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- 1 Detect change-point, trend, and seasonality in satellite time series data to track abrupt changes
- 2 and nonlinear dynamics: A Bayesian ensemble algorithm
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Abstract: Satellite time-series data are bolstering global change research, but their use to elucidate 18 land surface or vegetation dynamics is sensitive to algorithmic choices. Different algorithms often 19 give inconsistent or sometimes conflicting interpretations of the same data. This lack of consensus 20 21 has adverse implications and can be mitigated via ensemble modeling, an algorithmic paradigm that combines many competing models rather than choosing only a single "best" model. Here we report 22 one such time-series decomposition algorithm for deriving nonlinear ecosystem dynamics across 23 multiple timescales—A Bayesian Estimator of Abrupt change, Seasonal change, and Trend 24 (BEAST). As an ensemble algorithm, BEAST quantifies the relative usefulness of individual 25 decomposition models, leveraging all the models via Bayesian model averaging. We tested it upon 26 simulated, Landsat, and MODIS data. BEAST reliably detected changepoints, seasonality, and trends 27 in the data; it derived realistic nonlinear trend signals and credible uncertainty measures (e.g., 28 occurrence probability of changepoints over time)—some information difficult to derive by 29 conventional single-best-model algorithms but critical for interpretation of ecosystem dynamics and 30 31 detection of low-magnitude disturbances. The combination of many models enabled BEAST to 32 alleviate model misspecification, address algorithmic uncertainty, and reduce overfitting. BEAST is generically applicable to time-series data of all kinds, serving to improve robustness in uncovering 33 true time-series dynamics. It offers a new analytical option for changepoint detection and nonlinear 34 trend analysis and will help exploit environmental time-series data for probing patterns and drivers of 35 ecosystem dynamics. 36

Keywords: Changepoint; Bayesian changepoint detection; Disturbance ecology; Breakpoint; Trend
 analysis; Time series decomposition; Bayesian model averaging; Disturbances; Nonlinear dynamics; Regime
 shift

### 40 1. Introduction

Ecosystems are changing constantly, driven by natural forcings and human activities in 41 complex ways. Disentangling the complexity to build predictive biospheric sciences is a defining 42 43 theme of global change research (Franklin et al. 2016)—a goal hard to attain without reliable capabilities of monitoring lands over time (Pettorelli et al. 2014; Su et al. 2016; Zhao and Jackson 2014). 44 To date, such spatiotemporal data come primarily from satellites (Hu et al. 2017; Jetz et al. 2016). 45 Satellite time-series data, such as decades of Landsat, MODIS, or AVHRR imagery, have proven 46 particularly valuable for elucidating patterns and drivers of land and ecosystem dynamics (Hawbaker 47 et al. 2017; Li et al. 2018; Zhu and Woodcock 2014). 48

Despite existing successes in satellite time-series analyses, challenges remain. A notable issue 49 pertains to the diverging findings from the use of satellite data in addressing the same problem. For 50 example, there is controversy regarding how the Amazon forests respond to basin-wide droughts; 51 some satellite analyses suggested a green-up but others not (Huete et al. 2006; Samanta et al. 2010). 52 53 Inconsistencies like this are attributed partly to different algorithms and perspectives taken for data processing and analysis (Liu et al. 2018; Shen 2011; Tewkesbury et al. 2015). A preponderance of 54 satellite time-series analyses take a statistical modeling perspective, seeking a so-called best model out 55 56 of many candidates to decompose time series into vegetation dynamics such as trends and abrupt changes (Cai et al. 2017; Jonsson and Eklundh 2002). This single-best-model paradigm is broadly 57 embraced by practitioners (Powell et al. 2010; Zhao et al. 2018), but its use for seeking mechanistic 58 understandings of ecosystems is not necessarily safe (Chen et al. 2014; Grossman et al. 1996). 59 Mechanistic interpretations of time-series data are sensitive to choices of statistical 60 algorithms or models. When fitting a linear model to decades of AVHRR data, a greening trend in 61 vegetation was inferred and was attributed to global warming (Myneni et al. 1997). If using a piecewise 62 linear model with one changepoint instead, a greening was observed only for the first period whereas 63

a browning for the second, generating new explanations of climate-biosphere interactions (*Wang et al. 2011*). If piecewise models with multiple changepoints were fitted, the conclusion would change
again, giving alternative speculations on drivers of ecosystem changes (*Jong et al. 2012*). Similar
studies with diverging findings abound (*Alcaraz-Segura et al. 2010; Yu et al. 2010*). Extrapolation from
such findings is at stake if applied blindly to validate predictive models and inform resource
management.

Inconsistent or contradicting insights gained from different models are a common problem of 70 the single-best-model paradigm. The "best" models are often selected to optimize certain criteria 71 such as AIC and BIC. Depending on data quality and the choices of optimization algorithms and 72 model selection criteria, many "best" models are possible for the same time series (Banner and Higgs 73 74 2017; Cade 2015). The usefulness of these models is not dichotomous. Favoring one against others is an over-simplifying strategy that often overlooks the utility of alternative models and ignores model 75 76 uncertainties. Model selection in the single-best-model paradigm is also complicated by the 77 subjectivity in specifying data analysis models and the inability of simple models to represent complex time-series signals. Model structures with increased complexity are more likely to capture variations 78 79 in satellite data at multiple timescales, but they are also more likely to overfit the data and their 80 estimation entails sophisticated statistical techniques.

Many problems difficult to tackle by conventional methods can now be addressed by turning to Bayesian statistics—an inferential paradigm that can treat both model parameters and structures probabilistically and offer a unified framework to address uncertainties of various forms (*Denison* 2002; Ellison 2004; Finley et al. 2007; Zhao et al. 2008; Zhou et al. 2017). Unlike conventional criterion-based methods that choose only a single best model, the Bayesian paradigm can embrace all candidate models, evaluate how probable each of them is a true one, and synthesize the many models into an average model (*Denison 2002; Thomas et al. 2018; Zhao et al. 2013*). This scheme is known as Bayesian model averaging (BMA). It belongs to a category of multi-model techniques broadly called
ensemble learning. Consideration of many models helps BMA to capture model uncertainty, alleviate
model misspecification, and improve flexibilities and generalizability in modeling complex data.
These advantages of BMA have been exemplified in numerous case studies across disciplines (*Banner and Higgs 2017; Raftery et al. 2005; Zhang and Zhao 2012; Zhao et al. 2013*). Despite all the benefits of

Bayesian inference or BMA, its use for satellite time-series analysis remains rather limited, with
enormous potential to tap.

This study seeks to reliably decipher time-series data for via Bayesian modeling. Our aim is 95 (1) to introduce a generic Bayesian time-series decomposition algorithm for changepoint detection 96 and nonlinear trend analysis, and (2) to demonstrate its applications to satellite data for tracking land 97 and ecosystem nonlinear dynamics. We term the algorithm BEAST—a Bayesian Estimator of Abrupt 98 change, Seasonality, and Trend. BEAST features many advantages over conventional non-Bayesian 99 100 algorithms. Foremost, it forgoes the single-best-model paradigm and applies the Bayesian ensemble 101 modeling technique to combine numerous competing models and generate a rich set of information 102 unobtainable from non-Bayesian algorithms. BEAST can quantify various sources of uncertainties, detect abrupt changes of any magnitude, and uncover complex nonlinear dynamics from time-series 103 104 data. But due to the Bayesian computation needed, its applications to high-resolution imagery over large areas may be constrained by computer power. 105

106 In what follows, we further justify the value of Bayesian statistics for time-series analysis

107 (Sect 2; Fig. 1), then detail the formulation of our BEAST algorithm (Sect 3; Figs. 2-3), and test the

108 capabilities of BEAST using both simulated and real data (Sect 4 &5; Figs. 4-11). We also discuss the

109 many features of BEAST as contrasted to existing time-series decomposition algorithms, and explain

110 how ensemble learning and Bayesian modeling help to make BEAST a useful tool to capture,

111 monitor, and derive land surface dynamics from satellite data (Sect 6).

### 112 2. Why use Bayesian statistics?

We begin with extra backgrounds on how time-series data have been conventionally decomposed in non-Bayesian frameworks. Their potential weaknesses are then detailed to justify the needs for Bayesian algorithms. Below, our presentation focuses on time series of Normalized Difference Vegetation Index (NDVI)—a spectral variable measuring land surface greenness or vegetation vigor (Fig. 1a). But the reasoning applies equally to non-NDVI or non-satellite data, such as LAI, albedo, climate, streamflow, and social-ecological indicators.

Ecologically speaking, a NDVI time series captures landscape dynamics at three major 119 timescales (Kennedy et al. 2014): (1) seasonality or periodic variations as forced by intra-annual 120 climatic variations or phenological drivers; (2) gradual changes as driven by long-term environmental 121 trends, chronic disturbances, or successional dynamics; and (3) abrupt changes associated with severe 122 disturbances, sudden recoveries, regime shifts, or altered management practices (e.g., fire, insect, 123 logging, weeding, urbanization, re-vegetation, extreme weather, crop rotation, and climate shift). In 124 125 this decomposition, the time series is treated as the sum of the first two components-seasonal and trend signals (Fig. 1b). The third component—abrupt changes—do not stand out alone but is 126 embedded in seasonality and trends as changepoints (Fig. 1b, blue vertical bars). 127

Mathematically speaking, the search for ecological interpretations of a time series reduces to finding the relationship between NDVI (y) and time (t) from the observed data at n points of time  $\mathcal{D} = \{t_i, y_i\}_{i=1,...,n}$  via a statistical model  $\hat{y}(t) = f(t)$ . The model generally treats the time series  $y(t_i)$  as an addition of seasonal  $S(\cdot)$  and trend  $T(\cdot)$  signals(Fig. 1):

$$\hat{\mathbf{y}}(t_i) = f(t_i; \mathbf{\Theta}) = S(t_i; \mathbf{\Theta}_s) + T(t_i; \mathbf{\Theta}_T), i=1,...,n$$
(1)

where the parameters  $\Theta_s$  and  $\Theta_T$  specify the seasonal and trend signals; they also encode the abrupt changes implicitly. By analogy to linear regression, the time *t* and data *y* are independent and dependent variables, respectively;  $\Theta_s$  and  $\Theta_T$  are parameters to be estimated from the data  $\mathcal{D}$ .

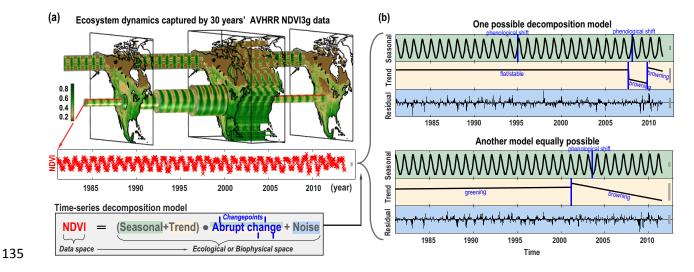


Fig. 1. Tracking land surface dynamics from space is treated here as a time-series decomposition problem. (a) A 3D 136 137 volumetric view of 30 years of AVHRR NDVI data depicts ecosystem dynamics at three timescales: seasonality, 138 trend (e.g., climate-driven responses or successional dynamics), and abrupt change (e.g., disturbance or 139 changepoint). Algorithmically speaking, decomposition of a time series into these three components is a model 140 selection problem, seeking an "optimal" model structure that best fits the time series. (b) But the use of different 141 inferential procedures or selection criteria yields different or even contradictory decompositions, with adverse 142 implications. For example, two "optimal" models in (b) can fit the same time series of (a) almost equally well, but 143 with inconsistent decompositions and ecological interpretations. Vertical blue bars denote changepoints in seasonal 144 dynamics or trends. The equal plausibility of the two "best" models highlights an inherent weakness of many 145 existing satellite time-series analyses for studying ecosystem changes.

(1) How many changepoints occur and when? Changepoints indicates any abrupt changes in trend/seasonal signals (*Jamali et al. 2015*). By "abrupt", we refer to not only sudden NDVI jumps (e.g., forest clearing or quick recovery) but also any turning points or breakpoints at which trend or seasonal signals start to deviate from the previous regular trajectories. This definition is broader and more inclusive than that assumed by other algorithms. As examples, a smooth recovery from tree stand-clearing is often associated with only one changepoint by many algorithms, but in our definition, the recovery trajectory may have many changepoints related to different succession stages

By decomposing a time series with Eq. 1, we seek to answer the following questions:

154 or rates of recovery. A subtle transition in vegetation dynamics caused by a shift in climate regime is rarely considered as a changepoint by many algorithms, but in our definition it is. 155

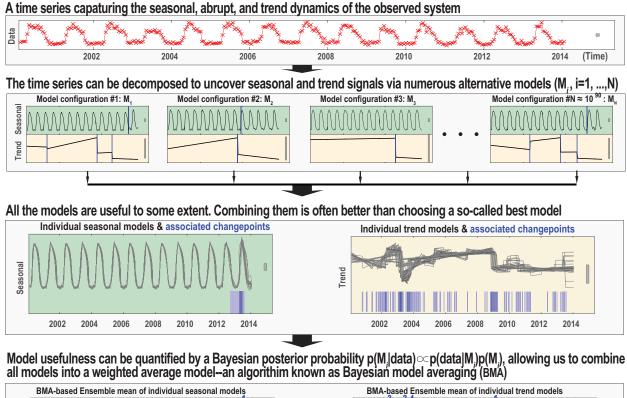
(2) What is the underlying trend? A trend is not just a linear line but can be a complex 156 157 nonlinear trajectory interspersed with changepoints. The transient trend trajectory at changepoints are rarely true discontinuous jumps but rather quasi-continuous sharp transitions. Detection of trends 158 with high fidelity is critical for inferring subtle drivers of ecosystem dynamics (e.g., climatic effects). 159 (3) What is the underlying seasonal signal? A seasonal signal may be also interspersed by 160 changepoints. Seasonal changepoints do not necessarily coincide with trend changepoints. Detection 161 of seasonal changepoints helps to identify potential drivers of phenology changes. 162 Any uncertainties or errors in inferring the model Eq. 1 will be translated to those in answering these 163 questions, thereby engendering contradictory or wrong ecological insights into ecosystem dynamics. 164 Existing methods to infer the model or relationship f come in many fashions (Brooks et al. 165 2014; Kennedy et al. 2010; Zhu and Woodcock 2014). Often, the trend is parameterized and 166 167 approximated by linear, piecewise-linear, or polynomial models (Browning et al. 2017). The seasonal signal is modeled via flexible basis functions, such as Fourier curves and wavelets (*Brooks et al. 2012*; 168 Jiang et al. 2010; Martínez and Gilabert 2009; Shu et al. 2017). Another alternative is to ignore 169 170 seasonal signals by fitting a trend model to a sub-time series (e.g., summertime NDVI only) (Wang et al. 2011). Moreover, abrupt NDVI changes are implicitly encoded in the parameters  $\Theta_T$  and  $\Theta_s$ . 171 These changepoints also need to be inferred from the data D (Chen et al. 2014). Such diverse options 172 for model configurations lead to a large or even infinite number of candidate models for analyzing the 173 same time series. Conventional methods aim to seek the "best" model and discard others based on 174 selection criteria, such as mean square error, Cp, AIC, anomaly threshold, or subjective criteria (Chen

et al. 2014; Wang et al. 2011). 176

177	These conventional methods have potential weaknesses that were not always articulated in
178	previous studies (Fig. 1). First, vegetation dynamics normally shows a nonlinear trend (Burkett et al.
179	2005; Jentsch et al. 2007), which is not guaranteed to be adequately approximated by a single linear,
180	piecewise-linear, or polynomial model. Second, many conventional analyses make too restrictive
181	model assumptions. For example, prior studies often assumed a prescribed number of changepoints
182	or a fixed harmonic order in seasonality (Lu et al. 2004; Wang et al. 2011), which is too arbitrary a
183	choice. Third, the true model for NDVI dynamics is essentially unknown so that model
184	misspecification is inevitable (Kennedy and O'Hagan 2001). The use of misspecified or wrong models
185	is of little concern for those applications on retrievals of biophysical variables (Shmueli 2010; Zhao et
186	al. 2018), but it becomes problematic for ecological interpretation of NDVI data simply because
187	different models imply contrasting or contradicting hypotheses. Such model uncertainties are
188	typically ignored by non-Bayesian approaches.
189	Fourth, even for the same class of model type, the final model chosen is sensitive to not only
190	model selection criteria but also data noises, thus opening up possibilities for inconsistent
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201	the Bayesian paradigm are being demonstrated by a growing body of theoretical and empirical
202	evidence (Denison 2002; Rankin et al. 2017; Reiche et al. 2015; Zhao et al. 2013; Zhou et al. 2017).
203	Foremost, Bayesian inference treats both model parameters and structures as random and therefore
204	characterizes them explicitly and probabilistically. As such, Bayesian inference tends not to deem any
205	single model configuration as the true model, but instead recognizes the relevance and usefulness of
206	all the potential models (Kennedy and O'Hagan 2001; Zhao et al. 2013). Specifically, each model is
207	assigned a probability being the true model (Fig. 2); this probability can be learned from data and then
208	used as an informative weight to synthesize all the models into a weighted average model. This
209	Bayesian model averaging scheme is flexible enough to approximate complex relationships that
210	cannot be represented by individual models (Fig. 2). It also alleviates the adverse consequences of
211	model misspecification and tackles model uncertainty (Zhao et al. 2013).
212	Computationally, Bayesian inference or BMA is implemented via stochastic sampling
213	algorithms known as Markov Chain Monte Carlo (MCMC) (Denison 2002; Green 1995). MCMC
214	sampling helps to effectively explore the enormous model space at a reasonable computation cost.
215	The use of MCMC circumvents analytical intractability and enables the Bayesian paradigm to handle
216	the complexity that conventional methods cannot handle. MCMC also generates various sample-
217	based statistics to test hypotheses that are difficult to tackle using the conventional paradigm.
218	Bayesian statistics can aid in inferring the model of Eq. 1, due especially to its additive nature:
219	a time series is the sum of seasonal and trend signals, with changepoints being inseparable parts of
220	them. Inference of the three— trend, seasonality, and changepoints,—is not separable. Any
221	estimation error in one will be leaked to bias the estimation of others. It is unlikely to correctly detect
222	changepoints if the trend or seasonality is not well modelled. Trend analysis and changepoint
223	detection are two sides of the same goal. It is also impossible to estimate true decomposition
224	uncertainties if not accounting for model misspecification simultaneously for the three components.

- 225 Therefore, reliable time-series decomposition requires sufficiently approximating the nonlinearity of
- both trend and seasonality and simultaneously incorporating model uncertainties of all sorts. These
- 227 issues are explicitly tackled by Bayesian inference, as detailed next.





229 Fig. 2. Illustration of BEAST—a Bayesian ensemble time-series decomposition algorithm. Our modeling philosophy 230 is that a time series can be fitted by numerous competing models, all of which are wrong but useful to some degree. 231 Conventional methods choose the "best" model, ignoring model uncertainty or misspecification and opening up room for fortuitous conclusions (Fig. 1). As a remedy, BEAST quantifies the relative usefulness of individual models 232 233 (i.e., model structures) and incorporates all the models into the inference via Bayesian model averaging. This 234 ensemble learning makes BEAST a universal approximator of complex nonlinear trends and allows BEAST to 235 account for uncertainties difficult to consider by non-Bayesian methods. For example, model uncertainty is explicitly 236 addressed (e.g., gray envelope around the fitted seasonal or trend signals are 95% credible intervals). BEAST not only

- 237 detects the changepoints but also quantifies their probabilities of being true changepoints, providing confidence
- 238 measures to guide informative interpretation of satellite time-series data.

### 239 3. BEAST: Bayesian estimator of abrupt change, seasonality & trend

- 240 This section describes the formulation and implementation of our BEAST time-series decomposition
- algorithm. The description is inevitably mathematical. Readers not interested in technical specifics
- 242 may skip to Section 4 while re-visiting Figs. 2 &3 or Section 2 for an overview of the concept and
- 243 capabilities of BEAST. The implemented software is available as both a Matlab library and an R
- 244 package (to be released upon acceptance of this ms).

### 245 **3.1 Parametric form of BEAST for time-series decomposition**

Our analysis considers a time series  $\mathcal{D} = \{t_i, y_i\}_{i=1,\dots,n}$  to be composed of three

components—seasonality, trend, abrupt changes—plus noise (Fig. 1b), which is formulated as a

248 rewriting of Eq. 1:

$$y_i = S(t_i; \Theta_s) + T(t_i; \Theta_T) + \varepsilon_i.$$
(2)

Here, we assume the noise  $\varepsilon$  to be Gaussian, capturing the remainder in the data not explained by the

- seasonal  $S(\cdot)$  and trend  $T(\cdot)$  signals. Following the common practice, we adopted general linear
- models to parameterize  $S(\cdot)$  and  $T(\cdot)$  (*Jiang et al. 2010; Verbesselt et al. 2010b*). Abrupt changes are
- implicitly encoded in the parameters  $\Theta_s$  and  $\Theta_T$  of the seasonal and trend signals.

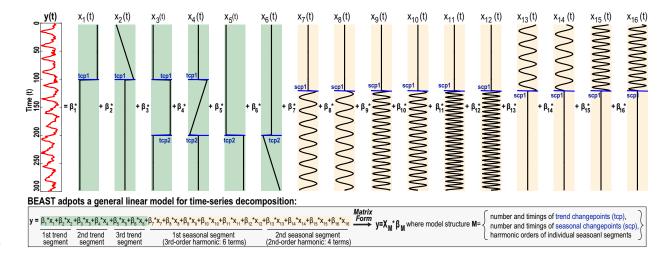


Fig. 3. How does BEAST decompose time series? BEAST is an additive model  $y = x_M \beta_M$ , formulating a time 254 series y(t) as the linear combination of many basis functions  $x_M$  (e.g., line segments  $x_1$ - $x_6$  or harmonics  $x_7$ - $x_{16}$  that are 255 256 zero-valued except for the active segments). These basis terms are specified by the model structure parameters M: 257 numbers and locations of seasonal/trend changepoints (i.e., horizontal blue bars such as tcp1 and scp1) and seasonal 258 harmonic orders (e.g., 3rd and 2nd in this example). The aim is to infer not only the coefficients  $\beta_M$  for a given M 259 but also the model structure M itself (i.e., changepoint and harmonic orders). The combinatorics of all possible 260 changepoints and harmonic orders gives an enormous model space with numerous candidate basis terms, making it 261 computationally impossible to pinpoint the true best model. BEAST infers M by randomly traversing the model 262 space via Bayesian model selection, so it is essentially a Bayesian general linear regression model. (The time axis is 263 oriented vertically for ease of displaying.) 264 Specifically, the seasonal signal S(t) is approximated as a piecewise harmonic model, defined with respect to p knots in time at  $\xi_k$ , k=1,...p (Fig. 3). These knots divide the time series into (p+1) 265 intervals  $[\xi_k, \xi_{k+1}]$ , j=0,...,p, where  $\xi_0 = t_0$  and  $\xi_{p+1} = t_n$  are the starting and ending times of the 266 data. The model is specified for each of the (p+1) segments  $[\xi_k, \xi_{k+1}]$ , k=0,...,p, taking the form of 267  $S(t) = \sum_{l=1}^{L_k} a_{k,l} \sin(\frac{2\pi lt}{P}) + b_{k,l} \cos(\frac{2\pi lt}{P}) \text{ for } \xi_k \le t < \xi_{k+1}, k = 0, \dots, p$ 268 Here, P is the period of the seasonal signal (i.e., one year in our cases);  $L_k$  is the harmonic order for 269

271  $\{a_{k,l}, b_{k,l}\}_{l=1,\dots,L_k}$  are the parameters for sins and cosines. This harmonic model is non-continuous as a 272 whole; the knots  $\xi_k$  indicate the changepoints at which abrupt seasonal changes may occur. Both the

total number of changepoints p and their timings  $\{\xi_k\}_{k=1,\dots,p}$  are unknown parameters to be

the k-th segment and is an unknown segment-specific parameter; and the coefficients

270

estimated. In short, we need the following parameters to fully specify the seasonal harmonic curve:

275 
$$\Theta_s = \{p\} \cup \{\xi_k\}_{k=1,\dots,p} \cup \{L_k\}_{k=0,\dots,p} \cup \{a_{k,l}, b_{k,l}\}_{k=0,\dots,p; l=1,\dots,L_k}$$

which includes the number and timings of changepoints, the harmonic orders for all the (p+1)

segments, and the coefficients of all the harmonic terms. All have to be estimated.

The trend T(t) is modeled as a piecewise linear function with respect to m knots at  $\tau_i$ ,

j=1,...m (Fig. 3), which divide the time span into (m+1) intervals  $[\tau_j, \tau_{j+1}]$ , j=0,...,p, with  $\tau_0 = t_0$  and  $\tau_{m+1} = t_n$  being the start and end of the time series. The trend knots or changepoints  $\tau_j$  are not necessarily the same as the seasonal changepoints  $\xi_k$ . The trend over each interval simply is a line segment (Fig. 2), defined by coefficients  $a_j$  and  $b_j$ :

283 
$$T(t) = a_j + b_j t \text{ for } \tau_j \le t < \tau_{j+1}, j = 0, ..., m$$

Similar to the seasonal signal, the number of changepoints m and their timings  $\{\tau_j\}_{j=1,\dots,m}$  are

unknown parameters to estimate. Hence, the full set of parameters specifying the trend T is

286 
$$\Theta_T = \{m\} \cup \{\tau_j\}_{j=1,...,m} \cup \{a, b_j\}_{j=0,...,m}$$

which comprises the number and timings of trend changepoints and the intercepts and slopes ofindividual line segments.

Both sets of the parameters,  $\Theta_s$  and  $\Theta_T$ , need to be estimated from the data  $\mathcal{D}$ . For ease of presentation, we re-classified the parameters  $\Theta_T$  and  $\Theta_s$  into two groups (Fig. 3):  $\{\Theta_T, \Theta_s\} = \{M, \beta_M\}$ . The first group M refers to model structure, including numbers and timings of trend and seasonal changepoints, and seasonal harmonic orders:

293 
$$\mathbf{M} = \{m\} \cup \{\tau_j\}_{j=1,\dots,m} \cup \{p\} \cup \{\xi_k\}_{k=1,\dots,p} \cup \{L_k\}_{k=0,\dots,p}.$$

294 The second group  $\beta_M$  is the segment-specific coefficient parameters used to determine exact shapes 295 of the trend and seasonal curves once the model structure M is given. Collectively,  $\beta_M$  is denoted by

296 
$$\boldsymbol{\beta}_{\mathrm{M}} = \left\{a, b_{j}\right\}_{j=0,...,m} \cup \left\{a_{k,l}, b_{k,l}\right\}_{k=0,...,p;l=1,...,L_{k}}.$$

297 The subscript M indicates the dependence of  $\beta_M$  on model structure M.

After this re-grouping, the original general linear model Eq. 2 becomes a familiar form:

$$y(t_i) = \mathbf{x}_{\mathsf{M}}(t_i)\boldsymbol{\beta}_{\mathsf{M}} + \boldsymbol{\varepsilon}_i \tag{3}$$

where  $\mathbf{x}_{M}(t_{i})$  and  $\boldsymbol{\beta}_{M}$  are dependent variables and associated coefficients, respectively. Again, the subscript M suggests that the exact form of  $\mathbf{x}_{M}$  and the coefficients in  $\boldsymbol{\beta}_{M}$  both depend on the model structure M (e.g., numbers and timings of changepoints). For example, column vectors of the design matrix  $\mathbf{x}_{M}(t_{i})$  are associated with individual segments of the piecewise linear and harmonic models (Fig. 3), with the number of coefficients in  $\boldsymbol{\beta}_{M}$  being  $2(m + 1) + 2\sum_{k=0}^{p} L_{k}$ .

304 As revealed in the re-formulated model of Eq. 3, the inference of vegetation dynamics now reduces to a model selection problem—determining an appropriate model structure M, including the 305 numbers and timings of changepoints and the harmonic orders. Identifying an optimal model 306 307 structure M for our problem is analogous to choosing the best subset of variables for simple linear regression. Once a model structure M is selected, its coefficients  $\beta_M$  are straightforward to estimate. 308 309 However, unlike simple linear regression, the number of possible model structures for Eq. 3 is extremely large. Even for a time series of moderate length (e.g., n >100), it takes billions of years' 310 computation to enumerate all possible models for finding the best one that optimizes certain criteria 311 (e.g., BIC). We circumvented this problem by resorting to Bayesian inference, as described next. 312

313

### 3.2 Bayesian formulation of BEAST

We extended the general linear model of Eq. 2 or 3 to build a Bayesian model for detecting abrupt change, seasonality, and trend from time-series data. In the Bayesian modeling, all the unknown parameters are considered random, including model structure M, coefficients  $\beta_M$ , and data noise  $\sigma^2$ . Given a time series  $\mathcal{D} = \{t_i, y_i\}_{i=1,...,n}$ , the goal is to get not just the best possible values of these parameters but more importantly, their posterior probability distribution  $p(\beta_M, \sigma^2, M|\mathcal{D})$ . By Bayes' theorem, this posterior is the product of a likelihood and a prior model:

$$p(\beta_{\mathrm{M}}, \sigma^2, \mathrm{M}|\mathcal{D}) \propto p(\mathcal{D}|\beta_{\mathrm{M}}, \sigma^2, \mathrm{M})\pi(\beta_{\mathrm{M}}, \sigma^2, \mathrm{M}).$$
 (4)

Here, the likelihood  $p(\mathcal{D}|\boldsymbol{\beta}_{M}, \sigma^{2}, M)$  is the probability of observing the data  $\mathcal{D}$  given the model parameters  $\boldsymbol{\beta}_{M}, \sigma^{2}$ , and M. Its form is governed by the general linear model  $y = \mathbf{x}_{M} \boldsymbol{\beta}_{M} + \varepsilon$  in Eq. 3. 322 Owing to the normality of error  $\varepsilon$ , the likelihood is simply Gaussian  $p(\mathcal{D}|\boldsymbol{\beta}_{M}, \sigma^{2}, M) =$ 

323 
$$\prod_{i=1}^{n} N(y_i; \mathbf{x}_{M}(t_i)\boldsymbol{\beta}_{M}, \sigma^2).$$

To complete our Bayesian formulation, what remains is to specify the second term of Eq. 4,  $\pi(\beta_M, \sigma^2, M)$ , which is called the prior distribution of the model parameters. By definition, we have

326 
$$\pi(\boldsymbol{\beta}_{M}, \sigma^{2}, M) = \pi(\boldsymbol{\beta}_{M}, \sigma^{2}|M)\pi(M)$$

327 Therefore, it suffices to elicit the conditional prior  $\pi(\beta_M, \sigma^2 | M)$  and the model prior  $\pi(M)$ 

328 separately. The priors encode our existing knowledge or beliefs in possible values of the model

329 parameters. Because of a lack of such general knowledge beforehand, our choices are flat priors, close

to being non-informative. First, for  $\pi(\beta_M, \sigma^2 | M)$ , we considered the normal-inverse Gamma

distribution and introduced an extra dispersion hyperparameter v into it to further reflect our vague

332 knowledge of the magnitude of model coefficients  $\beta_{M}$ . Second, for the prior on model structure

333  $\pi(M)$ , we assumed that the numbers of changepoints are any nonnegative integers that are equally

probable a prior. The exact formula of our priors are detailed in Appendix A.

335 Given our likelihood and prior models, the posterior of the model parameters becomes

$$p(\beta_{\mathsf{M}}, \sigma^2, \nu, \mathsf{M} | \mathcal{D}) \propto \prod_{i=1}^n N(y_i; \mathbf{x}_{\mathsf{M}}(t_i) \beta_{\mathsf{M}}, \sigma^2) \pi_{\beta}(\beta_{\mathsf{M}}, \sigma^2, \nu | \mathsf{M}) \pi(\mathsf{M}).$$
(5)

Its complete formulation after incorporating each component prior is expanded and presented inAppendix A, with more technical details explained there for interested readers.

338

## 3.3 Monte Carlo-based Inference

The posterior distribution  $p(\boldsymbol{\beta}_{M}, \sigma^{2}, v, \boldsymbol{M} | \boldsymbol{D})$  of Eq. 5 encodes all the information essential for inferring ecosystem dynamics. But it is analytically intractable, so we resorted to MCMC sampling to generate a realization of random samples for posterior inference. The MCMC sampling algorithm we used is a hybrid sampler that embeds a reverse-jump MCMC sampler (RJ-MCMC) into a Gibbs sampling framework, as briefly described below. The Gibbs framework samples the following three conditional posterior distributions inalteration for a total of N iterations.

$$p(\mathbf{M}^{(i+1)}|v^{(i)}, \mathcal{D});$$

$$p(\mathbf{\beta}_{\mathbf{M}}^{(i+1)}, \sigma^{2^{(i+1)}}|v^{(i)}, \mathbf{M}^{(i+1)}, \mathcal{D});$$

$$p(v^{(i+1)}|\mathbf{\beta}_{\mathbf{M}}^{(i+1)}, \sigma^{2^{(i+1)}}, \mathbf{M}^{(i+1)}, \mathcal{D});$$
(6)

346 These three conditional posteriors permit generating the (i+1)-th sample

 $\{\mathbf{M}^{(i+1)}, \mathbf{\beta}_{\mathbf{M}}^{(i+1)}, \sigma^{2^{(i+1)}}, v^{(i+1)}\} \text{ from the previous sample } \{\mathbf{M}^{(i)}, \mathbf{\beta}_{\mathbf{M}}^{(i)}, \sigma^{2^{(i)}}, v^{(i)}\}. \text{ In particular, the} \\ \text{second and third conditional posteriors are a normal-inverse Gamma distribution and a Gamma} \\ \text{distribution (Appendix A), which are easy to sample. In contrast, the first conditional posterior} \\ p(\mathbf{M}^{(i+1)}|v^{(i)}, \mathbf{D}) \text{ is difficult to sample because it is defined only up to an unknown proportionality} \\ \text{constant (Appendix A) and also because the dimension of } M \text{ varies from one model to another. These} \\ \text{two difficulties were tackled by using the RJ-MCMC algorithm ($ *Denison 2002; Green 1995* $). Details \\ \text{about RJ-MCMC are available in Zhao et al. (2013) and not given here.} \\ \end{cases}$ 

354

### 3.4 Posterior inference of changepoints, seasonality, and trends

355 The preceding MCMC algorithm generates a chain of posterior samples of length N  $\{\mathbf{M}^{(i)}, \boldsymbol{\beta}_{\mathbf{M}}^{(i)}, \sigma^{2^{(i)}}, v^{(i)}\}_{i=1,\dots,N}$ . The chain captures all the information essential for inference of land 356 357 dynamics, including trends, seasonal variations, and abrupt changes (Fig. 2). In particular, the sampled model structure  $\mathbf{M}^{(i)}$ , such as timings of changepoints and seasonal harmonic orders, can be 358 directly translated into the model's covariates  $\mathbf{x}_{\mathcal{M}^{(i)}}(t)$  (Fig.3), with their associated coefficients 359 being  $\boldsymbol{\beta}_{\mathbf{M}}^{(i)}$ . Each sampled model  $\mathbf{M}^{(i)}$  gives one estimate of the land dynamics,  $\mathbf{x}_{\mathbf{M}^{(i)}}(t) \cdot \boldsymbol{\beta}_{\mathbf{M}}^{(i)}$ . 360 Combining the individual estimates provides not only a final BMA estimate but also uncertainty 361 measures. The BMA estimate of time-series dynamics is the averaging of all the sampled models: 362

363  $\hat{y}(t) \approx \frac{\sum_{i=1}^{N} \mathbf{x}_{\mathbf{M}^{(i)}}(t) \beta_{\mathbf{M}}^{(i)}}{N}$ . The associated uncertainty is given as a sample-based variance estimate:  $v \widehat{a} r[\hat{y}(t)] \approx$ 364  $\frac{\sum_{i=1}^{N} [\mathbf{x}_{\mathbf{M}^{(i)}}(t) \beta_{\mathbf{M}}^{(i)} - \hat{y}(t)]^2}{N-1}$ .

Although each single model  $\mathbf{M}^{(i)}$  is a piecewise model, the combination of all the individual models enables the BMA estimate  $\hat{y}(t)$  to approximate arbitrary nonlinear signals. Moreover, because the covariates  $\mathbf{x}_{\mathbf{M}^{(i)}}(t)$  and model coefficients  $\boldsymbol{\beta}_{\mathbf{M}}^{(i)}$  are simply a coalescing of the individual elements of the trend and seasonal signals, these elements can be separated to recover the trend and seasonal components, respectively (Fig. 3).

# 370 More interestingly, the sampled model structure $\{\mathbf{M}^{(i)}\}_{i=1,\dots,N}$ , which is

 $\{m^{(i)}, \tau^{(i)}_{k=1,\dots,m^{(i)}}, p^{(i)}, \xi^{(i)}_{k=1,\dots,p^{(i)}}, L^{(i)}_{k=0,\dots,p^{(i)}}\}, \text{ allows making inference and testing hypothesis related to}$  $abrupt changes and land disturbances. Specifically, the chain <math>\{m^{(i)}\}_{i=1,\dots,N}$  or  $\{p^{(i)}\}_{i=1,\dots,N}$  gives an empirical distribution of the number of changepoints in the trend or seasonal signals; therefore, the mean total numbers of trend and seasonal changepoints can be estimated as  $\overline{m} = \frac{\sum_{i=1}^{N} m^{(i)}}{N}$  and  $\overline{p} = \frac{\sum_{i=1}^{N} p^{(i)}}{N}$ . For the seasonal signal, the chain of  $\{L^{(i)}_{k=0,\dots,p^{(i)}}\}_{i=1,\dots,N}$  can be used to compute the average harmonic order  $\overline{L}(t)$  needed to sufficiently approximate the seasonality for any given time t:

**377** 
$$\overline{L}(t) = \frac{\sum_{i=1}^{N} L_{k_i}^{(i)}}{N}, \text{ subject to } t \in [\xi_{k_i}^{(i)}, \xi_{k_i+1}^{(i)}]$$

The use of differing harmonic orders for different times or intervals is a strength distinguishing
BEAST from those algorithms that choose a pre-set, fixed order uniformly for the seasonal signal.

In addition, the chains  $\{\tau_{k=1,\dots,m^{(i)}}^{(i)},\xi_{k=1,\dots,p}^{(i)}\}_{i=1,\dots,N}$  indicate the exact timings at which the trend or seasonal changepoints occurred for the sampled individual models. From these chains, we can estimate the probability that a changepoint occurs at a time  $t_s$  or within a interval  $[t_s, t_e]$  by counting the frequency of the sample  $\{\tau_{k=1,\dots,m^{(i)}}^{(i)}\}_{i=1,\dots,N}$  containing the time  $t_s$  or falling into  $[t_s, t_e]$ :

384 
$$p(changepoint at t_s or within [t_s, t_e] | \mathbf{D}) \approx \frac{\# of \mathcal{M}^{(l)} that includes t_s or falls into [t_s, t_e]}{N}$$
.

Likewise, given an estimated changepoint, we can derive its credible interval. We can also calculate many more sophisticated statistics, such as what is the conditional probability of observing a changepoint in trend at a time if another changepoint has already occurred somewhere, and what is the joint probability of observing a changepoint in trend at one time and a seasonal changepoint at another time? All these sample-based statistics serve as important measures for statistical diagnostics such as uncertainty analysis and hypothesis testing. For example, a changepoint with an estimated occurrence probability of 3% is less likely to represent a true abrupt change.

### 392 3.5 Software Implementation

We implemented BEAST in the C programming language. The core is the MCMC sampler of Eq. 6, 393 an iterative process involving heavy matrix computation such as matrix multiplication and inversion. 394 We tested several matrix libraries and found that Intel's MKL was the fastest. We also implemented 395 an R and a Matlab interface to BEAST: an R package named "Rbeast" is forthcoming. To facilitate 396 algorithm assessment, we further developed a toolkit "trackEcoDyn" (Fig. 10). It offers a graphical 397 398 user interface (GUI) that allows interactively running BEAST and more importantly, manually analyzing and interpreting Landsat time series data in reference to other image sources (e.g., Landsat 399 images, and aerial photos). The tool is automatically linked with Google Earth and its high-resolution 400 401 historical imagery, facilitating visually cross-checking land histories among multiple sources. The purpose of trackEcoDyn is to aid in interpreting Landsat time series and collecting ground-reference 402 data for algorithm assessment, as used below in our second case study. 403

### 404 **4. Examples**

405 Three examples are given below to illustrate the basic usage and typical outputs of BEAST. To

406 highlight its differences from existing methods, we also compared BEAST to a community-endorsed

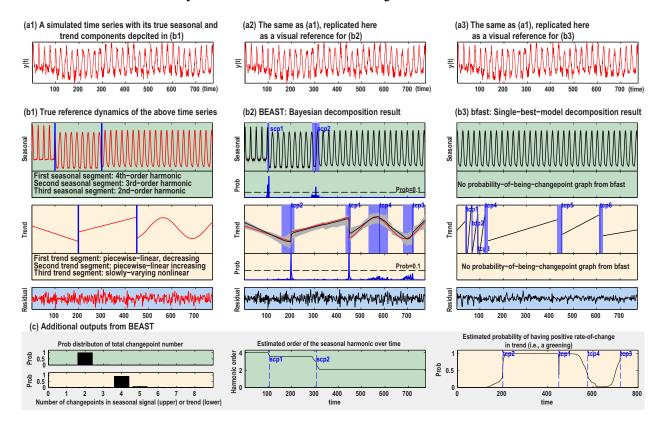
407 algorithm called bfast (Verbesselt et al. 2010a). Bfast is a criterion-based method seeking a single best

408 model, as opposed to the Bayesian inference with BEAST. Bfast and BEAST adopt the same general

- 409 linear model form, thus allowing us to isolate the effects of inference paradigms and remove other
- 410 confounding effects on the algorithm comparison. As shall be seen below, despite the use of the same
- 411 parametric model, BEAST and bfast disagreed on decomposition results.

### 412 **4.1 Example 1: A simulated time series**

- In Example 1, we simulated a time series of length n=774 with a period of P=24 (Fig. 4a1). In the
- simulation, the true reference seasonal signal has two seasonal changepoints (scp), giving three
- seasonal segments; the seasonality was simulated using different orders of harmonics for individual
- segments (Fig. 4-b1). The true trend has two trend changepoints (tcp), giving three trend segments:
- 417 The first two are piecewise-linear; the third is a slow-varying nonlinear continuous signal with no
- 418 abrupt jumps (Fig 3a). We chose such a continuous trend for the third segment because this is often
- the case for real ecosystem dynamics and the performances of conventional methods for such
- 420 nonlinear trends were rarely evaluated in the remote sensing time-series literature.



422 Fig. 4. Example 1: Use of a simulated time series (a1-a3) to illustrate BEAST. The true dynamics underlying the time 423 series (b1) were uncovered by BEAST accurately (b2). Specific information estimated by BEAST includes, but is not 424 limited to, seasonal and trend signals, seasonal and trend changepoints (seep or tcp, as denoted by vertical blue bars), 425 and harmonic orders of individual seasonal segments (c, middle). BEAST also provided an array of useful 426 uncertainty diagnostic statistics, such as credible intervals of the estimated signals (i.e., gray envelopes), the 427 probability of observing a scp or tcp at any given time, the probability distribution of total numbers of scp or tcp (c, 428 left), and the probability of having a positive rate-of-change in trend (c, right). For comparisons, the results from the 429 single-best-model algorithm "bfast" are given in (b3). Bfast detected no scp and six tcps. 430 Use of BEAST and bfast is sensitive to the specification of two hyperparameters: maximum number of changepoints (M<sub>max</sub>)—an upper limit imposed on how many changepoints are allowed in a 431 single model; minimum separation interval (h) —the minimum distance in time allowed between two 432 neighboring changepoints in a single model. In this example, we chose  $M_{max} = 8$  and h = 24 (one 433 period). (In bfast, h is expressed as the ratio of the interval to the time series length.) 434 BEAST uncovered the true dynamics from the simulated time series with high fidelity. The 435 detected signals correlated well with the true references [r=0.998 (seasonal) and 0.956 (trend), 436 437 n=774]. BEAST not only successfully pinpointed the two true scps but also correctly identified the 438 differing harmonic orders for the three seasonal segments (Fig. 4c, middle). In the trend, BEAST 439 precisely detected the two reference tcps associated with the piecewise-linear segments. For the third 440 nonlinear trend segment, BEAST additionally detected 2.2~2 tcps to capture the sinuous 441 nonlinearity. Because changepoints are defined as any timings at which the trend deviates from its previous linear trajectory (Sect 2), in theory, the nonlinear trend segment of this example is fraught 442 443 with changepoints through the time. This theoretical expectation aligns well with the BEASTestimated probability of changepoint occurrence (Fig. 4b2), wherein the estimated probability curve 444 was often nonzero with many small peaks over the third trend segment. All the probabilities were 445 446 small, indicating the very low likelihood of identifying high-intensity abrupt changes in this nonlinear

trend segment, except at the two turning points of the sinuosity. In contrast to BEAST, bfast detected 447 no scps and six tcps (Fig. 4b2). 448

BEAST also produced a rich set of uncertainty measures useful to guide the interpretation of 449 450 inferred dynamics (Figs. 4b2 & 4c). As examples, the synthesis of individual models allows BEAST to generate uncertainties that incorporate both data noises and model missspecification. The inferred 451 trend signal in Fig. 4b2 was not identical to the true signal, but the envelopes of 95% uncertainty 452 intervals enclosed the true signal almost completely, attesting to the utility and reliability of the 453 estimated credible intervals (Fig. 4b2). BEAST tells not only the most likely timings and numbers of 454 tcp or scps but also the probability of observing a scp or tcp for any given time as well as the 455 probability of detecting a certain total number of scps or tcps (Fig. 4c, left). In this example, the 456 probabilities of having 2 scps were 0.9963, leaving only a probability of 0.0037 to find other numbers 457 of scps and suggesting high confidence in pinpointing the two scps. 458

459 Likewise, BEAST can derive the probability distribution of harmonic orders needed to adequately model a seasonal segment. Another output important for ecological remote sensing is 460 pertinent to the rate of change in trend. For example, BEAST infers not only the sign of the change 461 (e.g., a greening or browning) but also the probability of having a greening or browning at any time 462 463 (Fig. 4c, right). In essence, for all parameters of interest, BEAST infers not only the most likely values but also the associated error bars and even more, the associated probability distributions, the 464 latter of which are generally impossible to estimate by non-Bayesian algorithms. 465

466

# 4.2 Example 2: A MODIS NDVI time series

Example 2 is based on 9-years' MODIS NDVI data at a forest site in Australia (Fig. 5), which 467 has been used by Verbesselt et al. (2010a) to test bfast. Despite being familiar to large audiences, its 468 true underlying seasonal and trend dynamics are unknown, except that we know that the site 469 experienced droughts in 2001 and 2002 and was harvested in 2004. With all trees removed, the 2004 470

- 471 harvest should have altered both the NDVI trend and seasonality. It remains untested whether the
- 472 drought effects are detectable from this time series. To run BEAST and bfast, we used a maximum
- 473 changepoint number of  $M_{max}$  =10 and a minimum inter-changepoint distance of h= .5 year.

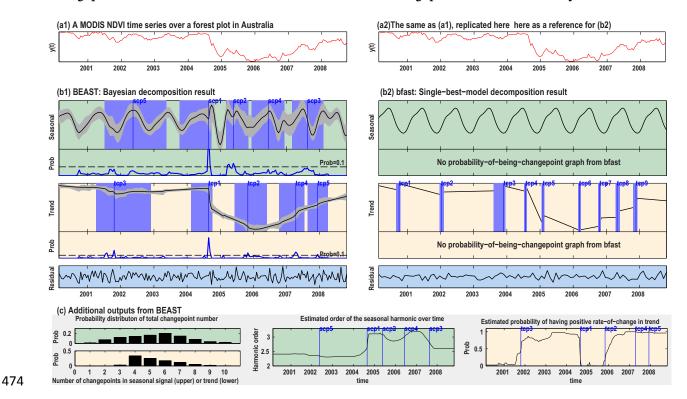
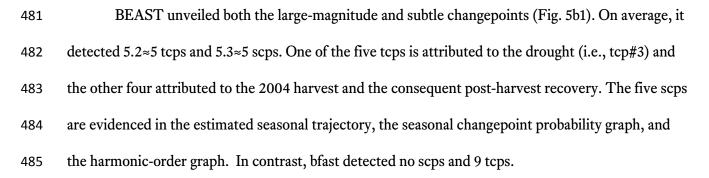


Fig. 5. Example 2: Use of a MODIS NDVI time series in the bfast R package to illustrate the use of BEAST. The true underlying seasonal and trend signals are unknown, except that we know that this site experienced droughts in 2001 and 2002 and was clear-cut in 2004. BEAST detected 5 scps and 5 tcps, uncovering not only the abrupt changes from the 2004 clear-cut but also the subtle disturbances associated with the 2001 drought. Phenological changes resulting from the 2004 clear-cut and the subsequent recovery and forest management activities were captured by a total of four scps (i.e., scp 1 to 4). For comparisons, bfast found no scp and 9 tcps detected (b2).

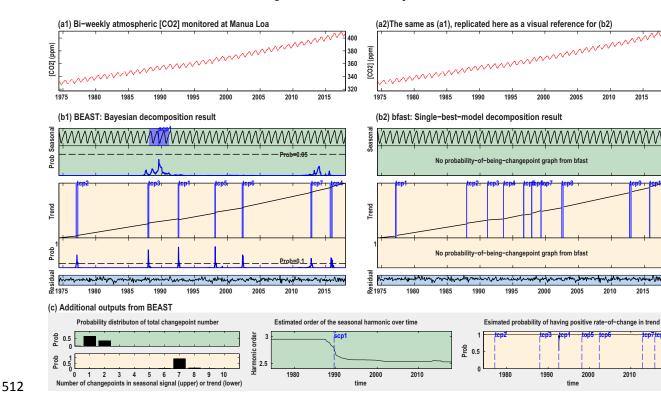


BEAST estimated a more parsimonious trend than bfast (i.e., 5.2 < 9). Despite the 486 parsimony, the BEAST trend captured a complex nonlinear dynamics (Fig. 6b1). As examples, the 487 low-intensity stresses of the 2001 and 2002 droughts were noticeable in the trend. The effect of the 488 489 2001 drought was found more severe and was associated with tcp#3 in Fig. 5.1. The rapid recovery past the year 2006 was uncovered by BEAST as a continuous nonlinear trajectory, which contrasts 490 with the bfast-detected discontinuous trajectory that has jumps with a browning trend after the year 491 2008. Another salient difference pertains to shifts in seasonality. With the 5 scps detected (Fig. 5b1), 492 BEAST was able to capture the phenological shifts caused by the 2002 drought (scp#5), the 2004 493 logging (scp#1), and the post-harvest recovery (scp#2, 3, &4). In contrast, bfast detected no scp and 494 uncovered a stable seasonal trajectory (Fig. 5b2), suggesting no phenological change before and after 495 the harvest. 496

497 **4.3 Example 3: CO2 time series at Manua Loa** 

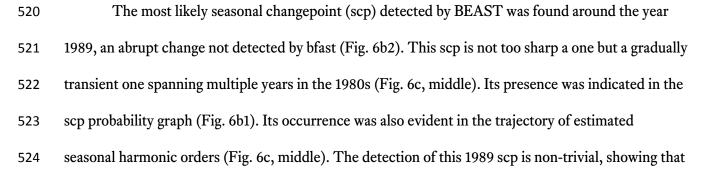
Example 3 is intended to demonstrate the use of BEAST as a generic algorithm. We considered 45 years' bi-weekly atmospheric CO2 measurements from the year 1974 to 2018 at Manua Loa (Fig. 7a1). The true trend or seasonal CO2 dynamics are unknown, except that we know there was a rising trend due to human activities and there was a regime shift in the Earth system in the 1980s (*Reid et al.* 2016), which should be reflected in the seasonal CO2 dynamics. This knowledge provides valuable information to assess the validity of the decomposition results. For both BEAST and bfast, we chose  $M_{max} = 10$  and h = 1 year.

505 Decomposition results of BEAST and bfast appeared visually similar, but the exact dynamics 506 uncovered by the two differed greatly (Fig. 6). On average, BEAST detected 1 seasonal changepoint 507 (scp) and 7 trend changepoints (tcps); bfast detected no scp and 10 tcps. One of the tcps—detected 508 by both BEAST and bfast—occurred around the year 1977, marking a heightened increase in CO2 509 and coinciding with the start of China's economic reform (Fig. 7b1). This finding is the first time that the carbon footprint of an economic policy has ever been directly pinpointed in a station-based CO2



time series. Exact drivers for other tcps need close scrutiny in future studies.

Fig. 6. Example 3: Use of 45 years' atmospheric CO2 data at Manua Loa (a1-a2) to illustrate BEAST for generic applications. On average, BEAST detected one seasonal changepoint (scp) and 7 trend changepoints (tcps). The true seasonal or trend CO2 dynamics are unknown, but the BEAST decomposition is consistent with known drivers. The CO2 trend shifted to a faster rising trajectory around the detected 1977 tcp [i.e., tcp2 in (b1)], coinciding with the end of China's Cultural Revolution and the start of its economic reform. More interestingly, the detected scp around the year 1989 (b1, top; c, middle) is consistent with the growing body of evidence that the Earth system saw a systematic regime shift in the 1980s. For comparisons, the bfast results detected no scp and 10 tcps.



525 the global carbon cycle was subject to a regime shift in the 1980s (Figs. 6b1 and 6c). The validity of this shift is supported by a converging body of observational and modeling evidence (*Reid et al. 2016*). 526 A comparison of the BEAST seasonal trajectories before and after 1989 indicates an intensified global 527 528 carbon cycle over time with a strengthened carbon sink. As a rough estimate, the amplitude in seasonal CO2 variation increased from 6.35 (pre-1989) to 6.58 ppm (post-1989), a 3.6% increase. The 529 magnitude of peak global carbon sink-estimated as the temporal derivative of the seasonal CO2 530 trajectories—was enhanced from 26.5 to 27.6 ppm/year. The post-1989 seasonal dynamics also 531 showed some enhanced springtime carbon sink, an advancing in peak sink, and a slight increase in 532 autumn carbon source, all consistent with the recognized effects of global warming on ecosystem 533 productivity (Piao et al. 2008). 534

### 535 5. Case Studies and Results

To evaluate BEAST and further exemplify its usefulness for remote sensing applications, we conducted three case studies using either simulated or real data (Figs. 7-11). These case studies were targeted at different aspects of BEAST; each chose a differing type of strategies or reference data for algorithm assessment:

(1) Case study 1 used simulated data with true reference dynamics precisely known. The aim is to test
how BEAST can uncover the true reference trend signals, an aspect critical for ecological remote
sensing but seldom tested before. A secondary aim is to quantify how the performance of BEAST
responds to data noises and relative magnitude of trend signals.

544 (2) Case study 2 used dense stacks of Landsat imagery. Ground-reference data on disturbances and

545 changepoints were visually derived from interpretation of multisource imagery following a protocol

546 similar to Cohen et al. (2011). The aim is to evaluate the ability of BEAST in detecting disturbances

547 from high-resolution data; trend signals is not evaluated here due to the impossibility of obtaining

548 true reference trend signals.

(3) Case study 3 used MODIS EVI data at 250-m resolution over a region where the extents and
timings of two large-scale disturbance events are known. Independent reference data were obtained
from aerial photos or Landsat imagery. The aim is to determine whether BEAST can help to reveal
the disturbance patterns from the MODIS data and also to assess the utility of the probabilistic
information derived by BEAST.

### 554 5.1 Case study 1: Simulated data

Simulated time-series data were generated by additively combining synthetic trend and seasonal 555 signals, abrupt changes, and random noises. The trends considered were piecewise linear, with 556 coefficients randomly sampled from a Gaussian distribution; the seasonal signals were piecewise 557 harmonics, with the order randomly sampled between 1 and 5. The simulation was based on varying 558 levels of data noises (2% to 20%), relative trend-to-seasonal signal strength (5% to 50%), and 559 changepoint number (0 to 10). For each combination, we replicated 1000 times with the time-series 560 length randomly chosen between 200 and 500, with a total of 110,000 time series generated. The use 561 562 of such well-controlled data is not only appealing but also necessary for algorithm evaluation because ground-truthing is rarely available at temporal and spatial scales commensurate with the satellite data. 563

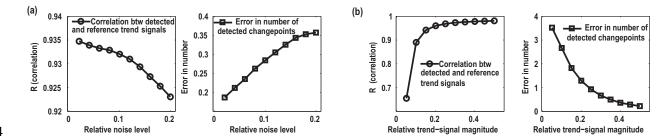


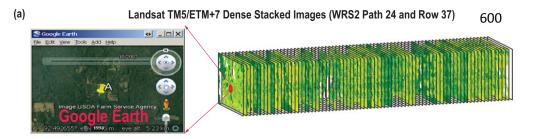
Fig. 7. Case study 1: Assessment of BEAST upon 110,000 simulated reference time series. Two performance metrics are plotted here—correlation between BEAST-detected and true trend signals and error in the number of detected changepoints. Positive errors indicate underestimates of the true changepoint numbers. Shown here are the performances of BEAST at different levels of data noises (a) and relative trend-signal magnitudes (b). Each data point plot here represents the averaging over 110,000/10=11,000 time series.

570	BEAST unveiled true trend signals accurately (Fig. 7). When tested upon the simulated data,
571	the estimated trends matched the true signals closely, with a correlation coefficient averaging 0.931.
572	Even for the noisy NDVI simulation with a noise magnitude of 20% (i.e., a signal-to-noise ratio of
573	5.0), BEAST could detect the true trend signals well; the correlation averaged 0.923 (Fig. 7a). In
574	contrast, the estimation of trends showed more sensitivity to relative magnitudes of the trend to
575	seasonal signals (Fig. 7b). For example, when the magnitudes of trends in simulated data were 5% of
576	those of seasonal signals, the correlation between the BEAST-detected and true trends was 0.67
577	(p<<0.001); if the relative trend magnitude increased to 10%, the correlation rose to 0.89 (p<<0.001).
578	Similarly, BEAST detected changepoints reliably, irrespective of the data noise levels
579	considered (Fig. 7a). However, when the true trend signals became weak and dwarfed by the seasonal
580	signals, detection of trend changepoints became difficult or impossible (Fig. 7b)—a data quality
581	problem that no algorithms can resolve. Therefore, the true changepoint numbers are increasingly
582	underestimated as the trend signal becomes weaker. The problem with weak trends also explains the
583	consistent underestimation pattern for all noise levels (Fig. 7a). The error depicted there at a given
584	noise level is the average over all possible levels of relative trend magnitude; therefore, this error is
585	contributed and dominated by the underestimation associated with those time series with weak trend
586	signals.

## 587 **5.2 Case Study 2: Dense Landsat Stack**

In Case study 2, we acquired 495 images of Landsat TM5 or Landsat 7 ETM+ (WRS2 Path 24/Row 37) over the Southern US. We corrected the images radiometrically and atmospherically into surface reflectance via the LEDAPS framework and the FMask cloud masking algorithm (*Schmidt et al. 2013; Zhu et al. 2015*); we then computed NDVI and stacked the results. The number of clear-sky dates in the stack averaged 191 across the scene. To assess BEAST, we randomly sampled 200 time series across the scene. This sample was interpreted independently by three analysts to manually

identify all potential changepoints to their full capacities using our GUI-based tool "trackEcoDyn"
(Sect 3.5 or Fig. 8). Any inconsistency among the three was reconciled if an agreement could be
reached and otherwise was simply not considered as changepoints. We used the final consensus set as
ground-reference data to assess how well BEAST detects changepoints in Landsat-type images. The
focus here is on evaluating changepoints rather than trend signals, due to the impossibility of
obtaining true reference trend signals.



(b)

trackEcoDyn: a GUI-based toolkit to interactively interpret Landsat stacked time series

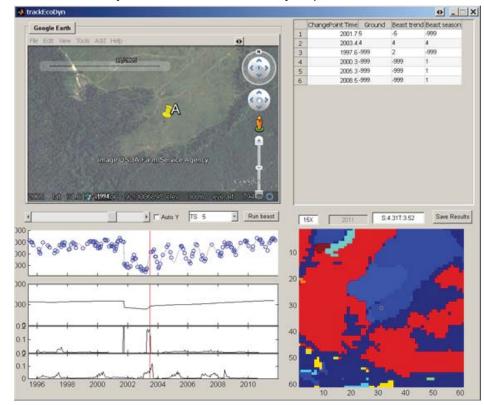


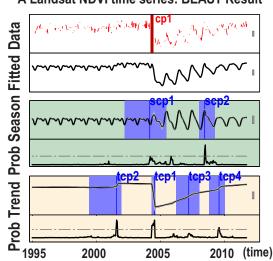
Fig. 8. Case study 2: Algorithm assessment based on dense Landsat stack of 495 scenes (WRS2 Path 24/Row 37)
over the Southern US. Shown in (a) is just a subset of the full scene. (b) To collect independent data of land

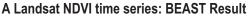
changes, we developed a GUI-based toolkit "trackEcoDyn" through the mixed use of Matlab and C to interactively
analyze and interpret Landsat time series. It integrates BEAST and ingests multiple external data sources. Google
Earth is also synchronized automatically. This toolkit was built here to help image analysts manually and visually
collect reference data for assessing the BEAST algorithm, but it can be equally applied to visually interpret or
automatically analyze other spatiotemporal data.

609 BEAST has detected most of the changepoints in the ground-reference data, though with 610 seemingly non-negligible omission and commission errors. In the ground reference for the 200 time series, there were a total of 368 changepoints pinpointed via visual interpretation, including 190 611 disturbance-type events (i.e., declining NDVI) and 178 recovery-type events (i.e., rising NDVI). 612 613 These reference changepoints were resolved to individual years. As for comparisons, BEAST detected 217 disturbance-type and 197 recovery-type changepoints, all of which were resolved to the 614 sub-monthly level. An automatic matching of the event years showed that the omission and 615 616 commission errors of BEAST were 17.7% (i.e., a producer accuracy of 82.3%), and 26.8% (i.e., a user 617 accuracy of 73.2%). Examined for disturbance-type events only, the omission and commission errors 618 are 9.5% (i.e., 18/190) and 20.7% (i.e., 45/217); for recovery-type events, the omission and 619 commission errors are 26.6% and 33.5%. It appears that BEAST had larger commission errors than 620 omission errors.

The assessment metrics reported above, especially the commission errors, are underestimates of the true capabilities and accuracies of BEAST. As a further evaluation, we manually paired and compared the BEAST results with the ground-reference data. The 18 omission errors out of the 190 disturbance-type reference changepoints, as labelled by the automatic matching, were not always true errors. Six of the 18 were not true omissions because BEAST correctly detected them to the submonthly level in years different from but immediately adjacent to the years in the ground references; the BEAST-detected timings were more accurate. Likewise, the commission errors reported above

628 are not always true algorithmic errors (Fig. 9). At least three of the 45 disturbance-type changepoints 629 labeled as commission errors are associated with data anomaly due to cloud contamination: we expected BEAST to detect these anomalies as changepoints, although they are not ecologically 630 631 meaningful. More importantly, many other commission errors are unlikely to be true errors because BEAST detected all kinds of changepoints of varying intensity but the ground-reference data 632 included only those visually conspicuous to the analysts. For example, in the recovery trajectory of a 633 forest plot (Fig. 9), BEAST identified three changepoints that demarcated contrasting succession 634 stages of the recovery, but the analysts could pinpoint only one changepoint. 635





636

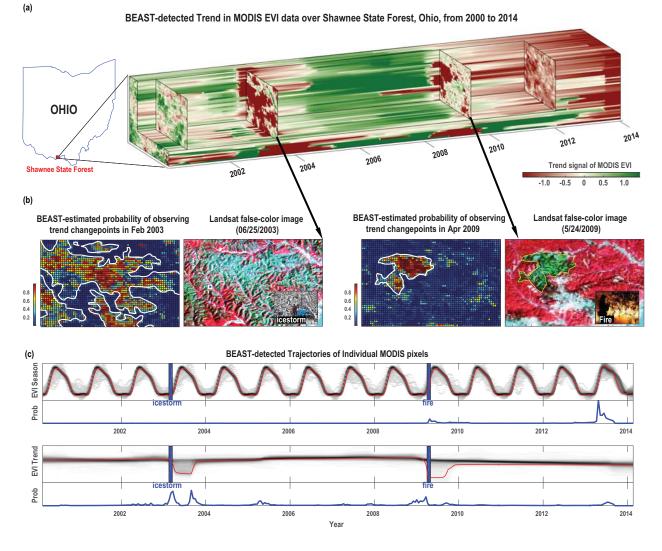
Fig. 9. Case study 2: BEAST decomposition of a Landsat time series at a forest pixel as an example to illustrate the artificial discrepancy in changepoint detection between BEAST and visual interpretation. BEAST found all types of changepoints—a total of four tcps, being abrupt or gradual. However, when interpreting visually, the three experts pinpointed only one changepoint (i.e., cp1--the sudden NDVI drop to forest logging). Hence, commission errors of BEAST in detecting changepoints in reference to the visually-interpreted ground reference are not always true errors. Illustrated also here is the capability of BEAST for filling data gaps in the Landsat time series.

643 5.3 Case Study 3: MODIS EVI

The study area chosen here is part of the Shawnee State Forest, Ohio, USA (Fig. 12a). This region 644 has been disturbed or frequently managed across various scales. In particular, the region was struck 645 by an ice storm in Feb 2003 and a fire in April 2009-Ohio's largest recorded wildfire (Eidenshink et 646 647 al. 2007). The data we examined were EVI data from MODIS's 16-day L3 data at 250-m resolution from year 2002 to 2014. To better characterize the disturbance patterns of the ice storm and fire, we 648 also complied Landsat-5 Thematic Mapper images at 30-m spatial resolution collected before or after 649 the disturbances. The perimeters of the regions disturbed by the ice storm and fire were manually 650 delineated from aerial photos (i.e., white polygons in Fig 10.b). We also calculated the Normalized 651 Burn Ratio from the pre-and post-fire Landsat images and took the difference – dNBR – as an 652 indicator of burn severity. These high spatial-resolution images and information provide independent 653 reference data to evaluate and interpret the MODIS results. 654

When applied to the MODIS data, BEAST uncovered spatiotemporal patterns of vegetation 655 dynamics that were consistent with the known disturbance history (Fig. 10). In particular, the two 656 657 major landscape-scale disturbances, the 2003 ice storm and 2009 fire, were detected successfully. The estimated disturbance timings matched closely with the true dates (Fig. 10c). The BEAST-658 detected locations and extents of the disturbances closely resembled those patterns revealed by the 659 660 post-disturbance Landsat images as well as those manually derived from independent high-resolution imagery. Within the perimeter of the disturbed regions, BEAST depicted the spatial heterogeneity in 661 disturbance magnitude. One such output is the probability of being a true changepoint. For example, 662 when tested for the burned region within the 2009 fire rim, the BEAST-estimated changepoint 663 probability strongly correlated with the independent Landsat-based dNBR (r=0.66, n=288, p-value 664 <<0.001) (Fig. 11a). Such probabilistic outputs enable BEAST to characterize not only those large-665 magnitude disturbances but also all other disturbances over a continuous range of magnitude. The 666

- 667 probabilistic results should be more informative and practically useful than the mere reporting of
- 668 binary outcomes about occurrence or not.



670 Fig. 10. Case study 3: MODIS EVI data from 2001 to 2014 over the Shawnee State Forest, Ohio where the forests 671 have been disturbed by many natural events and anthropogenic activities, for example, including an ice storm in 672 February 2003 and a fire in April 2009. Shown in (a) is a 3D volumetric view of the spatiotemporal patterns of forest 673 trend dynamics detected by BEAST; therein, brown areas indicate spatiotemporal locations where the forest 674 ecosystem is of low vitality. The ice storm and fire disturbance events are singled out to illustrate the detected 675 probability of changepoint occurrences. (b) Post-disturbance Landsat images together with manually-derived 676 disturbed regions (i.e., white polygons) are accompanied as visual references to assess the spatial patterns of 677 MODIS-based disturbances. Shown in (c) are density plots to depict individual trajectories of detected seasonal and

trend dynamics for all the MODIS pixels: the darker the color, the higher the trajectory density. Overlaid on the density plots are red solid curves to indicate the mean trajectories averaged over all the pixels. The "Prob" subplots show the mean changepoint-occurrence probabilities averaged over all the pixels (blue curves). The true timings of the ice storm and fire are indicated by vertical blue bars.

Ecologically speaking, the seasonal and trend dynamics uncovered by BEAST were 682 compatible with true vegetation responses to ice storm and fire. Sudden drops in NDVI were 683 detected by BEAST at the starts of the ice storm and fire, followed by rapid continuous transient 684 transitions for post-disturbance recovery. When uncovering seasonal dynamics, BEAST detected no 685 seasonal changepoints for the 2003 ice storm but some changepoints over part of the region for the 686 687 2009 fire (Fig. 10c). This result is corroborated by the contrasting damage severity of the two disturbances: the ice storm caused branch breakage and infrequent treefall; the fire was more 688 destructive and sometimes stand-replacing. The severe fire damages shifted the phenology at some 689 690 disturbed pixels (Fig. 10c).

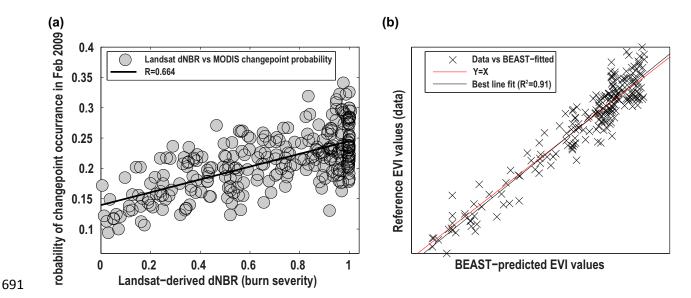


Fig. 11. Case study 3: (a) BEAST-estimated probabilities of changepoints occurring in Feb 2009 for
288 MODIS pixels within the fringe of the wildfire are correlated significantly with independently

derived Landsat burn severity dNBR. (b) True reference EVI values vs. BEAST-estimated values for
a selected MODIS time series based on the leave-one-out cross-validation.

From a regression standpoint, BEAST fitted the MODIS time series well and made accurate predictions within time-series data gaps. Averaged over all the pixels of the region, the correlation between the actual and fitted time series was 0.943 (Fig. 11a). The strong correlation highlights the predictive power of BEAST and supports its potential use as a gap-filling method. This capability is further confirmed by cross-validation. For example, in Fig. 11b, a leave-out-out cross-validation tested upon a MODIS time series showed that the estimated missing values matched the true reference values with high fidelity (R2=0.91).

703 6. Discussion

704 Leveraging the rapid growth of satellite time-series data to uncover the vagaries of landscape change is an area seeing a surge in algorithm development (Cohen et al. 2017; Wulder et al. 2012; Zhu 2017). 705 706 This advance leads to many new ecosystem dynamics products but, at the same time, opens new 707 research gaps (Cohen et al. 2017). The problem examined here is how to improve algorithmic 708 robustness and characterize algorithmic uncertainty. Cohen et al. (2017) stressed this problem by 709 noticing considerable discrepancies among seven algorithms, with a pixel-level agreement of only 710 0.2% in detected disturbances and a 1500% difference in estimated disturbance areas. Ensemble learning is touted as a remedy (Cohen et al. 2018; Healey et al. 2018) but was only partially explored. 711 The development of BEAST helps to bridge the gap by offering a generic tool that incorporates an 712 ensemble of models into time-series analysis. Our case studies provide experimental evidence on the 713 efficacy of BEAST in detecting abrupt change, seasonality, and trend. 714

715 6.1 What BEAST can and can't do?

BEAST is a Bayesian regression method to isolate periodic and trend signals from a time series and to
pinpoint abrupt shifts in the two isolated signals. It is intended primarily for trend analysis and

718 changepoint detection, targeted at questions like those elicited in Section 2. Are there any increasing 719 or decreasing trends, any changepoints, or any phenological shifts? What is the rate of change at a given time? Is the detected greening trend real? What is the probability of observing 3 changepoints 720 721 between 2001 and 2015, or both a seasonal and a tend changepoint in August 2009? Interpretations, connotations, validation of the answers to these questions are context-specific, depending on the 722 723 goals of applications (Cohen et al. 2017; Wulder et al. 2012). BEAST is applicable to any real-valued variables, such as LAI, temperature, soil moisture, gravity, and other biological or even 724 725 socioeconomic data; therefore, translating the results into insights is contingent on the natures of the 726 data and problems at hand. BEAST detects temporal dynamics but can't attribute drivers. Is a detected greening due to a 727 728 warming climate, post-disturbance recovery, or reduced grazing? Is a detected forest loss caused by fire, insect, hurricane, logging, or urbanization? Is a shift in phenology due to climate change, altered 729 management, crop rotation, succession, or land conversion? BEAST can't answer these attribution 730 731 questions directly. To a lesser extent, even a simple question like whether a detected NDVI drop 732 corresponds to a forest or grass loss can't be answered unless we know that the site observed is a 733 forest or a grassland. To answer the questions, we need to combine BEAST further with other 734 algorithms and ancillary information. For example, BEAST can be used to map extents, timings, and severity of gypsy moth infestation if we know that it is the disturbance agent. For applications on 735 736 mapping both changes and drivers, BEAST should be interfaced with a classifier that is trained empirically to relate BEAST-derived metrics with land-change classes or causative agents (Cohen et 737 al. 2017). The training and validation of the classifier can follow the good practices recommended for 738 mapping land cover (McRoberts 2011; Olofsson et al. 2014; Olofsson et al. 2013). 739 We envision that BEAST is particularly useful for three related but subtly different areas in 740

remote sensing. One area concerns ecosystem dynamics; the aim is to track vegetation changes over

742 time and understand their drivers. Current use of satellite data for such purposes is fraught with debates, for example, regarding how climate change has affected long-term vegetation growth, how 743 global warming alters land surface phenology, and how extreme weather impacts forests. The second 744 745 area pertains to mapping land disturbances and land conversion over time. Despite recent advances, the existing algorithms diverged greatly and produced inconsistent disturbance maps. With its proven 746 analytical capability, BEAST should be able to provide new perspectives into these two areas. A third 747 area of applications is to apply BEAST to fill temporal gaps in satellite data. BEAST can fit a 748 749 nonlinear curve to data with gaps and estimate the missing values.

#### 750 **6.2 BEAST vs. existing methods**

Numerous time-series methods have been introduced for applications in remote sensing or other
disciplines (*Brockwell and Davis 2016; Hamilton 1994; Zhu 2017*). Many of them were developed
under various names, such as trend analysis, seasonal decomposition, changepoint or breakpoint
analysis, signal segmentation, regime shift detector, anomaly detection, and structural change
(*Brockwell and Davis 2016; Denison 2002; Hamilton 1994; Harvey 1990*). Rigorous comparisons of
BEAST to the existing methods are complicated by the sheer number and diversity of algorithms and,
to some extent, a lack of consensus on nomenclature. For ease of comparisons, our discussion below

focuses only on two aspects of BEAST: trend analysis and changepoint detection.

BEAST extends conventional trend analyses in several ways. The majority of existing analyses—based mostly on NDVI—examined linear trends by fitting a global line to the data without considering seasonality, if any (*Brando et al. 2010; Myneni et al. 1997; Piao et al. 2006*). BEAST applies flexible basis functions to fit both linear and nonlinear trends and disentangle trends from seasonality. Some recent trend analysis methods attempted to address nonlinearity using piecewise linear models, but with a prescribed number of changepoints (*Chen et al. 2014; Wang et al. 2011*). A landmark study in this category is Wang et al. (*2011*) that applied a piecewise linear model with one changepoint to AVHRR data for new insights into climate-ecosystem interactions. Indeed, it is the one-changepoint
model of Wang et al. (2011) that motivated our algorithm development. BEAST goes beyond by
making the changepoint number an unknown parameter and letting the data tell what it is.
Statistically speaking, existing analyses were mostly based on frequentist methods, seeking only the
"best" model; BEAST employs Bayesian model averaging, embracing all candidate models rather
than selecting just one.

What distinguishes BEAST most from the existing trend analysis methods is its capability of 772 773 inferring nonlinear dynamics. BEAST provides a universal approximator of any arbitrarily complex trends. In contrast, most existing methods derive only linear or piecewise linear trends (Wang et al. 774 2011). True drivers of ecosystem dynamics are unlikely to be purely linear or piecewise-linear over 775 776 time but rather complex and nonlinear. For example, plant successional stages are known to largely follow a nonlinear recovery trajectory (Burkett et al. 2005). Long-term climate trends are confirmed to 777 be inherently nonlinear (Franzke 2014). With its better approximation power, BEAST is more likely 778 779 to find these true nonlinear trends than the existing methods. Improved fitting of trends can help with 780 changepoint detection because errors in fitting trends may be translated into errors in changepoint 781 detection.

782 For changepoint detection, existing algorithms are mostly heuristically-based, involving the testing or optimization of criteria (Cohen et al. 2017; Zhu 2017). For example, several well-known 783 algorithms, such as LandTrendr, VCT, and CCDC, rely on locally-based heuristic rules by checking 784 if some deviation metrics meet certain pre-set thresholds. They often iteratively analyze the time 785 786 series piece by piece or step by step (Huang et al. 2010; Kennedy et al. 2010; Zhu et al. 2012). In 787 contrast, BEAST is a parametric regression method. It does not require any threshold testing or criterion optimization but, instead, fits a global model to decompose the whole time series in one step 788 789 and uncover changepoint, trend, and seasonality altogether. As another key difference, many existing algorithms are hard detectors in that their outputs are limited to either 1 or 0—a changepoint or not;
BEAST is a soft/fuzzy detector capable of estimating the occurrence probability of changepoints over
time (*Cohen et al. 2017; Huang et al. 2010*). This difference is analogous to that between hard and
soft/fuzzy classifiers. To our knowledge, BEAST is the first fuzzy time-series algorithm ever
developed for remote sensing applications.

Of the existing algorithms, bfast is the one that shares the most commonality with BEAST 795 (Verbesselt et al. 2010a; Verbesselt et al. 2010b). The two have almost identical parametric models 796 797 except that bfast fixes the seasonal harmonic order to a constant of 3 or other constants but BEAST treats it as an unknown to be estimated for individual seasonal segments. This difference seems minor 798 but has substantial effects, partially explaining why BEAST detected more seasonal changepoints. 799 The varying harmonic order gives a flexible representation of seasonality and helps BEAST to 800 capture subtle variations difficult to represent by a fixed-order seasonal model (Fig. 6b1 vs Fig. 6b2). 801 The BEAST or bfast model is additive. If parts of the true seasonal dynamics are not captured by the 802 803 seasonal model S(t), these seasonal parts will be squeezed into the trend model T(t) or noises. As a 804 result, seasonal abrupt changes may be confused with trend changepoints. Likewise, parts of the true tend, if not adequately captured by T(t), will leak to contaminate the estimation of seasonality. This is 805 806 why we strived to make BEAST a flexible approximator of any arbitrary trends. In short, reliable detection of changepoints, especially those subtle ones, requires the accurate modeling of not only the 807 trend or seasonal component alone but both altogether. 808

Another key difference between BEAST and bfast or other algorithms lies in parameter estimation. Bfast treats the model parameters as unknown constants. BEAST treats them as random variables; its inferential goal is not only the best values of the parameters--number and timing of changepoints, harmonic orders, and coefficients--but also their probability distributions. BEAST tells not only a detection of 3 tcp but also a 71% probability for having 3 tcps, a 20% for 2 tcps, or a 5% for 1

tcp. Put differently, bfast seeks a single best model but BEAST embraces numerous models in terms

of a probability distribution over the model space. This is likened to the difference between CART

and Random Forests (*Friedman et al. 2001*). Bfast is like CART that finds only one decision tree;

817 BEAST is like Random Forests that uses many trees. As shown in the ecology and machine learning

818 literature, Random Forests is less likely to overfit and more likely to find ecologically-meaningful

819 relationships than does CART (*Breiman 2001a*). Similarly, as an ensemble modeling algorithm,

820 BEAST tends to generate more flexible and interpretable results.

#### 6.3 Ensemble learning: One plus one is more than two

BEAST is based on ensemble learning. Most other algorithms for satellite time-series analysis are not, 822 except two recent algorithms in Cohen et al. (2018) and Healey et al. (2018). But BEAST and these 823 two are not comparable. BEAST is a regression method for time-series decomposition wherein 824 ensemble learning is internalized into the Bayesian formulation. In contrast, the other two algorithms 825 826 are some classifiers that ingest the pool of multiple model outputs as predictors to classify disturbance 827 agents. More generally, ensemble learning comes in many other fashions, but the core is to combine many models or algorithms into a better one (Friedman et al. 2001). Experimental evidence is 828 829 unequivocal about the effectiveness and superiority of ensemble learning, compared to the single-830 best-model paradigm (Friedman et al. 2001). Recent years also saw a growing urge for better leveraging the paradigm of ensemble modeling or multi-model inference—a voice that is being heard 831 832 in many scientific disciplines and is reinforced again here.

833 Why does ensemble learning help with our time-series analysis? The answer lies in a familiar 834 example: the IPCC relies on many climate models instead of any single model to augment confidence 835 in climate prediction *(Solomon 2007)*. What is implicit here is George Box's aphorism "all models are 836 wrong", a creed that, if held, may help little with practical modeling but, if ignored, can engender 837 unwarranted epistemological debate *(Beven 2010)*. All remote sensing models, including radiative transfer models in operational use and our BEAST algorithm, are also wrong in the sense that they
are always simplifications and approximations of the true processes (*Schowengerdt 2006*). This is
connoted by the fact that remote sensing is fraught with the use of different algorithms or models to
decipher the same linkage or functional relationship (*Cohen et al. 2017*).

Since all models are wrong, the consideration of many models as in BEAST can reduce the 842 chance of deviating too far from the unknown truth, compared to the choice of just a "best" model. 843 When ranking models in terms of usefulness metrics such as AIC and BIC, the "best" ranked model 844 is not guaranteed to be closer to the truth than other models of lower ranks (Shmueli 2010; Zhao et al. 845 2013). As a rule of thumb, if two models have an AIC difference of <2.0, there is no strong evidence 846 that one should be favored over the other (Burnham and Anderson 2003). Similar rules exist for other 847 model selection criteria. In the current context, each candidate model is uniquely specified by the 848 model structure parameters, such as numbers and timings of changepoints. The entire model space 849 850 may comprise quadrillions of candidates or more. Not surprisingly, there can be numerous competing 851 models (e.g., millions) that are statistically indistinguishable from the "best" model in terms of AIC or BIC, a phenomenon called model equalfinality (Beven 2010). The lack of strong statistical power to 852 discriminate some models against others makes it safer to use the many models than a "best" model. 853 854 Even if not all models are wrong and the true model is in the space of candidate models, ensemble learning can still be more robust than single-best-model algorithms (Friedman et al. 2001; 855 Wintle et al. 2003; Zhao et al. 2013). Even in a simple scenario of linear regression, Zhao et al. (2013) 856 showed that many single-best-model regression procedures failed to recover the true linear model. 857 More generally, no model selection criterion guarantees finding the true model. The failure is 858 primarily due to two factors. First, the space of candidate models is so enormous that optimization 859 may be trapped at local minima, failing to find the real optimal model. Second, even if the real optimal 860 model is luckily found, it may still not be the true model: optimality is not equivalent to truth. The 861

true model may have worse AIC or BIC values than other models, for example, due to data noises or multicollinearity *(Friedman et al. 2001; Grossman et al. 1996)*. These difficulties justify the use of ensemble learning even if we can correctly parameterize the true model, let alone when we can't.

865 How can BEAST uncover arbitrary nonlinear vegetation dynamics, given that individual trend models are just piecewise-linear? A rigorous mathematical answer to this is beyond the current 866 scope. Intuitively speaking, the averaging of many piecewise irregular functions will smooth out the 867 irregularity and mold them into a more flexible function (Friedman et al. 2001). Indeed, for almost all 868 practical applications, the use of ensemble averaging is more flexible in fitting nonlinear functions 869 than any individual models. A familiar example again is Random Forests: each tree is a discontinuous 870 partition-based function, but the averaging of many trees is able to approximate complex functions 871 (Cogger 2010). This is what we call here as "the making of a stronger model from many weak models" 872 or "one plus one is more than two" (Friedman et al. 2001). It is this property that enables BEAST to 873 detect realistic vegetation trend dynamics. 874

# 875 6.4 Bayesian statistical modeling: To explain or predict?

885

876 BEAST fits a Bayesian regression model or a function curve to match the observed time series, with 877 time as the independent variable. In this regard, BEAST is the same as the many existing statistical 878 models relating remote sensing predictors to biophysical variables. However, their modeling purposes 879 are not the same (Shmueli 2010). Most of the statistical models are calibrated to minimize differences 880 between fitted and observed land variables and then estimate the variables for new data unused in the calibration, that is, to predict (Breiman 2001b; Zhao et al. 2018). The purpose of BEAST is not to 881 minimize the fitted-vs-observed differences or predict values at a new time but to identify the right 882 mechanisms underlying the observed time series, that is, to explain (Dashti et al. 2019; Thomas et al. 883 2018). Models that predict well may not explain well, and vice versa (Shmueli 2010). Black-box 884

machine learning models are such examples. Although the explain-vs-predict divide is not

dichotomous, future studies will garner more successes in designing robust statistical algorithms to
obtain useful vegetation dynamics information if we pay attention to the explaining nature of such
modeling efforts.

889 Bayesian modeling is of great value in mining complex data to find meaningful and interpretable relationships (Finley et al. 2008). A confirmatory example is our BEAST algorithm. 890 Bayesian inference is powerful particularly because of its explicit consideration of various sources of 891 uncertainty (Denison 2002; Kennedy and O'Hagan 2001). The time-series problem at hand is a 892 difficult one fraught with uncertainties, due to some apparent conflict. On one hand, model 893 misspecification is inevitable (in theory, true vegetation dynamics are unlikely piecewise-linear or – 894 harmonic); on the other hand, our aim is to use the misspecified model to capture the true vegetation 895 dynamics (the model should explain well). This conflict will be subtly translated into uncertainties in 896 the model parameters and structure. A full characterization of these uncertainties is practically 897 impossible with the conventional single-best-model paradigm, especially because it ignores model 898 899 uncertainty (Beven 2010; Kennedy and O'Hagan 2001). These uncertainties, however, can be 900 formalized and treated rigorously and systematically by the Bayesian paradigm. Despite the exceptional power of Bayesian modeling, its use in remote sensing remains 901 902 limited. Many factors contribute to this. Philosophically, the "subjective reasoning" label of Bayesian inference may deter many researchers from considering it seriously (Denison 2002): who wants to 903 sound subjective in the science enterprise? This concern is unwarranted, given the rising acceptance 904 of Bayesian statistics in essentially all fields after decades of philosophical debate (Ellison 2004; 905 Friedman et al. 2001). Even if its utility is realized, there is habitual inertia to overcome because 906 conventional statistical methods still find the dominant use. Moreover, the use of Bayesian methods 907 is often hampered more by practical factors, such as a dearth of easy-to-use Bayesian statistical 908 909 software, the unfamiliarity of these methods to the larger community, the inherent complexity of

Bayesian modeling, a lack of formal training in Bayesian statistics, and often enough, daunting

911 computation costs of Bayesian methods. Nonetheless, we hope that the demonstrated value of

912 BEAST provides an impetus to encourage future remote sensing applications of Bayesian techniques.

913 We envision that Bayesian techniques are particularly appealing in cases that data are complex or

noisy, characterization of uncertainty is pivotal, computation is not constraining, and the modeling

915 purpose is to explain (e.g., uncover the truth or test theories) rather than predict.

## 916 **6.5 How to validate time-series decomposition algorithms**

What should be validated or evaluated? The goal is to quantify the degrees to which estimated 917 dynamics and changepoints represent the truth. Because changepoints are parts of trend/seasonal 918 signals, validation of changepoints underpins that of trend or seasonal dynamics. In particular, 919 validation of changepoints should cover all the model structure parameters—numbers and timings of 920 changepoints, and harmonic orders. Changepoints here refer to abrupt shifts in both seasonality and 921 922 trend, be positive or negative in direction, that span a continuous spectrum of magnitude. The 923 changepoints referred to here are consistent with those in Wang et al. (2011) and Browning et al. 924 (2017). This range goes beyond the consideration of only large-magnitude disturbances (e.g., land 925 conversion, forest loss, and fire) that are characteristic of many Landsat-based algorithms (Cohen et 926 al. 2017; Huang et al. 2010). Estimated trend or seasonal dynamics, such as the sign and the rate of change, should be compared to true dynamics. 927

A full evaluation of time-series algorithms such as bfast and BEAST is critical but, often enough, difficult due to a lack of ground-truth (*Lu et al. 2004*). Take bfast as an example. In the MODIS data of Example 2, only the 2004 trend changepoint (tcp) was originally used to test bfast (Fig. 6) because the 2014 harvest was known precisely. The other tcps and scps were not assessed yet and are hard to test (Fig. 6b2). These tests are about whether the bfast-detected changepoints are real or artificial. A more difficult test is about how many true tcps and scps have been detected by bfast.

An even more difficult task is to test the veracity of the estimated trend or seasonal signal. (In Fig. 934 6b2, is the post-harvest browning after tcp#9 a real trend or an algorithmic artifact?) These validation 935 questions are difficult, if not impossible, to answer. The same difficulties apply to validation of 936 937 BEAST. Similar difficulties were also noted in Browning et al. (2017), which, though considering only 15 MODIS time series, is the first study to assess bfast with field-based vegetation dynamics data. But 938 even for that study, the validation was partial, limited to the testing of user accuracy for changepoints. 939 The aforementioned difficulties are manifested in other fashions. Current controversies 940 surrounding satellite-derived ecosystem dynamics could have been safely dismissed if the associated 941 time-series analyses had been validated. Even a seemingly simple question, like "is the NDVI trend a 942 greening or browning?", has been debated and largely unverifiable. Such issues are not confined to 943 remote sensing. Other fields, such as statistics, ecology, and econometrics, are also fraught with time 944 series analyses of the same nature as ours. We are unaware of any studies in these fields that 945 946 conducted full validation of changepoint algorithms when tested upon real-world data. For example, 947 many algorithms were applied to the river flow data of the Nile at Aswan (Balke 1993; Betken 2017; Denison 2002; Wu and Zhao 2007). Most of them gave similar but essentially different 948 decompositions. Even for this well-studied data, it is hard to test whether the algorithms uncovered 949 950 the true river flow dynamics.

Because we normally have no access to all the ground-truth needed, we recommend eight practical strategies for algorithm validation. First, a simple yet powerful strategy is to validate algorithms against synthetic data. If an algorithm cannot recover the known true dynamics from the synthetic data to which it is tailored, it unlikely applies well to real data. This test is the first filter that a useful algorithm must pass. Use of synthetic data also permits full assessments under various conditions (e.g., different noise levels) (Section 5.1). Second, algorithms can be validated qualitatively (not equal to "subjectively") with respect to some general known patterns. This is another filter that

958 useful algorithms must pass. If they detect a declining trend in the air CO2 data, a browning for forest 959 recovery, or no changepoints for a frequently-disturbed region, there must be some problems with the algorithms. Third, validation can be done using well-established knowledge, such as ecological 960 961 principles and empirical evidence. One example is the confirmation of the 2004 scp in the MODIS time series because forest clearing is known to change phenology. Another is the 1980s regime shift in 962 the air CO2 time series. Passing this test will enhance users' confidence in the algorithm. Fourth, as a 963 relative evaluation, an algorithm can be compared to other algorithms. Fifth, cross-validation is 964 another effective strategy, especially for those algorithms that apply parametric models to 965 approximate time series. 966

Sixth, validation can be done using known individual events (e.g., disturbance or land cover 967 change). One example is the evaluation of bfast upon the harvest/planting years over a region in 968 Australia. Our test of BEAST for the fire and ice storm events in Ohio was another example. Seventh, 969 970 validation can be done using reference data derived from independent sources. One example is 971 through photo-interpretation with TimeSync; another example is our tool trackEcoDyn, which is 972 functionally similar to TimeSync. As a caveat, such reference data are subject to errors and 973 uncertainties (Cohen et al. 2010), as explained in Figure 11. Eighth, validation can be done using proxy 974 data of all kinds. One example is the use of climate variables and field-based vegetation composition and biomass in Browning et al. (2011) to assess NDVI time series. Another example is our use of 975 976 dNBR to assess the BEAST-derived changepoint probability. As a third example, to test if surface evaporation sees an abrupt change at a time, we can check air temperature or moisture as proxies. 977 978 Overall, none of these validation strategies is complete and perfect. A compromise is to rely on as many strategies as possible. Indeed, to test BEAST, we employed all the eight strategies, each 979 emphasizing a differing aspect of BEAST. But in many existing satellite time-series analyses, the 980 practice was to focus only on one aspect of the algorithms (e.g., large-magnitude changepoint only, 981

trend only, or phenology only). Obviously, a comprehensive strategy that embraces more aspects of
the algorithms should be preferred because the various components of time-series decomposition do
not stand on their own but rather are linked: any errors in one component will be leaked to degrade
the estimation of others. Without such comprehensive evaluations, it becomes inevitable that
ecological interpretations of satellite time-series decomposition are laden with inconsistency or
controversies.

### 988 6.6 Caveats and future research

Several caveats are noted. First, BEAST detects anomalies and trends but doesn't attribute the 989 drivers. If data are contaminated by spurious errors (e.g., clouds) or systematic biases (e.g., gradual 990 sensor degradation) (Wang et al. 2012), these outliers and drifts can be misconstrued as true signals. 991 To reduce such commission errors, data artifacts should be removed or suppressed beforehand. 992 Second, BEAST makes inference via Monte Carlo sampling and therefore, requiring more 993 computation than many other algorithms (Kennedy and O'Hagan 2001). Applications of BEAST to 994 995 massive high-resolution data, such as the Landsat archive at the global scale, will demand daunting 996 computation. The recommended use of BEAST is for global coarse-resolution or local high-997 resolution (e.g., Landsat coverage of a county).

998 Third, BEAST explicitly quantifies how likely each point of time is a changepoint. The resultant probability appears indicative of disturbance severity (Fig. 11) and also captures low-999 1000 magnitude disturbances that may be missed by other algorithms. Interpretation of the probabilities is contingent data quality. An abrupt change will have a lower detection probability if data get noisier. 1001 All else being equal, the higher the signal-to-noise ratio, the larger the estimated probability of the 1002 1003 same disturbance. The interpretation is also confounded by sub-pixel heterogeneity. A changepoint 1004 detected with a 5% probability at a pixel, for example, may be due to either a low-magnitude disturbance across the whole pixel or contrastively, from a severe disturbance over a small fraction of 1005

the pixel. BEAST can't distinguish the two cases. The confounding can be resolved by turning to
finer-grained data (*Roy et al. 2014; Zhao et al. 2018*).

Fourth, the scale matters. When detecting changepoints, BEAST is scale-dependent. 1008 1009 Consider two adjacent pixels, one with a sudden NDVI drop and the other with a rise of the same magnitude at the same time. If applied separately, BEAST will detect a changepoint for each pixel. 1010 1011 But if the two pixels are combined into one, the two abrupt changes cancel out and the changepoint disappears at the aggregated scale. This scaling effect is an inherent characteristic of all algorithms. 1012 1013 On the contrary, we speculate that BEAST is scale-invariant when uncovering trends or seasonal 1014 dynamics. That is, applying BEAST to many pixels and then aggregating the individual detected trends should give the same overall trend as that obtained by first aggregating the individual pixels 1015 1016 into a large pixel and then applying BEAST to the aggregated pixel. This nice property is attributed to the additive nature of general linear models (Zhao et al. 2009). The scale-invariance permits the use of 1017 1018 BEAST across scales to infer trends without introducing artificial discrepancies, thereby facilitating 1019 fusion of multi-resolution data. For applications concerning only trends not changepoints, the use of 1020 BEAST at aggregated scales will also lessen the computation needed.

1021 Fifth, BEAST is applicable to any real-valued data. However, it is a univariate method and 1022 can't decompose multiple time series simultaneously or leverage the inter-correlatedness of the many 1023 time series (e.g., multispectral bands). Extending BEAST into a multivariate algorithm is 1024 conceptually easy but the implementation is complex—a future topic to be explored. Other extensions are also possible. Here we tested BEAST upon only dense time series to track both trend 1025 1026 and seasonality. It can be revised to handle sparser non-periodic time series (e.g., annual Landsat data 1027 with one observation per year) by simply suppressing the seasonal component in its formulation. BEAST can also be extended to handle data collected at irregular time intervals or data with duplicate 1028 1029 measurements at a single time. As an unsupervised decomposition algorithm, BEAST can't classify

1030 disturbance agents (Kennedy et al. 2015); therefore, another extension is to embed a supervised 1031 classifier into BEAST for simultaneously detecting changepoints and classifying disturbance types. Last, we highlighted the unique features of BEAST but our intent is not to favor or 1032 1033 discriminate one algorithm against others. All the algorithms have their own niches and offer different perspectives. Algorithmically speaking, there is no panacea for inferring true dynamics from noisy 1034 data (Breiman 2001b). The validity of the diverse or conflicting perspectives, therefore, needs to be 1035 1036 judged based on domain-specific knowledge and high-fidelity ground-truthing. Because BEAST is the 1037 first ensemble-based fuzzy time series decomposition algorithm ever developed for remote sensing applications and also because it is able to recover complex dynamics and characterize various types of 1038 uncertainty, its use can engender new insights not obtainable by other algorithms. Future studies may 1039 further test the utility of BEAST for various data, problems, and geographic regions. One example is 1040 1041 the analysis of AHVRR or MODIS data to detect disturbances and nonlinear long-term dynamics and 1042 determine how ecosystems have been driven by climate change and human activities, an area still 1043 fraught with many conflicting findings. Overall, BEAST serves a useful tool to derive observational 1044 information from satellite data, as a way to complement field surveys, controlled experiments, and computer models in quantifying ecosystem responses to environmental changes. 1045

# 1046 **7. Summary**

We presented a Bayesian algorithm—BEAST—for decomposition of time series into three contrasting components: abrupt change, periodic change, and trend. BEAST helps to leverage the increasing availability of multisource satellite time-series data for detecting land disturbances and tracking nonlinear ecosystem dynamics. Compared to many existing algorithms, BEAST explicitly addresses model uncertainties via ensemble learning, thereby alleviating inter-algorithm inconsistencies to some extent. Such inconsistencies were widely recognized and, if not addressed, would result in diverging or conflicting interpretations of the same data. Conceptually, BEAST

1054 combines many individual weak models into a better model via Bayesian model averaging.

1055 Mathematically, BEAST is rigorously formulated, with its key equations being analytically tractable.

1056 Practically, BEAST can estimate probabilities of changepoint occurrence, detect not only large but

1057 also low-magnitude disturbances, and uncover complex nonlinear trend dynamics, all of which are

1058 difficult to obtain by single-best-model algorithms. BEAST is generically applicable to not only

1059 remote sensing data but other environmental, ecological, or socioeconomic time-series data. Our

1060 initial experiments confirm the utility of BEAST. We envision that its use will offer new satellite-

1061 based insights into patterns and drivers of ecosystem dynamics.

1062 Appendix A.

Here we described more on the specification of the prior  $\pi(\beta_M, \sigma^2, M) = \pi(\beta_M, \sigma^2|M)\pi(M)$  for BEAST.

1065 First, we chose a normal-inverse Gamma distribution as the prior of model coefficients  $\beta_M$ 1066 and variance  $\sigma^2$  conditional on model configuration M:

$$\pi(\boldsymbol{\beta}_{\mathsf{M}}, \sigma^2 | \mathsf{M}) = \pi_{\boldsymbol{\beta}}(\boldsymbol{\beta}_{\mathsf{M}} | \sigma^2, \mathsf{M}) \pi_{\sigma^2}(\sigma^2) = \mathbb{N}(\boldsymbol{\beta}_{\mathsf{M}}; \mathbf{0}_{\mathsf{M}}, \sigma^2 \nu \mathbf{I}_{\mathsf{M}}) \cdot \mathbb{I}\mathbb{G}(\sigma^2; \underline{a}, \underline{b}).$$

where the conditional prior  $\pi_{\beta}(\beta_{M} | \sigma^{2}, M)$  is a Gaussian distribution  $\mathbb{N}(\beta_{M}; \mathbf{0}_{M}, \sigma^{2} v \mathbf{I}_{M})$ ; the prior 1067  $\pi_{\sigma^2}$  is an inverse-gamma distribution  $\mathbb{IG}(\sigma^2; \cdot, \cdot)$  that is independent of the model configuration M and 1068 is specified by two scalar hyperparameters <u>a</u> and <u>b</u>. To parameterize the Gaussian prior  $\pi_{\beta}(\cdot)$ , we set 1069 its prior mean to zeros  $0_M$ , a justifiable choice if the covariates are centered beforehand; the prior 1070 covariance we chose K is the ridge prior  $\sigma^2 v I_M$ . The subscript "M" in the zero-mean vector  $0_M$  and 1071 1072 the identity matrix I<sub>M</sub> indicates that their dimensions depend on the model structure M. Moreover, in the prior covariance for  $\pi_{\beta}(\cdot)$ , v is a scalar hyperparameter. Judicious values for v are not available in 1073 advance; therefore, we also treated v as random and further assigned it an inverse-gamma prior 1074

1075  $\pi_{v}(v) = \mathbb{I}\mathbb{G}(v; \underline{c}, \underline{d})$  with two hyperparameters  $\underline{c}$  and  $\underline{d}$ . This prior  $\pi_{v}(v)$  is a hyperprior because it is 1076 elicited at a level deeper than  $\beta_{M}$ . Consequentially, the full conditional prior of Eq. 5 is refurnished as

$$\pi(\beta_{\mathrm{M}}, \sigma^{2}, v | \mathrm{M}; \underline{a}, \underline{b}, \underline{c}, \underline{d})$$
$$= \pi_{\beta_{\mathrm{M}}}(\beta_{\mathrm{M}} | \sigma^{2}, v, \mathrm{M}) \pi_{\sigma^{2}}(\sigma^{2} | \underline{a}, \underline{b}) \pi_{v}(v | \underline{c}, \underline{d})$$

1077 where the hyperparameters  $\underline{a}, \underline{b}, \underline{c}$ , and  $\underline{d}$  are underlined and made explicit for the respective priors. 1078 Second, the prior on model structure  $\pi(M)$  is chosen to be vague in order to reflect a lack of 1079 prior knowledge on when and how many abrupt changes occur in an observed time series. Because of 1080 the separate parameterization for the trend and seasonal signals, it is reasonable to independently 1081 elicit the model priors for the trend and season signals:

1082 
$$\pi(M) = \pi\left(\{m\} \cup \{\tau_j\}_{j=1,\dots,m}\right) \pi\left(\{p\} \cup \{\xi_k\}_{k=1,\dots,p} \cup \{L_k\}_{k=0,\dots,p}\right).$$

1083 Firstly, the prior for the trend can be decomposed as

1084 
$$\pi \left( \{m\} \cup \{\tau_j\}_{j=1,...,m} \right) = \pi \left( \{\tau_j\}_{j=1,...,m} | m \right) \pi(m)$$

As a way to encode the vagueness of these model priors, we assume that the number of changepoints, m, takes any integer with an equal probability a priori. Meanwhile, we impose a constraint on the maximum number of changepoints allowable in a trend signal, as denoted by  $\underline{m_{max}}$ , which helps to preclude over-complicated models. The prior  $\pi(m)$  is therefore a uniform distribution over  $\{0,1,.., m_{max}\}$ :

1090 
$$\pi(m) = \begin{cases} 1/(\underline{\mathbf{m}_{max}} + 1) & \text{if } 0 \le m \le \underline{\mathbf{m}_{max}}\\ 0 & \text{if } m > \underline{\mathbf{m}_{max}} \end{cases}$$

1091 Further, given a total of m changepoints, their locations,  $\{\tau_j\}_{j=1,...,m}$  are assumed to take random 1092 values from the points of observation time  $\{t_i\}_{i=1,...,n}$ . This choice again represents a non-informative 1093 prior. As a practical constraint, we assume that any consecutive changepoints should be separated 1094 apart by at least a time interval T. Put together, the conditional prior for changepoint locations is

1095 
$$\pi\left(\left\{\tau_{j}\right\}_{j=1,\dots,m}|m\right) \propto \begin{cases} 1 & if \max_{(i,j)}|\tau_{i}-\tau_{j}| < \underline{T} \\ 0 & \text{otherwise} \end{cases}$$

1096 Secondly, the prior on the seasonal model structure can be re-written as

1097 
$$\pi(\{p\} \cup \{\xi_k\}_{k=1,\dots,p} \cup \{L_k\}_{k=0,\dots,p}) = \pi(\{\xi_k\}_{k=1,\dots,p} | p)\pi(p) \prod_{k=0}^p \pi(L_k)$$

1098 where the priors on the number and locations of changepoints,  $\pi(p)$  and  $\pi(\{\xi_k\}_{k=1,\dots,p}|p)$ , take the 1099 same forms as those of the trend signal, except that the maximum number of changpoints allowable is 1100  $\underline{p_{max}}$  rather than  $\underline{m_{max}}$  and that the minimum separable distance between adjacent changepoints is 1101  $\underline{W}$  rather than  $\underline{T}$ . Similarly, the prior on the order of the piecewise harmonic model,  $\pi(L_k)$ , is also 1102 considered non-informative in that  $L_k$  randomly takes any value between pre-defined lower and upper 1103 limits of the allowable orders ( $\underline{L_{min}}$  and  $\underline{L_{max}}$ ):

1104 
$$\pi(L_k) = \begin{cases} 1/(\underline{L_{max}} - \underline{L_{min}} + 1) & \text{if } \underline{L_{min}} \le L_k \le \underline{L_{max}} \\ 0 & \text{otherwise} \end{cases}$$

1105 In the prior above, the model parameters { $\beta_M$ ,  $\sigma^2$ , v, **M**} are of inferential interest and are all 1106 considered random. In contrast, the ten underlined hyperparameters

 $\{\underline{a}, \underline{b}, \underline{c}, \underline{d}, \mathbf{m}_{max}, \mathbf{p}_{max}, \underline{T}, \underline{W}, L_{min}, L_{max}\}$  are treated as fixed and should be pre-specified, although it 1107 is permissible to additionally treat them as random variables by further eliciting hyperpior 1108 1109 distributions at higher levels in a manner similar to the treatment of v. There are no general rules on how to specify the values of these hyperparameters. The setup in this study was chosen as  $\underline{a} = \underline{b} =$ 1110  $0.01, \underline{c} = \underline{d} = 0.02, \underline{T} = \underline{W} = 1$  year,  $L_{min} = 0, L_{max} = 10, m_{max} = p_{max} = \max(n/P, 30)$  with 1111 n and P being the total number of observations and the period of the NDVI signal, respectively. Such 1112 1113 choices for the inverse gamma priors are almost equivalent to non-informative priors for practical purposes, reflecting our vague knowledge on  $\sigma^2$  or v a priori. Preliminary trials with various datasets 1114 suggest that the resulting predictive performances are insensitive to the settings of these 1115

1116	hyperparameters as long as $\underline{m_{max}}$ , $\underline{p_{max}}$ , and $\underline{L_{max}}$ assumes a moderately large value (e.g., $\underline{m_{max}} >$
1117	15, and $\underline{L_{max}} > 6$ ), { $\underline{a}$ , $\underline{b}$ , $\underline{c}$ , $\underline{d}$ } take small values, and the data are standardized beforehand.
1118	As a recap of the Bayesian formulation for BEAST, the likelihood Eq. 4 and the priors Eqs.5
1119	and 7 combine to reach the full posterior of our formulation according to Eq. 3:
1120	$p(\boldsymbol{\beta}_{\mathbf{M}}, \sigma^2, v, \mathbf{M}   \boldsymbol{\mathcal{D}}) \propto$
1121	$\prod_{i=1}^{n} N(y_{i}; \mathbf{x}_{M}(t_{i})\boldsymbol{\beta}_{M}, \sigma^{2}) \pi_{\beta}(\boldsymbol{\beta}_{M}   \sigma^{2}, v, M) \pi_{\sigma^{2}}(\sigma^{2}   \underline{a}, \underline{b}) \pi_{v}(v   \underline{c}, \underline{d}) \pi\left(\{\tau_{j}\}_{j=1,\dots,m}, m   \underline{\mathbf{m}_{max}}, \underline{\mathbf{T}}\right) \pi\left(\{\xi_{k}\}_{k=1,\dots,p}, p   \underline{p_{max}}, \underline{W}\right) \prod_{k=0}^{p} \pi(L_{k}   p, L_{min}, L_{max}).$
1122	It can be further factored into three conditional posteriors:
1123	$p(M v, \mathcal{D}) \propto p(\mathcal{D} v, M) \cdot \pi(M);$
1124	$p(\boldsymbol{\beta}_{M},\sigma^{2} \boldsymbol{v},M,\boldsymbol{\mathcal{D}}) = \mathbb{N}\left(\boldsymbol{\beta}_{M};  \mathbf{V}_{M}^{*}  \mathbf{X}_{M}^{\mathrm{T}} \mathbf{y},\sigma^{2} \mathbf{V}_{M}^{*}\right) \cdot \mathbb{I}\mathbb{G}\left(\sigma^{2}; \underline{a} + \frac{n}{2}, \underline{b} + \left[\mathbf{y}^{T} \mathbf{y} - \mathbf{y}^{T}  \mathbf{X}_{M} \mathbf{V}_{M}^{*}  \mathbf{X}_{M}^{\mathrm{T}} \mathbf{y}\right]\right);$
1125	$p(v \boldsymbol{\beta}_{M},\sigma^{2},M,\boldsymbol{\mathcal{D}}) = \mathbb{I}\mathbb{G}\left(v;\underline{c}+\frac{p_{M}}{2},\underline{d}+\frac{\sum_{k=1}^{p_{M}}\beta_{k,M}^{2}}{2}\right)$
1126	where we have $\mathbf{V}_{M}^{*} = (v^{-1}\mathbf{I}_{M} + \mathbf{X}_{M}^{T}\mathbf{X}_{M})^{-1}$ and $p_{M}$ is the total number of coefficients collected for all
1127	segments of the piecewise linear and harmonic models. These three conditional posteriors were
1128	sampled iteratively to simulate a chain of posterior samples using our hybrid Gibbs MCMC sampler.
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