

# POPAN-6: exploring convergence and estimate properties with SIMULATE

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**ABSTRACT** We describe some developments in the POPAN system for the analysis of mark-recapture data from Jolly-Seber (JS) type experiments. The latest version, POPAN-6, adopts the Design Matrix approach for specifying constraints and then uses it in the constrained maximization of the likelihood. We describe how this is done and the difference it makes to convergence and parameter identifiability over the constraint contrast-equation methods used in POPAN-5. Then we show how the SIMULATE capabilities of POPAN can be used to explore the properties of estimates, including their identifiability, precision, and robustness to model misspecification or capture heterogeneity.

## 1 Introduction

Over the last two EURING meetings, we have described the evolution of the POPAN system for the analysis of mark-recapture data using models of the Jolly-Seber type (Schwarz, 2000). At Patuxent in 1994, we described POPAN-4 (Arnason & Schwarz, 1995), the first version to implement the unified model (Schwarz and Arnason, 1996) that allowed general user-specified constraints. The unified model produces a tractable likelihood using the logits of the fundamental parameters that describe the dynamics of sampling and population change in an open population. The fundamental parameters in a  $k$ -sample experiment are:

- $p_i$  the probability of capture at sample time  $i$ ,  $i = 1, \dots, k$ ,
- $\phi_i$  the probability of an animal surviving between sample time  $i$  and sample time  $i + 1$  given it was alive at sample time  $i$ ,  $i = 1, \dots, k - 1$ ,

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$b_i$  the proportion of animals (out of a total recruitment of  $N$  animals) that enter after sample time  $i$  and survive to sample time  $i + 1$ ,  $i = 0, \dots, k - 1$ . The first parameter,  $b_0$ , is used to estimate the initial stock of animals just before the first sample is taken.

The  $b_i$  are the net birth proportions for each sample interval out of the total net recruitment  $N$ , and formulating the likelihood in terms of these parameters was key to finding a tractable means of imposing constraints. In POPAN-4 you could impose three kinds of constraints: (i) *fixed* value constraints (e.g. setting  $\phi_i$  to 1.0 or  $b_i$  to 0.0 to specify no losses or recruitment in interval  $i$ ); (ii) *sameness* constraints (e.g. constrain survival or survival per unit time to be the same over some sample times); (iii) *covariate* model constraints (e.g. the capture rates are a linear or quadratic function of known sampling effort at each time).

One of the advantages of the unified model is that it is possible to impose non-linear constraints just as easily as linear constraints. The per-unit-time adjustments to survival require this, since constraints have to be imposed on  $\phi_i^{1/\delta_i}$  where  $\delta_i$  is the time between sample  $i$  and  $i + 1$ . Constraints on the fundamental parameters are easily translated into equivalent constraints on their logits, the model parameters. Once the model has been fit and the parameters estimated, further derived parameters of interest to the biologist can be estimated and standard errors (SEs) formed using the delta method and the numeric variance-covariance matrix that drops out automatically with a numeric scoring algorithm for maximizing the likelihood. These included, in POPAN-4, the abundance and net and gross births, defined as:

- $N_i = n_i/p_i$  the abundance at sample time  $i$ ,  $i = 1, \dots, k$ ,  
 $B_i = N b_i$  the net births defined as the number of animals that enter after sample time  $i$  and survive to sample time  $i + 1$ ,  $i = 1, \dots, k - 1$ .  
 $B_0 = N_1$ , the initial population size,  
 $B_i^* = g(\phi_i)B_i$  the gross births where  $g(\phi_i) = \ln(\phi_i)/(\phi_i - 1)$  is the net to gross adjustment, assuming the recruitment and survival per unit time is uniform, or in practice changing only slowly, over the sample interval.

In POPAN-4, you could place sameness or covariate model constraints on net but not on gross births. If you have unequal time intervals, you want to equate or model the gross births per unit time, and this, over short uniform intervals, is:  $g(\phi_i)B_i/\delta_i$ . These constraints are difficult to impose as they are non-linear and a function of more than one fundamental parameter, but they are important to biologists who model total escapements of fish (Schwarz *et al.*, 1993) and to those who model total emergence of insects (N. Schtickzelle, personal communication). Such constraints are possible in POPAN-5.

POPAN-5 was introduced at the 1997 EURING meeting at Norwich (Arnason & Schwarz, 1998, 1999). It extended the unified model fit (called procedure UFIT in POPAN) to groups so that sameness and covariate models could be imposed both over time (temporal constraints) or over groups. This now brings to Jolly-Seber models the ability to fit general temporal and group constraints of the types usually designated using the notation of Lebreton *et al.* (1992): group time interaction models  $g^*t$ ; group effect models  $g$ ; time effect models  $t$ ; and constant parameter models ( $\bullet$ ). So for example, POPAN-5 can fit the model  $(p_g, \phi_{g^*t}, b_i)$  where capture rates are constant over time but different among groups, survival is different at

every time in each group, and the recruitment pattern varies over time but is the same in every group.

As in POPAN-4, constraints are specified by contrast equations but with group extensions (e.g. G1P1-G2P3 means that the parameter at time 1 in group 1 should be constrained to equal the parameter at time 3 in Group 2). These contrasts are used to generalize the scoring method used to maximize the likelihood. This method has advantages (gone into in Arnason & Schwarz, 1999) but also some limitations, which we explore below.

POPAN-5 lets you define the cohort groupings on the fly by specifying logical conditions on fixed cohort attributes supplied with the animal encounter histories. Thus, if you supplied attributes for gender, year class, and initial weight, you could explore models using cohorts defined as any combination of these attribute values without re-entering the data. In sampling breeding populations where samples are annual and animals are marked in their year of birth, then year class is given by the time of first capture. POPAN lets you define groups based on this attribute too, so the familiar age-dependent models of Lebreton *et al.* (1992) can be fit. To fit this and other grouping models, POPAN had to be extended to account for groups and to allow for sample times that may have sample size 0. This can happen by design (e.g. there are no 1997 year class animals in the 1996 sample) or by chance when one of the groups happens to be small or hard to capture. We showed how POPAN handles this for the age-design models (in Arnason & Schwarz, 1999) and in this paper we will discuss how to handle the by-chance cases. These missing samples create identifiability problems that need to be resolved by fixing appropriate parameters.

When you have data on multiple groups, there are additional models and constraints that are of interest. For example, additive models where parameters are constrained to follow the same pattern over time but at possibly different levels in different groups. Additive models on the natural, log and logit scale were added in POPAN-5. Meta-constraints (not involving the fundamental parameters directly) such as imposing equal slopes or intercepts or both across groups in a linear covariate model are also of interest. These are also available in POPAN-5 but a problem with POPAN-5 is that covariate models are applied across all sample times and cannot be restricted to a sub-set of the sample times. In principle, this is resolvable using the unified model, but in practice, the means of implementing this gets increasingly complex using the contrast equation approach in POPAN-5. Such meta-models are not a problem for the Design Matrix (DM) approach used to specify such constraints on survival or capture rates in Program MARK (White & Burnham, 1999) and SURGE (Pradel & Lebreton, 1993).

In order to circumvent such problems, and in order to incorporate the UFIT procedure into Mark, POPAN-6 abandons the contrast equation method and adopts the DM approach. In this paper, we describe how the DM approach is implemented, compared to the contrast equation method, and discuss the advantages and disadvantages of switching approaches. We also show how the method is generalized to adapt to arbitrary parameter transformations such as the log and natural (anti-logit) transformations as well as such non-linear and cross-parameter transformations as required for time adjustment of survival and gross birth rates.

We also discuss the convergence and identifiability problems that can occur because of chance small-sample problems. Then we give an example of how the integration of UFIT with a general SIMULATE procedure, capable of doing both deterministic and stochastic simulations, can be used to explore identifiability, precision, and robustness of estimates to model misspecification and assumption failures.

## 2 Constraint implementation

To compare how POPAN-5 and POPAN-6 fit constrained models, it is helpful to consider a specific model: say  $(p_g, \phi_i, b_{g^{\text{in}(t)}})$  with  $g = 2$  (groups, say females and males) and  $k = 4$  samples. The birth proportions  $b_i$  are modelled as linear in time ( $t = i = 1, 2, 3$ ) and initially we might look at models with different intercepts and slopes for males and females and then see if models with common slope between the sexes are supported. In the general  $g$ -group,  $k$ -sample model there are  $g(3k - 1)$  parameters and we let  $\theta$  be the vector of parameters in standard order:

$$p_{11}, \dots, p_{1k}, \phi_{11}, \dots, \theta_{1k-1}, b_{10}, \dots, b_{1k-1}, p_{21}, \dots, b_{2k-1}, p_{g1}, \dots, b_{gk-1}$$

where the first subscript now indicates group. Standard order is the  $p$ ,  $\phi$  and  $b$  for group 1, followed by those for group 2, etc. Not all these parameters are identifiable in the unconstrained case, but in our constrained example, just 11 of the  $2(3 \times 4 - 1) = 22$  full set of parameters are different and all 11 of the reduced set are, it turns out, identifiable. If we call this reduced set the vector  $\beta$ , then

- $\beta_1$  and  $\beta_2$  are the capture rates for males and females respectively,
- $\beta_3, \beta_4$  and  $\beta_5$  are the survival rates at times 1, 2 and 3 (common to both sex groups),
- $\beta_6, \beta_7$  and  $\beta_8$  are  $b_0$  and the intercept and slope for females ( $g = 1$ ), and
- $\beta_9, \beta_{10}$  and  $\beta_{11}$  are  $b_0$  and the intercept and slope for males ( $g = 2$ ).

Note that  $b_0$  is modelled as a separate parameter and not as part of the linear model since this represents the initial proportion of the entries that are present just prior to the first sample. All the other  $b_i$  are for the proportion of entries between two samples and if samples are equally spaced, we might expect a consistent pattern among these, but unrelated to  $b_0$ . The relationship between the full and reduced parameter set is  $\theta = \mathbf{D}\beta$ . In Table 1, we show the form of  $\mathbf{D}$ , the 22 row by 11 column full design matrix;  $\theta$ , the 22 by 1 vector of the full parameters in standard order; and  $\beta$  the 11 by 1 vector of reduced parameters.

In POPAN-6, as in MARK, it is easier to specify the sameness constraints (here, on  $p$  and  $\phi$ ) using a parameter index matrix (PIM). This is an array of integer indexes, one for each parameter in standard order, and if the index is the same for two parameters, it means they are to be constrained to be the same. The user then specifies only a reduced DM for the remaining covariate and fixed constraints if any. For this example, the PIM is shown in Table 2.

The DM only has to specify the covariate model to impose further constraints on the parameters with index (we call it, redundantly, the PIM index) numbers 7...9 and 11...13 to reduce the 13 parameters to 11 as before, or, as shown in Table 2, to the 10-parameter common slopes model.

It is straightforward to reconstruct a full design matrix,  $\mathbf{D}$ , from a PIM and a reduced DM. Fixing parameters is done by adding a first column to the reduced DM to contain the value to fix the parameter to (and all other cells in that row must be empty).

In POPAN-6, the maximization algorithm iteratively selects values for the  $\beta$  parameters in its search to maximize the log likelihood. We can derive the method of doing this from the scoring method for finding the unconstrained model parameters by applying a chain rule. The scoring method used in POPAN-5, ignoring

TABLE 1. Full design matrix where the rows give the full parameters ( $\theta_{row}$ ) in standard order and the columns give the reduced parameters ( $\beta_{col}$ ). The meaning of the reduced parameters is indicated as  $p(g,t)$  with a dot replacing the group  $g$  or time  $t$  to indicate a sameness constraint; or as  $int(g)$  and  $sl(g)$  to indicate the parameters in group  $g$  are fitted by a linear model with this intercept and slope

	$\beta_1 =$ $p(1,.)$	$\beta_2 =$ $p(2,.)$	$\beta_3 =$ $\phi(. , 1)$	$\beta_4 =$ $\phi(. , 2)$	$\beta_5 =$ $\phi(. , 3)$	$\beta_6 =$ $b(1,0)$	$\beta_7 =$ $int(1)$	$\beta_8 =$ $sl(1)$	$\beta_9 =$ $b(2,0)$	$\beta_{10} =$ $int(2)$	$\beta_{11} =$ $sl(2)$
$\theta_1 = p_{1,1}$	1	0	0	0	0	0	0	0	0	0	0
$\theta_2 = p_{1,2}$	1	0	0	0	0	0	0	0	0	0	0
$\theta_3 = p_{1,3}$	1	0	0	0	0	0	0	0	0	0	0
$\theta_4 = p_{1,4}$	1	0	0	0	0	0	0	0	0	0	0
$\theta_5 = \phi_{1,1}$	0	0	1	0	0	0	0	0	0	0	0
$\theta_6 = \phi_{1,2}$	0	0	0	1	0	0	0	0	0	0	0
$\theta_7 = \phi_{1,3}$	0	0	0	0	1	0	0	0	0	0	0
$\theta_8 = b_{1,0}$	0	0	0	0	0	1	0	0	0	0	0
$\theta_9 = b_{1,1}$	0	0	0	0	0	0	1	1	0	0	0
$\theta_{10} = b_{1,2}$	0	0	0	0	0	0	1	2	0	0	0
$\theta_{11} = b_{1,3}$	0	0	0	0	0	0	1	3	0	0	0
$\theta_{12} = p_{2,1}$	0	1	0	0	0	0	0	0	0	0	0
$\theta_{13} = p_{2,2}$	0	1	0	0	0	0	0	0	0	0	0
$\theta_{14} = p_{2,3}$	0	1	0	0	0	0	0	0	0	0	0
$\theta_{15} = p_{2,4}$	0	1	0	0	0	0	0	0	0	0	0
$\theta_{16} = \phi_{2,1}$	0	0	1	0	0	0	0	0	0	0	0
$\theta_{17} = \phi_{2,2}$	0	0	0	1	0	0	0	0	0	0	0
$\theta_{18} = \phi_{2,3}$	0	0	0	0	1	0	0	0	0	0	0
$\theta_{19} = b_{2,0}$	0	0	0	0	0	0	0	0	1	0	0
$\theta_{20} = b_{2,1}$	0	0	0	0	0	0	0	0	0	1	1
$\theta_{21} = b_{2,2}$	0	0	0	0	0	0	0	0	0	1	2
$\theta_{22} = b_{2,3}$	0	0	0	0	0	0	0	0	0	1	3

TABLE 2. Parameter Index Matrix (PIM) for the sameness constraints specified in Table 1 and the design matrix for two reduced models based on the PIM parameterization. Notation for reduced parameters is as in Table 1

PIM	$p_{g,1}$	$p_{g,2}$	$p_{g,3}$	$p_{g,4}$	$\phi_{g,1}$	$\phi_{g,2}$	$\phi_{g,3}$	$b_{g,0}$	$b_{g,1}$	$b_{g,2}$	$b_{g,3}$
(a) PIM											
$g = 1$	1	1	1	1	3	4	5	6	7	8	9
$g = 2$	2	2	2	2	3	4	5	10	11	12	13

	Different slopes DM				Common slope DM		
	$\beta_1 =$ $int(1)$	$\beta_2 =$ $sl(1)$	$\beta_3 =$ $int(2)$	$\beta_4 =$ $sl(2)$	$\beta_1 =$ $int(1)$	$\beta_2 =$ $sl(.)$	$\beta_3 =$ $int(2)$
(b) Reduced models							
$\theta_1 = PIM_7$	1	1	0	0	1	1	0
$\theta_2 = PIM_8$	1	2	0	0	1	2	0
$\theta_3 = PIM_9$	1	3	0	0	1	3	0
$\theta_4 = PIM_{11}$	0	0	1	1	0	1	1
$\theta_5 = PIM_{12}$	0	0	1	2	0	2	1
$\theta_6 = PIM_{13}$	0	0	1	3	0	3	1

constraints for the moment, gets parameter estimates at iteration  $j + 1$  from the previous estimates at iteration  $j$  using

$$\theta_{j+1} = \theta_j + H_{\theta}^{-1}(\theta_j) S_{\theta}(\theta_j) \quad (1)$$

where  $\theta$  is the vector of model parameters in standard order, of dimension  $n$  by 1, where  $n = g(3k - 1)$ , and  $S_{\theta}(\theta_j)$  is the  $n$  by 1 score vector of derivatives of the log likelihood evaluated at the current parameter values  $\theta_j$ ; and  $H_{\theta}^{-1}(\theta_j)$  is the inverse Hessian evaluated at the current values. The Hessian is the  $n$  by  $n$  array of second partial derivatives of the log likelihood with respect to the  $n$  model parameters. In POPAN-6, the iteration is on the  $\beta$  vector of length  $m$ , say, using

$$\beta_{j+1} = \beta_j + H_{\beta}^{-1}(\beta_j) S_{\beta}(\beta_j) \quad (2)$$

but it is possible to derive the three arrays in this equation from the design matrix and the original score and Hessian matrix. First we get the current full parameters from  $\theta_j = \mathbf{D}\beta_j$  (some of these will be the same, but we can always compute the full  $n$  model parameters given the  $\beta$  and the full design matrix). We can also find the beta score function from the old score function, since one application of the chain rule gives

$$S_{\beta}(\beta_j) = \mathbf{D}' S_{\theta}(\theta_j) \quad (3)$$

and a second application gives the method of deriving the Hessian from the old Hessian:

$$H_{\beta}(\beta_j) = \mathbf{D}' H_{\theta}(\theta_j) \mathbf{D} \quad (4)$$

Applying these three substitutions to equation (2) gives equation (1), which shows that both methods are equivalent in maximizing the log likelihood but since at each step we are iterating on the  $\beta$ , the constraints specified by the full design matrix are being maintained on the  $\theta = \mathbf{D}\beta$  at each iteration; hence at the expense of a couple of matrix operations, the size of the Hessian to be inverted can be greatly reduced (from 22 to 11 in our example) and a constrained maximization algorithm is converted to the equivalent of an unconstrained search.

The method in equation (2) generalizes to allow the method to apply to any transformation of the parameters provided the transformation is differentiable with respect to model parameters. This includes the per-unit-time (delta) transformation of survival rates and the substitution of derived rates and other scales for model parameters (e.g. constraints and covariate models on gross births instead of on birth proportions; additive or covariate models on the log or natural scale rather than on the logit scale), or on relative rates such as dilution or seniority rates (described below). If  $\theta_j^{(\text{new})} = T_j(\theta)$  is the transform function for replacing  $\theta_j$  by its transformed value, then equation (3) becomes

$$S_{\beta}(\beta_j) = \mathbf{D}' \mathbf{T} S_{\theta}(\theta_j)$$

and equation (4) becomes

$$H_{\beta}(\beta_j) = \mathbf{D}' \mathbf{T}' H_{\theta}(\theta_j) \mathbf{T} \mathbf{D}$$

where  $\mathbf{T}$  is the  $n$  by  $n$  array of partials  $\mathbf{T} = [t_{ij} = \partial T_i(\theta) / \partial \theta_j]$ . Thus imposing different transformations on different parameters just requires the computation of the  $\mathbf{T}$  array and some extra matrix operations at each step of the iteration. Simple univariate transformations, such as the delta, log, or anti-logit transform, are easier to implement because they result in a diagonal  $\mathbf{T}$ . We have not yet decided whether

POPAN-6 will impose transformations globally or whether we will let the user specify them on a parameter by parameter basis. In POPAN-5 you specify them globally (e.g. BIRTHS = GROSS) and then the transform is applied to all birth parameters at all times and in all groups so that any constraints are on the gross births rather than on the birth proportions. One can imagine situations in which one wanted transformations for some parameters and a different transformation for other parameters but this may give the user a bit too much flexibility (i.e. rope with which to hang oneself on the gallows of non-identifiability).

In POPAN-5, the imposition of constraints actually makes the score and Hessian larger than  $n$ , because the constraints are imposed by the method of Lagrange operators. The iteration from step  $j$  to step  $j + 1$  becomes

$$\begin{bmatrix} \theta_{j+1} \\ \bullet \end{bmatrix} = \begin{bmatrix} \theta_j \\ \bullet \end{bmatrix} + \begin{bmatrix} H(\theta_j) & -C(\theta_j) \\ -C'(\theta_j) & 0 \end{bmatrix}^{-1} \begin{bmatrix} S(\theta_j) \\ c(\theta_j) \end{bmatrix}$$

where  $c(\theta) = 0$  is the vector of  $c$  contrast equations for the constrained model and  $C(\theta)$  is the  $n \times c$  array of partial derivatives of each constraint with respect to each parameter. (The terms indicated by  $\bullet$  are Lagrange values that need not concern us here.) For our example, there are 11 constraints. Six of these specify the group-effect constraint on the  $p_{gi}$  (i.e. the capture rates are constant over time but different for females and males; note that each constraint is expressed as a parenthesized contrast expression which is to evaluate to 0):

$$(p_{11} - p_{12})(p_{12} - p_{13})(p_{13} - p_{14})(p_{21} - p_{22})(p_{21} - p_{23})(p_{23} - p_{24})$$

Three specify the time-effect on the  $\phi_{gi}$  (i.e. survival is the same for males and females at each time but varies over time):

$$(\phi_{11} - \phi_{21})(\phi_{12} - \phi_{22})(\phi_{13} - \phi_{23})$$

and the last two constraints come from the covariate model for each sex (once the slope and intercept is determined, the remaining  $(k - 1) - 2$  birth parameters are determined by their covariate values).

It is important to see how POPAN-5 casts a covariate model into such constraints because it leads to very different convergence properties than the DM method in POPAN-6. To take a slightly different example, suppose we had  $g = 1$  and  $k = 5$  and we wished to model capture rate in terms of known effort (say  $e_i$  is the measure of effort for sample  $i$ ). Now at each iteration, the values of  $p_1$  and  $p_2$  allow us to solve for a slope ( $\beta_1$ ) and intercept ( $\beta_2$ ) using the equations:

$$p_1 = \beta_1 + \beta_2 e_1$$

$$p_2 = \beta_1 + \beta_2 e_2$$

In matrix form, we could write this as  $p_{1:2} = \mathbf{X}_{1:2}\beta$  where  $\mathbf{X}$  is the 2 by 2 coefficient matrix

$$\begin{bmatrix} 1 & e_1 \\ 1 & e_2 \end{bmatrix}.$$

The solution for the model coefficients is then

$$\beta = \mathbf{X}_{1:2}^{-1} \mathbf{p}_{1:2}. \quad (5)$$

The remaining  $k - 2$  parameters are modelled as

$$p_3 = \beta_1 + \beta_2 e_3$$

$$p_4 = \beta_1 + \beta_2 e_4$$

$$p_5 = \beta_1 + \beta_2 e_5$$

or, in matrix form:

$$\mathbf{p}_{3:5} = \mathbf{X}_{3:5} \beta$$

Given the current  $\beta$  and the known effort at these three times, these are our three constraints. The meta-constraints (e.g. equal slopes between two groups) can also be cast as a contrast equation since, from equation (5) above it is clear that the  $\beta$  can be viewed as a linear function of the fundamental parameters and hence any sameness constraint between them is also a linear function. SEs for the  $\beta$  are also derived using equation (5), the delta method and the variance-covariances of the parameters ( $p_1$  and  $p_2$  in the example above).

A disadvantage of this method is that the matrix  $\mathbf{X}$  in equation (5) can be singular. This would happen in our example if  $e_1 = e_2$ . This problem can be circumvented in theory by choosing 2 other parameters to solve for  $\beta$  but POPAN does not do this for you because it is just too messy to detect and implement. Instead you can apply a small jitter to  $e_2$ , which usually works, but introduces a small amount of error.

Constraints and covariate models involving transformations of parameters are easy to implement as there is no requirement that the constraints  $c(\theta)$  be univariate or linear in the model parameters. However, it is more difficult to develop a single means of letting the user specify such transformations and to then implement them (including deriving SEs). In POPAN-5 the user is allowed to choose from a pre-specified set of global transformations that apply to certain constraint models, and then ad hoc code derives the necessary constraints and SEs. Constraints and their partial derivatives for any meta-constraints need to be derived and programmed explicitly. It certainly lacks the generality and ease-of-implementation of the DM approach.

The constraint approach of POPAN-5 has one advantage over DM when fitting covariate models: it almost always converges even if the covariate model is over-specified or misspecified, or if the covariate coefficients are imprecisely determined by the data. If samples are large enough that fundamental parameter estimates are reasonably precise and if the matrix  $\mathbf{X}$  in equation (5) is invertible, then you always get estimates of the covariate  $\beta$  coefficients at each iteration, because the iteration is updating the model parameters and then deriving the  $\beta$  coefficients from them. With the DM approach, you are iterating on the  $\beta$  coefficients directly, and if the likelihood surface is flat or ill-shaped (e.g. ridges to infinity reflecting the inability to separately identify two coefficients) in these parameters then the model may not converge.

This difference showed up when running the TESTUSIM example from the POPAN-5 test suite (Table 3). This is a stochastic simulation with  $g = 1$ ,  $k = 6$  and different covariate models for each of the parameters  $p$ ,  $\phi$  and  $b$ . The model for  $p$



TABLE 3. Example of a POPAN-5 UFIT analysis of Simulated data to test convergence and check for bias in covariate models. The SIMULATED population is chosen so that it is correctly modelled by the specified UFIT model

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C THIS IS PROGRAM 'TESTUSIM.POP'

UFIT,
C first specify the UFIT analysis to be applied in later (replicated)
simulations
C Covariate 1 (C1) might just be day number and
C Covariate 2 (C2) might be sampling effort on each day
C Use 6 samples (days)

    LSEL = 6;
    C1 = (1.0, 2.0, 3.0, 4.0, 5.0, 6.0) ;
    C2 = (5.0, 2.0, 1.0, 1.0, 2.0, 5.0);

C Capture rate model, linear and interaction effects of C1 and C2
  CPCONST = P - (CO,C1,C2,C12);

C Survival rate model, additive effects of C1 and C2 (no realism here)
  SPCONST = P - (C1,C2);
C simulated data is assumed equally spaced so adjust has no effect
  ADJUST = NO ;

C Entry rate model, quadratic time effect (peaked entry curve)
  BPCONST = P - (CO, C1, C11) ;

C Use minimal tracing and save UFIT keywords for later Simulation
C Initial estimates from the Jolly_Dickson full model with constant p

C trace bit 123456789012345678
  TRACE = 010000000000000000;    SAVE = UFIT;
  ANALYSIS = 9; TITLE = 'Fitting Covariate Models';/

SIMULATE,
C LSEL must match that in the UFIT paragraph
  LSEL = 6;    TITLE = 'SIMULATION TEST - CALLING UFIT FROM SIMULATE';

C Specify the capture rates to be used, these are the values that would result
C if the CP covariate model has (true) coefficients = 0.02 for each term
  CMECHANISM = VECTOR(0.24, 0.18, 0.16, 0.20, 0.36, 0.84);

C Specify the survival rates, these are for the SP covariate
C model with all coefficients = 1/8 (except the last...non-estimable)
  SMECHANISM = VECTOR(0.75, 0.5, 0.5,0.625,0.875, 0.99);

C Assume no tag loss or losses on capture (but maybe change this later
C to see if they have an effect)
  TMECHANISM = FIXED(0.0);    LMECHANISM = FIXED(0.0);

C The true model for new entries is, -40 + 240 C1 - 40 C1*C1)  c1=1..5
C NET Ntot = 2000, giving pent(0..5)=0.4, 0.08, 0.14, 0.16, 0.14, 0.08
  NEWENTRIES = VECTOR(800, 160, 280, 320, 280, 160);

C No age or group effects in this population
  AMECHANISM = FIXED(0);
  ATYPE = FIXED;    GROUP = NONE;

C Specify the (latent) UFIT analysis and set the usual run parameters
  SEED = 123456789;    RUN = YES;    ANALYSIS = UFIT;
  REPLICATIONS = 16;    WRITE = NO;    SAVE = NO;/

```

---

involves two covariates and four  $\beta$  coefficients and these coefficients are poorly determined by the data. Nevertheless, in all 16 iterations of the model, there was no convergence failure, the estimates of  $p$  were precise (CV around 15%) and unbiased, while estimates of the  $\beta$  coefficients, while unbiased, were quite imprecise (CV over 100% in most cases) but this was clear from the SEs (also unbiased but imprecise). On the other hand, when a number of these stochastically generated data sets were run through POPAN-6, none of them converged. It was simply impossible to estimate the coefficients. This is potentially a serious problem since, in analysing real data, we do not know the correct model, so we typically try a flexible but likely over-specified model (say a cubic model in a covariate) and then fit a nested set of more restrictive models (quadratic, linear) until the LRT or AIC model selection rules tell us we have gone too far. If fitting over-specified models is going to be a problem, then covariate model selection becomes difficult in the DM approach.

To summarize then, the advantages of the DM approach of POPAN-6 over the constraint approach of POPAN-5 include:

- more generality and flexibility in specifying constraints, especially on transformed or derived parameters. Also, applying models such as covariate or additive models to selected times or groups is easily accomplished,
- ease of implementation: reduced array sizes and a simple consistent method of applying transformations and link functions; builds on existing iteration by adding a few matrix operations, and permits a general algorithm to be used for extracting derived parameters and their SEs.

Disadvantages include:

- appears to be much slower (the extra matrix operations are costly),
- may have more difficulty fitting over-specified or poorly-determined covariate models.

### 3 Available estimates and their identifiability

Not all of the  $g(3k - 1)$  parameters are identifiable. A parameter is non-identifiable if it always occurs in the likelihood function in some fixed combination with another parameter. This is a very dangerous situation because the estimates of non-identifiable parameters may be plausible, but are in fact meaningless. Non-identifiability can also cause convergence problems, but this can be resolved by imposing some additional constraints. What is identifiable depends on what further constraints are imposed but, for the full time-dependent model,  $b_0$  and  $p_1$  are not separately estimable, nor are  $\phi_{k-1}$  and  $p_k$ . In POPAN's UFIT, the user can resolve this by constraining  $p_1$  and  $p_k$  to be 1, but must realize, as we discuss below, that this affects the interpretation of these and other estimates. POPAN includes a keyword (AUTOMATIC) to impose these constraints in each group in addition to any user-specified constraints.

POPAN automatically constrains the entry rates,  $b_i$ , to sum to 1 (within each group). The user can specify equality or closure ( $b_i = 0$ ) constraints on  $b_i$  for  $i = 0 \dots k - 1$  but they cannot all be constrained to 0 as they must sum to 1.0. Note that if you constrain  $b_i$  to 0 for the first  $x$  sample times ( $i = 0 \dots x - 1$ ) then the population size will also be 0 until time  $x$  and you must also take steps to constrain the  $p_i$  and  $\phi_i$  at these times as well, since they are non-identifiable. Within

a group, you can constrain the proportion of entries at two times to be equal and this will cause the estimated Net births at those two times to be equal. However if you specify equality constraints on birth rates in two different groups, the Net birth estimates will not be equal; this is because the total entries,  $N$ , is different for each group (and cannot be constrained to be equal) and consequently constraints on Net births are determined only within a constant of proportionality. This means that when you constrain  $b_i$  across groups you are hypothesizing that the relative rather than absolute birth patterns are the same but this is generally what you want to do. As noted earlier, the  $b_0$  should not be involved in sameness or covariate constraints as they represent initial populations rather than entry rates. You can constrain either the net or the gross rates and adjust on a per unit time basis, but equalities are still relative when across groups (keywords ADJUST and BIRTHS control this).

Deficiencies in the data can also produce non-identifiability and convergence problems. Sometimes this is due to small samples, high turnover, or low recapture rates, but sometimes, as in age-structured models, it happens because a group is empty at certain times. We dealt with the age-structured models in Arnason & Schwarz (1999). Here we give some brief guidelines on the first situation.

The completely unrestricted model ( $p_{g^*t}$ ,  $\phi_{g^*t}$ ,  $b_{g^*t}$ ) has the following non-identifiability problems:

- $p_k \phi_{k-1}$  cannot be separated
- $p_1^* b_0$  cannot be separated
- A complicated function of  $b_1$ ,  $p_1$  and  $\phi_1$ , cannot be separated.

This has implications for counting the number of parameters and for model fitting. In the model ( $p_{g^*t}$ ,  $\phi_{g^*t}$ ,  $b_{g^*t}$ ), the restrictions  $p_1 = 1$  and  $p_k = 1$  can be set automatically (using AUTO = BOTH) to remove the non-identifiability and avoid convergence problems, but they introduce inference problems. These restrictions imply that, in each group,  $\phi_{k-1}$ ,  $b_0$  and  $b_1$  now estimate some confounded parameters (see Schwarz & Arnason, 1996). If reduced models are fit, you need to pay careful attention to what other restrictions you apply; e.g. if you fit the model  $\phi_i$  where survival is equal over groups, then  $\phi_{k-1}$  should not be included in the restriction because it is actually estimating  $p_k^* \phi_{k-1}$  and it is unlikely that this quantity is the same over all groups. In the next section we show how simulation can be used to show this sort of effect.

Additional non-identifiabilities can be introduced when certain summary statistics are 0. The main problems occur when a complete sample is zero ( $n_i = 0$  and hence the number of marks in the sample,  $m_i$ , and the number returned to the population,  $s_i$  is also 0, as are the number of later recoveries from those returned,  $r_i = 0$ ) but problems can also occur if there are no marked recaptures in samples after the first ( $m_i = 0$  for  $i > 1$ ), no subsequent recoveries after a sample ( $r_i = 0$ ) or there are no uncaptured but known-alive animals ( $z_i = 0$  for  $i > 1$  and  $i < k$ ). We deal with these case by case.

**(i)  $m_i = 0, n_i > 0$  for  $i > 1$ : No marked animals captured in a recapture sample**

This could be a problem because the likelihood estimate for the population size could be infinite. However, the  $u_i$  provide some information about the true population size and, in many cases, the program does converge properly. If the

program seems to be driving  $b_{i-1}$  to 1.0 then you need to constrain  $b_{i-1}$  to some value.

(ii)  $n_i = 0$  (and hence  $m_i, s_i, r_i = 0$ )  $z_i > 0$ : *null sample*

Usually caused by no samples taken at a particular sample time. This can often happen by chance in any multi-group analysis where one of the groups (e.g. females) is small or hard to catch relative to other groups. POPAN must analyse the same set of sample times for all groups, so these samples cannot be eliminated (e.g. by OMIT or GROUP in SELECT) without eliminating what might be large numbers of captures of animals in the other groups. Nevertheless, the best solution is usually to eliminate such problem times so one should always consider re-mapping the sample histories (in SELECT) or redefining the groups (in UFIT) to make them larger and so eliminate these small-sample problems, provided there is not too much loss of precision and insight. Sometimes this cannot be done (e.g. covariates like effort may be hard to define if samples are pooled). When there is a null sample at time  $i$  the following holds.

$\phi_{i-1}\phi_i$  can be estimated. Constrain  $\phi_i = 1$  and interpret  $\phi_{i-1}$  as the product.

$b_{i-1} + b_i$  can be estimated. Constrain  $b_i = 0$  and use  $b_{i-1}$  as the sum.

$p_i = 0$ . Constrain  $p_i = 0$ . There will be no estimate of abundance at  $i$ .

(iii)  $z_i = 0, r_i > 0$

This situation is usually caused by poor sample sizes or high turnover rates. It seems to indicate there are no marked animals left in the population except those caught in the current sample. If convergence problems occur, try restricting  $p_i = 1$  using the design matrix.

(iv)  $z_i = 0, r_i = 0$

Usually caused by poor sample sizes. Program should converge when restricting  $\phi_i = 0$ , but this causes problems in estimating the gross births.

### 3.1 *Derived estimates added in POPAN-6*

UFIT provides for multiple starting points in the likelihood maximization search using automatic or user-specified initial parameter values. The user can modify the convergence criteria and can ask for different levels of detail in tracking the search process in case there are problems in converging to the maximum. On convergence, it prints out the maximized likelihood and the number of actual restrictions used in the fit (excluding redundant constraints). This permits the user to use likelihood ratio or Akaike Information Criterion (AIC) methods for model selection.

UFIT then reports the statistics and PIM mapping used and then provides estimates of the fundamental parameters ( $p, \phi, b$ ), the derived parameters (net and gross births including total recruitment, and abundances) and their SEs (as was done in POPAN-5). There is an option to see the full set of model (logit) parameter estimates and their SEs. In POPAN-6 the (reduced DM)  $\beta$  estimates and their SEs are reported and the estimate table includes derived estimates for relative rates of change in births and abundance: gamma, called the seniority rate (Pradel, 1996) between two times  $\gamma_{i+1} = N_i\phi_i/N_{i+1}$  is the inverse of Jolly's (1965) dilution rate; and lambda, the finite rate of population change between two times is

$\lambda_i = N_{i+1}/N_i$ . These estimates are known to be much more robust to capture heterogeneity than the absolute birth and abundance estimates (Schwarz, 2000) and are important in their own right for assessing demographic trends in populations. Eventually, it will be possible in POPAN-6 to constrain these derived parameters through the DM, permitting the testing of hypotheses about the stationarity of a population ( $\lambda = \text{constant}$ ). This is more general than testing for stable population size ( $\lambda = 1$ ), which can be done in POPAN-5 by using the covariate model ( $p_i - cn_i$ ) where the sample size  $n_i$  is used as a covariate in a no-intercept linear model. The estimated slope  $c$  is an estimate of  $1/N$ .

POPAN creates standard Estimate Tables for output of all parameter estimates and their SEs. This ensures that UFIT can be integrated with the POPAN SIMULATE paragraph for exploring the properties of estimates and their SEs over replicated probabilistic simulations of a specified sampling and demographic model.

#### 4 Explorations of estimate properties using SIMULATE

The SIMULATE paragraph provides a general means of generating replicated, stochastic sampling experiments applied to a population with user-specified demographic rates. To use it with UFIT, you first specify the constrained analysis (by a PIM and DM in POPAN-6) but designate that the procedure is to be saved (SAVE = UFIT) rather than being executed immediately as is usually done for real data. You then specify a SIMULATE procedure giving mechanisms for capture, survival and entry rates (see TESTUSIM in Table 3 for an example). Mechanisms can be specified that satisfy, or that violate, assumptions such as homogeneity of rates over individuals. SIMULATE then uses the mechanisms to generate an encounter history file and passes this as input to UFIT, which analyses it as if it were real data. SIMULATE traps the Statistics and Estimate tables and rather than print them out, it accumulates sums and sums of squares so that after the last replication, it can report means and standard deviation (SD) of every estimate and every SE over the replications. Comparison of these estimate means with their true value can reveal the magnitude of bias in estimates. The mean of a SD helps predict precision for a given sampling scheme imposed on a hypothesized population with given turnover rates. The mean of a SE can be compared with the SD of the estimate over replications to look for bias in the SE. The RANK keyword lets the user provide an observed maximized log likelihood (*mll*) and the simulation will then report the percentile rank of that value among the simulated *mll* values. This is the parametric bootstrap estimate of Goodness-of-Fit of the data to that model.

Violations that can be modelled in SIMULATE include tag-loss, temporary emigration, marking and handling effects on survival and subsequent capture rates. Heterogeneity due to age and other cohort effects can be modelled and group effects are allowed. You can investigate bias due to model misspecification by using a UFIT procedure whose constraints do not match the mechanisms specified in SIMULATE. However, if there are no sources of rate heterogeneity other than group and time effects, investigations of bias and precision can be investigated more efficiently by a non-stochastic mean value (MV) analysis. This is possible in POPAN because UFIT can accept either encounter histories or a table of summary statistics as input.

In a MV analysis, the expected values of the statistics (the  $n$ ,  $m$ ,  $s$ ,  $r$ ,  $z$  for each sample time in each group) given the mechanisms are generated by SIMULATE and these are passed to a UFIT procedure to be analysed as if they were

real summary statistics (the expected values need not be whole numbers but, unfortunately, POPAN stores them as integers, thus losing some accuracy in the rounding). This is the numerical equivalent of the technique used by Carothers (1973) and many later authors to investigate the bias and precision of mark-recapture estimates.

In Table 4 we show a POPAN-6 program that carries out a simple MV analysis. The true parameter values used to drive the simulation for this six-sample experiment are shown in Table 5(a) in the form they appear in SIMULATE's preliminary report: Capture Probability ( $CP(I) = p_i$ ); Survival Probability ( $SP(I) = \phi_i$ ), and New Entries ( $NE(I) = N b_{i-1} = B_{i-1}$ ). These result in the expected abundance shown under  $CN(I)$  and expected sample size, shown under  $N(I)$ . POPAN also reports the remaining expected summary statistics (for  $m, s, r$ , etc) but we have not reported them here.

When the first UFIT paragraph is run, POPAN imposes the AUTOMATIC constraint on  $p_1$  and  $p_6$  ( $CP(1)$  and  $CP(6)$  in Table 5(a)) which leads to confounded estimates for  $\phi_5$  ( $SP(5)$ ) and also for  $B_1$  and  $B_5$ . Excerpts of the estimate table are given in Table 5(b). We will now use the POPAN notation for the parameters, as defined in Table 5, because it distinguishes between the true value of the parameter (e.g.  $SP(5)$  in Table 5(a)) and the MV of its estimate (e.g.  $PHI(5)$  in Tables 5(b)-(d)). Notice first that most of the estimates are, to three significant figures or more, exactly equal to their true values (disagreement is partly because the expected statistics are rounded on input to the nearest whole number). The obvious exceptions are the confounded parameters:  $PHI(5)$  which clearly estimates the product  $SP(5) \times CP(6) = 0.8 \times 0.5 = 0.4$ ; and  $BH(1)$  and  $BH(5)$ , whose meaning is a bit more complicated. First note that the derived parameters  $NH(1)$  and  $NH(6)$ , which are derived from  $PH$  using  $NH(I) = N(I)/PH(I)$  are also confounded. Because  $PH(1) = PH(6) = 1$ , we have that  $NH(1) = N(1)$  and  $NH(6) = N(6)$ . Then,  $BH$  is derived from the  $NH$  and  $PHI$  as follows:

$$\begin{aligned} BH(I) &= NH(I+1) - PHI(I) + (NH(I) - N(I) + S(I)) \\ &= NH(I+1) - PHI(I) \times NH(I) \text{ when there are no losses on capture.} \end{aligned}$$

Thus, substituting the confounded value for  $NH(1)$ , we see that  $BH(1)$  is an estimate of

$$CN(2) - SP(1) \times N(1)$$

which, in this case, is  $1000 - 0.9 \times 500 = 550$ , a seriously biased estimate of the true value for  $B_1 = NE(2) = 100$ . For  $BH(5)$ , substituting the confounded values for both  $PHI(5)$  and  $NH(6)$  shows that  $BH(5)$  is an estimate of

$$N(6) - SP(5) \times CP(6) \times CN(5)$$

which is  $558.8 - 0.8 \times 0.5 \times 1272.0 = 50.0$ ; again not very close to the true value of  $NE(6) = 100$ .

Finally, note that the last estimate in the  $BH$  column is for the total net births over the experiment (we can denote it  $BH(\text{tot})$  rather than  $BH(6)$ ). It is derived as:

$$BH(\text{tot}) = NH(1) + \sum_{I=1}^{k-1} BH(I)$$

and so is also confounded whenever  $NH(1)$  or any of the  $BH$  is confounded.

TABLE 4. Example of a POPAN-6 Mean Value analysis using SIMULATE and UFIT. In the SIMULATE paragraph, expected statistic (XSTAT) data are generated from the one-group model ( $p_i, \phi_i, b_i$ ) and passed to three UFIT analyses, the first two from the correct model (without and with confounding removed) and the second from the almost correct model ( $p, \phi, b$ )

---

```

C   THIS IS PROGRAM 'TESTMVAL.POP'

SIMULATE:
  TITLE = ' EXAMPLE USING SAVE=XSTAT' ;
C   DEFINE A POPULATION OF 1000 ANIMALS (INITIALLY) AND TOTAL
C   NET ENTRIES OF 2000
  LSEL = 6 ;
  NEWENT = VECTOR(1000,100,250, 300, 250, 100) ;
C   CAPTURE RATES NOT QUITE CONSTANT...CHECK FOR BIAS IN CP=CONST MODEL
  CMECH = VECTOR(0.50,0.45,0.55, 0.45, 0.55,0.50) ;
C   SURVIVAL IS INITIALLY 0.9 AND DECLINES
  SMECH = VECTOR(0.90, 0.90, 0.85, 0.80, 0.80, 0.70) ;
C   DEFINE RUN TIME PARAMETERS
  SEED = -1410983851 ; RUN = YES ; WRITE = NO ; REP = 1 ;
C   USE AN J-D CONSTANT CAPTURE RATE ANALYSIS AND SAVE XSTATS.
  SAVE = XSTAT ; DATASET='test/mvxstat.tbl' ;
  ANALYSIS = 9 ;/

UFIT:
C   FIRST UFIT TASK IS UNCONSTRAINED J-S Full Model (with usual estimates
confounded)
C   UNGROUPED UFIT OF EXPECTED STATISTICS GENERATED BY SIMULATE
  TITLE='CONFOUNDED MV ANALYSIS OF UNGROUPED EXPECTED STATISTICS' ;
  LSEL = 6 ; INPUT = 'test/mvxstat.tbl' ;
  OUT = TABLE ; SUPP = BO ;
  TRACE = 1000000000000000000 ;
C   123456789012345678
  AUTO = YES ;
  WRITE = NO ;/

UFIT:
C   SECOND UFIT TASK REMOVES CONFOUNDED USING LINEAR CONSTRAINTS
  TITLE='UNCONFOUNDED MV ANALYSIS OF UNGROUPED EXPECTED STATISTICS' ;
  LSEL = 6 ; INPUT = 'test/mvxstat.tbl' ;
  OUT = TABLE ; SUPP = BO ;
C   DO P1 PK CONSTRAINTS MYSELF
  AUTO = NO ;
C   PIM MATRIX SETS P1=P6 TO RESOLVE NON-IDENTIFIABILITY OF CP(1)
C   and Phi(4) = Phi(5) TO RESOLVE NON-IDENTIFIABILITY OF CP(6)
C   i = ( 0, 1, 2, 3, 4, 5, 6 ) rows for p, phi and b
  PIM = ( 1, 2, 3, 4, 5, 1 ),
        ( 6, 7, 8, 9, 9 ),
        (10, 11, 12, 13, 14, 15 )
  WRITE = NO ;/

UFIT:
C   THIRD UFIT FITS CONSTANT CAPTURE RATE (APPROXIMATELY CORRECT) MODEL
  TITLE='OVER-CONSTRAINED BUT UNCONFOUNDED MV ANALYSIS OF EXPECTED
STATISTICS' ;
  LSEL = 6 ; INPUT = 'test/mvxstat.tbl' ;
  OUT = TABLE ; SUPP = BO ;
C   DO P1 PK CONSTRAINTS MYSELF
  AUTO = NO ;
C   GLOBAL CONSTRAINTS STILL WORK AS IN POPAN-5
C   TRY THE MODEL WITH CONSTANT CAPTURE TO SEE BIAS EFFECT OF NON-CONSTANT P
  CPCON = CONSTANT ;
  WRITE = NO ;/

```

---

TABLE 5. Selected output from the example in Table 4. The notation of this paper is given in the column headings to explain the POPAN notation below it (in uppercase letters).  $E(parm)$  and  $SE(parm)$  are the expected value and SE of the estimated  $parm$  computed by the mean value analysis

$i$	$p_i$	$\phi_i$	$Nb_{i-1}$	$N_i$	$n_i = N_i p_i$			
I	CP(I)	SP(I)	NE(I)	CN(I)	N(I)			
(a) Preliminary Report (parameters and expected statistics)								
1	0.5000	0.9000	1000.0	1000.0	500.0			
2	0.4500	0.9000	100.0	1000.0	450.0			
3	0.5500	0.8500	250.0	1150.0	632.5			
4	0.4500	0.8000	300.0	1277.5	574.9			
5	0.5500	0.8000	250.0	1272.0	699.6			
6	0.5000	0.7000	100.0	1117.6	558.8			
$i$	$E(p_i)$	$SE(p_i)$	$E(\phi_i)$	$SE(\phi_i)$	$E(Nb_i)$	$SE(Nb_i)$	$E(N_i)$	$SE(N_i)$
I	PH(I)	S(PH(I))	PHI(I)	S(PHI(I))	BH(I)	S(BH(I))	NH(I)	S(NH(I)!N)
(b) First UFIT (correct model, confounding not removed)								
1	1.0000 G	0.0000	0.9007	0.0257	547.9847	45.2717	500.0000	19.1970
2	0.4507	0.0259	0.8994	0.0278	252.8680	48.3365	998.3530	50.4905
3	0.5501	0.0237	0.8499	0.0309	299.8265	44.6376	1150.7405	44.2887
4	0.4500	0.0223	0.8001	0.0362	250.3713	40.6372	1277.8608	53.4390
5	0.5506	0.0263	0.4000	0.0185	50.4295	15.0682	1272.7928	55.6019
6	1.0000 G	0.0000	0.0000 U	0.0000 U	1901.4801	23.3154	559.5477	19.8718
(c) Second UFIT (correct model, confounding removed)								
1	0.4999	0.0391	0.9007	0.0257	97.4963	86.2650	1000.1340	87.2729
2	0.4507	0.0259	0.8994	0.0278	252.8674	48.3539	998.3538	50.7495
3	0.5501	0.0237	0.8499	0.0309	299.8258	44.6640	1150.7404	44.6801
4	0.4500	0.0223	0.8001	0.0362	250.3736	40.6577	1277.8593	53.8391
5	0.5506	0.0263	0.8001	0.0362	100.8706	30.1186	1272.7980	55.9841
6	0.4999	0.0391	0.0000 U	0.0000 U	2001.5677	31.7782	1119.2454	83.3283
(d) Third UFIT (approximately correct model, confounding removed)								
1	0.4988	0.0122	0.8844	0.0233	50.8901	40.6524	1002.3600	45.9738
2	0.4988	0.0122	0.9368	0.0257	344.8791	36.8731	937.3544	35.7344
3	0.4988	0.0122	0.8033	0.0250	218.6320	33.4788	1222.9871	40.1051
4	0.4988	0.0122	0.8698	0.0295	322.5935	34.7327	1201.0051	38.8143
5	0.4988	0.0122	0.7688	0.0347	70.5670	28.3493	1367.2290	45.1705
6	0.4988	0.0122	0.0000 U	0.0000 U	2009.9218	28.1885	1121.7512	48.7772

There are many ways to resolve the confounding: the simplest is to use a linear constraint on  $p_6$  or  $\phi_5$  at the one end, or a linear constraint on  $p_1$  or on  $b_1$  at the other. Note that you cannot constrain  $b_0$ , but any constraint that resolves the confounding of  $b_1$  (and hence  $B_1$ ) should also resolve the confounding of  $p_1$ . In many situations, a closure constraint on  $b_1$  is a reasonable restriction. Other ways are a covariate model for any of the three parameter types ( $p$ ,  $\phi$ ,  $b$ ) although a covariate model for  $\phi$  only resolves  $p_6$  and you would still need to constrain  $p_1$ . The second UFIT (Table 4) uses sameness constraints specified by a PIM to resolve all parameters. The constraints are artificially chosen using knowledge of the correct model to show (Table 5(c)) that all the estimates can now be determined and BH(tot) is unbiased for the true total (2000). In analysing real data, we would have to guess reasonable parameter constraints that will resolve confounding and carefully assess their validity using goodness of fit and other model fit diagnostics.

MV analysis can also be used to investigate the expected precision of estimates and their sensitivity to incorrect constraints. Note that while precision is expected



to be good for the capture rate and survival estimates (S(PH( $I$ )) and S(PHI( $I$ )) in Table 5), it is rather poor for the net births S(BH( $I$ )). In the last UFIT in Table 4, we fit the constant capture probability model CPCON = CONST. This will resolve the confounding but it introduces bias because the capture rates are not, in fact, constant. The degree of bias in the model parameters and the derived parameters NH and BH(tot) can be judged by comparing the expected value of the estimates in Table 5(d) with the true values in Table 5(a). Bias in the overall recruitment is negligible although individual recruitment and population estimates are more severely biased.

## 5 Discussion

We expect that open models of the Jolly-Seber (JS) type will become increasingly important in bird studies now that the software to analyse data from JS experiments is readily available in MARK and in POPAN. The UFIT method in POPAN provides a means of modelling the birth and recruitment process, in addition to the survival and capture rates, and thence derives estimates of population size and total recruitment. Temporal and group constraints on births can be imposed in a fashion that will be familiar to those who model survival and capture rates using CJS models in MARK. Age constraints can also be imposed (i.e. where groups are year classes in annually sampled populations) but the group by time parameter structure in POPAN is rectangular, not triangular as in annual CJS and band-recovery studies so special steps have to be taken to deal with structural zeros among the sample sizes (Arnason and Schwarz, 1999).

The birth process is both more complex and more difficult to model than the survival process. As with survivals, the user needs to consider occasions when there is closure (no births and/or losses) and model these as fixed constraints, and to adjust for unequal sample time intervals in imposing sameness or covariate constraints between times. Unlike survival rates, sameness and covariate constraints that involve more than one group are not absolute, but constrain the relative recruitment patterns in the two groups. Estimates of gross births are available and can be adjusted to a per-unit-time basis and can be modelled and constrained, but the user has to consider whether the conditions for deriving gross births apply and, because gross births is a function of both survival and birth rates, whether confounding in the  $\phi$  estimates makes some of the gross births meaningless; e.g. if the confounding of  $\phi_{k-1} p_k$  is artificially resolved (as in the MV example in Table 4) by fixing  $p_k$  to 1, then  $\phi_{k-1}$  is biased and hence so is  $B_{k-1}^*$ . Total net and gross recruitment are available over the entire sampling experiment (the initial population estimate plus the sum of the  $B_i$  or  $B_i^*$ ) but to obtain this, the non-identifiability of initial population size and  $b_0$  has to be resolved by imposing constraints, usually on  $p_1$  or (in emergence and escapement studies) by starting sampling early enough that it is reasonable to assume that  $b_0 = 0$ . When the conditions for estimating total recruitment apply, the JS model can allow derivation of average staging time (mean time spent on the area when arrival and departure of birds are the sole sources of 'births' and 'deaths') using Little's Law (Allen, 1990): the average staging time = total standing population/total arrivals =  $(\sum N_i)/(\sum B_i^*)$

The use of a DM in POPAN-6 to obtain the constrained maximum of the open-model likelihood makes it easy to obtain and constrain other derived parameters, such as the fecundities ( $B_i/N_i$ ) and the seniorities ( $\gamma_i$ ) and finite rates of change ( $\lambda_i$ ) defined above. However, just because these parameters can be constrained,

does not mean it makes biological sense; for example what does it mean to model or constrain the  $\gamma_i$ , a complex function of the birth and death rates, especially if the underlying ( $b_i$ ,  $\phi_i$ ) rates are not constrained? The biologist needs to consider what effects influence the population dynamics and which mechanisms they operate on. On the other hand, fitting a constraint on a derived parameter, such as constraining the  $\lambda_i$  to be fixed, is a useful smoothing trick (in this case, to approximate the change in population size over time by a linear trend) even if we do not believe there is a complex balancing of births and mortalities needed to achieve this. Alternatively one might fit a random effects model in which the  $\lambda_i$  vary about a common  $\lambda$  as implemented for  $\phi$  in MARK.

There may be technical difficulties in getting the more complex JS models to fit. There are  $gk$  more parameters to estimate than in an equivalent CJS model, and these additional birth parameters are notorious for being imprecise, even in experiments where the capture and survival rate estimates are quite precise. We have noted in this paper that there may be difficulty in obtaining convergence of the iterative maximization when there are unresolved parameter confoundings, small statistics problems, or mis- or over-specified covariance models. We have suggested here some technical solutions to try when these problems arise: fixing parameters (which may create interpretation problems); adding constraints (which may introduce bias), or regrouping sample times and cohort groups (which may increase sample and summary statistic sizes but risks introducing heterogeneity). As we have shown here, these effects can be investigated using simulation. MV simulations are useful for estimating precision and bias and the effects of parameter confounding and model over-simplification on these. It can also be used to get an idea of the ability to discriminate among candidate models by comparing the (expected) deviances obtained with different MV simulations models run with one set of input statistics. Stochastic simulations can be used to determine if convergence is likely to occur reliably for the chosen candidate model when fit to data with given (guessed) population and sample sizes and turnover rates. As we have described above, it can also be used to perform a parametric bootstrap goodness-of-fit test of a fitted model.

Another useful strategy in fitting JS models is to ignore the birth component initially and use CJS models in MARK to fit the survival and capture components using the AIC and goodness-of-fit criteria to select the most appropriate model. One can then use POPAN to explore models involving different candidates for modelling the  $b$  while keeping the ( $p$ ,  $\phi$ ) part of the model fixed at the final model determined in the CJS analyses. We have done a number of experiments with simulated data that show this is a reasonable strategy and yields much the same model selection criteria ( $\Delta$ AIC) and estimates, at least when there are no serious violations of the assumptions of capture and survival homogeneity (see the TESTMARK suite of examples available from the Downloads page of the POPAN web site: [www.cs.umanitba.ca/~popan](http://www.cs.umanitba.ca/~popan)).

Finally, the most important consideration in using JS rather than CJS methods is to ensure that the sample design supports meaningful estimates of recruitment and abundance. Because CJS models derive estimates entirely from the marked animals and do not take account of the numbers of unmarked animals encountered, the biologist does not have to be particularly concerned with how unmarked animals are added to the sample. As long as the animals chosen and marked can be considered representative in their survival and recapture rates of some wider population of interest, it does not matter if samples are drawn from a well-defined

target population. In JS experiments, having a well-defined target population and having a proper probability sample from that population, become crucial. For example, recruitment estimates could be meaningless if the study area is expanded over time, thus changing the ‘population at risk’ of capture. Similarly, siting sampling locations in a small sub-area of a larger, unbounded population can create time-varying differences in the population at risk and in the biasing influence of transient animals and those whose home range only partly overlaps the sub-area and so are at reduced risk of capture. And using the derived relative rates is not a solution. While it is known that the  $b_i$ ,  $\gamma_i$  and  $\lambda_i$  are more robust to capture heterogeneity than the  $B_i$  and  $N_i$  (Schwarz, 2000), they can still be rendered meaningless by an ill-defined population and inadequate sample coverage of that population in space and time.

Despite these difficulties, the unified open JS model opens up new methods for studying the dynamics of populations. POPAN-5 provides one method of fitting the unified model that is particularly strong when trying to fit environmental covariates and group effects. POPAN-6 provides another method that is particularly convenient for providing user flexibility in constraint definition and ease of implementing derived estimates. In the future, the likelihood can be redeveloped by computing the contribution to the likelihood from each encounter history, rather than from the summary statistics; this would then allow the use of individual covariates. Eventually, we may see it used with Bayesian approaches to model estimation and selection, and this may provide another unified approach to parameter interval estimation, model selection, and random effects modelling.

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### REFERENCES

- ALLEN, A. O. (1990) *Probability, Statistics, and Queueing Theory with Computer Science Applications* 2nd edn (San Diego, Academic Press).
- ARNASON, A. N. & SCHWARZ, C. J. (1995) POPAN-4. Enhancements to a system for the analysis of mark-recapture data from open populations, *Journal of Applied Statistics*, 22, pp. 785-800.
- ARNASON, A. N. & SCHWARZ, C. J. (1998) POPAN-5: a data maintenance and analysis system for mark-recapture data. Scientific Report, Department of Computer Science, University of Manitoba, Winnipeg, viii + 318 pp.
- ARNASON, A. N. & SCHWARZ, C. J. (1999) Using POPAN-5 to analyse banding data, *Bird Study*, 46(suppl.), pp. S157-168.
- CROTHERS, A. D. (1973) The effects of unequal catchability on Jolly-Seber estimates, *Biometrics*, 29, pp. 79-100.
- JOLLY, G. M. (1965) Explicit estimates from capture-recapture data with both death and immigration—stochastic model, *Biometrika*, 52, pp. 225-247.
- LEBRETON, J.-D., BURNHAM, K. P., CLOBERT, J. & ANDERSON, D. R. (1992) Modeling survival and testing biological hypotheses using marked animals: a unified approach with case studies, *Ecological Monographs*, 62, pp. 67-118.
- PRADEL, R. (1996) Utilization of capture-mark-recapture for the study of recruitment and population growth rates, *Biometrics*, 52, pp. 703-709.
- PRADEL, R. & LEBRETON, J.-D. (1993) User's manual for program SURGE Version 4.2. Centre d'Ecologie Fonctionnelle et Evolutive-CNRS, Montpellier, France.

- SCHWARZ, C. J. (2000) The Jolly-Seber model: more than just abundance, *Journal of Agricultural, Biological, and Environmental Statistics*, in press.
- SCHWARZ, C. J. & ARNASON, A. N. (1996) A general methodology for the analysis of capture-recapture experiments in open populations, *Biometrics*, 52, pp. 860-873.
- SCHWARZ, C. J., BAILEY, R. E., IRVINE, J. E. & DALZIEL, F. C. (1993) Estimating salmon spawning escapement using capture-recapture methods, *Canadian Journal of Fisheries and Aquatic Sciences*, 50, pp. 1181-1191.
- WHITE, G. C. & BURNHAM, K. P. (1999) Program MARK—survival estimation from populations of marked animals, *Bird Study*, 46(suppl.), pp. S120-139.