# Supplementary Materials for "Interval Estimation of Thermal Summation Parameters in Forensically Important Insects"

**Jędrzej Wydra**[1,2,*]**, Łukasz Smaga**[3]**, and Szymon Matuszewski**[1,2]

[1]Laboratory of Criminalistics, Adam Mickiewicz University, al. Niepodległości 53, Poznań 61-714, Poland
[2]Center for Advanced Technologies, Adam Mickiewicz University, ul. Uniwersytetu Poznańskiego 10, Poznań 61-614, Poland
[3]Department of Mathematical Statistics and Data Analysis, Adam Mickiewicz University, ul. Uniwersytetu Poznańskiego 4, Poznań 61-614, Poland
[*]corresponding author: jedrzej.wydra@amu.edu.pl

## ABSTRACT

Estimating time of death based on entomological evidence commonly relies on the "law of total effective temperature", which requires developmental parameters of specific insect taxa. These are often calculated using the method of Ikemoto and Takai. However, this approach has key limitations. It assumes a homogeneous population and does not provide meaningful interval estimates, despite substantial variation within species and even populations. Moreover, by aggregating raw data before analysis, it discards valuable information, potentially reducing accuracy.

In this study, we propose an alternative method that addresses both issues. It estimates interval values for developmental parameters while simultaneously identifying component populations within a dataset. The method involves fitting a finite mixture of Weibull distributions to development time data using the Expectation-Maximization (EM) algorithm. This allows for the inclusion of individual-level variability in the estimation process.

We tested the method using previously published developmental data on two forensic beetle species, *Creophilus maxillosus* and *Necrodes littoralis* (Staphylinidae). Our approach yielded 95% intervals with coverage close to the nominal level, in contrast to Ikemoto and Takai's method, which captured only 75% and 59% of actual cases, respectively. These findings suggest that our method improves the reliability of insect-based postmortem interval estimates in forensic entomology.

## Content of the Supplement

This document provides additional content related to the article titled "Interval Estimation of Thermal Summation Parameters in Forensically Important Insects". It includes: (1) full results for *Creophilus maxillosus*, (2) a practical application example based on *Necrodes littoralis* data (3) interval estimates for the parameter $k$ calculated at levels lower than 95% for both *Necrodes littoralis* and *Crephilus maxillosus*, and (4) technical details of the applied methods that were omitted from the main text for brevity.

## Results for *Creophilus maxillosus*

### Coefficients of the Fitted Model

For *Creophilus maxillosus*, our algorithm distinguished two component populations, fitting each to a Weibull distribution. The coefficients of the fitted distribution are presented in Table 1. The separation of these populations is illustrated in Figure 1.

|  | Blue population | Red population |
|---|---|---|
| $w_l$ | 0.87 | 0.13 |
| $\kappa_l$ | 14.03 | 6.72 |
| $\lambda_l$ | 442.74 | 556.66 |
| $t_0^{(l)}$ | 11.25 | 11.15 |

**Table 1.** Coefficients of mixture model of Weibull's distribution for *Creophilus maxillosus* dataset.
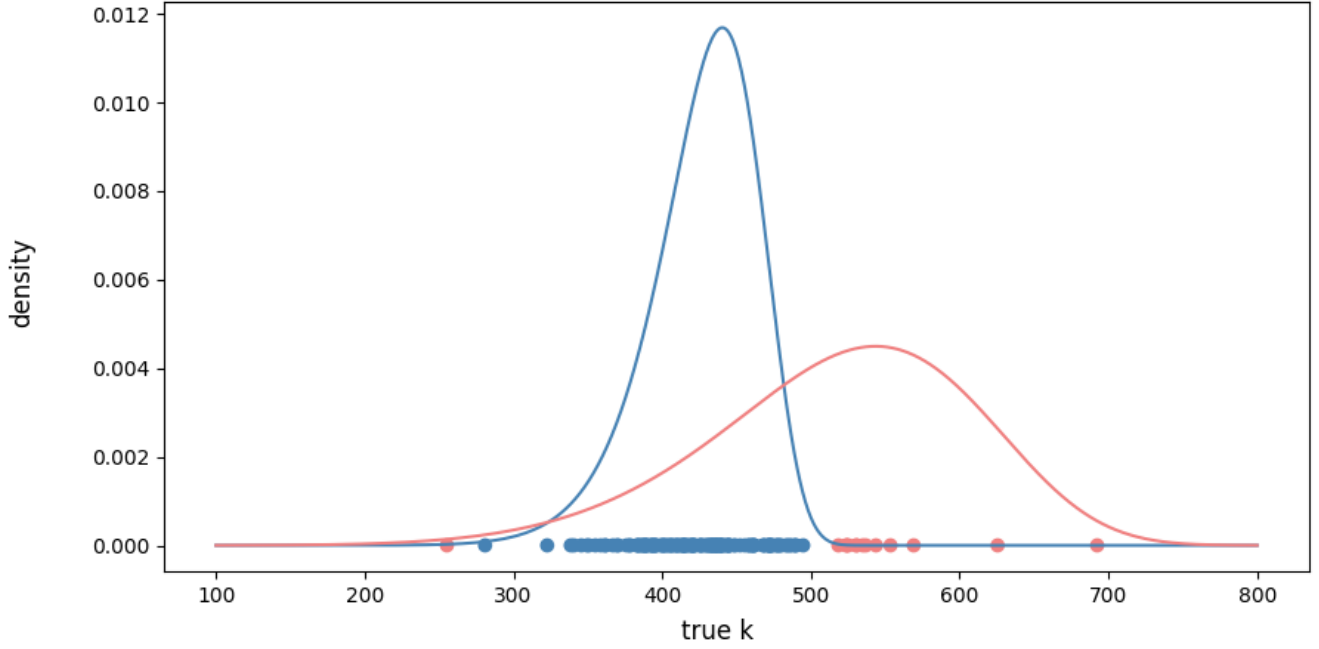
**Figure 1.** Density functions for the detected populations in the *Creophilus maxillosus* dataset. The regular experiment results are marked in blue, and outliers are marked in red.

### Component populations

The size of the red population is much smaller than that of the blue population (see the $w_l$ coefficients in Table 1). According to the U-test, there were no significant differences in size (Table 2, $p$-value $> 0.7$). Also, according to chi-squared test, there were no significant differences in the proportion of males and females between populations ($p$-value $> 0.5$). Additionally, the red population exhibits extreme or outlier values of $k$ and DI (Figures 1 and 2). Therefore, we consider the blue population to represent the regular experimental results, while the red population is treated as outlier observations.

The standard deviation of $K$ is about 30% smaller in the blue population compared to the combined population.

|  | Length [mm] |
|---|---|
| Blue population | 19.57 |
| Red population | 19.21 |

**Table 2.** Mean insect length in each population.

### Confidence interval

The 95% confidence interval for the parameter $k$ estimated using the Ikemoto and Takai method is $[378, 456]$ (for the calculation details, see the technical details below), while its empirical counterpart derived from the bootstrap sample is $[405, 423]$. The empirical coverage probability of this 95% confidence interval is 1. The standard error of the Ikemoto and Takai estimator is 19.52, while the bootstrap standard error is 4.96 (Table 3).

For the new method, the 95% confidence interval of the estimator for the expected value of $K$ (the counterpart of the parameter $k$ from the Ikemoto and Takai's method) is $[416.641, 428.709]$, while its empirical counterpart derived from the bootstrap sample is $[416.972, 428.709]$. The empirical coverage probability of this 95% confidence interval is 0.96. The standard error of the new estimator is 3.02, whereas the bootstrap equivalent is 3.06 (Table 3).

### Interval estimate

For the Ikemoto and Takai method, the interval estimate is $[378, 456]$, with an empirical coverage probability of 0.75. In the case of the new method, the interval estimate is $[341, 486]$, and its empirical coverage probability is 0.94 (Table 4). While both methods declare covering 95% of observations.
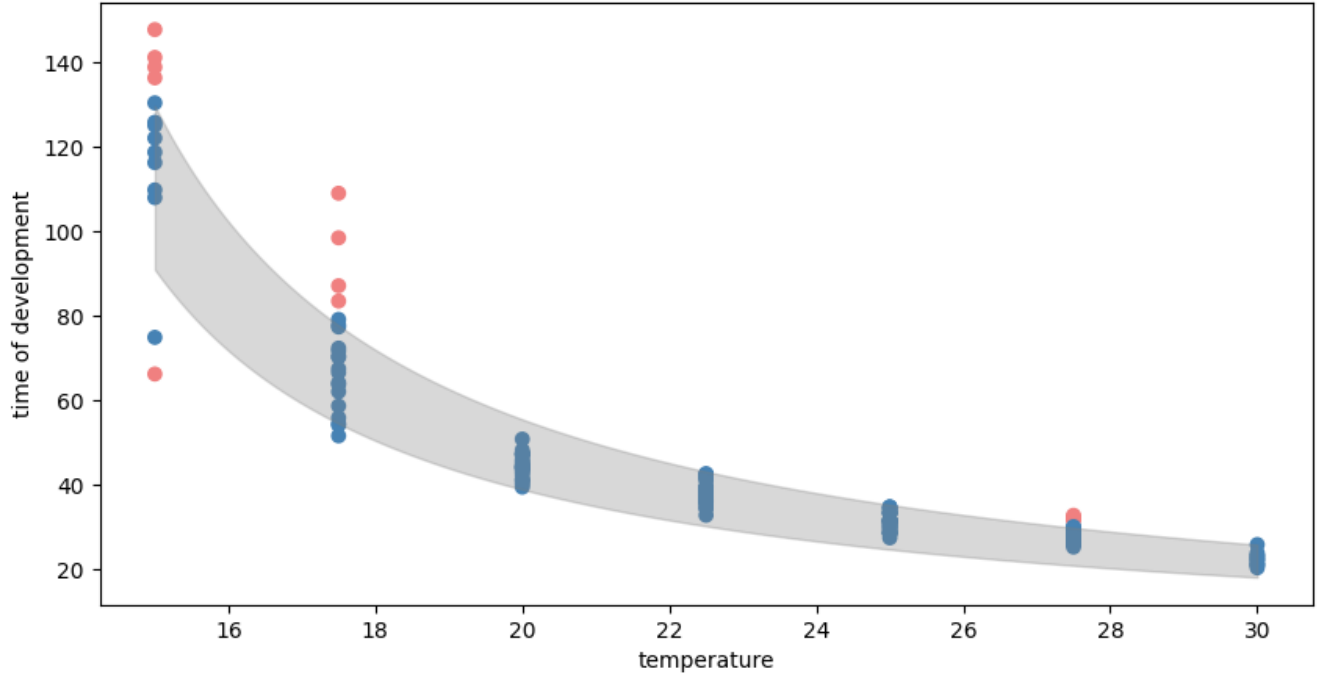
**Figure 2.** Time of development vs. temperature in the *Creophilus maxillosus'* dataset. Blue points are regular results of the experiment, red points are outliers, and the shaded area is an interval estimate.

| Method | 95% confidence interval | Interval's width | Coverage probability of the 95% interval |
|---|---|---|---|
| Ikemoto and Takai | $[378, 456]$ | 78 | 1 |
| This paper | $[416.641, 428.709]$ | 12.069 | 0.96 |

**Table 3.** Comparison of confidence intervals for *Creophilus maxillosus* derived using different methods.

## Practical application using *Necrodes littoralis* data

### Estimation of time of development

Suppose an expert found a freshly eclosed individual of the species *Necrodes littoralis* on the cadaver, measuring 18 mm in length, and the average preceding temperature was 22 degrees Celsius, hence $T = 22$. Let $k_l$ and $k_u$ denote the lower and upper bounds of the interval estimate of $K$, respectively. The values calculated using the Ikemoto and Takai method are $k_l = 420$, $k_u = 518$ (Table 8), and $t_0 = 8.49$[1]. Ultimately, the interval estimate of the development time is:

$$\left[ \frac{k_l}{T - t_0}, \frac{k_l}{T - t_0} \right] = \left[ \frac{420}{22 - 8.49}, \frac{518}{22 - 8.49} \right] = [31.01, 38.34] \tag{1}$$

In our dataset on *Necrodes littoralis*[2], at a temperature of 22°C, two individuals (approximately 2%) with a length of 18 mm or more developed within the interval $[31.01, 38.34]$ days. According to Table 8, on average, the intervals calculated in this way for different temperatures and sizes cover 59% of cases.

Considering the same scenario but using the values calculated with the method from this paper, namely $k_l = 306$, $k_u = 431$ (Table 8), and $t_0 = 9.52$ (Table 9). In this case, the parameters of the blue population should be used, as the length of the examined individual exceeds the average length of individuals in the blue population (Table 10). The interval estimate of the development time is:

$$\left[ \frac{k_l}{T - t_0}, \frac{k_l}{T - t_0} \right] = \left[ \frac{306}{19 - 9.52}, \frac{431}{19 - 9.52} \right] = [24.52, 34.54] \tag{2}$$

| | 95% interval estimate of $k$ | Interval's width | Coverage probability of 95% interval estimate of $k$ |
|---|---|---|---|
| Blue population | $[341, 486]$ | 145 | 0.94 |
| Ikemoto and Takai | $[378, 456]$ | 78 | 0.75 |

**Table 4.** Interval estimates for parameter $k$ for *Creaphilus maxillosus*.

In the dataset, all individuals measuring 18 mm or more at a temperature of 22°C developed within the interval $[24.52, 34.54]$ days. According to Table 8, on average, the intervals calculated in this way for different temperatures and sizes cover between 96% and 100% of cases.

## Controlling width of the interval

According to the assumption adopted in the article, the above intervals should cover approximately 95% of the actual cases. Matuszewski and Mądra-Bielewicz[3] suggest that in some cases, using narrower intervals may be more practical. With the Ikemoto and Takai method, it is not possible to control how many actual cases will be covered by the interval. In contrast, with the new method, intervals covering any desired proportion of cases can be calculated using the quantiles of the Weibull distribution with parameters from Table 9. Table 5, Table 6 and Table 7 contain examples.

| Quantile orders of the interval limits | Interval estimate | Theoretical coverage probability |
|---|---|---|
| $[0.025, 0.975]$ | $[324, 466]$ | 0.95 |
| $[0.05, 0.95]$ | $[341, 459]$ | 0.90 |
| $[0.1, 0.9]$ | $[360, 451]$ | 0.80 |
| $[0.15, 0.85]$ | $[371, 444]$ | 0.70 |

**Table 5.** Examples of interval estimates of $k$ for *Necrodes littoralis* smaller than 17.34.

| Quantile orders of the interval limits | Interval estimate | Theoretical coverage probability |
|---|---|---|
| $[0.025, 0.975]$ | $[306, 431]$ | 0.95 |
| $[0.05, 0.95]$ | $[322, 425]$ | 0.90 |
| $[0.1, 0.9]$ | $[338, 418]$ | 0.80 |
| $[0.15, 0.85]$ | $[348, 412]$ | 0.70 |

**Table 6.** Examples of interval estimates of $k$ for *Necrodes littoralis* larger than 17.34.

| Quantile orders of the interval limits | Interval estimate | Theoretical coverage probability |
|---|---|---|
| $[0.025, 0.975]$ | $[341, 486]$ | 0.95 |
| $[0.05, 0.95]$ | $[358, 479]$ | 0.90 |
| $[0.1, 0.9]$ | $[377, 470]$ | 0.80 |
| $[0.15, 0.85]$ | $[389, 463]$ | 0.70 |

**Table 7.** Examples of interval estimates of $k$ for *Creophilus maxillosus.*

## Technical details

### Assumptions
We assumed that $(D, T)$ is a bivariate random variable, where the variables $D$ and $T$ are related according to the formula:

$$K = D(T - t_0), \tag{3}$$

where $K$ is a random variable of a development parameter $k$, whereas $k$ is a realization of $K$.

We assumed that combined population $K_c$ consists of component populations $K_1, K_2, \ldots, K_L$. Each $K_i$ is distributed accoring to Weibull distribution (as the Weibull distribution is used for modeling time-to-event data[4] and $K$ is a time, normalized by temperature, to completion of development), and consequently, the combined population follows a finite mixture model[5] of Weibull distributions, i.e.:

$$\begin{aligned}
K_1 &\sim \text{Weib}(k_1, \kappa_1, \lambda_1), \\
K_2 &\sim \text{Weib}(k_2, \kappa_2, \lambda_2), \\
&\vdots \\
K_L &\sim \text{Weib}(k_L, \kappa_L, \lambda_L), \\
K_c &\sim \sum_{i=1}^{L} w_i \, \text{Weib}(k_i, \kappa_i, \lambda_i)
\end{aligned} \tag{4}$$

where $K_i$ are random variables, $k_i$ are their realizations, weib is the density of the Weibull distribution, $\kappa_i$ and $\lambda_i$ are the parameters of the Weibull distribution, $\sum_{i=1}^{L} w_i = 1$.

Moreover, we assume that $k_i = d(t - t_0^{(i)})$, where d is a realization of the random variable $D$, $t$ is a realization of random variable $T$, $t_0^{(i)}$ is a parameter that distinguishes populations. In consequence:

$$\begin{aligned}
K_1 &= D(T - t_0^{(1)}) \sim c_1 \, \text{Weib}(d(t - t_0^{(1)}), \kappa_1, \lambda_1), \\
K_2 &= D(T - t_0^{(2)}) \sim c_2 \, \text{Weib}(d(t - t_0^{(2)}), \kappa_2, \lambda_2), \\
&\vdots \\
K_L &= D(T - t_0^{(L)}) \sim c_L \, \text{Weib}(d(t - t_0^{(L)}), \kappa_L, \lambda_L), \\
K_c &\sim \sum_{i=1}^{L} w_i \, c_i \, \text{Weib}(d(t - t_0^{(i)}), \kappa_i, \lambda_i)
\end{aligned} \tag{5}$$

where $c_i$ are normalization constants, the remaining notations are as previously defined.

Finally, our goal is to estimate the parameters of the distribution of the combined population, i.e. $t_0^{(i)}$, $\kappa_i$, and $\lambda_i$, for $i = 1, \ldots, L$.

### Fitting model
We applied the EM (Expectation–maximization) algorithm[6]. It is iterative, so we randomly chose starting values for the parameters. Let

$$
\begin{aligned}
\mathbf{w} &= (w_1,\ldots,w_L) \\
\boldsymbol{\kappa} &= (\kappa_1,\ldots,\kappa_L) \\
\boldsymbol{\lambda} &= (\lambda_1,\ldots,\lambda_L) \\
\mathbf{t_0} &= \left(t_0^{(1)},\ldots,t_0^{(L)}\right) \\
{}^{(j-1)}\mathbf{w} &= \left({}^{(j-1)}w_1,\ldots,{}^{(j-1)}w_L\right) \\
{}^{(j-1)}\boldsymbol{\kappa} &= \left({}^{(j-1)}\kappa_1,\ldots,{}^{(j-1)}\kappa_L\right) \\
{}^{(j-1)}\boldsymbol{\lambda} &= \left({}^{(j-1)}\lambda_1,\ldots,{}^{(j-1)}\lambda_L\right) \\
{}^{(j-1)}\mathbf{t_0} &= \left({}^{(j-1)}t_0^{(1)},\ldots,{}^{(j-1)}t_0^{(L)}\right) \\
\mathbf{d} &= (d_1,\ldots,d_n) \\
\mathbf{t} &= (t_1,\ldots,t_n)
\end{aligned}
\tag{6}
$$

The vectors $\mathbf{w}$, $\boldsymbol{\kappa}$, $\boldsymbol{\lambda}$, and $\mathbf{t_0}$ are the vectors of parameters we want to estimate. The vectors $\mathbf{w}^{(j-1)}$, $\boldsymbol{\kappa}^{(j-1)}$, $\boldsymbol{\lambda}^{(j-1)}$, and $\mathbf{t_0}^{(j-1)}$ are the approximations of these parameters in the $(j-1)$-th iteration. The vectors $\mathbf{d}$ and $\mathbf{t}$ represent the data.

The EM algorithm maximizes the $Q$-function. In our case, it is of the following form:

$$
Q\left(\mathbf{w},\boldsymbol{\kappa},\boldsymbol{\lambda},\mathbf{t_0} \mid {}^{(j-1)}\mathbf{w}, {}^{(j-1)}\boldsymbol{\kappa}, {}^{(j-1)}\boldsymbol{\lambda}, {}^{(j-1)}\mathbf{t_0}, \mathbf{d}, \mathbf{t}\right) =
$$
$$
\sum_{i=1}^{n}\sum_{l=1}^{L} v_{i,l}\left({}^{(j-1)}\mathbf{w}, {}^{(j-1)}\boldsymbol{\kappa}, {}^{(j-1)}\boldsymbol{\lambda}, {}^{(j-1)}\mathbf{t_0}\right)\left[\log(w_l) + \log\left(c_l\,\mathrm{Weib}(d_i(t_i - t_0^{(l)}), \kappa_l, \lambda_l)\right)\right]
\tag{7}
$$

where

$$
v_{i,r}\left({}^{(j-1)}\mathbf{w}, {}^{(j-1)}\boldsymbol{\kappa}, {}^{(j-1)}\boldsymbol{\lambda}, {}^{(j-1)}\mathbf{t_0}\right) = \frac{{}^{(j-1)}w_r\, c_r\, \mathrm{Weib}\left(d_i(t_i - {}^{(j-1)}t_0^{(r)}), {}^{(j-1)}\kappa_r, {}^{(j-1)}\lambda_r\right)}{\sum_{l=1}^{L}{}^{(j-1)}w_l\, c_l\, \mathrm{Weib}\left(d_i(t_i - {}^{(j-1)}t_0^{(l)}), {}^{(j-1)}\kappa_l, {}^{(j-1)}\lambda_l\right)}
\tag{8}
$$

We then manually computed the partial derivatives of the $Q$-function with respect to each parameter. (This is a minor difference from the approach described by McLachlan et al.[5]. They did not differentiate with respect to the parameter w, but we did). In each iteration, we computed the value of the $Q$-function and found its stationary point by founding the zeros of the partial derivatives using the bisection method. The stationary point was then used as the parameter values for the next iteration. The loop terminated when the difference in the $Q$-function values between consecutive iterations was less than $10^{-6}$.

We denote the estimated values of the parameters as $\widehat{w}_i$, $\widehat{t}_0^{(i)}$, $\widehat{\kappa}_i$, and $\widehat{\lambda}_i$.

**Clustering**

To separate the combined population into component populations, we performed a clustering based on the following principle: a point $(d_i, t_i)$ belongs to population $l$ if:

$$
\widehat{w}_l\, c_l\, \mathrm{Weib}\left(d_i(t_i - \widehat{t}_0^{(l)}), \widehat{\kappa}_l, \widehat{\lambda}_l\right) = \max\left(\widehat{w}_1\, c_1\, \mathrm{Weib}(d_i(t_i - \widehat{t}_0^{(1)}), \widehat{\kappa}_1, \widehat{\lambda}_1), \ldots, \widehat{w}_L\, c_L\, \mathrm{Weib}(d_i(t_i - \widehat{t}_0^{(L)}), \widehat{\kappa}_L, \widehat{\lambda}_L)\right)
\tag{9}
$$

From now on, we refer to $k_i = d_i(t_i - t_0^{(l)})$ as the "true k".

**Choosing number of populations**

To determine the number of component populations, we applied the EM algorithm four times with $L$ set to 1, 2, 3, and 4, respectively. We then selected the optimal value of $L$ using the Bayesian Information Criterion (BIC) and the elbow rule[7]. The formula for BIC was as follows:

$$\text{BIC}(m,n,f,\mathbf{d},\mathbf{t}) = m\ln(n) - 2\sum_{i=1}^{n}\ln\big(f(d_i,t_i)\big) \tag{10}$$

where $m$ is the number of parameters, $n$ is the number of observations, $f$ is the density of the combined population, and $\mathbf{d}$, $\mathbf{t}$ are vectors of data as previously defined.

**Choosing the best population**

Our goal in this part is to select one population, which we then use to calculate both the interval estimate and the confidence interval.

If, in a given case, the value $w_l$ for a certain component population was much higher than for the others, we treated the population $l$ as representing the desirable experimental results, and the remaining populations as outlier observations. The meaning of "much higher" is subjective and arbitrary.

If the values $w_i$ for several populations were high and similar, we used a Mann-Whitney U-test to assess the significance of differences in the sizes of individuals belonging to different populations. From further analyses, both the outlier population and the population of small insects were excluded.

**Bootstrap sampling**

We compared the results of both methods with the results of bootstrap simulations to assess which are more reliable. For the new method, we drew a sample with replacement equal in size to the dataset, transformed the data using the formula $d_i(t_i - t_0^{(l)})$, and then calculated the arithmetic mean. We repeated this sampling 1,000 times, obtaining a bootstrap sample, which we used to determine an empirical confidence interval for the mean. We refer to this confidence interval as the empirical counterpart derived from the bootstrap sample ("counterpart" because we calculate the confidence interval using the proposed method). In the case of the Ikemoto and Takai method, we also drew a sample with replacement equal in size to the dataset and then applied the Ikemoto and Takai method to this new sample. By repeating this sampling 1,000 times, we obtained a bootstrap sample, which we used to determine an empirical confidence interval for the parameter $k$. We also refer to this confidence interval as the empirical counterpart derived from the bootstrap sample, which should not lead to misunderstandings (again "counterpart" because we calculate the confidence interval using the Ikemoto and Takai's method).

It is easy to show that both approaches lead to a distribution of the mean which, based on the central limit theorem, converges to a normal distribution as the sample size increases. However, these distributions differ because the Ikemoto and Takai method manipulates the sample size, which slows down the convergence.

**Coverage probability of confidence interval**

To evaluate whether the presented method is more precise than the Ikemoto and Takai[8] method, we calculated the empirical coverage probability for the population $l$, selected as described earlier.

We computed the confidence intervals for the expected value of the variable $D(T - t_0^{(l)})$ based on the sample $\big(d_1(t_1 - t_0^{(l)}),\ldots,d_n(t_n - t_0^{(l)})\big)$ using the Central Limit Theorem, i.e.:

$$\left[\overline{k} - 1.96\,\frac{\widehat{s}}{\sqrt{n}},\ \overline{k} + 1.96\,\frac{\widehat{s}}{\sqrt{n}}\right] \tag{11}$$

where $\overline{k}$ and $\widehat{s}$ are the sample mean and the sample standard deviation of $\big(d_1(t_1 - t_0^{(l)}), d_2(t_2 - t_0^{(l)}), \ldots, d_n(t_n - t_0^{(l)})\big)$. Then we calculated the empirical coverage probability using bootstrap sampling as the proportion of elements of the bootstrap sample that fall inside this interval relative to the total number of elements.

For the Ikemoto and Takai method, we calculated the confidence intervals for the estimated development parameter $k$, assuming the 95% interval takes the form $[\widehat{k} - 1.96\,s_e,\ \widehat{k} + 1.96\,s_e]$, where $\widehat{k}$ is the parameter estimate and $s_e$ is the standard error, both computed using the Ikemoto and Takai method. For comparison, as we described earlier, we also calculated the empirical coverage probability using bootstrap sampling.

**Coverage probability of interval estimate**

Let the random variable $X$ be distributed according to some distribution $P$. We define the interval estimate capturing 95% of the realizations $x$ as $[x_l, x_u]$, where $x_l$ is the 0.025 quantile of the distribution $P$, and $x_u$ is the 0.975 quantile of the distribution $P$.

We computed the interval estimate for the realization $k$ of the random variable $K$ for the presented method as follows: we selected the population $l$ according to the criteria mentioned earlier and then used the identity:

$$\text{Weib}\big(d_i(t_i - t_0^l), \kappa_l, \lambda_l\big) = \text{Weib}(k_i, \kappa_l, \lambda_l) \tag{12}$$

Then we calculated the quantiles of the Weibull distribution with parameters $\kappa_l$ and $\lambda_l$. Therefore, the interval $[k_l, k_u]$ (such that $k_l$ is the 0.025 quantile and $k_u$ is the 0.975 quantile) is our interval estimate that captures 95% of the realizations of $k$. From now on, we will skip the phrase "captures 95% of the realizations" as obvious. All our interval estimates should be understood as 95% coverage intervals.

For the Ikemoto and Takai method, we used its confidence interval computed in the previous section just for illustration that it does not perform well in real-life estimations.

To compare these two intervals, we computed the proportion of observations within these intervals relative to all observations. We refer to this proportion as the empirical coverage probability of the interval estimate.

|  | 95% interval estimate of $k$ | Interval's width | Coverage probability of 95% interval estimate of $k$ |
|---|---|---|---|
| Large insects (blue population) | $[306, 431]$ | 125 | 1 |
| Small insects (red population) | $[324, 466]$ | 142 | 0.96 |
| Combined population | $[306, 466]$ | 160 | 0.98 |
| Ikemoto and Takai | $[420, 518]$ | 98 | 0.59 |

**Table 8.** Interval estimates for parameter $k$ of *Necrodes littoralis* (reproduced from the main article, Table 6)

|  | Blue population | Red population |
|---|---|---|
| $w_l$ | 0.41 | 0.59 |
| $\kappa_l$ | 14.57 | 13.67 |
| $\lambda_l$ | 394.44 | 423.95 |
| $t_0^{(l)}$ | 9.52 | 10.21 |

**Table 9.** Coefficients of mixture model of Weibull's distribution for *Necrodes littoralis* dataset (reproduced from the main article, Table 3).

|  | Length [mm] |
|---|---|
| Blue population | 17.75 |
| Red population | 16.96 |

**Table 10.** Mean insect length in each population of *Necrodes littoralis* (reproduced from the main article, Table 4)

# References

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## Author contributions statement

J.W.: Conceptualization, Writing – review & editing, Software, Investigation, Data curation, Formal analysis, Validation, Visualization, Writing – original draft. Ł.S.: Conceptualization, Writing – review & editing, Supervision. S.M.: Conceptualization, Writing – review & editing, Supervision.

## Data availability statement

The data analyzed in this study were obtained from previously published works and are not publicly available due to copyright and data sharing restrictions. Access to these data can be requested from the corresponding authors of the respective publications:

1. Frątczak-Łagiewska, K., Grzywacz, A. & Matuszewski, S. Development and validation of forensically useful growth models for central european population of Creophilus maxillosus l. (coleoptera: Staphylinidae). Int. J. Leg. Medicine 134, 1531–1545, (2020), https://doi.org/10.1007/s00414-020-02275-3

2. Gruszka, J. & Matuszewski, S. Temperature models of development for Necrodes littoralis l. (coleoptera: Silphidae), a carrion beetle of forensic importance in the palearctic region. Sci. Reports 12, 9689, (2022), DOI: https://doi.org/10.1038/s41598-022-13901-y

The datasets were used with appropriate permissions solely for the purposes of this analysis. All additional data, materials, and code generated during this study are openly available in the GitHub repository (https://github.com/Jedrzej-Wydra/survival_analysis_em) and in supplementary materials.

## Additional information

The authors declare no competing interests.