

DEB-in-Practice Advanced data analysis

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Amsterdam Institute for Life and Environment

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Empirical cycle



Avoid thinking in terms of "the" model -> families of related models

"All models are wrong, some are useful"



Modular Framework



 possible to develop and test modules independently -> walk up and down levels of complexity

AmP procedure







5

"Augmented" loss function



Like et al 2020 The use of augmented loss functions for estimating dynamic energy budget parameters. Ecol Model

Combining different entries



a continuum between parameters being the same or different: parameters are allowed to vary between (related) species, but not that much

extension of the loss function is a function of weight coefficients and parameters, but not of data or predictions.

DEB theory takes parameter values to be individual-specific, but the differences are small enough for the mean values to represent the species, eco-type or population.

If enough is known about each individual, the different entries might even represent individuals, rather than species

essential feature for DEB theory, since evolutionary selection is at the level of individuals, and treating parameters as individual-specific evolutionary changes in parameter values, as studied in the field of adaptive dynamics, can be included naturally By fitting each species one-by-one, large differences in parameter values can show up. But is this the result of real differences between species or an artifact caused by data not determining parameters accurately

How much can we reduce the differences in parameter values, without affecting the goodness of fit too much? Since, in our view, parameter values represent species diversity, we are looking for a reduction in this diversity that is still allowed by data

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RESEARCH ARTICLE



Tomos Potter¹ | David N. Reznick² | Tim Coulson¹







Augmented loss function

$$F_{sb} = \sum_{i=1}^{n} \sum_{j=1}^{n_i} \frac{w_{ij}}{n_i} \frac{(d_{ij} - p_{ij})^2}{d_i^2 + p_i^2} + \sum_{k=1}^{N} \frac{w_k \operatorname{var}(\theta_k)}{\operatorname{mean}(\theta_k)^2}$$

with $d_i = \frac{1}{n_i} \sum_{j=1}^{n_i} d_{ij}$ and $p_i = \frac{1}{n_i} \sum_{j=1}^{n_i} p_{ij}$

"Augmented" loss function

```
run pet
                                                  list of pets
close all;
                                                  estimation options
global pets
pets = { ...
         'Clarias gariepinus', ...
          'Clarias gariepinus x Heterobranchus longifilis', ...
          'Heterobranchus_longifilis', ...
          'Heterobranchus longifilis x Clarius gariepinus', ...
       };
estim options('default');
estim options('max step number', 1e3);
estim options('max fun evals',5e3);
```

```
estim_options('pars_init_method', 1);
estim_options('results_output', 3);
%estim_options('method', 'no');
```

```
pets = { ...
    'Clarias_gariepinus', ...
    'Clarias_gariepinus_x_Heterobranchus_longifilis', ...
    'Heterobranchus_longifilis', ...
    'Heterobranchus_longifilis_x_Clarius_gariepinus', ...
};
```





Parameters with reduced variance in the Augmented loss function procedure



11

function [par, metaPar, txtPar] = pars init group(metaData)

metaPar.model = {'abj', 'abj', 'abj', 'abj'}; metaPar.cov rules = ''; % see function parGrp2Pets metaPar.weights.E Hb = 0; metaPar.weights.E Hj = 0; metaPar.weights.E Hp = 0; metaPar.weights.h a = 0; metaPar.weights.kap = 0;metaPar.weights.p M = 2;metaPar.weights.v = 2;metaPar.weights.z = 0; metaPar.weights.del M = 0; metaPar.weights.f tW = 5;

$$F_{sb} = \sum_{i=1}^{n} \sum_{j=1}^{n_i} \frac{w_{ij}}{n_i} \frac{(d_{ij} - p_{ij})^2}{d_i^2 + p_i^2} + \sum_{k=1}^{N} \frac{w_k \operatorname{var}(\theta_k)}{\operatorname{mean}(\theta_k)^2}$$

with $d_i = \frac{1}{n_i} \sum_{j=1}^{n_i} d_{ij}$ and $p_i = \frac{1}{n_i} \sum_{j=1}^{n_i} p_{ij}$

parameter θ_k is

different

 w_k large

$$w_k = 0$$
 parameter θ_k is the same

function [par, metaPar, txtPa:

par.z = [17.2809]



10.9743 12.9022

11.952]; free.z = [1 1 1 1]; units.z = '-';

Application of the augmented loss function to understand differences in morphotypes



ECOLOGICAL

Ecological Modelling 430 (2020) 109088



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Can DEB models infer metabolic differences between intertidal and subtidal morphotypes of the Antarctic limpet *Nacella concinna* (Strebel, 1908)?



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Application of the augmented loss function to understand differences in morphotypes



Some overall results:

- Minor differences in temperature-corrected parameter values between both populations
- Despite the known morphological difference between the populations, the difference in shape coefficients was small

Application of the augmented loss function to understand differences in morphotypes



Authors ran "merging trials" gradually increasing the weight of the parameter:

they tried to merge the models into a single one, parameter by parameter, to evaluate the contrasts in parameters between the types

models were merged without generating significant changes in MRE and loss function values

=> There is still a lot to understand with this approach

Augmented loss function in the context of multiple compounds







OECD guidelines 232 Collembolan Reproduction Test in Soil



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MODELING THE EFFECTS OF BINARY MIXTURES ON SURVIVAL IN TIME

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(Received 25 August 2006; Accepted 8 January 2007)

deb ► AmPtox ► OECD232_Cd_Cu_Pb_Zn

mydata_OECD232_Cd_Pb.m
 mydata_OECD232_Cd_Zn.m
 mydata_OECD232_Cu_Cd.m
 mydata_OECD232_Cu_Pb.m
 mydata_OECD232_Zn_Cu.m
 mydata_OECD232_Zn_Pb.m

predict_OECD232_Cd_Pb.m
 predict_OECD232_Cd_Zn.m
 predict_OECD232_Cu_Cd.m
 predict_OECD232_Cu_Pb.m
 predict_OECD232_Zn_Cu.m
 predict_OECD232_Zn_Pb.m

Modeling effects of mixtures. For the exposure to two compounds simultaneously, the effects are described by the toxicity parameters of the individual compounds, extended with an interaction parameter called d_{AB} , which is expressed as

Effect ~ [A] + [B] + d_{AB} [A][B]

pars_init_group parameters for all pets weight coefficients of the augmented term

%% parameters

% stress

par h = 0.01277: free h = 1: units h = $\frac{1}{d}$: label h = 'hazard rate in the bl



More generally, for mixtures the model contains three parameters per compound describing the effect of the individual compound, a control mortality rate for the experiment, and one interaction parameter for each pair of compounds. So for a mixture of *k* compounds, a total of 1 (control mortality) + 3k (effect parameters for the three compounds) + k(k - 1)/2 interaction parameters are required.



%% parameters

% stress par.c_0Cd = 1.0929; free.c_0Cd = 1; units.c_0Cd = 'mg/g'; label.c_0Cd = 'No-Ef par.c_0Cu = 3.0546; free.c_0Cu = 1; units.c_0Cu = 'mg/g'; label.c_0Cu = 'No-Ef par.c_0Pb = 0.00029355; free.c_0Pb = 1; units.c_0Pb = 'mg/g'; label.c_0Pb = 'N par.c_0Zn = 4.0419; free.c_0Zn = 1; units.c_0Zn = 'mg/g'; label.c_0Zn = 'No-Ef par.b_Cd = 0.044493; free.b_Cd = 1; units.b_Cd = 'g/d.mg'; label.b_Cd = 'killin par.b_Cu = 0.21539; free.b_Cu = 1; units.b_Cu = 'g/d.mg'; label.b_Cu = 'killin par.b_Pb = 0.085115; free.b_Pb = 1; units.b_Pb = 'g/d.mg'; label.b_Db = 'killin par.b_Zn = 0.4856; free.b_Zn = 1; units.b_Zn = 'g/d.mg'; label.b_Zn = 'killin par.k_eCd = 56.0527; free.k_eCd = 1; units.k_eCd = '1/d'; label.k_eCd = 'elimi par.k_ePb = 0.0054207; free.k_ePb = 1; units.k_ePb = '1/d'; label.k_ePb = 'eli par.k_eZn = 569.9706; free.k_eZn = 1; units.k_eZn = '1/d'; label.k_eZn = 'elim par.d_xy = [7.1001e-06 0.0064216 0.074399 0.00085962 0.00047524 0.001 % other

par.h = 0.01277; free.h = 1; units.h = '1/d'; label.h = 'hazard rate in the bl

Binary compound alone:



OECD232_Cd_Pb

author: Bas Kooijman institution: VU University Amsterdam email: bas.kooijman@vu.nl date: 2022 3 1 toxTest: OECD232 species: Folsomia candida casno: 7440-43-9 & 7439-92-1 compound: Cd & Pb endpoint: # surviving individuals target: hazard rate DEBpars: NA DEBmodel: NA



elasticities

bibliography



TKTD model

Toxicokinetic assumptions

- · The temperature, food density and external concentrations (i.e. in the water) are constant
- · The uptake rates are proportional to the external concentrations
- The elimination rates k_e are proportional to the internal concentrations

Toxicodynamic assumptions

- Effects are linked to the internal concentrations c_x and c_y, scaled such that they have the dimension of external concentrations
- The hazard rate equals h+b_x*max(0,c_x-c_0x)+b_y*max(0,c_y-c_0y)+d_xy*max(0,c_x-c_0x)*max(0,c_y-c_0y) for no-effect concent of the hazard rate equals h+b_x*max(0,c_x-c_0x)+b_y*max(0,c_y-c_0y)+d_xy*max(0,c_x-c_0x)*max(0,c_y-c_0y) for no-effect concent of the hazard rate equals h+b_x*max(0,c_x-c_0x)+b_y*max(0,c_y-c_0y)+d_xy*max(0,c_x-c_0x)*max(0,c_y-c_0y)+d_y*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)*max(0,c_y-c_0x)*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)*max(0,c_y-c_0x)+d_y*max(0,c_y-c_0x)*max(0,c_y-c_0x)+d_y*max(0,c_y-c

Discussion

· Growth is neglected

Facts

"Philosophy of modelling effects"



Choose your reference model and parameters Effects modelled as a change in a well chosen parameters

- Goal: understanding instead of describing data
- AmP procedure can be used to obtain control model and parameters.

RESEARCH

Open Access

CrossMark



Modelling effects of time-variable exposure to the pyrethroid beta-cyfluthrin on rainbow trout early life stages

Elke I. Zimmer^{1*}, Thomas G. Preuss², Steve Norman³, Barbara Minten⁴ and Virginie Ducrot²

AmP entry for rainbow trout Control model and parameters

Availability of data and materials

All data generated or analysed during this study are included in this published article and its Additional file.

The physiological model for rainbow trout and the data used for its parameterization are available from: https://www.bio.vu.nl/thb/deb/deblab/add_my_pet/entries_web/Oncorhynchus_mykiss/Oncorhynchus_mykiss_res. html, Version: 20170527.



Prediction of long-term variation in offspring metabolism due to BPA in eggs in rainbow trout using the DEB model

B. Sadoul^{a,b,*,1}, S. Augustine^{c,1}, E. Zimmer^d, M.-L. Bégout^e, M.M. Vijayan^a

Table 1

Primary parameter values estimated in this study at reference temperature (20 °C) and uploaded online (AmP version 20171030).

Symbol	Value	Unit	Description
{ <i>p</i> _{Am} }	2512	J/d/cm ²	Maximum surface area specific assimilation rate
$\{\dot{F}_m\}$	6.5	l/d/cm ²	Maximum specific searching rate
KX	0.8	1.77	Digestion efficiency of food to reserve
Кр	0.1	-	Faecation efficiency of food to faeces
v	0.03	cm/d	Energy conductance
κ	0.62	_	Allocation fraction to soma
KR	0.95	-	Reproduction efficiency
[p _M]	344	J/d/cm ³	Volume specific somatic maintenance
<i>k</i> _I	0.002	1/d	Maturity maint rate coefficient
$[E_G]$	5268	J/cm ³	Specific cost for structure
E_{H}^{b}	43	J	Maturity at birth
EH	854	J	Maturity at metamorphosis
EHP	388 10 ⁴	J	Maturity at puberty
<i>h</i> a	$3.004 \ 10^{-24}$	$1/d^2$	Weibull aging acceleration
SG	10	-	Gompertz stress coefficient

Parameters $\{\dot{F}_m\}$, κ_X , κ_P , κ_R , \dot{k}_J , \ddot{h}_a and s_G were fixed.

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Regulation of reproductive processes with dynamic energy budgets



Erik B. Muller^{1,2} | Konstadia Lika³ | Roger M. Nisbet⁴ | Irvin R. Schultz⁵ | Jérôme Casas⁶ | André Gergs⁷ | Cheryl A. Murphy⁸ | Diane Nacci⁹ | Karen H. Watanabe¹⁰

2.2 | Dynamic energy budget theory

This study uses the standard model of dynamic energy budget (std-DEB) theory as a reference. Since Kooijman (2010) has described

	Interpretation	Value	Source	
(c) Fixed parameters (T = 11°C)				
d _M	C-mole to dry weight conversion	24.6 g/C-mole	AmP	
dw	Wet weight to dry weight conversion	0.2	AmP	
f	Scaled food density	0.9	See text ^b	
i _M	Specific maintenance rate	0.025/day	AmP	
k _j	Maturity maintenance coefficient	0/day	See text	
m _{F0}	Initial density of reproductive matter (stdDEB+)	0 ^c	See text	
m _{Gm}	Maximum density of reproductive matter (stdDEB+)	6.60	See text	
M _{Vm}	Maximum structural biomass	1.12 C-mole	AmP	
y _F	Conversion efficiency general reserve to reproductive buffer	0.95	AmP	
У _G	Conversion efficiency reproductive reserve to gonads (stdDEB+)	1	See text	
Y _{RE}	Conversion efficiency general to reproductive reserve	0.95	AmP	
y _v	Conversion efficiency general reserve to structure	0.88	AmP	
ĸ	Fraction reserves allocated to soma (stdDEB+)	0.56	AmP	

"Effects" as deviations from a well chosen reference



Here the strategy is to have some parameters fixed because estimated from data, and then estimate parameters from modules which can be removed.

Trajectory reconstruction



Option 1 : Adopt the same strategy outlined before. Choose a reference set of parameters, and back estimate past food and temperature conditions:

in the reference growth is a function of food

for the trajectory reconstruction : write out food as a function of growth. Treat growth parameters as "given". Estimate the food parameters.

Option 1 : Adopt the same strategy outlined before. Choose a reference set of parameters, and back estimate past food and temperature conditions:





Journal of Sea Research



What can the shell tell about the scallop? Using growth trajectories along latitudinal and bathymetric gradients to reconstruct physiological history with DEB theory

Check for updates

Romain Lavaud^{a,b,*}, Aurélie Jolivet^b, Eric Rannou^c, Fred Jean^b, Øivind Strand^d, Jonathan Flye-Sainte-Marie^b

Step 1: "reference parameters"





Predictions & Data for this entry

Model: abj	climate: MC	migrate:	phylum: Mollusca
COMPLETE = 2.5	ecozone: MANE	food: biPp	class: Bivalvia
MRE = 0.047	habitat: 0jMp, jiMb	gender: D	order: Ostreoida
SMSE = 0.009	embryo: Mp	reprod: O	family: Pectinidae

Three sites:

Brest Celtic Sea Træna



















Problem formulation



- \dot{p}_A : Assimilation
- \dot{p}_C : Mobilization
- κ : Fraction of \dot{p}_C mobilized towards growth and somatic maintenance
- \dot{p}_S : Somatic maintenance
- \dot{p}_J : Maturity maintenance
- \dot{p}_G : Growth
- \dot{p}_R : Maturity then Reproduction

The DEB parameters are treated as known – they are the reference



Energy fluxes:

Energy fluxes:

$$\dot{p}_{A} = f(X) \{\dot{p}_{Am}\} V^{2/3}$$

$$\dot{p}_{C} = E \left(\frac{[E_{G}] \dot{v} V^{2/3} + \dot{p}_{S}}{\kappa E + [E_{G}] V} \right)$$

$$\dot{p}_{S} = [\dot{p}_{M}] V + \{\dot{p}_{T}\} V^{2/3}$$

$$\dot{p}_{G} = \kappa \dot{p}_{C} - \dot{p}_{S}$$

$$\dot{p}_{J} = \dot{k}_{J} E_{H}$$

$$\dot{p}_{R} = (1 - \kappa) \dot{p}_{C} - \dot{p}_{J}$$



Reconstruct the past food level

Energy fluxes:

$$\dot{p}_{A} = f(X) \{\dot{p}_{Am}\} V^{2/3}$$

$$\dot{p}_{C} = E \left(\frac{[E_{G}] \dot{v} V^{2/3} + \dot{p}_{S}}{\kappa E + [E_{G}] V} \right)$$

$$\dot{p}_{S} = [\dot{p}_{M}] V + \{\dot{p}_{T}\} V^{2/3}$$

$$\dot{p}_{G} = \kappa \dot{p}_{C} - \dot{p}_{S}$$

$$\dot{p}_{J} = \dot{k}_{J} E_{H}$$

$$\dot{p}_{R} = (1 - \kappa) \dot{p}_{C} - \dot{p}_{J}$$



Approach

Growth is a function of food

Food is a function of growth



Approach:

- Step 1: download parameter values
- Step 2: modify the 4-user defined files
- Step 3: Estimate



Adapt the AmP code





Steps for making your code

- Step 1: create folder with the 4-user defined files
- <u>Step 2</u>: edit the run file (define the knot-abscissa for the f that is being estimated - pass the knot abscissa as globals)
- <u>Step 3</u>: edit the pars_init file: fix the core DEB parameters, auxiliary parameters, and insert an f parameter for each of the knot abscissa defined in the run file (hint: pass the knot abscissa as a global)
- <u>Step 4</u>: modify the predict: remove unnecessary predictions, put prediction for length as function of time-varying food and temperature
- **<u>Step 5</u>**: create additional plots at the end of the run-file

Step 3: edit the pars_init file:



Put results_Pecten_maximus.mat in your working directory

mat2pars_init('Pecten_maximus',1)

insert an f parameter for each of the knot abscissa defined in the run file (hint: pass the knot abscissa as a global)



Questions to explore:

- Interval of knot functions
- Interpolation of temperature and food
- Initial conditions
- Starting values for free parameters
- Comparing across sites

add-my-pet/AmPtox



DEB2023_reconstruction	6/7/2023 11:02 PM	File folder	
docs	3/13/2023 3:53 AM	File folder	
no_pet	6/7/2023 8:03 PM	File folder	
OECD201_LAS	6/7/2023 8:04 PM	File folder	
OECD202_dichromate	6/7/2023 8:05 PM	File folder	
OECD203_dieldrin	5/23/2023 4:57 AM	File folder	
OECD210_PAH	5/23/2023 4:57 AM	File folder	
OECD221_Cd	3/13/2023 3:53 AM	File folder	
OECD222_Cu	3/13/2023 3:53 AM	File folder	
OECD232_Cd_Cu_Pb_Zn	5/23/2023 4:57 AM	File folder	
OECD232_Cd_Pb	6/7/2023 8:59 PM	File folder	
OECD232_Cd_Zn	3/13/2023 3:53 AM	File folder	
OECD232_Cu_Cd	3/13/2023 3:53 AM	File folder	
OECD232_Cu_Pb	5/10/2023 4:25 AM	File folder	
OECD232_Zn_Cu	3/13/2023 3:53 AM	File folder	
OECD232_Zn_Pb	5/23/2023 4:57 AM	File folder	



Pecten_maximus
 reconstruction_brest
 reconstruction_celtic
 reconstruction_traena

6/7/2023 11:02 PM 6/7/2023 11:02 PM 6/7/2023 11:02 PM 6/7/2023 11:02 PM File folder File folder File folder File folder

Start with Celtic





Contents lists available at ScienceDirect

Journal of Sea Research

journal homepage: www.elsevier.com/locate/seares

What can the shell tell about the scallop? Using growth trajectories along latitudinal and bathymetric gradients to reconstruct physiological history with DEB theory



OURNAL OF

Romain Lavaud^{a,b,*}, Aurélie Jolivet^b, Eric Rannou^c, Fred Jean^b, Øivind Strand^d, Jonathan Flye-Sainte-Marie^b

For full discussion. This was just to illustrate.

Options:



Option 1 : Adopt the same strategy outlined before. Choose a reference set of parameters, and back estimate past food and temperature conditions:

Option 2 : Integrate your reconstruction directly into the "main" estimation

Many examples in collection of



option 2:

you can find a list in the collection by looking for predict files where food level is splined.

often knots are chosen within the predict, and the knot abcissa (parameters) are defined in pars init.





Different "nomenclatures" - statistical nomenclature is followed here

zerounibitri-

of independent variables !

multi- more than 1 dependant variables !

Final slide



Questions?