

Appendix: Multi-model inference of mate choice effects from an information theoretic approach

S-1) Mutual Mating Propensity Models

SEXUAL SELECTION MODELS

Female sexual selection

The model is $q'_{ij} = m_{ij}q_{ij}$ with

$$m'_{11} = m'_{12} = \dots = m'_{1k_2} = a_1$$

$$m'_{21} = m'_{22} = \dots = m'_{2k_2} = a_2$$

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$$m'_{(k_1-1)1} = m'_{k_12} = \dots = m'_{k_1k_2} = a_{k_1-1}$$

$$m'_{k_11} = m'_{k_12} = \dots = m'_{k_1k_2} = 1 \quad (\text{A1})$$

and restriction $a_i > 0 \forall i$.

Note that the relationships among the propensities will not be altered if we divide by a_{k_1} so that we have fixed $a_{k_1} = 1$. Thus, under female sexual selection models we can consider $H_1 \in [1, k_1 - 1]$ different parameters.

The normalization factor is the mean propensity $M = \sum m'_{ij}q_{ij}$. Now, if we compute the marginal female and male propensities we see that

$$m_{\text{Fem}_1} = a_1/M; m_{\text{Fem}_2} = a_2/M \dots; m_{\text{Fem}_{k_1}} = 1/M$$

$$m_{\text{Male}_1} = m_{\text{Male}_2} = m_{\text{Male}_3} = \dots = m_{\text{Male}_{k_2}} = M/M = 1$$

Thus, the model just depends on the parameters a_i . Let the number of different parameters be $H_1 = k_1 - 1$. By derivation of (A1), equating to zero and checking it is a maximum, we obtain the maximum likelihood estimate of the parameter a_h

$$\hat{a}_h = \left(\frac{1 - \sum_i^{H_1} p_{1i}}{p_{1h}} \right) \frac{\sum_j^{k_2} x_{hj}}{n - \sum_i^{H_1} \sum_j^{k_2} x_{ij}} = \frac{\lambda(a_h)}{\lambda(1)}$$

$\lambda(\theta)$ is defined in general for any set A of mating pair types having the same value of propensity θ as

$$\lambda(\theta) = \frac{\sum_t^A x_t}{\sum_{t_1 t_2}^A p_{1t_1} p_{2t_2}} \quad (\text{A2})$$

So, $\lambda(a_h)$ expresses the sum of the observed matings having expected propensity a_h divided by the sum of the product of the population frequencies from each partner type.

In the particular case of having $k_1 - 1$ parameters then the observed matings with propensity a_h are just $\sum x_{hj}$ with the sum over all male types. The sum of the product of frequencies is $\sum p_{1h} \times p_{2j} = p_{1h} \sum p_{2j} = p_{1h}$.

In the opposite case, having only one parameter the sum of observed matings having propensity a , implies $\sum \sum x_{hj}$ where the first summatory is for all the female types except females of type k_1 , and the second is over all male types. The sum of the product of frequencies is $1 - p_{1k_1}$.

Similarly, $\lambda(1)$ corresponds to the sum of the observed matings having expected propensity 1 divided by the sum of the corresponding products of population frequencies.

The general case for any parameter a_h , $1 \leq h < k_1$, is expressed as $\lambda(a_h)$ applying (A2).

Therefore, for any given number of parameters H_1 , the maximum likelihood estimate of the parameters under the female sexual selection models is

$$\hat{a}_h = \frac{\lambda(a_h)}{\lambda(1)}$$

SEXUAL ISOLATION MODELS

We could define sexual isolation models in which the homotype mating has absolute propensity of 1 while the different heterotypes have absolute value of a_{ij} . The maximum likelihood estimate is

$$\hat{a}_{h_1 h_2} = \frac{\lambda(a_{h_1 h_2})}{\lambda(1)}$$

The number of parameters in this type of model is $K - \min\{k_1, k_2\} - \sum_S (C_s - 1)$ where the sum is over the set of different heterotype matings and C_s is the cardinality of each set.

DOUBLE EFFECT MODELS

The following models have double effect even when the population frequencies are uniform.

Double effect models with sexual selection in one sex under uniform frequencies

The simplest approach consists to build a new model from the symmetric one by setting $m'_{ii} = 1$ and $m'_{jj} = 1 + c$. Then, if we desire isolation jointly with sexual selection only in females we additionally set $m'_{ij} = 1 - c$ on the contrary, if we desire selection only in males we set $m'_{ji} = 1 - c$ with $-1 < c < 1$. If the frequencies are not uniform the model generates isolation jointly with sexual selection in both sexes.

In the case of the mixed model with $m'_{ij} = 1 - c$ (female sexual selection if frequencies are uniform) the maximum likelihood estimate of c is one of the roots of the quadratic

$$(x_{jj} - x_{ij} + n'D) - c[x_{ij} + x_{jj} + D(x_{jj} - x_{ij})] - c^2 D[n' - (x_{ij} + x_{jj})] = 0$$

where $D = q_{ij} - q_{jj}$ and $n' = \sum x_{ij}$ is the number of matings (sample size).

If the frequencies are uniform and $k_1 = k_2$, i.e. $p_{1i} = p_{1j} = p_{2i} = p_{2j} \forall i, j$ then

$$\hat{c} = \frac{x_{jj} - x_{ij}}{x_{jj} + x_{ij}}$$

The case for male sexual selection is obtained simply by interchanging x_{ij} by x_{ji} and q_{ij} by q_{ji} in the formulas.

The above model has only one parameter c ; we can introduce a more complex two parameter model, $M_{(a,c)}$ by setting $m'_{ii} = a$, $m'_{jj} = 1 + c$ and $m'_{ij} = 1 - c$, for female sexual selection (or $m'_{ji} = 1 - c$ for male sexual selection). For obtaining the MLE of this two parameter mixed model, with restrictions $a > 0$, $c < |1|$, we have used a numerical bounded Nelder-Mead simplex algorithm (Press 2002; Singer and Singer 2004; Gao and Han 2012).

Double effect models with sexual selection in both sexes under uniform frequencies

To get isolation jointly with sexual selection in both sexes under uniform frequencies, we just need to combine the above uniform one parameter models of each sex, so that

$$m'_{ii} = 1, \quad m'_{jj} = 1 + c \text{ and } m'_{ij} = m'_{ji} = 1 - c.$$

The maximum likelihood estimate of c involves the solution of the quadratic

$$[x_{jj} - x_s + n'D_2] - c[x_{jj} + x_s + D_2(x_{jj} - x_s)] + c^2 D_2[x_{jj} + x_s - n'] = 0$$

where $x_s = x_{ij} + x_{ji}$ and $D_2 = q_{ij} + q_{ji} - q_{jj}$.

However, we can set even a more simplistic mixed model with sexual selection in both sexes, $m'_{ii} = m'_{ij} = m'_{ji} = 1$ and $m'_{jj} = a$. The estimate of a under this model is $\lambda(a) / \lambda(1)$.

General double effect models

We can also define a set of general models where any propensity m'_{ij} has parameter θ_{ij} with at least one propensity having value of 1. The MLE of the parameters of this kind of model is

$$\hat{\theta}_{ij} = \frac{\lambda(\theta_{ij})}{\lambda(1)}$$

where $\lambda(\theta_{ij})$ is defined as in (A2).

The most parameterized model defined in this way has $K-1$ parameters and coincides with the saturated model so that the estimates are the corresponding pair total indices (PTI).

All the above derived MLE formulae have also been checked by a numerical bounded Nelder-Mead simplex algorithm (Press 2002; Singer and Singer 2004; Gao and Han 2012). The set of described models jointly with their effects are summarized in Table S1.

Table S1. Propensity-based mating models for any number of mating traits k_1 and k_2 , as defined by different parameters and their effects

Name (abbreviation)	Model	Number of Parameters and MLE	Effect
Random (M_0)	$m'_{ij} = 1$	0	Random mating
Multiplicative Sexual Selection Models			
Female sexual selection (S_{Fem} -1P, -2P...)	$i < k_1: m'_{ij} = m'_{ij+1} = \dots = m'_{ik_2} = a_i > 0$	$[1, k_1 - 1]$	Non-freq-dep sexual selection in

	else $m'_{kij} = 1$		females
		$a_i = \lambda(a_i) / \lambda(1)$	
Male sexual selection ($S_{\text{Male-1P, -2P...}}$)	$j < k_2: m'_{ij} = m'_{i+1j} = \dots = m'_{kij} = b_j > 0$ else $m'_{ik2} = 1$	$[1, k_2 - 1]$	Non-freq-dep sexual selection in males
		$b_i = \lambda(b_i) / \lambda(1)$	
Two sex sexual selection ($S2-2P, \dots$)	combine female and male sexual selection models:	$[2, k_1+k_2 - 2]$	Non-freq-dep sexual selection in both sexes
	$i < k_1$ and $j < k_2:$ $m'_{ij} = a_i b_j$ else		
	$i < k_1: m'_{ik2} = a_i$ else	$a_i = \lambda_{\text{fem}}(a_i) / \lambda_{\text{fem}}(1)$	
	$j < k_2: m'_{kij} = b_j$ else $m'_{k1k2} = 1$	$b_i = \lambda_{\text{male}}(b_i) / \lambda_{\text{male}}(1)$	
Sexual Isolation Models	non-multiplicative		Isolation freq-dep
Symmetric sexual isolation ($I-1p$)	$m'_{ii} = a > 0 \forall i$ and $m'_{ij} = 1$	1	Isolation UF
Full sexual isolation ($I-Hp$)	$m'_{ii} = a_i > 0; m'_{ij} = 1$	$H = \min(k_1, k_2)$ $a_i = \lambda(a_i) / \lambda(1)$	Isolation freq-dep
Double effect Models: uniform frequencies			Isolation + sexual selection under UF
Double-1: Isolation + one sex selection ($D_{\text{Fem-c1p}}, (D_{\text{Male-c1p}}$)	$m'_{ii} = 1; m'_{ij} = 1+c;$	1	Isolation + 1 sex selection UF
	m'_{ij} or $m'_{ji} = 1 - c;$ $ c < 1$	$c = (x_{ij} - x_{ji}) / (x_{ij} + x_{ji})$	
Double -1: Isolation + two sex selection ($D2-c1p$)	$m'_{ii} = 1; m'_{ij} = 1+c;$	1	Isolation + 2 sex selection UF
	$m'_{ij} = m'_{ji} = 1 - c;$ $ c < 1$	$Ac^2 + Bc + D = 0$	
Double -2: Isolation + one sex selection ($D_{\text{Fem-c2p}}, (D_{\text{Male-c2p}}$)	$m'_{ii} = a; m'_{ij} = 1+c;$	2	Isolation + one sex selection UF
	m'_{ij} or $m'_{ji} = 1 - c;$ $ c < 1; a > 0$	numerical	
General Double Effect Models ($D-gp$)		$g \in [1, K-1]$	Isolation+Sex Sel

		$a_i = \lambda(a_i) / \lambda(1)$	
Saturated (M_{sat})	$m'_{ij} = a_{ij}; m'_{k_1 k_2} = 1$	$K - 1$	

k_1 : number of female categories; k_2 : number of male categories; UF: under uniform frequencies; $K = k_1 \times k_2$; x_{ij} : number of matings $i \times j$.

S-2) Monte Carlo simulation of mating tables

MODELS

Relying on the mutual mating propensity parameters we can generate various effects models (see some examples in Table S1 and Fig S1) and produce distinct mating tables under these models.

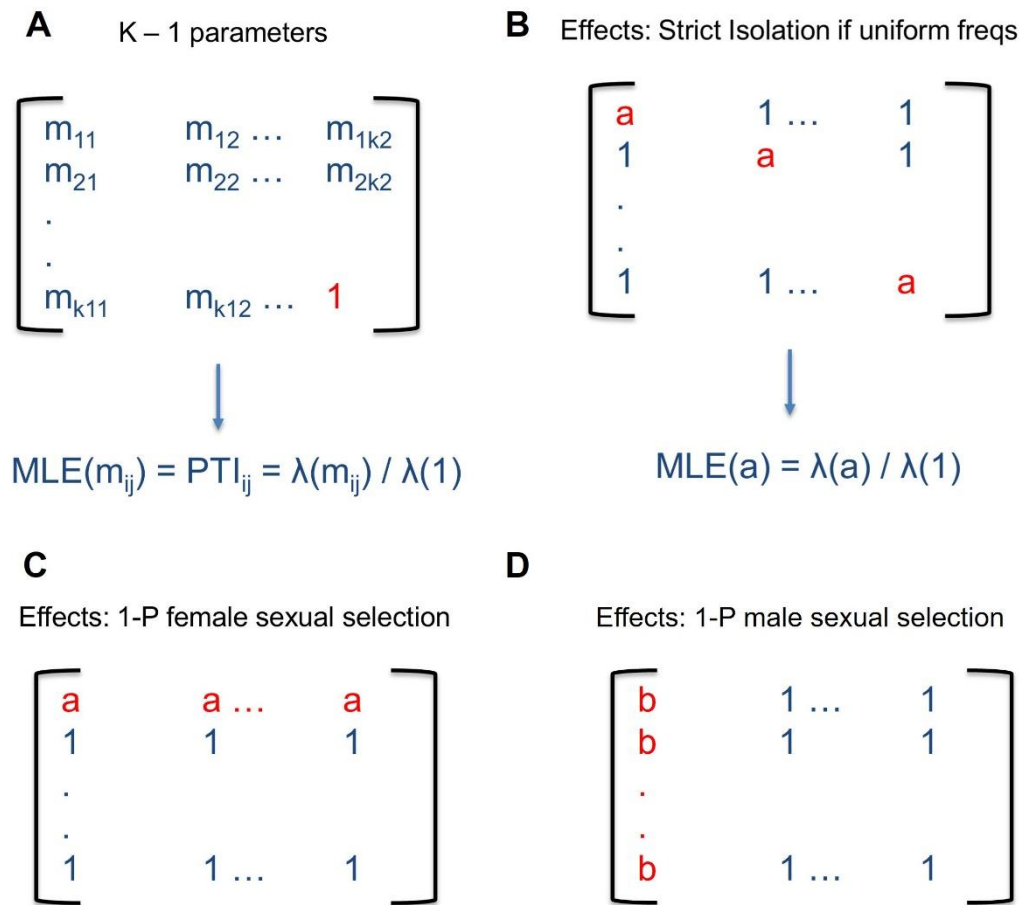


Fig. S1. Mating models as defined by their effects. A: The saturated model with $K-1$ free parameters; this model produces double effect of sexual isolation plus sexual selection. B: One-parameter model generating only sexual isolation (intersexual selection), or with sexual selection, depending if the frequencies are uniform or not. C: One-parameter model producing female selection model. D: One-parameter model producing male selection model. The ML estimates in C and D are obtained by the same formula as in B.

MATING TABLES

The mating tables for the simulation experiments were generated by the program

MateSim (Carvajal-Rodriguez 2018) available at

<http://acraaj.webs.uvigo.es/MateSim/matesim.htm>.

We ran 1,000 runs for each case. For each run we first generated the number of premating males and females from a given population size. For example, if the population size consisted in n_1 females and n_2 males, we got $n_{1A} = n_1 \times U$ females of the A type and $n_{1B} = n_1 - n_{1A}$ females of the B type. Where U is a value sampled from the standard uniform. The premating males were obtained similarly.

Then, the female population frequencies were $p_{1i} = n_{1i} / n_1$ and $p_{2i} = n_{2i} / n_2$ for the male ones.

Finally, we obtained a sample of n' matings where the number of counts for each mating type $i \times j$ was

$$Q(i,j) = n' \times p_{1i} \times p_{2j} \times m'_{ij} / M$$

where m'_{ij} are the mating propensity parameters as defined for each kind of model and

$$M = \sum p_{1i} \times p_{2j} \times m'_{ij}.$$

The format of the obtained tables was the same as the JMating (Carvajal-Rodriguez and Rolan-Alvarez 2006) input files (Fig S2).

```
# format number
0
# num of types
2
#premating male numbers
1626      3374
#premating female numbers
917      4083
# matings by rows (females)
30      62
133      275
```

Fig. S2. Example of a table generated by the simulations. The format is the same as for the JMating software.

Table S2. Average (standard error) parameter estimates for different simulated models under sample size 100.

Model		m'_{11}	m'_{12}	m_{21}	m_{22}
M₀	Expected	1	1	1	1
	AICc	1.0±0.000	1.0±0.000	1.0±0.000	1.0±0.000
	KICc	1.0±0.000	1.0±0.000	1.0±0.000	1.0±0.000
	BIC	1.0±0.000	1.0±0.000	1.0±0.000	1.0±0.000
Isol	Expected	2	1	1	2
	AICc	2.0±0.005	1.2±0.148	1.0±0.001	2.1±0.028
	KICc	2.0±0.005	1.1±0.108	1.0±0.001	2.1±0.023
	BIC	2.0±0.008	1.0±0.000	1.0±0.000	2.1±0.007
SS_{Fem}	Expected	2	2	1	1
	AICc	1.8±0.094	1.8±0.142	1.0±0.043	1.0±0.013
	KICc	1.7±0.164	1.6±0.209	1.1±0.068	1.0±0.014
	BIC	1.5±0.217	1.4±0.209	1.1±0.083	1.0±0.0157
SS_{Fem}U	Expected	2	2	1	1

AICc	2.0±0.000	2.0±0.000	1.0±0.000	1.0±0.000
KICc	2.0±0.000	2.0±0.000	1.0±0.000	1.0±0.000
BIC	2.0±0.000	2.0±0.000	1.0±0.000	1.0±0.000

M_0 : Random mating model. Isol: isolation model; SS_{Fem} : Female sexual selection model. SS_{FemU} : Female sexual selection model with uniformly distributed population frequencies $p_{1i}=1/k_1$ and $p_{2j}=1/k_2$.

Table S3. *Littorina saxatilis* data. Mutual-propensity estimates from multimodel inference under the KICc. Values are the average over the two years plus minus the standard error.

		Males		
		RB	HY	SU
	RB	1.8±0.17	1.6±0.32	0.6±0.30
Females	HY	0.6±0.30	1.1±0.70	1±0
	SU	0.16±0.01	0.6±0.30	1.5±0.30

Table S4. *Littorina saxatilis* data. Mutual-propensity estimates from multimodel inference under the BIC. Values are the average over the two years plus minus the standard error.

		Males		
		RB	HY	SU

	RB	1.9±0.10	1.5±0.32	0.6±0.29
Females	HY	0.6±0.29	1.1±0.61	1±0
	SU	0.18±0.00	0.6±0.29	1.5±0.30

S-3) Example

```

# format number
0
# num of types
3
#premating male numbers
173 69 234
#premating female numbers
175 78 345
# matings by rows (females)
13 7 7
4 2 6
2 2 30

```

Fig. S3. Input file for the *Littorina saxatilis* example (year 1999, data kindly provided by E. Rolán-Alvarez). The format is the same as for the JMating software.

References

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