Supporting information for: All individuals are not created equal; accounting for inter-individual variation in fitting life-history responses to toxicants.

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January 7, 2013

1 Log-likelihood function

The parameter vector for the basic parameters $\boldsymbol{\theta}$ (in this case r_B and L_m) follows a k-variate normal distribution, with a vector of mean values $\boldsymbol{\mu}$ and a covariance matrix $\boldsymbol{\Sigma}$:

$$\boldsymbol{\theta} \sim \mathcal{N}_k(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \tag{1}$$

The $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are here defined by the individuals in the control treatment only.

For each individual i in the treatments, the likelihood $\mathcal{L}$ of its basic parameter vector $\boldsymbol{\theta}_i$, given the data set for that individual ($\boldsymbol{Y}_i$ with n_i data points) is given by the probability density of the parameter set ($\boldsymbol{\theta}_i$) from the multi-variate normal (f_k) multiplied by the product of the probability density for each observation $Y_{i,j}$ from the univariate normal (f_1):

$$\mathcal{L}(\boldsymbol{\theta}_i | \boldsymbol{Y}_i, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\theta}_t) = f_k(\boldsymbol{\theta}_i | \boldsymbol{\mu}, \boldsymbol{\Sigma}) \prod_{j=1}^{n_i} f_1(Y_{i,j} | \boldsymbol{\theta}_t, \boldsymbol{\theta}_i) \tag{2}$$

where $\boldsymbol{\theta}_t$ is the global set of toxicity parameters (in this case k_e, c_0 and c_T). Thus, I assume that the observations for one individual are independent (hence the product). This yields the log-likelihood function:

$$\ell(\boldsymbol{\theta}_i | \boldsymbol{Y}_i, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\theta}_t) = \ln f_k(\boldsymbol{\theta}_i | \boldsymbol{\mu}, \boldsymbol{\Sigma}) + \ln \left(\prod_{j=1}^{n_i} f_1(Y_{i,j} | \boldsymbol{\theta}_t, \boldsymbol{\theta}_i) \right) \tag{3}$$

The probability density of the basic parameter vector $\boldsymbol{\theta}_i$ (first term in the equation) follows from the multivariate normal distribution:

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$$f_k(\boldsymbol{\theta_i}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{k/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{\theta_i} - \boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta_i} - \boldsymbol{\mu})\right) \tag{4}$$

$$\ln f_k(\boldsymbol{\theta_i}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{1}{2}\ln|\boldsymbol{\Sigma}| - \frac{1}{2}(\boldsymbol{\theta_i} - \boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta_i} - \boldsymbol{\mu}) + C \tag{5}$$

where C collects all of the additive terms that do not depend on the model parameters, and can be ignored. We interpret the deviations between model prediction and measurements for each individual as 'measurement error' here. Therefore, we assume normal independent distributions with for all individuals (second term in the log-likelihood equation). Treating the standard deviation of that error as a nuisance parameter (see [1, 2]):

$$\ln\left(\prod_{j=1}^{n_i} f_1(Y_{i,j}|\boldsymbol{\theta_t}, \boldsymbol{\theta_i})\right) = -\frac{n_i}{2}\ln\sum_{j=1}^{n_i}\left(Y_{i,j} - \hat{Y}_{i,j}(\boldsymbol{\theta_t}, \boldsymbol{\theta_i})\right) + C \tag{6}$$

Again, C collects all of the additive terms that do not depend on the model parameters. The overall log-likelihood is the sum of the optimal log-likelihoods over all N individuals:

$$\ell(\boldsymbol{\theta_t}|\boldsymbol{Y}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{i=1}^{N}\ell(\hat{\boldsymbol{\theta}}_i|\boldsymbol{Y}_i, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\theta_t}) \tag{7}$$

We can thus optimise the likelihood of the toxicity parameters $\boldsymbol{\theta_t}$, given the data $\boldsymbol{Y}$ and the multivariate distribution of the control parameters (specified by $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$).

In principle, it should be possible to also optimise $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ using the complete data set (control and treatments), however in practice this runs into problems. When $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are also estimated, the optimisation routine converges towards a very high correlation between the two parameters. This increases the probability density for the parameter combinations on an almost straight line (for the case of two parameters). The increase in probability density is more than enough to compensate for the poorer fit on the body size data. This is clearly an issue that requires some further study.

2 Additional plots: controls

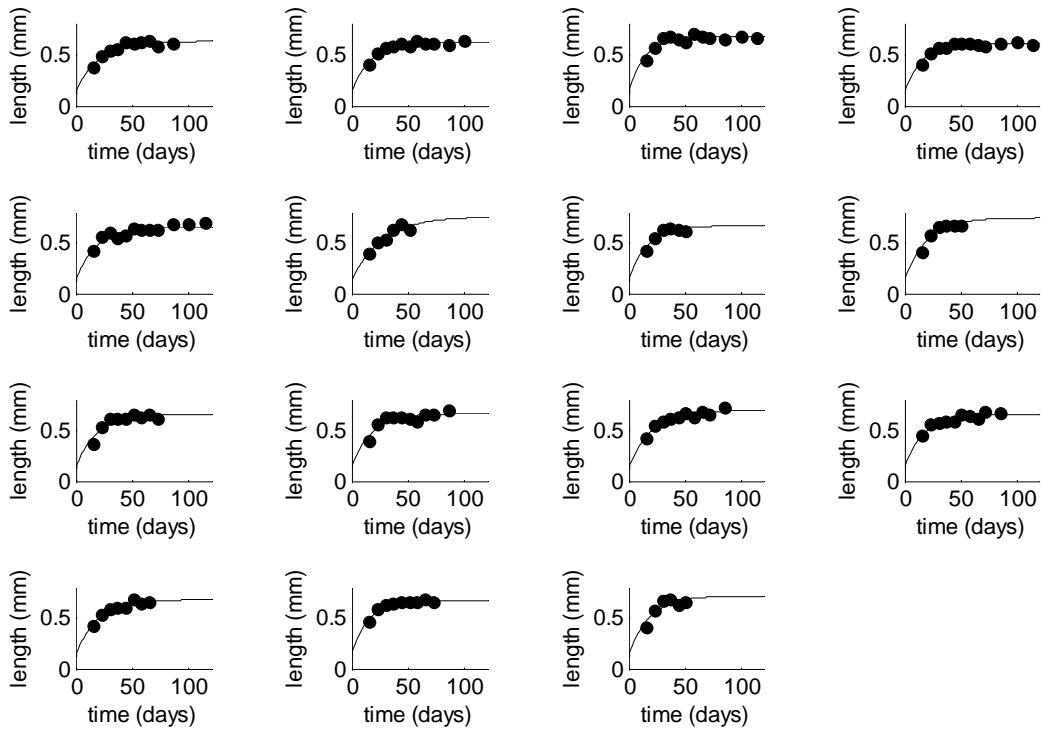In all cases, length is expressed as volumetric length (cubic root of body volume).

Figure 1: Individual fits for the animals in controls.
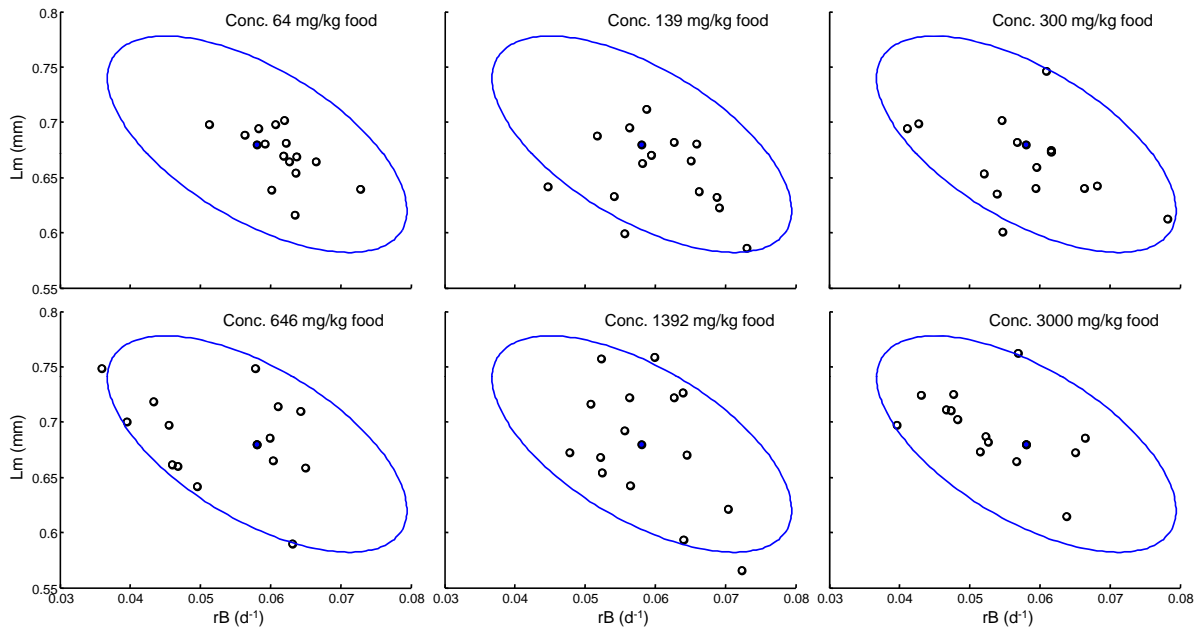
3 Additional plots: treatments

Figure 2: Values for the two basic model parameters for each individual in each treatment. The ellipse and the filled symbol are the 95% coverage and the mean from the control fits, respectively.

On the next pages, the individual fits in the treatments are provided. In all cases, length is expressed as volumetric length (cubic root of body volume).
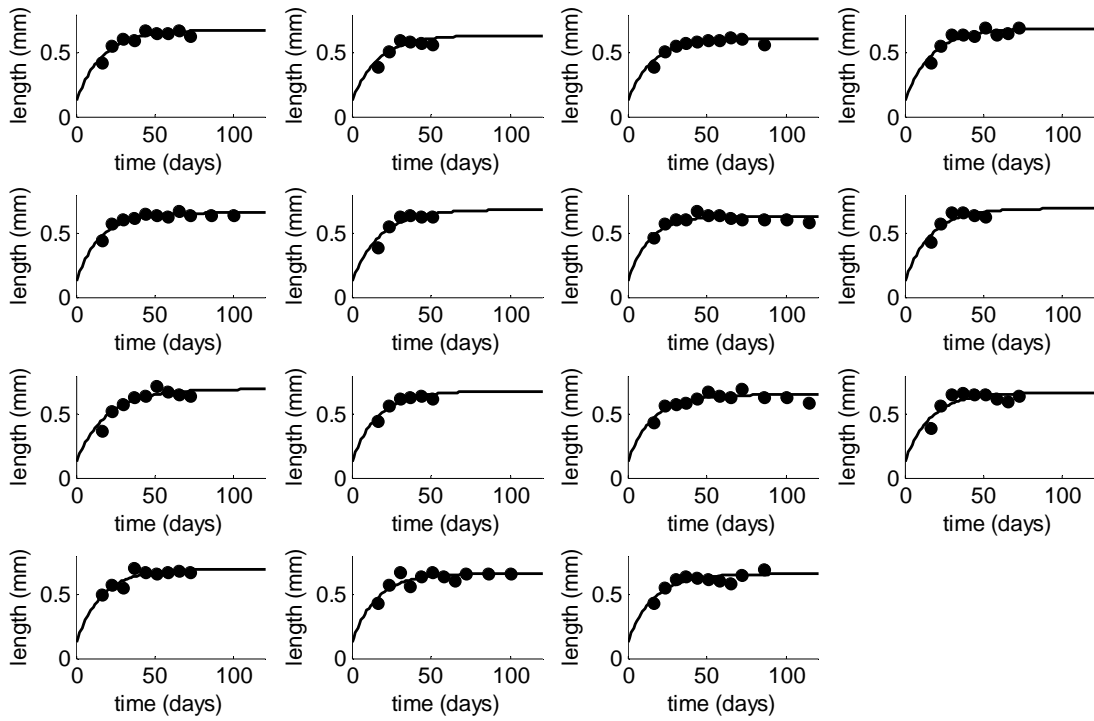
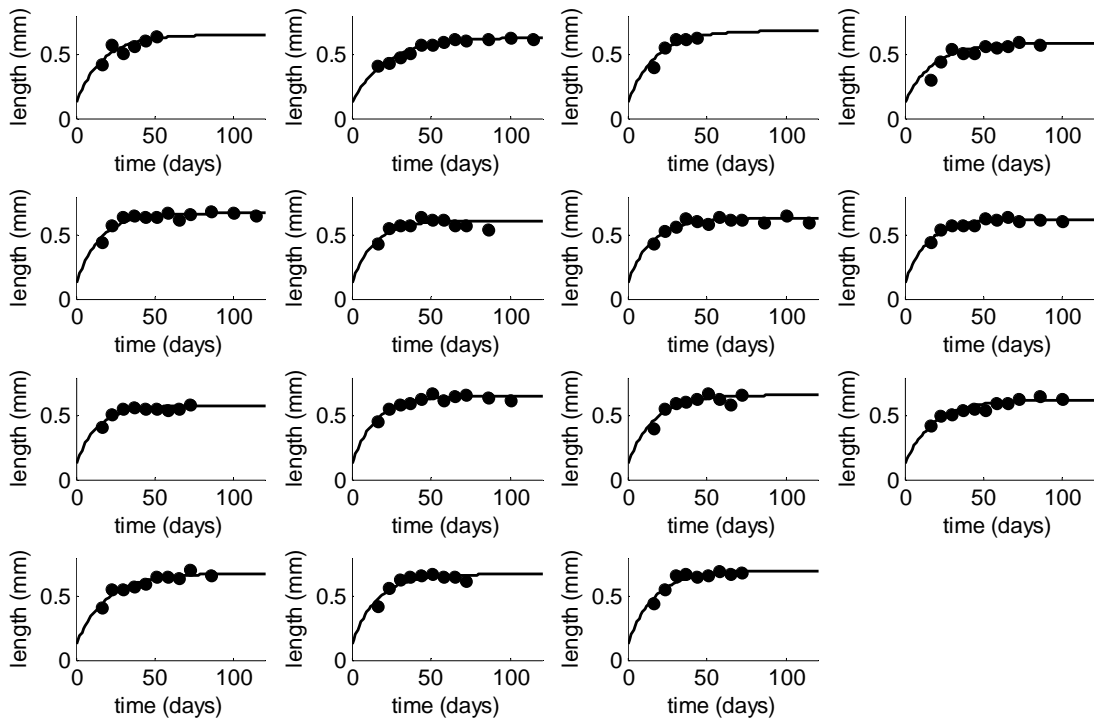Figure 3: Individual fits for the animals in treatment 64 g/kg food.

Figure 4: Individual fits for the animals in treatment 139 g/kg food.
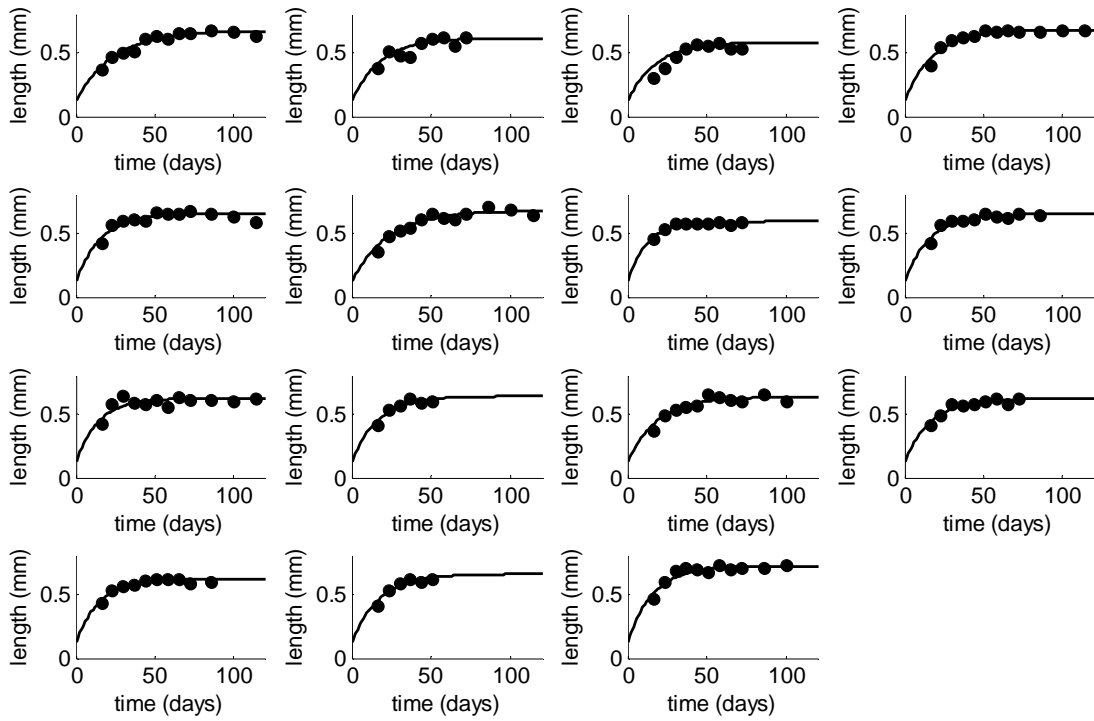
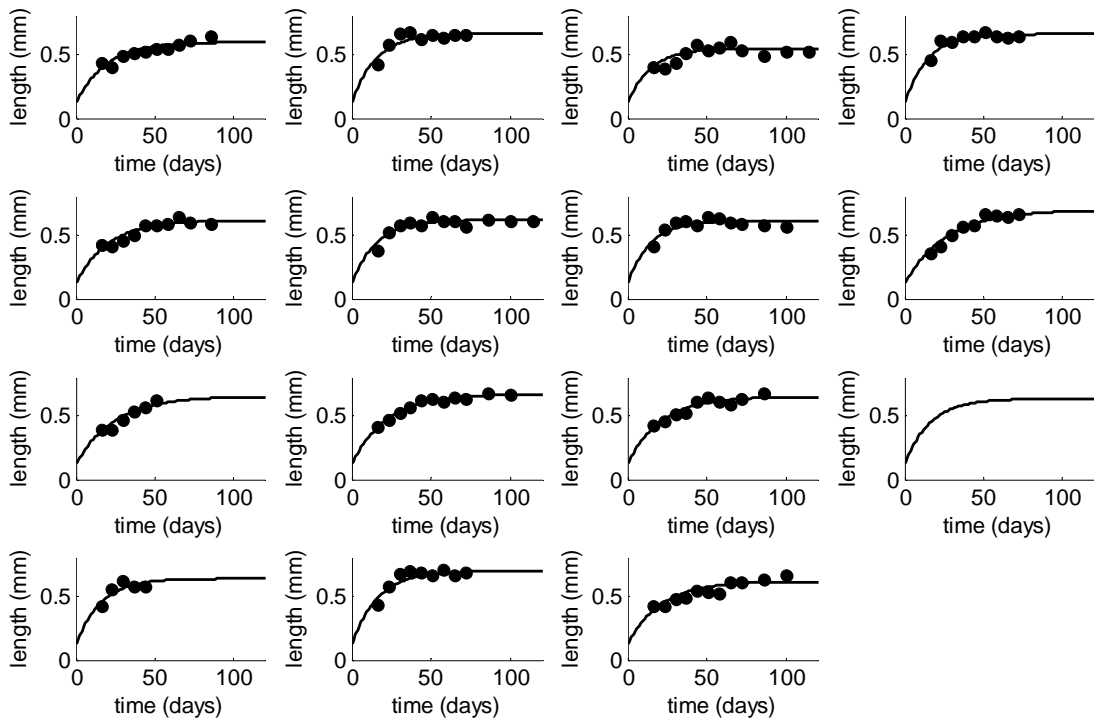Figure 5: Individual fits for the animals in treatment 300 g/kg food.

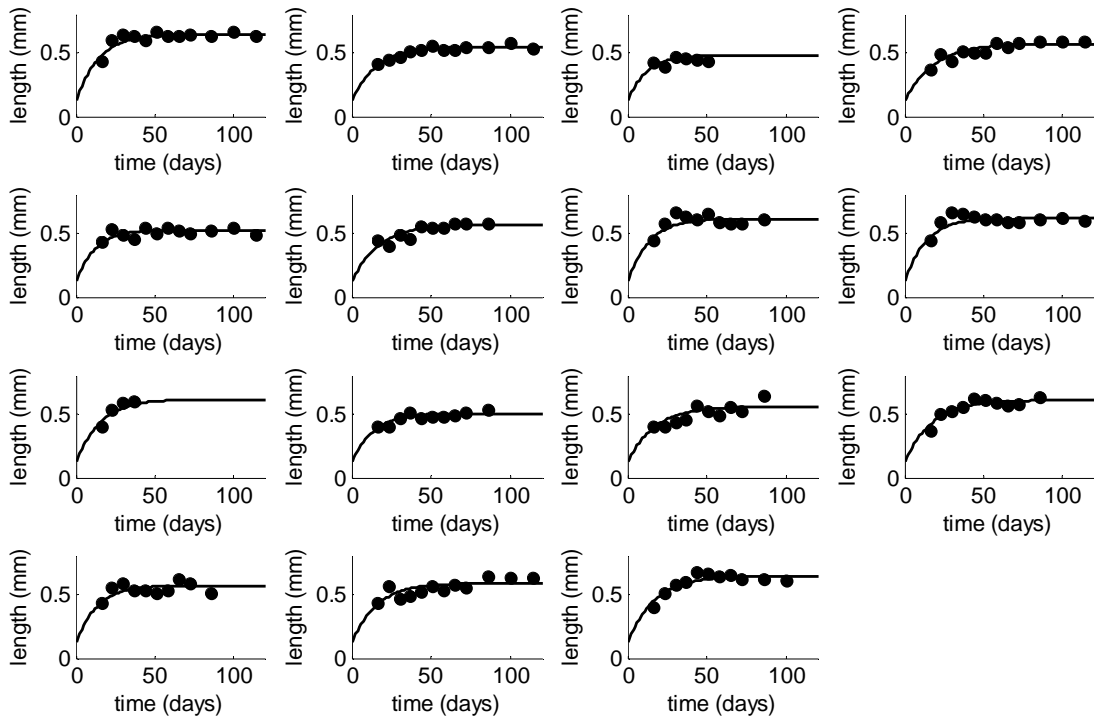Figure 6: Individual fits for the animals in treatment 646 g/kg food.

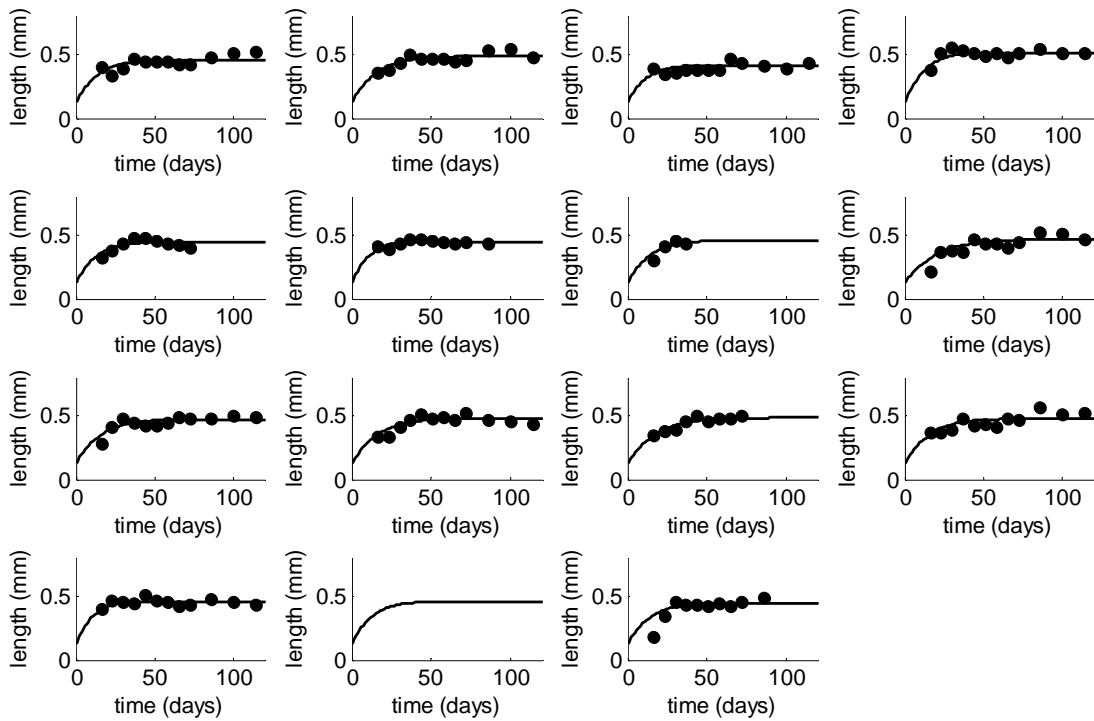Figure 7: Individual fits for the animals in treatment 1392 g/kg food.

Figure 8: Individual fits for the animals in treatment 3000 g/kg food.

References

[1] T. Jager and E. I. Zimmer. Simplified dynamic energy budget model for analysing ecotoxicity data. *Ecological Modelling*, 225:74–81, 2012.

[2] Y. Pawitan. *In all likelihood: statistical modelling and inference using likelihood.* Oxford University Press, Oxford, UK, 2001.