

Initialize Step (Step 1/3)

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Algorithm:

Inputs: $w \sim \text{Unif}(0,1)$

$l_k(x^*) = \log(g_l(x^*))$

$u_k(x^*) = \log(g_u(x^*))$

$h(x^*) = \log(g(x^*))$

$s_k(x) = \exp(u_k(x)) / (\int_D u_k(x') dx') = g_u(x) / (\int_D g_u(x') dx')$

The lower bound of $h(x)$ is $l_k(x)$, which connects the values of function h on abscissas. The function of $l_k(x)$ between two consecutive abscissas x_j and x_{j+1} is $l_k(x) = \frac{(x_{j+1}-x)h(x_j) + (x-x_j)h(x_{j+1})}{x_{j+1}-x_j}$

Let T be the domain of abscissas, H be the domain of the realized function H at abscissas, H_prime be the domain of the realized first derivative of function H at abscissas.

$$h'(x) = \frac{d \log(g(x))}{dx} = \frac{g'(x)}{g(x)}$$

Step 1: If $w < \exp(l_k(x^*) - u_k(x^*))$

- Accept x^* when the condition is satisfied. Draw another x^* from $s_k(x)$

- Reject x^* when the condition is not satisfied.

Step 2: These two procedures can be done in parallel.

- Evaluate $h(x^*), h'(x^*)$. Update $l_k(x), u_k(x), s_k(x)$, which are now include x^* as an element. - Accept x^* if $w < \exp(h(x^*) - u_k(x^*))$. Otherwise, reject.

Example: Start with $g(x) = 3 \cdot N(0,1)$.

$$g(x) = \frac{3}{\sqrt{2\pi}} e^{-(x)^2/2}$$

```
#Create
#install.packages("Ryacas")
#install.packages("Deriv")
#install.packages("distr")
#install.packages("truncnorm")
library(truncnorm)
library(Ryacas)
library(Deriv)
```

```
##
```

```
## Attaching package: 'Deriv'
```

```
## The following object is masked from 'package:Ryacas':
```

```
##
```

```
## Simplify
```

```
#library(distr)
```

```
#####
```

```
#User supplied parameters
```

```
#User supplied g-function
```

```
g <- function(x){
```

```

sigma <- 1
mu <- 0
val <- 3/sqrt(2*pi*sigma^2)*exp(-(x-mu)^2/(2*sigma^2))
}

#Examples for function g
g(0)
g(1)
g(-1)

#Number of starting points
k_start=2

#Bounds for x
x.Bound=c(-Inf,Inf)

#####
#Test default deriv() function + Simplify() function
sigma <- 1
mu <- 0

x <- Sym("x")
f <- 1/sqrt(2*pi*sigma^2)*exp(-(x-mu)^2/(2*sigma^2))
#print(f)
dx <- eval(deriv(g(x),Sym("x"))); #Derivative of f in terms of x
print(dx)

## expression(-1.1968268412 * (exp(-x^2/2) * (2 * x))/2)
dxSimp <- Ryacas::Simplify(deriv(g(x),"x")) #Simplified version of derivative (collapse terms)...
print(dxSimp)

## expression(-2.3936536824 * (exp(-x^2/2) * x)/2)
s = deriv(~a^2,'a',func = T) #Create function s(a)=a^2
#s(5) #5^2

#####
#Internally created functions
g_d <- function(x){
  as.numeric(eval(Deriv(~g(X),"X")))
}
#h function
h <- function(x){
  log(g(x))
}

#Examples for function h
#h(1)
#h(-1)
#h(0)

#h' function
h_d <- function(X){

```

```

#print("X:")
#print(X)

#print("Original:")
#print(h(X))

#print("Derivative - deriv()")
#print(deriv(log(g(x)), "x"))

#print("Derivative - Deriv() Unevaluated")
#print(Deriv(~log(g(X)), "X"))

#print("Derivative - Deriv() Evaluated")
#print(eval(fun))
#deriv(log(g(x), 1))

#return(as.numeric(eval(Deriv(~log(g(X)), "X"))))
return(as.numeric(1/g(X)*eval(Deriv(~g(X), "X"))))
}

#Examples for function h'...
#h_d(0)
#h_d(-0.5)

#Initial function (main)
Initial <- function(k_start, x.Bound, g, QC=FALSE){
  #print(all.equal(x.Bound, c(-Inf, Inf)))

  upBd <- x.Bound[length(x.Bound)]
  lowBd <- x.Bound[1]
  if (lowBd != -Inf){
    needPosHprime <- FALSE
  } else{
    needPosHprime <- TRUE
  }
  if (upBd != Inf){
    needNegHprime <- FALSE
  } else{
    needNegHprime <- TRUE
  }
  upBdInit <- upBd #Upper bound for initialization points
  lowBdInit <- lowBd #Lower bound for initialization points
  if (0==1){

    if (QC==TRUE){
      print("Lower & upper bound pairs")
      print(lowBd)
      print(upBd)

      print(upBdInit)
      print(lowBdInit)
    }
  }
}

```

```

k <- 0
X <- c()

#print(paste0("Begin: Find initialization points"))
while (k < k_start){
  samp <- rtruncnorm(1,a=lowBdInit,b=upBdInit)
  hPrime <- h_d(samp)
  if (QC==TRUE){
    print(paste0("Initialization bounds: ",lowBdInit," ",upBdInit))
    print(paste0("Need positive / negative h'? ",needPosHprime," ",needNegHprime))

    print(paste0("Sampled point x: ",samp))
    print(paste0("h'(x): ",h_d(samp)))
  }

  if (hPrime >0 & needPosHprime==TRUE){
    needPosHprime <- FALSE
    X <- append(X,samp,length(X))
    k <- k+1
    #print(paste0("Appended X with h'(X) > 0"))

    if (needNegHprime==TRUE) {
      lowBdInit <- samp
      #print(paste0("Changed lower initialization bound to sampled point"))
    }
    else {
      lowBdInit <- lowBd
      #print(paste0("Changed lower initialization bound to distribution lower bound"))
    }
  }
  else if (hPrime < 0 & needNegHprime==TRUE) {
    needNegHprime <- FALSE
    X <- append(X,samp,0)
    k <- k+1
    #print(paste0("Appended X with h'(X) < 0"))

    if (needPosHprime == TRUE) {
      upBdInit <- samp
      #print(paste0("Changed upper initialization bound to sampled point"))
    }
    else {
      upBdInit <- upBd
      #print(paste0("Changed upper initialization bound to distribution upper bound"))
    }
  }
  else if (k < (k_start-needPosHprime-needNegHprime)){
    X <- append(X,samp,length(X[X<samp]))
    k <- k+1
    #print(paste0("Appended X; no h' requirements met"))
  }
  else {

```

```

        #print(paste0("Sampled point does not satisfy any initialization requirements. Sample again. "))
    }
}
#print(paste0("Finished: Find initialization points"))

H <- h(X)
H_d <- h_d(X)
Z <- c(lowBd, upBd)
return(list(X, H, H_d, Z))
}

```

Normal distribution (2 starting pts)

```

#User supplied g-function
g <- function(x){
  sigma <- 1
  mu <- 0
  val <- 3/sqrt(2*pi*sigma^2)*exp(-(x-mu)^2/(2*sigma^2))
}

Initial(k_start=2, x.Bound=c(-Inf, Inf), g
        #, QC=TRUE
        )

```

```

## [[1]]
## [1] 2.4119015 -0.1000012
##
## [[2]]
## [1] -2.7289608 0.1746736
##
## [[3]]
## [1] -2.4119015 0.1000012
##
## [[4]]
## [1] -Inf Inf

```

```

system.time(Initial(k_start=2, x.Bound=c(-Inf, Inf), g
        #, QC=TRUE
        ))

```

```

## user system elapsed
## 0.287 0.003 0.305

```

Exponential distribution (2 starting pts)

```

g <- function(x){
  lam <- 1
  value <- lam*exp(-lam*x)
}

```

```

#a <- AbscontDistribution(d=g,low=0,low1=0)
#print(g(1))
Initial(k_start=2,x.Bound=c(0,Inf),g
      #,QC=TRUE
      )

```

```

## [[1]]
## [1] 0.8800005 1.1956156
##
## [[2]]
## [1] -0.8800005 -1.1956156
##
## [[3]]
## [1] -1 -1
##
## [[4]]
## [1] 0 Inf

```

Normal distribution (5 starting pts)

```

#User supplied g-function
g <- function(x){
  sigma <- 1
  mu <- 0
  val <- 3/sqrt(2*pi*sigma^2)*exp(-(x-mu)^2/(2*sigma^2))
}
Initial(k_start=5,x.Bound=c(-Inf,Inf),g
      #,QC=TRUE
      )

```

```

## [[1]]
## [1] 0.07065779 -1.46264688 -0.66467338 -0.56187684 0.33905853
##
## [[2]]
## [1] 0.17717749 -0.88999420 -0.04122160 0.02182096 0.12219341
##
## [[3]]
## [1] -0.07065779 1.46264688 0.66467338 0.56187684 -0.33905853
##
## [[4]]
## [1] -Inf Inf

```

```

print(system.time(Initial(k_start=5,x.Bound=c(-Inf,Inf),g
      #,QC=TRUE
      )))

```

```

## user system elapsed
## 0.484 0.035 0.587

```

Gamma distribution (5 starting pts)

```
#User supplied g-function
g <- function(x){
  alpha <- 1
  beta <- 1
  val <- beta^alpha/gamma(alpha)*x^(alpha-1)*exp(-beta*x)
}

Initial(k_start=5,x.Bound=c(0,Inf),g
      #,QC=TRUE
      )
```

```
## [[1]]
## [1] 0.3903494 0.5107521 0.5438679 0.9327843 2.2745782
##
## [[2]]
## [1] -0.3903494 -0.5107521 -0.5438679 -0.9327843 -2.2745782
##
## [[3]]
## [1] -1 -1 -1 -1 -1
##
## [[4]]
## [1] 0 Inf
```

Beta distribution (10 starting pts)

```
#User supplied g-function
g <- function(x){
  alpha <- 1
  beta <- 3
  val <- x^(alpha-1)*(1-x)^(beta-1)/(gamma(alpha)*gamma(beta)/gamma(alpha+beta))
}

Initial(k_start=10,x.Bound=c(0,1),g
      #,QC=TRUE
      )
```

```
## [[1]]
## [1] 0.06867557 0.07863842 0.21166391 0.21881569 0.33182613 0.37132615
## [7] 0.71521893 0.73841366 0.77456309 0.91411376
##
## [[2]]
## [1] 0.9563171 0.9348068 0.6229507 0.6047240 0.2921986 0.1703269
## [7] -1.4134568 -1.5833695 -1.8808176 -3.8108511
##
## [[3]]
## [1] -2.147479 -2.170700 -2.536989 -2.560215 -2.993233 -3.181300
## [7] -7.022939 -7.645659 -8.871662 -23.286618
##
## [[4]]
## [1] 0 1
```

```
system.time(Initial(k_start=10,x.Bound=c(0,1),g
  #,QC=TRUE
))
```

```
##      user  system elapsed
## 0.838   0.015   0.879
```