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

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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
gldrm.control <- function(eps=1e-10, maxiter=100, returnfTiltMatrix=TRUE,
                            returnfOScoreInfo=FALSE, print=FALSE,
                           betaStart=NULL, f0Start=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$returnfTiltMatrix</pre>
    returnfOScoreInfo <- gldrmControl$returnfOScoreInfo</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>
    weightsMatrix[cbind(1:n, ySptIndex)] <- weights</pre>
```

 $Date \colon \mathsf{March}\ 7,\ 2021.$ 

```
# 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,</pre>
                        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)
betaTemp <- rep(NA, nBeta)</pre>
betaTemp[!naID] <- beta</pre>
beta <- betaTemp
## 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>
          }
File defined by 1, 4, 6, 10.
"../R/wgldrm.R" 4\equiv
          #' Beta optimization routing
          #' @param 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.
          #' Cparam fO Current values of fO.
          #' Oparam linkinv Inverse link function.
          #' Cparam 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}
          #'@param betaControl A "betaControl" object returned from the \code{beta.control}
          #,
          #' 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
          #' \code{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
        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)
```

```
## 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
                      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) {
                      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, 10.
"../R/wgldrm.R" 6\equiv
          ## Computes log(sum(exp(x))) with better precision
          logSumExp <- function(x)</pre>
          {
              i <- which.max(x)</pre>
              m <- x[i]
              lse \leftarrow log1p(sum(exp(x[-i]-m))) + m
```

## We need to solve for beta such that I(betaHat) %\*% beta = Score(betaHat),

```
lse
}
## 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.
#'@param 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.
#'
#' @return 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.
#' \item \code{fTiltSW} Matrix containing the exponentially tilted distribution for each
#' observation, conditional on that observation being sampled, i.e. f(y|X=x, S=1).
#' If \code{sampprobs=NULL}, then \code{fTiltSW} matches \code{fTilt}.
#' \item \code{bPrimeSW} Vector containing the mean for each observation, conditional
#' on that observation being sampled. If \code{sampprobs=NULL}, then \code{bPrimeSW}
#' matches \code{bPrime}.
#' \item \code{bPrime2SW} Vector containing the variance for each observation, conditional
#' on that observation being sampled. If \code{sampprobs=NULL}, then \code{bPrime2SW}
#' 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.")
    logit <- thetaControl$logit</pre>
    eps <- thetaControl$eps</pre>
    maxiter <- thetaControl$maxiter</pre>
    maxhalf <- thetaControl$maxhalf
    maxtheta <- thetaControl$maxtheta</pre>
    logsumexp <- thetaControl$logsumexp</pre>
    ## 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>
        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)")
```

```
## Value does not change
gMu \leftarrow g(mu, m, M)
## Initialize values
theta <- thetaStart # initial values required
thetaOld <- bPrimeErrOld <- rep(NA, n)
conv <- rep(FALSE, n)
maxedOut <- rep(FALSE, n)</pre>
if (logsumexp) {
    logf0 \leftarrow log(f0)
    logfUnstd <- logf0 + tcrossprod(spt, theta)</pre>
    logb <- apply(logfUnstd, 2, logSumExp)</pre>
    fTilt <- exp(logfUnstd - rep(logb, each=sptN))
    normfact <- colSums(fTilt)</pre>
    normss <- which(normfact != 1)</pre>
    fTilt[, normss] <- fTilt[, normss, drop=FALSE] / rep(normfact[normss], each=sptN)</pre>
} else {
    fUnstd <- f0 * exp(tcrossprod(spt, theta)) # |spt| x n matrix of tilted f0 values
    b <- colSums(fUnstd)</pre>
    fTilt <- fUnstd / rep(b, each=sptN) # normalized
bPrime <- colSums(spt*fTilt) # mean as a function of theta
bPrime2 <- colSums(outer(spt, bPrime, "-")^2 * fTilt) # variance as a function of theta
bPrimeErr <- bPrime - mu # used to assess convergence
## Update theta until convergence
conv <- (abs(bPrimeErr) < eps) |</pre>
    (theta==maxtheta & bPrimeErr<0) |
    (theta==-maxtheta & bPrimeErr>0)
s <- which(!conv)
iter <- 0
while(length(s)>0 && iter<maxiter) {</pre>
    iter <- iter + 1
    bPrimeErrOld[s] <- bPrimeErr[s] # used to assess convergence</pre>
    ## 1) Update theta
    thetaOld[s] <- theta[s]</pre>
    if (logit) {
        tPrimeS <- (M-m) / ((bPrime[s]-m) * (M-bPrime[s])) * bPrime2[s]
            # t'(theta) from paper: temporary variable
            # only needed for the subset of observations that have not converged
        tPrimeS[is.na(tPrimeS) | tPrimeS==Inf] <- 0</pre>
            # If bPrime is on the boundary, then bPrime2 should be zero.
            # Exceptions are due to rounding error.
        thetaS <- theta[s] - (g(bPrime[s], m, M) - gMu[s]) / tPrimeS</pre>
        thetaS <- theta[s] - bPrimeErr[s] / bPrime2[s]</pre>
    }
    thetaS[thetaS > maxtheta] <- maxtheta</pre>
    thetaS[thetaS < -maxtheta] <- -maxtheta</pre>
    theta[s] <- thetaS
    ## 2) Update fTilt, bPrime, and bPrime2 and take half steps if bPrimeErr not improved
    ss <- s
    nhalf <- 0
    while(length(ss)>0 && nhalf<maxhalf) {</pre>
        ## 2a) Update fTilt, bPrime, and bPrime2
```

if (logsumexp) {

```
logfUnstd[, ss] <- logf0 + tcrossprod(spt, theta[ss])</pre>
                           logb[ss] <- apply(logfUnstd[, ss, drop=FALSE], 2, logSumExp)</pre>
                           fTilt[, ss] <- exp(logfUnstd[, ss, drop=FALSE] - rep(logb[ss], each=sptN))
                           normfact <- colSums(fTilt[, ss, drop=FALSE])</pre>
                           normss <- which(normfact != 1)</pre>
                           fTilt[, ss[normss]] <- fTilt[, ss[normss], drop=FALSE] / rep(normfact[normss], each=sptN)
                       } else {
                           fUnstd[, ss] <- f0*exp(tcrossprod(spt, theta[ss])) # |spt| x n matrix of tilted f0 value
                           b[ss] <- colSums(fUnstd[, ss, drop=FALSE])</pre>
                           fTilt[, ss] <- fUnstd[, ss, drop=FALSE] / rep(b[ss], each=sptN) # normalized
                       bPrime[ss] <- colSums(spt*fTilt[, ss, drop=FALSE]) # mean as a function of theta
                       bPrime2[ss] <- colSums(outer(spt, bPrime[ss], "-")^2 * fTilt[, ss, drop=FALSE]) # variance a
                       bPrimeErr[ss] <- bPrime[ss] - mu[ss] # used to assess convergence
                       ## 2b) Take half steps if necessary
                       ss <- ss[abs(bPrimeErr[ss]) > abs(bPrimeErrOld[ss])]
                       if (length(ss) > 0) nhalf <- nhalf + 1
                       theta[ss] <- (theta[ss] + thetaOld[ss]) / 2</pre>
                  ## If maximum half steps are exceeded, set theta to previous value
                  maxedOut[ss] <- TRUE</pre>
                  theta[ss] <- thetaOld[ss]</pre>
                  ## 3) Check convergence
                  conv[s] <- (abs(bPrimeErr[s]) < eps) |</pre>
                       (theta[s] == maxtheta & bPrimeErr[s] < 0) |</pre>
                       (theta[s] == -maxtheta & bPrimeErr[s] > 0)
                  s <- s[!conv[s] & !maxedOut[s]]
              }
              fTiltSW <- fTilt
              bPrimeSW <- bPrime
              bPrime2SW <- bPrime2
              ## Calculate log-likelihood
             # llik <- sum(log(fTiltSW[cbind(ySptIndex, seq_along(ySptIndex))]))</pre>
              fTiltSW.extracted <- fTiltSW[cbind(ySptIndex, seq_along(ySptIndex))]</pre>
              llik <- sum(weights[fTiltSW.extracted>0] * log(fTiltSW.extracted[fTiltSW.extracted>0]))
              list(theta=theta, fTilt=fTilt, bPrime=bPrime, bPrime2=bPrime2,
                    fTiltSW=fTiltSW, bPrimeSW=bPrimeSW, bPrime2SW=bPrime2SW,
                   llik=llik, conv=conv, iter=iter)
          }
File defined by 1, 4, 6, 10.
"../R/wgldrm.R" 10 \equiv
          #' Control arguments for f0 update algorithm
          \#' This function returns control arguments for the eqn{f_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.
#'Cparam maxhalf Maximum number of half steps allowed per iteration if
#' log-likelihood does not improve between iterations.
#'Cparam 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}
#'@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.
#' @return 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
maxlogstep <- f0Control$maxlogstep
f0 <- f0Start # assumes sum(f0Start) = 1 and sum(f0Start * spt) = mu0
th <- thStart
llik <- th$llik
score.log <- NULL
smm <- outer(spt, mu, "-")</pre>
ymm <- 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>
    fTiltSWSums <- rowSums(th$fTiltSW)</pre>
    fTiltSWSumsWeighted <- apply(th$fTiltSW, MARGIN=1, function(x) sum(weights * x))
    smmfTiltSW <- smm * th$fTiltSW</pre>
    ystd <- ymm / th$bPrime2SW
    ystdWeighted <- weights * ystd
    ystd[yeqmu] <- 0 # prevent 0/0
    ystdWeighted[yeqmu] <- 0 # prevent 0/0</pre>
    score.logT1 <- sptFreq.weighted</pre>
    score.logT2 <- fTiltSWSumsWeighted</pre>
    score.logT3 <- c(smmfTiltSW %*% 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(fTiltSWSumsWeighted) # max inverse diagonal of first information term, on log scal
        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)</pre>
        # 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)</pre>
    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$llik
conv <- abs((llik - llikold) / (llik + 1e-100)) < eps</pre>
# If log-likelihood does not improve, change step direction to be along gradient
# Take half steps until likelihood improves
# Continue taking half steps until log likelihood no longer improves
nhalf <- 0
if (llik<llikold) {</pre>
    llikprev <- -Inf
    while ((llik<llikold || llik>llikprev) && nhalf<maxhalf) {</pre>
        nhalf <- nhalf + 1
        # Set previous values
        llikprev <- llik
        thprev <- th
        fOprev <- f0
        infoinvBFGS.logprev <- infoinvBFGS.log</pre>
        f0 \leftarrow \exp((\log(f0) + \log(f0)) / 2)
        f0 \leftarrow f0 / sum(f0)
        f0 <- getTheta(spt=spt, f0=f0, mu=mu0, weights=weights, ySptIndex=1,</pre>
                        thetaStart=0, thetaControl=thetaControl)$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 <- paste0("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$bPrimeSW, "-")</pre>
                   ymm \leftarrow y - th$bPrimeSW
                   yeqmu <- which(abs(ymm) < 1e-15)</pre>
                     fTiltSWSums <- rowSums(th$fTiltSW)</pre>
             fTiltSWSumsWeighted <- apply(th$fTiltSW, MARGIN=1, function(x) sum(weights * x))
             smmfTiltSW <- smm * th$fTiltSW</pre>
            ystd <- ymm / th$bPrime2SW
            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 <- fTiltSWSumsWeighted</pre>
             score.logT3 <- c(smmfTiltSW %*% ystdWeighted)</pre>
             score.log <- score.logT1 - score.logT2 - score.logT3</pre>
             # Final info calculation
             info.logT1 <- diag(fTiltSWSumsWeighted)</pre>
             info.logT2 <- tcrossprod(th$fTiltSW)</pre>
             info.logT3 <- tcrossprod(smmfTiltSW, smmfTiltSW) * rep(ystdWeighted, each=nrow(smmfTiltSW)))</pre>
             info.log <- info.logT1 - info.logT2 - info.logT3</pre>
               list(f0=f0, llik=llik, th=th, conv=conv, iter=iter, nhalf=nhalf,
                    score.log=score.log, info.log=info.log)
          }
File defined by 1, 4, 6, 10.
```