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D8.3

Empirically parameterized and verified rotation scale models for gene frequencies

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Dissemination Level	
PU Public	PU
PP Restricted to other programme participants (including the Commission Services)	
RE Restricted to a group specified by the consortium (including the Commission Services)	
CO Confidential, only for members of the consortium (including the Commission Services)	

1. Introduction

Model 'parameterization' is the step in model development, in which the mathematical expressions and their parameters are defined, by which to describe a real-world system. In this case, we developed a generic model of herbicide-resistant and herbicide-susceptible weed populations in an agricultural field undergoing crop rotation.

Once a model has been parameterized and the parameter values have been estimated, model 'verification' is carried out to check that the model behaves in a sensible way. For this purpose, parameter values are estimated roughly only, and model output is judged only informally.

Model parameterization and verification, as reported here, is the result of a two-day workshop held at CNR in Padova, 4-5 February 2015, with participants from AU, CNR and WU.

2. Model description

The number of seeds in the soil seed bank (N_b ; m⁻²) decrease with time due to the processes of seed mortality (μ ; y⁻¹) and seedling emergence (ε ; y⁻¹) and, increase due to net seed production (ΔP ; m⁻²),

$$\Delta N_b = -(\mu + \varepsilon)N_b\Delta t + \Delta P$$

with a time step (Δt ; y) of one year.

The number of seedlings (N_s ; m⁻²) equals the emergence,

$$N_s = \varepsilon N_b \Delta t$$

of which a certain proportion (σ ; y⁻¹) survives into mature plants (N_w ; m⁻²),

$$N_w = \sigma N_s \Delta t$$

The above-ground weed biomass (M_w ; g m⁻²) scales to weed density (N_w), taking intraspecific and interspecific competition with the crop (N_c ; m⁻²) into account,

$$M_w = \frac{N_w}{b_0^{-1} + b_w N_w + b_c N_c}$$

with parameters for biomass per weed plant at no competition (b_0^{-1} ; g⁻¹ m²) and coefficients for intraspecific (b_w ; g⁻¹ m²) and interspecific competition (b_c ; g⁻¹ m²).

Weed seed production (ΔS ; m⁻¹) is proportional to weed biomass:

$$\Delta S = \frac{\rho M_w}{s}$$

with parameters for reproductive effort (ρ ; g/g) and individual seed weight (s ; g).

Of the seeds produced only a proportion ($\pi; \text{y}^{-1}$) will survive as the net seed production (ΔP) that enters the soil seed bank (N_s),

$$\Delta P = \pi \Delta S$$

3. Model parameterization

The final model will describe *Echinochloa crus-galli* in a maize-dominated crop rotation and *Alopecurus myosuroides* in a winter wheat-dominated crop rotation. However, to verify the model it was concluded that a case of a single weed in one crop would be a sufficiently test of model robustness. Hence *E. crus-galli* in continuous maize was chosen as the concrete case. Parameters were estimated by their typical values or, in case of uncertainty or natural variance, by their typical interval (Table 1).

Table 1. Model parameter estimates for *Echinochloa crus-galli* (herbicide-susceptible) in continuous maize.

Parameter	Value	Source
Seed bank mortality ($\mu; \text{y}^{-1}$)	0.14	Literature
Seedling emergence ($\varepsilon; \text{y}^{-1}$)	[0.05; 0.1]	CNR experts
Seedling survival ($\sigma; \text{y}^{-1}$)	[0.01; 0.02]	CNR experts
No competition ($b_0; \text{g}^{-1} \text{m}^2$)	0.0006	CNR experiments
Intraspecific competition ($b_w; \text{g}^{-1} \text{m}^2$)	0.0004	CNR experiments
Interspecific competition ($b_c; \text{g}^{-1} \text{m}^2$)	[0.0001; 0.0003]	Workshop experts
Reproductive effort ($\rho; \text{g/g}$)	[0.15 ; 0.26]	CNR experiments
Individual seed weight ($s; \text{g}$)	[0.0015 ; 0.0020]	CNR experiments
Survival of new seeds ($\pi; \text{y}^{-1}$)	[0.7 ; 1]	Workshop experts

4. Model verification

The model was implemented in R. Each simulation lasted 30 years starting out with an initial seed bank of 50 seeds per m². For those parameters estimated as an interval, a random value inside that interval was chosen before the simulation. The simulation was repeated 100 times, yielding 100 different outcomes due to the randomly chosen parameter values. The predicted weed population dynamics were summarized by quantile spline regressions (10%, 50%, 90%) (*qsreg* of the *fields* R package). The influence of each parameter was visualised by plotting its value against the asymptotic outcomes of the model; the data points were summarised by Loess-smoothed curves (*geom_smooth* of the *ggplot2* R package), including standard errors.

Table 2. Model outcomes (i.e. model variables) for *Echinochloa crus-galli* in continuous maize.

Model variable
Seed bank density (N_b ; m ⁻²)
Seedling density (N_s ; m ⁻²)
Weed mass density (M_w ; g m ⁻²)
Weed plant density (N_w ; m ⁻²)
Reproduction total (ΔS ; m ⁻¹)

The simulations (Fig. 1) quickly resulted in a much too large seed bank: more than 1 million seeds per m² compared to the maximum of 80,000 seeds per m² observed in the field by CNR. Consequently, other model outcomes such as weed plant density and biomass were also too large. Yet, the response of the model to changes in model parameters (Fig. 2) made sense. For example, the first row of sub-figures in Fig. 2 shows how the ultimate size of the seed bank depends mostly on the reproductive investment (positively), seed size (negatively) and seed survival (positively). Obviously, the more that is invested in reproduction and the higher the survival of the seeds, the larger the seed bank. And, the larger the seeds are, the fewer seeds will be reproduced from the reproductive investment, and hence the smaller the seed bank can get in the long run.

Field data from CNR revealed the cause of the over-estimated growth of the weed population: *E. crus-galli*, like most weeds, emerges in flushes. The inter-specific competition coefficient (b_c) was estimated for the case when the weed emerges simultaneously with the crop. However, this first flush is controlled chemically nearly 100%. The weeds that emerge in subsequent flushes, and which make up the seed-setting population, will endure a much stronger competition.

To verify that the model would react sensibly to an increased pressure of competition from the crop, b_c was multiplied by 50. In the resulting simulations (Fig. 3), the seed bank was growing much slower and for many years remained below the observed maximum of 80,000 seeds per m². Similarly, the other state variables of the weed population were reduced. The sensitivity of model outcomes to parameter values remained much the same (Fig. 4).

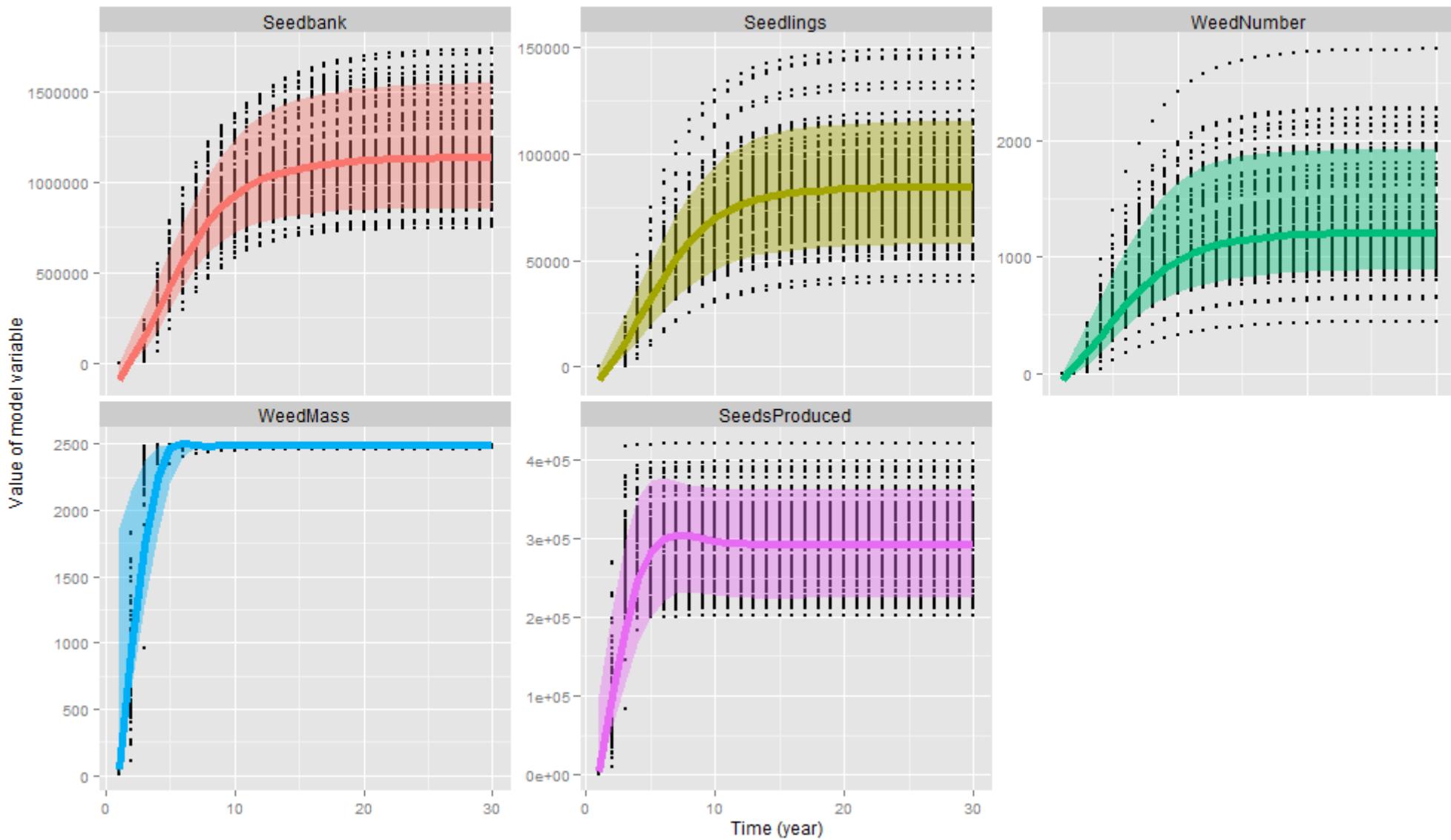


Figure 1. Simulated dynamics of *Echinochloa crus-galli* in continuous maize over 30 years. The 100 replicate simulations are summarised by their median value (line) and 10%-90% percentile span (coloured area).

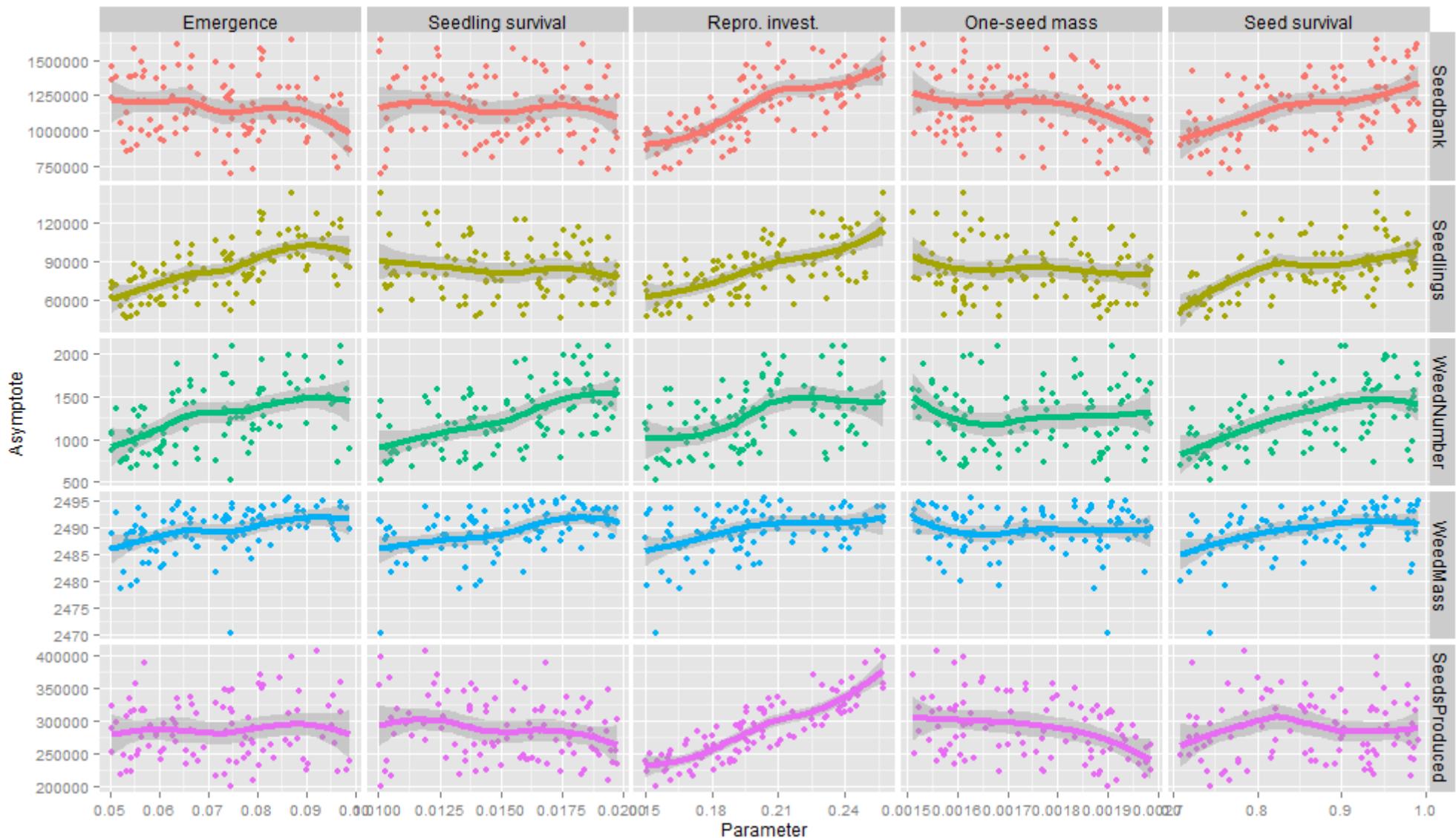


Figure 2. Asymptotic values (from Fig. 1) of simulated dynamics of *Echinochloa crus-galli* in continuous maize over 30 years, depending on the value of model parameters. Data summarised by Loess-smoothed curves with standard error (grey bands).

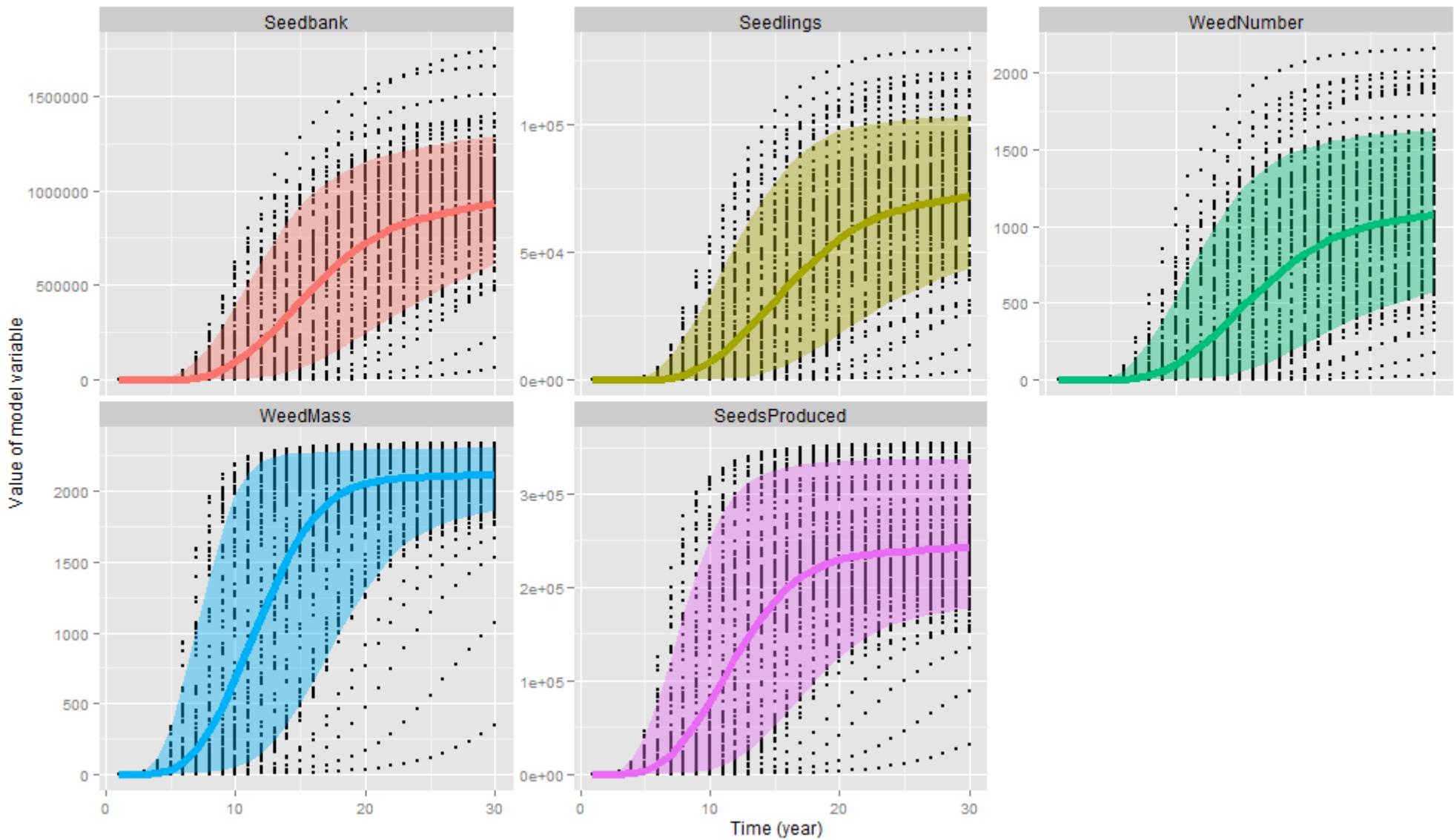
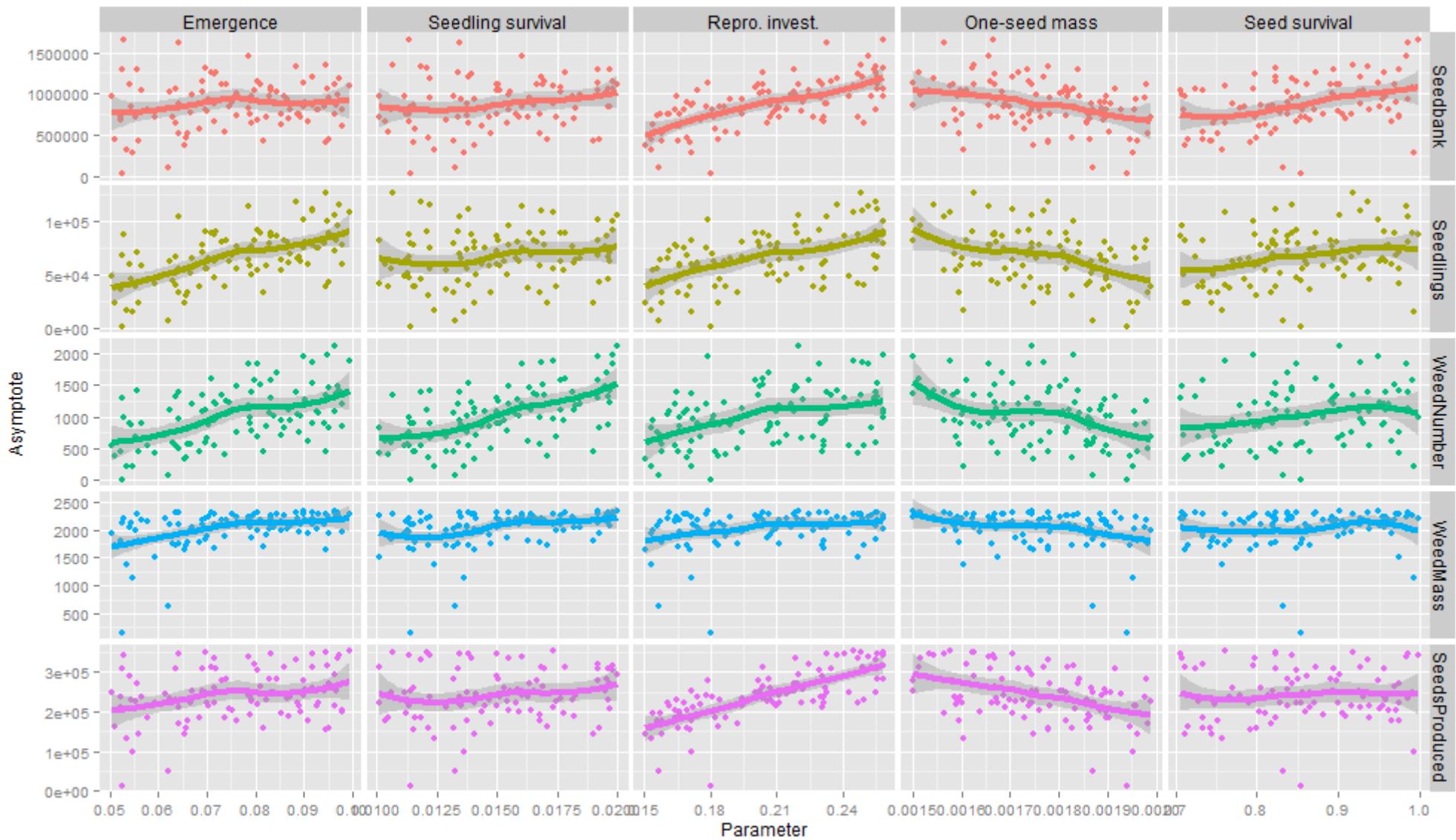


Figure 3. As Fig. 1 but with inter-specific competition increased by a factor 50.

**Figure 4.** Asymptotic values (from Fig. 3), otherwise as Fig. 2.

5. Conclusions and further work

The model was verified to work sensibly in the one-weed one-crop case. The effect of delayed emergence of the weed relative to the crop could be accommodated by increasing the interspecific competition coefficient.

The addition of another weed will not change the structure of the model, only add competition terms insofar as the two weeds (herbicide-resistant and herbicide-susceptible) differ in their competitive ability. In addition, crop rotation can be accommodated simply by switching between different parameter sets, one set for each crop.

The completed model will be based on parameter estimates obtained from empirical work of the present project in combination with estimates from literature. The model will be used to analyse how fitness penalties suffered by herbicide-resistant weeds, *E. grubs-galli* and *A. myosuroides*, can be exploited as part of integrated weed management strategies.

A joint publication on this work is being written by researchers from AU, CNR and WU.