## GENERALIZED LINEAR DENSITY RATIO MODEL (GLDRM) WITH FREQUENCY WEIGHTS

## ANIKO SZABO

The code is based on the gldrm package, with minor changes to incorporate frequency weights. The code is simplified a bit as well by removing some options:

- sampling weights are removed
- there is no variance/standard error calculation, and no inference against the null
- "../R/wgldrm.R"  $1 \equiv$

```
#' Main optimization function
ж,
#' This function is called by the main \code{gldrm} function.
#' @keywords internal
#' @importFrom stats lm.fit lm.wfit weighted.mean
gldrm.control <- function(eps=1e-10, maxiter=100, returnfTiltMatrix=TRUE,</pre>
                           returnfOScoreInfo=FALSE, print=FALSE,
                           betaStart=NULL, fOStart=NULL)
{
    gldrmControl <- as.list(environment())</pre>
    class(gldrmControl) <- "gldrmControl"</pre>
    gldrmControl
}
gldrmFit <- function(x, y, linkfun, linkinv, mu.eta, mu0=NULL, offset=NULL, weights=NULL,
                      gldrmControl=gldrm.control(), thetaControl=theta.control(),
                      betaControl=beta.control(), f0Control=f0.control())
{
    ## Extract control arguments
    if (class(gldrmControl) != "gldrmControl")
        stop("gldrmControl must be an object of class \'gldrmControl\' returned by
               gldrmControl() function.")
    eps <- gldrmControl$eps</pre>
    maxiter <- gldrmControl$maxiter</pre>
    returnfTiltMatrix <- gldrmControl$returnfTiltMatrix</pre>
    returnf0ScoreInfo <- gldrmControl$returnf0ScoreInfo</pre>
    print <- gldrmControl$print</pre>
    betaStart <- gldrmControl$betaStart</pre>
    f0Start <- gldrmControl$f0Start</pre>
    ## Tabulation and summary of responses used in estimating f0
    n <- length(y)</pre>
    spt <- sort(unique(y)) # observed support</pre>
    ySptIndex <- match(y, spt) # index of each y value within support
    # sptFreq <- table(ySptIndex)</pre>
    # attributes(sptFreq) <- NULL</pre>
    # create a weight matrix for score.logT1 calculation
    weightsMatrix <- matrix(0, nrow=n, ncol=length(spt))</pre>
```

Date: December 23, 2021.

```
weightsMatrix[cbind(1:n, ySptIndex)] <- weights</pre>
# weighted version of "sptFreq"
sptFreq.weighted <- colSums(weightsMatrix)</pre>
## Initialize offset
if (is.null(offset))
    offset <- rep(0, n)
## Initialize muO if not provided by user
if (is.null(mu0)) {
   mu0 <- weighted.mean(y, weights)</pre>
} else if (mu0<=min(spt) || mu0>=max(spt)) {
    stop(pasteO("muO must lie within the range of observed values. Choose a different ",
                "value or set mu0=NULL to use the default value, weighted.mean(v,weights)."))
}
## Initialize f0
if (is.null(fOStart)) {
  # weighted version of initial value for baseline distribution
    f0 <- sptFreq.weighted / sum(sptFreq.weighted)</pre>
    if (mu0 != weighted.mean(y,weights))
        f0 <- getTheta(spt=spt, f0=f0, mu=mu0, weights=weights, ySptIndex=1, thetaStart=0,
                        thetaControl=thetaControl)$fTilt[, 1]
} else {
    if (length(fOStart) != length(spt))
        stop("Length of fOStart should equal number of unique values in the response.")
    if (any(fOStart <= 0))</pre>
        stop("All values in fOStart should be strictly positive.")
    f0 <- f0Start / sum(f0Start)</pre>
    f0 <- getTheta(spt=spt, f0=f0, mu=mu0, weights=weights, ySptIndex=1, thetaStart=0,
                   thetaControl=thetaControl)$fTilt[, 1]
}
## Initialize beta
## The starting values returned by lm.fit guarantee that all mu values are
## within the support range, even if there is no intercept.
## Offset could still create problems.
lmcoef <- stats::lm.wfit(x=x, y=linkfun(mu0) - offset, weights)$coef</pre>
if (is.null(betaStart)) {
    beta <- lmcoef
} else {
    if (length(betaStart) != ncol(x))
        stop("Length of betaStart should equal the number of columns in the model matrix.")
 beta <- betaStart
}
## Drop coefficients if x is not full rank (add NA values back at the end)
naID <- is.na(lmcoef)</pre>
beta <- beta[!naID]</pre>
x <- x[, !naID, drop=FALSE]</pre>
eta <- c(x %*% beta + offset)
mu <- linkinv(eta)</pre>
if (ncol(x) >= n)
stop("gldrm requires n > p.")
if (any(mu<min(spt) | mu>max(spt)))
stop("Unable to find beta starting values that do not violate convex hull condition.")
## Get initial theta and log likelihood
```

```
th <- getTheta(spt=spt, f0=f0, mu=mu, weights=weights, ySptIndex=ySptIndex,
               thetaStart=NULL, thetaControl=thetaControl)
llik <- th$llik
conv <- FALSE
iter <- 0
while (!conv && iter <= maxiter)</pre>
    iter <- iter+1
    betaold <- beta
    f0old <- f0
    llikold <- llik
    ## update beta (mu) and theta, with fixed f0:
    bb <- getBeta(x=x, y=y, spt=spt, ySptIndex=ySptIndex, f0=f0,
                  linkinv=linkinv, mu.eta=mu.eta, offset=offset, weights=weights,
                  betaStart=beta, thStart=th,
                  thetaControl=thetaControl, betaControl=betaControl)
    th <- bb$th
    llik <- bb$llik
    mu <- bb$mu
    beta <- bb$beta
    ## update f0 and theta, with fixed beta (mu)
    ff <- getf0(y=y, spt=spt, ySptIndex=ySptIndex,</pre>
                weights-weights, sptFreq.weighted=sptFreq.weighted, mu=mu, mu0=mu0, f0Start=f0, thSta
                thetaControl=thetaControl, fOControl=fOControl, trace=FALSE)
    th <- ff$th
    llik <- ff$llik
    f0 <- ff$f0
    ## Check convergence
    del <- abs((llik - llikold) / llik)
    if (llik == 0) del <- 0
    conv <- del < eps
    if (print) {
        cat("iteration ", iter,
            "\nrelative change in log-likelihood = ", del,
            " (eps = ", eps, ")\n")
    }
}
## Final values
eta <- linkfun(mu)</pre>
dmudeta <- mu.eta(eta)</pre>
llik <- ff$llik
theta <- th$theta
bPrime <- th$bPrime
bPrime2 <- th$bPrime2
fTilt <- th$fTilt[cbind(ySptIndex, seq_along(ySptIndex))]</pre>
## Add NA values back into beta vector and varbeta if covariate matrix is not full rank
nBeta <- length(beta) + sum(naID)</pre>
betaTemp <- rep(NA, nBeta)</pre>
betaTemp[!naID] <- beta</pre>
beta <- betaTemp
```

4

```
## Return gldrm object
              attributes(beta) <- NULL
              attributes(f0) <- NULL
              fit <- list(conv=conv, iter=iter, llik=llik,</pre>
                           beta=beta, mu=mu, eta=eta, f0=f0, spt=spt, mu0=mu0,
                           theta=theta, bPrime=bPrime, bPrime2=bPrime2, fTilt=fTilt, weights=weights)
              if (returnfTiltMatrix)
                  fit$fTiltMatrix <- t(th$fTilt)</pre>
              if (returnf0ScoreInfo) {
                  fit$score.logf0 <- ff$score.log</pre>
                  fit$info.logf0 <- ff$info.log</pre>
              class(fit) <- "gldrm"</pre>
              fit
          }
File defined by 1, 4, 6, 11.
"../R/wgldrm.R" 4\equiv
          #' Beta optimization routing
          #,
          #' Oparam x Covariate matrix.
          #' @param y Response vector.
          #' Cparam spt Vector of unique observed support points in the response.
          #' @param ySptIndex Index of each \code{y} value within the \code{spt} vector.
          #' @param f0 Current values of f0.
          #' Oparam linkinv Inverse link function.
          #' @param mu.eta Deriviative of inverse link function.
          #' Oparam offset Vector of known offset values to be added to the linear
          #' combination (x' beta) for each observation. Mostly intended for likelihood ratio
          #' and score confidence intervals.
          #'@param sampprobs Optional matrix of sampling probabilities.
          #'@param betaStart Starting values for beta (typically the estimates from the
          #' previous iteration).
          #'@param thStart Starting theta values. Needs to be a list of values matching
          #' the output of the \code{getTheta} function.
          #'@param thetaConrol A "thetaControl" object returned from the \code{theta.control}
          #' function.
          #'@param betaControl A "betaControl" object returned from the \code{beta.control}
          #' function.
          #' Oreturn A list containing the following:
          #' \itemize{
          #' \item \code{beta} Updated values.
          #' \item \code{mu} Updated mean for each observation.
          #' \item \code{th} Updated list returned from the \code{getTheta} function.
          #' \item \code{llik} Updated log-likelihood.
          #' \item \code{iter} Number of iterations until convergence. (Will always be
          #' one unless \code{maxiter} is increased to something greater than one using the
          #' \code{betaControl} argument.)
          #' \item \code{conv} Convergence indicator. (Will always be FALSE unless
          \mbox{\tt\#'}\ \mbox{\tt \code}\{\mbox{\tt maxiter}\} is increased to something greater than one using the
          #' \code{betaControl} argument.)
```

```
#'}
#'
#' @keywords internal
beta.control <- function (eps = 1e-10, maxiter = 1, maxhalf = 10)
    betaControl <- as.list(environment())</pre>
    class(betaControl) <- "betaControl"</pre>
    betaControl
}
getBeta <- function(x, y, spt, ySptIndex, f0, linkinv, mu.eta, offset, weights,</pre>
                     betaStart, thStart,
                     thetaControl=theta.control(), betaControl=beta.control())
{
    ## Extract control arguments
    if (class(betaControl) != "betaControl")
      stop("betaControl must be an object of class betaControl returned by betaControl() function.")
    eps <- betaControl$eps</pre>
    maxiter <- betaControl$maxiter</pre>
    maxhalf <- betaControl$maxhalf</pre>
    sptMin <- min(spt)</pre>
    sptMax <- max(spt)</pre>
    beta <- betaStart
    th <- thStart
    llik <- th$llik
    conv <- FALSE
    maxhalfreached <- FALSE
    iter <- 0
    while (!conv && !maxhalfreached && iter < maxiter)
    {
        iter <- iter+1
        ## Update mean vector and related quantities
        eta <- c(x %*% beta + offset)
        mu <- linkinv(eta)</pre>
        dmudeta <- mu.eta(eta)</pre>
        betaold <- beta
        muold <- mu
        thold <- th
        llikold <- llik
        ## Compute weighted least squares update
        w <- weights * dmudeta^2 / th$bPrime2</pre>
        ymm \leftarrow y - mu
        r <- ymm / dmudeta
        yeqmu <- which(abs(ymm) < 1e-15)</pre>
        w[yeqmu] <- 0 # prevent 0/0</pre>
        r[yeqmu] <- 0  # prevent 0/0
        if (any(w==Inf)) break
        betastep <- unname(coef(lm.wfit(x, r, w)))</pre>
        betastep[is.na(betastep)] <- 0</pre>
        ## Let q = b''*(theta) / b''(theta)
        ## W = diag{dmudeta^2 / b''(theta) * q}
```

```
## r = (y - b'*(theta)) / (q * dmudeta)
                  ## We need to solve for beta such that I(betaHat) %*% beta = Score(betaHat),
                  ## or equivalently, X'WX = X'Wr, or equivalently W^{1/2}X = W^{1/2}r.
                  ## The linear system can be solved using qr.coef().
                  ### Update beta and take half steps if log-likelihood does not improve
                  beta <- beta + betastep
                  eta <- c(x %*% beta + offset)
                  mu <- linkinv(eta)</pre>
                  if (min(mu)<sptMin || max(mu)>sptMax) {
                      llik <- -Inf
                  } else {
                      th <- getTheta(spt=spt, f0=f0, mu=mu, weights=weights, ySptIndex=ySptIndex,
                                      thetaStart=thold$theta, thetaControl=thetaControl)
                      llik <- th$llik
                  nhalf <- 0
                  while ((llik<llikold) && (nhalf<maxhalf)) {</pre>
                      nhalf <- nhalf + 1</pre>
                      beta <- (beta + betaold) / 2
                      eta <- c(x %*% beta + offset)
                      mu <- linkinv(eta)</pre>
                      if (min(mu)<sptMin || max(mu)>sptMax) {
                           llik <- -Inf
                      } else {
                           th <- getTheta(spt=spt, f0=f0, mu=mu, weights=weights, ySptIndex=ySptIndex,
                                          thetaStart=thold$theta, thetaControl=thetaControl)
                          llik <- th$llik
                      }
                  }
                  if (llik < llikold) {</pre>
                      beta <- betaold
                      mu <- muold
                      th <- thold
                      llik <- llikold
                      conv <- FALSE
                      maxhalfreached <- TRUE
                  } else {
                      del <- (llik - llikold) / llik
                      if (llik == 0) del <- 0 # consider converged if model fit is perfect
                      conv <- del < eps
                  }
              }
              return(list(beta=beta, mu=mu, th=th, llik=llik, iter=iter, conv=conv))
          }
File defined by 1, 4, 6, 11.
"../R/wgldrm.R" 6\equiv
          ## usethis namespace: start
          #' @useDynLib exchreg, .registration = TRUE
          #' @importFrom Rcpp sourceCpp
          ## usethis namespace: end
```

```
## Computes log(sum(exp(x))) with better precision
logSumExp <- function(x)</pre>
₹
    i <- which.max(x)</pre>
    m \leftarrow x[i]
    lse \leftarrow log1p(sum(exp(x[-i]-m))) + m
}
## g function (logit transformation from appendix)
g <- function(mu, m, M) log(mu-m) - log(M-mu)
#' Control arguments for \eqn{\theta} update algorithm
#'
#' This function returns control arguments for the \eqn{\theta} update algorithm.
#' Each argument has a default value, which will be used unless a different
#' value is provided by the user.
#'@param eps Convergence threshold for theta updates. Convergence is
#' evaluated separately for each observation. An observation has converged when
#' the difference between \eqn{b'(\theta)} and \eqn{\mu} is less than \code{epsTheta}.
#'@param maxiter Maximum number of iterations.
#'@param maxhalf Maximum number of half steps allowed per iteration if the
#' convergence criterion does not improve.
#'@param maxtheta Absolute value of theta is not allowed to exceed \code{maxtheta}.
#'@param logit Logical for whether logit transformation should be used. Use of
#' this stabilizing transformation appears to be faster in general. Default is TRUE.
#'@param logsumexp Logical argument for whether log-sum-exp trick should be used.
#' This may improve numerical stability at the expense of computational time.
#'
#' @return Object of S3 class "thetaControl", which is a list of control arguments.
#'
#' @keywords internal
theta.control <- function(eps=1e-10, maxiter=100, maxhalf=20, maxtheta=500,
                          logit=TRUE, logsumexp=FALSE)
{
    thetaControl <- as.list(environment())</pre>
    class(thetaControl) <- "thetaControl"</pre>
    thetaControl
}
#' getTheta
#' Updates theta. Vectorized but only updates observations that have not converged.
#'@param spt Support of the observed response variable. (This is the set of
#' unique values observed, not the set of all possible values.)
#'@param f0 Values of the baseline distribution corresponding to the values of spt
#'@param mu The fitted mean for each observation. Note these values must lie
#' strictly within the range of the support.
#'@param sampprobs Matrix of sampling probabilities. The number of rows should
#' equal the number of observations, and the number of columns should equal
#' the number of unique observed support points.
#'@param ySptIndex Vector containing index of each obervation's response value
#' within the \code{spt} vector. This is only needed to calculate the log-likelihood
#' after each update.
#'Oparam thetaStart Vector of starting values. One value per observation. If
#' \code{NULL}, zero is used as the starting value for each observation.
#'@param thetaControl Object of class \code{thetaControl}, which is a list of
#' control arguments returned by the \code{thetaControl} function.
```

```
#'
#' Oreturn List containing the following:
#' \itemize{
#' \item \code{theta} Updated values.
#' \item \code{fTilt} Matrix containing the exponentially tilted distribution for each
\#' observation, i.e. f(y|X=x). Each column corresponds to an observation and sums to one.
#' \item \code{bPrime} Vector containing the mean of the exponentially tilted distribution
#' for each observation. Should match \code{mu} argument very closely.
#' \item \code{bPrime2} Vector containing the variance of the exponentially tilted
#' distribution for each observation.
#' matches \code{bPrime2}.
#' \item \code{llik} Semiparametric log-likelihood, evaluated at the current beta
#' and f0 values. If sampling weights are used, then the log-likelihood is conditional
#' on each observation being sampled.
#' \item \code{conv} Convergence indicator.
#' \item \code{iter} Number of iterations until convergence was reached.
#'}
#'
#' @keywords internal
getTheta <- function(spt, f0, mu, weights, ySptIndex, thetaStart=NULL, thetaControl=theta.control())</pre>
    ## Extract control arguments
    if (class(thetaControl) != "thetaControl")
        stop("thetaControl must be an object of class \'thetaControl\' returned by
             thetaControl() function.")
    ## Define value from inputs
    sptN <- length(spt)</pre>
    m <- min(spt)
    M <- max(spt)
    n <- length(mu)
    ## Format arguments
    spt <- as.vector(spt)</pre>
    f0 <- as.vector(f0)</pre>
    mu <- as.vector(mu)</pre>
    if (!is.null(thetaStart)) {
        thetaStart <- as.vector(thetaStart)</pre>
    } else {
        thetaStart <- rep(0, n)
    ## Argument checks
    if (length(f0) != sptN)
        stop("spt and f0 must be vectors of equal length.")
    if (any(f0 < 0))
        stop("f0 values cannot be negative.")
    if (min(mu)<m || max(mu)>M)
        stop("mu starting values must lie within the range of spt.")
    if (length(thetaStart) != n)
        stop("thetaStart must be a vector with length equal length(mu)")
    res <- getThetaC(spt, f0, mu, thetaStart, thetaControl)</pre>
    ## Calculate log-likelihood
    fTilt.extracted <- res$fTilt[cbind(ySptIndex, seq_along(ySptIndex))]</pre>
    llik <- sum(weights[fTilt.extracted>0] * log(fTilt.extracted[fTilt.extracted>0]))
    list(theta=c(res$theta), fTilt=res$fTilt, bPrime=c(res$bPrime), bPrime2=c(res$bPrime2),
```

The computationally intensive part of getTheta is implemented in C++. For now, only the logsumexp = FALSE and logit = FALSE settings are implemented.

```
"../src/getTheta.cpp" 9\equiv
```

```
#include <RcppArmadillo.h>
using namespace Rcpp;
using namespace arma;
// [[Rcpp::depends(RcppArmadillo)]]
// Computes log(sum(exp(x))) with better precision
double logSumExp(arma::vec x){
 uword i = x.index_max();
 double m = x(i);
 x.shed_row(i);
 double lse = log1p(sum(exp(x-m))) + m;
 return lse;
}
// g function (logit transformation from appendix)
arma::vec g(arma::vec mu, double m, double M){
 arma::vec res = log(mu-m) - log(M-mu);
 return res;
}
// [[Rcpp::export]]
List getThetaC(arma::vec spt, arma::vec f0, arma::vec mu,
              arma::vec thetaStart, List thetaControl){
// bool logit = thetaControl["logit"];
 double eps = thetaControl["eps"];
 int maxiter = thetaControl["maxiter"];
 double maxhalf = thetaControl["maxhalf"];
 double maxtheta = thetaControl["maxtheta"];
// bool logsumexp = thetaControl["logsumexp"];
 int sptN = spt.size();
// double m = min(spt);
// double M = max(spt);
 int n = mu.size();
  //initialize values
  arma::vec theta = thetaStart:
 arma::vec thetaOld(n);
 arma::vec bPrimeErrOld(n);
 uvec conv(n, fill::zeros);
 uvec maxedOut(n, fill::zeros);
 arma::rowvec oo(sptN, fill::ones);
 mat fUnstd = exp(spt * theta.t());
 {\tt fUnstd.each\_col()} %= f0; // |spt| x n matrix of tilted f0 values
 rowvec b = oo * fUnstd; //column sums;
```

```
mat fTilt = fUnstd.each_row() / b; // normalized
 colvec bPrime = fTilt.t() * spt; \ // mean as a function of theta
 colvec bPrime2(n); // variance as a function of theta
 for (int j=0; j< n; j++){
                                //iterate over the columns of fTilt
   bPrime2(j) = 0;
   for (int i=0; i<sptN; i++){ //iterate over the rows of fTilt
     bPrime2(j) += pow(spt(i) - bPrime(j), 2.0) * fTilt(i,j);
 }
 colvec bPrimeErr = bPrime - mu; // used to assess convergence
 conv = (abs(bPrimeErr) < eps) || (theta==maxtheta && bPrimeErr<0) ||</pre>
     (theta==-maxtheta && bPrimeErr>0);
 uvec s = find(conv == 0);
 int iter = 0;
while(s.size() > 0 && iter < maxiter) {</pre>
   bPrimeErrOld(s) = bPrimeErr(s); // used to assess convergence
// 1) Update theta
   thetaOld(s) = theta(s);
   colvec thetaS = theta(s) - bPrimeErr(s) / bPrime2(s);
   thetaS(find(thetaS > maxtheta)).fill(maxtheta);
   thetaS(find(thetaS < -maxtheta)).fill(-maxtheta);</pre>
   theta(s)= thetaS;
// 2) Update fTilt, bPrime, and bPrime2 and take half steps if bPrimeErr not improved
   uvec ss = s;
   int nhalf = 0;
   while(ss.size() > 0 && nhalf < maxhalf) {</pre>
// 2a) Update fTilt, bPrime, and bPrime2
     fUnstd.cols(ss) = exp(spt * theta(ss).t());
     fUnstd.each\_col(ss) \ \%= \ f0; \ \ // \ |spt| \ x \ n \ matrix \ of \ tilted \ f0 \ values
     b = oo * fUnstd.cols(ss); //column sums;
     mat tmp = fUnstd.cols(ss);
     fTilt.cols(ss) = tmp.each_row() / b; // normalized
     bPrime(ss) = fTilt.cols(ss).t() * spt; // mean as a function of theta
     for (uword j=0; j<ss.size(); j++){</pre>
                                              //iterate over the columns of fTilt[,ss]
        bPrime2(ss(j)) = 0;
        for (int i=0; i<sptN; i++){ //iterate over the rows of fTilt[,ss]</pre>
          bPrime2(ss(j)) += pow(spt(i) - bPrime(ss(j)), 2.0) * fTilt(i,ss(j));
        }
      }
     bPrimeErr(ss) = bPrime(ss) - mu(ss);
// 2b) Take half steps if necessary
      ss = ss(find(abs(bPrimeErr(ss)) > abs(bPrimeErrOld(ss))));
      if (ss.size() > 0){
        nhalf++;
     theta(ss) = (theta(ss) + thetaOld(ss)) / 2;
// If maximum half steps are exceeded, set theta to previous value
   maxedOut(ss).fill(1);
   theta(ss) = thetaOld(ss);
```

```
// 3) Check convergence
              conv(s) = (abs(bPrimeErr(s)) < eps) || (theta(s)==maxtheta && bPrimeErr(s) < 0) ||</pre>
                (theta(s)==-maxtheta && bPrimeErr(s) > 0);
              s = s(find(conv(s) == 0 \&\& maxedOut(s) == 0));
           }
           List res;
           res["theta"] = theta;
           res["fTilt"] = fTilt;
           res["bPrime"] = bPrime;
           res["bPrime2"] = bPrime2;
           res["conv"] = conv;
           res["iter"] = iter;
           return res;
          0
"../R/wgldrm.R" 11\equiv
          #' Control arguments for f0 update algorithm
         #'
         #' This function returns control arguments for the \neq 0 update algorithm.
          #' Each argument has a default value, which will be used unless a different
          #' value is provided by the user.
          #'
         #'@param eps Convergence threshold. The update has converged when the relative
          #' change in log-likelihood between iterations is less than \code{eps}.
         #' absolute change is less than \code{thesh}.
          #'@param maxiter Maximum number of iterations allowed.
          #'@param maxhalf Maximum number of half steps allowed per iteration if
          #' log-likelihood does not improve between iterations.
          #'@param maxlogstep Maximum optimization step size allowed on the
          #' \code{log(f0)} scale.
          #,
          #' @return Object of S3 class "fOControl", which is a list of control arguments.
          #' @keywords internal
          f0.control <- function(eps=1e-10, maxiter=1000, maxhalf=20, maxlogstep=2)</pre>
              f0Control <- as.list(environment())</pre>
              class(f0Control) <- "f0Control"</pre>
              f0Control
          #' f0 optimization routine
          #'
          #'@param y Vector of response values.
          #'@param spt Vector of unique observed support points in the response.
          #'@param ySptIndex Index of each \code{y} value within \code{spt}.
          #'@param sptFreq.weighted Vector containing weighted frequency of each \code{spt} value.
          #'@param mu Fitted mean for each observation. Only used if \code{sampprobs=NULL}.
          #'Oparam muO Mean constraing for fO.
          #'@param fOStart Starting fO values. (Typically the estimate from the previous
          #' iteration.)
          #'@param thStart Starting theta values. Needs to be a list of values matching
```

```
#' the output of the \code{getTheta} function.
#'@param thetaControl A "thetaControl" object returned from the \code{theta.control}
#' function.
#'@param f0Control An "f0Control" object returned from the \code{f0.control}
#' function.
#' trace Logical. If TRUE, then progress is printed to terminal at each iteration.
#' Oreturn A list containing the following:
#' \itemize{
#' \item \code{f0} Updated values.
#' \item \code{llik} Updated log-likelihood.
#' \item \code{th} Updated list returned from the \code{getTheta} function.
#' \item \code{conv} Convergence indicator.
#' \item \code{iter} Number of iterations until convergence.
#' \item \code{nhalf} The number of half steps taken on the last iteration if the
#' initial BFGS update did not improve the log-likelihood.
#' \item \code{score.log} Score function with respect to log(f0) at convergence.
#' \item \code{info.log} Information matrix with respect to log(f0) at convergence.
#'}
#,
#' @keywords internal
getf0 <- function(y, spt, ySptIndex, weights, sptFreq.weighted, mu, mu0, f0Start, thStart,
                  thetaControl=theta.control(), f0Control=f0.control(), trace=FALSE)
    ## Extract theta control arguments
    if (class(f0Control) != "f0Control")
        stop("f0Control must be an object of class f0Control returned by f0Control() function.")
    eps <- f0Control$eps
    maxiter <- f0Control$maxiter</pre>
    maxhalf <- f0Control$maxhalf</pre>
    maxlogstep <- f0Control$maxlogstep
    f0 <- f0Start # assumes sum(f0Start) = 1 and sum(f0Start * spt) = mu0
    th <- thStart
    llik <- th$llik
    score.log <- NULL</pre>
    smm <- outer(spt, mu, "-")</pre>
    ymm \leftarrow y - mu
    yeqmu <- which(abs(ymm) < 1e-15)</pre>
    conv <- FALSE
    iter <- 0
    while (!conv && iter<maxiter) {</pre>
        iter <- iter + 1
        # Score calculation
        score.logOld <- score.log</pre>
        fTiltSums <- rowSums(th$fTilt)</pre>
        fTiltSumsWeighted <- apply(th$fTilt, MARGIN=1, function(x) sum(weights * x))
        smmfTilt <- smm * th$fTilt</pre>
        ystd <- ymm / th$bPrime2</pre>
        ystdWeighted <- weights * ystd</pre>
        ystd[yeqmu] <- 0 # prevent 0/0</pre>
        ystdWeighted[yeqmu] <- 0 # prevent 0/0</pre>
        score.logT1 <- sptFreq.weighted</pre>
```

```
score.logT2 <- fTiltSumsWeighted</pre>
score.logT3 <- c(smmfTilt %*% ystdWeighted)</pre>
score.log <- score.logT1 - score.logT2 - score.logT3</pre>
# Inverse info, score step, and f0 step are on the log scale (score is not)
if (iter == 1) {
    d1 <- min(fTiltSumsWeighted) # max inverse diagonal of first information term, on log scale
    d2 <- max(abs(score.log)) / maxlogstep</pre>
    d \leftarrow max(d1, d2)
    infoinvBFGS.log <- diag(1/d, nrow=length(f0))</pre>
} else {
    scorestep.log <- score.log - score.logOld</pre>
   # f0step.log <- log(f0) - log(f0old)
    # to prevent the 0/0 situation
    ratiof0f0old <- f0 / f0old
    ratiof0f0old[is.na(ratiof0f0old)] <- 1</pre>
    f0step.log <- log(ratiof0f0old)</pre>
    sy <- sum(f0step.log * scorestep.log)</pre>
    yiy <- c(crossprod(scorestep.log, infoinvBFGS.log %*% scorestep.log))</pre>
    iys <- tcrossprod(infoinvBFGS.log %*% scorestep.log, f0step.log)</pre>
    infoinvBFGS.log <- infoinvBFGS.log + ((yiy - sy) / sy^2) * tcrossprod(f0step.log) - (1 / sy)
logstep <- c(infoinvBFGS.log %*% score.log)</pre>
# Cap log(f0) step size
logstep.max <- max(abs(logstep))</pre>
if (logstep.max > maxlogstep)
    logstep <- logstep * (maxlogstep / logstep.max)</pre>
# Save values from previous iteration
f0old <- f0
thold <- th
llikold <- llik
# Take update step
f0 \leftarrow exp(log(f0) + logstep)
# Scale and tilt f0
f0 <- f0 / sum(f0)
f0 <- getTheta(spt=spt, f0=f0, mu=mu0, weights=weights, ySptIndex=1,</pre>
                thetaStart=0, thetaControl=thetaControl)$fTilt[, 1]
# Update theta and likelihood
thold <- th
llikold <- llik
th <- getTheta(spt=spt, f0=f0, mu=mu, weights=weights, ySptIndex=ySptIndex,
                thetaStart=th$theta, thetaControl=thetaControl)
llik <- th$llik
conv <- abs((llik - llikold) / (llik + 1e-100)) < eps</pre>
# If log-likelihood does not improve, change step direction to be along gradient
# Take half steps until likelihood improves
# Continue taking half steps until log likelihood no longer improves
nhalf <- 0
if (llik<llikold) {</pre>
    llikprev <- -Inf
    while ((llik<llikold || llik>llikprev) && nhalf<maxhalf) {</pre>
        nhalf \leftarrow nhalf + 1
        # Set previous values
```

llikprev <- llik

```
thprev <- th
               fOprev <- f0
               infoinvBFGS.logprev <- infoinvBFGS.log</pre>
               f0 \leftarrow \exp((\log(f0) + \log(f0)) / 2)
               f0 <- f0 / sum(f0)
               f0 <- getTheta(spt=spt, f0=f0, mu=mu0, weights=weights, ySptIndex=1,
                               thetaStart=0, thetaControl=thetaControl)$fTilt[, 1]
               th <- getTheta(spt=spt, f0=f0, mu=mu, weights=weights, ySptIndex=ySptIndex,
                               thetaStart=th$theta, thetaControl=thetaControl)
               llik <- th$llik
               infoinvBFGS.log <- infoinvBFGS.log / 2</pre>
           }
           if (llik < llikprev) {</pre>
               nhalf <- nhalf - 1
               llik <- llikprev
               th <- thprev
               f0 <- f0prev
               infoinvBFGS.log <- infoinvBFGS.logprev</pre>
           conv <- abs((llik - llikold) / (llik + 1e-100)) < eps</pre>
      }
      if (llik < llikold) {</pre>
           f0 <- f0old
           th <- thold
           llik <- llikold
           conv <- TRUE
      }
      if (trace) {
          printout <- pasteO("iter ", iter, ": llik=", llik)</pre>
           if (nhalf > 0)
               printout <- pasteO(printout, "; ", nhalf, " half steps")</pre>
           cat(printout, "\n")
      }
  }
  # Final score calculation
      smm <- outer(spt, th$bPrime, "-")</pre>
      ymm <- y - th$bPrime
      yeqmu <- which(abs(ymm) < 1e-15)</pre>
        fTiltSums <- rowSums(th$fTilt)</pre>
fTiltSumsWeighted <- apply(th$fTilt, MARGIN=1, function(x) sum(weights * x))
smmfTilt <- smm * th$fTilt</pre>
ystd <- ymm / th$bPrime2
ystdWeighted <- weights * ystd</pre>
ystd[yeqmu] <- 0 # prevent 0/0
ystdWeighted[yeqmu] <- 0 # prevent 0/0</pre>
ystd[yeqmu] <- 0 # prevent 0/0</pre>
score.logT1 <- sptFreq.weighted</pre>
score.logT2 <- fTiltSumsWeighted</pre>
score.logT3 <- c(smmfTilt %*% ystdWeighted)</pre>
score.log <- score.logT1 - score.logT2 - score.logT3</pre>
```