Tutorial: quantile g-and-k

EB, PJ, MG, CR June 10, 2017

```
# load package
library(winference)
# register parallel cores
registerDoParallel(cores = detectCores())
# remove all
rm(list = ls())
# apply preferences for ggplotting
require(gridExtra)
theme_set(theme_bw())
# set RNG seed
set.seed(11)
```

Setting

This script illustrates the calculation of the likelihood in a g-and-k example, then runs an MCMC algorithm to approximate the posterior. The g-and-k distribution is defined through its quantile function:

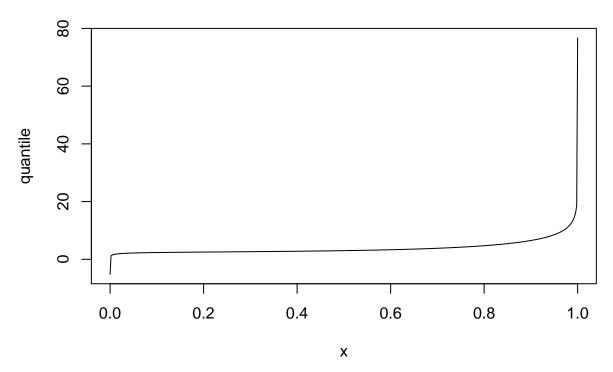
$$r \in (0,1) \mapsto a + b \left(1 + 0.8 \frac{1 - \exp(-gz(r))}{1 + \exp(-gz(r))} \right) \left(1 + z(r)^2 \right)^k z(r),$$

with parameters (a, b, g, k). We define the data-generating parameter $(a_{\star}, b_{\star}, g_{\star}, k_{\star}) = (3, 1, 2, 0.5)$.

```
#include <Rcpp.h>
using namespace Rcpp;
// [[Rcpp::export]]
NumericVector gandk_quantile(NumericVector x, NumericVector theta){
   NumericVector z = qnorm(x);
   double A = theta(0);
   double B = theta(1);
   double c = 0.8;
   double g = theta(2);
   double k = theta(3);
   return A + B * (1 + c * (1 - exp(- g * z)) / (1 + exp(- g * z))) * pow((1 + pow(z, 2.0)), k) * z;
}
```

We plot the quantile function associated with that parameter.

```
# parameter of data-generating process
theta_star <- c(3, 1, 2, 0.5)
# define associated quantile function
quantile_star <- function(r) {
    gandk_quantile(r, theta_star)
}
# plot function
curve(sapply(x, FUN = function(v) quantile_star(v)), from = 1e-10, to = 1 -
    1e-10, n = 500, ylab = "quantile")</pre>
```



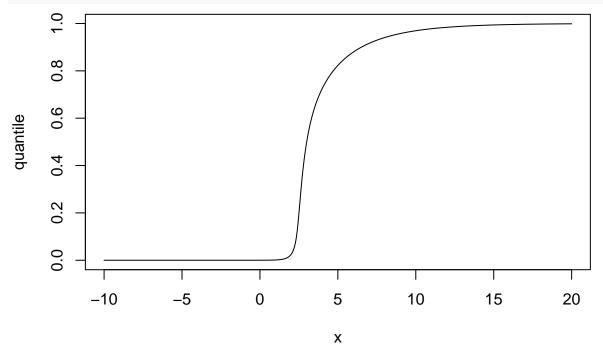
To compute the likelihood, we need to get the pdf of the g-and-k distribution. The pdf is the derivative of the cdf, which is the inverse of the quantile function. We first get the cdf, by numerical inversion of the quantile function. We use a simple binary search scheme.

```
#include <Rcpp.h>
using namespace Rcpp;
// [[Rcpp::export]]
double gandk_cdf(double y, NumericVector theta, int maxsteps = 1000,
                 double tolerance = 1e-10, double lower = 1e-20, double upper = 1-1e-20){
  double A = theta(0);
  double B = theta(1);
  double c = 0.8;
  double g = theta(2);
  double k = theta(3);
  int istep = 0;
  double current_try = (upper + lower) / 2;
  double current_size = (upper - lower) / 4;
  NumericVector dd(1);
  dd(0) = current_try;
  NumericVector z = qnorm(dd);
  double fattempt = A + B * (1 + c * (1 - \exp(-g * z(0)))) / (1 + \exp(-g * z(0)))) *
    pow((1 + pow(z(0), 2.0)), k) * z(0);
  while (!(fattempt > y-tolerance && fattempt < y+tolerance) && (istep < maxsteps)){</pre>
   istep++;
    if (fattempt > y-tolerance){
      current_try = current_try - current_size;
      dd(0) = current_try;
      NumericVector z = qnorm(dd);
      fattempt = A + B * (1 + c * (1 - \exp(-g * z(0)))) / (1 + \exp(-g * z(0)))) *
        pow((1 + pow(z(0), 2.0)), k) * z(0);
      current_size = current_size / 2;
```

```
} else {
    current_try = current_try + current_size;
    dd(0) = current_try;
    NumericVector z = qnorm(dd);
    fattempt = A + B * (1 + c * (1 - exp(- g * z(0))) / (1 + exp(- g * z(0)))) *
        pow((1 + pow(z(0), 2.0)), k) * z(0);
        current_size = current_size / 2;
    }
}
return current_try;
}
```

We can now plot the cdf.

```
# plot cdf
curve(sapply(x, FUN = function(v) gandk_cdf(v, theta_star)), from = -10, to = 20,
    n = 500, ylab = "quantile")
```



Finally we can get the pdf by numerical differentiation, e.g. using the numDeriv package.

```
library(numDeriv)
```

```
## Warning: package 'numDeriv' was built under R version 3.2.5

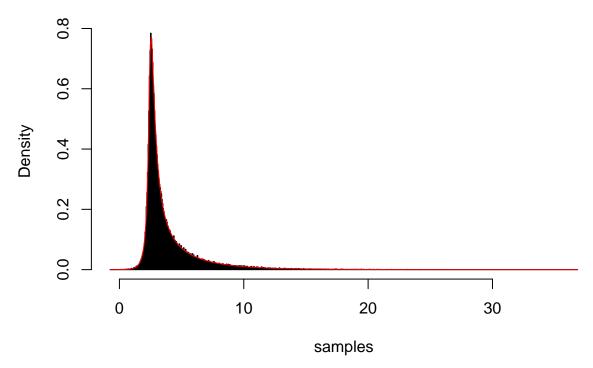
cdf_ <- function(z) sapply(z, FUN = function(v) gandk_cdf(v, theta_star))

pdf <- function(x) {
    return(grad(cdf_, x))
}

# test: sample from the distribution
samples <- gandk_quantile(runif(1e+05), theta_star)

# plot the histogram and overlay pdf
hist(samples, prob = TRUE, nclass = 1000)
curve(pdf(x), add = TRUE, col = "red", n = 500)</pre>
```

Histogram of samples



Once we get the pdf, we can simply compute the likelihood by multiplying the pdf evaluated at each observation. However, we can be more efficient by sorting the observations, and inverting the quantile function for each observation in increasing order. Indeed, we can then successively reduce the range of the search within the interval [0, 1]. Such an implementation of the g-and-k likelihood is provided below.

```
# this function computes the likelihood of ys, given each theta each theta
# being a row in the matrix 'thetas'
loglikelihood <- function(thetas, ys, ...) {</pre>
    n <- length(ys)
    evals <- rep(0, nrow(thetas))
    for (itheta in 1:nrow(thetas)) {
        11 \leftarrow function(ys, h = 1e-05, tolerance = 1e-10) {
            all_ys <- c(ys - h, ys + h) # for finite difference differentiation
            o <- order(all ys)
            x <- rep(0, length(all ys))
            x[o[1]] \leftarrow gandk\_cdf(y = all\_ys[o[1]], theta = thetas[itheta,],
                 tolerance = tolerance)
            for (i in 2:length(all_ys)) {
                 x[o[i]] <- gandk_cdf(y = all_ys[o[i]], theta = thetas[itheta,
                   ], tolerance = tolerance, lower = x[o[i - 1]])
            }
            return(sum(log((x[(n + 1):(2 * n)] - x[1:n])/(2 * h))))
        }
        evals[itheta] <- 11(ys)
    return(evals)
}
```

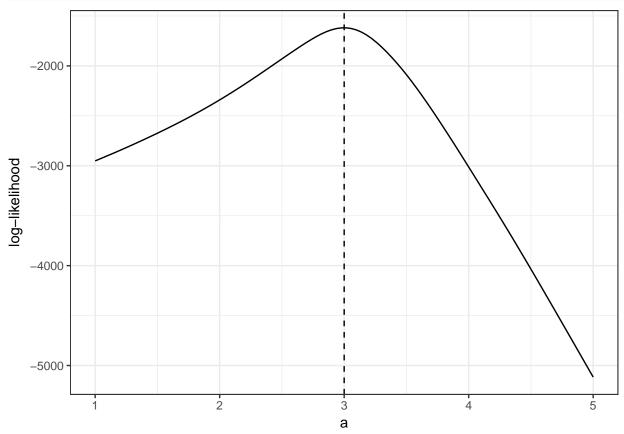
Define the model, and generate some data.

We can now plot the likelihood of the observations, e.g. as follows, as a function of a, the other parameters

being fixed.

```
nthetas <- 100
thetas <- matrix(nrow = nthetas, ncol = 4)
as <- seq(from = 1, to = 5, length.out = nthetas)
lls <- rep(0, nthetas)
for (i in 1:nthetas) {
    thetas[i, ] <- theta_star
    thetas[i, 1] <- as[i]
}
lls <- loglikelihood(thetas, obs)

qplot(x = as, y = lls, geom = "line") + geom_vline(xintercept = theta_star[1],
    linetype = 2) + xlab("a") + ylab("log-likelihood")</pre>
```



We can perform MCMC, as follows. This might take a few minutes.

```
g2 <- ggplot(chain.df %>% filter(iteration > burnin, iteration%%10 == 1), aes(x = iteration,
    y = X.2, group = ichain)) + geom_line() + geom_hline(yintercept = theta_star[2],
    col = "red", linetype = 2)
g3 <- ggplot(chain.df %>% filter(iteration > burnin, iteration%%10 == 1), aes(x = iteration,
    y = X.3, group = ichain)) + geom_line() + geom_hline(yintercept = theta_star[3],
    col = "red", linetype = 2)
g4 <- ggplot(chain.df %>% filter(iteration > burnin, iteration%%10 == 1), aes(x = iteration,
    y = X.4, group = ichain)) + geom_line() + geom_hline(yintercept = theta_star[4],
    col = "red", linetype = 2)
grid.arrange(g1, g2, g3, g4, ncol = 2)
   3.10
                                                  1.2
   3.05
                                                  1.1
₹ 3.00
   2.95
                                                  0.9
   2.90
                  4000
                              6000
                                         8000
                                                                 4000
       2000
                                                     2000
                                                                             6000
                                                                                         8000
                      iteration
                                                                     iteration
   2.3
                                                  0.6
ლ
× 2.1
                                                  0.5
      2000
                  4000
                              6000
                                         8000
                                                     2000
                                                                 4000
                                                                             6000
                                                                                         8000
                      iteration
                                                                     iteration
```

Finally we can run the WABC approach and compare to the posterior. We run the method for 3 minutes, and plot the resulting marginal approximations of the posteriors.

```
# sort observations
obs_sorted <- sort(obs)
# function to compute distance between observed data and data generated
# given theta this corresponds to the 1-Wasserstein distance
compute_d <- function(y_fake, metric = metricL2) {
    y_fake_sorted <- sort(y_fake)
    return(mean((abs(obs_sorted - y_fake_sorted))))
}
# algorithmic parameters
param_algo <- list(nthetas = 1024, nmoves = 1, proposal = mixture_rmixmod(),
    minimum_diversity = 0.5, R = 2, maxtrials = 1e+05)
results <- wsmc(compute_d, target, param_algo, maxtime = 3 * 60)</pre>
```

```
# let's look at the marginal distributions
wsmc.df <- wsmc_to_dataframe(results)</pre>
nsteps <- length(results$thetas_history)</pre>
g1 <- ggplot(chain.df %% filter(iteration > burnin), aes(x = X.1))
g1 <- g1 + geom_density(aes(y = ..density.., fill = "Posterior"), alpha = 0.5)
g1 <- g1 + geom_density(data = wsmc.df %>% filter(step == nsteps), aes(x = a,
    y = ..density.., fill = "WABC"), alpha = 0.5)
g1 <- g1 + scale_fill_manual(name = "", values = c(Posterior = "black", WABC = "darkblue"))
g1 <- g1 + xlab(expression(a)) + geom_vline(xintercept = theta_star[1])</pre>
g2 <- ggplot(chain.df %>% filter(iteration > burnin), aes(x = X.2))
g2 <- g2 + geom_density(aes(y = ..density.., fill = "Posterior"), alpha = 0.5)
g2 <- g2 + geom_density(data = wsmc.df %% filter(step == nsteps), aes(x = b,
    y = ..density.., fill = "WABC"), alpha = 0.5)
g2 <- g2 + scale_fill_manual(name = "", values = c(Posterior = "black", WABC = "darkblue"))
g2 <- g2 + xlab(expression(b)) + geom_vline(xintercept = theta_star[2])</pre>
g3 <- ggplot(chain.df %>% filter(iteration > burnin), aes(x = X.3))
g3 <- g3 + geom_density(aes(y = ..density.., fill = "Posterior"), alpha = 0.5)
g3 <- g3 + geom_density(data = wsmc.df %% filter(step == nsteps), aes(x = g,
    y = ..density.., fill = "WABC"), alpha = 0.5)
g3 <- g3 + scale_fill_manual(name = "", values = c(Posterior = "black", WABC = "darkblue"))
g3 <- g3 + xlab(expression(g)) + geom_vline(xintercept = theta_star[3])
g4 <- ggplot(chain.df %>% filter(iteration > burnin), aes(x = X.4))
g4 <- g4 + geom_density(aes(y = ..density.., fill = "Posterior"), alpha = 0.5)
g4 <- g4 + geom density(data = wsmc.df %>% filter(step == nsteps), aes(x = k,
    y = ..density.., fill = "WABC"), alpha = 0.5)
g4 <- g4 + scale_fill_manual(name = "", values = c(Posterior = "black", WABC = "darkblue"))
g4 <- g4 + xlab(expression(k)) + geom_vline(xintercept = theta_star[4])
grid.arrange(g1, g2, g3, g4, ncol = 2)
```

