric ICAR approach successfully recovered the 'true' time-sequence of p used to generate the simulated dataset 2 (Fig. 2c), indicating that available sample size should be able to recover accurately and fairly precisely at least a couple of cycles of diffusion at millennium scale.
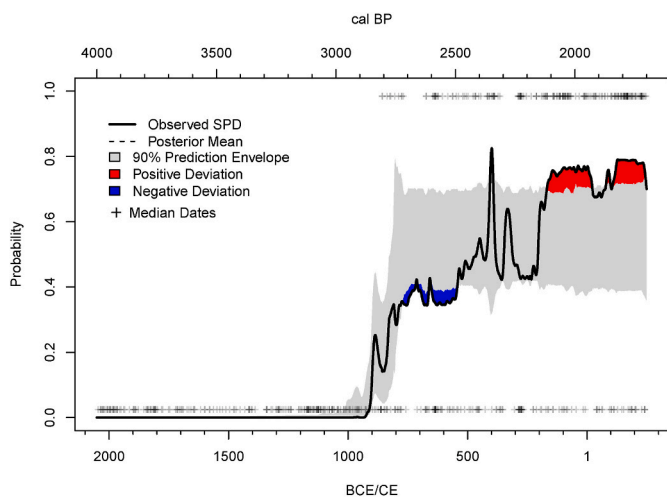

Fig. 4. Posterior predictive check of the fitted hierarchical Model on observed proportion SPD of ^{14}C dates on wheat and barley over dates on wheat, barley, and hazelnut in Britain (case study 1b).

Table 1
Posterior estimates and convergence diagnostics on key parameters for case studies 1a and 1b (r: diffusion rate, m: inflection point; μ: modal equilibrium value of probability cap k; φ: concentration parameter for k).

Region	Parameter	Median	90% HPD	Rhat
Japan (Case study 1a)	r	0.1023	0.0131–0.3378	1.0003
	m	844 BCE	893–809 BCE	0.9999
	μ	0.703	0.476–0.937	0.9999
	φ	0.75	0.17–1.67	1.0004
Britain (Case study 1b)	r	0.0136	0.0015–0.0382	1.0005
	m	4053 BCE	4361–3857 BCE	1.0003
	μ	0.182	0.01–0.42	1.0001
	φ	0.31	0.1–0.57	1

Our empirical case study revealed the existence of two major cycles of diffusion and abandonment of cremation; one peaking in the Late Neolithic at around 2900 BCE and the other in the Early to Middle Bronze Age around 1900-1200 BCE (Fig. 5). The ICAR model also identified key shifts in the probability of a date being associated with cremation, with the most notable case identified at the turn of the 2nd

Fig. 3. Posterior predictive check of the fitted hierarchical Model on observed proportion SPD of ^{14}C dates on rice over dates on rice and nuts in Japan (case study 1a).
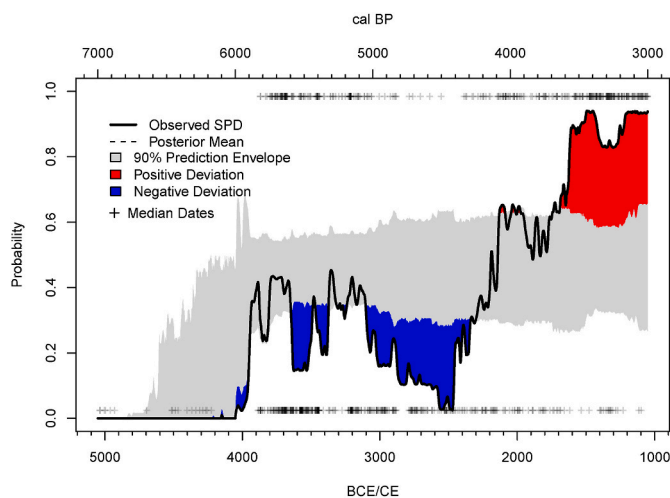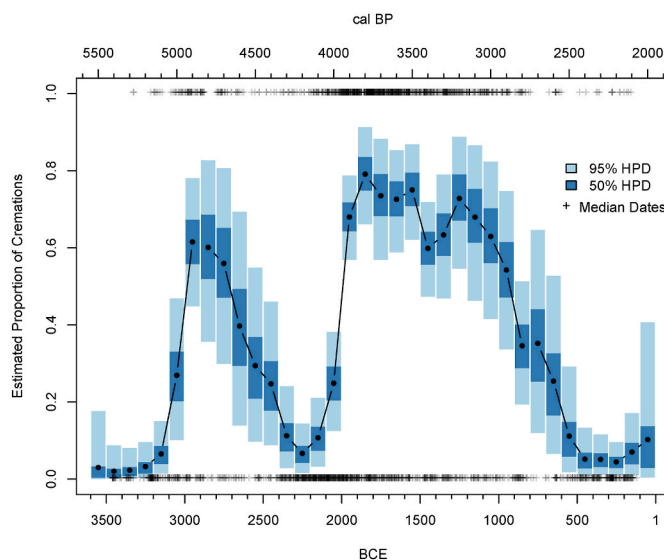

Fig. 5. Estimated proportion of cremation dates in Britain (case study 2).

millennium BCE when the cremation proportion increases sharply following a period of low prevalence that corresponds with the appearance of Beaker phenomenon inhumation rites across Britain.

6. Discussion

The new suite of Bayesian inferential tools we introduced has successfully managed to infer DOI curves based on the time-frequency of radiocarbon dates from both simulated and empirical datasets. Our solution overcomes several problems that affect current approaches based on SPDs, including sampling error, calibration-based artefacts, and overdispersion arising from inter-site variation in both sampling practices and past behaviour.

Albeit applicable in most contexts, the two approaches we present — the parametric hierarchical model and the non-parametric ICAR model — were developed with different purposes in mind. The parametric model can provide numerical estimates such as diffusion rate (r) or average diffusion cap (μ), which can potentially be associated with independent explanatory variables to evaluate specific hypotheses concerning diffusion drivers. In contrast, the non-parametric ICAR solution provides a visual descriptive tool that may be used to characterise more complex diffusion dynamics. This flexibility inevitably comes with a cost, as specific hypotheses cannot be assessed, and key summary statistics are not inferred from the empirical data.

Our case studies on the diffusion of agriculture in prehistoric Japan and Britain showcase the many challenges in fitting a s-shaped diffusion curve on empirical datasets. Despite the added flexibility of our hierarchical approach, neither of the two studies showed a good fit between the data and the model, and instead highlighted significant deviations between the observed and expected proportion SPDs. While this might be interpreted as a negative result, we highlight that our posterior predictive check provided means to identify whether and, more importantly, how the empirical data deviates from the expectation. It is important to note that predictive intervals are conditioned by the extent of uncertainty and variability in the data. Smaller sample sizes and high overdispersion (i.e. high inter-site variability in k) typically generate wider posterior intervals, decreasing the chance of observing significant departures of the observed SPD from the prediction envelope. As noted above, our simulation datasets demonstrated that an accurate and precise recovery of the data-generating parameters is possible with the available sample sizes. It follows that the bulk of the variability of the posterior envelope in Figs. 3 and 4 are dictated primarily by the low concentration parameters. While we cannot determine the extent by which such estimated variability in k was due to variation in sampling practices or genuine variations in the role of farming across different sites, the added flexibility was not sufficient to explain the range of fluctuations in observed SPDs, suggesting that we have robust signals of deviations from sigmoid diffusion curves.

In both Japan and Britain, archaeological evidence provides some clues on why a sigmoid diffusion curve did not fit the observed data. In the case of Japan, the dispersal of rice agriculture is known to have been characterised by episodes of significant regional accelerations and slowdowns (Crema et al., 2022), which might explain why the observed diffusion curve (Fig. 3) can be described as a double s-shape. These shapes imply an initial stage with a fast diffusion rate followed by a drastic slowdown (a saddle point in the curve), followed again by an accelerated diffusion rate. Several explanations have been proposed in the literature (Cadavid and Cardona, 2014; Lefebvre, 1995; Reader, 2004), with the most common interpretation centred on the idea that these shapes signal the existence of community structure, with the saddle point being the consequence of intervals when the innovation is transmitted across different metapopulations. Indeed, the interval between 500 and 200 BCE, when the empirical diffusion curve is fairly flat and does not show positive or negative deviations, corresponds exactly to the timing of the most prominent slowdown in the dispersal of farming in Japan (cf. transition from region V to VI on Fig. 3 in Crema

et al., 2022).

As with the Japanese case, the diffusion curve for farming in Britain and its deviations from the sigmoid curve are not unexpected. Previous studies (Bevan et al., 2017; Stevens et al., 2022; Stevens and Fuller, 2012, 2015) have already revealed a shift in subsistence towards total reliance on pastoralism and wild food resources, accompanied in many regions of mainland Britain by the abandonment of crops and cultivation. Agricultural crops reappear in the Beaker period/Early Bronze Age accompanied by genetic evidence for the appearance of peoples whose ancestors originated in the Eastern Steppe (Patterson et al., 2022), with declining evidence for wild foods in the 2nd millennium BCE along with many cultural elements associated with fully agricultural societies (Stevens and Fuller 2012; Stevens et al., 2022).

Although based on a different methodology, our approach still highlights this pattern, providing a more accurate estimate of when we observe a lower-than-expected proportion of dates associated with farming. The British agricultural diffusion case study also demonstrates how the model is sensitive to the exact distribution of available dates in determining its parameters. For example, the relative lack of ^{14}C dates around the crucial centuries before and after 4000 BCE (Fig. 4), which corresponds to the earliest occurrence of domesticates in Britain, had most likely limited the estimates of r and m as there was virtually no information available on the proportion of dates associated with wheat and barley. Finally, it is worth noting that the interpretation of the model parameters should always account for the model's goodness of fit. For example, the midpoint parameter m in Japan is a biased estimator of when half the population adopted rice agriculture, given that we observe positive deviations of the empirical curve around proportions above the estimated average cap μ right at the end of our window of analysis. Similarly, the overall low diffusion rate r in Britain is largely impacted by the presence of a temporary abandonment of farming, and as such, it reflects just the average long-term rate of diffusion.

The flexibility of the non-parametric model provides a clear advantage under these conditions and, more generally, in cases where we do not expect an s-shaped diffusion curve to begin with. The case of burial customs in Britain is a typical example where our primary goal is exploratory and our objective is to determine the timing of the repeated adoption and abandonment of one cultural trait across several millennia. Our model has confirmed the existence of two such major cycles, one in the Neolithic between 3200 and 2300 BCE and one in the Bronze Age from 2200 to 500 BCE.

The first of these cycles reflects the adoption and abandonment of Later Neolithic cremation practices across Britain. The radiocarbon evidence for this period is relatively sparse, indicated by the larger error bars in this portion of the plot; some Late Neolithic cemetery sites such as Stonehenge in Wiltshire (Willis et al., 2016) and Fortevoit in Perth and Kinross (Noble et al., 2017) have produced many cremation dates, but cremated remains from this period have been historically under-valued and under-studied (Mckinley, 1994). The abandonment of this phase of cremation, following its peak in around 3000-2900 BCE, is often presumed to be associated with the advent of the Beaker period. However, the decline in cremation is marked from 2800 BCE onwards and thus pre-dates Beaker inhumation practices in Britain by several centuries, suggesting that this decline may reflect endogenous factors rather than external influences.

The second major cycle of cremation customs reflects a well-attested series of Early Bronze Age traditions that arose after the inhumation-focused Beaker period. Although some cremation activity persists across the Beaker period (Bloxam and Parker Pearson, 2022) the rites that proliferate during the second cycle are associated with new material culture and monument forms, and indicate the development of a new cremation practice rather than a return of rites from the previous cycle.

From 2200 BCE onwards cremation sees a rapid increase in prevalence with a longer-lasting period of predominance than in the first cycle: cremation rites remain the most common practice for the subsequent millennium. A key finding for this cycle is the speed at which a

transition from ~10% to ~80% prevalence occurs, the century 2050–1950 BCE seeing a particularly rapid shift in practices; this is in marked contrast to the slow decline in prevalence seen at the end of each cycle, which is drawn out over several centuries. The variable speed of these processes in each cycle provides evidence to support future study of how different drivers of change, including the role of cultural versus demic diffusion, might influence the rate of adoption of novel funerary practices. Further, it can be used to support further investigations of the variable timing of post-depositional re-engagement with burials observed across later prehistory (Appleby, 2013; Booth and Brück, 2020; Brück and Booth, 2022).

As noted above, the inferential framework introduced in section 3 can theoretically be extended to incorporate other elements. Equation [5] can include covariates allowing users, for example, to account for the time of dispersal (m) to be conditioned by the distance from the point of origin of an innovation, or to determine the extent to which environmental settings promote or inhibit the diffusion of farming practices (e. g. by associating covariates to the diffusion rate r). The relationship between time and p does not need to follow a sigmoid curve. One could potentially model the different curves to estimate cycles of adoption (e. g. using a sine wave function) or account for population structure (e.g. using a double-stage sigmoid curve), and even different transmission biases (Henrich, 2001), although a non-parametric model might be more useful during early stages of data exploration.

It is worth noting that the inferential power of the two methods is inevitably conditioned by the underlying shape of the diffusion curve, the sample size, and the specific idiosyncrasies of the calibration curve. Our two examples on the diffusion of farming provide instances of longer (Britain) and shorter (Japan) term dynamics, with the latter at least in part conditioned by the calibration plateau around 800-400 BCE. Similarly, case study 2 (British burials) encompasses several intervals with calibration plateaus. Yet a comprehensive assessment of all factors conditioning the inferential power of the approach we propose is not possible. Simulation studies like those presented here where artificial datasets with the same sample size, sample structure, and temporal window of analyses as the observed data are examined in detail can reveal the extent to which the inferential engine can or cannot recover hypothetical patterns. Such *what-if* experiments (Buck and Meson, 2015) are paramount for properly determining whether the available samples are appropriate for the specific question posed.

Lastly, all empirical case studies presented here covered a comparatively wide geographic and chronological window where the assumption of a stationary diffusion process can be difficult to justify. As evidenced in both case studies on the diffusion of farming, one should expect variations in diffusion dynamics within larger spatial and temporal windows where the assumption of a sigmoid curve might hold only for particular intervals and locations. Curves fitted over these datasets should be examined with care, as they capture averaged trends and obscure potential variations. There is inevitably a trade-off; smaller spatial and temporal windows are more likely to follow a sigmoid curve but are also limited by smaller sample sizes and lower inferential power. Furthermore, defining a meaningful geographic subdivision is a challenge itself, given potential issues such as the modifiable areal unit problem (Openshaw, 1984). A possible solution to this is to employ models that formally account for the spatial structure of the data, such as Gaussian Process regression (Rasmussen and Williams, 2006). These potential directions would still require sufficient sample sizes to be viable, but the growing number of large databases of radiocarbon dates might give hope that such opportunities are not that far away. It is further worth noting that the assumption of stationarity was made also for the site level random effect k_j. In the British dataset for case study 1b, 11% (36 out of 314) of the sites have calibrated dates spanning an interval of over 1000 years, making the assumption of the same value for k_j potentially problematic. Employing different aggregation units, possibly adding multiple levels (e.g. context or phase and site) may address this issue, particularly when additional covariates at such a level might help

inform the model in estimating sensible values of k_j.

7. Conclusions

The last decade saw an increasing effort in synthesising large collections of radiocarbon dates to provide new insights into the human past. While much of the focus has been centred on paleo-demographic inferences, there are increasing opportunities to investigate other phenomena, each with its own methodological and theoretical challenges. Here we introduced and explored the application of a Bayesian pipeline for modelling DOI curves. Results on both simulated and empirical datasets have revealed that our method can accurately recover the temporal dynamics of the diffusion process and identify instances where observed patterns deviate from a typical s-shaped curve. Both empirical case studies on the diffusion of farming did indeed show such deviations. In Japan, this was most likely the consequence of a slow-down in the dispersal of rice agriculture in the northern regions of the archipelago, whilst, in Britain, this was the result of a temporary increase in pastoralism and consumption of wild plants. Whilst both phenomena were known from previous studies, our analyses provided an independent assessment of these events and a more accurate estimate of their timing. Our third case study on the temporal changes in the burial customs in Britain showcased how our non-parametric model can be used in instances where we should not expect a sigmoid curve to begin with but are interested in simply recovering the shape of fashion cycles. Although exploratory by nature, this approach can still provide numerical estimates of the magnitude of diffusion events and the timing of when abrupt changes might have occurred.

CRediT authorship contribution statement

E.R. Crema: Conceptualization, Data curation, Formal analysis, Funding acquisition, Methodology, Software, Writing – original draft, Writing – review & editing, Visualization. **A. Bloxam:** Data curation, Funding acquisition, Writing – original draft, Writing – review & editing. **C.J. Stevens:** Data curation, Writing – review & editing, Writing – original draft. **M. Vander Linden:** Data curation, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jas.2024.105962.

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