**Methods. 3000 words max (Nature format)**

To disentangle the relative contributions of cultural diffusion and takeover to the modern

distribution of cultural traits, we simulated the evolution and global spread of agriculture. Our model simulates an initial colonization of the world by hunter-gathers and subsequently allows agriculture to arise and spread from a limited number of known historical. Different model variants allow for different mechanisms to drive these processes. The most basic variant simulates spread of agriculture solely via vertical transmission. More complex variants allow for diffusion, takeover, or both. The outputs of these simulations are then summarized through 19 highly-targeted phylogenetic and spatial statistics (each model variant is replicated 160K times). The actual values computed from the current distribution of 6000 real societies can then be compared to the resulting distributions.

The model is divided into three modules that are run independently but in sequence so that there are natural breaks in running the model. Module one accepts input parameters and produces a simulation from those inputs. Module one returns a realized landscape and the associated phylogenetic tree for that realization. Module two accepts simulation replicates (landscapes and trees) and calculates a targeted list of summary statistics to describe those simulations. Module two returns a list of summary statistics from those simulated worlds. Module three accepts the summary statistics from module 2 and the summary statistics from the realized human history and returns estimates for which of the four simulation types the realized human history more closely resembles.

**Module 1: Produce simulations**

Simulations are initiated as two data storage objects, a spatial layout and a phylogenetic tree, that are updated each time step as the simulation progresses. The spatial layout object is a set of ~6000 points marking the centroids of all extant languages that are linked together using a forced-connection network defining available neighbors for each point. This object is stored as a matrix where each row contains the latitude, longitude, a list of neighbors for that point, and labels (tip and trait) for matching locations to the phylogenetic tree. Each of these points is then assigned an agricultural habitat suitability score based on the number of domesticated species found at a particular centroid location compared to the global pool of domesticated species. This integer value is converted to a binary indicator (1, 0) of agricultural suitability (good for farming or not) according to the method outlined in Vilela et al. (*in prep*). Each location has at least 7 defined neighbors but some can have more connections because symmetrical connections are forced between all points and that occasionally requires identifying more than 7 neighbors. Societies can only be assigned a single trait state (agriculturalist or foraging society) and a single state of environmental suitability (1, 0). Each simulation starts by choosing a single random location to assign as the first foraging society and all other societies radiate from that single origin as the simulation progresses.

The phylogenetic tree object is a matrix object where each row contains the name of a single node, the parent node from which that node came, and the daughter nodes directly connected to it. During the simulation, all the evolutionary relationships are tracked using this phylogenetic tree. These initialized objects are identical between replicate simulation, so all simulations begin under the same conditions. The branch lengths (*BL*) correspond to the sum of time steps from the origin of a node (*k*) or tip to the current time of the simulation (*BLk = Ti - Tk*). During a speciation process (through the Speciation or Takeover module) one society will bifurcate into two new societies in the phylogenetic tree so the tree is always binary and non-reticulated. All society extinctions (through the Extinction or Takeover module) will be pruned from the phylogenetic tree. At the end of each time step, all the tip lengths are extended by adding the current time step so that the tree is always ultrametric. The final phylogenetic tree will always be binary and ultrametric. The output tree will include all extant societies but no extinct societies that have been trimmed from the tree.

Replicate simulations each start with identical initial conditions and then they are subjected to a series of simulation rule sets to modify both the spatial and phylogenetic objects each time the simulation progresses. Each time step, these objects are modified a maximum of 5 times by up to 5 separate and randomly ordered simulation modules named: arisal, speciation, extinction, diffusion, and takeover. Each of these modules simulates a single process contributing to the spatial spread and persistence of a trait. The number of modules used is defined by the model type run. The basic model uses only the arisal, speciation, and extinction modules. The diffusion model adds the diffusion module to the set of basic modules, while the takeover model adds the takeover module to the set of basic modules instead. The full model includes all 5 modules. These modules are randomly reordered each step as an experimental control because there is no intrinsic hierarchical relationship between them and we didn’t want to introduce a bias artificially assuming an ordered relationship between these causes.

Rule sets within each module cannot be applied to all centroid locations at the same time because the modification of one point can interfere with the modification of the next, so points are sampled without replacement and modified one by one. This sampling scheme randomly reorders the sequence of spatial points each time a new module is applied and prevents spatial bias when applying rule sets.

Each rule set module accepts a 2x2 matrix of probabilities defining how those rules are applied throughout a particular replicate simulation. These matrices are created before the simulation begins by drawing random numbers from a uniform distribution to populate each of the boxes in 5 separate 2x2 matrices. The rows of these matrices define the trait identity for the source population (forager of domesticator) that is trying to expand into a neighboring centroid. In the modules defining the basic model (speciation, extinction, and arisal), the column values define the environmental suitability for target areas and the modules extending the basic model (takeover, diffusion, and both) define their columns as the target societies’ susceptibility to receiving a trait through diffusion or takeover. The cells of these matrices define the individual probabilities for each possible outcome (e.g. domesticator in good environment for domestication, domesticator in a bad environment for domestication, a forager in a good environment for foraging, and a forager in a bad environment of domestication). These numbers are redrawn for each replicate simulation but they stay the same across time within a given replicate. The values in each box defines a probability threshold for triggering an action or not. Within a module, a random number is drawn from a uniform distribution. If that drawn value is less than the value defined in the probability matrix, then the module takes its defined action. If the drawn value is greater than the value provided in the matrix, then the module action is skipped for that time step.

**Rule sets:**

Arisal – Every society has a chance to change their trait from foraging to farming at every time step.

Speciation – Every society has a chance to expand into un-colonized neighbor locations at each time step. Because societies can only occupy one location, a speciation occurs when a society expand into a new location, and a new society is created (Speciation module). The decedent society will keep the same trait of the parent society.

Extinction – Every society has a chance to go extinct at each time step.

Diffusion – Every society has a chance to diffuse their trait to other neighbor society at every time step

Takeover – Every society has a chance to takeover a neighbor society (with speciation of the source society and extinction of the target society) at every time step (Takeover module). Takeover only happens when all neighbor cells are occupied [Note that because the Speciation module requires empty neighbors, while Takeover only occurs in the absence of them, only one of these two modules will happen at each time step per society. This avoids an artificial inflation of the speciation rate with Takeover]. Farming societies will always prefer to invade locations suitable for farming if they are available.

**Module 2: Calculate summary statistics**

The spatial layout object and phylogenetic tree are both passed directly to this module without modification. These objects are immediately trimmed to match the 1200 societies in the realized history dataset. Those trimmed objects are then passed to 19 individual functions which each produce a single summary statistic. Those statistics are then aggregated into a single list and returned as the output of this module. The statistics used in this module are organized according to their basic unit of measurement and the type of summary they represent. There are 5 subcategories of analysis:

1. Branch Length (richness and divergence)

The basic unit of measurement for this section is the branch length, which is the unit length between each node. Phylogenetic diversity (*PD*) is the summation of all branch lengths connecting species together (Faith 1992). This is an anchor test, which means it is regularly used, well understood, and we should use it to anchor our work to past work. PD is a richness measure, it tells us how much evolutionary history is associated with a set of tips. Average phylogenetic diversity (*avPD*) (Clarke and Warwick 2001) is the mean branch length calculated as *PD* divided by the total number of tips in the tree.

1. Pairwise distance between tips (richness, divergence, and regularity)

The basic unit of measurement for this section is the pairwise distance. This is the patristic distance, meaning the sum of the branch lengths following the shortest distance between two tips in a tree, implemented as a distance matrix where every tip is compared to every other tip. The sum of all pairwise distances, *F*, is more formally called ‘Extensive quadratic entropy’. (Izsak and Papp 2000). Just as it was with branch lengths, this is a richness measure and, accordingly, describes the amount of distance between compared tips. The divergence metric for pairwise distance is mean pairwise distance, *MPD* (a.k.a. *AvTD*, and *Δ+*), which is the mean inter-species distances between species. (R. Clarke and Warwick 1998; Webb et al. 2002; Webb, Ackerly, and Kembel 2008; Kembel et al. 2010). Variance in pairwise distances, *VPD* (a.k.a. *VarTD and Λ+*), is a regularity indices. (Clarke and Warwick 2001) Variance is relative to tips, not to total branches. These are the residuals to the mean pairwise distance, they compare each individual pairwise connection to the overall mean.

1. Phylogenetic isolation (divergence and regularity)

A phylogenetic isolation index represents the relative isolation of a given species within a phylogenetic tree. Several indices have been proposed so far but we focus here on the evolutionary distinctiveness index called ‘Fair Proportion’ as proposed by Redding (2003) and Isaac et al. (2007). The sum of phylogenetic isolation units is evolutionary distinctiveness (*ED*), which is a richness indices. It can be useful to note that *ED* is not equal to Faith’s *PD* because the EDi are computed from the regional pool of species and summed across a given assemblage (i.e. a subset of the regional species pool) (Tucker et al. 2016; Safi et al. 2013; Redding 2003; Isaac et al. 2007).

1. Tree topology

Tree topology is a measure of the shape of the overall tree. The tree can be lopsided side-to-side or root-to-tip. Our most trusted index for the tippy vs trunky of a tree is the gamma index, γ. The index characterizes the distribution of branching events within the tree. Trees with γ < 0 have relatively longer branches towards the tips of the phylogeny (tippy trees), whereas trees with γ > 0 have relatively longer inter-nodal distances towards the root of the phylogeny (stemmy trees). tk represents an ‘evolutionary period’ (limits are given by two speciation events) or equivalently an internode distance (Pybus and Harvey 2000).

1. Spatial analyses
2. Macro evolutionary tree metrics (rate and rate change in tree units)

**Module 3: Classification**

Module three accepts the list of summary statistics produced by module two and uses a random forest machine learning algorithm to first classify all of the replicate simulations according to model type and then use the decision trees created during that classification to categorize the realized cultural phylogeny estimated from historical, linguistic, and archeological data. Module three returns a list ranking the value each summary statistic brings to classifying each simulation, a matrix describing how good each decision tree in the random forest was at classifying each simulation, and a list recording the classifications that all of the individual decision trees assigned to the realized historical phylogeny. This final count represents the probability that the realized historical phylogeny came from each of the proposed mechanisms.

**Running the simulation using High-performance computing clusters**

We ran the simulations from 17 January 2016 to 15 May 2016 across 4 separate high-performance computer cluster at three different institutions.