THE LAPLACE MOTION IN PHYLOGENETIC COMPARATIVE METHODS

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ABSTRACT

The majority of current phylogenetic comparative methods assume that the stochastic evolutionary process is homogeneous over the phylogeny or offer relaxations of this in rather limited and usually parameter expensive ways. Here we make a preliminary investigation, by means of a numerical experiment, whether the Laplace motion process can offer an alternative approach.

INTRODUCTION – PHYLOGENETIC COMPARATIVE METHODS

It is by now well established that when doing a between species analysis (of some traits common to these species) one needs to take into consideration that the data points (usually means of a number of individuals from each species) could potentially come from a dependent sample. This dependence is due to the species’ shared evolutionary history. Due to phylogenetic inertia species which diverged more recently are expected to have more similar trait values. This was noticed from the very birth of the theory of evolution [4] but only recent availability of computational power and genomic data, from which we can derive evolutionary histories, allowed us to start developing and using phylogenetic comparative methods in practice. The main challenge with comparative data is the type of sample we observe. We do not observe a time series trajectory but we only (with some exceptions e.g. where fossil data is included, but in this situation one runs into dating issues) observe the trait values of currently alive species which contain a (better or worse estimated) branching structure behind them. This means that we do not have a natural way of exploiting independent increments between observations.

The first proposed model [7] of continuous trait (labelled $X$) evolution was a Brownian motion model, $dX(t) = \sigma dB_t, X(0) = X_0$, where $B_t$ is the Wiener process and $X_0$ is the trait value of the common ancestor of all of the studied species. If we denote by $T = \begin{bmatrix} t_{a_{i,j}} \end{bmatrix}_{1 \leq i,j \leq n}$ the matrix of between species divergence times ($t_{a_{i,j}}$ is the time of divergence of species $i$ and $j$) then under this model the mean and variance of our trait sample $\bar{x} = [x_i]_{1 \leq i \leq n}$ are $E[\bar{x}] = X_0 \bar{1}_n$ and $\text{Var}[\bar{x}] = \sigma^2 T$. This simple form makes the Brownian motion model tractable. Its major drawback however is that with time the variance will be going to infinity and other models based on the Ornstein–Uhlenbeck process have been studied [1,3,8,10,12,16]. One is naturally interested in estimating the process parameters and then discussing to what biological properties they correspond to. In the current study we will however not consider models more complicated
than Brownian motion as we will be concentrating on another aspect of phylogenetic comparative methods.

**UNCERTAINTY IN THE PHYLOGENY, RELAXING PROCESS HOMOGENEITY**

The vast majority of programs for phylogenetic comparative analysis assume that the provided phylogeny is completely resolved and are limited in allowing process parameters to vary over different parts of the phylogenetic tree. The current wealth of sequence data will provide us with better and better phylogenies but uncertainty is something that will never be completely removed. The majority of current methods e.g. [3, 20, 22] advocate to use an ensemble of (plausible) phylogenies, on each one run the analysis and then weight the results (either uniformly or with some prescribed weights to each phylogeny e.g. posterior probabilities from a Bayesian tree estimation procedure). Alternatively one can run a joint MCMC that samples both the phylogeny and stochastic process parameters that evolve on it [13, 14, 21]. These approaches are unfortunately computationally very demanding.

One can also question the assumption of process homogeneity over the whole tree. It is of course possible to study models where the parameters differ over different parts of the phylogeny [3, 16, 20]. This however causes an inflation in the number of parameters which results in more difficult and unreliable (due to small sample sizes) estimation. One approach to this was suggested in [17] where it is proposed to rescale each branch length by a random variable from e.g. a gamma(ν/2, ν/2) or log–normal(1, σ) distribution (see also [5]). This can be interpreted as that on each branch the trait will have its unique speed of evolution but only at the cost of a single parameter describing the distribution. This sort of time change can also be viewed as uncertainty in the phylogeny — in the branch length estimates. Another possibility is presented in [6], where a Bayesian model selection procedure searches for Brownian motion rate changes over the phylogeny.

**LAPLACE MOTION**

The Laplace motion (also known as the variance gamma process) can be represented as a Brownian motion with drift with a random time change given by a gamma process [18]. Following [18] let $B_{\theta,\sigma}(t)$ be a Brownian motion with drift,

$$ B_{\theta,\sigma}(t) = \theta t + \sigma B(t), \quad (1) $$

and then we define, again after [2, 15, 18], the gamma process $\gamma_{\nu,\beta}(t)$ as the process of independent gamma increments over non–overlapping time intervals. The density of the increment $g = \gamma_{\nu,\beta}(t + h) - \gamma_{\nu,\beta}(t)$ over a time interval of length $h$ is given by the gamma density with shape parameter $h/\nu$ and scale parameter $\beta$,

$$ f_{h;\nu,\beta}(g) = \left( \Gamma \left( \frac{h}{\nu} \right) \right)^{-1} \beta^{h}\sigma^{-h} g^{h-1} e^{-\beta g} \quad (2) $$

Now we define the Laplace motion as,

$$ X_{\theta,\sigma,\nu}(t) = X_0 + B_{\theta,\sigma}(\gamma_{\nu,\nu}(t)), \quad (3) $$

In our particular application we consider the Laplace motion with no drift, $\theta \equiv 0$, also known as the symmetric variance gamma process [18, 19], for which given a fixed $t$ the following equality in distribution holds,

$$ X_{\sigma,\nu}(t) = B_{\sigma}(\gamma_{\nu,\nu}(t)) \overset{D}{=} X_0 + \sqrt{\gamma_{\nu,\nu}(t)}\sigma B(t). \quad (4) $$

Naturally a non–zero drift has biological interest however at this point we do not consider it. The idea of using a Laplace motion is closely related to the suggestion of [17], but it is put in a formal mathematical framework of Lévy processes.
LAPLACE MOTION ESTIMATION

To estimate the model parameters of interest, $X_0$, $\sigma^2$ and $\nu$, we use an EM algorithm, following [15], which exploits the representation in Eq. (4) of the Laplace motion by treating the unobservable gamma random variables for the branch lengths (variances) as missing values. We also exploit that we only have observations of the tip species. Due to this, from the perspective of a phylogenetic comparative method, a Laplace motion is equivalent to changing each branch $i$ of length $t_i$ to a gamma random variable with mean $t_i$ and variance $\nu t_i$. Notice that in this parametrization of a gamma random variable, $\sigma^2$ is not a superfluous parameter as it will not “disappear” into the gamma process’ scale parameter due to us forcing a relationship between the shape and scale. Multiplying a gamma random variable by a constant is equivalent to multiplying the scale by the same value but it does not relate to the shape. In the limit as $\nu \to 0$ we arrive at the original tree. The main computational challenge is how to effectively do the expectation (E) step as we do not observe a time series process. The main aim of this work is an initial consideration of introducing the Laplace motion so we made do with an approximate numerical treatment of the problem. For the maximization step we employ a simulated annealing type of search. We used R 2.15 [24] (on an Intel Core i5 2.3GHz machine running Suse Linux 12.1) to implement the estimation procedure described in Alg. [1]. In it we allow for a non–homogeneous Laplace motion, i.e. we allow the parameter $\nu$ describing it to vary over predefined by the user branches of the phylogeny (regimes). A user is free to specify a specific value for each branch but then we run into obvious estimation problems. The natural approach is to group branches (v/8) according to some shared trait/environmental variable (see the biological example where we have one $\nu$ for each breeding group size).

DATA EXAMPLE CERVIDAE FEMALE BODY SIZE

As a proof of concept example we re–analyze a portion of the Cervidae data set of [23]. The data set consists of averages of measurements of male antler length (mm), male body mass (kg), female body mass (kg) in 31 deer species along with their phylogeny derived from [9]. In addition the breeding group size (discrete variable with three levels: 1–2, 3–5 and > 5) of each species is recorded and also the mating tactic (discrete variable with four levels: harem, territorial, tending and monogamous) is recorded (missing in Megamuntiacus vuquangensis). The aim of [23] was to study how male antler length depends on the remaining measured variables. In [1] we were able to improve on this analysis due to our newly developed mvSLOUCH R software. We found that both male antler length and male body mass were jointly responding to changes in female body mass and breeding group size. The logarithm of female body mass was found to be best explained (AICc) by a Brownian motion. The results and biological conclusions are consistent with those of [23] except that a more refined model provides better explanation for them. In this study we consider just the female body mass and see whether it can be better explained by a Brownian motion with different rates for different breeding group sizes or by a Laplace motion with one $\nu$ parameter or a different one for each breeding group size. We also checked whether the diffusion parameter of the Brownian motion aids estimation in the Laplace motion models. The female body size and deer phylogeny is presented in Fig. [1]. The estimation results are presented in Tabs. [1] and [2].

Using the AICc to choose between competing models we can see that, from the set of candidate models, the homogeneous Laplace motion with $\sigma^2$ unknown best explains the female body size data. This suggests that the rate of trait evolution is not homogeneous but currently available methods would not detect this as they would have to be overly parametrized.

CONCLUSIONS AND FUTURE WORK

The aim of this work was to describe how the Laplace motion model would fit in the phylogenetic comparative methods field and whether it could be a potential alternative to models with different
A detailed analytical study is required in order to achieve a stabler and more formal estimation example. This work is however only a preliminary investigation to gain intuitions for the model. Paying too much in parameters. Such a situation was seen in the presented here Cervidae data. The Laplace motion allows one to relax the process homogeneity assumption without diffusion coefficients on different parts of the phylogeny. Such models are expensive in terms of parameters and with commonly small samples could be rejected in favour of a homogeneous model. The Laplace motion allows one to relax the process homogeneity assumption without paying too much in parameters. Such a situation was seen in the presented here Cervidae data example. This work is however only a preliminary investigation to gain intuitions for the model. A detailed analytical study is required in order to achieve a stabler and more formal estimation

\begin{algorithm}
\textbf{Algorithm 1} Approximate EM algorithm for MLE of phylogenetic Laplace motion
\begin{align*}
i &:= 1, \mathcal{L}_0 = -\infty, \nu_1 = \text{starting value}, \tau_0 = 50 \\
\text{while } i \leq 60 \text{ and } |\mathcal{L}_i - \mathcal{L}_{i-1}| > \epsilon \text{ do} \\
&\quad \text{if previous iteration was rejected then} \\
&\quad \quad \mathcal{L}_i = \mathcal{L}_{i-1} \\
&\quad \end{align*}
\begin{algorithmic}[1]
\State $\forall k = 1$ to 1000 do
\State $\text{Tree}_k := \text{Original Tree}, \mathcal{L}_{T_k} = 0$
\For {each branch $j$ in $\text{Tree}_k$}
\State $t_j = \Gamma(\text{shape} = T_j/\nu[j], \text{scale} = \nu[j])$ \{ $T_j$ is branch $j$'s length in the original tree\}
\State $\mathcal{L}_{T_k} += \log(f_{T_j, \nu}(t_j))$ \{ $f_{T_j, \nu}(\cdot)$ is the appropriate gamma density\}
\EndFor
\State $(\hat{X}_{01k}, \hat{\sigma}^2_{1k}) = \text{MLE conditional on } \text{Tree}_k \text{ and trait data vector } \vec{x}$ \under the Brownian motion model by mvSLOUCH \[1\]
\State $\mathcal{L}_{x_k} = \log\text{–likelihood of } (\hat{X}_{01k}, \hat{\sigma}^2_{1k}) \text{ conditional on } \vec{x}$ and $\text{Tree}_k$
\EndFor
\State $\mathcal{L}_T = \sum_k \mathcal{L}_{T_k}$ \{The following four are heuristic formulae that were found to work well\}
\State $\mathcal{L}_i = \sum_k (\mathcal{L}_{T_k} + \mathcal{L}_{x_k} - \mathcal{L}_T)$
\State $\hat{X}_{01i} = \sum_k \hat{X}_{01k} \cdot \exp(\mathcal{L}_{T_k} + \mathcal{L}_{x_k} - \mathcal{L}_T - \mathcal{L}_i)$
\State $\hat{\sigma}^2_i = \sum_k \hat{\sigma}^2_{ik} \cdot \exp(\mathcal{L}_{T_k} + \mathcal{L}_{x_k} - \mathcal{L}_T - \mathcal{L}_i)$
\If {$\mathcal{L}_i \leq \mathcal{L}_{i-1}$ \text{ and } $U > \exp((\mathcal{L}_i - \mathcal{L}_{i-1})/\tau_i)$ \{ $U$ is uniform on $[0, 1]$ \}}
\State $\hat{X}_{01i} = \hat{X}_{01i-1}, \hat{\sigma}^2_i = \hat{\sigma}^2_{i-1}$ \{do not update\}
\EndIf
\State $\nu_{i+1} = \exp(\log(\nu_i) + \zeta |Z|)$ \{ $Z$ is normal with mean 0 and variance dependent on $\nu_i$, $\zeta \in \{-1, 1\}$ depending which direction seems better locally\}
\State $\tau_{i+1} = \tau_i / \nu_i$
\State $i += 1$
\EndWhile
\end{algorithmic}
\end{algorithm}

Table 1. Summary of Cervidae model comparisons. Model marked with * was analyzed with Brownie \[20\], remaining by a front–end to mvSLOUCH. In Fig. 2 we can see the relationships between the models.

| Model          | df | Log–likelihood | AIC   | AICc  |
|----------------|----|----------------|-------|-------|
| BM             | 2  | -36.140        | 76.279| 76.708|
| BM + BGS *     | 4  | -34.815        | 77.629| 79.168|
| Laplace        | 3  | -34.798        | 75.596| 76.484|
| Laplace + BGS  | 5  | -34.741        | 79.481| 81.881|
| Laplace ($\sigma^2 = 1$) | 2  | -37.017        | 78.034| 78.463|
| Laplace + BGS ($\sigma^2 = 1$) | 4  | -36.945        | 81.890| 83.429|
Figure 1. Left: Cervidae phylogeny [9], right: logarithm of female body size and breeding group size.

Table 2. Summary of Cervidae estimation. Values marked with * were estimated by Brownie [20], remaining by a front–end to mvSLOUCH. Notice that $\sigma^2$ is a relative value as we set the tree’s height as 1.

| Parameter  | BM    | BM+BGS | Laplace | Laplace + BGS | Laplace $(\sigma^2 = 1)$ | Laplace + BGS $(\sigma^2 = 1)$ |
|------------|-------|--------|---------|---------------|--------------------------|-------------------------------|
| $X_0$      | 3.835 | 3.459* | 3.838   | 3.878         | 3.767                    | 3.792                        |
| $\sigma^2$ | 1.396 | —      | 1.379   | 1.269         | —                        | —                             |
| $\sigma^2_{small}$ | — | 0.642* | —       | —             | —                        | —                             |
| $\sigma^2_{medium}$ | — | 2.568* | —       | —             | —                        | —                             |
| $\sigma^2_{large}$ | — | 1.251* | —       | —             | —                        | —                             |
| $\nu$      | —     | —      | 0.897   | —             | 0.604                    | —                             |
| $\nu_{small}$ | — | —       | —       | 0.712         | —                        | 0.248                        |
| $\nu_{medium}$ | — | —       | —       | 1.006         | —                        | 0.100                        |
| $\nu_{large}$ | — | —       | —       | 0.816         | —                        | 0.049                        |

Figure 2. Relationships between models, an arrow from model $i$ to $j$ indicates that model $i$ is a direct submodel of $j$ (we do not indicate transitive relationships).

procedure, find its estimability properties and be able to couple the variance gamma process with Ornstein–Uhlenbeck type evolutionary processes.
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