

Bayesian Quantile Matching Estimation

Rajbir-Singh Nirwan^{1,a,b} and Nils Bertschinger^{2,a,b}

^aGoethe University, Frankfurt am Main, Germany

^bFrankfurt Institute for Advanced Studies, Frankfurt am Main, Germany

Abstract

Due to increased awareness of data protection and corresponding laws many data, especially involving sensitive personal information, are not publicly accessible. Accordingly, many data collecting agencies only release aggregated data, e.g. providing the mean and selected quantiles of population distributions. Yet, research and scientific understanding, e.g. for medical diagnostics or policy advice, often relies on data access. To overcome this tension, we propose a Bayesian method for learning from quantile information. Being based on order statistics of finite samples our method adequately and correctly reflects the uncertainty of empirical quantiles. After outlining the theory, we apply our method to simulated as well as real world examples. In addition, we provide a python-based package that implements the proposed model³.

1 Introduction

Due to data protection laws sensitive personal data cannot be released or shared among businesses as well as scientific institutions. While anonymization techniques are becoming increasingly popular, they often raise security concerns and have been re-identified in some cases [Narayanan and Shmatikov \(2010\)](#). To be on the safe side, big data collecting organisation such as Eurostat (statistical office of the European Union) or the World Bank only release aggregated summaries of their data. Instead of individual salary data only selected quantiles of the population distribution are available. Thus, for exploratory analysis as well as statistical modeling, the need for methods which work on aggregated data is there. This need can be further expected to grow as data privacy rules (e.g. GDPR ([European Commission, 2018](#))) are becoming more widespread.

Here, we will in particular put emphasis on data where only some quantile values are available. The matching of quantiles has already been explored in other contexts. So far, most of the work in this area has been built upon a nonlinear regression model where the mean squared error (MSE) between the cumulative density function (CDF) and the observed quantile values is minimized. In particular, the Federal Institute for Risk Assessment in Germany has open sourced an R-package ([Belgorodski et al., 2017](#)) that fits quantile data using this approach. Similarly, [Sgouropoulos et al. \(2015\)](#) and [Dominicy and Veredas \(2013\)](#) propose to minimize the quadratic distance between quantile statistics of modeled and actual data. Indeed, [Karian and Dudewicz \(2003\)](#) show that moment matching might be more reliable when using quantiles instead of other moments.

In this paper, we propose another method for quantile matching estimation that is based on the theory of order statistics. Order statistic is used a lot in the frequentists domain. [Cohen \(1998\)](#) used order statistics to estimate threshold parameters and [Chuiv and Sinha \(1998\)](#) estimated parameters of known distributions. [Geisser \(1998\)](#) made use of Bayesian analysis and order statistics for outlier detection. Our model also uses order statistics within the Bayesian framework to estimate parameters by matching observed quantiles. To the best of our knowledge, this method has not

¹nirwan@fias.uni-frankfurt.de

²bertschinger@fias.uni-frankfurt.de

³<https://github.com/RSNirwan/bqme>

been used in this context, but leads to a sound and intuitive noise model. In particular, we compare this model with other noise models, e.g.: the Gaussian noise model, which corresponds to the MSE fit mentioned earlier. We show that our noise model derived from order statistic puts more emphasis on the tails of the distribution and also captures the parameter uncertainty better than the Gaussian noise model.

Overall, the goal of this paper is to provide an alternative and principled approach to quantile matching estimation. For that we utilize the theory of order statistics. We start by defining the problem in section 2. Section 3 introduces the mathematical background needed to understand our approach. It starts with the uncertainty of the sample quantiles related to the uniform distribution and extends it further to non-uniform distributions. In section 4 we conduct experiments to show how our proposed approach performs compared to other approaches. Finally, section 5 concludes the paper.

2 Problem Definition

Suppose we are given M quantiles $\mathbf{q} = (q_1, \dots, q_M)$, e.g. for $M = 3$ we might be given the 25, 50 and 75% quantiles, and their corresponding empirical values $\mathbf{x} = (x_1, \dots, x_M)$ in a sample of N data points drawn from a distribution p . The task is to infer the underlying distribution from this information⁴. Note that the quantile values \mathbf{x} are calculated from the samples and thus are not the true values of the underlying distribution. Other N samples from the same distribution p will result in different values of \mathbf{x} for fixed quantiles \mathbf{q} . That means the quantile values \mathbf{x} themselves are noisy and need to be treated as such. The resulting uncertainty is shown in the left panel of Figure 2.1 showing 100 empirical CDFs of a standard Gaussian. For each CDF, we sampled 20 values from a standard Gaussian, ordered them from low to high, which results in the values of \mathbf{x} . The corresponding q -value is just the index m of the ordered vector \mathbf{x} divided by the total number of samples $N = 20$, $q_m = m/N$. The width (variance) of the CDFs for a fixed quantile q_m is the uncertainty associated with the corresponding x_m . So, for a fixed quantile q , we have a distribution $p(x|q)$ over x , that we want to model. This distribution is shown in the right panel of Figure 2.1 for $q = 0.25, 0.50, 0.95$ and 0.99 for the standard Gaussian distribution. Note that around the center ($q = 0.5$) the uncertainty associated with the empirical quantile values \mathbf{x} is lower than the uncertainty at the tails ($q = 0.95$ and 0.99). This difference in the uncertainty of different quantiles q is exactly what we want our model to capture.

Quantile matching methods as the Gaussian noise model (described in section 3.5) do have other prior assumptions for the uncertainty. In particular, minimizing the MSE between theoretical and observed quantiles can be considered as assuming a fixed Gaussian noise around the fitted CDF (independent of q). That, as we see in the right panel of Figure 2.1, is obviously not true⁵. This assumption, however, leads to a model that under emphasizes the uncertainty of the tails and implicitly downweights the information coming from the samples from the tails. As we describe in the next section, this problem can be handled using order statistics.

3 Order Statistics

In order to give a solution of the above stated problem, we need to review some literature on order statistics. In this section we start by looking at the order statistics of the uniform distribution

⁴In particular, we have no access to any of the N individual samples, e.g. due to reasons of data protection.

⁵Furthermore, it corresponds to a distribution $p(q|x)$, i.e. considering the quantile itself as variable. Instead, in most practical applications the quantiles \mathbf{q} are chosen a-priori and their corresponding values \mathbf{x} are reported. In contrast, our noise model correctly reflects this data generating process.

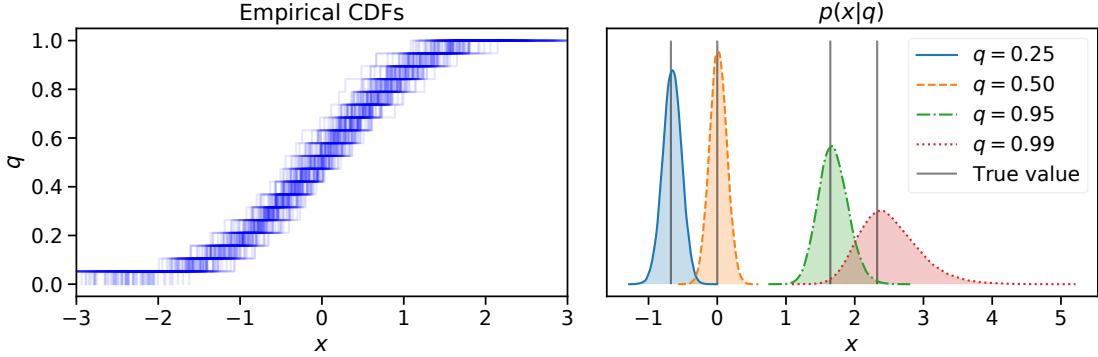


Figure 2.1: The left panel shows 100 empirical CDFs, each created with 20 samples from the standard Gaussian distribution. The right panel shows the distribution $p(x|q)$ of the quantile value x for $q = 0.25, 0.50, 0.95$ and 0.99 . This corresponds to the cut of the left panel at the given q -values.

and then generalize to non-uniform distributions. At the end of this section we also introduce the CDF-regression model with Gaussian noise. In section 4 we will compare the approach for the regression via order statistics to the CDF-regression model with Gaussian noise.

3.1 Order Statistics of a Uniform Distribution

To fix notation, assume we are given n real-valued iid observations (X_1, \dots, X_n) from some continuous distribution and the ordered series of the observations $(X_{(1)}, \dots, X_{(n)})$, where $X_{(1)} \leq \dots \leq X_{(n)}$. The k -th order statistic of that sample is equal to its k -th smallest value $X_{(k)}$. As stated in the problem definition (section 2) we are interested in the distribution of the order statistic $p(X_{(k)}|k)$ ⁶.

To get an intuition of the order statistics we will start with the uniform distribution on the interval $[0, 1]$. Thus, let (X_1, \dots, X_n) be iid samples from a $\text{Uniform}(0, 1)$ distribution. We want to find the PDF $p(X_{(k)})$ and the CDF $P(X_{(k)})$ of the k -th order statistics $X_{(k)}$. For $x \in [0, 1]$, the CDF $P(X_{(k)}) = P(X_{(k)} < x)$ has the following interpretation: if the event $X_{(k)} < x$ occurs, then there are at least k many X_i 's that are smaller or equal to x . Thus, drawing all the samples (X_1, \dots, X_n) can be seen as Bernoulli trials, where success is defined as $X_i < x \forall i \in \{1, \dots, n\}$. $P(X_{(k)} < x)$ is then defined as at least k successes and has the following form

$$P(X_{(k)} < x) = \sum_{i=k}^n \binom{n}{i} x^i (1-x)^{n-i}. \quad (3.1)$$

The PDF is given by the derivative of equation (3.1) and takes the form

$$p(X_{(k)} = x) = n \binom{n-1}{k-1} x^{k-1} (1-x)^{n-k}, \quad (3.2)$$

which is the Beta distribution $\text{Beta}(k, n - k + 1)$. It has also a convenient interpretation: All n samples that can result in the k -th order statistic, one of them becomes $X_{(k)}$ and out of the $n - 1$ left, there must be exactly $k - 1$ successes (defined as $X_i < X_{(k)}$). So, for samples from a standard Uniform distribution the k -th order statistic $X_{(k)}$ is Beta-distributed $X_{(k)} \sim \text{Beta}(k, n - k + 1)$.

⁶Note that the maximum, minimum, median and other quantiles are also order statistics, since $X_{(1)} = \min(X_1, \dots, X_n)$, $X_{(n)} = \max(X_1, \dots, X_n)$, $X_{((n+1)/2)} = \text{median}(X_1, \dots, X_n)$ for odd n . There is an ambiguity for even n . But that is not important for us right now.

3.2 Generalization of Uniform Order Statistics

In the more general case, where $X_{(i)}$ s are random samples drawn from a continuous non-uniform distribution with density f_x , we again ask for the k -th order statistics $p_x(X_{(k)})$. In this case, we just transform the samples such that they become uniformly distributed samples and then use the procedure described in the previous section. However, since we are transforming a random variable, we have to correct for the resulting change of measure by multiplying with the absolute Jacobian.

Given the cumulative distribution function F_x , we obtain $U_i = F_x(X_i)$. U_1, \dots, U_n correspond to samples from the standard uniform distribution. Again, $U_{(k)}$ will be Beta distributed

$$U_{(k)} = F_x(X_{(k)}) \sim \text{Beta}(F_x(X_{(k)})|k, n-k+1) := p_u(U_{(k)}). \quad (3.3)$$

Given a probability $p_u(u)$ on u and an invertible map g , so that $u = g(x)$, the density $p_x(x)$ on x is given by

$$p_x(x) = p_u(g(x)) \left| \frac{dg(x)}{dx} \right|. \quad (3.4)$$

In our case the invertible map is the cumulative distribution function F . So, we get

$$p_x(X_{(k)}) = p_u(F_x(X_{(k)})) \left| \frac{dF_x(x)}{dx} \right|_{x=X_{(k)}}. \quad (3.5)$$

Using eq. (3.3) and since $|dF_x(x)/dx| = f_x(x)$, we obtain

$$p_x(X_{(k)}) = \text{Beta}(F_x(X_{(k)})|k, n-k+1) f_x(X_{(k)}), \quad (3.6)$$

which is the k -th order statistic of any random variable X with the PDF f_x and CDF F_x .

3.3 Joint Distribution of the Order Statistics

Even if the underlying samples are independent, their order statistics will not be. Thus, in order to learn from observed (quantile values) $\mathbf{x} \in \mathbb{R}^M$ and their corresponding order $\mathbf{k} \in \mathbb{N}^M$ we need to know the joint PDF of the order statistics $p_x(X_{(1)}, \dots, X_{(M)}|\theta) \neq \prod_k p_x(X_{(k)}|\theta)$. In particular, if $i < j$, $X_{(i)}$ will for sure be smaller than $X_{(j)}$. We start with the joint distribution of two such observations.

The application of the CDF F to all of the observed quantile values \mathbf{x} , leads to a uniformly distributed random vector $\mathbf{U} = (U_1, \dots, U_M)$. The joint PDF of two order statistics $U_{(i)}$ and $U_{(j)}$, where $U_{(i)} < U_{(j)}$ then takes the following form

$$p_{U_{(i)}, U_{(j)}}(u, v) = n! \frac{u^{i-1}}{(i-1)!} \frac{(v-u)^{j-i-1}}{(j-i-1)!} \frac{(1-v)^{n-j}}{(n-j)!}, \quad (3.7)$$

where u and v correspond to the observed values of $U_{(i)}$ and $U_{(j)}$, the first fraction $u^{i-1}/(i-1)!$ is proportional to the binomial distribution of $i-1$ of the samples being smaller than u . The second term $(v-u)^{j-i-1}/(j-i-1)!$ corresponds to $j-i-1$ of the samples being in the interval (u, v) and the last term $(1-v)^{n-j}/(n-j)!$ corresponds to $(n-j)$ samples being greater than v . This process is illustrated in Figure 3.1.

The procedure can be extended to M observed values from a uniform distribution $\mathbf{u} = (u_1, \dots, u_M) \in \mathbb{R}^M$ with their order $\mathbf{k} = (k_1, \dots, k_M) \in \mathbb{N}^M$ and leads to the following joint PDF

$$p_{\mathbf{U}}(\mathbf{u}|\mathbf{k}) = c u_1^{k_1-1} (1-u_M)^{n-k_M} \prod_{m=2}^M (u_m - u_{m-1})^{k_m - k_{m-1}-1}, \quad (3.8)$$

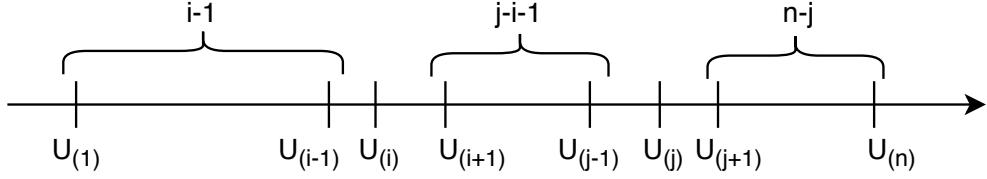


Figure 3.1: Illustration of the PDF of the joint order statistics (equation 3.7).

where the normalization constant c is given by (see Appendix A)

$$c = \frac{n!}{(k_1 - 1)!(n - k_m)! \prod_{m=2}^M (k_m - k_{m-1} - 1)!}. \quad (3.9)$$

From here, it is easy to extend equation (3.8) to samples from a non-uniform distribution with PDF f and CDF F . As already mentioned earlier, applying F to the samples will convert them to the desired samples from a uniform distribution and we can use equation (3.8) adjusted with the Jacobian correction. So, for observations $\mathbf{x} \in \mathbb{R}^M$ from a PDF f , their corresponding order $\mathbf{k} \in \mathbb{N}^M$ and the total number of observations n , we get the following joint order statistics

$$p_{\mathbf{X}}(\mathbf{x}|\mathbf{k}) = cF(x_1)^{k_1-1}(1-F(x_M))^{n-k_M} \prod_{m=2}^M (F(x_m) - F(x_{m-1}))^{k_m - k_{m-1} - 1} \prod_{m=1}^M f(x_m). \quad (3.10)$$

If instead of the order \mathbf{k} we are given the corresponding quantile information $\mathbf{q} = (q_1, \dots, q_M) \in [0, 1]^M$, we just need to replace the k_m with nq_m in equation (3.10).

3.4 Fit of Non-Uniform Distributions given Quantile Information

By utilizing the order statistics of a random variable, we can now use the observed quantiles and infer the underlying distribution. Given M observed quantiles, which are based on N samples, we denote as $\mathbf{q} = (q_1, q_2, \dots, q_M) \in [0, 1]^M$ the quantiles and $\mathbf{x} = (x_1, x_2, \dots, x_M) \in \mathbb{R}^M$ their corresponding empirical values. k as defined previously, is simply the product of a quantile q_i and the number of total samples N , i.e.: $k_i = q_i N$ ⁷.

With these definitions, the model likelihood becomes

$$\begin{aligned} p_{\mathbf{X}}(\mathbf{x}|\mathbf{q}, \boldsymbol{\theta}, N) &= cF_{\boldsymbol{\theta}}(x_1)^{q_1 N - 1}(1 - F_{\boldsymbol{\theta}}(x_M))^{N - q_M N} \\ &\quad \prod_{m=2}^M (F_{\boldsymbol{\theta}}(x_m) - F_{\boldsymbol{\theta}}(x_{m-1}))^{q_m N - q_{m-1} N - 1} \\ &\quad \prod_{m=1}^M f_{\boldsymbol{\theta}}(x_m), \end{aligned} \quad (3.11)$$

where $F_{\boldsymbol{\theta}}$ is the CDF parameterized by $\boldsymbol{\theta}$. From here on, one can either maximize equation (3.11) with respect to the parameter $\boldsymbol{\theta}$, or infer the full posterior $p(\boldsymbol{\theta}|\mathbf{x}, \mathbf{q}, N)$. We choose the latter, since it provides the full distribution of all parameters and thus also includes their estimation

⁷Note k_i is a positive integer but q_i can be any number between 0 and 1. Thus, by not setting k_i as $\lfloor q_i N \rfloor$ or $\lceil q_i N \rceil$ but as $k_i = q_i N$ we have an interpolation.

uncertainty. For the fully Bayesian treatment of the model, we assign a prior distribution $p(\boldsymbol{\theta})$ over the parameters $\boldsymbol{\theta}$ and infer the posterior. The posterior is then given by Bayes rule

$$p(\boldsymbol{\theta}|\mathbf{x}, \mathbf{q}, N) = \frac{p(\mathbf{x}|\boldsymbol{\theta}, \mathbf{q}, N)p(\boldsymbol{\theta})}{p(\mathbf{x})}, \quad (3.12)$$

which is intractable. There are several methods to approximate the posterior e.g.: Markov Chain Monte Carlo (MCMC), Variational Bayes (VB), etc.. We implement the model in the probabilistic programming language Stan ([Carpenter et al., 2017](#)), where both, MCMC (NUTS version of HMC) and VB with Gaussian approximation to the posterior, can be used out of the box. For our experiments we use MCMC.

3.4.1 Generative Model

Given N , \mathbf{q} , \mathbf{x} and the probability function $f_{\boldsymbol{\theta}}$, parameterized by $\boldsymbol{\theta}$, we obtain the following generative model:

$$\begin{aligned} \boldsymbol{\theta} &\sim p(\boldsymbol{\theta}) \\ \mathbf{x} &\sim p_{\mathbf{X}}(\mathbf{x}|\mathbf{q}, \boldsymbol{\theta}, N), \end{aligned} \quad (3.13)$$

where $F_{\boldsymbol{\theta}}$ is the CDF of $f_{\boldsymbol{\theta}}$. $p(\boldsymbol{\theta})$ is the prior distribution for our parameters and $p_{\mathbf{X}}(\mathbf{x}|\mathbf{q}, \boldsymbol{\theta}, N)$ is the likelihood given in equation (3.11). For all the experiments in section 4 we took a very broad Gaussian prior for all parameters (see below). The Stan code for the model is provided in the supplementary material. In addition, we have written a BQME-package in python (<https://github.com/RSNirwan/bqme>). The package allows for an easy specification of the model (prior and likelihood) and inference in just a few lines of code. After inference, it also allows the user to generate new samples and evaluate the density of unseen data.

For all presented examples and most practical purposes, i.e. where M is small, the code runs almost instantaneously. In particular, by equation (3.11), computing the likelihood has linear complexity requiring $O(M)$ CDF and PDF evaluations.

3.5 CDF Regression Model

Another approach for quantile-matching estimation (QME) which is widely used nowadays, is based on fitting the CDF to observed quantiles via mean squared error (MSE) minimisation. Given the quantiles \mathbf{q} and the values at the quantiles \mathbf{x} , the idea is to choose a parametric form of the distribution $f_{\boldsymbol{\theta}}$ (parameterized by $\boldsymbol{\theta}$) and find the parameters such that the MSE

$$\min_{\boldsymbol{\theta}} \sum_{m=1}^M (q_m - F_{\boldsymbol{\theta}}(x_m))^2 \quad (3.14)$$

is minimized. Thus, one basically fits the CDF $F_{\boldsymbol{\theta}}$ of $f_{\boldsymbol{\theta}}$ to the observed data (\mathbf{q}, \mathbf{x}) . Note that the MSE error function corresponds to the log-likelihood of a Gaussian noise model. Thus, we can equivalently consider the maximum likelihood estimate (MLE) for the parameters $\boldsymbol{\theta}$ for a model with likelihood

$$p(\mathbf{q}|\boldsymbol{\theta}, \mathbf{x}, \sigma_{\text{noise}}^2) = \prod_{m=1}^M \mathcal{N}(q_m | F_{\boldsymbol{\theta}}(x_m), \sigma_{\text{noise}}^2). \quad (3.15)$$

By comparing equation (3.15) to (3.11), we see that the modelling of the uncertainty is quite different. Whereas the regression of quantiles puts the noise on the quantiles \mathbf{q} (equation 3.15),

the solution with the order statistics treats the observed quantile values \mathbf{x} as noisy (equation 3.11). On the one hand, this reverses the data generating process where in practice the quantiles \mathbf{q} are chosen a-priori and their corresponding values \mathbf{x} are reported. On the other hand, it leads to a different penalty for the deviation of the regression function. As already stated in section 2, this model assumes a fixed Gaussian noise around the fitted CDF, which is independent of q or x . This assumption, however, leads to an underestimation of the noise uncertainty, especially at the tails and leads to another fit than the order statistics. We further discuss these points in the next section.

4 Experiments

In this section we conduct experiments on quantile matching estimations and discuss the results. We will start by looking at the posterior distribution of the parameters of the PDF for both noise models (order statistics and the Gaussian noise model). Subsequently, we will discuss their sensitivity to the change of single data points, which is also related to the robustness of the models. At the end, we analyse how the 2 noise models emphasise different regimes (tails or the center of the PDF) of the observed data. The prior on the parameters of both models in all experiments is set to a very broad Gaussian with mean 0 and standard deviation 100. The code for the simulations is available on Github: https://github.com/RSNirwan/BQME_experiments.

4.1 Bayesian Quantile Matching Estimation

In this subsection we will deal with the case of correctly specified models, where the data generating distribution is from the same class as the distribution that we use to fit the data. In real world applications one does not know the data generating distribution and the model distribution may differ from it. In section 4.2 we consider the case of misspecified models and discuss how this situation can be detected.

4.1.1 Gaussian Fit

We will start by fitting a Gaussian distribution to the observed data. The data are generated by taking N samples from a Gaussian with known parameters μ and σ . Afterwards we take M quantile values $\mathbf{x} \in \mathbb{R}^M$ for given quantiles $\mathbf{q} \in \mathbb{R}^M$. The tuple $(\mathbf{x}, \mathbf{q}, N)$ is the “observed data” that we fit by a Gaussian PDF. This is done with order statistics (equation 3.11) as well as with the Gaussian noise model (equation 3.15).

Figure 4.1 shows the sampled posterior for μ and σ . The kernel density estimate (KDE) of the samples is plotted and true values of the data generating distribution (which is also a Gaussian) are shown with vertical black line and were set to $\mu = 3.0$ and $\sigma = 1.5$. The top row shows the results for $N = 200$ and $M = 10$ and the bottom row shows the results for $N = 500$ and $M = 100$. \mathbf{q} is chosen equidistantly between 5% and 95% for both plots. As one can see, the Gaussian noise model clearly underestimates the uncertainty for μ compared to the order statistic model. The probability mass the Gaussian noise model puts on the true value is almost zero, which is not a desirable property for any model.

4.1.2 Dependency on N

When we fit a distribution to some observed quantile values, we would ideally expect an effect of the number of samples the observed quantile values are based on. The higher the sample size, the closer (less uncertain) observed sample quantile values will be to the true quantile values of the

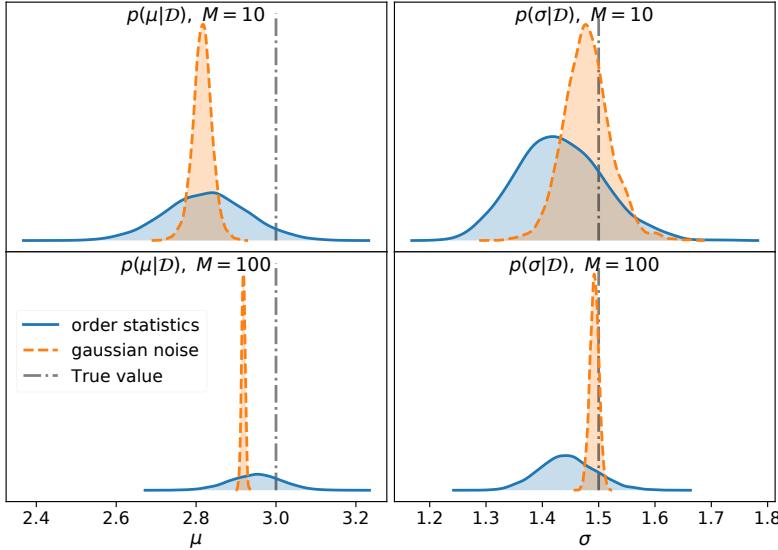


Figure 4.1: The posterior parameter distribution for a fit with a Gaussian distribution. Top row shows the results for μ and σ for $M = 10$ and the bottom row for $M = 100$. q s were chosen equidistantly between 5% to 95%, $N = 200$ for $M = 10$ and $N = 500$ for $M = 100$ and the true values for μ and σ are 3.0 and 1.5, respectively.

underlying distribution. This is taken care of in the order statistic. The likelihood of the order statistics (equation 3.11) is dependent on N . The higher N , the more accurate the parameters of the fitted distribution will be. In this subsection we will look at the change of the posterior distribution as a function of N . We fix M and q . x is set to the true quantile values of a Gaussian. The only parameter we change is N .

Figure 4.2 shows the results for $\mu = 3.0$ and $\sigma = 1.5$, M was set to 10 and the quantiles q were chosen equidistantly between 5% and 95%. As expected, with higher N the uncertainty in the posterior is decreasing. This is driven by the model likelihood in equation (3.11) which exactly and correctly captures the dependency on N in the uncertainty of the empirical quantiles. In contrast, the Gaussian noise model would only indirectly respond to increasing sample sizes as the empirical CDF more closely tracks the theoretical one and the MSE is reduced, i.e. $\sigma_{\text{ML}}^2 \rightarrow 0$ for $N \rightarrow \infty$.

4.2 Penalty for OS and CDF-fit

As already mentioned, the penalty of the observed data points (q, x, N) to the regression function is quite different by choosing either the order statistics error probability (equation 3.11) or the Gaussian error probability (equation 3.15). This can be illustrated by looking at the true and the matched quantile plots.

We take N samples from the data generating distribution, calculate M quantile values x for given quantiles q . Subsequently, we fit the desired distribution to (q, x, N) via the order statistics and the Gaussian error function. Ideally, one would take the same distribution to fit the data as the data generating distribution, but this cannot be guaranteed, since for most real world cases one rarely knows its form.

Figure 4.3 shows the results for a fit with the Gaussian probability function. Left hand side shows the result for a correctly specified model, where the fitted distribution is from the same

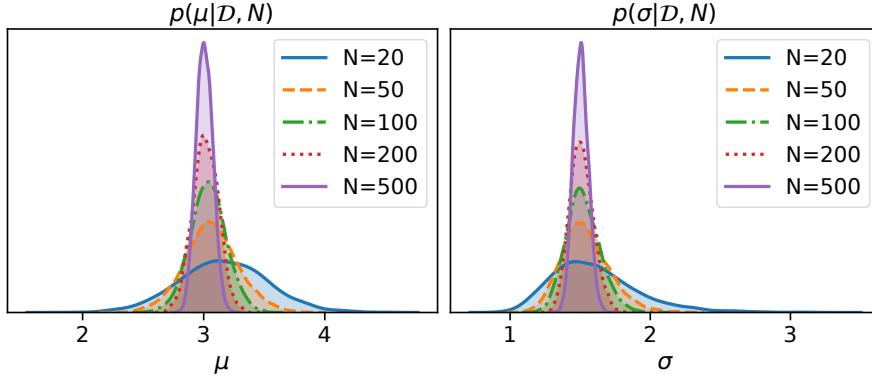


Figure 4.2: Posterior parameter distribution for a Gaussian fit for different N . With higher N the uncertainty in the posterior is reduced significantly.

class as the data generating distribution. Here, both are Gaussian and the location and scale parameters for the data generating Gaussian distribution were set to 3.0 and 1.5. The right hand side shows the results for a misspecified model, where the data generating distribution is not from the same class as the distribution that we fit to the data. Here, the data generating distribution was a Cauchy with location and scale parameters set to 3.0 and 1.5 and we fitted a Gaussian to the observed quantile values. In each case, we took $N = 200$ and 20 equidistant quantile values in the range from 5% to 95%. Note that since the Cauchy distribution is heavy tailed, the scale of the coordinate axes is not the same in both figures.

Both models perform quite well in the case of the specified model, but the order statistics clearly capture the uncertainty better than the Gaussian noise model, which underestimates it. In the misspecified case, each of the model focuses on different parts of the data. While the Gaussian noise model emphasises the central part of the distribution, the tails are better captured by the order statistics.

Note, that we are fitting data from a Cauchy distribution with a Gaussian distribution. Because of the very different tail behavior (heavy tails of Cauchy and light tails of the Gaussian) those will never be fitted correctly. The Gaussian noise model, which corresponds to the MSE function, does not put much emphasis on the tails. In the tails the difference between even the CDF of a very heavy tailed distribution (as the Cauchy) and a very light tailed distribution (as the Gaussian) is negligible compared to their differences around the mode. Thus, the contribution of the tails to the overall MSE is very small and leads to the neglect of the tails. In contrast, the order statistics correctly weights the information from all observations and strives to increase the variance of the Gaussian to capture some of the heavy tail behavior. This is shown in Figure 4.4. We plotted the likelihood of the order statistics (blue) and the Gaussian noise model (orange) for a standard Gaussian $\mathcal{N}(0, 1)$ with PDF $f(x)$ and CDF $F(x)$. In particular, we plotted the likelihoods (normalized such that the maximum is at 1) as a function of x

$$p_{\text{os}}(x|q) \propto F(x)^{qN-1} (1 - F(x))^{N-qN} f(x) \quad (4.1)$$

$$p_{\text{gn}}(q|x) \propto \exp \left\{ -\frac{1}{2\sigma_{\text{noise}}^2} (F(x) - q)^2 \right\} \quad (4.2)$$

for three fixed quantiles $q \in \{0.1, 0.01, 0.001\}$. p_{os} is the likelihood for the order statistics and p_{gn} is the likelihood for the Gaussian noise model. The black vertical line shows the quantile value x_{true} for the fixed quantile q_{true} and the blue and orange lines show the score that an estimated value

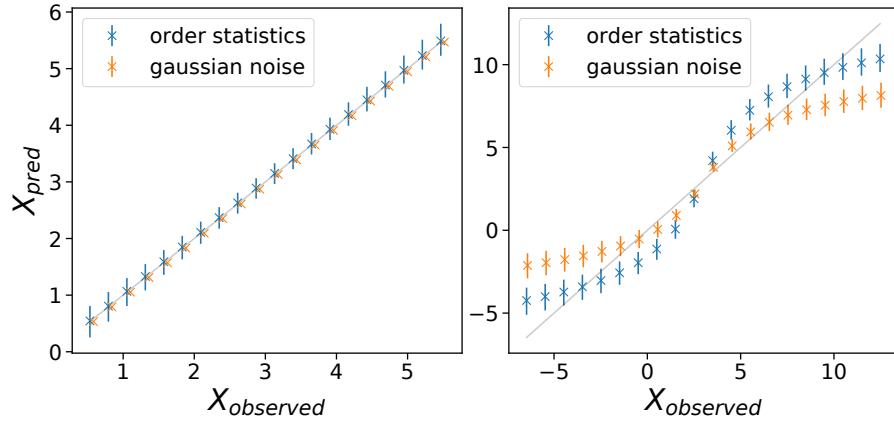


Figure 4.3: Correctly specified (left) and misspecified model (right) fitted with the order statistics and Gaussian noise. In the specified case, both models perform quite well, but the Gaussian noise underestimates the uncertainty. In the misspecified case, both models put emphasis on different parts of the data.

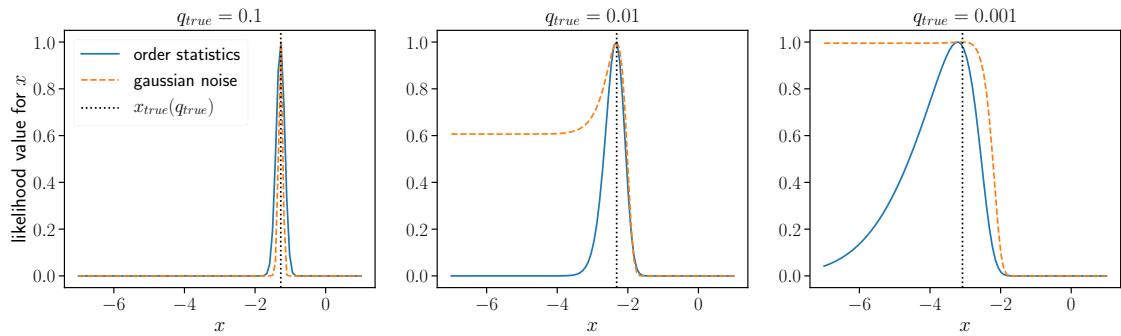


Figure 4.4: Likelihood of Gaussian noise model and order statistics as a function of x at different fixed quantiles q . Note that the likelihood of the Gaussian noise model does not decrease to zero even for arbitrarily large deviations from the true value x_{true} in the (left) tail.

Table 1: Aggregated salary data of some European countries from 2016. Columns 25, 50 and 75 are the corresponding quantiles of the yearly salary of individuals. “Sample Size” indicates number of total samples of the survey.

COUNTRY	SAMPLE SIZE	25	50	75
EL	12918	4930	7500	11000
ES	19177	8803	13681	20413
FR	21325	16185	21713	29008
IT	24969	10699	16247	22944
LU	10292	23964	33818	48692
NL	12748	16879	22733	30327
SE	11635	17794	25164	33365
UK	17645	14897	21136	30151

Table 2: The mean of the log likelihood samples for different models and countries. Best fits to the salary quantile data (bold numbers) are given by the Weibull, lognormal and gamma distribution. The + and - values show the distance to the 95 and 5 % quantile of the posterior log-likelihood distribution.

COUNTRY	WEIBULL	LOGNORMAL	GAMMA	INV_GAMMA	FRECHET	CHI_SQUARE	EXPONENTIAL
EL	$-6.9^{+0.9}_{-2.1}$	$4.3^{+0.9}_{-2.0}$	10.2 $^{+1.0}_{-2.0}$	$-31.5^{+0.9}_{-2.0}$	$-81.1^{+1.0}_{-2.2}$	$-2063.9^{+0.5}_{-1.3}$	$-1416.4^{+0.5}_{-1.3}$
ES	$-13.4^{+1.0}_{-1.9}$	$-0.2^{+1.0}_{-2.1}$	10.1 $^{+0.9}_{-1.8}$	$-58.9^{+1.0}_{-2.0}$	$-130.4^{+1.0}_{-2.1}$	$-2776.2^{+0.5}_{-1.4}$	$-1854.7^{+0.5}_{-1.4}$
FR	$-57.7^{+1.0}_{-2.0}$	13.0 $^{+0.9}_{-2.0}$	$3.5^{+1.0}_{-2.2}$	$-4.4^{+1.0}_{-2.1}$	$-76.8^{+0.9}_{-2.0}$	$-5847.6^{+0.5}_{-1.4}$	$-4554.3^{+0.5}_{-1.4}$
IT	9.1 $^{+0.9}_{-2.0}$	$-48.9^{+0.9}_{-2.0}$	$5.3^{+0.9}_{-2.0}$	$-155.2^{+0.9}_{-2.0}$	$-290.0^{+1.0}_{-2.1}$	$-4500.3^{+0.5}_{-1.4}$	$-3139.8^{+0.5}_{-1.4}$
LU	$-47.7^{+1.0}_{-2.0}$	9.3 $^{+1.0}_{-2.1}$	$-9.3^{+0.9}_{-2.1}$	$9.1^{+0.9}_{-2.0}$	$-10.9^{+0.9}_{-1.9}$	$-2062.3^{+0.5}_{-1.4}$	$-1524.1^{+0.5}_{-1.4}$
NL	$-23.3^{+0.9}_{-1.9}$	11.6 $^{+1.0}_{-2.0}$	$9.0^{+0.9}_{-1.9}$	$-1.9^{+1.0}_{-2.0}$	$-49.4^{+1.0}_{-2.1}$	$-3473.8^{+0.5}_{-1.4}$	$-2698.1^{+0.5}_{-1.4}$
SE	11.4 $^{+1.0}_{-2.0}$	$-21.2^{+0.9}_{-2.0}$	$3.9^{+1.0}_{-2.0}$	$-63.0^{+1.0}_{-2.0}$	$-138.7^{+0.9}_{-2.0}$	$-2910.8^{+0.5}_{-1.3}$	$-2191.0^{+0.5}_{-1.4}$
UK	$-62.8^{+0.9}_{-2.0}$	12.1 $^{+1.0}_{-2.0}$	$-8.1^{+1.0}_{-2.0}$	$0.5^{+0.9}_{-1.9}$	$-45.6^{+0.9}_{-1.9}$	$-3582.7^{+0.5}_{-1.3}$	$-2641.1^{+0.5}_{-1.3}$

x corresponding to a q would get. The order statistics show a peak at the true value x_{true} and decreases on both sides even if x_{true} is set further in the tails ($q = 0.1, 0.01, 0.001$). The Gaussian noise model on the other hand does not decrease to zero even far away from the true quantile value (middle and right plot). The reason being, that the likelihood (equation 4.2, specifically $(F(x) - q)^2$) does not change much for a large change in x . This is the case, in particular, in the tails. Therefore, a bad estimate, e.g., of $q = F(x) = 0.0001$ for $q_{\text{true}} = 0.001$ leads to almost the same likelihood score as the correct value $q = F(x) = 0.001 = q_{\text{true}}$. Because of that, the CDF regression with Gaussian noise is totally not suitable for applications where tails of the distribution are important. Order statistics is a better choice here.

4.3 Real World Data

Due to data privacy acts, many times the data are not available on an individual basis but only in aggregated forms. Whenever this is the case, traditional machine learning techniques are not very useful. In the case of medical data, one cannot simply publish private data of individual

patients. But the the data are published in aggregated form. The same is true for other sensitive data sources, e.g.: economic data. Here also data is provided in aggregated form. As an example we take the distribution of income of European countries. Table 1 shows the salary values for 25, 50 and 75% quantiles and the total number of samples of the survey⁸.

Before fitting the data as explained in section 3, we normalize it by dividing the salaries by the median (50% quantile) of each country. The normalized data are then fitted by various distributions. The goodness of the fits measured by the log-likelihood is shown in table 2. Each row corresponds to one particular country and contains the log-likelihood values for several models. The highest log-likelihood value (best fit to the data from the particular country) is emphasised in bold writing. The corresponding fit for the cumulative density (posterior predictive cumulative density) of the salary is also shown in Figure 4.5, i.e.

$$P(X < x') = \int F_{\theta}(x') p(\theta | \mathbf{x}, \mathbf{q}, N) d\theta . \quad (4.3)$$

Bandourian et al. (2002) suggests to use a Weibull distribution to fit salary data. However, the data they use are not as aggregated as ours are. Table 2 shows that Weibull as well as lognormal and gamma distributions provide reasonable fits to the data. However, also in this case we should keep in mind that we try to fit the whole distribution from just 3 quantiles, which might not contain enough information to pinpoint one single distribution. Given the predictive distribution, questions like the following can be answered very easily: What is the threshold for the 99% quantile (earnings of the top 1%)? In the supplementary material we provide a table estimating the 99% quantile of the predictive distribution for the best fits for each country. In addition, a similar plot to Figure 4.3 is included in the supplementary material for UK. While being based on three quantiles $q = 0.25, 0.5, 0.75$ only (where we know the empirical salaries) the log-normal model shows no sign of misspecification in contrast to the other considered models.

5 Conclusion

We proposed an alternative approach for quantile matching estimation. In contrast to the widely used procedure of minimizing the MSE between the theoretical and empirical CDF, our Ansatz is based on the order statistics of the samples. This leads to a principled noise model combining the information contributed from several quantiles. In particular, we showed that our model correctly accounts for the higher uncertainty of tail quantiles, whereas the Gaussian noise model – corresponding to MSE minimization – overemphasises the central part of the distribution. Furthermore, our Bayesian approach allows for a principled assessment of model uncertainty and model comparison. As an example, we fitted income data from several European countries with our proposed method and compared several candidate distributions.

References

- Bandourian, R., Turley, R., and McDonald, J. (2002). A Comparison of Parametric Models of Income Distribution across Countries and over Time. LIS Working papers 305, LIS Cross-National Data Center in Luxembourg.
- Belgorodski, N., Greiner, M., Tolksdorf, K., Schueller, K., Flor, M., and Göhring, L. (2017). rriskDistributions: Fitting distributions to given data or known quantiles.

⁸The data are downloaded from the Eurostat homepage (Distribution of income by quantiles - EU-SILC and ECHP surveys) at <https://ec.europa.eu/eurostat/>. Information about the sample size is also available on the website (EU and national quality reports).

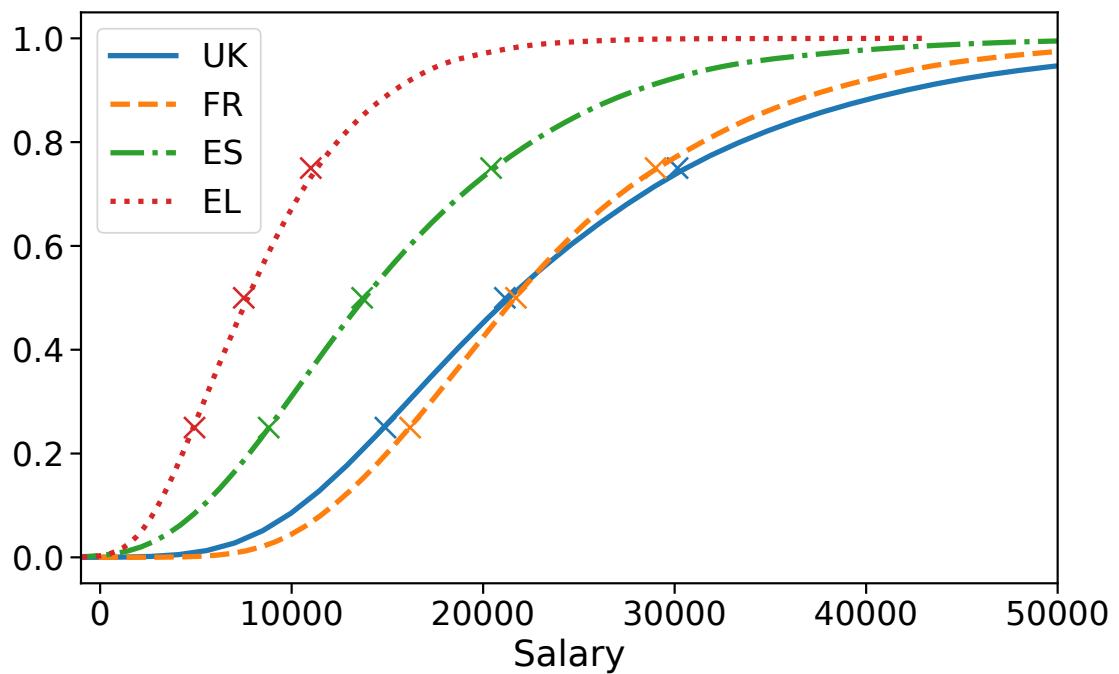


Figure 4.5: Posterior predictive cumulative distribution. Observed data are marked by crosses. Different colors indicate observed data and learned distribution for different countries.

- Bishop, C. M. (2006). *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Springer-Verlag, Berlin, Heidelberg.
- Carpenter, B., Gelman, A., Hoffman, M., Lee, D., Goodrich, B., Betancourt, M., Brubaker, M., Guo, J., Li, P., and Riddell, A. (2017). Stan: A probabilistic programming language. *Journal of Statistical Software, Articles*, 76(1):1–32.
- Chuiv, N. N. and Sinha, B. K. (1998). On some aspects of ranked set sampling in parametric estimation. In *Order Statistics: Applications*, volume 17 of *Handbook of Statistics*, pages 337 – 377. Elsevier.
- Cohen, A. C. (1998). The role of order statistics in estimating threshold parameters. In *Order Statistics: Applications*, volume 17 of *Handbook of Statistics*, pages 283 – 314. Elsevier.
- Dominicy, Y. and Veredas, D. (2013). The method of simulated quantiles. *Journal of Econometrics*, 172(2):235 – 247. Latest Developments on Heavy-Tailed Distributions.
- European Commission (2018). 2018 reform of EU data protection rules.
- Geisser, S. (1998). Some uses of order statistics in Bayesian analysis. In *Order Statistics: Applications*, volume 17 of *Handbook of Statistics*, pages 379 – 400. Elsevier.
- Karian, Z. A. and Dudewicz, E. J. a. (2003). Comparison of GLD fitting methods: Superiority of percentile fits to moments in l^2 norm. *Journal of the Iranian Statistical Society*, 2(2).
- Narayanan, A. and Shmatikov, V. (2010). Myths and fallacies of “personally identifiable information”. *Commun. ACM*, 53(6):24–26.
- Sgouropoulos, N., Yao, Q., and Yastremiz, C. (2015). Matching a distribution by matching quantiles estimation. *Journal of the American Statistical Association*, 110(510):742–759. PMID: 26692592.

Supplementary Material

A Normalization Constant

To verify that equation (3.9) is indeed the normalization constant, we have to integrate equation (3.8) with respect to all u 's

$$\frac{1}{c} = \int_0^{u_2} \int_{u_1}^{u_3} \cdots \int_{u_{M-1}}^1 u_1^{k_1-1} (1-u_M)^{n-k_M} \prod_{m=2}^M (u_m - u_{m-1})^{k_m - k_{m-1}-1} du_1 du_2 \dots du_M . \quad (\text{A.1})$$

For the integration of a particular u_i , however, only the following term is relevant

$$\int_{u_{i-1}}^{u_{i+1}} (u_i - u_{i-1})^{k_i - k_{i-1}-1} (u_{i+1} - u_i)^{k_{i+1} - k_i - 1} du_i . \quad (\text{A.2})$$

The rest is constant with respect to u_i . To solve this integral we substitute $u = \frac{u_i - u_{i-1}}{u_{i+1} - u_{i-1}}$ for u_i and get

$$\begin{aligned} & \int_{u_{i-1}}^{u_{i+1}} (u_i - u_{i-1})^{k_i - k_{i-1}-1} (u_{i+1} - u_i)^{k_{i+1} - k_i - 1} du_i \\ &= (u_{i+1} - u_{i-1})^{k_{i+1} - k_{i-1}-1} \int_0^1 u^{k_i - k_{i-1}-1} (1-u)^{k_{i+1} - k_i - 1} du \\ &= (u_{i+1} - u_{i-1})^{k_{i+1} - k_{i-1}-1} \frac{\Gamma(k_i - k_{i-1}) \Gamma(k_{i+1} - k_i)}{\Gamma(k_{i+1} - k_{i-1})} . \end{aligned} \quad (\text{A.3})$$

Note that the integrand in the second step is a unnormalized beta distribution, where we already know the normalization constant (Bishop, 2006). $\Gamma(\cdot)$ is the Gamma-function, which, for integer input has the form $\Gamma(n+1) = n!$.

By integrating out u_i , the resulting expression has still a similar form. Thus, by successive applications of the above result, we obtain the normalization constant as in equation (3.9).

B Stan code for Bayesian Quantile Matching Estimation

Below is the stan code to fit a Weibull distribution to the data.

```

1  functions{
2    real orderstatistics(int N, int M, vector q, vector U){
3      real lpdf = 0;
4      lpdf += lgamma(N+1) - lgamma(N*q[1]) - lgamma(N-N*q[M]+1);
5      lpdf += (N*q[1]-1)*log(U[1]);
6      lpdf += (N-N*q[M])*log(1-U[M]);
7      for (m in 2:M){
8        lpdf += -lgamma(N*q[m]-N*q[m-1]);
9        lpdf += (N*q[m]-N*q[m-1]-1)*log(U[m]-U[m-1]);
10    }
11    return lpdf;
12  }
13 }
14 data{
15   int N;           // total sample size
16   int M;           // number of observed quantiles
17   vector[M] q;    // quantiles
18   vector[M] X;    // quantile values
19 }
20 parameters{
21   real<lower=0> shape;
22   real<lower=0> scale;
23 }
24 transformed parameters{
25   vector[M] U;
26   for (m in 1:M)
27     U[m] = weibull_cdf(X[m], shape, scale);
28 }
29 model{
30   shape ~ normal(0, 100);
31   scale ~ normal(0, 100);
32   target += orderstatistics(N, M, q, U);
33   for (m in 1:M)
34     target += weibull_lpdf(X[m] | shape, scale);
35 }
36 generated quantities {
37   real<lower=0> predictive_dist = weibull_rng(shape, scale);
38   real log_prob = orderstatistics(N, M, q, U);
39   for (m in 1:M)
40     log_prob += weibull_lpdf(X[m] | shape, scale);
41 }
```

To fit a lognormal, for example, instead of a weibull, we only need to change the following lines:
Line 27 to

```
U[m] = lognormal_cdf(X[m], mu, sigma);
```

Line 34 to

```
target += lognormal_lpdf(X[m] | mu, sigma);
```

Line 37 to

```
real<lower=0> predictive_dist = lognormal_rng(mu, sigma);
```

Line 40 to

```
log_prob += lognormal_lpdf(X[m] | mu, sigma);
```

In addition, we assume that the `shape` and `scale` parameters have been renamed to `mu` and `sigma` within the code.

C Predicted earnings of the top 1% of the population

Table 3: The earnings of the top 1% according to the best model based on the log-likelihood score. The + and - values show the distance to the 95 and 5 % quantile of the posterior predictive distribution.

COUNTRY	BEST MODEL	99% QUANTILE
EL	GAMMA	23268.6 $^{+406.8}_{-400.4}$
ES	GAMMA	44343.5 $^{+701.7}_{-633.7}$
FR	LOGNORMAL	59331.9 $^{+834.6}_{-838.8}$
IT	WEIBULL	41096.2 $^{+483.8}_{-467.6}$
LU	LOGNORMAL	115693.5 $^{+3038.5}_{-2796.1}$
NL	LOGNORMAL	62265.1 $^{+1185.3}_{-1142.6}$
SE	WEIBULL	53926.5 $^{+754.0}_{-744.5}$
UK	LOGNORMAL	71466.4 $^{+1294.2}_{-1280.7}$

D In sample and out of sample predictions for UK

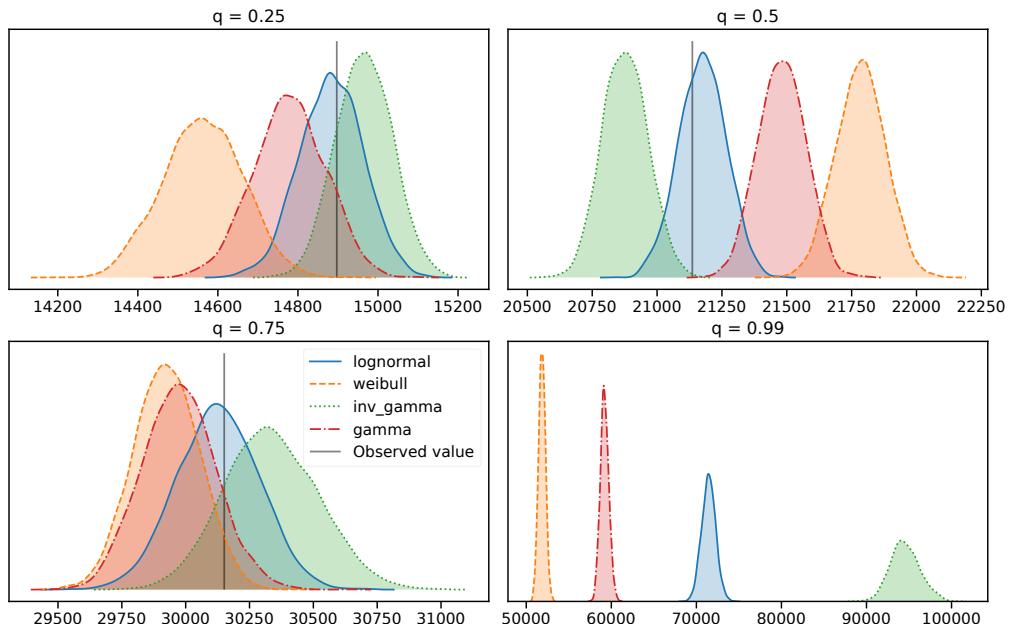


Figure D.1: The top row and the left side of the bottom row shows the predictions made for the quantile that we also observed and the bottom right plot shows an out of sample prediction for the 99% quantile. Different colors indicate different models. The best model according to the log-likelihood value was the lognormal distribution. This figure visually validates that result.