

The tenets of indirect inference in Bayesian models

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Abstract

This paper extends the application of Bayesian inference to probability distributions defined in terms of its quantile function. We describe the method of *indirect likelihood* to be used in the Bayesian models with sampling distributions which lack an explicit cumulative distribution function. We provide examples and demonstrate the equivalence of the “quantile-based” (indirect) likelihood to the conventional “density-defined” (direct) likelihood. We consider practical aspects of the numerical inversion of quantile function by root-finding required by the indirect likelihood method. In particular, we consider the problem of ensuring the validity of an arbitrary quantile function with the help of Chebyshev polynomials and provide useful tips and implementation of these algorithms in Stan and R. We also extend the same method to propose the definition of an *indirect prior* and discuss the situations where it can be useful.

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Contents

1	Introduction	3
1.1	Aims of the paper	3
1.2	Paper structure	3
1.3	Paper contribution	5
2	Distribution specification	5

26	2.1	Essential functions	5
27	2.2	Derivatives of the inverses and numerical approximation	6
28	2.3	Quantile distributions	7
29	3	Bayesian inference with quantile functions	8
30	3.1	Direct and indirect likelihood	8
31	3.2	Direct and indirect prior	10
32	4	Indirect likelihood with a non-analytically invertible sampling distribution	12
33	5	Numerical inversion of quantile function	15
34	5.1	Target function	15
35	5.2	Root-finding algorithms	15
36	5.3	Generalized g-and-h distribution and the normal QDF	17
37	5.4	Root bracketing with grid-matching	18
38	6	Validation of quantile functions	20
39	6.1	Parameter conditions	21
40	6.2	Grid-checking	22
41	6.3	Global minimum check	22
42	6.4	Direct root-finding	23
43	6.5	Proxy root-finding	23
44	7	Discussion and conclusion	24
45		Miscellaneous	25
46		Acknowledgments	25
47		Data Availability Statement	25
48		Supplemental materials	25
49		ORCID	25
50		Appendix A. Distributions used in the paper	25
51		Exponential distribution	25
52		Rayleigh distribution	26
53		Govindarajulu distribution	26
54		Generalized exponential distribution	27
55		Appendix B. Dealing with false roots	27
56		Appendix C. Practical tips for implementing quantile distributions in Stan	

You have to start looking at the world in a new way.
 – Priya in TENET by Christopher Nolan

1 Introduction

1.1 Aims of the paper

Quantile distributions are a special class of distributions with explicit quantile functions that are not analytically invertible (Gilchrist, 2000). There have been a number of published articles where quantile distributions have been used in a context of the likelihood-free approximate Bayesian computation (Allingham et al., 2009; Drovandi and Pettitt, 2011; Karabatsos and Leisen, 2018; Fearnhead and Prangle, 2012; Bernton et al., 2019; McVinish, 2012), but the classical Bayesian inference applications have been limited (Haynes and Mengersen, 2005; Rayner and MacGillivray, 2002).

This article attempts to build on the ideas of Rayner and MacGillivray (2002) and Nair et al. (2020) and systematically present and illustrate Bayesian inference using quantile functions. We call this method of inference “indirect” because it deals with *intermediate cumulative probabilities* (which we call *depths*¹) corresponding to observations (given the parametrized model). Our aim is to show that the indirect Bayesian inference using intermediate depths, leads to the same posterior beliefs, as the conventional, density-based inference. We highlight and discuss practical challenges related to inverting the non-invertible quantile functions and propose a novel application of the proxy root-finding algorithm for validation of quantile functions.

The proposed concept of *indirect inference*, although shares the name with the likelihood-free method described in Heggland and Frigessi (2004) and Drovandi and Pettitt (2011) and the method of auxiliary parameter estimation in time-series models presented in Smith Jr. (1993) and Gourieroux et al. (1993) has no connection with those contributions.

1.2 Paper structure

Section 2 revisits the functions and identities for characterizing the distribution of a continuous random variable. Then in Section 3 we introduce the terms of *indirect likelihood* and *indirect prior* and show that likelihood (and prior) can be expressed without the use of the probability density function (PDF). Section 4 presents an example of a Bayesian model with

¹Because they indicate how “deep” an observation is into the distribution.

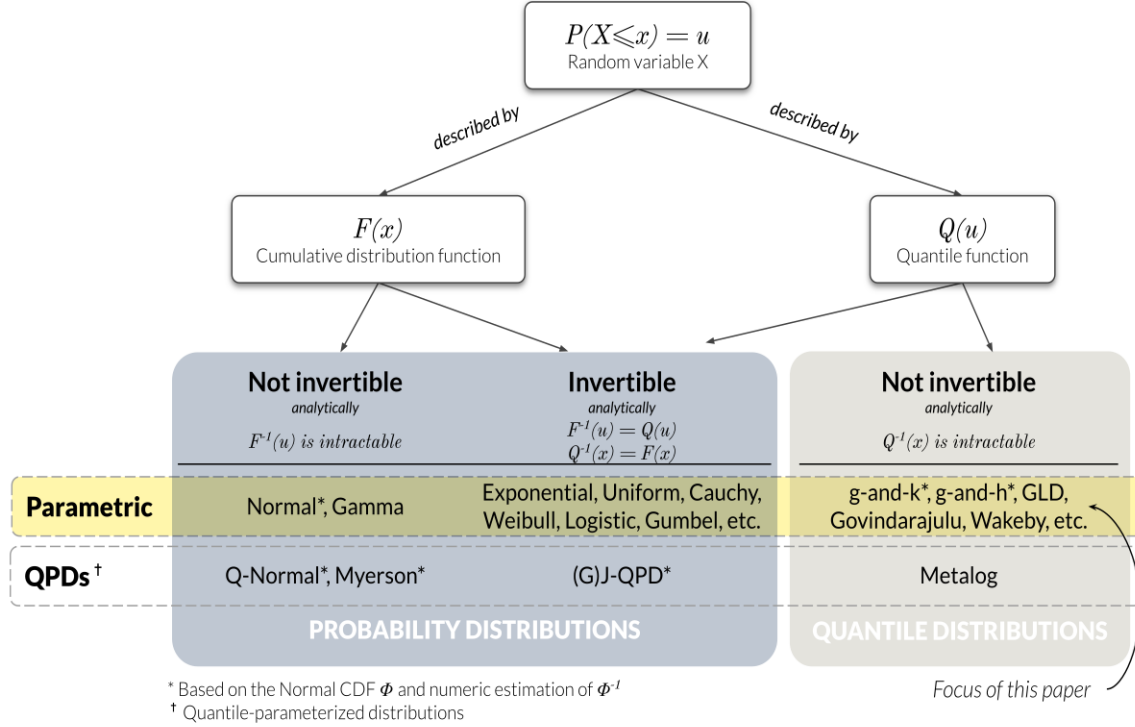


Figure 1: Probability distributions, quantile distributions and parameterization.

indirect likelihood expressed by a non-invertible quantile distribution implemented using Hamiltonian Monte Carlo in Stan (Stan Development Team, 2021a).

Section 5 discusses the computational aspects of estimating the intermediate depths in indirect likelihood expressed by a quantile distribution. We discuss root-finding algorithms and provide an example model with the indirect generalized *g-and-h* (Haynes et al., 1997) likelihood. We used the Robust Adaptive Metropolis MCMC algorithm by Vihola (2012) interfaced by the `fmcmc` package (Vega Yon and Marjoram, 2019) and a built-in bracketing root-finding algorithm for inverting a quantile function in R (R Core Team, 2021).

Section 6 discusses a problem of ensuring that the particular combination of parameters produces a valid quantile function. We propose a proxy-root-finding algorithm based on Chebyshev polynomials and discuss challenges and computational cost associated with finding the roots of a QDF. We illustrate the use of Chebyshev polynomials for proxy root-finding by approximating the quantile density function of the *g-and-k* distribution and provide custom functions in R implementing the two methods of approximation proposed by Boyd (2013).

We conclude the paper by discussion and summary of the results in Section 7. The definitions of the distributions used in this paper are provided in Appendix A.

1.3 Paper contribution

Although the description of indirect likelihood (Rayner and MacGillivray, 2002; King, 1999) and prior (Nair et al., 2020) appeared in the literature before, they were presented in the context of the specific distributions and not as a general principle of inference. In their recent work, Nair et al. (2020) presented Bayesian inference with quantile functions, but their presentation of what we describe here as *indirect prior* lacked the necessary adjustment to the likelihood due to the non-linear transformation of the parameters involved (see Section 3.2). Furthermore, although the numerical inversion of quantile functions was discussed in Gilchrist (2000), Nair and Sankaran (2009) and Nair et al. (2020), the discussion was limited to the description of the Newton-Raphson method. In this paper we discuss both bracketing and non-bracketing methods (Section 5.2) and provide Stan and R code for numerical inversion of quantile functions for various distributions (Supplementary Materials). Finally, the application of proxy root-finding using Chebyshev polynomials for validation of quantile functions (Section 6 and Appendix B), is, to the best of our knowledge, novel and can be applied in situations beyond those discussed in the paper as a general approach to ensuring the validity of quantile distributions (as defined in Section 2 below).

2 Distribution specification

In this section we briefly review the different ways of specifying a probability distribution to set the scene for the discussion of direct and indirect Bayesian inference. We review the use of the inverse cumulative distribution function (quantile function) to describe statistical distributions and discuss several examples of distributions defined by the quantile function (“quantile distributions”) found in the scientific literature (Figure 1).

2.1 Essential functions

Let X be a continuous random variable. It can be expressed via the distribution function, also known as the *cumulative distribution function* (CDF):

$$F_X(x|\theta) = Pr(X \leq x|\theta), \quad \theta \in \mathcal{A} \subset \mathbb{R} \quad (1)$$

Alternative way of describing the random variable X is via the *quantile function* (QF).

$$Q_X(u|\theta) = \inf\{x : F_X(x|\theta) \geq u\}, \quad 0 \leq u \leq 1 \quad (2)$$

129 If $F_X(x)$ is continuous and strictly monotonically increasing over the support of X , then
 130 $Q_X(u|\theta)$ is simply the inverse of $F_X(x|\theta)$. Therefore, the quantile function is often referred
 131 to as the “inverse CDF”, i.e.

$$Q_X(u|\theta) = F_X^{-1}(x|\theta) \quad (3)$$

132 Not all CDFs are analytically invertible. A distribution whose quantile function $Q_X(u|\theta)$ is
 133 not analytically invertible is called a *quantile distribution* (Figure 1).

134 The derivative of the CDF is the *probability density function* (PDF) denoted by

$$f_X(x|\theta) = \frac{dF_X}{dx} \quad (4)$$

135 Similarly, the derivative of the QF is the *quantile density function* (QDF) denoted by

$$q_X(u|\theta) = \frac{dQ_X}{du}, \quad 0 \leq u \leq 1 \quad (5)$$

136 The reciprocal of the QDF $[q_X(u|\theta)]^{-1} = f(Q_X(u|\theta))$ is referred to as the *density quantile*
 137 *function* (Parzen, 1980) or *p-pdf* (Gilchrist, 2000).

$$f(Q(u)) = \frac{dF(Q(u))}{dQ(u)} = \frac{dF(Q(u))/du}{dQ(u)/du} = \frac{dF(F^{-1}(u))/du}{q(u)} = \frac{du/du}{q(u)} = [q(u)]^{-1} \quad (6)$$

138 Here and for the rest of the article we will often omit the subscript $_X$ and the conditioning
 139 on θ to simplify notation.

140 2.2 Derivatives of the inverses and numerical approximation

141 Following the inverse function theorem (Price, 1984), for a function to be invertible in the
 142 neighborhood of a point it should have a continuous non-zero derivative at that point. If the
 143 function is invertible, the derivative of the inverse is reciprocal to the function’s derivative.
 144 Formally, if dy/dx exists and $dy/dx \neq 0$, then dx/dy also exists and $dx/dy = [dy/dx]^{-1}$.
 145 Therefore, for a quantile function $Q(u) = x$, if a QDF $q(u)$ exists and $q(u) \neq 0$, then PDF
 146 $f(x)$ also exists and it is equal to $f(x) = [q(u)]^{-1}$ (Figure 2). In Section 3 of this paper,
 147 we rely on the density quantile function (DQF) $[q(u|\theta)]^{-1}$, a quantile form of the PDF, to
 148 define the likelihood in a Bayesian model based on the quantile distribution.

149 Even though quantile distributions lack the closed-form CDF $F_X(x|\theta) = u$, in most cases,

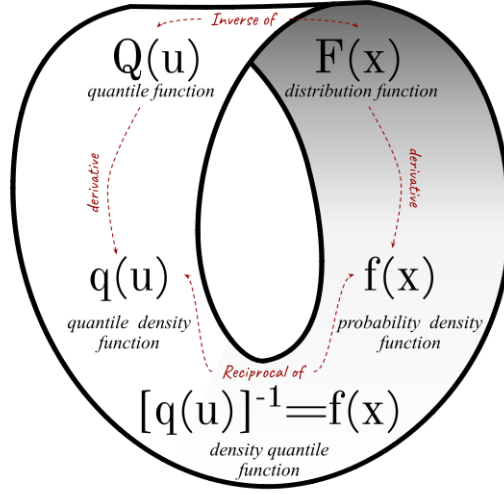


Figure 2: Moebius strip of probability functions.

the depths u can be approximated by numerically inverting the $Q_X(u|\theta)$. We denote the numerically inverted quantile function as $\widehat{Q}_X^{-1}(x|\theta)$ or $\widehat{F}_X(x|\theta)$. The inverse of a quantile function $Q(u|\theta)$ at point u , corresponding to the observation x , is obtained by minimizing the difference between the actual observation x and $Q_X(u|\theta)$ by iteratively refining the depth u . The details of the numerical inversion algorithms are discussed in Section 4.

2.3 Quantile distributions

Statistical methods utilizing QF and QDF were pioneered by the seminal work of Parzen (1979). Today the research area of quantile distributions is an active field of interest for many scientists. The most popular quantile distributions covered in the literature are generalized g -and- h and its sibling g -and- k distribution (Haynes and Mengersen, 2005; Jacob, 2017; Prangle, 2017; Rayner and MacGillivray, 2002), Generalized Lambda Distribution, known as GLD (Aldeni et al., 2017; Chalabi et al., 2012; Dedduwakumara et al., 2021; Fournier et al., 2007; Freimer et al., 1988), Wakeby distribution (Rahman et al., 2015) and Govindarajulu distribution (Nair et al., 2012, 2013). Multivariate version of the quantile distributions have been explored in the past (Field and Genton, 2006; Serfling, 2002), but they are not widely adopted in the the scientific literature.

Although in this paper we focus on the parametric quantile distributions, the quantile distributions parameterized by the quantile-probability pairs (“quantile-parametrized” quantile distributions) are also worth a mention. The most prominent examples are the Myerson distribution (Myerson, 2005) Johnson QPD (J-QPD) and its generalization (Hadlock and

Bickel, 2017, 2019), as well as the Simple Q-Normal(Keelin and Powley, 2011) and meta-log distribution (Keelin, 2016). These distributions play an important role in representing expert beliefs about the variables, parameters or quantities of interest, although they don't lend themselves easily as sampling distributions due to the special nature of their parameterization.

3 Bayesian inference with quantile functions

In this section we adopt the Bayesian updating approach proposed by Rayner and MacGillivray (2002) and Nair et al. (2020) and apply it to the classical gamma-exponential model. Rayner and MacGillivray (2002) describe the three-step process of calculating the log-likelihood for a quantile distribution and use it for maximum likelihood estimation of parameters in *g-and-k* and generalized *g-and-h* distribution. Nair et al. (2020) performed quantile function substitutions both for observables $x_i = Q(u_i|\theta)$, $u_i \in [1..N]$ and for parameters $\theta = Q(v)$ and computed Bayes estimator under the squared error loss for Govindarajulu likelihood. In this section we try to summarize this approach and introduce the terms of *direct* and *indirect* likelihood based on the identities and substitutions introduced in Section 2 and show the equivalence of the two ways of expressing likelihood in Bayesian models.

3.1 Direct and indirect likelihood

Traditional Bayesian inference formula can be restated using the substitutions involving quantile functions. Assume that the prior information about the scalar parameter θ can be summarized by the prior distribution over the parameter space, Θ . Then, given a random sample of $\underline{x} = \{x_1, x_2, \dots, x_n\}$, the posterior distribution of θ can be expressed as:

$$f(\theta|\underline{x}) \propto \mathcal{L}(\theta; \underline{x})f(\theta) \quad (7)$$

where $f(\theta|\underline{x})$ is the posterior distribution of θ after having observed the sample \underline{x} , $f(\theta)$ is the prior distribution of θ , and $\mathcal{L}(\theta; \underline{x}) = \prod_{i=1}^n f(x_i|\theta)$ is the likelihood, which is a function of θ . We refer to this form of likelihood as “direct”, because the observed \underline{x} are used as input to the likelihood function directly.

Given the random sample of \underline{x} , we can use the quantile function to compute $\underline{Q} = \{Q_1(u_1), Q_2(u_2), \dots, Q_n(u_n)|\theta\}$, such that $u_i = F(x_i|\theta)$, $i = 1, 2, \dots, n$. The depths u_i , which we denote by $\underline{u}|\theta$ are degenerate random variables, because they are fully

determined given the observables \underline{x} and parameter θ . Since $Q(u_i|\theta) = x_i$ we can substitute \underline{Q} for \underline{x} . Then the Bayesian inference formula (7) becomes:

$$f(\theta|\underline{Q}) \propto \mathcal{L}(\theta; \underline{Q})f(\theta) \quad (8)$$

We refer to the likelihood $\mathcal{L}(\theta; \underline{Q}) = \prod_{i=1}^n f(Q(u_i|\theta)) = \prod_{i=1}^n [q(u_i|\theta)]^{-1}$ as “indirect”, because it relies on computing intermediate depths $u_i = F(x_i|\theta)$, $i = 1, 2, \dots, n$. As we have shown, the two forms of likelihood $\mathcal{L}(\theta; \underline{Q})$ and $\mathcal{L}(\theta; \underline{x})$ are equal to each other. Therefore, following the likelihood principle, the posterior beliefs about θ are equivalent.

Since the likelihood in the Equation (8) is expressed in terms of $\underline{Q} = Q(\underline{u}|\theta)$, an additional transformation is required to arrive at $\underline{u} = F(\underline{x}|\theta)$. In case a closed form of the CDF $F(\underline{x}|\theta)$ is not available, the numeric approximation of $\widehat{Q}^{-1}(\underline{x}|\theta)$ may be used. We discuss the details of the numerical approximation of the inverse quantile function in Section 5 of this paper.

To illustrate the equivalence of the two ways of specifying likelihood in Bayesian models, we use the example from Klugman et al. (2004)² regarding the distribution of the insurance claim amounts (referred to hereinafter, as the Claims Example).

Klugman et al. (2004) model the claim amounts using exponential distribution with the mean of $1/\lambda$, where parameter λ is given the gamma prior distribution with the shape $\alpha = 4$ and the scale $\beta = 0.001$. Given three observations of the claim amounts $\underline{x} = \{100, 950, 450\}$, we sample from the posterior distribution of the parameter λ using the Hamiltonian Monte Carlo “No U-Turn” sampler implemented in Stan (Stan Development Team, 2021a). Since gamma prior is conjugate to the exponential sampling distribution (Pratt et al., 1995) we can verify the distribution of the posterior draws using the analytic solution as $f(\lambda|\underline{x}) = \text{Gamma}(\lambda|\alpha + N, \beta + \sum_{i=1}^n x_i)$, where α and β are the parameters of gamma distribution and x_i , $i = 1, 2, \dots, N$ is the sample of observations of size N .

Table 1 and Figure 3 present the posterior distribution of θ from the two gamma-exponential models: one with a direct and another one with an indirect likelihood, along with the posterior from the conjugate model. Stan programs for the corresponding examples are provided in the Supplementary Material.

The posterior distributions of parameter λ from the two models are equivalent and match the analytic solution from the conjugate model within a Monte Carlo error.

²Example 16.17 on p.544

Table 1: Posterior sample comparison for the models

model	mean	median	q5	q95	rhat
direct likelihood	0.0028	0.0027	0.0013	0.0048	1.000
indirect likelihood	0.0028	0.0027	0.0014	0.0048	1.001

Gamma-Exponential model

Comparing posterior distributions of λ from models with direct and indirect likelihoods

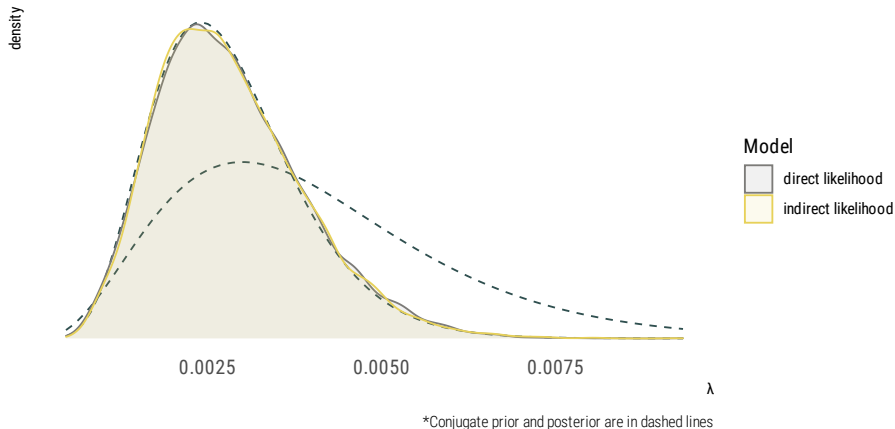


Figure 3: Distribution of posterior samples from the gamma-exponential model with direct and indirect likelihood

3.2 Direct and indirect prior

It is possible to extend the same logic of substitution using quantile functions to define the *direct* and *indirect* prior. In this section we discuss the transformation of parameters required for implementing the quantile prior and show its connection to the inverse transform used for non-uniform sampling.

The Bayesian inference formula can also be restated using the quantile form of the prior (Nair et al., 2020). Assume that the prior distribution of θ can be described using the invertible CDF $F_{\Theta}(\theta) = v$, so that $Q_{\Theta}(v) = \theta$. Substituting the quantile values $Q_{\Theta}(v)$ for values of θ , prior beliefs about the parameter(s) of the distribution of θ can be expressed *indirectly* using the distribution of the quantile values corresponding to the random variate v , given hyperparameter(s) of the prior distribution as $f(Q_{\Theta}(v)) = [q_{\Theta}(v)]^{-1}$. We refer to such formulation of the prior as the *indirect prior* because it describes the prior distribution of the random variate v corresponding to the parameter θ and not the distribution of the parameter θ itself.

241 Likewise, the likelihood $\mathcal{L}(Q_{\Theta}(v); \underline{x})$ will also rely on the parameter transformation $\theta =$
 242 $Q_{\Theta}(v)$. However, the likelihood with such non-linear parameter transformation requires a
 243 Jacobian adjustment (Andrilli and Hecker, 2010), which is equal to the absolute derivative of
 244 the transform, i.e. $J(Q_{\Theta}(v)) = |dQ_{\Theta}(v)/dv| = |q_{\Theta}(v)|$. Provided that the $Q_{\Theta}(v)$ is a valid
 245 (non-decreasing) quantile function, meaning that $q_{\Theta}(v)$ is non-negative on $v \in [0, 1]$, the
 246 quantile density term representing the prior and the Jacobian adjustment can be dropped
 247 as they are reciprocal to each other.

$$\begin{aligned} [q_{\Theta}(v|\underline{x})]^{-1} &\propto \mathcal{L}(Q_{\Theta}(v); \underline{x}) [q_{\Theta}(v)]^{-1} |q_{\Theta}(v)| \implies \\ [q_{\Theta}(v|\underline{x})]^{-1} &\propto \mathcal{L}(Q_{\Theta}(v); \underline{x}) \end{aligned} \quad (9)$$

248 where $[q_{\Theta}(v|\underline{x})]^{-1}$ is the quantile form of the posterior, and the quantile prior $[q_{\Theta}(v)]^{-1}$ is
 249 implied. The quantile function transform $Q_{\Theta}(v) = \theta, v \in [0, 1]$ (given the relevant hyperpa-
 250 rameters) hints at the shape of the prior.

251 Indirect prior can also be used in combination with an indirect likelihood, since, as we showed
 252 previously, regardless of the form of likelihood used, the posterior beliefs about the parameter
 253 θ (and, consequently, v) will be the same. In such a case, neither prior nor likelihood would
 254 require the existence of the closed-form PDF and, therefore, both of them can be represented
 255 by quantile distributions.

256 In the Claims Example the prior belief about the distribution of the exponential parameter
 257 λ was represented by the gamma distribution, which is not easily invertible (Figure 1).
 258 In order to illustrate the indirect specification of the prior, we pick an invertible prior as
 259 representation of the expert’s beliefs about the exponential parameter λ . The shape of
 260 the new prior *Rayleigh*(0.003) is comparable to the gamma prior *Gamma*(4, 0.001) used
 261 previously (Figure 4).

Table 2: Summary of the posterior samples of the parameter lambda from the Rayleigh-Exponential model with direct and indirect prior and likelihood

model	mean	median	q5	q95	rhat
direct prior, direct likelihood	0.0027	0.0026	0.0011	0.0048	1.001
direct prior, indirect likelihood	0.0027	0.0025	0.0011	0.0048	1.001
indirect prior, direct likelihood	0.0027	0.0026	0.0011	0.0047	1.000
indirect prior, indirect likelihood	0.0027	0.0026	0.0011	0.0048	1.001

262 Table 2 and Figure 5 compare the posterior distribution of θ from the gamma-exponential
 263 model with direct and indirect likelihood. Stan programs for corresponding examples are

Prior distribution of λ

Non-invertible distribution (Gamma) substituted with the invertible distribution (Rayleigh)

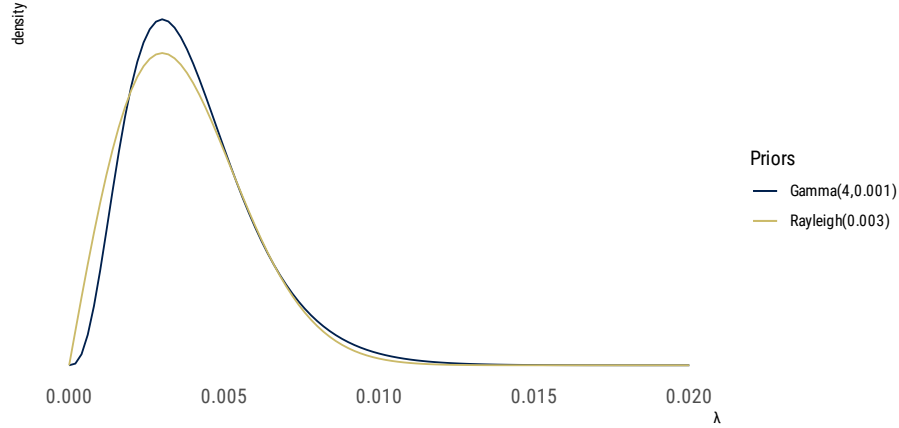


Figure 4: Substitution prior for the rate parameter

provided in the Supplementary Material.

4 Indirect likelihood with a non-analytically invertible sampling distribution

The models we have used in the previous sections allowed us to choose between *direct* or *indirect* likelihood because the (exponential) sampling distribution was easily invertible. The main advantage of using the *indirect* form of the likelihood is that it allows us to adopt the data generative model based on non-invertible (quantile) distributions. Below, we show an example of updating the parameters of a bathtub-shaped Govindarajulu distribution, which does not have a closed-form CDF or PDF.

We take the dataset provided in Aarset (1987) on time-to-failure of 50 devices (Figure 6). Lifetime reliability data are often modeled using specialized distributions (Nadarajah, 2009) or 2(3)-component mixtures. Nair et al. (2020) used the Bayes estimator under the squared error loss function to estimate the posterior mean of the parameter γ in the Govindarajulu distribution (Nair et al., 2012), given the generalized exponential prior (Gupta and Kundu, 2007). We extend their approach to estimate the full posterior distribution of both parameters in the Govindarajulu likelihood, implementing it in Stan (Stan Development Team, 2021a).

Rayleigh-Exponential model

Comparing posterior distributions from models with direct and indirect prior and likelihoods

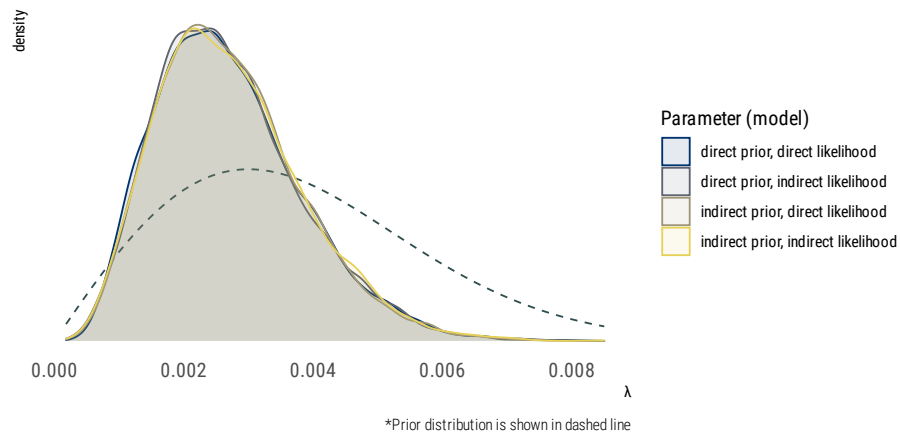


Figure 5: Distribution of the posterior samples from the Rayleigh-Exponential model with direct and indirect prior and likelihood

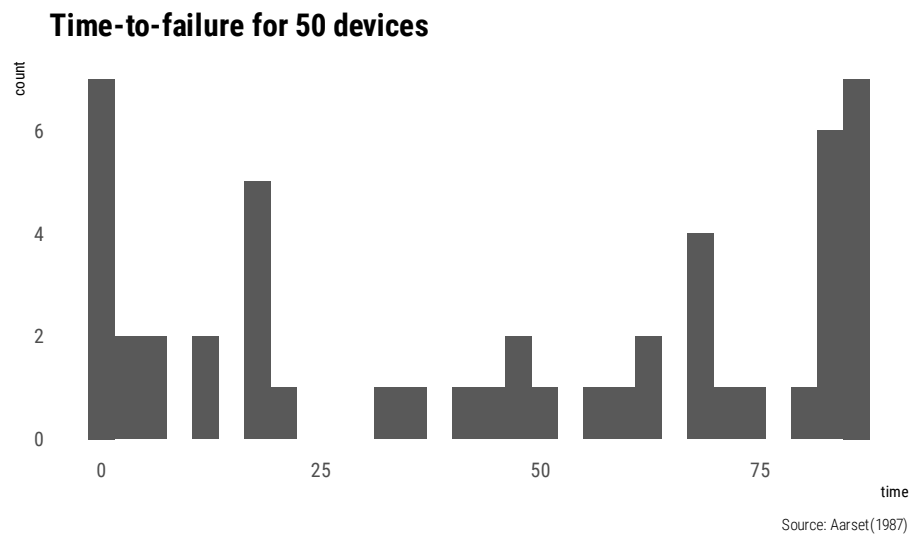


Figure 6: Histogram of the time to failure data

281 We adopt the generalized exponential prior for the parameter γ of Govindarajulu distribution
282 with hyperparameters $\alpha = 5$ and $\lambda = 1$. The parameter σ of the Govindarajulu distribution
283 can not be lower than the maximum of the observed times-to-failure. Therefore, we defined
284 a shifted exponential prior with PDF $\lambda e^{-\lambda(x-l)}$ with the rate $\lambda = 1$ and varying lower bound
285 l corresponding to the highest time to failure (in our example equal to 86). The Jacobian
286 for adding a constant to the sampled parameter σ is equal to one, so there is no impact on
287 the log density, as the shifting transform produces a Jacobian derivative matrix with a unit
288 determinant.

Table 3: Summary of the posterior samples from the GenExp-Govindarajulu model using indirect likelihood

parameter	mean	median	q5	q95	rhat
gamma	2.0355	2.0067	1.5749	2.5978	1.001
sigma	86.0225	86.0004	86.0000	86.1240	1.001

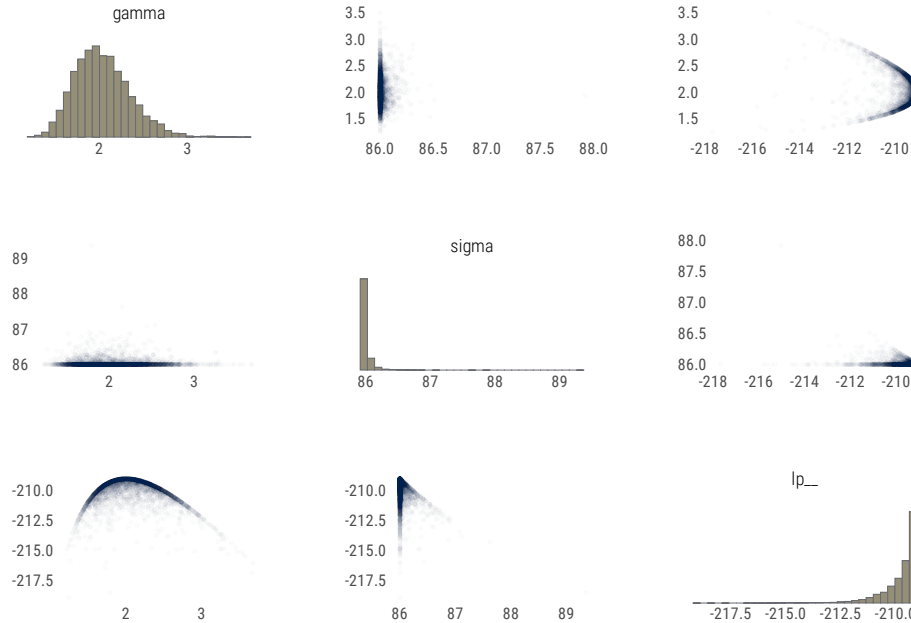


Figure 7: Posterior distribution of parameters in GenExp-Govindarajulu model

289 Table 3 and Figure 7 summarize the posterior distribution of the parameters σ and γ of
290 Govindarajulu distribution. We used 2500 post-warmup iterations and 4 chains (see Figure
291 8 for NUTS parameter plots).

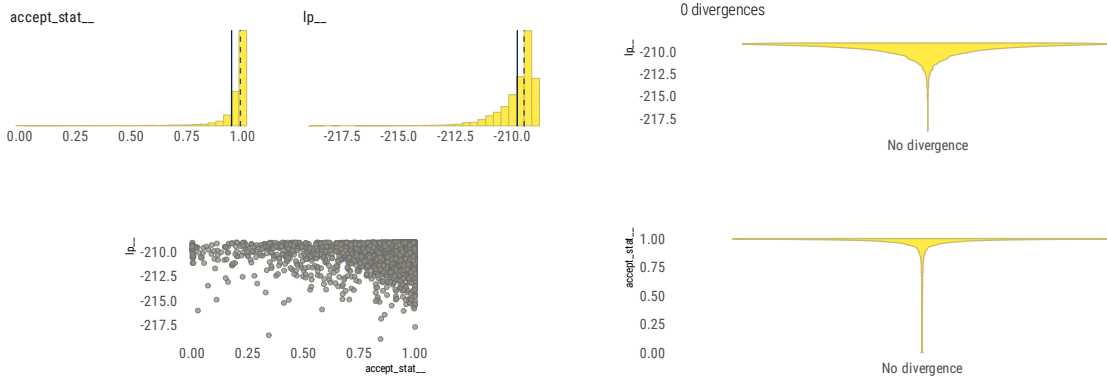


Figure 8: NUTS parameters for GenExp-Govindarajulu model

5 Numerical inversion of quantile function

The core element of the *indirect* likelihood method is the use of the intermediate depths \underline{u} , corresponding to the observables \underline{x} given the parameter θ . These values can either be found analytically, as $Q^{-1}(x) = F(x)$ for probability distributions, or, numerically via root-finding algorithm, as $\widehat{Q}_X^{-1}(x) = \widehat{F}_X(x)$ e.g. in case of quantile distributions (Figure 1).

5.1 Target function

The problem of inverting a quantile function is tantamount to finding the root of a target function

$$\Omega(u; x, \theta) = [x - Q_X(u|\theta)] \quad (10)$$

where x is a known observation, θ is the parameter value, and $u|\theta$ is the depth. Provided that the $Q(u|\theta)$ is a non-decreasing function and x is a fixed observable value, the target function $\Omega(u; x, \theta)$ is non-increasing. The root-finding algorithm uses the target function to take an observable x and “pull in” its inverted equivalent $Q(u|\theta)$ until the two values exactly meet by iteratively adjusting u .

5.2 Root-finding algorithms

In principle, the choice of the algorithms for finding the zeros of a target function Ω includes two broad groups of methods: *bracketing* and *non-bracketing* (Atkinson, 2008; Burden and Faires, 2011).

309 The bracketing methods, such as bisection, Lagrange polynomial and Brent method, require
310 a pair of values around the root, i.e. two values of u^+ and u^- , such that $\Omega(u^+; x, \theta) > 0$
311 and $\Omega(u^-; x, \theta) < 0$. In order for the algorithm to rapidly converge on a true value of
312 probability u faster, the interval $[u^+, u^-]$ needs to be relatively narrow. One way of ensuring
313 that the starting interval is small is via the method, which we call “grid-matching”. Because
314 $Q^{-1}(x) = F(x)$ is a non-decreasing function, the interval of depths $[u^+, u^-]$ enclosing the
315 true value u corresponding to the observable x , can be found by matching the observable x
316 to the sorted grid of K quantile values $Q_k^{grd} = Q_X(u_k^{grd}|\theta)$, $k \in 1..K$, where $\forall u_k^{grd}, k \in$
317 $(1 \dots K) : 0 < u_k^{grd} < 1$, $u_k^{grd} < u_{k+1}^{grd}$ come from a sorted grid of depths. Once x is matched
318 to the grid of quantiles Q_k^{grd} , the quantile value immediately preceding the observable x
319 and immediately following it, such that $Q_m^{grd} \leq x \leq Q_{m+1}^{grd}$ can be determined and the
320 corresponding depths u_m^{grd} and u_{m+1}^{grd} can be returned. The interval formed by these depths
321 can be adopted as $[u^+, u^-]$, as it is guaranteed to contain the value of u corresponding to
322 the root of the target function $\Omega(u; x, \theta)$.

323 The non-bracketing methods do not require the initial values to be on both sides of the root,
324 but also do not guarantee that the root will be found. The simplest of these methods, secant,
325 requires two initial guess values and approximates the slope of the function near the root
326 by secant lines. More complex non-bracketing methods are gradient-based. For example,
327 Newton-Raphson method, requires a single “initial guess” value $u_{(i)}$ and the derivative of a
328 target function $\Omega'(u_{(i)}; x, \theta)$. Following this method the “improved” value u^* can found as:

$$u^* \approx u_{(i)} - \frac{\Omega(u_{(i)}; x, \theta)}{\Omega'(u_{(i)}; x, \theta)} \quad (11)$$

329 Substituting the target function Ω , the Newton-Raphson formula for finding the inverse of
330 the quantile function becomes:

$$u^* \approx u_{(i)} - \frac{x - Q_X(u_{(i)}|\theta)}{d[x - Q_X(u_{(i)}|\theta)]/du_{(i)}} = u_{(i)} + \frac{x - Q_X(u_{(i)}|\theta)}{q_X(u_{(i)}|\theta)} \quad (12)$$

331 where $u_{(i)}$ is the initial value of the probability (the “depth”) u , corresponding to the obser-
332 vation x given θ , u^* is the new (improved) value of $u_{(i)}$ after an iteration and $q_X(u_{(i)}|\theta)$ is the
333 QDF of X , which is the first derivative of the QF $Q_X(u_{(i)}|\theta)$ with respect to the depth $u_{(i)}$.
334 The procedure can be repeated by taking the approximated u^* as a new initial value $u_{(i)}$
335 and recomputing the value of u^* , until $|\Omega(u_{(i)}; x, \theta)| < \epsilon$, where ϵ is some small value. The
336 method has been used in the literature for approximating CDFs of several known quantile
337 distributions (see p.99 in [Gilchrist, 2000](#); p.345 in [Nair et al., 2013](#)).

For faster convergence it is desirable that the initial guess value $u_{(i)}$ be as close to the true root as possible. Gilchrist (2000) describes the Newton-Raphson method for inverting the quantile function and recommends using $u_{(i)r} = r/(n + 1)$ as the initial guess of the depth corresponding to the r -th order statistic from the sample of size n . The implicit assumption is that if the sample is covering quantile function range fairly evenly, then the depth $u_{(i)r}$ corresponding to the r -th order statistic will not be too far from $r/(n + 1)$. The limitation of this approach to initializing the Newton-Raphson algorithm is that for parameter values θ far from the median of the posterior the observations will not cover the range of the quantile function and most initial values will end up being far from the true root value, which can cause problem with root-finding. We recommend using grid-matching to set the initial values of the depth $u_{(i)}$ to improve the chances of finding the true root values using non-bracketing methods.

The Newton-Raphson represents the first-order Householder’s method (Householder, 1970), suitable for finding the roots of the double-differentiable functions. The Householder methods of higher order require higher degree of differentiability. For example, the Halley method requires two derivatives and can be used to find roots of triple-differentiable scalar functions (Scavo and Thoo, 1995).

There are other optimization methods which can be adapted for finding the zeros of a function, even though they may have been developed for a different purpose. In the absence of other built-in root-finders, we used Stan’s `algebra_solver()`, intended for finding the roots of systems of equations, to numerically determine the depths corresponding to the observable times-to-failure (see example in Section 4 above). Stan’s algebra solver is based on the Powell hybrid method, initially developed for finding the local minimum of functions. Powell’s hybrid method combines the advantages of Newton’s method with the steepest descent method, which guarantees stable convergence (Powell, 1970).

The rest of the section illustrates how to use the bracketing root-finding algorithm implemented in R for inverting the quantile function of the generalized *g-and-h* distribution (Rayner and MacGillivray, 2002). The `stats::uniroot()` function in R implements Brent’s method, also known as the Brent-Dekkert algorithm, which combines the features of the bisection and secant methods with the inverse quadratic interpolation. Brent’s algorithm performance ranks it only slightly behind more recent Riddler and Zhang methods (Stage, 2013; Zhang, 2011).

5.3 Generalized *g-and-h* distribution and the normal QDF

The generalized *g-and-h* distribution is defined by the quantile function:

$$Q_{gnh}(u) = A + Bz[1 + C \tanh(gz/2)] \exp(hz^2/2) \quad (13)$$

where $z = z(u) = \Phi^{-1}(u|0, 1)$ is the standard normal quantile function, $B > 0$ and $h > 0$. The parameter g is responsible for skewness, i.e. when $g < 0$ the distribution is skewed left, and when $g > 0$, it is skewed right. The parameter h is responsible for kurtosis. For all values of kurtosis greater than that of the normal distribution, i.e. $h \geq 0$, regardless of value of g , the parameter $C \leq 0.83$ (approximately) results in a proper distribution. In practice the parameter C is often set to 0.8 (Haynes and Mengersen, 2005; Rayner and MacGillivray, 2002).

The challenge with g -and- h distribution is that it is expressed in terms of $z(u)$ and not in terms of u itself. In order to differentiate the g -and- h QF with respect to u we can use the chain rule $q(u) = \frac{dQ}{du} = \frac{dQ_{gnh}(z)}{dz} \frac{dz}{du}$. The second part of this expression is the QDF of the standard normal $\frac{dz}{du} = \frac{d\Phi^{-1}(u)}{du} = q_{norm}(u)$.

Even though normal distribution does not have a closed-form QF, we can exploit the fact that Stan and R have built-in functions for calculating the $\Phi^{-1}(u)$ and derive QDF (and DQF) of the normal distribution in terms of the normal QF:

$$\frac{d\Phi^{-1}(u)}{du} = q_{norm}(u) = [f_{norm}(Q_{norm}(u))]^{-1} = [f(\Phi^{-1}(u))]^{-1} \quad (14)$$

Therefore the QDF of the generalized g -and- h distribution

$$q_{gnh}(u) = \left(0.5B \exp(hz^2/2)[1 + C \tanh(gz/2)](1 + hz^2) + \frac{Cgz}{2 \cosh^2(gz/2)} \right) q_{norm}(u) \quad (15)$$

where $z = Q_{norm}(u|0, 1)$ is the QF of standard normal and $q_{norm}(u)$ is the QDF of standard normal.

5.4 Root bracketing with grid-matching

The `pgnh()` function in `qpd` package (Perepolkin, 2019) implements $\widehat{Q}_{gnh}^{-1}(x)$ using the grid-matching method to find a pair of values bracketing the root. We use R's built-in `findInterval()` function for locating the index m of the sorted grid of K quantile values $Q_k^{grd} = Q(u_k^{grd}|\theta)$, $k \in 1..K$, such that $Q_m^{grd} \leq x \leq Q_{m+1}^{grd}$. In order to make the search of the root for the target function more numerically stable, we perform the search on the scale of z -values, i.e. the standard normal quantile values corresponding to the depth u (Rayner

396 and MacGillivray, 2002). Once the root is found, the value of z corresponding to the root
 397 of the target function can be converted back to the depth using the standard normal CDF
 398 $\Phi(z) = u$.

399 The following R code snippet implements the $\widehat{Q}_{gnh}^{-1}(x)$ inverse quantile function (approximate
 400 CDF) for g -and- h distribution

```
pgnh <- function(q, A,B,C=0.8,g,h, n_grid=100L, s_grid=5L, tol=1e-15, maxiter=1e3){
  # target function
  afun <- function(z, q, A,B, C, g, h) {q - qgnh(z,A,B,C,g,h, zscale=TRUE)}
  stopifnot(B>0 && h>=0)
  # service function for producing a grid of values on [0,1]
  p_grd <- make_pgrid(n=n_grid, s=s_grid)
  q_grd <- qgnh(p_grd, A,B,C, g,h, zscale=FALSE)
  idx_lower <- findInterval(q, q_grd, all.inside = TRUE)
  idx_upper <- idx_lower+1L
  int_lower <- stats::qnorm(p_grd[idx_lower]) # convert to z-scale
  int_upper <- stats::qnorm(p_grd[idx_upper]) # convert to z-scale

  zs <- mapply(function(.q, .il, .iu) { # do this for every element in q
    tmp_zs <- NULL
    tmp_zs <- stats::uniroot(afun, q=.q, A=A, B=B, C=C, g=g, h=h,
                             interval=c(.il,.iu), extendInt="downX",
                             check.conv=TRUE, tol = tol, maxiter = maxiter)
    if(is.null(tmp_zs)) res <- NA_real_ else res <- tmp_zs$root
    res #return the value of the root
  }, q, int_lower, int_upper)

  ps <- stats::pnorm(zs) # convert the z values back to probability scale

  ps[!is.finite(ps)] <- NA_real_
  ps
}
```

401 We take a random sample of 100 values from the g -and- h distribution with parameters $A=5$,
 402 $B=5$, $C=0.8$, $g=5$ and $h=0.25$. The distribution of simulated values is shown in Figure 9.

403 We assumed that the parameters A and B of g -and- h distribution are known, and defined
 404 a normal prior for parameter g as $Normal(3,1)$ and Rayleigh prior for parameter h as

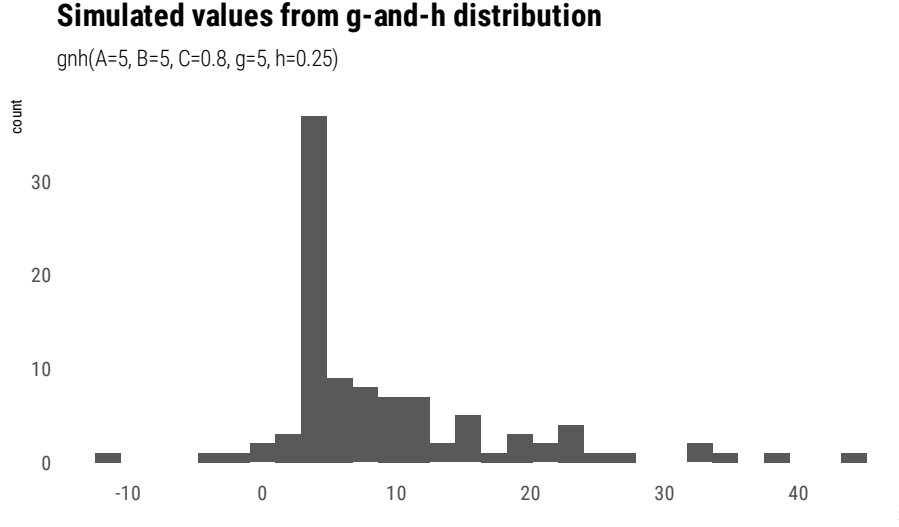


Figure 9: Simulated data from g-and-h distribution

405 *Rayleigh*(0.3). We performed Bayesian inference using Robust Adaptive Metropolis MCMC
 406 algorithm by Vihola (2012) interfaced by the `fmcmc` package (Vega Yon and Marjoram, 2019)
 407 in R. Table 4 and Figure 10 summarize the posterior distribution of parameters g and h .

Table 4: Posterior summary of parameters in g-and-h distribution

parameter	mean	median	q5	q95	rhat
g	5.0063	5.0136	4.5932	5.3759	1.003
h	0.4223	0.4165	0.2912	0.5732	1.004

408 6 Validation of quantile functions

409 The flexibility of quantile distributions can become a curse, as certain combinations of pa-
 410 rameters may produce an invalid quantile function. In order for the quantile function to
 411 be valid, it needs to be continuous and non-decreasing. The violation of the QF feasibility
 412 condition manifests itself in the negative values of the QDF, measuring the rate of change
 413 in the quantile function. An invalid shape of the quantile function can cause the CDF ap-
 414 proximation to fail both because the root-finding algorithm, such as Newton-Raphson, can
 415 get stuck in the local minimum and because the QDF can produce an invalid gradient.

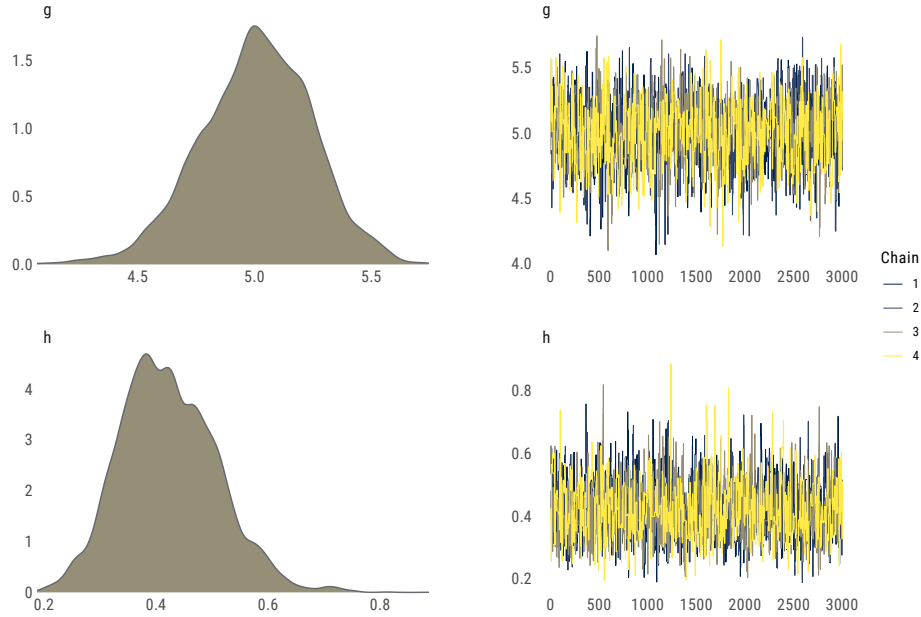


Figure 10: Posterior distribution and traceplot of parameters in g-and-h distribution

6.1 Parameter conditions

In some instances it is possible to avoid problematic cases by limiting the allowable range of parameter values. However, in highly parameterized quantile distribution, parameters may be mutually dependent, which makes it impossible to limit the problematic cases by imposing restrictions on each parameter independently. For example, Wakeby distribution has five parameter conditions, four of which are related to more than one parameter (simultaneous conditions), some of which are mutually exclusive, e.g. “either $\beta + \sigma > 0$ or $\beta = \gamma = \delta = 0$ ”. These complex conditions and bounds imposed on parameters may also be difficult to implement in MCMC samplers.

Expressing parameter conditions requires a good understanding of the distribution, and even then there might be some combinations of parameters which produce an illegal quantile function. For example, [Prangle \(2017\)](#) and [Rayner and MacGillivray \(2002\)](#) discuss the range of valid parameter values for the *g-and-k* distribution. The parameter k should be larger than -0.5 , but some values of $-0.5 < k < 0$ can also lead to a quantile function being invalid. The irregularities can be difficult to spot on the quantile function graph, but the effect on the derivative functions (QDF and DQF) can be quite dramatic.

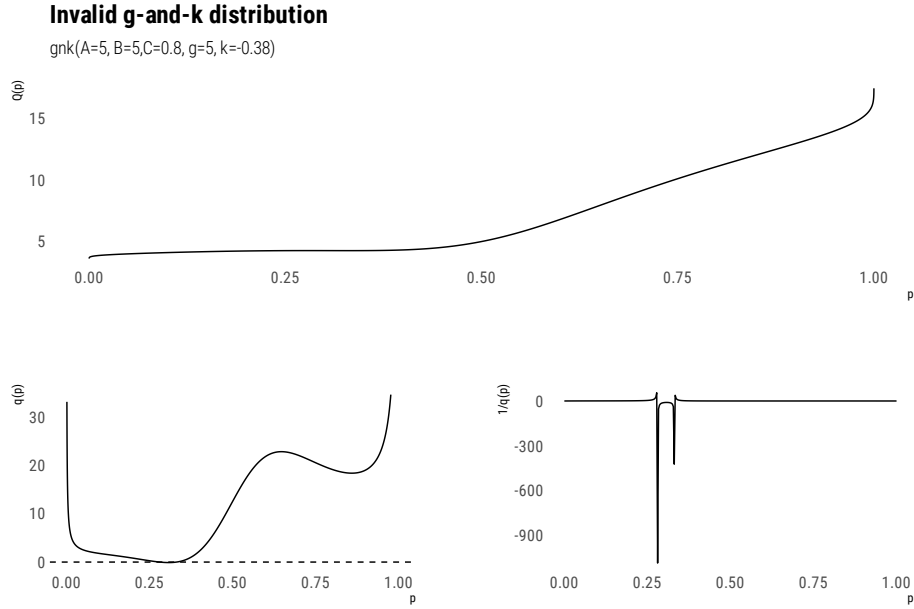


Figure 11: Some combination of parameters of g-and-k distribution may lead to an invalid quantile function

6.2 Grid-checking

The validity of the quantile function can also be checked by computing the QDF values corresponding to the tight grid of probabilities spread across the $[0,1]$ range. Should any one of the QDF values be negative we can reject the quantile function with their parameters as invalid. This requires that the probability grid is tight enough to eliminate the possibility of the QDF “dipping” below zero between the grid values. If the cost of computing the quantile function is relatively low, and the distribution is relatively smooth (no sharp wiggles) this strategy can be reasonable. For a very tight probability grid, though, this method can become computationally expensive.

6.3 Global minimum check

An alternative approach may include finding the global minimum of the QDF and checking if it is positive. However, given the complex shape of the QDF (Figure 11), this may prove to be computationally expensive, as well.

6.4 Direct root-finding

A QDF can also be checked for roots. The values between the roots (or, if only one root is found, on one side of the root) are likely to be negative. Therefore if the roots are found this can indicate that the corresponding QF is invalid. The challenge with finding the QDF roots is that in most cases we can not use any of the bracketing methods, because the presence of roots is not known a-priori. The Newton-Raphson method can also be problematic, due to difficulties of finding the “good” initial value. Also gradient-based methods, such as Newton-Raphson, would require a derivative “quantile convexity function” (QCF) which may not be available, should the QDF be invalid. When validating the quantile function we are not interested in finding the roots of the QDF per se, but rather in using them as an indication that a QDF may take negative values on the range $[0,1]$ and thus, that the corresponding QF is invalid.

6.5 Proxy root-finding

Finally, we can represent the QDF with a proxy function, the roots of which can be computed analytically. This method is referred to in the literature as the “proxy root-finding” and has been studied extensively (Boyd, 2013). Chebyshev polynomials are known for their ability to approximate functions of arbitrary complexity (Boyd and Gally, 2007). In order to increase the precision of the approximation either higher degree polynomials should be used or the function range should be partitioned, keeping the degree of the polynomials applied on the subdivisions low (Boyd, 2006). The main computational load of the Chebyshev polynomial method is computing the eigenvalues of the Chebyshev-Frobenius companion matrix (Boyd, 2013). The logic of the method relying on a large number of partitions is that it might be computationally cheaper to find eigenvalues of many small matrices, than finding eigenvalues of a large matrix. The `qpd` package (Perepolkin, 2019) implements several functions for computing the coefficients, finding roots and evaluating the Chebyshev polynomial of arbitrary degree on any interval of a function. For QPD the full range of the function is $(0,1)$, but `qpd::is_qdf_valid()` can check a QDF function passed by the user using arbitrary number of subdivisions fitting the Chebyshev polynomial of a user-defined degree to every partition. Another strategy discussed in Boyd (2013) is “recursive partitioning”, where the algorithm starts by fitting a single polynomial to the whole function range and comparing the goodness of fit (e.g. the sum of squares) to some small value. If the error exceeds the threshold, the range is split in two and polynomials are fit to each subsegment, repeating the algorithm recursively.

Given the shape of the QDF function (most likely U-shaped) the largest error will be in the tails, so it might be a smart idea to make more splits toward the tails and less splits

in the middle of the function range. We implemented an S-shaped subdivision scheme in `qpd::is_qdf_valid()` and compared its performance to the linearly partitioned quantile function. In Appendix B we compare the two schemes of proxy root-finding (degree of polynomial vs number of partitions) and discuss different approaches for dealing with false roots, which are an inevitable byproduct of polynomial approximation.

7 Discussion and conclusion

Quantile distributions expand the menu of options available to the scientists and offer a wide selection of distributions to be used as likelihoods and/or priors. Hadlock (2017) summarizes the ideas from Gilchrist (2000) and Powley (2013) and provides a useful overview of properties of quantile functions. Using these properties and transformation rules, new distributions can be created on demand (Rodrigues et al., 2020; Midhu et al., 2014; Sankaran et al., 2016; Sankaran and Dileep Kumar, 2018; Yang and Zhang, 2009; Smithson and Shou, 2017).

In the past 20 years many examples using quantile distributions in approximate Bayesian computation (ABC) appeared in the literature (Allingham et al., 2009; Drovandi and Pettitt, 2011; Dunson and Taylor, 2005; McVinish, 2012; and Smithson and Shou, 2017). ABC methods normally do not require computation of the likelihood, which in case of quantile distributions is convenient, as they lack an explicit CDF and PDF.

The first application of likelihood-based Bayesian inference for quantile distributions that we could identify was proposed by Rayner and MacGillivray (2002). The method proposed by the authors is very similar to the *indirect likelihood* method, but the authors used it for maximum likelihood estimation. Later Haynes and Mengersen (2005) used this method to estimate the parameters in *g-and-k* distribution using a custom MCMC algorithm. Recently, Nair et al. (2020) offered the formulae for likelihood and prior expressed using the transformations involving the quantile functions, although applying it only to closed-form Bayes estimator of the posterior mean in Govindarajulu model. In this paper we summarized the ideas proposed by Rayner and MacGillivray (2002) and Nair et al. (2020) and presented an *indirect inference* method which makes quantile distributions usable as sampling distributions or priors. We also offered examples and implementation in STAN demonstrating the equivalence of using indirect likelihood and prior to the Bayesian inference using the traditional (density-based) likelihood and prior.

A class of quantile distributions, which we did not cover in this paper, namely, quantile-parameterized distributions (Keelin and Powley, 2011; Hadlock and Bickel, 2017; Keelin, 2016) can be especially useful as priors, given their highly interpretable parameterization. Further research is required in applying the principles of indirect likelihood to quantile-

parametrized quantile distributions to make them useful as sampling distributions.

Embracing and expanding the use of quantile distributions in Bayesian inference can enable new solutions for old problems and enrich the toolkit available to scientists for performing hard inference tasks. We hope that the *indirect* inference methods presented in this paper can contribute to expanding the body of knowledge in Bayesian statistics and fuel further research in the area of quantile distributions.

Miscellaneous

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Data Availability Statement

The `qpd` R package used in this paper is available on Github at <https://github.com/dmi3kno/qpd>. Contact corresponding author Dmytro Perepolkin (Dmytro.Perepolkin@cec.lu.se) for requests for data.

Supplemental materials

Supplemental materials contain R and Stan code for all examples used in the article.

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Appendix A. Distributions used in the paper

Exponential distribution

The exponential distribution function $F(x)$ and the probability density function $f(x)$ are given by

$$\begin{aligned} F(x) &= 1 - e^{-\lambda x} \\ f(x) &= \lambda e^{-\lambda x} \end{aligned} \tag{16}$$

540 where $\lambda > 0$ and $x \in [0, \infty)$.

541 The exponential quantile function $Q(u)$ and quantile density function $q(u)$ are

$$\begin{aligned} Q(u) &= -\frac{\ln(1-u)}{\lambda} \\ q(u) &= \frac{dQ(u)}{du} = \frac{1}{\lambda(1-u)} \end{aligned} \tag{17}$$

542 where $\lambda > 0$ and $u = F(x), u \in [0, 1]$

543 **Rayleigh distribution**

544 The Rayleigh distribution function $F(x)$ and probability density function $f(x)$ are:

$$\begin{aligned} F(x|\sigma) &= 1 - \exp(-x^2/(2\sigma^2)) \\ f(x|\sigma) &= \frac{x}{\sigma^2} \exp(-x^2/(2\sigma^2)) \end{aligned} \tag{18}$$

545 where $\sigma > 0$ is Rayleigh scale parameter.

546 The Rayleigh quantile function $Q(p)$ and quantile density function $q(p)$ are:

$$\begin{aligned} Q(p|\sigma) &= \sigma \sqrt{-2 \ln(1-p)} \\ q(p|\sigma) &= \frac{\sigma}{\sqrt{2} \sqrt{-\ln(1-p)}(1-p)} \end{aligned} \tag{19}$$

547 where $\sigma > 0$ and $p \in [0, 1]$.

548 **Govindarajulu distribution**

549 The Govindarajulu distribution defined by the quantile function has the following QF and
550 QDF:

$$\begin{aligned} Q_X(u) &= \sigma \gamma u^\gamma (1 + \gamma^{-1} - u) \\ q_x(u) &= K u^{\gamma-1} (1 - u) \end{aligned} \tag{20}$$

551 where $K = \sigma \gamma (\gamma + 1)$, and $\gamma > 0$.

552 The distribution has support on $(Q(0), Q(1)) = (0, \sigma)^3$.

553 Generalized exponential distribution

554 The generalized exponential distribution has the following CDF and PDF:

$$\begin{aligned} F(x) &= (1 - e^{-\lambda x})^\alpha \\ f(x) &= \alpha \lambda (1 - e^{-\lambda x})^{\alpha-1} e^{-\lambda x} \end{aligned} \quad (21)$$

555 where $x, \alpha, \lambda > 0$.

556 Appendix B. Dealing with false roots

557 When using high degree polynomials on complex QPDs, false-positives are not uncommon.
 558 [Boyd \(2006\)](#) suggests using the roots identified by the proxy-root-finding method as starting
 559 values for the Newton-Raphson algorithm to refine (or refute) the roots. This adds to
 560 computational complexity and requires the presence of a valid QCF. The method we adopted
 561 in the `qpd` package is based on the idea of using the proxy roots as subdivisions of a QDF
 562 (0,1) range and checking a value from every segment of the function range formed by the
 563 proxy roots (e.g. if only one proxy root is found, checking one value on each side of the
 564 root). This way the number of evaluations required for assuring non-negativity of QDF can
 565 be significantly reduced.

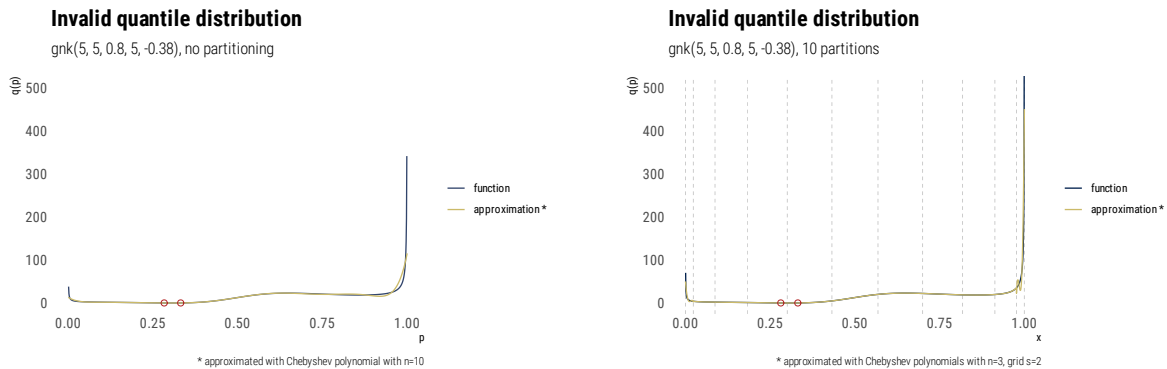


Figure 12: Chebyshev polynomial approximation: valid QDF and true-positive proxy roots

566 Figure 12 illustrates the ideas presented in this section. The *g-and-k* distribution
 567 $GnK(5, 5, 0.8, 5, -0.38)$ has an invalid QF. Graph on the left shows an approximation

³For definition of the Govindarajulu distribution with shifted support see [Nair et al. \(2012\)](#)

568 of QDF with Chebyshev polynomials of degree 10 without partitioning the range. Two
 569 roots are identified and they are correctly highlighting the area where QDF takes negative
 570 values. The function range can also be partitioned as shown on the graph to the right. Here
 571 partitioning is performed using the S-shaped scheme implemented in `qpd::make_pgrid()`.
 572 The parameter `s` is passed to the beta inverse transform so that the partitions are made
 573 at the points corresponding to $Q_{beta}(\{u_{(M)}\}, s, s)$, where $\{u_{(M)}\}$ is a uniformly distributed
 574 grid of M points. Uneven grid facilitates better fit in the tails of the QDF, but most
 575 importantly, allows us to use lower degree polynomials. In the partitioned case presented
 576 on the right, we used cubic Chebyshev polynomial fit on each of the 10 segments.

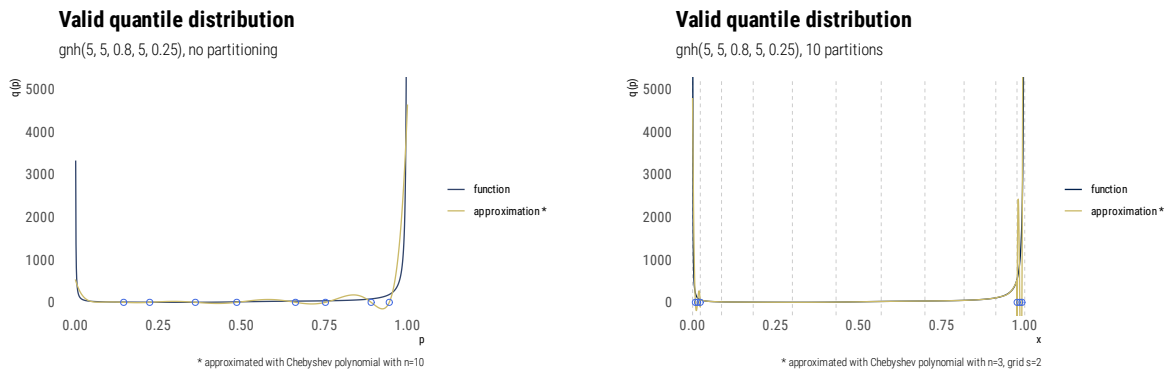


Figure 13: Chebyshev polynomial approximation: valid QDF and false-positive proxy roots

577 Unfortunately, not all quantile functions are behaving as nicely. Figure 13 presents a valid
 578 *g-and-h* distribution which we also approximated with a Chebyshev polynomial of degree
 579 10. All roots are false. They appear because of extreme curvature of the QDF in the tails.
 580 When the range is partitioned, the false roots move into the outermost bins, which are in
 581 fact “safest” areas of the QDF curve (above the y-axis) even by visual inspection. We need
 582 to evaluate the function less than 10 times to refute the roots and assure ourselves that the
 583 function is valid. Increasing the degree of the fitted polynomial (or increasing the number
 584 and/or density of the QDF range partitions) might reduce the number of false roots and
 585 move them even further out towards the tails. Given the low number of roots, and relatively
 586 inexpensive evaluation of QDF, these strategies may not be justifiable.

Appendix C. Practical tips for implementing quantile distributions in Stan and in R.

We implemented several quantile distributions in R (see `qpd` package) and in Stan (see Supplementary Materials) using certain conventions which might simplify their usage in other applications. First of all, we followed the prefix convention in R for naming probability functions “p” for CDF (e.g. `pnorm()`), “q” for QF (e.g. `qnorm()`), “d” for PDF (`dnorm()`) and “r” for random number generators (`rnorm()`). We extended the prefix list for quantile distributions: “f” for QDF (e.g. `fnorm()`), “dq” for DQF (e.g. `dqnorm()`) and “ff” for QCF, second derivative of QF (e.g. `ffnorm()`). Moreover, all approximate inverse QF (or CDF) functions have *tolerance* and *maximum number of iterations* arguments exposed (with reasonable default values), which indicate that even though the “p”-prefixed function is available, it is based on the approximation. We used bracketing root-finding algorithm with grid-matching to provide initial values to the target function (exposing the control over the grid to the user).

In Stan, custom functions are implemented in the `functions{}` block. In most cases we had to implement a QF (for various transformations, including inside target function), sometimes both vectorized and scalar version, because user functions in Stan can have only one signature. We also implemented a QDF to be used, for example, in the Newton-Raphson method, and as a service function inside the DQF. Because DQF is used in likelihood, Stan requires that the function name ends with `_lpdf` suffix. Should the tilde sampling notation be used, the suffix can be omitted. We hope that in the future quantile density suffix `_ldqf` will be accepted as well, but until that time we opted for double-suffixing.

As we mentioned, Stan allows only one signature for user function per name. Although it is possible to implement a vectorized log-DQF function to be used for likelihood, we opted for the scalar version (and therefore use it inside the loop over the observations). Implementing a scalar version of the log-density-quantile function is unavoidable for specification of the indirect prior, so in order to minimize the code repetition we used the scalar version for the likelihood as well. In the process of testing the Stan code, none of our custom probability functions caused problems or divergences. Challenges were more often caused by the lookup function (which performs the grid-matching) or the root-finding functions (we used built-in `algebra_solver()`). We could not get the recently implemented `algebra_solver_newton()` to work inside the indirect likelihood without divergences, so we used the default Powell hybrid algorithm. When implementing custom functions that will be used outside of the `transformed data{}` block, the usage of step-like functions should be minimized, in order to avoid possible issues with divergent transitions (see Section 3.7 in

622 Stan Development Team (2021b) for details).

623 We calculated the depths \underline{u} directly in the model block inside the likelihood loop and not
624 as `transformed parameters{}`. The cost of computing the depths $u_i \in \underline{u}$ depends on how
625 close are the initial guess values `u_guess` to the root of the target function $\Omega(u; x, \theta)$ and
626 the precision settings in the root-finding algorithm. The HMC algorithm implemented in
627 Stan requires calculation of the derivative of the log-likelihood function. Our experience
628 shows that as long as the initial guess values are close to the true values of the depths, the
629 numerically inverted quantile function is smooth and the “autodiff” algorithm built into Stan
630 is able to compute the derivative of the indirect log likelihood without divergences. Below
631 is the example of the `model{}` block from our GenExp-Govindarajulu model.

```
632 model {  
633   vector[N] u;  
634   // create grid of quantile values  
635   vector[M] xs_grd = govindarajulu_v_qf(ys_grd, gamma, sigma);  
636   // look-up u corresponding to closes value from the grid  
637   vector[N] u_guess = vlookup(x_srt, xs_grd, ys_grd);  
638   // priors  
639   target += genexp_s_lpdf(gamma | genexp_alpha, genexp_lambda);  
640   target += exponential_lpdf(dsigma | exp_lambda);  
641   // likelihood  
642   for (i in 1:N){  
643     // numerical inversion  
644     u[i] = approx_govindarajulu_cdf_algebra(x_srt[i], u_guess[i], gamma, sigma, rel_tol,  
645     // likelihood statement  
646     target += govindarajulu_s_ldqf_lpdf(u[i] | gamma, sigma);  
647   }  
648 }
```

649 We found that when using *indirect* inference (both in Stan and in R), good initial values are
650 essential. We tried to cue initial values closer to the mode of the prior to facilitate better
651 mixing of MCMC chains. The most important consideration is that the initial values be
652 within the admissible range (i.e. unit parameters should have specified upper and lower
653 bound), but also that the MCMC chain could successfully start exploring the parameter
654 space, meaning that the first few transitions are valid. A good approach could be to generate
655 a few samples from the prior distribution (given hyperparameters) and take the mean or
656 median value from it, as an initial value for the parameter.

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