A parametric interpretation of Bayesian Nonparametric Inference from Gene Genealogies: linking ecological, population genetics and evolutionary processes

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Abstract

Using a nonparametric Bayesian approach Palacios and Minin (2013) dramatically improved the accuracy, precision and biological adequacy of Bayesian inference of population size trajectories from gene genealogies. These authors proposed an extension of a Gaussian Process (GP) nonparametric inferential method for the intensity function of non-homogeneous Poisson processes. The authors found that not only the statistical properties of the estimators were improved with their method, but also, that key aspects of the demographic histories were recovered. The authors' work represents the first Bayesian nonparametric solution to this inferential problem because they specify a convenient prior belief without a particular functional form on the population trajectory. Their approach works so well and provides such a profound understanding of the biological process, that the question arises as to how truly 'nonparametric' (*i.e.* "biology-free") their approach really is. Using well-known concepts of stochastic population dynamics, here I demonstrate that in fact, Palacios and Minin's GP model can be cast as a parametric population growth model with density dependence and environmental noise. Making this link between population genetics and stochastic population dynamics modeling provides novel insights into eliciting biologically meaningful, parametric, priors for the trajectory of the effective population size. The results presented here also bring novel understanding of GP as models for the evolution of a trait. Thus, the ecological principles

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foundation of Palacios and Minin (2013)'s prior adds to the conceptual and scientific value of these authors' inferential approach. I then conclude this note by listing a series of insights brought about by this connection with Ecology to illustrate why Palacios and Minin (2013)'s article is a very stimulating reading.

Keywords Demographic Stochasticity, Environmental variability, Gaussian Process, Gene Genealogies, Ornstein Uhlenbeck process, Population Size Trajectories.

1 Introduction

Palacios and Minin (2013) propose a Bayesian nonparametric methodology to reconstruct past population dynamics using genomic data and the Coalescent process. This non homogeneous Markov death process specifies the relationship between ancestral genealogies of a random sample of genes and effective population size. Because changes in population size result in changes on the genetic pool in a population, at any point in time genomic data carries information regarding past demographic processes and population dynamics. Although estimating the effective population size amounts to estimating the total population size in an idealized Wright-Fisher model without selection, studying in changes in this parameter remains important because of its interpretation as a metric of relative genetic diversity.

Motivated by the lack of statistical methods to infer past population dynamics from a sample of genes that didn't depend on strong parametric assumptions, Palacios and Minin (2013) proposed a transformed Gaussian Process (GP) as the prior for past population trajectories. These authors justify their choice because such process "does not adhere to a particular functional form, or hypothesis on past population dynamics" (Palacios and Minin, 2013). In this article, I borrow results from theoretical ecology, to show that Palacios and Minin (2013) prior choice can be interpreted as a class of stochastic population dynamics models, albeit one previously not studied and hence, one that brings novel insights into both, population genetics and statistical ecology.

Engen et al. (1998) published in *Biometrics* what now is considered one of the standard references to understand the concepts of "demographic stochasticity" and "environmental variability" in population dynamics modeling. These authors drew their ideas from the stochastic processes models of Keiding (1975) and Lud-

wig (1976) which incorporated two main sources of variability: stochasticity due to random births and deaths, known as demographic stochasticity; and temporal variability in any of the demographic rates (*e.g.* good years/bad years for survival, etc...). Traditional ecological concepts, such as density-dependence were also explicitly incorporated in these models. Operationally, formulating a model with the so called 'demographic stochasticity' amounted to specify, for instance, a Branching Process (BP) model with a density dependent offspring distribution of individuals. To add temporal variability into one of the demographic rates, or what came to be known as 'environmental stochasticity' (Lewontin and Cohen, 1969), a temporally uncorrelated random shock was added to the mean of the offspring distribution (often assumed to be Poisson). The result was a density-dependent, BP in Random Environments (PBRE) model (Tier and Hanson, 1981). At that time, various properties of simpler BPRE's had already been worked out by Athreya and Karlin (1971b,a).

Diffusion approximations of the PBRE models later opened the door to the study of animal abundance fluctuations as modeled by realistic, stochastic population dynamics models (Keiding, 1975; Ludwig, 1976; Tier and Hanson, 1981) (see Appendix 1). Straightforward analytical expressions of the properties of the density-dependent BPRE models (such as stopping times and quasi-extinction probabilities) are often too unwieldy or difficult to obtain. Their approximation by means of diffusion processes however, have led to a remarkable improvement in the understanding of how stochasticity from demographic events (births, deaths, etc.) and hence persistence, are affected when the rates themselves are allowed to vary randomly over time. To date, research in this field has yielded a plethora of results that guide the decisions and questions of wildlife managers, population biologists and theoretical ecologists alike (Dennis et al., 1991; Dennis and Taper, 1994; Dennis et al., 1995; de Valpine and Hastings, 2002; Staples et al., 2005; Dennis et al., 2006; Sæther et al., 2007; Lele et al., 2007; Melbourne and Hastings, 2008; Nichols et al., 2009; Knape and de Valpine, 2012; Sæther et al., 2013; Lebreton and Gimenez, 2013; Dennis and Ponciano, 2014; Ferguson and Ponciano, 2014, 2015).

The diffusion approximation of ecological BP models are usually presented as a Stochastic Differential Equation (SDE) model (Tier and Hanson, 1981). The infinitesimal mean of these models usually corresponds to one of the well-known deterministic ODE models of population growth, such as the logistic equation. If only demographic stochasticity is considered (*i.e.*, if a BP model in constant environments is approximated with a diffusion), then the infinitesimal variance of the process scales proportionally to population size, whereas including both, environ-

mental and demographic stochasticities results in an infinitesimal variance with two terms, one proportional to population size and one that scales like the square of population size (see Dennis (2002) and citations therein). Finally, a density-dependent (or density-independent) SDE model of population abundances where the infinitesimal variance scales only like the square of population size has been shown to correspond to a model that assumes no demographic variability and only environmental stochasticity. In what follows, I briefly summarize first the approximation of BPRE's with diffusions. I then expose the relationship between a simple transformation of the Ornstein-Uhlenbeck process and stochastic demography, as well as Palacios and Minin (2013)'s GP prior and stochastic demography. I conclude by showing how, unbeknownst to Palacios and Minin (2013), their GP model brings about novel parametric understanding of stochastic population dynamics.

2 Stochastic demography and Palacios and Minin's model

2.1 Diffusion approximation of density-dependent PB in random environments

In this section I briefly summarize the work of numerous authors, which work under different hypotheses and notations (Goel and Richter-Dyn, 1974; Keiding, 1975; Ludwig, 1976; Turelli, 1977; Tier and Hanson, 1981; Braumann, 1983b,a; Ethier and Kurtz, 1986). This account is accompanied by a detailed appendix and is the basis for a later discussion of the key assumptions of the diffusion approximation of a BPRE, and its relation to Palacios and Minin (2013)'s GP-based model for $N_e(t)$. These author's prior for $N_e(t)$ is given by the transformation

$$N_e(t) = \left[\frac{\lambda}{1+\exp\{-f(t)\}}\right]^{-1}, \tag{1}$$

where $f(t)$ is a Gaussian Process (GP). By so doing, the authors posit a priori sigmoidal, scaled logistic function of a GP with a restricted range between $(0, \lambda)$ for $1/N_e(t)$. Their approach to build a prior is then purportedly phenomenological in nature. For the sake of computational tractability, the authors use a Markovian GP and compare, for one of their examples, the performance of Brownian motion,

an Ornstein-Uhlenbeck (OU) process and a higher order integrated Brownian motion. In the case of the Brownian and OU diffusion processes, because a smooth transformation of a diffusion process is also a diffusion (see Karlin and Taylor (1981), Theorem 2.1 p. 173), then Palacios and Minin (2013)'s prior for $N_e(t)$ is also a diffusion. The key point of this note is to show that the resulting diffusion prior for $N_e(t)$ is in fact a class of well known diffusion processes representing density-dependent, stochastic population growth. Hence, Palacios and Minin (2013)'s priors for $N_e(t)$ are in fact, parametric, in the sense that can be made to represent different hypotheses regarding population growth, density dependence and the structure of variability in a population.

Diffusions that model stochastic population growth are usually presented as SDEs of the form

$$dY_t = m(y)dt + \sqrt{\sigma^2(y)}dW_t,$$

where $m(y)$ is the infinitesimal mean of the diffusion, $\sqrt{\sigma^2(y)}$ is its infinitesimal variance and $dW_t \sim \mathrm{N}(0, dt)$. Both, $m(y)$ and $\sigma^2(y)$ are continuous functions of y. In these models, the infinitesimal mean is usually given by the deterministic skeleton of an ODE, logistic-type model. The authors above have shown that a suitable diffusion approximation of a BP with a density dependent offspring distribution has an infinitesimal variance of the the form $\sigma^2(y) = y\alpha$ ($\alpha > 0$), whereas a diffusion approximating a BPRE has an infinitesimal variance of the form $\sigma^2(y) = y\alpha + (y\beta)^2, \beta > 0$. Thus, if the mean of the offspring distribution of a BP varies randomly every generation, then the infinitesimal variance of the corresponding approximating diffusion scales like the square of population size. This scaling then represents random fluctuations in the quality of the environment (*i.e.*, for instance, if there are good/bad years for reproduction), and is analogous to the variance scaling brought about by random, temporal changes in selection of population genetics models (Karlin and Taylor, 1981). As I show in the following sections, the model for $N_e(t)$ that Palacios and Minin (2013) present as a transformed GP is in fact, to a very close approximation, a stochastic Gompertz-like model with only environmental fluctuations.

In ecology, a plethora of sigmoidal mathematical models describing population growth as a function of continuous time have been reported in the literature (*e.g.* Turner et al. (1976)). In light of empirical data, and among many equations in a large family of models related to Malthus' "law of geometric growth", it has been shown that the Gompertz equation emerges as one of the best models of the growth of population size as a function of time (see citations in Vereecken et al. (2000) and in Dennis and Ponciano (2014); Ferguson and Ponciano (2015)).

In bacterial growth research for instance, the Gompertz model has served as a golden reference to which models that account for various idiosyncratic phenomena of microbial cultures have been compared (Baranyi and Roberts, 1994). The solution of the Gompertz ODE model $dy_t/dt = \theta y_t[\log \kappa - \log y_t]$, where κ is the carrying capacity and θ is the speed of equilibration is given by $y_t = \kappa \exp\left(e^{-\theta t} \log(y_0/\kappa)\right)$, where y_0 is the initial population size. This solution has an inflection point at κ/e, provided y_0 is below the carrying capacity. The stochastic Gompertz diffusion written in SDE form is given by (Dennis and Ponciano, 2014)

$$dY_t = \theta Y_t[\log \kappa - \log Y_t]dt + \sqrt{\alpha Y_t + \beta^2 Y_t^2} dW_t. \tag{2}$$

The construction of this diffusion starts with a family of BP's $\left(Z_k^N\right)_{k=0,1,2,\ldots}$, indexed by some arbitrarily large population size N. The idea is then to accelerate time by N (*i.e.* so that N generations of the original process occur in one new unit of time) and scale the state by a factor $1/N$. Writing the scaled process as $Y_t^N \equiv \frac{1}{N} X^N([Nt])$, where $[Nt]$ is the smallest integer close to Nt, then our diffusion Y_t is defined as $\lim_{t\to\infty} Y_t^N$. Now, such approximation works provided

i) $\frac{1}{1/N}\mathrm{E}[Y^N_{t+\frac{1}{N}} - Y_t^N | Y_t^N = \frac{z}{N}] \to m(y)$,

ii) $\frac{1}{1/N}\mathrm{E}[(Y^N_{t+\frac{1}{N}} - Y_t^N)^2 | Y_t^N = \frac{z}{N}] \to \sigma^2(y)$,

iii) $\frac{1}{1/N}\mathrm{E}[(Y^N_{t+\frac{1}{N}} - Y_t^N)^4 | Y_t^N = \frac{z}{N}] \to 0$

as $N \to \infty$ and $z/N \to y$ (Karlin and Taylor, 1981), where $m(y)$ and $\sigma^2(y)$ are continuous functions of y. To obtain the diffusion approximation, the moments of the one-step differences in the unscaled process Z_k (dropping the superscript N for simplicity) are first computed. Then, the process' time unit and state are rescaled, and this allows the calculation of the infinitesimal moments and checking if the limits above (conditions ***i-iii***) hold. In the Appendix, I present as an example the steps leading to the construction of the stochastic Gompertz diffusion model with environmental and demographic stochasticity (eq. 2).

2.2 The Gompertz SDE and the OU process

Let Y_t be a Gompertz diffusion with environmental variability and no demographic stochasticity (Dennis and Ponciano, 2014). Then, its infinitesimal mean

and variance are given by $m_Y(y) = \theta y[\ln \kappa - \ln y]$ and $\sigma^2_Y(y) = \beta^2 y^2$ respectively. In SDE form we write

$$dY_t = \theta Y_t[\ln \kappa - \ln Y_t]dt + \beta Y_t dW_t. \tag{3}$$

Let $X_t = g(Y_t)$ be a smooth invertible transformation of Y_t. Then, it immediately follows that X_t is also a diffusion with infinitesimal mean and variance given by $m_X(x) = m_Y(y)g'(y) + \frac{1}{2}\sigma^2_Y(y)g''(y)$ and $\sigma^2_X(x) = \sigma^2_Y(y)\left[g'(y)\right]^2$ respectively (Karlin and Taylor, 1981), where $y = g^{-1}(x)$. In particular, setting $g(y) = \ln y$ yields $m_X(x) = \theta(\mu - x)$, where $\mu = \ln \kappa - \frac{\beta^2}{2\theta}$, and $\sigma^2(X)_x = \beta^2$. Thus, written in SDE form the diffusion X_t becomes

$$dX_t = \theta(\mu - X_t)dt + \beta dW_t, \tag{4}$$

which is a special OU process, one where the mean is a function of both, the strength of return to the mean, given by θ, and the scaling of the environmental variance of the original process. Conversely, if we start with the OU process defined in eq. 4 and transform it using $y = g(x) = e^x$, then we retrieve the Gompertz diffusion with environmental noise (eq. 3). These results suggest that Palacios and Minin (2013)'s transformation (eq. 1), when applied to an OU process, should result in a population growth diffusion under density-dependence and either environmental noise, demographic stochasticity or both. This Itô transformation is explored in the next section.

2.3 Palacios and Minin's prior on $N_e(t)$ as an SDE model

Let $n = g(x) = \frac{1}{\lambda} + \frac{1}{\lambda}\exp\{-x\}$, which is Palacios and Minin (2013)'s model for $N_e(t)$ as a function of a gaussian process. Then $g^{-1}(n) = \ln\left(\frac{1}{n\lambda - 1}\right)$ and applying an Itô transformation of the OU process in eq. 4 gives the infinitesimal mean and variance of the $N_e(t)$ process. The infinitesimal mean is

$$\begin{aligned} m_N &= m_X g'(x) + \frac{1}{2}\sigma^2_X(x)g''(x) \\ &= \theta\left(n - \frac{1}{\lambda}\right)\left(\ln\left(\frac{1}{\lambda n - 1}\right) - \mu + \frac{\beta^2}{2\theta}\right) \qquad (5) \\ &= \frac{\theta}{\lambda}\left(\ln\kappa - \ln(n\lambda - 1)\right)(n\lambda - 1). \qquad (6) \end{aligned}$$

This expression is readily recognized as a translated Gompertz growth equation, one where the state space n is defined so that $n\lambda - 1 > 0$. The solution of the

ODE $dn/dt = \frac{\theta}{\lambda}\left(\ln\kappa - \ln(n\lambda - 1)\right)(n\lambda - 1)$ is also readily found to be

$$n(t) = \frac{\kappa}{\lambda}\exp\left\{e^{-\theta t}\ln\left(\frac{n_0\lambda - 1}{\kappa}\right)\right\} + \frac{1}{\lambda}.$$

The infinitesimal variance of the resulting $N_e(t)$ diffusion is $\sigma^2_{N_e}(n) = \frac{\beta^2}{\lambda^2}(\lambda n - 1)^2$. Because the process is re-scaled to have a lower bound, then this form of the infinitesimal variance is immediately recognized as the variance of a diffusion model where the quantity $n\lambda - 1$ is growing as in the logistic model with added environmental variation (see Appendix 1). Thus, Palacios and Minin (2013)'s prior can be cast as a recognizable stochastic population dynamics model, one that bears specific biological hypotheses regarding population size trajectories and their associated structure of variability.

Besides having a direct connection with a continuous time stochastic, density dependent process, the OU process and its transformation according to eq. 1 has a direct connection with a class of discrete-time population dynamics models. This class of population trajectory models consists of discrete-time, density-dependent stochastic models, which Melbourne and Hastings (2008) and Ferguson and Ponciano (2014) show to be very flexible and accurately represent various biological systems. The connection between the OU and this class of models is possible because, as shown byDennis and Ponciano (2014), the OU process (eq. 4) has also a one-to-one transformation with the discrete-time, stochastic Gompertz model Dennis et al. (2006) with environmental variability, whose one-step changes are given by:

$$N_{t+1}|(N_t = n_t) = n_t\exp\left\{a + b\ln n_t + E_t\right\},$$

where $E_t \sim \mathrm{N}(0, \sigma^2)$. Setting $c = b + 1$ and $X = \ln N$, the transition probabilities of the log-transformed Gompertz process and of the OU process coincide by setting $a = \mu(1 - e^{-\theta}); c = e^{-\theta}; \sigma^2 = (1 - e^{-2\theta})\beta^2(2\theta); \mu = a/(1 - c)$ and $\beta^2 = -[2\sigma^2\ln c]/(1 - c^2)$. Although the connection with both, the continuous-time and the discrete-time ecological model is a rare and particular property of the Gompertz equation, it opens the door to the investigation of wether other, discrete-time ecological models can be suitably approximated by continuous processes. If carefully treated, the topic of finding equivalent, continuous-time stochastic models for these processes could lead to the construction of a biologically rich (and parametric) class of priors for $N_e(t)$. To exemplify this claim, in what follows we briefly outline two possible multivariate prior for a set of jointly varying $N_e(t)^{(i)}, i = 1, 2, \ldots, p$.

2.4 Two parametric multivariate priors

The results presented here also hint at the construction of multivariate GP-based priors for a set of jointly varying $N_e(t)^{(i)}, i = 1, 2, \ldots, p$ values for p gene populations. The stochastic Gompertz model with environmental stochasticity can readily be written in multivariate form to study the joint fluctuation of population abundances of a set of p species (Ives et al., 2003). According to this model, the set of effects of each population in each other's rate of change, or interaction coefficients, specified as the elements of the "interactions matrix" in Ives et al. (2003) formulation, determines the joint response and fluctuations of population trajectories in the face of environmental buffeting. Interestingly, this set of coefficients determines the strength of the variability of the fluctuations, the rate of approach to (multivariate) stationary behavior and the speed of return to stationarity following an external perturbation of population sizes. Ives et al. (2003) go as far as eliciting novel "stochastic stability" measures for multivariate time series of population trajectories. These stochastic stability measures and the corresponding multivariate prior for jointly fluctuating effective population sizes could find many applications in the study of joint gene genealogies.

The diffusion approximation of BPREs hinges on assuming individuals with *iid* offspring distributions. Here I show how accounting for individual dependencies results in a potentially useful multivariate prior. Starting with single population trajectories, suppose we use independent $\text{Poisson}(\lambda p_t)$ offspring distributions to formulate a discrete-time population process, where p_t is the density-dependent survival probability of newborns, which can take the forms

$$p_t \propto \begin{cases} e^{-bn_t} & \text{for the Ricker model,} \\ \exp\left\{-b\, n_t^{\theta}\right\} & \text{for the theta Ricker model,} \\ \exp\{-b \ln n_t\} & \text{for the Gompertz model,} \\ 1/(1 + b\, n_t)^c & \text{for the Hassell model,} \\ 1/(1 + (a-1)(n_t/K)^{\beta}) & \text{for the Below model.} \end{cases}$$

Thus, this Poisson model includes stochastic reproduction and density-dependent survival of potential recruits (Melbourne and Hastings, 2008; Ferguson and Ponciano, 2014). When environmental noise is added, the mean of these offspring distributions, λ, is assumed to be itself the outcome of a random, environmental process. If, for instance, the environmental process is modeled with a gamma distribution $\lambda \sim \text{Gamma}(k, \alpha)$, then integrating it over the joint Poisson offspring distributions gives the Negative-Binomial process Melbourne and Hastings

(2008):

$$P(N_{t+1} = n_{t+1}|N_t = n_t) = \frac{\Gamma(n_{t+1}+k)}{\Gamma(k)n_{t+1}!}\left(\frac{\alpha}{n_t p_t+\alpha}\right)^k\left(\frac{n_t p_t}{n_t p_t+\alpha}\right)^{n_{t+1}}.$$

This derivation, however, ignores the possibility of the environmental process creating a dependency in the demographic response, *i.e.*, in the offspring distributions. If, for instance, the environmental process is modeled with a gamma distribution, then integrating it over the joint Poisson offspring distributions $X_1, X_2 \ldots X_{n_t}$ gives the Multivariate Negative-Binomial process for the total number of surviving offspring from every individual. Letting the total number of individuals born and surviving for next generation being denoted by $N_{t+1} = \sum_{i=1}^{n_t} X_i$, the joint distribution of survivors is given by

$$\begin{aligned} P(X_1 = x_1, X_2 = x_2, \ldots, X_{n_t} = x_{n_t}) &= \int_0^\infty \prod_{i=1}^{n_t} \frac{e^{-\lambda p_t}(\lambda p_t)^{x_i}}{x_i!}\frac{\alpha^k}{\Gamma(k)}\lambda^{k-1}e^{-\alpha\lambda}d\lambda \\ &= \frac{n_{t+1}!}{x_1!x_2!\ldots x_{n_t}!}\frac{\Gamma(n_{t+1}+k)}{n_{t+1}!\Gamma(k)}\left(\frac{1}{n_t p_t+\alpha}\right)^{x_1} \\ &\ldots \left(\frac{1}{n_t p_t+\alpha}\right)^{x_{n_t}}\left(\frac{\alpha}{n_t p_t+\alpha}\right)^k. \end{aligned} \tag{7}$$

which has a well-defined covariance structure and is also known as the sum symmetric power series distribution (Sibuya et al., 1964). This distribution is also known as the negative multinomial distribution. To the best of my knowledge, this non-independent population dynamics model has never been elicited nor used. This model is a probabilistic account for the rate of change of the total size of a population that accounts for demographic variability, environmental noise and a covariance structure among the elements (individuals) composing the population. As a consequence, the transitional mean and variance of total population size process is radically different from the model assuming independence among individuals. In the context of gene genealogies, this multivariate model could then be used to elicit priors for $N_e(t)$ that specify a structure in its total variability that reflects dependencies among its components.

3 Discussion

In this note I show that Palacios and Minin (2013)'s prior for $N_e(t)$, when obtained as a transformation of an OU process, belongs to a class of well-known stochastic

population dynamics models and as such, is well rooted in a family of ecological parametric models. In ecology, the different variance scalings brought about by either type of stochasticity have enabled the separation of the contribution of environmental and demographic processes to the rate of change of the population size. If we adopt the cautious interpretation of the effective population size as a measure of the relative genetic diversity (see Palacios and Minin (2013)), then using the population dynamics SDE models presented here would allow the specification of different hypotheses regarding the nature of the variance components of the rate of change of genetic diversity.

Palacios and Minin (2013)'s prior is indeed general because any GP, Markovian or not, can be substituted in their transformation. Thus, the nonparametric labeling of the inference they propose remains valid as well as generally applicable. However, without prior information or guidance as to what constitutes a good candidate GP, practitioners are left with a plethora of possibilities. One possibility is however, to posit as priors for $N_e(t)$ an array of models exhibiting all different combinations of the type of density dependence and structure of variability in its growth rate (demographic, environmental or both).

Besides opening the door to new, obvious candidate priors (like the flexible theta-logistic model with both environmental and demographic variabilities), the results presented here also suggest novel approaches with applications in both, gene genealogies inference and stochastic population dynamics modeling in ecology. The derivation in the appendix evidences two key assumptions that have been long forgotten (but see Engen et al. (1998)): first, that environmental variability is assumed to affect only the mean of the offspring distribution in the original BP, but not the variance and second, that the individual's offspring distribution are independent among themselves. Relaxing these two assumptions may lead to novel, meaningful population trajectories models that could be applicable both in population genetics as well as in population dynamics and conservation biology (Ferguson and Ponciano, 2014).

The work presented here also reveals a first-principles justification of using the OU process to model the evolution of a quantitative trait. This process has been extensively used to model the evolution of a quantitative trait, or as it is often the case, the *logarithm* of a quantitative trait Butler and King (2004); Pennell and Harmon (2013). Considerable amount of work is devoted to improve and expand this model capabilities with phenomenological modifications to the original process (*e.g* Beaulieu et al. (2012)), and aiming to understand its benefits and limitations. It is in that respect that the connection presented here between Palacios and Minin (2013)'s transformation of the OU process and stochastic population

dynamics brings novel understanding into the evolution of a quantitative trait: because exponentiating an OU process results in a stochastic Gompertz model with environmental variability and no demographic stochasticity, by modeling the logarithm of a trait with the OU process, a biologist is in fact hypothesizing that the trait, in its original scale grows over evolutionary time in a Gompertz-like manner (*i.e.*, 'size-dependent') and with a random, epochal rate of change. Furthermore, by excluding demographic stochasticity this model is stating that the total trait size is composed of equal, non-random partitions. Including 'demographic' stochasticity would amount to hypothesizing that the trait is composed by a sum of random, unequal contributions at any point in time.

The Itô transformation of the stochastic Gompertz model with environmental noise also reveals why it is difficult to tease apart the parameter estimates θ, μ, β^2 of the OU process, when used in contexts like modeling the evolution of a trait (Ané et al., 2014). The parameter μ in eq. 4 is in fact, itself a function of the other two parameters and the carrying capacity κ of the process in its original scale. If what is being modeled is the logarithm of a quantitative trait, then the carrying capacity denotes a limiting size or constraint of the value of the trait. In fact, thinking of the branching process formulation, and because the model has no demographic stochasticity, this model is implicitly hypothesizing that a trait as a whole is conformed by the sum of individual contributions that are identical in size, and eventually converge to a given biological constrained size. A model for the evolution of a trait that includes both, the analogous of demographic stochasticity and environmental noise is thus, easily conceivable as a reasonable alternative to the OU process. Other forms of 'density-dependence' besides Gompertz can be considered too.

Finally, it could be argued that simple logistic-type models are themselves phenomenological descriptions of population growth dynamics, and thus that, the SDE Gompertz model with environmental noise that results from the transformation (eq. 1) is itself phenomenological and hence, non-parametric. However, a full body of research in mathematical biosciences exists illustrating "first-principles" derivations of logistic-type models (see for instance Vellekoop and Högnäs (1997)).

3.1 Concluding remarks:

Using well-known concepts of stochastic population dynamics, here I demonstrate that in fact, Palacios and Minin's GP model is a special case of a population growth model with density dependence and environmental noise. One of the main

advantages of the Bayesian approach is the ability to include meaningful *a priori* information to conduct inference. However, eliciting priors is by far one of the most challenging problems that practitioners in population genetics and ecology face. It is in that sense that I hope that the parametric interpretation brought about by this contribution proves to be a useful, constructive critique. Finally, although the OU process has been shown to be insufficient and a current need of new parametric models has been expressed (Pennell and Harmon, 2013), its connection with stochastic, logistic-like growth pointed in this note opens the door to a plethora of other models for the evolution of a trait. Thus, Palacios and Minin (2013)'s transformation has deep implications for the advancement of other areas of modeling in evolution.

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A

A.1 Diffusion approximation of an ecological density-dependent branching process in random environments

Let Z_k be the total pop. size at time k and B_i be the (density-dependent) offspring distribution such that $p_j(z) = P(B_i = j|Z_k = z)$. According to the standard definition of a branching process, we let the population size in generation $n+1$ be given by $Z_{k+1} = \sum_{i=1}^{Z_k} B_i$. Let also denote the conditional mean and variance of the offspring distribution as $E[B_i|Z_k = z] = h(z)$ and $V[B_i|Z_k = z] = v(z)$ respectively. The idea behind the diffusion approximation is to scale both, the process by some reference population size and then time. Once both, the process and the original time unit have been re-scaled, in order for the diffusion approximation to hold, the first and second moment of a small increment in the process have to converge to continuous functions of the scaled process and the new time scale (see Karlin and Taylor (1981) eqs. 1.2 and 1.3 page 159 and eqs. 1.21 and 1.22 page 169). These two continuous functions are then the infinitesimal mean and variance of the diffusion process. The first and second moment of a one-step change in population size for the branching process above is given by:

$$\begin{aligned} E[\Delta Z_k|Z_k = z] &= E[(Z_{k+1} - Z_k)|Z_k = z] = E[\sum_{i=1}^{z}(B_i|Z_k = z)] - z = z[h(z) - 1], \\ E[(\Delta Z_k)^2|Z_k = z] &= E[(Z_{k+1} - Z_k)^2|Z_k = z] = Var\left[\left(\sum_{i=1}^{z}(B_i|Z_k = z)\right) - z\right] \\ &\quad + \left\{E\left[\left(\sum_{i=1}^{z}(B_i|Z_k = z)\right) - z\right]\right\}^2 = zv(z) + \{z(h(z) - 1)\}^2. \end{aligned} \tag{8}$$

Once these moments are computed, we accelerate time by N (*i.e.* so that N generations of the original process occur in one new unit of time) and scale the state by a factor $1/N$. Recall that the scaled process is denoted as $Y_t^N \equiv \frac{1}{N}X^N([Nt])$, where $[Nt]$ is the smallest integer close to Nt. With the process re-scaled, in order to find the infinitesimal mean and variance of the approximating diffusion, if it exists, we compute the infinitesimal moments and limits presented as conditions ***i-iii*** in the main text. For the first condition we get that

$$\begin{aligned} \frac{1}{1/N}\mathrm{E}\left[Y^N_{t+\frac{1}{N}} - Y^N_t|Y^N_t = \frac{z}{N}\right] &= \frac{1}{1/N}\mathrm{E}\left[\frac{Z([Nt]+1)}{N} - \frac{Z([Nt])}{N}\Big|\frac{Z([Nt])}{N} = \frac{z}{N}\right] \\ &= \frac{N}{N}\mathrm{E}\left[Z([Nt]+1) - Z([Nt])\Big|\frac{Z([Nt])}{N} = \frac{z}{N}\right] \\ &= N \times \frac{z}{N}(h(z) - 1). \end{aligned} \tag{9}$$

Keiding (1975); Ludwig (1976); Tier and Hanson (1981) all require that small changes in the scaled process occur in small time increments (*i.e.* that the offspring mean is close to replacement) because they set $h(z) = 1 + \frac{1}{N}\mu\left(\frac{z}{N}\right)$. Thus, the deviations from perfect replacement are of the order $\frac{1}{N}$. Their function $\mu(x)$, on the other hand, takes the form of the per capita growth rate given by any deterministic, single species ODE model with density dependence. Assume, for instance, that population growth conforms to the Gompertz equation shown in the main text. Then $\mu(x) = \theta x[\log\kappa - \log x]$. Substituting this expression for the rescaled offspring mean in eq. 9 and simplifying we get that $\frac{1}{1/N}\mathrm{E}\left[Y^N_{t+\frac{1}{N}} - Y^N_t \middle| Y^N_t = \frac{z}{N}\right] = \frac{z}{N}\mu\left(\frac{z}{N}\right) \to y\mu(y) = m(y)$ as $N \to \infty$ and $z/N \to y$. Thus, re-scaled first difference moments converge to a continuous function of y, the infinitesimal mean $m(y)$ of the diffusion. Under the hypotheses imposed by the form of $h(z)$, the infinitesimal mean of the diffusion can be made equal to the deterministic trend of any single species ODE model. This fact opens the door to the possibility of specifying a wide array of biological hypotheses in the form of logistic-like population growth. The second condition becomes

$$\begin{aligned}
\frac{1}{1/N}\mathrm{E}\left[\left(Y^N_{t+\frac{1}{N}} - Y^N_t\right)^2 | Y^N_t = \frac{z}{N}\right] &= \frac{1}{1/N}\mathrm{E}\left[\left(\frac{Z([Nt]+1) - Z([Nt])}{N}\right)^2 \middle| \frac{Z([Nt])}{N} = \frac{z}{N}\right] \\
&= N \times \frac{1}{N^2}\left(zv(z) + (z(h(z)-1))^2\right) \\
&= \frac{z}{N}v(z) + \frac{1}{N}\left(\frac{z}{n}\mu\left(\frac{z}{N}\right)\right)^2, \qquad (10)
\end{aligned}$$

which converges to $yd(y)$ as $N \to \infty$ and $z/N \to y$, where following Keiding (1975); Ludwig (1976) and Tier and Hanson (1981) we denote $v(z)$ with the unspecified function of the scaled process, $d(\frac{z}{N})$. Thus, the infinitesimal variance of the diffusion is $\sigma^2(y) = yd(y)$. Therefore, both the first and the second moment converge to finite functions of y and t. The simplest assumption regarding the general function $d(y)$ is to make it equal to a constant, say $\alpha > 0$, which we will adopt in what follows for simplicity. Lipow (1977) formally proved the convergence to a diffusion of a BP so defined. Then, the infinitesimal variance will be written as $y\alpha$. Besides these two conditions, it is necessary for higher order moments to be negligible, *i.e.* that

$$\lim_{\frac{1}{N}\to 0} \frac{1}{1/N} E[\left(Y^N_{t+\frac{1}{N}} - Y^N_t\right)^j | Y_t = x] = O[(1/N)^{j/2-1}],\ j > 2,$$

which has been done formally elsewhere Keiding (1975); Ludwig (1976); Lipow (1977). Adding environmental stochasticity amounts to adding random fluctuations to the mean of the offspring distribution. Operationally, this is achieved by

adding an iid process denoting random environmental fluctuations at time k. We denote this process with W_k, and let $E(W_k) = 0$ and $V(W_k) = 1$, and assume that the W_k are independent from the Z_m, $m < k$. Then, the probabilities of the offspring distribution are defined as

$$p_j(z, w) = P(B_i = j | Z_k = z, W_k = w).$$

Again, $h(z, w)$ and $v(z, w)$ are the conditional mean and variance of the offspring distribution. To get the marginal mean and variance, using conditional expectation we average the mean and the variance of the offspring distribution over the environmental process. For the variance, authors to date have writen $E[v|Z_k = z] = E[E[v|Z_k = z, W_k]] = d\left(\frac{z}{N}\right)$. This is the expected value of the variance of the offspring distribution over the environmental process. This is then, by definition, the average demographic variance. As for the mean, adding the environmental fluctuation results in its conditional form being written as $h(z, w) = 1 + \frac{1}{N}\mu\left(\frac{z}{N}\right) + \sqrt{\frac{1}{N}e\left(\frac{z}{N}\right)}w$, where the fluctuations due to the environment are of order $\sqrt{\frac{1}{N}}$ (a sum of a large number of iid random variables) and $e(.)$ is a general function of the scaled process. As with the function $d(.)$ above, the simplest assumption is to set $e(z/N)$ equal to a constant, say β^2 . Authors that have adopted such assumptions, like Tier and Hanson (1981) have therefore implicitly stated that only the mean of the offspring distribution is affected by the environmental process. This assumption, however, has been recently questioned (see Ferguson and Ponciano (2015) and citations therein). The diffusion approximation of a BPRE has then been found by computing the infinitesimal mean and variance of the re-scaled process as in eqs. 9 and 10. For the first moment, and averaging over the environmental process we get that:

$$\frac{1}{1/N}\mathrm{E}\left\{\mathrm{E}\left[Y^N_{t+\frac{1}{N}} - Y^N_t \middle| Y^N_t = \frac{z}{N}, W_t\right]\right\} = NE\left[\frac{z}{N}(h(z) - 1)\right] = \frac{z}{N}\mu\left(\frac{z}{N}\right) \to y\mu(y) = m(y), \tag{11}$$

whereas for the second moment

$$\begin{aligned}\frac{1}{1/N}\mathrm{E}\left\{\mathrm{E}\left[\left(Y^N_{t+\frac{1}{N}} - Y^N_t\right)^2 \middle| Y^N_t = \frac{z}{N}, W_t\right]\right\} &= N\frac{1}{N^2}E\left[zv(z) + (z(h(z) - 1))^2\right] \\ &= \frac{z}{N}v(z) + \left(\frac{z}{N}\right)^2 e\left(\frac{z}{N}\right) \to yd(y) + y^2e(y).\end{aligned} \tag{12}$$

For simplicity, we assume that the functions $d(x)$ and $e(x)$ are constants equal to α and β^2 respectively. Note that in the equation for the environmental variance, $y\alpha$ is the expected value of the variance of the offspring distribution: this term specifies

on average, how much does the offspring distribution varies. The term $y^2\beta^2$ in turn represents the variance of the expected value of the offspring distribution: it quantifies how much does the mean of the offspring distribution changes over time.