**OVERVIEW**

This document details methods for studying time series of high-dimensional data. Our specific motivating context is the study of ecological communities comprised of species, where samples of organisms are collected over time (Christensen *et al.* 2018). We are interested in determining if the composition of communities changes over the course of the study, and if it does, we seek to quantify those dynamics. However, ecological communities are typically composed of many species relative to the number of samples collected (*i.e.,* the data are high-dimensional), which presents a challenge to time series modeling. To address this problem, we reduce the dimensionality of the community data prior to time series analysis (Christensen *et al.* 2018).

We accomplish this through a two-stage analysis referred to here as LDATS. The first stage (LDA) uses Latent Dirichlet Allocation (Blei *et al*. 2003)—a so-called “topic model”—to find a latent, simplified representation of the data, which is then analyzed in the second stage (TS) using multinomial Time Series models built upon the changepoint time series model of Western and Kleykamp (2004).

The LDA model derived and developed by Blei *et al*. (2003) has been successfully applied to ecological data by Valle *et al*. (2014) and Christensen *et al*. (2018). In relation to the linguistic models that motivated the original LDA description and notation (Blei *et al.* 2003), species are like terms (word options) in a vocabulary, communities are like linguistic topics, samples are like documents using the terms, and organisms within a sample are like words within documents (Valle *et al*. 2014). For the sake of maintaining the relationship between our LDATS model and the topic model derivation of LDA, we retain the original naming scheme (*i.e.*, observations of words within documents, latent grouping of terms into topics).

Here, the TS models include discrete (changepoint) and continuous temporal changes as well as covariate impacts and are fit using parallel tempering Markov Chain Monte Carlo (ptMCMC) methods (Earl and Deem 2005). To align our approach with existing topic models

This document describes the two-stage LDATS model in a unified mathematic setting and accompanies the codebase (Simonis *et al*. *In Development*). Because of the overlap in notation between classical LDA (Blei *et al.* 2013) and the time series models used here (Western and Kleykamp 2004) (*e.g.*, both use but with different meanings), we create a new notational set for use here and within the LDATS code and curate a translational list of terms (Table 1). Given that LDATS specifically uses LDA as the first stage and that our methods build upon topic models, in instances of notational overlap between the LDA and TS components, we defer to the original LDA usage.

We do make one important deviation from the original LDA notation (Blei *et al.* 2003) to clarify the dimensionality of parameters. Specifically, we use the lowercase, regular type letter (*e.g.,* ) to indicate a singular value; the lowercase, boldface letter (*e.g.,* )to indicate a vector of values; and the capital, boldface letter (*e.g.,* ) to indicate a matrix of values.

**STAGE ONE: DIMENSION REDUCTION**

The first stage of the analysis is focused on reducing the raw, high-dimensional data to a lower dimensional representation of the information contained in the data using Latent Dirichlet Allocation (Blei *et al*. 2003). This section describes the application of the Variational Expectation Maximization version of the LDA model derived and developed by Blei *et al*. (2003), with no novel developments.

A corpus (set of documents) consists of total documents comprising total words from total terms. Each document (in ) consists of words ( in ) assigned to one of in terms. The total number of words in the corpus is the sum of the words within each document:

LDA involves grouping the terms into in total latent (unobserved) component topics, such that “component topic” means a group of terms that tend to be found together in specific proportions. The allocation process (Blei *et al.* 2003)allows that individual terms can be assigned to multiple component topics. The total number of latent topics is also unknown, and for the present approach is fixed *a priori* within a given Stage 1 (LDA) model in .

Each word within a document has an observed term identity, notated as , and a latent topic membership, notated as . Because there are varying numbers of words in each document, we use a vector structure to hold word-level data across the study. The term identities of all words within document are (or just ) and the term identities of all words across all documents are (or simply ), an -length vector. Similarly, the topic identities of all words in document are represented as (or simply ) and the topic identities of all words across all documents are (or just ), an -length vector. Across all words from all documents, is the latent state (topic identity) and is what is observed (term identity).

For a specific model with a total number of topics , the word-level topic distribution within a document (*i.e.*, the allocation of an words among the possible topics) is a -dimension categorical random variable (equivalent to a multinomial variable with sample size 1) described by probabilities held in vector () and collated across samples into -dimension matrix . Thus, the topic identity of a word within a document is

The vector of topic probabilities within a document () is described by a -dimensional Dirichlet distribution with concentration parameters ,which we assume do not change among documents (*i.e.*, ). Further, we assume that the concentration parameters are symmetric (*i.e.,* ), thereby reducing the distribution to reliance on a single parameter :

which is an unknown parameter to be estimated.

The word-level topic distribution within a document (*i.e.*, the allocation of an words among the possible terms) is a -dimension categorical random variable contingent upon the topic identity of the word and defined by probabilities , where the sum across terms within a topic for a given document is 1 (*i.e.*, ). The probabilities across all topics within a document are held in a -dimension matrix (), which we assume is constant across documents, (), thus the term state of an word within a document is

which is equivalent to a categorical variable defined by the row of interest in given topic identity

The components of are unknown parameters to be estimated.

The inferential problem of interest lies in determining the posterior distribution of the latent quantities (the topic probabilities and states ), given the observations () and fitted parameters ( and )

an equation which obviously necessitates an estimation of the parameters and . From a parameter estimation standpoint, we are concerned with the probability of the suite of observations () given the parameters and , or the likelihood () of the parameters given the data:

However, for fitting purposes, we are interested in the log-likelihood () of the parameters, given the data

The log-likelihood of (the data across all samples) is the sum of the logged probabilities of each document’s data given the parameters (under the assumption that all documents are derived from the same parameters):

The probability of a document’s data given the parameters () can be decomposed into the product of [1] the word-by-word term-identity distributions () and [2] the sample-level community distribution (), integrated over the uncertainty in the latent community distribution, :

The word-level topic-identity distribution can be further decomposed into the product of [1] the term identity distribution given the topic identity and the unknown parameter matrix () and [2] the topic identity distribution given the latent topic distribution (), integrated (summed due to discreteness) over the uncertainty in topic type

The probability of a single document’s observations can therefore be decomposed into the product of [A] the product of the word-by-word topic distributions, each integrated over the uncertainty in topic type (which are themselves the product of [1] the term identity given the topic identity and the unknown parameters and [2] the community identity given the latent parameter ) and [B] the probability of the latent parameter given the unknown parameter , integrated over the uncertainty in

This is then scaled up to the probability of the entire corpus under the unknown parameters and , which is the product of the sample-level probabilities given those parameters:

The probabilities for in cannot be tractably estimated due to the coupling of (and thus ) and in the summation over latent topics (Blei *et al*. 2003). To address this, we use a variational approximation to the equations that decouples the parameters, and which we fit using the expectation-maximization routine (aka VEM for Variational Expectation Maximization; Blei *et al*. 2003).

To accomplish this, we endow the model with free variational parameters ( and ) that characterize a family of distributions (notated by to distinguish from ) which provide a lower bound on the log likelihood. is an -dimension matrix similar to . However, the rows of (row corresponding to document : or simply ) correspond to the concentration parameters of a -dimension Dirichlet distribution and therefore are not constrained to sum to 1. is an -dimensional matrix, where the rows correspond to the words across documents (indexed akin to and ) and the columns correspond to the topics. describes the probability that word within document is from topic , and (or simply ) is a -length vector of probabilities that define the categorical distribution controlling that word’s topic identity, where . is composed of document-specific matrices, where the matrix for a specific document is -dimensional and notated .

In comparison to and , the variational parameters are document-specific (able to vary among documents), and so are found separately for each document. For a specific document , the variational distribution is

As the Expectation Step (“E-Step”) in the VEM algorithm, the distribution can be used to find a tight lower bound on by optimizing the variational parameters and (*i.e.*,find and , where the asterisks notate optimal values) with respect to minimizing the Kullback-Leibler Divergence () between and the true posterior :

Minimization of the distance is achieved through an iterative fixed-point method, where the derivative of the is set to zero, producing a pair of update equations. First, the parameters describing the topic allocation of each word () are updated based on the topic distribution for the document ():

where the expected value of the (log-scale) topic probability is calculated using the digamma function (), which is the logarithmic derivative of the gamma function (), a quantity that is calculated through Taylor approximation:

And then, the parameters describing the topic distribution for the document () are updated based on the word-level topic distributions for the sample ():

The update equations are alternated until the bound converges (*i.e.*, the updates do not yield changes to the parameters), at which point the document-specific variation parameters have been optimized ( and have been found) for the set of main parameters ().

Similarly to the overall log likelihood for the set of documents being equal to the sum of the log likelihoods for the individual documents, the variational lower bound () for all of the documents is equal to the sum of the variational lower bounds for the individual documents:

The complete E-Step maximizes this overall lower bound with respect to the full variational parameters and (*i.e.*, given the main model parameters). The Maximization Step (“M-Step”) maximizes the overall lower bound with respect to the main model parameters and (*i.e.*, given the optimal variational parameters). This corresponds to obtaining maximum likelihood values of the model parameters using expected sufficient statistics for each sample under the approximate posterior calculated in the E-Step.

The update for the topic-level term distribution () can be written analytically:

where is an indicator variable based on the term identity () of the observed word ():

The update for the concentration parameter underlying the document-level topic distribution () requires an iterative approach to find a stationary point estimate. The optimization is conducted using the Newton-Raphson method (Ronning 1989), which repeats

(where is the hessian matrix and is the gradient) until convergence. Having updated the main model parameters (the M-Step), a new iteration of the E-Step followed by the M-Step is conducted, and the E-Step and M-Step are alternated until the lower bound of the log-likelihood converges. Thus, the VEM approach can be considered coordinate ascent in (the space defined by the lower bound).

Once the log-likelihood has converged, the VEM algorithm has arrived at approximate maximum likelihood estimates for the model parameters ( and ) given the full set of observations () for the specific Stage 1 model (notated by the component in the superscripts), which forms the basis of Stage 1 model selection to determine the most parsimonious number of topics . Specifically, we use as our Stage 1 model selection criterion, defined for a specific LDA model :

where is the number of parameters in the model: corresponding to and corresponding to each entry in , a -dimensional matrix (Grün and Hornik 2011). If small sample size is a concern with respect to the degrees of freedom being used, we can use the correction based on the number of observations, here corpus size (, Grün and Hornik 2011):

Because of the use of multiple iterative optimization routines (which require starting values to be drawn at random) to solve otherwise intractable likelihood functions, it is critical to account for the potential influence of starting values on analytical results. Here, we accomplish this by running multiple models with the same number of topics () using different starting values, assigned through the random number generator seed ().

Specifically, we use replicates ( in ) at each number of topics from 2 to , the total number of topics to be explored. The minimal number of topics is set to 2 by the current coding implementation of the LDA algorithm (Blei *et al.* 2003, Grün and Hornik 2011), although it is possible to generalize the code to include the limiting case of a single topic. Thus, the total number of models in the Stage 1 () is

The optimal (according to ) LDA model () is determined by

and has a corresponding set of parameters:

Having found the optimal model, we can obtain the posterior point estimates for the document-level topic probabilities (held in a -length vector) by normalizing the vector of optimal values of the variational Dirichlet concentration parameters (taken from the final step of the VEM algorithm in model ) for the document () so it sums to one and is thereby a proper proportion (notated by the bar accent ):

The posterior point estimates of the topic proportions across the documents are then held in an -dimension matrix , corresponding to the optimal (from an “ based on VEM inference”-perspective) decomposition of the word-level data to topic-level data. This matrix forms the multivariate response variable analyzed in the time series model, as outlined in the next section.

**MULTINOMIAL TIME SERIES MODEL**

The approach we take in analyzing the temporal topic dynamics leverages change point time series analyses (Western and Kleykamp 2004) that allow for continuous and discrete changes in dynamics, combined with multinomial generalized regression (Ripley 1996, Venables and Ripley 2002) to manage the proportional nature of the response variable (document-level topic compositions).

The output from the decomposition detailed in the previous section () is a matrix of multinomial variables corresponding to proportions of each topic in present in each document in . Further, each document has a weight , which is a function of the number of words relative to the maximum number of words across all documents:

thereby allowing us to account for variable efforts (numbers of words) among documents (with vector ).

We are interested in quantifying changes in topic composition over time, and so we define the time of document to be and the vector of all document times to be or simply . defines the temporal relationship among documents, and must be a discrete variable. In addition, we collate total covariates, indexed as in and measured for each document. The value of a particular covariate for a specific document is and the set of covariates for the document is a vector or simply . All of the covariates (including the intercept) across all of the documents are held in , an -dimensional matrix.

Although the analysis of the topic proportions is via “time series” models, the time of the document () *per se* does not necessarily enter every Stage 2 (time series) model ( in ) directly. Rather, depending upon the model, the time of the documents may control the application of the predictor variables in the model (in the case of discrete change points) or may directly influence quantitative values of predictors (in the case of continuous time impacts). Future developments of the model will allow time to also impact the non-independence of the data via autocorrelation structures, but presently autocorrelation is not included.

A given Stage 2 model has a non-negative integer number of discrete change points () that divide the time series into distinct segments or “chunks” ( in ), where the number of chunks () is always one more than the number of change points (). If there are change points (*i.e.,* ), then their locations (for the in change points) are unknown parameters to be estimated. A specific change point ’s location is represented by and the set of change points are represented by the –length vector or simply .

To define the full deconstruction of the time series into chunks, we augment the vector of change point locations with the time before the minimum () and maximum times () in the series, generating the –length vector , where the over brace accent references the addition of the fixed time range to the unknown change points. In the instance that there are no change points (*i.e.,* ), is still defined, but now is simply a length-2 vector including the minimum and maximum times, and therefore includes no unknown change point locations to be determined.

We use the locations to assign the documents to specific chunks via a document ↔ segment indicator function (), which returns an indication if document belongs to chunk (0 for no or 1 for yes) that we notate as . operates on the timestamp of the document () and the start and end time of a given chunk , defined by its start time and end time :

This indicator function allows us to identify to which chunk each document belongs and we use this identity to deconstruct the full output matrix from the first stage model () into matrices ( in ), each of which is analyzed separately. For each chunk in , the function produces an -length vector of 0s and 1s ( or simply ). is a submatrix of :

where we use the parenthetical notation to mean “of chunk ” and the square bracket indicates the subset of the matrix as , such that only the rows corresponding to 1s in are included, and all columns are included.

We note an important distinction between the original change point model (Western and Kleykamp 2004) and our model here with respect to the application of the change points to the regression. In Western and Kleykamp’s (2004) model, the indicator function is only applied within the “fixed-effect” component of a singular regression fit, such that all chunks have the same error terms. In our model, however, the data are fully separated into multiple independent regression fits, as a result applying the indicator to both the “fixed-effect” and error components.

Further, the original change point model (Western and Kleykamp 2004) assumed a univariate normal response variable, whereas our response data are multivariate and non-normal. Specifically, our response variable is a set of multinomial probabilities, each of which must be non-negative and which must sum to 1. To accommodate this structure, we take a generalized linear model approach and, within each given chunk of time, model the data using a log-linear multinomial (aka multinomial logit, softmax) regression (Ripley 1996, Venables and Ripley 2002).

Within chunk of time , we are interested in describing the proportion of each topic in in a document in . We notate this proportion as , which is the probability that a word in document comes from topic . Following general linear modeling, we wish to define the proportion in terms of predictor covariates (, a vector of covariates—including the intercept—for document ) and coefficients (, a vector of the coefficients associated with the specific topic during this chunk of time).

However, we must acknowledge the two constraints on the response variable (proportions): that each be non-negative and that they sum to 1. We accommodate the non-negative constraint by using a log-linear model that relates the log of the proportion to the linear predictors. We handle the sum-to-1 constraint by subtracting a “constant” value for the document (, where is known as the partition function) from all topics’ proportions:

or, with respect to the raw proportions,

where is a row matrix and is a column matrix.

Given the sum-to-1 (), we can define :

Thus, the specific equation for the proportion of topic in document can be written as

replacing the with in the denominator summation to avoid confusion with the focal topic .

However, because of the sum-to-1 constraint, only of the proportions ( in ) are uniquely identifiable (and, by extension only of the parameter vectors in are uniquely identifiable). Thus, we define the augmented parameter vectors in in relation to the parameters of the first topic ():

This sets the parameters associated with the first topic to be 0 (, and thus ), thereby reducing the number of free parameter vectors (and by extension the number of proportions that are estimated), by 1 to the that we are able to fit. This results in the modified equation

where . Thus, the parameters in the vectors to are the unknowns to be fit for this specific chunk of time . This equation is known as the softmax function, and so we also can write

For notational condensation, we combine all of the parameter vectors to (including the vector of 0s in ) into a matrix ( is capital ), which has rows and a number of columns equal to the number of coefficients in the model including the intercept (*i.e.*, the length of ). This allows us to further condense the probability equation to

thereby facilitating use of the linear modeling framework. We expand the model to predict the proportions across all of the topics within the document, which means we can drop the input and produce the full set of values from the softmax, which is a vector that needs to be transposed after the softmax calculation to conform to the existing dimensionality to the response variable when scaled up ()

( indicates transpose). Next, we expand the model across all documents within the chunk of time

where the covariates are held in a matrix () with the number of rows equal to the number of coefficients and the number of columns equal to the number of documents in the chunk. That is, is a series of column vectors.

As stated earlier, it is at this level (time chunks of documents) where the regression parameters are estimated, which differs from the original model formulation of Western and Kleykamp (2004), which fits the parameters across all observations within a single model. Thus, while we can continue to expand the model up across time chunks, it will be with a formulation that differs slightly from Western and Kleykamp (2004) with respect in particular to parameter estimation. Most specifically, in our model, there is no covariance among regression parameters fit in different chunks, whereas the Western and Kleykamp (2004) model allows for covariance among all of the regression parameters.

To do this, we first define an expanded version of the parameter matrix , which has rows and a number of columns equal to the number of coefficients across all of the time chunks:

We next expand the covariates to the matrix , which has a number of rows equal to the number of coefficients across all of the time chunks and columns:

Finally, we compute the full matrix of topic-by-document proportions:

Now can move to the rest of what W and K use to describe the model

Add the var-cov matrix and the distributions of the priors and the change points

fit using a single-hidden-layer neural network with skip-layer connections

Changepoint model (Western and Kleykamp 2004)

Parallel tempering MCMC (Earl and Deem 2005)

**LITERATURE CITED**

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