

Sample size for estimating organism concentration in ballast water: a Bayesian approach

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Abstract

Estimation of microorganism concentration in ballast water tanks is important to evaluate and possibly to prevent the introduction of invasive species in stable ecosystems. For such purpose, the number of organisms in ballast water aliquots must be counted and used to estimate their concentration with some precision requirement. **Poisson and negative binomial models have been employed to describe the organism distribution in the tank, but determination of sample sizes required to generate estimates with pre-specified precision is still not well established. A Bayesian approach is a flexible alternative to accommodate adequate models that account for the heterogeneous distribution of the organisms and may provide a sequential way of enhancing the estimation procedure by updating the prior distribution along the ballast water discharging process. We adopt such an approach to compute sample sizes required to construct credible intervals obtained via two optimality criteria that have not been employed in this context. Such**

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intervals may be used in the decision with respect to compliance with the D-2 standard of the Ballast Water Management Convention. We also conduct a simulation study to verify whether the credible intervals obtained with the proposed sample sizes satisfy the precision criteria.

Keywords: average coverage criterion, average length criterion, Poisson/gamma distribution, negative binomial/Pearson Type VI distribution.

1 Introduction

Evaluation of ballast water discharges from ships is a topic of current interest because the possible introduction of invasive species in stable ecosystems may bring serious environmental and economic consequences. Estimates of damage costs of invasive species may vary from 0.4 to 220 billion USD per year in 2008 prices (Marbuaah *et al.*, 2014, Table 1). Among other requirements, the D-2 standard of the Ballast Water Management (BWM) Convention requires that deballasted water should contain less than 10 viable organisms (referred to simply as organisms in the remainder) per mL , sized ≥ 10 and $< 50 \mu m$ in minimum dimension (IMO, 2004). This class of organisms comprise zooplankton and phytoplankton. An overview of research in ballast water in the last thirty years is presented in Bailey (2015).

Given the large amount of ballast water (up to thousands of tons) transported by big vessels, one has to rely on sampling methods to verify whether the standard is satisfied. This is a difficult task, especially for organisms sized ≥ 10 and $< 50 \mu m$ in minimum dimension. Recently, Jang *et al.* (2019) mention that there is no established sampling methodology for such microorganisms. Although this topic has attracted the attention of many researchers,

very few papers deal with sample sizes required to verify compliance with the D-2 norm. Exceptions are Basurko & Mesbahi (2011), Miller *et al.* (2011) and Frazier *et al.* (2013), who discuss the problem but do not provide a formal solution. Costa *et al.* (2015, 2016) attacked the problem with a more formal approach, defining the sample as a set of n aliquots (sub-samples) in each of which the number of organisms is counted. The volume of each sample, say w , depends on the specific counting procedure (Casas-Monroy *et al.*, 2020). The sampling process is based on a probabilistic model and on a criterion according to which one must compute the number of aliquots of ballast water with volume w mL needed to decide **with a certain margin of error** whether the D-2 standard is complied with. One of the difficulties with this approach relates to the heterogeneous nature of the organism concentration in the ballast water tank (Murphy *et al.*, 2002; Carney *et al.*, 2013; Casas-Monroy *et al.*, 2020). Based on frequentist methods, Costa *et al.* (2015, 2016) adopted models that take this heterogeneity into account. In particular, Costa *et al.* (2015) consider Poisson and negative binomial distributions and specify probabilities for Type I and II errors to test the hypothesis that the mean organism concentration in the tank is smaller than 10 organisms per mL . Costa *et al.* (2016), on the other hand, consider the same probability distributions and specify a lower bound to the probability that the difference between the mean concentration and its estimate be less than a fixed value. Costa (2017) suggests the adoption of more flexible models that may possibly incorporate knowledge acquired over time. Bayesian models are excellent candidates to incorporate such characteristics because that information may be considered in the prior distribution which may also be updated when more data is obtained.

Two criteria are widely used in the Bayesian literature, but not in

the setup under investigation for sample size determination, namely, the average coverage and the average length of credible intervals (ACC and ALC, respectively). In both cases, we choose the smallest sample size that satisfies the condition imposed on some specified average characteristic of the posterior distribution of the parameter of interest.

For the ACC we compute the posterior probability of a highest posterior density (HPD) interval with fixed length for each sample \mathbf{x}_n of size n and weigh it by the marginal distribution of the data. This average probability must be not smaller than a specified lower bound. For the ALC, on the other hand, we compute the length of an interval with fixed credible degree for each (\mathbf{x}_n, n) and weigh it by the same marginal distribution. The average length must not be larger than a specified upper bound.

Adcock (1987, 1988) uses the ACC (with a different label) to determine sample sizes required to estimate multinomial probabilities under Dirichlet prior distributions as well as to estimate the mean and the variance of normal distributions with prior normal or chi-squared distributions for the cases where the variance is known or unknown, respectively. Joseph *et al.* (1995) and Joseph *et al.* (1997) use both the ACC and the ALC, among other Bayesian criteria for estimating the proportion and the difference between two proportions under binomial distributions with beta prior distributions.

Wang & Gelfand (2002) use the same criteria to determine the sample size for the estimation of parameters of distributions belonging to the exponential family, of parameters in Weibull survival models as well as of parameters in logistic regression models. M'Lan *et al.* (2006) use the ACC and ALC criteria in the context of case-control studies; Stamey *et al.* (2006) also consider these criteria to estimate the parameters of Poisson distributions as well to estimate the difference or the ratio of the parameters of two Poisson

distributions. We may also cite Joseph & Bélisle (1997), Joseph & Wolfson (1997), Rahme *et al.* (2000), De Santis (2007), M'Lan *et al.* (2008) for related work.

We consider a Bayesian approach to compute minimum sample sizes required to obtain lower and upper limits of credible intervals for the mean organism concentration in a ballast water tank with specified average coverage or average length. Letting \mathbf{x}_n denote a sample of size n determined according to the proposed approach, the credible intervals defined by the lower [say, $a(\mathbf{x}_n)$] and upper [say, $b(\mathbf{x}_n)$] limits will have in average, the specified coverage or length. Given this interval, the ship from which the sample was collected is declared not compliant with the D-2 standard if $a(\mathbf{x}_n) \geq 10$ or compliant, if $b(\mathbf{x}_n) < 10$. Otherwise, if $a(\mathbf{x}_n) < 10 \leq b(\mathbf{x}_n)$, more data are needed to make a decision.

In Section 2 we describe the adopted Bayesian models. Sample size determination under both the ACC and the ALC criteria is discussed and implemented in Section 3. A simulation study to evaluate whether HPD intervals constructed with the proposed sample sizes satisfy the adopted optimality criteria is presented in Section 4. The last section discusses the results obtained from the computation of the minimum sample sizes as well as from the simulation study. Algorithms for sample size computations, written with the R language (R Core Team, 2016), are presented in the Supplementary Material.

2 Bayesian models

2.1 Poisson model with a gamma prior distribution

Given that the expected organism concentration (per unit of volume) in the tank is λ , let X be the number of organisms in an aliquot of volume w ; in this aliquot, we expect to find $\mathbb{E}[X|\lambda] = w\lambda$ organisms. Suppose that the organisms are homogeneously distributed in the ballast water tank, and that, given λ , X follows a Poisson distribution with mean $w\lambda$.

The natural (conjugate) choice for the prior distribution is a gamma distribution with parameters θ_0 and λ_0 , namely $\lambda \sim G(\theta_0, \theta_0/\lambda_0)$, for which the probability density function is

$$h(\lambda) \propto \lambda^{\theta_0-1} \exp(-\theta_0\lambda/\lambda_0).$$

This implies that $\mathbb{E}[\lambda] = \lambda_0$ and $\text{Var}[\lambda] = \lambda_0^2/\theta_0$. In this context, λ_0 represents a prior expected concentration and θ_0 controls the variability of λ around λ_0 . The gamma distribution provides ample flexibility to model the shape of the prior knowledge on the mean concentration λ . In Figure S1 of the Supplementary Material we present gamma density functions with different shapes.

Consider a random sample $\mathbf{x}_n = (x_1, \dots, x_n)$ of size n of $X|\lambda$ and a gamma prior distribution for λ . We may write the Bayesian Poisson/gamma model hierarchically as follows

$$X_i|\lambda \stackrel{\text{iid}}{\sim} \text{Poi}(w\lambda), \quad i = 1, 2, \dots, n; \quad (1)$$

$$\lambda \sim G(\theta_0, \theta_0/\lambda_0). \quad (2)$$

The posterior distribution of λ is also gamma, with parameters $\theta_0 + s_n$

and $nw + \theta_0/\lambda_0$, where $s_n = \sum_{i=1}^n x_i$, *i.e.*, $\lambda|\mathbf{x}_n \sim G(\theta_0 + s_n, nw + \theta_0/\lambda_0)$. An example of prior and posterior densities is presented in Figure 1. The effect of the observed data is clearly observed to lead to a posterior distribution more concentrated than the prior distribution.

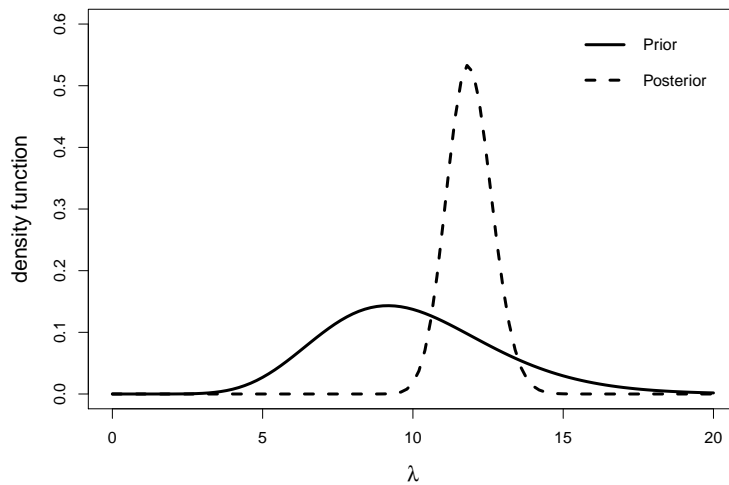


Figure 1: Prior gamma distribution $G(\theta_0, \theta/\lambda_0)$ and posterior gamma distribution $G(\theta_0 + s_n, nw + \theta_0/\lambda_0)$ with $w = 1$, $\lambda_0 = 10$, $\theta_0 = 12$, $n = 20$ and $s_n = 240$.

2.2 Negative binomial model with a Pearson Type VI prior distribution

In contrast with the homogeneity assumption for the organism distribution in the tank inherent to the Poisson model, consider a more realistic situation where the organisms are distributed heterogeneously. A reasonable model for the organism distribution in this case is the negative binomial distribution, which may be motivated as follows.

Suppose that the organism concentration varies in the tank according to a gamma distribution with parameters ϕ and ϕ/λ . Consider n aliquots

with volume w randomly selected from the tank and let λ_i denote the corresponding organism concentration, $i = 1, \dots, n$. Assume that given λ_i , the corresponding number of organisms, X_i , follows a Poisson distribution with mean $w\lambda_i$. Thus, given λ and ϕ , X_i follows a negative binomial distribution with $\mathbb{E}[X_i|\lambda, \phi] = w\lambda$ and $\text{Var}[X_i|\lambda, \phi] = w\lambda + (w\lambda)^2/\phi$, where ϕ is a shape (or agglomeration) parameter. This is denoted as $X_i|\lambda, \phi \sim NB(w\lambda, \phi)$ and the probability function can be written as

$$f(x_i|\lambda, \phi) = \frac{\Gamma(\phi + x_i)}{\Gamma(x_i + 1)\Gamma(\phi)} \left(\frac{w}{\phi}\lambda\right)^{x_i} \left(1 + \frac{w}{\phi}\lambda\right)^{-\phi - x_i}.$$

For inferences on the parameter of interest λ we consider ϕ fixed (taking on several values in the following analysis). A natural conjugate prior distribution for the parameter λ of the negative binomial distribution is a Pearson Type VI distribution (Johnson *et al.*, 1994a,b), also known as a generalized beta prime distribution with a further scale factor ϕ/w , for which the kernel of the probability density function is

$$h(\lambda) \propto \frac{w}{\phi} \left(\frac{w}{\phi}\lambda\right)^{\theta_0 - 1} \left(1 + \frac{w}{\phi}\lambda\right)^{-\theta_0 - (\theta_0/\lambda_0 + 1)},$$

with location parameter 0, scale parameter ϕ/w and shape parameters θ_0 and $\theta_0/\lambda_0 + 1$, where λ_0 and θ_0 are known positive fixed constants (hyperparameters). We use the notation $\lambda \sim PVI(0, \phi/w, \theta_0, \theta_0/\lambda_0 + 1)$. In this case, $\mathbb{E}[\lambda] = (\phi/w)\lambda_0$ and $\text{Var}[\lambda] = (\lambda_0^2/\theta_0)[\phi^2(\lambda_0 + 1)/(w^2(1 - \lambda_0/\theta_0))]$, for $\lambda_0 < \theta_0$.

In the Poisson model with gamma prior distribution, we have $\mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X|\lambda]] = \mathbb{E}[w\lambda] = w\lambda_0$, *i.e.*, the expected number of organisms when collecting an aliquot depends only on the hyperparameter λ_0 . This makes sense since we are assuming homogeneity for the concentration, and regardless

of the location where we collect an aliquot in the ballast water tank, we expect to find the same number of organisms. On the other hand, if we consider the negative binomial model with a Pearson Type VI prior distribution, we have $\mathbb{E}[X] = \phi\lambda_0$ so that the expected number of organisms in an aliquot depends on the parameter ϕ that controls the heterogeneity of the organisms in the tank. Note that ϕ is also a scale parameter for the prior distribution and the larger its value, the more spread out is the distribution with the other parameters fixed, indicating a vague prior knowledge about the parameter of interest. Furthermore, we can set the other parameters in such a way that the prior distribution may represent cases where there is high probability associated to an interval even when the value of ϕ increases. When λ_0 and θ_0 are fixed and ϕ increases, we have distributions representing cases with large variability. **Examples are presented in Figures S2 and S3 of the Supplementary Material.**

Consider a random sample of size n from $X|\lambda, \phi$, and a Pearson Type VI prior distribution for λ . We may write the model hierarchically as follows

$$X_i|\lambda, \phi \stackrel{\text{iid}}{\sim} NB(w\lambda, \phi), \quad i = 1, 2, \dots, n; \quad (3)$$

$$\lambda \sim PVI(0, \phi/w, \theta_0, \theta_0/\lambda_0 + 1). \quad (4)$$

The posterior distribution of λ is Pearson Type VI, with the same location and scale parameters as the prior distribution, and shape parameters $\theta_0 + s_n$ and $\theta_0/\lambda_0 + n\phi + 1$, *i.e.*, $\lambda|\mathbf{x}_n \sim PVI(0, \phi/w, \theta_0 + s_n, \theta_0/\lambda_0 + n\phi + 1)$.

We must emphasize that ϕ plays two roles in model (3)-(4). In (3), it plays the role of a dispersion (or agglomeration) parameter. The larger is ϕ , the more homogeneous is the organism concentration in the tank. In the prior distribution (4), ϕ plays the role of scale parameter. Keeping the other

parameters fixed, the larger is ϕ , the less precise is the prior knowledge about the parameter of interest (see Figure S2 of the Supplementary Material). This does not mean that if ϕ (previously known) is large we may only assign prior distributions with large variability, because we may specify the parameters λ_0 and θ_0 to adjust the precision of the prior knowledge even with large values of ϕ (see Figure S3 of the Supplementary Material).

3 Sample size determination

We consider two criteria to determine the minimum sample size, *i.e.*, **minimum number of aliquots**, required to estimate λ with a pre-specified precision.

3.1 Average coverage criterion (ACC)

The objective is to obtain the minimum sample size n such that the credible interval $R(\mathbf{x}_n)$ for λ has a pre-specified length with posterior probability at least equal to $1 - \rho$, *i.e.*,

$$\int_{R(\mathbf{x}_n)} h(\lambda|\mathbf{x}_n)d\lambda \geq 1 - \rho,$$

where \mathbf{x}_n is a sample of size n and $R(\mathbf{x}_n)$ is a subset (an interval in our case) of the parameter space. Since the sample size determination precedes the actual sampling, we must consider all possible outcomes for \mathbf{x}_n to achieve the objective. In this direction we may weigh each outcome by its probability, *i.e.*,

$$\int_{\mathcal{X}^n} \left[\int_{R(\mathbf{x}_n)} h(\lambda|\mathbf{x}_n)d\lambda \right] g(\mathbf{x}_n)d\mathbf{x}_n \geq 1 - \rho,$$

where \mathcal{X}^n is the sample space associated to \mathbf{x}_n and $g(\mathbf{x}_n)$ is the marginal probability function of the outcomes.

For models (1)-(2) and (3)-(4), the credible region **in general is an interval** and in this case, we consider the highest posterior density (HPD) interval to define $R(\mathbf{x}_n) = [a(\mathbf{x}_n), b(\mathbf{x}_n)]$. We fix the length $\ell > 0$ of the **desired** HPD intervals for λ , specify the minimum Bayesian coverage probability, $1 - \rho$ and determine the minimum sample size as well as the bounds $a(\mathbf{x}_n)$ and $b(\mathbf{x}_n) = a(\mathbf{x}_n) + \ell$ such that

$$\int_{\mathcal{X}^n} \left[\int_{a(\mathbf{x}_n)}^{b(\mathbf{x}_n)} h(\lambda|\mathbf{x}_n) d\lambda \right] g(\mathbf{x}_n) d\mathbf{x}_n \geq 1 - \rho. \quad (5)$$

Given $a(\mathbf{x}_n)$, $b(\mathbf{x}_n)$ and the parameters of the posterior distribution, the inner integral in (5) may be obtained computationally; the outer integral may be estimated via Monte Carlo simulation. An algorithm to obtain the minimum sample size satisfying the criterion is outlined in the Supplementary Material.

In Tables 1 and 2 we present sample sizes computed via ACC (5) **setting the length of the required credible interval $\ell = 2$** for models (1)-(2) and (3)-(4), respectively. **In Tables S1 and S2 of the Supplementary Material we present the same scenario for $\ell = 4$.** Note that for model (3)-(4) we consider $\lambda_0 = 10(w/\phi)$ to make the prior expected value equal to 10 in order to allow a comparison with model (1)-(2) for which we fixed $\lambda_0 = 10$. **The values considered for the parameter ϕ were chosen to cover the range of estimates obtained from real data and reported in Casas-Monroy *et al.* (2020) as well as more extreme cases to mimic low and high aggregation of the organisms in the ballast water tank. For the Poisson/gamma model, the values considered for θ_0 were chosen to cover its parameter space in such a way that large and small prior variances were contemplated. For the negative binomial/Pearson Type VI model the values for θ_0 were chosen according to the constraint**

imposed by the prior variance, $\lambda_0 < \theta_0$.

Table 1: ACC (5) based minimum sample size (n) computed under the Poisson/gamma model (1)-(2) with $\lambda_0 = 10$, $\rho = 0.05$ and $\ell = 2$.

Aliquot volume (w)	Shape parameter (θ_0)				
	1.0	2.5	5.0	7.5	10.0
0.5	77	77	76	76	75
1.0	39	39	38	38	38

Table 2: ACC (5) based minimum sample size (n) computed under the negative binomial/Pearson Type VI model (3)-(4) with $\lambda_0 = 10(w/\phi)$, $\rho = 0.05$ and $\ell = 2$.

Aliquot volume (w)	ϕ	Shape parameter (θ_0)			
		11	25	50	75
0.5	1	465	458	452	445
	8	123	121	116	110
	13	104	102	97	92
	22	93	90	85	80
	30	88	85	80	75
1.0	1	430	424	420	417
	8	86	84	82	79
	13	68	66	64	61
	22	55	54	52	49
	30	51	49	47	44

3.2 Average length criterion (ALC)

An alternative criterion used to determine sample sizes is based on the average length of the posterior credible intervals. The rationale here is to set the minimum Bayesian coverage probability $1 - \rho$ and obtain the minimum sample size n by requiring that the length of the posterior credible region $\ell'(\mathbf{x}_n, n) = b(\mathbf{x}_n) - a(\mathbf{x}_n)$ be such that

$$\int_{\mathcal{X}^n} \ell'(\mathbf{x}_n, n)g(\mathbf{x}_n)d\mathbf{x}_n \leq \ell_{\max}, \quad (6)$$

where ℓ_{\max} is the maximum admissible length for the posterior credible region. The lower and upper bounds of the **desired** HPD interval may be obtained via numerical methods and the integral by Monte Carlo simulation. An algorithm to obtain the minimum sample size satisfying this criterion is outlined in the Supplementary Material.

Based on the ideas of M'Lan *et al.* (2008), who used a binomial model with a beta prior distribution, we may obtain the sample size using the ALC under the model (1)-(2) with no need for numerical methods via the following result.

Theorem 1 *Consider the Poisson/gamma model and (1)-(2) the average length criterion (6). Based on large sample approximation, the minimum n , to guarantee that the posterior credible interval average length is smaller than ℓ_{\max} is the smallest integer such that*

$$n \geq \frac{\theta_0}{w\lambda_0} \left\{ \left[\frac{\lambda_0}{\theta_0} \frac{2z_{\rho/2}}{\ell_{\max}} \frac{\Gamma(\theta_0 + 1/2)}{\Gamma(\theta_0)} \right]^2 - 1 \right\},$$

where $z_{\rho/2}$ is the quantile of order $1 - \rho/2$ of the standard normal distribution.

The proof of Theorem 1 is presented in the Supplementary Material. In Tables 3 and 4 we present sample sizes computed using ALC (6) **setting $\ell_{\max} = 2$** for models (1)-(2) and (3)-(4); in Table 3 (**and S3 of the Supplementary Material**) we present corresponding sample sizes (within parentheses) computed using Theorem 1. **In Tables S3 and S4 of the Supplementary Material we present the same scenario for $\ell_{\max} = 4$.**

The results displayed in both subsections of Section 3 are commented in Section 5.

Table 3: ALC (6) based minimum sample size (n) computed under the Poisson/gamma model (1)-(2) (and also using Theorem 1) with $\lambda_0 = 10$, $\rho = 0.05$ and $\ell_{\max} = 2$.

Aliquot volume (w)	Shape parameter (θ_0)				
	1.0	2.5	5.0	7.5	10.0
0.5	77 (61)	77 (70)	76 (73)	76 (73)	75 (73)
1.0	38 (31)	38 (35)	38 (37)	38 (37)	38 (37)

Table 4: ALC (6) based minimum sample size (n) computed under the negative binomial/Pearson Type VI model (3)-(4) with $\lambda_0 = 10(w/\phi)$, $\rho = 0.05$ and $\ell_{\max} = 2$.

Aliquot volume (w)	ϕ	Shape parameter (θ_0)			
		11	25	50	75
0.5	1	459	453	450	445
	8	123	120	115	110
	13	104	101	97	92
	22	92	90	85	79
	30	88	85	80	75
1.0	1	424	419	418	414
	8	85	84	82	79
	13	67	66	63	61
	22	56	54	51	49
	30	50	49	46	44

4 Simulation study

We conduct a simulation study to verify whether the credible intervals obtained with the sample sizes proposed in Section 3 satisfy the precision criteria.

For each (prior distribution) scenario and sample size obtained via the ACC (5) displayed in Table 1 (and S1 of the Supplementary Material) we drew 1000 samples from a Poisson/gamma model (1)-(2) with values of λ fixed at the quantiles of order 1/6, 2/6, 3/6, 4/6 and 5/6 of the corresponding prior distribution. Then, for each sample we obtained the lower $[a(\mathbf{x}_n)]$ and

upper $[b(\mathbf{x}_n)]$ limits of the HPD credible interval for the mean organism concentration in a ballast water tank with pre-specified average coverage probability ($1 - \rho = 0.95$) and computed the proportion of intervals containing the fixed value of λ . The results are displayed in Tables 5 and S5. We expect that the estimates of the HPD Bayesian coverage probability to be at least 0.95.

Under the same model, but using sample sizes displayed in Tables 3 and S3, obtained via the ALC (6), we conducted a similar simulation study, the results of which are displayed in Tables 6 and S6. In this case, we expect that the estimates of length of the HPD intervals to be at most 2 (or 4).

The same strategy was conducted for data obtained via the negative binomial/Pearson Type VI model (3)-(4) using the sample sizes provided in Tables 2, 4, S2 and S4. The results are provided in Table 7, 8 and in Tables S7-S10 of the Supplementary Material.

Table 5: ACC based Bayesian coverage probability of HPD intervals estimated via simulation for some scenarios under the Poisson/gamma model (1)-(2) using sample sizes displayed in Table 1 for $\ell = 2$.

Aliquot volume (w)	θ_0	n	Probability quantile used to fix λ				
			1/6	2/6	3/6	4/6	5/6
0.5	1.0	77	1.00	1.00	0.98	0.94	0.85
	2.5	77	0.99	0.99	0.97	0.95	0.88
	5.0	76	0.99	0.98	0.95	0.94	0.92
	7.5	76	0.98	0.97	0.96	0.94	0.91
	10.0	75	0.97	0.98	0.95	0.95	0.93
1.0	1.0	39	1.00	1.00	0.98	0.95	0.86
	2.5	39	0.99	0.99	0.97	0.93	0.88
	5.0	38	0.99	0.98	0.97	0.94	0.90
	7.5	38	0.98	0.98	0.95	0.94	0.90
	10.0	38	0.98	0.96	0.95	0.96	0.92

Table 6: ALC based length of HPD intervals estimated via simulation for some scenarios under the Poisson/gamma model (1)-(2) using sample sizes displayed in Table 3 for $\ell_{\max} = 2$.

Aliquot volume (w)	θ_0	n	Probability quantile used to fix λ				
			1/6	2/6	3/6	4/6	5/6
0.5	1.0	77	0.85	1.27	1.66	2.09	2.66
	2.5	77	1.30	1.60	1.86	2.13	2.49
	5.0	76	1.52	1.75	1.93	2.12	2.37
	7.5	76	1.61	1.79	1.94	2.10	2.30
	10.0	75	1.67	1.83	1.96	2.10	2.27
1.0	1.0	38	0.86	1.28	1.67	2.10	2.68
	2.5	38	1.31	1.61	1.87	2.14	2.50
	5.0	38	1.52	1.74	1.93	2.12	2.37
	7.5	38	1.61	1.80	1.95	2.10	2.30
	10.0	38	1.66	1.82	1.95	2.08	2.26

For illustrative purposes, we consider two sets of hypothetical data and obtain the corresponding HPD intervals under both proposed models. The first set mimics a case with extreme heterogeneity in the organism concentration and the second, a case with where the organisms are homogeneously distributed. This kind of severe aggregation occurs when individuals of the same species are physically attached to each other forming colonies as indicated in Rajakaruna *et al.* (2018).

We first determined the sample size required to satisfy the ACC with $\ell = 2$ assuming a Poisson/gamma model with a prior distribution having $\lambda_0 = 10$ and $\theta_0 = 0.01$. This choice corresponds to a large prior variance. Setting $w = 1$ and $\rho = 0.01$, the required sample size is $n_P = 104$. We then generated 104 observations from a negative binomial model with $\lambda = 9$, $\phi = 0.1$ and $w = 1$. The generated counts are displayed in Table 9 where the heterogeneity induced by the negative binomial model is evident.

The sum of the counts is $s_{n_P} = s_{104} = 1173$ so that the corresponding HPD intervals (obtained via the algorithms described described in Subsections

Table 7: ACC based Bayesian coverage probability of HPD intervals estimated via simulation for some scenarios under the negative binomial/Pearson Type VI model (3)-(4) using sample sizes displayed in Table 2 setting $w = 0.5$ and $\ell = 2$.

ϕ	θ_0	n	Probability quantile used to fix λ				
			1/6	2/6	3/6	4/6	5/6
1	11	465	0.999	0.996	0.989	0.963	0.853
	25	458	0.998	0.990	0.983	0.947	0.843
	50	452	0.992	0.989	0.970	0.946	0.878
	75	445	0.986	0.975	0.968	0.938	0.881
8	11	123	0.994	0.975	0.962	0.956	0.892
	25	121	0.978	0.972	0.959	0.943	0.905
	50	116	0.969	0.979	0.968	0.958	0.920
	75	110	0.967	0.971	0.961	0.955	0.927
13	11	104	0.984	0.976	0.942	0.944	0.916
	25	102	0.977	0.959	0.961	0.950	0.908
	50	97	0.968	0.965	0.953	0.958	0.929
	75	92	0.961	0.976	0.959	0.955	0.937
22	11	93	0.976	0.964	0.964	0.926	0.909
	25	90	0.975	0.964	0.968	0.938	0.928
	50	85	0.962	0.973	0.976	0.947	0.930
	75	80	0.967	0.957	0.979	0.962	0.944
30	11	88	0.982	0.973	0.954	0.935	0.903
	25	85	0.971	0.963	0.959	0.948	0.926
	50	80	0.970	0.964	0.962	0.949	0.933
	75	75	0.961	0.972	0.969	0.958	0.948

1.1.1 and 1.2.1 of the Supplementary Material) are, respectively, (10.3, 12.3) for the Poisson/gamma model setting $\lambda_0 = 10$ and $\theta_0 = 0.01$, and (8.81, 10.81) for the negative binomial/Pearson Type VI model [for which we set $\phi \approx 0.1213$ (obtained via maximum likelihood), $\lambda_0 = 10(w/\phi) \approx 82.4$ and $\theta_0 = \lambda_0 + 1$, in order to obtain a large variance]. The first interval does not contain the organism concentration ($\lambda = 9$) used to generate the data and suggest (erroneously) non-compliance with the D-2 regulation. The second interval, on the other hand, contains the value $\lambda = 9$ (even with the sample size obtained under the Poisson/gamma model) and suggests (correctly)

Table 8: ALC based length of HPD intervals estimated via simulation for some scenarios under the negative binomial/Pearson Type VI model (3)-(4) using the sample sizes in Table 4 with $w = 0.5$ and $\ell_{\max} = 2$.

ϕ	θ_0	n	Probability quantile used to fix λ				
			1/6	2/6	3/6	4/6	5/6
1	11	459	0.909	1.202	1.526	1.990	2.845
	25	453	1.211	1.488	1.768	2.126	2.723
	50	450	1.425	1.655	1.877	2.143	2.549
	75	445	1.529	1.730	1.922	2.142	2.458
8	11	123	1.489	1.705	1.911	2.139	2.465
	25	120	1.666	1.820	1.956	2.107	2.311
	50	115	1.769	1.884	1.979	2.083	2.221
	75	110	1.818	1.906	1.984	2.068	2.174
13	11	104	1.559	1.758	1.934	2.130	2.402
	25	101	1.718	1.852	1.972	2.099	2.272
	50	97	1.800	1.900	1.980	2.067	2.178
	75	92	1.840	1.918	1.985	2.052	2.136
22	11	92	1.608	1.790	1.950	2.119	2.348
	25	90	1.745	1.866	1.970	2.081	2.224
	50	85	1.825	1.907	1.983	2.056	2.151
	75	79	1.872	1.940	1.996	2.052	2.126
30	11	88	1.626	1.799	1.949	2.111	2.319
	25	85	1.760	1.879	1.976	2.078	2.214
	50	80	1.836	1.920	1.986	2.054	2.142
	75	75	1.874	1.936	1.990	2.042	2.110

compliance with the D-2 regulation.

For the second scenario, we generated 104 observations via a Poisson model with $\lambda = 9$ and $w = 1$. The generated counts are displayed in Table 9 and shows the more homogeneous distribution of the organisms. The sum of the corresponding counts is $s_{n_P} = s_{104} = 859$ so that the associated HPD intervals are (7.29, 9.29) for both the Poisson/gamma model with parameters $\lambda_0 = 10$ and $\theta_0 = 0.01$ and the negative binomial/Pearson Type VI model with parameters $\phi \approx 233$ (obtained via maximum likelihood), $\lambda_0 = 10(w/\phi) \approx 0.043$ and $\theta_0 = \lambda_0 + 0.01$. Both intervals contain the organism concentration $\lambda = 9$ suggesting (correctly) compliance with the

Table 9: Simulated counts of the example via the negative binomial (NB) model ($\phi = 0.1$, $\lambda = 9$ and $w = 1$) and via Poisson (P) model ($\lambda = 9$ and $w = 1$).

	0	0	2	65	0	0	0	19	0	6	0	1	2	0	10	27	4	0	41	0	53
	0	0	0	0	0	0	0	72	6	0	1	1	55	0	12	1	0	0	0	0	0
NB	4	0	3	0	0	248	20	1	0	5	0	0	16	0	0	7	208	0	94	0	0
	1	0	0	0	0	13	0	0	0	4	0	2	1	1	2	0	0	0	0	6	0
	75	0	50	6	0	0	5	0	8	1	0	0	4	0	0	8	0	2	0	0	0
	5	10	10	10	12	10	3	7	10	9	10	9	7	13	7	12	7	7	6	7	7
	7	6	4	7	12	9	13	12	4	9	7	7	9	6	11	6	7	17	12	9	10
P	7	10	8	9	10	9	7	11	5	7	11	9	6	9	9	11	6	12	12	4	7
	3	7	11	7	9	4	9	6	13	3	11	5	9	8	5	7	10	14	9	6	9
	6	13	8	7	6	13	6	13	6	6	5	9	7	4	7	11	4	9	7	6	6

D-2 regulation.

These examples suggest that the negative binomial/Pearson Type VI model accommodates both homogeneous and extreme heterogeneous situations while the Poisson/gamma model fails in the latter case. We must recognize, however, that both models behave quite similarly when heterogeneity is not extreme. This raises the question of eliciting prior information on the organism aggregation, but this depends on historical data which is not yet available.

5 Discussion

The results in Tables 1 and S1 obtained under the Poisson/gamma model indicate that the sample size does not decrease much when θ_0 increases, *i.e.*, when the variance of the prior distribution decreases. This may be explained by the homogeneity assumption for the expected concentration which is intrinsic to the adopted model. Unless we consider a precise prior distribution, the sample size required to satisfy the ACC will not change much. This feature is also visible when we compute the sample size under the same model using the ALC (see Tables 3 and S3).

On the other hand, under model (3)-(4) using either the ACC or the

ALC with a fixed value for ϕ , the precision of the prior knowledge, controlled by θ_0 here, directly affects the required sample size. This also happens when we consider a fixed θ_0 and vary ϕ , that plays the role of a scale parameter in the prior distribution (see Tables 2, 4, S2 and S4).

Assuming that ϕ is known may be a disadvantage but we can circumvent this problem in a practical manner without considering a prior distribution for this parameter. The first and simpler way is to consider ϕ as small as possible, *e.g.*, $\phi = 1$. Since the sample size n decreases as ϕ increases, when we take ϕ as the minimum, we are being conservative, in the sense that the corresponding n is enough or more than enough to achieve the pre-specified criteria settings. The second alternative is to consider a naive sequential procedure in which samples are selected one by one (or by lots). Observe that sample sizes obtained under a Poisson/gamma model (n_P) are always smaller than those obtained by a negative binomial/Pearson VI model (n_{NB}), with respective parameters fixed and write $n_{NB} = n_P + K$, where K is a positive integer. For fixed w , ℓ (or ℓ_{\max}) and fixed hyperparameters, we may compute the sample size under a Poisson model, proceed with the sample collection obtaining n_P organism counts (\mathbf{x}_{n_P}). Using these n_P organism counts we may compute an estimate for ϕ by maximum likelihood or by the method of moments (see Ludwig & Reynolds, 1988, eq. 3.5, for example) and with this estimate we may obtain n_{NB} and consequently K , which is the required number of additional aliquots. Since the prior distributions used in both models are different, we must choose the hyperparameters for the Pearson Type VI distribution which represent “equivalent prior knowledge” to those fixed in the gamma distribution. Given w , λ_0 and the estimate of ϕ , we may choose θ_0 such that the plot of the Pearson Type VI distribution is similar to the plot of the gamma distribution with previous hyperparameters

used to obtain n_P .

The standard approach, on the other hand, would be to consider a prior distribution for ϕ which implies including at least an additional hyperparameter so that we must deal with another integral in order to obtain the marginal distribution of λ . This introduces further computational effort and is object of future research.

As in Inoue *et al.* (2005), we compare sample sizes obtained under different perspectives. Under the Bayesian approach fixing either ℓ or ℓ_{\max} (Tables 2, 4, **S2 and S4**), the sample sizes are, in general, smaller than those computed under a frequentist approach with ϵ_a (maximum absolute error estimation) equal to 1 or 2 (see Tables 2 and 3 in Costa *et al.*, 2016). This may be justified by the additional information provided by the prior distribution relatively to that considered in the frequentist approach, where only lower and upper bounds for the parameter of interest are given.

For the ALC we also present a result (Theorem 1) which allows the computation of sample sizes under model (1)-(2) without the need for numerical and/or simulation methods. The corresponding sample sizes are consistently smaller than those obtained via Monte Carlo replicates, although the differences are not large. Note that since this theorem is based on large sample approximations, we expect a difference between the corresponding sample sizes and those obtained directly from the proposed criterion.

The simulation results (Tables 5-7 and Tables S5-S10 of the Supplementary Material) show similar **results** to those obtained under the simulation study presented in Costa *et al.* (2016). For smaller values of λ , the coverage criterion is attained well above the limit but the results are reversed for the larger values and the minimum fixed coverage is not attained. A similar conclusion holds when using the ALC. We also note that for values

of λ smaller or equal to the median, the estimated coverage probability is larger than the proposed one. This is expected, but may not happen for values of λ greater than the median, mainly for the quantiles of order 5/6 or higher, *i.e.*, in some cases the posterior interval does not contain λ , and this happens with estimated coverage probability smaller than the specified one. To justify this, note that for the Poisson/gamma model, given λ , S_n follows a sampling Poisson distribution with mean and variance $nw\lambda$. When the value of λ (*i.e.*, the prior quantile) increases, the variance of S_n also increases and consequently the variability of the posterior expected value increases, generating more HPD intervals that do not contain the true value of λ . The same happens for the negative binomial/Pearson Type VI model, where the sampling variance of S_n is $nw\lambda + n(w\lambda)^2/\phi$. When λ increases we observe the same behavior as in the Poisson/gamma model, but here, additionally, when ϕ increases, the sampling variance of S_n decreases. This may explain the increase (decrease) of the coverage probability (length) of HPD intervals when λ is fixed at the the 5/6 quantile of the prior distribution. Also, note that ϕ is scale and shape parameter of the posterior distribution and this may explain the reversed behavior for the other quantiles (see Tables 7, 8, S7 and S8). This suggests that in practice, if the goal is a minimum coverage with probability $1 - \rho$, we should consider a sample size n corresponding to a minimum coverage probability greater than $1 - \rho$ in order to prevent or minimize this problem.

Although, for simplicity, we mention only one of the requirements of the D-2 standard, the proposed procedure is also valid for the requirement that deballasted water should contain less than 10 viable organisms per m^3 , sized $\geq 50 \mu m$ in minimum dimension, provided the aliquot volume w is changed accordingly.

Practical issues related to the actual collection of the ballast water aliquots have been addressed by many authors (Carney *et al.*, 2013; First *et al.*, 2013; Gollasch & David, 2017). In a recent paper, Casas-Monroy *et al.* (2020) compares different methods for obtaining the sample, concluding that among three available competitors the in-line method may be the best one. Given that the BWM Convention requires ships to install a sampling port after their ballast water treatment system, the pipes within the required machinery may be used to collect aliquots along the entire deballasting process. The aliquots (with, say, 10 mL) are then integrated into a single volume from which the organisms are counted and the corresponding credible interval is computed.

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