Adaptive Rejection Sampling

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General Methodology

Code

Helper Functions

```
calc_s_j <- function (m, b, z) {</pre>
  ## Calculate beta values and weights
  ## needed to sample from u(x)
  ##
  ## Arguments
  ## m, b: slope/offset for piecewise u_j(x)
  ## z: bounds z_j for piecewise function u_j(x)
  ## Value (list)
  ## beta: amplitude of each piecewise segment in u(x)=beta*exp(m*x)
  ## w: area of each segment
 L <- length(z)
  eb <- exp(b) # un-normalized betas</pre>
  eb <- ifelse(is.finite(eb), eb, 0.0) # Inf/Nan -> 0
  ## treat m=0 case
  nz < (m != 0.0)
  nz_sum \leftarrow sum((eb[nz]/m[nz])*(exp(m[nz]*z[2:L][nz]) - exp(m[nz]*z[1:L-1][nz])))
  z_{sum} \leftarrow sum(eb[!nz]*(z[2:L][!nz] - z[1:L-1]))
  ## Normalize beta
  beta <- eb/(nz_sum + z_sum)
  ## Calculate weights for both m!=0 and m=0 cases
  w \leftarrow ifelse(nz, (beta/m)*(exp(m*z[2:L]) - exp(m*z[1:L-1])), beta*(z[2:L] - z[1:L-1]))
 return (list(beta = beta, w = ifelse((w > 0) & is.finite(w), w, 0.0)))
calc_z_j <- function (x, h, dh, bounds) {</pre>
 ## Calculate intercepts of piecewise u_j(x)
  ##
  ## Arguments
  ## x, h, dh: evaluated x, h(x) and h'(x)
  ## bounds: bounds of distribution h(x)
  ##
  ## intercepts (bounds) of piecewise u_j(x)
 L <- length(h)
```

```
z \leftarrow (h[2:L] - h[1:L-1] - x[2:L]*dh[2:L] + x[1:L-1]*dh[1:L-1])/(dh[1:L-1] - dh[2:L])
 return (append(bounds[1], append(z, bounds[2])))
}
calc_u <- function (x, h, dh) {</pre>
 ## Calculate slope/intercept for piecewise u_j(x)
 ## Arguments
  ## x, h, dh: evaluated x, h(x), and h'(x)
 ## Value (list)
 ## m, b: slope/intercept of u(x)
 return (list(m = dh, b = h - x*dh))
}
calc_l <- function (x, h) {</pre>
  ## Calculate slope/intercept for piecewise l_j(x)
  ## Arguments
  ## x, h: evaluated x, and h(x)
 ## Value (list)
 ## m, b: slope/intercept of l(x)
 L <- length(h)
 m \leftarrow (h[2:L] - h[1:L-1])/(x[2:L] - x[1:L-1])
 b \leftarrow (x[2:L]*h[1:L-1] - x[1:L-1]*h[2:L])/(x[2:L] - x[1:L-1])
 return (list(m = m, b = b))
}
draw_x <- function (N, beta, m, w, z) {</pre>
  ## Sample from distribution u(x), by selecting segment j
       based on segment areas (probabilities), and then sample
  ##
       from exponential distribution within segment using
  ##
       inverse CDF sampling.
  ##
  ## Arguments
  ## N: number of samples
  ## beta, m, w: parameters of u_j(x)
  ## z: intercepts (bounds) of u_j(x)
  ##
  ## Value (list)
  ## x: samples from u(x)
 ## J: segment index j of each sample
  J <- sample(length(w), N, replace = TRUE, prob = w) # choose random segments with probability w
  u <- runif(N) # uniform random samples</pre>
  ## Inverse CDF sampling of x
  x \leftarrow ifelse(m[J] != 0, (1.0/m[J])*log((m[J]*w[J]/beta[J])*u + exp(m[J]*z[J])), z[J] + w[J]*u/beta[J])
```

```
return (list(x = x, J = J))
}
```

Main Function

```
ars <- function (f, N, x0 = c(-1.0, 1.0), bounds = c(-Inf, Inf), ...) {
 ## Input sanity check
 if (!is.function(f)) {
    stop('f is not a function.')
 if (length(bounds) != 2) {
    stop('Length of bounds must be 2! (upper and lower bounds required)')
  if (bounds[1] == bounds[2]) {
    warning('Same upper and lower bounds, replacing them by default: bounds=c(-Inf, Inf)')
    bounds <- c(-Inf, Inf)</pre>
  }
  if (!all((x0 > bounds[1]) & (x0 < bounds[2]))) {</pre>
    stop('Bad inputs: x0 must be inside bounds.')
  }
  ## define h(x) = log(f(x))
 h <- function(x) {
   return (log(f(x, ...)))
  }
  ## helper variables
  dx \leftarrow 1E-8 # mesh size for finite difference approximation to h'(x)
  max_iters <- 10000 # prevent infinite loop</pre>
  current_iter <- 0</pre>
  bds_warn <- FALSE # Flag for boundary warning in main while loop
  ## initialize vectors
  x0 <- sort(x0) # Ensures x0 is in ascending order
  x_j <- c() # evaluated x values
  h_j \leftarrow c() # evaluated h(x) values
  dh_j <- c() # evaluated h'(x) values
  x <- c() # accepted sample vector
  ## compute/check h(x0)
 h0 \leftarrow h(x0)
  x0 <- x0[is.finite(h0)]</pre>
 h0 <- h0[is.finite(h0)]</pre>
  ## Error if no good x0 values
  if (length(h0) == 0) {
   stop('h(x0) either infinite or NaN.')
```

```
}
## compute h'(x0)
##
## normalizing h(x0) values gives better accuracy
## in finite difference approximation to h'(x)
avg <- mean(h0)
if (abs(avg) < dx) {</pre>
  avg <- 1.0
## Finite difference approximation to h'(x)
dh0 \leftarrow avg*((h(x0 + dx)/avg) - (h0/avg))/dx
## ARS requires either finite bounds or at least
## one positive and one negative derivative
if (!(dh0[1] > 0 || is.finite(bounds[1]))) {
  stop('dh(x0)/dx must have at least one positive value, or left bound must be greater than -infinity
}
if (!(dh0[length(dh0)] < 0 || is.finite(bounds[2]))) {</pre>
  stop('dh(x0)/dx must have at least one negative value, or right bound must be less than infinity.')
##### MAIN LOOP #####
## Loop until we have N samples (or until error)
while (length(x) < N) {
  ## Track iterations, 10000 is arbitrary upper bound
  current_iter <- current_iter + 1</pre>
  if (current_iter > max_iters) {
    stop('Maximum number of iterations reached.')
  ## Vectorized sampling in chunks
  ## Chunk size will grow as square of iteration,
  ## up until it is the size of the sample (\mathbb{N})
  ## This ensures small samples at first, while
  ## u(x) is a poor approximation of h(x), and
  ## large samples when the approximation improves.
  chunk_size <- min(c(N, current_iter**2))</pre>
  ##### INITIALIZATION AND UPDATING STEP #####
  ## only re-initialize if there are new samples
  if (length(x0) > 0) {
    ## Update with new values
    x_j \leftarrow append(x_j, x0)
```

```
h_j <- append(h_j, h0)</pre>
  dh_j <- append(dh_j, dh0)</pre>
  x0 <- c()
  h0 < -c()
  dh0 <- c()
  ## Sort so that x_j's are in ascending order
  srtd <- sort(x_j, index.return = TRUE)</pre>
  x_j <- srtd$x
  h_j <- h_j[srtd$ix]</pre>
  dh_j <- dh_j[srtd$ix]</pre>
  L <- length(dh_j)
  ## Check for duplicates in x and h'(x)
  ## This prevents discontinuities when
  ## computing z_j's
  while (!all(((dh_j[1:L-1] - dh_j[2:L]) > dx) & ((x_j[2:L] - x_j[1:L-1]) > dx))) {
    ## Only keep values with dissimilar neighbors
    ## Always keep first index (one is always unique)
    dup \leftarrow append(TRUE, (((dh_j[1:L-1] - dh_j[2:L]) > dx) & ((x_j[2:L] - x_j[1:L-1]) > dx)))
    x_j \leftarrow x_j[dup]
    h_j \leftarrow h_j[dup]
    dh_j <- dh_j[dup]
    L <- length(dh_j)
    if (L == 1) {
      break
    }
  }
  ## Ensure log-concavity of function
  if(!all(dh_j[2:L] \leftarrow dh_j[1:L-1])) {
    stop('Input function f not log-concave.')
  ## pre-compute z_j, u_j(x), l_j(x), s_j(x)
  z_j \leftarrow calc_z_j(x_j, h_j, dh_j, bounds)
  u_j \leftarrow calc_u(x_j, h_j, dh_j)
  m_u <- u_j$m
  b_u <- u_j$b
  l_j \leftarrow calc_l(x_j, h_j)
  m_1 <- 1_j$m
  b_1 <- 1_j$b
  s_j \leftarrow calc_s_j(m_u, b_u, z_j)
  beta_j <- s_j$beta
  w_j <- s_j$w
}
```

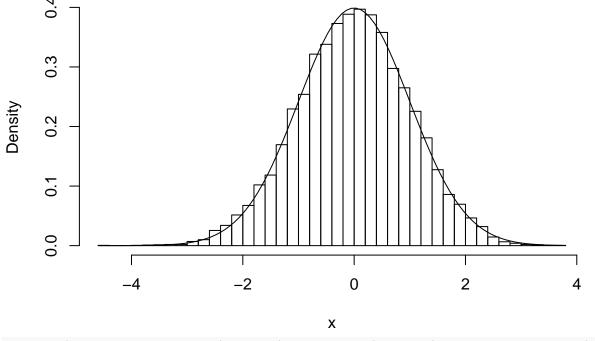
```
##### SAMPLING STEP #####
## draw x from exp(u(x))
draws <- draw_x(chunk_size, beta_j, m_u, w_j, z_j)</pre>
x s <- draws$x
J <- draws$J
## random uniform for rejection sampling
w <- runif(chunk_size)</pre>
## Warn if samples were outside of bounds
## This happens if bounds given don't reflect
## the actual bounds of the distribution
if (!all((x_s > bounds[1]) & (x_s < bounds[2]))) {</pre>
  ## Flag so warning only happens once
  if (!bds_warn) {
    warning('Sampled x* not inside bounds...please check bounds.')
    bds_warn <- TRUE
  ## Only keep x values within bounds
  ibd <- ((x_s > bounds[1]) & (x_s < bounds[2]))
  J \leftarrow J[ibd]
  x s \leftarrow x s[ibd]
  w <- w[ibd]
## Index shift for l_j(x)
J_1 \leftarrow J - ifelse(x_s < x_j[J], 1, 0)
## only use x-values where l_j(x) > -Inf
ibd <- (J_1 \ge 1) & (J_1 < length(x_j))
## Perform first rejection test on u(x)/1(x)
y \leftarrow \exp(x_s[ibd]*(m_1[J_1[ibd]) - m_u[J[ibd]]) + b_1[J_1[ibd]] - b_u[J[ibd]])
acc \leftarrow (w[ibd] \leftarrow y)
## Append accepted values to x
x <- append(x, x_s[ibd][acc])</pre>
## Append rejected values to x0
x0 <- append(x_s[!ibd], x_s[ibd][!acc])</pre>
if (length(x0) > 0) {
  ## Evaluate and check h(x0)
  h0 \leftarrow h(x0)
  isnum <- is.finite(h0)</pre>
  ## Cut to finite values
  x0 <- x0[isnum]
  h0 <- h0[isnum]
  w <- append(w[!ibd], w[ibd][!acc])[isnum]</pre>
  J <- append(J[!ibd], J[ibd][!acc])[isnum]</pre>
```

```
## compute h'(x0)
    ##
    ## normalizing h(x0) values gives better accuracy
    ## in finite difference approximation to h'(x)
    avg <- mean(h0)</pre>
    if (abs(avg) < dx) {</pre>
      avg <- 1.0
    ## Finite difference approximation to h'(x)
    dh0 \leftarrow avg*((h(x0 + dx)/avg) - (h0/avg))/dx
    ## Perform second rejection test on u(x)/h(x)
    acc \leftarrow (w \leftarrow exp(h0 - x0*m_u[J] - b_u[J]))
    ## Append accepted values to x
    x <- append(x, x0[acc])</pre>
  }
}
## Only return N samples (vectorized operations makes x sometimes larger)
return (x[1:N])
```

Example Usage

```
x <- ars(dnorm, 10000)
hist(x, breaks = 50, freq = FALSE)
xr <- seq(min(x), max(x), length = 100)
lines(xr, dnorm(xr))</pre>
```

Histogram of x



```
x <- ars(dgamma, 10000, x0 = c(0.1, 2.5), bounds = c(0.0, Inf), shape = 3, rate = 2)
hist(x, breaks = 50, freq = FALSE)
xr <- seq(min(x), max(x), length = 100)
lines(xr, dgamma(xr, shape = 3, rate = 2))</pre>
```

Histogram of x

