Putting life history theory to the test - the estimation of reproductive values from field data

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Abstract

Quantifying fitness is important to understand adaptive evolution. Reproductive values are useful for making fitness comparisons involving different categories of individuals, like males and females. By definition, the reproductive value of a category is the expected *per capita* contribution of the members of that category to the gene pool of future generations. Life history theory reveals how reproductive values can be determined from life-history parameters, but this requires matrix algebra. Recently, a more intuitive, pedigree-based method has become popular. It estimates genetic contributions of individuals to future generations by tracking their descendants. Here we compare both methods. We implement various life-history scenarios (for which the "true" reproductive values can be calculated) in individual-based simulations, use this data to estimate reproductive values with both methods, and compare the results with the true reproductive values. We show that the pedigree-based estimation of reproductive values is either systematically biased (and hence inaccurate), or very imprecise. This holds even for simple life histories and under idealized conditions. The traditional algebraic method estimates reproductive values with accuracy, and the precision of estimates can be determined by sensitivity analyses. However, these estimates can be biased as well when they are based on inadequate life-history models.

Keywords

Class-structured population, fitness in a life history context, life-history model, pedigree-based reproductive value

Introduction

Quantifying fitness is important to understand how natural selection affects evolution. Estimating fitness in the wild is, however, a difficult task. Studies often measure survival, recruitment rate or number of hatchlings as a proxy for fitness. In some well-monitored populations, lifetime reproductive success can be determined. Expected lifetime reproductive success is often a good proxy for fitness (Brommer et al., 2004), but even this measure is incomplete as it does not account for the rate of reproduction and the fact that different types of offspring (e.g. females and males; different size classes) can be produced.

A fitness measure that does include all components of fitness is reproductive value (Fisher, 1930), which is defined as the expected contribution to the future gene pool of an individual of a certain class (Grafen, 2006). Reproductive value is influenced by all kinds of life-history decisions, like age at first reproduction, trade-offs between survival and fecundity, risk-taking behaviour, or the kind of offspring produced (e.g. sons or daughters). Reproductive values are a particularly useful tool in behavioural ecology, as they allow the evolutionary costs and benefits of fitness-relevant individual decisions to be quantified. For example, Tinbergen and Daan (1990) used an RV approach to predict the optimal clutch size in passerine birds on the basis of the trade-off between current and future reproduction. Reproductive values also play an important role in predicting the optimal sex ratio (Pen and Weissing, 2002).

While the definition of reproductive value is straightforward, its measurement is not. As briefly reviewed below, RVs can be derived from a life-history model by solving an eigenvector equation that contains all relevant life-history parameters (Caswell 1982). In line with this, most applications of RVs in empirical systems first estimate life-history parameters and subsequently obtain RVs by inserting these parameters in the eigenvector equation (Leverich and Levin, 1979; Schulman and Chapais, 1980; Tinbergen and Daan, 1990; Newton and Rothery, 1997; Pen et al., 1999; Bonduriansky and Brassil, 2002; van de Pol et al., 2007; Bouwhuis et al., 2012). Hereafter, we will call the RVs thus obtained “model-based reproductive values” (mRV). Obtaining a good estimate of reproductive values along these lines can, however, be difficult in natural systems, since it requires a good understanding of all relevant life-history transitions and because life-history parameters can often only be estimated with limited accuracy and precision.

Recently, reproductive values have been estimated with a more intuitive method, based on genetic pedigree data (Barton and Etheridge, 2011; Chen et al., 2019; Hunter et al., 2019; Reid et al., 2019). In this method, the average *per capita* number of descendants of the members of a certain class of individuals is used as an estimate of the reproductive value of that class. Hereafter, we will call the RVs thus obtained

"pedigree-based reproductive values" (pRV). The pRV method closely reflects Fisher's definition of reproductive value. This method requires the availability of sufficiently deep and complete pedigrees, but if such pedigrees are available it has the big advantage that no detailed knowledge of life-history transitions or estimates of life-history parameters are required. Therefore, the pRV method could potentially be a great substitute for the mRV method. However, whether the pRV method matches the mRV method in accuracy and precision when applied to field data has yet to be determined.

In this theoretical study, we will test the performance of both methods when applied to organisms with a relatively simple life history. To this end, we use individual-based simulations to produce several generations of individuals on the basis of a life-history model. The simulation data can be used to construct a pedigree (complete or incomplete) and to estimate life-history data such as survival probabilities and fecundities. Subsequently, reproductive values can be estimated by both methods (mRV and pRV) and compared with the "true" reproductive values (which are well-defined for the simulated populations). This allows us to judge the accuracy and precision of both estimates and to address questions like: how deep and complete must a pedigree be in order to get a reliable pRV estimate? How well must the life-history model be known, and how well do we need to know the life-history parameters in order to get reliable mRV estimates?

Before approaching the estimation problem, we first give some theoretical background by briefly reviewing some basal insights of life history theory.

Theoretical considerations: why are reproductive values useful?

In a population with discrete, non-overlapping generations and only one type of individual (e.g. no sex differences), expected lifetime reproductive success (ELRS) is an adequate fitness measure, as alleles that enhance the lifetime reproductive output of their bearers have a selective advantage. The situation is different in populations with different classes of individuals (e.g. females and males; breeders and helpers; workers, soldiers and reproductives). In such cases, alleles inducing their bearers to produce a maximal number of offspring throughout their lifetime are not necessarily favoured. The reason is that different types of offspring may differ in the efficiency with which they spread genes to future generations. For example, in a population with a 4:1 female-biased sex ratio (4 females per male), the reproductive success per male is on average four times greater than the reproductive success per female (because each offspring has one mother and one father). Therefore, an allele inducing the lifetime production of two sons has a lower ELRS than an allele inducing the lifetime production of four daughters, but a higher

"fitness": it spreads more efficiently to future generations, as the expected reproductive success of two sons is twice the expected reproductive success of four daughters (for the given sex ratio). Similarly, adding up potential offspring does not result in a suitable fitness measure when generations are overlapping, and different age classes coexist. In this situation, the timing of reproduction matters: for example, it may be advantageous to produce offspring as early in life as possible (even if this leads to a lower lifetime production of offspring), as early-born offspring can more quickly contribute to the spread of their parental genes.

Quantifying fitness in a life-history context (i.e., in a population with different categories of individuals) is therefore not an easy task. Fortunately, life-history theory is a well-developed branch of evolutionary biology (Roff, 1992; Stearns, 1992; Caswell, 2001), and various fitness concepts are available (Brommer, 2000). A typical life-history model starts with a life-cycle graph (see figure 1 for examples) that includes all life history "stages" (e.g. all age classes) and the transitions between these stages (e.g. survival to the next age class; production of offspring). If the number of stages is finite, this graph can be translated into a "stage transition matrix" which in the case of three stages looks like this:

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \qquad (1)$$

Matrix element a_{ij} is the *per capita* contribution of a member of stage *j* to the number of individuals in stage *i* in the next time step. For example, the stage transition matrix of an age-structured population with three age classes has the special form of a "Leslie matrix":

$$\mathbf{A} = \begin{pmatrix} F_1 & F_2 & F_3 \\ P_1 & 0 & 0 \\ 0 & P_2 & 0 \end{pmatrix}. \qquad (2)$$

Here, P_1 is the probability to survive from age class 1 to age class 2, P_2 is the probability to survive from age 2 to age 3, and F_1, F_2, and F_3 is the expected number of surviving offspring (surviving till age class 1) produced per individual of the respective age class.

Life-history matrices are a very useful tool, as they determine the dynamics of a stage-structured population (Stearns, 1992). In most cases, such a population will converge to a "stable stage distribution" (in the case of an age-structured population: a stable age distribution; in the case of a population with two sexes: a stable sex ratio), that is, to a state where the ratio between the number of individuals in the

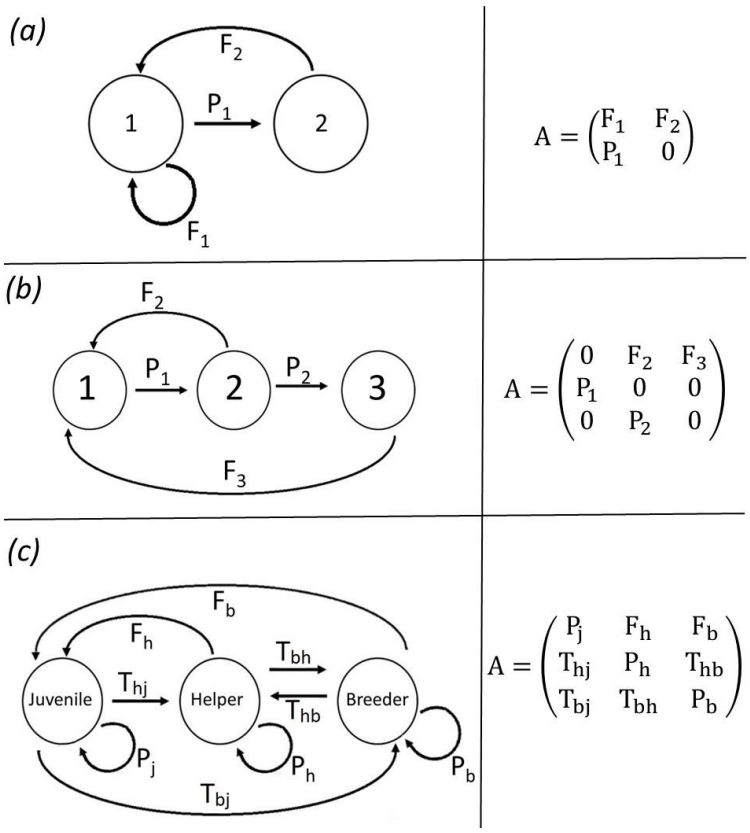

Figure 1. Life cycle graphs and matrices used in our simulations. (a) A two-stage life cycle with two age classes. One-year-old individuals survive to their second year with probability P_1, second-year-old individuals die after reproduction. F_1 and F_2 denote the expected number of offspring (surviving to their first year) produced by one- and two-year-old individuals, respectively. **(b)** A three-stage life cycle with three age classes. Only two- and three-year-old individuals can reproduce (with expected fecundity F_2 and F_3), and one- and two-year-old individuals survive to their next year with probabilities P_1 and P_2, respectively. **(c)** A three-stage life cycle with behavioural stages. A juvenile can either stay juvenile for another time unit (probability P_j), promote to helper status (probability T_{hj}), promote to breeder status (probability T_{bj}), or die. A helper can either stay a helper for another time unit (probability P_h), promote to breeder status (probability T_{bh}), or die. A breeder can stay a breeder (probability P_b) or die. Both helpers and breeders can reproduce with expected fecundity (number of offspring surviving to juvenile stage) F_h and F_b, respectively.

stages ($n_1 : n_2 : n_3$) does not change anymore. Once the stable stage distribution is reached, the population as a whole grows with a characteristic "population growth factor λ". When λ=1, the population size will stay constant over time, while the population size will increase exponentially when λ>1, and decrease exponentially when λ<1.

The population growth factor λ is the most fundamental fitness measure in a stage-structured population (Brommer, 2000): if we consider a population with transition matrix **A** and corresponding λ, a mutant

inducing a slightly different transition matrix $\mathbf{A_m}$ with growth factor λ_m can be expected to successfully invade the population if $\lambda_m > \lambda$, while mutants with $\lambda_m < \lambda$ will go extinct. Mathematically, λ is the "dominant eigenvalue" of the stage-transition matrix **A**, and there are recipes to calculate λ for a given matrix **A**. Unfortunately, the eigenvalue equation determining λ is an "implicit" equation (in case of an age-structured population the so-called "Euler-Lotka equation" (Otto and Day, 2007)), which even for simple life histories can only be solved numerically and does not provide much insight into the factors governing evolution. It is therefore useful to look out for an alternative fitness measure.

At this point reproductive values come into play. Conceptually, the "reproductive value" v_i of a stage *i* is the expected genetic contribution of a member of stage *i* to the gene pool of future generations (Grafen, 2006). Mathematically, the vector $\mathbf{v}^T = (v_1, v_2, v_3)$ of reproductive values satisfies the equation $\mathbf{v}^T \cdot \mathbf{A} = \lambda \cdot \mathbf{v}^T$, which means that it is a "left eigenvector" with respect to the dominant eigenvalue λ. Reproductive values have many useful properties (e.g., Taylor & Frank, 1996; Brommer, 2000; Pen & Weissing, 2000b, 2002; Otto & Day 2007). Take, for example, an age-structured population, where the matrix **A** is given by eqn (2). If we focus on a stationary population ($\lambda = 1$), the eigenvector equation $\mathbf{v}^T \cdot \mathbf{L} = \lambda \cdot \mathbf{v}^T$ is actually a set of three equations (one per age class):

$$v_i = F_i v_1 + P_i v_{i+1}. \qquad (3)$$

This equation has a clear-cut interpretation. An individual of age *i* contributes genes to the next time step in two ways, by producing offspring and by survival. On average, it generates $F_i v_1$ units of reproductive value via reproduction (the expected number of offspring F_i multiplied by the reproductive value v_1 of each of these offspring) and $P_i v_{i+1}$ units via its own survival (the survival probability P_i multiplied by the reproductive value v_{i+1} of this individual if it happens to survive to the next age class *i*+1). In case of a non-stationary population, the contribution $F_i v_1 + P_i v_{i+1}$ to the next time step has to be divided by the population growth factor λ (Otto & Day 2007), in order to ensure that reproductive values represent the *relative* contribution of a given type of individuals to the gene pool of future generations.

Why is an equation like this useful? Assume that we want to know whether selection will favour the production of *b* additional offspring at age *i*, when this 'benefit' is associated with a 'cost' *c* in terms of reduced parental survival. Since natural selection will maximize the reproductive value of each age class (Schaffer, 1974), eqn (3) tells us that the benefits will outweigh the costs if

$$(F_i + b)v_1 + (P_i - c)v_{i+1} > F_i v_1 + P_i v_{i+1} \qquad (4)$$

(see Taylor & Frank, 1996; Pen & Weissing, 2000c; or Otto & Day, 2007 for a formal justification). This inequality can be rewritten as:

$$b/c > v_{i+1}/v_1 \,. \qquad (5)$$

Hence, for a given benefit-cost ratio those age classes should be more inclined to take the survival risk if their future fitness expectation v_{i+1} is relatively small. In other words, only those age classes that have 'not much to lose' should take the risk (see Wolf et al., 2007 for various implications of this 'asset protection principle').

As illustrated by these calculations, reproductive values are extremely useful tools in translating intricate fitness considerations into transparent cost-benefit comparisons (see Pen & Weissing 2000a, 2000b, 2002 for other examples). Cost-benefit considerations are further simplified by the fact that reproductive values are *relative* attributes that are only determined up to a constant factor. This implies that they can be normalized in the most convenient manner, for example by equating one of the reproductive values to one (e.g. $v_1 = 1$, which would simplify eqn (5)) or by equating the sum of all reproductive values to one.

Finally, we would like to remark that classical life history theory is ecologically not consistent, in that its models predict exponential growth (when $\lambda>1$) or exponentially decline (when $\lambda<1$) in populations. To cope with this problem, density dependence needs to be incorporated into a life history model. It is important to realize that this has to be done in an explicit manner, as the form of density dependence can have major implications for the course and outcome of evolution (Mylius and Diekman, 1995; Pen and Weissing, 2000b). Below we show how to introduce various forms of density dependence in the models. Rather than complicating the models, this actually simplifies calculations, as the inclusion of density dependence has two benefits: (a) it allows the assumption that $\lambda=1$ at ecological equilibrium and (b) it reduces the dimensionality of the parameter space (thus making it easier to classify the evolutionary outcomes).

Methods

Simulations for the pedigree-based estimation of reproductive values

All individual-based simulations were based on a specific life-history scenario, as in figure 1. Time proceeds in discrete steps, where one time step corresponds to a reproductive season. During a time step *t*, each individual is in a certain state (either an age class or a breeding state), which can change from one time step to the next. Reproduction takes place at the start of each time step. If, according to the life history scenario, F_X is the expected fecundity in state X, each individual of that stage produces *f* offspring, where *f* is drawn from a Poisson distribution with mean F_X. Offspring enter the population at time *t*+1, and they belong to age class 1 in the age-based scenarios and to the juvenile state in the breeder-helper scenario. After reproduction, all individuals present at time *t* change their state stochastically (including death and staying in the same state), according to the probability assigned to their state by the life-history model. Each simulation was repeated for a fixed number of time steps *T* (typically *T*=20). For each life-history scenario, simulations were run for various parameter combinations, and in each case the simulations were repeated at least 100 times. To ensure that our results were not biased by start-up effects, we initialized all populations in demographic equilibrium.

We used a "gene-dropping" approach (MacCluer et al., 1986) to estimate pRVs. At the start of the simulation (*t*=0), every individual is endowed with a unique marker (corresponding to a unique allele at a locus with infinite alleles). At each reproduction event, the offspring inherit their marker from their parent. This allowed us to identify the descendants of each individual of the initial population in all future time steps. For each life history state *X* and each time *t*, we determined the average *per capita* number of descendants at time *t* for those individuals in the initial population that started in state *X*. We interpret this number, $pRV_X(t)$, as the pedigree-based estimate of the RV of individuals in state *X*: according to the definition of RV ("*per capita* contribution to the gene pool of future generations") $pRV_X(t)$ should, for large *t*, approximate the "true" reproductive value of state *X*. We then normalize all reproductive values so that the RV of the "first" state (age class 1 in the age-structured scenarios; juvenile state in the helper-breeder scenario) is scaled to 1. To achieve this, the values $pRV_X(t)$ were divided by $pRV_1(t)$, the estimated reproductive value of the first state. For simplicity, we assumed that marker inheritance is based on asexual reproduction. In Appendix B we show that, for the same life-history scenarios, identical results are obtained if the marker is inherited from parents to offspring in a randomly mating sexual population of diploid individuals.

To prevent exponential growth or exponential decline of the simulated populations, we made the reasonable assumption that population sizes are kept in check by density dependent processes. In the fixed-parameter scenarios 1 to 3, this was done by choosing the life-history parameters in such a way that the resulting population is expected to be stationary (λ=1; see above). In scenario 4, where the life-history parameters are fluctuating in time, it was more complex to set the parameters correctly to satisfy λ=1, therefore we added density regulation more directly by assuming that the survival probability from age 1 to age 2 is density dependent:

$$P_1 = P_1(N) = \frac{1}{1+\alpha N}, \qquad (6)$$

where *N* is population size and α indicates the intensity of density dependence. We also used this method in scenario 1 for some simulations, to compare if both methods of density regulation resulted in similar pRV estimates. To ensure that the simulated populations did indeed start in demographic equilibrium when density regulations were added as in eqn. (6), we first let each simulation run for 100 time steps (from t=-100 until t=-1) before gene dropping was initiated (at t=0). Unless indicated otherwise, we chose the initial population size (scenarios 1 to 3) or the parameter α in such a way that the population size of the resulting stationary population was N=1,000. Note that this means that about 1,000 individuals are present at every time step. If the life expectancy per individual is about two time units (a typical value in scenarios 1 and 4), a pedigree with a time horizon of 20 time steps therefore encompasses about 10,000 individuals.

Four scenarios

<u>Scenario 1 – A population with two age classes.</u> This simple scenario, with only two life-history states and three life-history parameters, is characterized by Figure 1(a). Both one- and two-year-old individuals can reproduce (with fecundity F_1 and F_2). One-year-old individuals survive to their second year with probability P_1; all individuals die after their second year. A simple calculation reveals that a stationary population (λ=1) is only achieved if the life-history parameters satisfy the requirement:

$$F_1 + P_1 \cdot F_2 = 1. \qquad (7a)$$

In this case, the "true" reproductive values are given by:

$$v_1 = 1,\ v_2 = F_2. \qquad (7b)$$

Both equations make intuitive sense. The left-hand side of (7a) corresponds to the expected lifetime production of surviving offspring, which needs to be 1 in a stationary population. Eqn (7b) may be viewed as a special case of eqn (3): the RV of a two-year-old is equal to its fecundity, as the *future* RV of a two-year-old is zero in this scenario.

Condition (7a) for "ecological consistency" will not be satisfied for arbitrary values of the life-history parameters. However It will be satisfied if we assume that (some of) these parameters decline with population density, thus enforcing condition (7a) at population dynamic equilibrium. Here, we considered two ways of enforcing a stationary population: by choosing two of the three life-history parameters (e.g. F_1 and F_2) and (i) determining the third parameter (P_1) in such a way that eqn (7a) is met; or (ii) by making the third parameter density dependent (as described in eqn (6)), which eventually will also result in a stationary population.

<u>Scenario 2 – A population with three age classes.</u> This scenario, with three life-history states and four life-history parameters, is described in Figure 1(b). Two- and three-year-old individuals can reproduce (with fecundity F_2 and F_3). One- and two-year-old individuals can survive to their next year (with probabilities P_1 and P_2); all individuals die after their third year. Now the condition for a stationary population and the reproductive values are given by:

$$P_1 \cdot F_2 + P_1 \cdot P_2 \cdot F_2 = 1 . \qquad (8a)$$

$$v_1 = 1,\ v_2 = F_2 + P_2 F_3,\ v_3 = F_3 . \qquad (8b)$$

Ecological consistency (a stationary population) was ensured by either of the two methods described in Scenario 1.

<u>Scenario 3 – A population with three behavioural classes.</u> This scenario, which is characterized in Figure 1(c), includes three life-history states (juveniles, helpers, breeders) and a full set of nine life-history parameters. All newly produced individuals start as juveniles. A juvenile either stays in juvenile state for another time period (with probability P_j), or it becomes a helper (with probability T_{hj}) or a breeder (with probability T_{bj}), or it dies (with probability $1 - P_j - T_{hj} - T_{bj}$). Likewise, a helper either stays in the helper state for another period (probability P_h), or it becomes a breeder (probability T_{bh}), or it dies. A breeder either stays in the breeding state for another time step (probability P_b), or it loses its position and becomes a helper (probability T_{hb}.), or it dies. Helpers and breeders can both produce offspring (fecundities F_h and

F_b per timestep). As before, the condition for a stationary population and the reproductive values can be calculated, but as the equations inspire little insight they are not given here.

Scenario 4 – A population with two age classes in a temporarily changing environment. This is identical to Scenario 1, but now the fecundities F_1 and F_2 change systematically in time. To this end, we think of a population in a seasonal environment, having three breeding periods (= time steps) per year. To be more specific, the fecundity of two-year-olds oscillates around $\overline{F}_2$, returning to the same pattern after three time steps:

$$F_2(t) = \overline{F}_2 + \sin(\tfrac{2}{3}\pi t)\,. \qquad (9)$$

The fecundity F_1 of one-year-olds oscillates in parallel with F_2: $F_1(t) = \frac{1}{3} \cdot F_2(t)$. The survival probability P_1 of one-year-olds is density dependent and given by eqn (6).

When the environment fluctuates, the different periods interact with each other. For example, if at time step 1 many one-year-old individuals are produced and at time step 2 the then two- year-old individuals reproduce a lot, the population will increase vastly, even if at time step 1 two-year-olds barely reproduce. To get a full overview of the system, the stage-transition matrices of three subsequent time steps have to be multiplied: the "true" reproductive values can then be determined from this "overall" matrix (see Appendix D for details).

The pedigree-based estimation of reproductive values might depend on the period (= time of year) when the pedigree is initiated. To check for this, we initiated gene dropping at three different times (corresponding to t=0, t=1, and t=2).

Model-based estimation of RVs under uncertainty

Parameter uncertainty: If for a natural population (a) the life-history states and their transitions are well characterized by a model, and (b) all life-history parameters of the model are fully known, then the "true" RVs of all states can be calculated by standard methods. In reality neither condition (a) nor condition (b) is ever satisfied. Deviations from condition (b) can be tackled in a straightforward manner. As described by (Caswell, 2001, 2019), the "sensitivity" of the population growth rate λ and the reproductive values to uncertainty of a given life-history parameter can be determined with methods from vector calculus. However, the equations for the sensitivity of reproductive values are intricate and not very insightful. We therefore determined the implications of parameter uncertainty by means of parameter randomisation. This approach assumes that the life-history parameters of a given scenario are not known exactly, but

have to be estimated with considerable sampling error. To this end, we considered a fixed set of parameters, representing the "true" values. We assumed that only estimates of these values are available that are only known with 10% (resp. 20%) uncertainty (that is, the coefficient of variation of each parameter is 0.1 or 0.2). We created 1,000 parameter sets, where the value for each parameter was drawn at random from a normal distribution with a mean corresponding to the "true" parameter value and a standard deviation corresponding to 10% (resp. 20%) of the mean. Whenever an estimated parameter did not make biological sense (e.g. if a parameter representing a transition probability was outside of the unit interval or if a parameter representing fecundity was negative), it was discarded and a new estimate was drawn. For each set of parameter estimates thus created, we determined the mRVs. These 1,000 sets of RVs were subsequently compared with the "true" RV, that is, the RV of the model that is determined by the set of "true" parameters.

Life-history model uncertainty: It is much more challenging to investigate deviations from condition (a) above. All models are at best approximations to the "true" situation in nature; accordingly, every life-history model is "wrong". The problem is that it is very difficult to judge which aspects of a model need particular attention in order to avoid misleading conclusions. In life-history models, already the basal classification of life-history stages in discrete categories may be inadequate (e.g. because states are "pooled" that are clearly different from the organism's perspective), leading to a model structure that misrepresents the system under study. Here, we investigate another aspect that may lead to a "wrong" model: overlooking systematic environmental variation. To this end, we consider a situation as in scenario 4, where the environment changes regularly in time. We ask to what extent it matters if the researcher overlooks these oscillations, considering them as stochastic variation, rather than a recurrent pattern. To this end, we consider both perspectives and compare their predictions of RVs.

Technical note

Simulations were written in C++ and ran in Visual Studio Enterprise 2019 (version 16.8). Figures were made using R 3.4.1 (R Core Team, 2021), with the packages ggplot2 (Wickham, 2016) and cowplot (Wilke, 2019).

Results

Pedigree-based estimation of reproductive values

Effects of stochasticity. Figure 2a shows that stochasticity in individual reproductive success is extensive. For example, two of the three individuals that started in age class 1 have not left any descendants after 20 years, while the third individual (Individual 2) leaves about 20 descendants. Similar patterns are seen

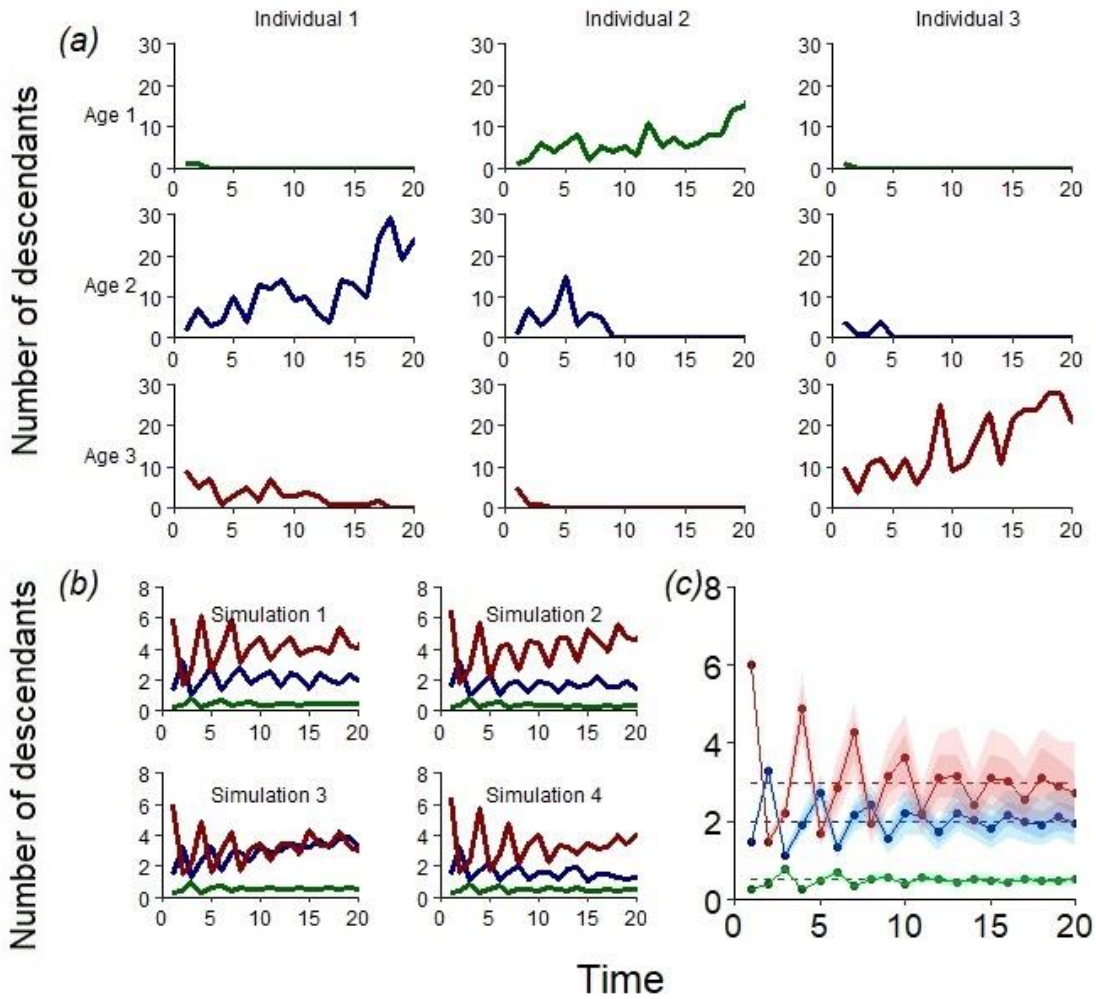

Figure 2. Stochasticity in life-history processes. Example simulations based on Scenario 2 (three age classes; Fig. 1(b)) illustrate stochasticity within and across simulations. **(a)** Number of descendants at a given time step (0 to 20) from nine individuals (three per age class) that were present in the same simulation at time zero. **(b)** For four replicate simulations, the panels show the number of descendants at a given time step of the three cohorts at the start of the simulation (t=0): one-year olds (green), two-year olds (blue), and three-year olds (red). **(c)** Summary of 100 simulations. Dashed horizontal lines correspond to the "true" RVs. The dots connected by solid lines indicate the median of the 100 simulations. The 50% (respectively 90%) central values of the simulations are represented by the darker (respectively lighter) shaded area around the medians. Parameter values: P_1=0.25, P_2=0.5, F_2=1 and F_3=6.

for the other age classes. Estimating RV based on a single individuals is therefore highly inaccurate, since these values mainly reflect stochasticity, rather than the capability of the individual to spread its genes to future generations. When using estimates based on entire cohorts (or behavioural groups in later scenarios), this stochasticity partially gets averaged out. Yet, as shown in figure 2b, each simulation still creates a unique pattern of numbers of descendants per age group (i.e. a different answer). Note that one simulation corresponds to one field population of size *N* = 1,000. Therefore, the variation across simulations already indicates that even extensive pedigrees provide inaccurate RV estimates. To get an impression of this variation, we ran 100 replicate simulations, resulting in figure 2c, which shows the median values and the 50% and 90% central values of these 100 simulations. On a short time horizon ($t<10$), the simulations agree with each other reasonably well, but the pedigree-based estimates $pRV_j(t)$ (for $j=1,2,3$) deviate substantially and systematically from their target value, the "true" RVs v_j. These deviations occur despite of the fact that the populations are reasonably large and all simulations were started in demographic equilibrium. In Appendix A of the Supplement, we show that large deviations are *always* to be expected for small values of *t*. For example, for the shown 3x3 Leslie model the expected values of the pRVs at $t=1$ are given by $pRV_1(1)=F_1+P_1=0.25$, $pRV_2(1)=F_2+P_2=1.5$, and $pRV_3(1)=F_3=6$, while the true reproductive values are $v_1=\frac{1}{2}$, $v_2=\frac{1}{2}\left(F_2+P_2F_3\right)=2$, $v_3=\frac{1}{2}F_3=3$ (see figure 2c). On a longer time horizon ($t\geq 10$) the median pRVs approximate the true RVs, but now the simulations differ considerably from one another.

<u>Effects of population size</u>. Figure 3 illustrates the effect of population size on the estimation of pRV, for the simple case of a population with two age classes (scenario 1, illustrated in figure 1a). From now on, we follow the standard practice in life history theory and report *normalised* reproductive values, where the reproductive value of stage 1 is normalised to one (i.e., $v_1=1$). We can therefore focus on age class 2, which is given by $v_2=F_2=2$. The pRV values are normalized accordingly, by dividing $pRV_2(t)$ by $pRV_1(t)$. For all three population sizes considered in figure 3, the pedigree-based estimates of v_2 differ considerably from their target value in the first few time steps. The length of this period differs considerably depending on the life-history scenario and the life-history parameters (see Figure A1 in Appendix A for an example). On a longer time horizon, the median value of the 100 estimates agrees well with v_2, but the simulations differ a lot from each other, even for $t=20$ or $t=100$ (see Appendix B). The precision of the estimates is improved considerably at larger population sizes, but even for this simple life history quite large populations (e.g., *N* = 5,000 as in figure 3c) are needed for achieving narrow confidence intervals. In field studies, pedigrees often include much fewer individuals. Figure 3a shows the implications of this for a

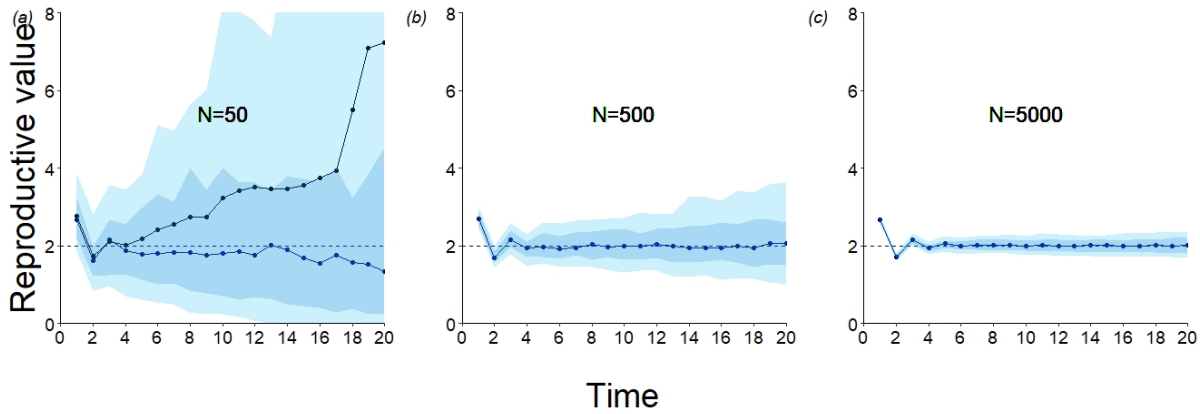

Figure 3. Effect of population size and density regulation on the accuracy and precision of pedigree-based estimations of RV (pRV). Each panel shows the (normalised) pRV in 100 simulations based on Scenario 1 (two age classes; Fig. 1(a)). In all cases, the "true" RV of two-year-olds is $v_2 = F_2 = 2$ (dashed line). **(a)** to **(c)** simulations start with population sizes of 50, 500, and 5000 individuals for the parameter setting $F_1 = 0.5$, $P_1 = 0.25$, $F_2 = 2$. For this setting, the population size remains approximately constant (since λ=1). Blue dots connected by solid lines indicate the median pRV of the 100 simulations. The 50% (respectively 90%) central values of the 100 pRVs are represented by the darker (respectively lighter) shaded area around the medians. The black points connected with a solid black line in (a) show the arithmetic mean of the 100 pRVs.

population size of $N = 50$. Although the median pRV estimate stays reasonably close to $v_2 = 2$ for $t \leq 20$ (it later drops rapidly due to the extinction of descendants from one of the two age groups; see Appendix B), the variation across simulations gets so large that a single simulation does not provide any meaningful information. This is illustrated by the fact that the arithmetic mean of the pedigree-based estimates of v_2 is a factor 4 larger than the true value at $t = 20$.

<u>Precision and accuracy of the estimates.</u> Figure 4 shows the pedigree-based estimates of (normalised) RVs for two scenarios with a three-stage life cycle. Both scenarios confirm our earlier conclusions: on a short time period the estimates are very inaccurate, as the pRV values (including their median) differ substantially and systematically from the true RVs (Appendix A, especially figure A2). On a longer time horizon, the accuracy increases (the median pRVs approach the true RVs), but now the estimates are very unprecise, as the individual simulations differ considerable from each other. As shown in Appendix B, the precision of the estimate decreases with the time horizon *t*. As one simulation corresponds to a single field study, this results in the unfortunate conclusion that pedigree-based estimation of RVs is either

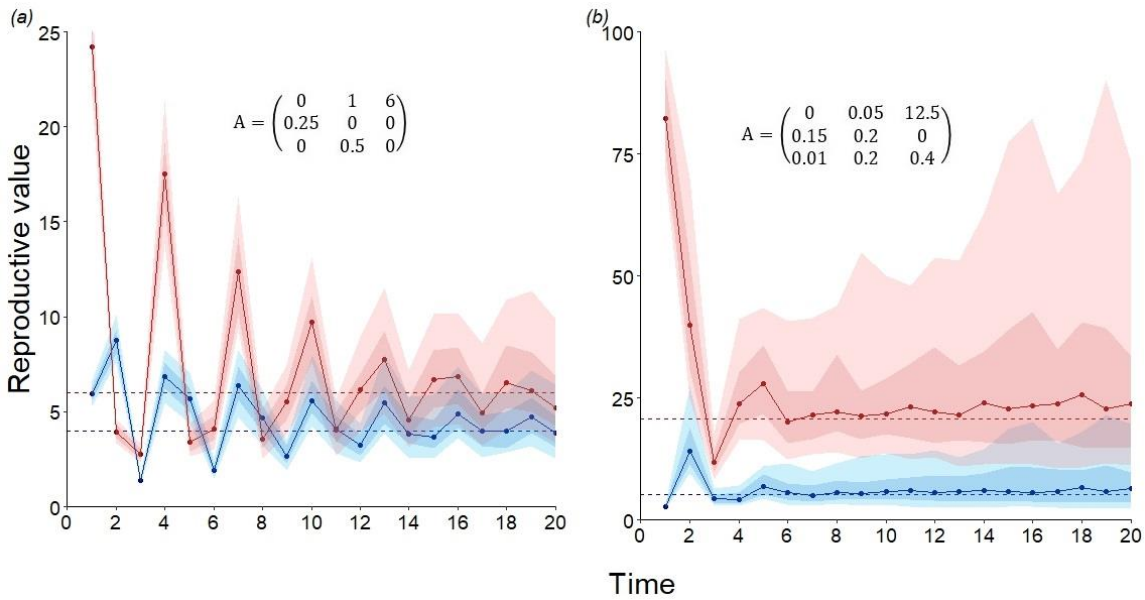

Figure 4. Accuracy and precision of pedigree-based estimates of RV in two scenarios with a three-stage life cycle. Pedigree-based estimation of two (normalised) RVs in 100 replicated simulations based on **(a)** Scenario 2 (three age classes; Fig. 1(b)) and **(b)** Scenario 3 (juvenile-helper-breeder; Fig. 1(c)). The matrix inserts show the parameter settings. The "true" RVs are represented by dotted lines: $v_2 = 4$ and $v_3 = 6$ in (a) (see eqn (8b)); $v_h = 5.3$ and $v_b = 20.8$ in (b). Dots connected by solid lines indicate the median pRV of the 100 simulations; the 50% (resp. 90%) central values of the 100 pRVs are represented by the darker (respectively lighter) shaded area around the medians. Blue: pRVs of two-year-olds in (a) and helpers in (b); red: pRVs of three-year-olds in (a) and breeders in (b). Please note the difference in scale on the y-axis.

inaccurate (in case of short time horizons) or unprecise (in case of long time horizons), even in case of a relatively large study population (N = 1,000 in the simulations shown in figure 4).

Reproductive values in a fluctuating environment. Until now, we considered a constant environment. Determining RVs under fluctuating conditions is quite challenging, even in a simple situation as considered in scenario 4, where there are only two stages and where the environment oscillates regularly between three states (see Appendix D). Figure 5 illustrates that in a scenario like this, the pedigree-based estimation of RVs can be strongly biased, even on a long-term perspective. Moreover, the pRVs strongly depend on the timing of gene-dropping. The inserts in figure 5 indicate at what moment (i.e. at which value of $F_2(t)$) gene dropping occurred. Even in the cases considered in figures 5b and 5c, the bias in the estimate of v_2 is considerable, but it is an order of magnitude larger in figure 5a.

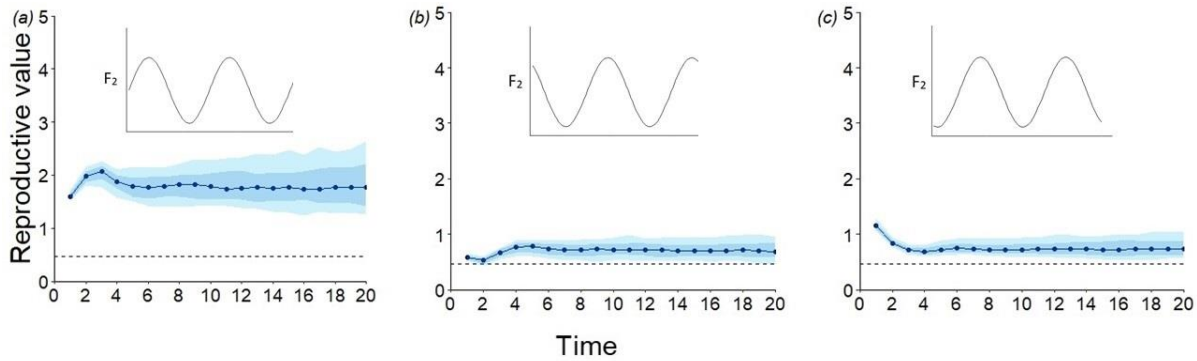

Figure 5. Effect of pedigree initialization on pedigree-based RV estimation in a changing environment. Each panel shows the pedigree-based estimation of the (normalised) RV of two-year-olds in 100 replicate simulations based on Scenario 4 (two age classes, oscillating environment). All simulations use the same life-history parameters, and the "true" RV is the same in all cases ($v_2 = 0.47$, indicated by a dashed line). Panels **(a)**, **(b)** and **(c)** only differ in the timing of gene dropping (the time of pedigree initialization) in relation to the environmental oscillations (as indicated by the insets). In all three cases, pRV systematically overestimates the true RV, but the degree of the estimation bias strongly depends on the timing of gene dropping. Parameter setting: $\overline{F_2} = 1.25$, and α was chosen such that population size stabilized at $N = 1{,}000$. Blue dots connected by solid lines indicate the median pRV of the 100 simulations. The 50% (respectively 90%) central values of the 100 pRVs are represented by the darker (respectively lighter) shaded area around the medians.

Model-based estimation of reproductive values

Parameter uncertainty. Figure 6 shows for two life-history scenarios how the (model-based) estimation of the population growth rate λ and the reproductive values are affected by uncertainty about the life-history parameters. The matrices on top of the panels show the true parameter values, and the corresponding "true" values of λ, v_2 and v_3 are indicated by dashed lines. The boxplots show how the model-based estimates of λ, v_2 and v_3 vary if the life-history parameters are not known exactly but with two degrees of uncertainty (coefficient of variation 10% resp. 20%). In all cases, the median estimate of 100 simulations corresponded well with the true values of λ, v_2 and v_3. However, there is considerable variation across the simulations, especially if *all* life-history parameters can only be estimated with "20% uncertainty" (i.e. $cv = 0.2$). Yet, the model-based estimates of RVs seem generally more accurate ("on target") and precise (less variable) than the pedigree-based estimates for the same life-history scenarios. Figure 6 also shows how sensitive the (model-based) estimates of λ, v_2 and v_3 are regarding uncertainty of a single parameter. In line with more general results from life-history theory (Caswell, 2001, 2019), the mRV of the final age class is most sensitive to uncertainty concerning the fecundity of that age class (i.e.

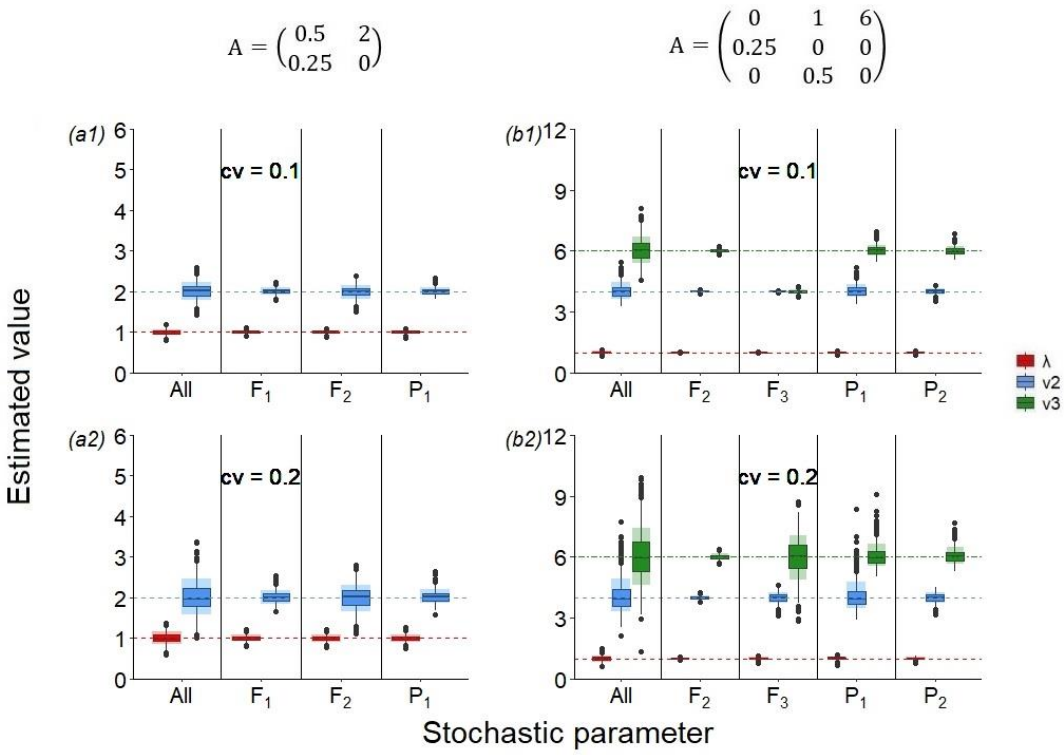

Figure 6. Effects of parameter uncertainty on the model-based estimation of reproductive values and population growth factor. Parameters were estimated by drawing 1000 random samples from a normal distribution with the true value as a mean and a coefficient of variation (cv) of either 0.1 or 0.2. These estimated values were used to calculate the population growth rate λ and the (normalised) reproductive values. The effect of parameter uncertainty on λ and the reproductive values are indicated by boxplots, where the box shows the centre 50% of values and the shaded area the 90% central values. **(a1)** and **(a2)** show the results for a two-stage life cycle (see figure 1a) and **(b1)** and **(b2)** show the results for a three-stage life cycle (see figure 1b). Note the differences in scale on the vertical axes.

v_2 is most sensitive to fluctuations in F_2 in the two-stage life history in fig. 6a, while v_3 is most sensitive to fluctuations in F_3 in the three-stage life history in fig. 6b).

Life-history model uncertainty. A life history model is a simplified, and hence inaccurate, representation of a real system. It is very difficult to evaluate the implications of the unavoidable deviation between a stylized model and the typically more intricate situation in the field. To get at least some idea about these implications, we considered the following thought experiment. Assume that the "true" situation in the field is represented by scenario 4, where some of the life history parameters are not constant but systematically changing, as in a seasonal environment. Assume further that the researchers do not include

these oscillations in their model, but instead view them as random fluctuations ('noise'). How would this affect the estimation of RVs? This question is answered in Appendix D. For the life history scenario considered in figure 4, the RV of two-year olds would be estimated as $v_2 = 1.25$ if the oscillations of the fecundity parameters were misinterpreted as random fluctuations. As shown in Figure D1, the true value of v_2 (which is obtained by taking the oscillations into account) is much smaller than this estimate. The discrepancy between the (wrong) estimate and the true value increases linearly with the amplitude of the oscillations. For an amplitude of 1, the true value is $v_2 = 0.25$, and thus five times smaller than the estimated value.

Discussion

Reproductive values are a very useful theoretical tool (Taylor and Frank, 1996), as they can help to answer questions like: what is the optimal clutch size (Tinbergen and Daan, 1990)? What is the optimal investment in male versus female offspring (Fisher, 1930, Pen and Weissing, 2002)? Under which circumstances should offspring stay on their natal territory and help their parents raise additional offspring (Pen and Weissing, 2000c)? However, we need to be able estimate RVs with accuracy and precision if we are to use them to test predictions of life-history theory.

Reproductive values are increasingly estimated by making use of pedigree information from long term studies (e.g. Chen et al., 2019; Hunter et al., 2019; Reid et al., 2019). In essence, the *per capita* number of descendants of the members of a certain life-history stage is used to estimate the reproductive value of that stage. This method is intuitively appealing, as it closely reflects Fisher's (1930) definition of "reproductive value". However, our study clearly reveals that the method has important drawbacks in practice, even if the pedigree includes many individuals (hundreds or even thousands) per timestep. The analytical arguments (Appendix A) and simulations outlined in the results show that pedigree-based estimates are strongly and systematically biased if the pedigree encompasses a short time horizon (say, $t < 10$). In other words, the estimates are highly inaccurate. On a longer time horizon, the median estimates of RV of 100 replicate simulations match the "true" RVs reasonably well, but the individual simulations tend to diverge considerably from each other with increasing "depth" of the pedigree. As one simulation corresponds to one field study, this implies that the pedigree-based estimate of RV is typically way "off target" if it is only based on one, or a small number of, field studies.

Our findings concur with the patterns reported in natural populations. In both Soay sheep (*Ovis aries*, Hunter et al., 2019) and Florida Scrub-Jays (*Aphelocoma coerulescens*, Chen et al., 2019) estimates of RV

428 based on individuals did not stabilise, just as in our simulations. Moreover, the pedigree-based estimates
429 showed a similar initial "zig-zag" pattern as in our study (e.g. Fig. 4a). Last, but not least, when the
430 estimation was repeated for the same population by applying the gene-dropping method to different
431 cohorts, the RV estimates obtained varied a lot (Hunter et al., 2019). It is conceivable that the precision
432 and accuracy of pedigree-based RV estimation could be improved by estimating RVs for several cohorts
433 and subsequently averaging over cohorts.

434 Our study confirms that the more traditional, model-based calculation of reproductive values on the basis
435 of estimates of the life-history parameters has some desirable statistical properties. Typically, the bias in
436 the estimate gained using this method is relatively small (see Fig. 6), and the precision of the estimates
437 can be judged using a sensitivity analysis (Caswell, 2019). Still, these estimates can have a low degree of
438 confidence if some, or all, life history parameters cannot be determined well. For example, estimating
439 survival probabilities can be difficult in open populations, where mortality can easily be confounded with
440 emigration.

441 Here, we point to another difficulty of the model-based approach: the use of the wrong life-history model.
442 We illustrated this by a simple example (Appendix D), where a season-related systematic pattern in the
443 fecundities remained unnoticed and was misinterpreted as random fluctuations. As shown in Figure D1,
444 such a seemingly small misjudgement can create a substantial bias in the estimation of RVs. However,
445 systematic spatio-temporal patterns of the environment can also have major effects on the pedigree-
446 based method. As shown in Figure 5, pedigree-based estimates can be systematically biased; moreover,
447 the degree of bias may strongly depend on the exact initiation time of the pedigree.

448 We purposely kept our model assumptions as simple as possible. We focussed on very simple life-
449 histories, assuming that estimation issues that arise in simple scenarios will most likely be even worse in
450 more complex life-histories. We assumed that our populations are closed (no emigration or immigration),
451 that pedigree information is complete, and that the life-history parameters remained constant over time
452 (with the exception of the regular oscillations in Scenario 4). Again, it is likely that RV estimates get worse
453 when the situation is less ideal (as is the case for most field studies). Most of our simulations assume
454 asexual reproduction, but as shown in Appendix C they equally apply to randomly mating sexual
455 populations. However, they are not necessarily representative for more complicated situations, such as
456 kin interactions, inbreeding or inbreeding avoidance, and sexual selection. But again, one might argue
457 that methods that do not work well in a very simple context will most likely also fail in more intricate
458 situations.

Life history theory is one of the most advanced branches of evolutionary biology, with sophisticated tools and methods and a well-established fitness concept (Taylor and Frank, 1996, Brommer, 2000). Individual-based simulations are rarely used in life-history studies, perhaps because analytical techniques are readily available. Yet, such simulations can provide valuable additional information. First, simulation models are very flexible and can easily be tailored to the intricacies encountered in real-world situations. For example, it is quite difficult to include sex- and age-structure, non-random mating, and kin interactions in a life history model without compromising analytical solvability, while this is straightforward in a simulation approach. Second, running replicated simulations gives researchers a good idea on the kind and degree of variation to be expected. Individual-based simulations are therefore a useful tool for judging the validity of empirical methods, such as the pedigree-based estimation of reproductive values.

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Author Contributions

MJB and FJW designed the experiment and interpreted the data. MJB built the simulations and analysed all data. MJB and FJW wrote the manuscript; JK and DSR revised it critically multiple times. All authors have approved on publication of the manuscript. All authors agree to be accountable for their aspects of the work.

Data availability

All data will be archived on the University of Groningen Dataverse, which is publicly accessible. The data is not publicly available yet, but will be as soon as the manuscript is published.

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