

Package ‘SQUAREM’

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Title Squared Extrapolation Methods for Accelerating EM-Like Monotone Algorithms

Description Algorithms for accelerating the convergence of slow, monotone sequences from smooth, contraction mappings such as the EM algorithm. It can be used to accelerate any smooth, linearly convergent scheme. A tutorial-style introduction is available in vignette(“SQUAREM”). See also: Varadhan & Roland (2008) <[doi:10.18637/jss.v092.i07](https://doi.org/10.18637/jss.v092.i07)>.

Depends R (>= 4.0)

Suggests setRNG, interval

License GPL (>= 2)

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fpiter

*Fixed-Point Iteration Scheme***Description**

A function to implement the fixed-point iteration algorithm. This includes monotone, contraction mappings including EM and MM algorithms

Usage

```
fpiter(par, fixptfn, objfn=NULL, control=list( ), ...)
```

Arguments

par	A vector of parameters denoting the initial guess for the fixed-point iteration.
fixptfn	A vector function, F that denotes the fixed-point mapping. This function is the most essential input in the package. It should accept a parameter vector as input and should return a parameter vector of same length. This function defines the fixed-point iteration: $x_{k+1} = F(x_k)$. In the case of EM algorithm, F defines a single E and M step.
objfn	This is a scalar function, L , that denotes a "merit" function which attains its local minimum at the fixed-point of F . This function should accept a parameter vector as input and should return a scalar value. In the EM algorithm, the merit function L is the log-likelihood. In some problems, a natural merit function may not exist, in which case the algorithm works with only <code>fixptfn</code> . The merit function function <code>objfn</code> does not have to be specified, even when a natural merit function is available, especially when its computation is expensive.
control	A list of control parameters to pass on to the algorithm. Full names of control list elements must be specified, otherwise, user-specifications are ignored. See <i>*Details*</i> below.
...	Arguments passed to <code>fixptfn</code> and <code>objfn</code> .

Details

`control` is list of control parameters for the algorithm.

control A list of control parameters. Default settings: `list(tol = 1.e-07, maxiter = 1500, trace = FALSE, intermed = FALSE)`. See details below for descriptions of individual elements.

tol A small, positive scalar that determines when iterations should be terminated. Iteration stops when $\|x_k - F(x_k)\| \leq tol$. Default is `1.e-07`.

maxiter An integer denoting the maximum limit on the number of evaluations of `fixptfn`, F . Default is `1500`.

trace A logical variable denoting whether intermediate results should be displayed. Default is `FALSE`.

intermed A logical variable denoting whether intermediate results should be returned. If TRUE, returns a matrix with parameters at each iteration and corresponding fixed-point residuals. Default is FALSE.

Value

A list with the following components:

par	Parameter, x^* that are the fixed-point of F such that $x^* = F(x^*)$, if convergence is successful.
value.objfn	The value of the objective function L at termination.
fpevals	Number of times the fixed-point function <code>fixptfn</code> was evaluated.
objfevals	Number of times the objective function <code>objfn</code> was evaluated.
convergence	An integer code indicating type of convergence. 0 indicates successful convergence, whereas 1 denotes failure to converge.

References

R Varadhan and C Roland (2008), Simple and globally convergent numerical schemes for accelerating the convergence of any EM algorithm, *Scandinavian Journal of Statistics*, 35:335-353.

C Roland, R Varadhan, and CE Frangakis (2007), Squared polynomial extrapolation methods with cycling: an application to the positron emission tomography problem, *Numerical Algorithms*, 44:159-172.

See Also

[squarem](#)

Examples

```
#####
# Example 1: EM algorithm for Poisson mixture estimation
poissmix.em <- function(p,y) {
# The fixed point mapping giving a single E and M step of the EM algorithm
#
pnew <- rep(NA,3)
i <- 0:(length(y)-1)
zi <- p[1]*exp(-p[2])*p[2]^i / (p[1]*exp(-p[2])*p[2]^i + (1 - p[1])*exp(-p[3])*p[3]^i)
pnew[1] <- sum(y*zi)/sum(y)
pnew[2] <- sum(y*i*zi)/sum(y*zi)
pnew[3] <- sum(y*i*(1-zi))/sum(y*(1-zi))
p <- pnew
return(pnew)
}

poissmix.loglik <- function(p,y) {
# Objective function whose local minimum is a fixed point \
# negative log-likelihood of binary poisson mixture
i <- 0:(length(y)-1)
loglik <- y*log(p[1]*exp(-p[2])*p[2]^i/exp(lgamma(i+1)) +
```

```

(1 - p[1])*exp(-p[3])*p[3]^i/exp(lgamma(i+1)))
return ( -sum(loglik) )
}

# Real data from Hasselblad (JASA 1969)
poissmix.dat <- data.frame(death=0:9, freq=c(162,267,271,185,111,61,27,8,3,1))
y <- poissmix.dat$freq
tol <- 1.e-08

# Use a preset seed so the example is reproducible.
require("setRNG")
old.seed <- setRNG(list(kind="Mersenne-Twister", normal.kind="Inversion",
  seed=54321))

p0 <- c(runif(1),runif(2,0,4)) # random starting value

# Basic EM algorithm
pf1 <- fpiter(p=p0, y=y, fixptfn=poissmix.em, objfn=poissmix.loglik, control=list(tol=tol))

#####
# Example 2: Accelerating the convergence of power method iteration for
# finding the dominant eigenvector of a matrix

power.method <- function(x, A) {

# Defines one iteration of the power method
# x = starting guess for dominant eigenvector
# A = a square matrix

ax <- as.numeric(A %*% x)
f <- ax / sqrt(as.numeric(crossprod(ax)))
f
}

# Finding the dominant eigenvector of the Bodewig matrix
# This is a famous matrix for which power method has trouble converging
# See, for example, Sidi, Ford, and Smith (SIAM Review, 1988)
#
# Note: there are two eigenvalues that are equally dominant,
# but have opposite signs.
# Sometimes the power method finds the eigenvector corresponding to the
# large positive eigenvalue, but other times it finds the eigenvector
# corresponding to the large negative eigenvalue
b <- c(2, 1, 3, 4, 1, -3, 1, 5, 3, 1, 6, -2, 4, 5, -2, -1)
bodewig.mat <- matrix(b,4,4)
eigen(bodewig.mat)

p0 <- rnorm(4)

# Standard power method iteration
ans1 <- fpiter(p0, fixptfn=power.method, A=bodewig.mat)
# re-scaling the eigenvector so that it has unit length

```

```
ans1$par <- ans1$par / sqrt(sum(ans1$par^2))
ans1
```

squarem	<i>Squared Extrapolation Methods for Accelerating Slowly-Convergent Fixed-Point Iterations</i>
---------	--

Description

Globally-convergent, partially monotone, acceleration schemes for accelerating the convergence of *any* smooth, monotone, slowly-converging contraction mapping. It can be used to accelerate the convergence of a wide variety of iterations including the expectation-maximization (EM) algorithms and its variants, majorization-minimization (MM) algorithm, power method for dominant eigenvalue-eigenvector, Google's page-rank algorithm, and multi-dimensional scaling.

Usage

```
squarem(par, fixptfn, objfn, ... , control=list())
```

Arguments

par	A vector of parameters denoting the initial guess for the fixed-point.
fixptfn	A vector function, F that denotes the fixed-point mapping. This function is the most essential input in the package. It should accept a parameter vector as input and should return a parameter vector of same length. This function defines the fixed-point iteration: $x_{k+1} = F(x_k)$. In the case of EM algorithm, F defines a single E and M step.
objfn	This is a scalar function, L , that denotes a "merit" function which attains its local maximum or minimum at the fixed -point of F . Also see the control parameter <code>minimize</code> which determines whether the objective function is minimized or maximized. The objective function should accept a parameter vector as input and should return a scalar value. In the EM algorithm, the merit function L is the either log-likelihood or its negative. In some problems, a natural merit function may not exist, in which case the algorithm works with only <code>fixptfn</code> . The merit function function <code>objfn</code> does not have to be specified, even when a natural merit function is available, especially when its computation is expensive.
control	A list of control parameters specifying any changes to default values of algorithm control parameters. Full names of control list elements must be specified, otherwise, user-specifications are ignored. See <i>*Details*</i> .
...	Arguments passed to <code>fixptfn</code> and <code>objfn</code> .

Details

The function `squarem` is a general-purpose algorithm for accelerating the convergence of *any* slowly-convergent (smooth) fixed-point iteration. Full names of control parameters must be specified; otherwise, user specifications are ignored.

Default values of control are: `K = 1`, `method = 3`, `minimize = TRUE`, `square = TRUE`, `step.min0 = 1`, `step.max0 = 1`, `mstep = 4`, `objfn.inc = 1`, `kr = 1`, `tol = 1e-07`, `maxiter = 1500`, `trace = FALSE`, `intermed = FALSE`.

`K` An integer denoting the order of the SQUAREM scheme. Default is 1, which is a first-order scheme developed in Varadhan and Roland (2008). First-order schemes are adequate for most problems. `K = 2, 3` may provide greater speed in some problems, although they are less reliable than first-order schemes.

`method` Either an integer or a character variable that denotes the particular SQUAREM scheme to be used. When `K = 1`, `method` should be an integer: 1, 2, or 3. These correspond to the 3 schemes discussed in Varadhan and Roland (2008). Default is `method = 3`. When `K > 1`, `method` should be a character string, either "RRE" or "MPE". These correspond to reduced-rank extrapolation or squared minimal polynomial extrapolation (see Roland, Varadhan, and Frangakis (2007)). Default is "RRE".

`minimize` A logical variable. By default it is set to TRUE for minimization of the objective function. If the objective function is to be maximized (commonly the case for likelihood estimation), set to FALSE.

`square` A logical variable indicating whether a squared extrapolation scheme should be used. Squared extrapolation schemes are typically faster and more stable than unsquared schemes. Default is TRUE.

`step.min0` A scalar denoting the minimum steplength taken by a SQUAREM algorithm. Default is 1. For contractive fixed-point iterations (e.g., EM and MM), this default works well. In problems where an eigenvalue of the Jacobian of F is outside of the interval $(0, 1)$, `step.min0` should be less than 1 or even negative in some cases.

`step.max0` A positive-valued scalar denoting the initial value of the maximum steplength taken by a SQUAREM algorithm. Default is 1. When the steplength computed by SQUAREM exceeds `step.max0`, the steplength is set equal to `step.max0`, but then `step.max0` is increased by a factor of `mstep`.

`mstep` A scalar greater than 1. When the steplength computed by SQUAREM exceeds `step.max0`, the steplength is set equal to `step.max0`, but `step.max0` is increased by a factor of `mstep`. Default is 4.

`objfn.inc` A non-negative scalar that dictates the degree of non-monotonicity. Default is 1. Set `objfn.inc = 0` to obtain monotone convergence. Setting `objfn.inc = Inf` gives a non-monotone scheme. In-between values result in partially-monotone convergence.

`kr` A non-negative scalar that dictates the degree of non-monotonicity. Default is 1. Set `kr = 0` to obtain monotone convergence. Setting `kr = Inf` gives a non-monotone scheme. In-between values result in partially-monotone convergence. This parameter is only used when `objfn` is not specified by the user.

`tol` A small, positive scalar that determines when iterations should be terminated. Iteration stops when $\|x_k - F(x_k)\| \leq tol$. Default is $1e-07$.

- `maxiter` An integer denoting the maximum limit on the number of evaluations of `fixptfn`, F . Default is 1500.
- `trace` A logical variable denoting whether intermediate results of iterations should be displayed. Default is FALSE.
- `intermed` A logical variable denoting whether intermediate results of iterations should be returned. If set to TRUE, the function will return a matrix where each row corresponds to parameters at each iteration, along with the corresponding log-likelihood value. When `objfn` is not specified, it will return the fixed-point residual instead of the objective function values. Default is FALSE.

Value

A list with the following components:

- | | |
|--------------------------|--|
| <code>par</code> | Parameter, x^* that are the fixed-point of F such that $x^* = F(x^*)$, if convergence is successful. |
| <code>value.objfn</code> | The value of the objective function $\$L\$$ at termination. |
| <code>fpevals</code> | Number of times the fixed-point function <code>fixptfn</code> was evaluated. |
| <code>objfevals</code> | Number of times the objective function <code>objfn</code> was evaluated. |
| <code>convergence</code> | An integer code indicating type of convergence. 0 indicates successful convergence, whereas 1 denotes failure to converge. |
| <code>p.intermed</code> | A matrix where each row corresponds to parameters at each iteration, along with the corresponding log-likelihood value. This object is returned only when the control parameter <code>intermed</code> is set to TRUE. It is not returned when <code>objfn</code> is not specified. |

References

R Varadhan and C Roland (2008), Simple and globally convergent numerical schemes for accelerating the convergence of any EM algorithm, *Scandinavian Journal of Statistics*, 35:335-353.

C Roland, R Varadhan, and CE Frangakis (2007), Squared polynomial extrapolation methods with cycling: an application to the positron emission tomography problem, *Numerical Algorithms*, 44:159-172.

Y Du and R Varadhan (2020), SQUAREM: An R package for off-the-shelf acceleration of EM, MM, and other EM-like monotone algorithms, *Journal of Statistical Software*, 92(7): 1-41. <doi:10.18637/jss.v092.i07>

See Also

[fpiter](#)

Examples

```
#####
# Also see the vignette by typing:
# vignette("SQUAREM", all=FALSE)
#
# Example 1: EM algorithm for Poisson mixture estimation
```

```

poissmix.em <- function(p,y) {
# The fixed point mapping giving a single E and M step of the EM algorithm
#
pnew <- rep(NA,3)
i <- 0:(length(y)-1)
zi <- p[1]*exp(-p[2])*p[2]^i / (p[1]*exp(-p[2])*p[2]^i + (1 - p[1])*exp(-p[3])*p[3]^i)
pnew[1] <- sum(y*zi)/sum(y)
pnew[2] <- sum(y*i*zi)/sum(y*zi)
pnew[3] <- sum(y*i*(1-zi))/sum(y*(1-zi))
p <- pnew
return(pnew)
}

poissmix.loglik <- function(p,y) {
# Objective function whose local minimum is a fixed point
# negative log-likelihood of binary poisson mixture
i <- 0:(length(y)-1)
loglik <- y*log(p[1]*exp(-p[2])*p[2]^i/exp(lgamma(i+1)) +
(1 - p[1])*exp(-p[3])*p[3]^i/exp(lgamma(i+1)))
return ( -sum(loglik) )
}

# Real data from Hasselblad (JASA 1969)
poissmix.dat <- data.frame(death=0:9, freq=c(162,267,271,185,111,61,27,8,3,1))
y <- poissmix.dat$freq
tol <- 1.e-08

# Use a preset seed so the example is reproducible.
require("setRNG")
old.seed <- setRNG(list(kind="Mersenne-Twister", normal.kind="Inversion",
seed=54321))

p0 <- c(runif(1),runif(2,0,4)) # random starting value

# Basic EM algorithm
pf1 <- fpiter(p=p0, y=y, fixptfn=poissmix.em, objfn=poissmix.loglik, control=list(tol=tol))

# First-order SQUAREM algorithm with SqS3 method
pf2 <- squarem(par=p0, y=y, fixptfn=poissmix.em, objfn=poissmix.loglik,
control=list(tol=tol))

# First-order SQUAREM algorithm with SqS2 method
pf3 <- squarem(par=p0, y=y, fixptfn=poissmix.em, objfn=poissmix.loglik,
control=list(method=2, tol=tol))

# First-order SQUAREM algorithm with SqS3 method; non-monotone
# Note: the objective function is not evaluated when objfn.inc = Inf
pf4 <- squarem(par=p0,y=y, fixptfn=poissmix.em,
control=list(tol=tol, objfn.inc=Inf))

# First-order SQUAREM algorithm with SqS3 method;
# objective function is not specified

```

```

pf5 <- squarem(par=p0,y=y, fixptfn=poissmix.em, control=list(tol=tol, kr=0.1))

# Second-order (K=2) SQUAREM algorithm with SqRRE
pf6 <- squarem(par=p0, y=y, fixptfn=poissmix.em, objfn=poissmix.loglik,
               control=list (K=2, tol=tol))

# Second-order SQUAREM algorithm with SqRRE; objective function is not specified
pf7 <- squarem(par=p0, y=y, fixptfn=poissmix.em, control=list(K=2, tol=tol))

# Comparison of converged parameter estimates
par.mat <- rbind(pf1$par, pf2$par, pf3$par, pf4$par, pf5$par, pf6$par, pf7$par)
par.mat

# Compare objective function values
# (note: `NA's indicate that \code{objfn} was not specified)
c(pf1$value, pf2$value, pf3$value, pf4$value,
  pf5$value, pf6$value, pf7$value)

# Compare number of fixed-point evaluations
c(pf1$fpeval, pf2$fpeval, pf3$fpeval, pf4$fpeval,
  pf5$fpeval, pf6$fpeval, pf7$fpeval)

# Compare number of objective function evaluations
# (note: `0' indicate that \code{objfn} was not specified)
c(pf1$objfeval, pf2$objfeval, pf3$objfeval, pf4$objfeval,
  pf5$objfeval, pf6$objfeval, pf7$objfeval)

#####
# Example 2: Same as above (i.e. Poisson mixture)
# but now showing how to "maximize" the log-likelihood

poissmix.loglik.max <- function(p,y) {
# Objective function which is to be *maximized*
# Log-likelihood of binary poisson mixture
i <- 0:(length(y)-1)
loglik <- y*log(p[1]*exp(-p[2])*p[2]^i/exp(lgamma(i+1)) +
(1 - p[1])*exp(-p[3])*p[3]^i/exp(lgamma(i+1)))
return ( sum(loglik) )
}

# Maximizing the log-likelihood
# Note: the control parameter `minimize' is set to FALSE
#
pf.max <- squarem(par=p0, y=y, fixptfn=poissmix.em, objfn=poissmix.loglik.max,
                 control=list(tol=tol, minimize=FALSE))
pf.max

#####
# Example 3: Accelerating the convergence of power method iteration
# for finding the dominant eigenvector of a matrix

power.method <- function(x, A) {
# Defines one iteration of the power method

```

```
# x = starting guess for dominant eigenvector
# A = a square matrix
ax <- as.numeric(A %*% x)
f <- ax / sqrt(as.numeric(crossprod(ax)))
f
}

# Finding the dominant eigenvector of the Bodewig matrix
b <- c(2, 1, 3, 4, 1, -3, 1, 5, 3, 1, 6, -2, 4, 5, -2, -1)
bodewig.mat <- matrix(b,4,4)
eigen(bodewig.mat)

p0 <- rnorm(4)

# Standard power method iteration
ans1 <- fpiter(p0, fixptfn=power.method, A=bodewig.mat)
# re-scaling the eigenvector so that it has unit length
ans1$par <- ans1$par / sqrt(sum(ans1$par^2))
ans1

# First-order SQUAREM with default settings
ans2 <- squarem(p0, fixptfn=power.method, A=bodewig.mat, control=list(K=1))
ans2$par <- ans2$par / sqrt(sum(ans2$par^2))
ans2

# First-order SQUAREM with a smaller step.min0
# Convergence is dramatically faster now!
ans3 <- squarem(p0, fixptfn=power.method, A=bodewig.mat, control=list(step.min0 = 0.5))
ans3$par <- ans3$par / sqrt(sum(ans3$par^2))
ans3

# Second-order SQUAREM
ans4 <- squarem(p0, fixptfn=power.method, A=bodewig.mat, control=list(K=2, method="rre"))
ans4$par <- ans4$par / sqrt(sum(ans4$par^2))
ans4
```

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