Package ‘EMpeaksR’

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Type Package

Title Conducting the Peak Fitting Based on the EM Algorithm

Version 0.2.0

Description The peak fitting of spectral data is performed by using the frame work of EM algorithm. We adapted the EM algorithm for the peak fitting of spectral data set by considering the weight of the intensity corresponding to the measurement energy steps (Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019 and 2021) <doi:10.1080/14686996.2019.1620123> and <doi:10.1080/27660400.2021.1899449>
age efficiently estimates the parameters of Gaussian mixture model during iterative calculation between E-step and M-step, and the parameters are converged to a local optimal solution. This package can support the investigation of peak shift with two advantages: (1) a large amount of data can be processed at high speed; and (2) stable and automatic calculation can be easily performed.

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R topics documented:

show_dsgmm_curve *Visualization of the result of spect_em_dsgmm*

Description

Visualization of the result of spect_em_dsgmm().

Usage

```
show_dsgmm_curve(spect_em_dsgmm_res,
                 x,
                 y,
                 mix_ratio_init,
                 mu_init,
                 sigma_init,
                 alpha_init,
                 eta_init)
```

Arguments

`spect_em_dsgmm_res`	data set obtained by spect_em_dsgmm()
`x`	measurement steps
`y`	intensity
`mix_ratio_init`	initial values of the mixture ratio of the components
`mu_init`	initial values of the mean of the components
`sigma_init`	initial values of the standard deviation of the components
`alpha_init`	initial values of the asymmetric parameter of the components
`eta_init`	initial values of the mixing ratio of Gauss and Lorentz distribution

Details

Perform a visualization of fitting curve estimated by Doniach-Sunjic-Gauss mixture model.

Value

Show the fitting curve and variation of the parameters.

References

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019). Spectrum adapted expectation-maximization algorithm for high-throughput peak shift analysis. Science and technology of advanced materials, 20(1), 733-745.

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2021). Spectrum adapted expectation-conditional maximization algorithm for extending high–throughput peak separation method in XPS analysis. Science and Technology of Advanced Materials: Methods, 1(1), 45-55.

Examples

```
#generating the synthetic spectral data based on three component Doniach-Sunjic-Gauss mixture model.
x               <- seq(0, 100, by = 0.5)
true_mu         <- c(20, 50, 80)
true_sigma      <- c(3, 3, 3)
true_alpha      <- c(0.1, 0.3, 0.1)
true_eta        <- c(0.4, 0.6, 0.1)
true_mix_ratio  <- rep(1/3, 3)
degree          <- 4

#trancated Doniach-Sunjic-Gauss
truncated_dsg <- function(x, mu, sigma, alpha, eta) {
                 ((eta*(((gamma(1-alpha)) /
                 ((x-mu)^2+(sqrt(2*log(2))*sigma)^2)^((1-alpha)/2)) *
                 cos((pi*alpha/2)+(1-alpha)*atan((x-mu) /
                 (sqrt(2*log(2))*sigma))))) + (1-eta)*dnorm(x, mu, sigma)) /
                 sum( ((eta*(((gamma(1-alpha)) /
                 ((x-mu)^2+(sqrt(2*log(2))*sigma)^2)^((1-alpha)/2)) *
                 cos((pi*alpha/2)+(1-alpha)*atan((x-mu) /
                 (sqrt(2*log(2))*sigma))))) + (1-eta)*dnorm(x, mu, sigma)))
}

y <- c(true_mix_ratio[1]*truncated_dsg(x = x,
                                       mu = true_mu[1],
                                       sigma = true_sigma[1],
                                       alpha = true_alpha[1],
                                       eta = true_eta[1])*10^degree +
       true_mix_ratio[2]*truncated_dsg(x = x,
                                       mu = true_mu[2],
                                       sigma = true_sigma[2],
                                       alpha = true_alpha[2],
                                       eta = true_eta[2])*10^degree +
       true_mix_ratio[3]*truncated_dsg(x = x,
                                       mu = true_mu[3],
                                       sigma = true_sigma[3],
                                       alpha = true_alpha[3],
                                       eta = true_eta[3])*10^degree)

plot(y~x, main = "genrated synthetic spectral data")

#Peak fitting by EMpeaksR
#Initial values
K <- 3
mix_ratio_init <- c(0.2, 0.4, 0.4)
mu_init        <- c(20, 40, 70)
sigma_init     <- c(4, 3, 2)
alpha_init     <- c(0.3, 0.2, 0.4)
eta_init       <- c(0.5, 0.4, 0.3)

#Coducting calculation
SP_ECM_DSG_res <- spect_em_dsgmm(x = x,
                                 y = y,
```

```
                                 mu = mu_init,
                                 sigma = sigma_init,
                                 alpha = alpha_init,
                                 eta = eta_init,
                                 mix_ratio = mix_ratio_init,
                                 conv.cri = 1e-6,
                                 maxit = 100)

#Plot fitting curve and trace plot of parameters
show_dsgmm_curve(SP_ECM_DSG_res,
                 x,
                 y,
                 mix_ratio_init,
                 mu_init,
                 sigma_init,
                 alpha_init,
                 eta_init)

#Showing the result of spect_em_dsgmm()
print(cbind(c(mu_init),
            c(sigma_init),
            c(alpha_init),
            c(eta_init),
            c(mix_ratio_init)))

print(cbind(SP_ECM_DSG_res$mu,
            SP_ECM_DSG_res$sigma,
            SP_ECM_DSG_res$alpha,
            SP_ECM_DSG_res$eta,
            SP_ECM_DSG_res$mix_ratio))

print(cbind(true_mu,
            true_sigma,
            true_alpha,
            true_eta,
            true_mix_ratio))
```

`show_gmm_curve` *Visualization of the result of spect_em_gmm*

Description

Visualization of the result of spect_em_gmm().

Usage

```
show_gmm_curve(spect_em_gmm_res, x, y, mix_ratio_init, mu_init, sigma_init)
```

Arguments

spect_em_gmm_res
: data set obtained by spect_em_gmm()

x
: measurement steps

y
: intensity

mix_ratio_init
: initial values of the mixture ratio of the components

mu_init
: initial values of the mean of the components

sigma_init
: initial values of the standard deviation of the components

Details

Perform a visualization of fitting curve estimated by Gaussian mixture model.

Value

Show the fitting curve and variation of the parameters.

References

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019). Spectrum adapted expectation-maximization algorithm for high-throughput peak shift analysis. Science and technology of advanced materials, 20(1), 733-745.

Examples

```
#generating the synthetic spectral data based on three component Gausian mixture model.
x              <- seq(0, 100, by = 0.5)
true_mu        <- c(35, 50, 65)
true_sigma     <- c(3, 3, 3)
true_mix_ratio <- rep(1/3, 3)
degree         <- 4

y <- c(true_mix_ratio[1] * dnorm(x = x, mean = true_mu[1], sd = true_sigma[1])*10^degree +
      true_mix_ratio[2] * dnorm(x = x, mean = true_mu[2], sd = true_sigma[2])*10^degree +
       true_mix_ratio[3] * dnorm(x = x, mean = true_mu[3], sd = true_sigma[3])*10^degree)

plot(y~x, main = "genrated synthetic spectral data")

#Peak fitting by EMpeaksR
#Initial values
K <- 3

mix_ratio_init  <- c(0.2, 0.4, 0.4)
mu_init         <- c(20, 40, 70)
sigma_init      <- c(2, 5, 4)

#Coducting calculation
SP_EM_G_res <- spect_em_gmm(x, y, mu = mu_init, sigma = sigma_init, mix_ratio = mix_ratio_init,
                            conv.cri = 1e-8, maxit = 100000)
```

```
#Plot fitting curve and trace plot of parameters
show_gmm_curve(SP_EM_G_res, x, y, mix_ratio_init, mu_init, sigma_init)

#Showing the result of spect_em_gmm()
print(cbind(c(mu_init), c(sigma_init), c(mix_ratio_init)))
print(cbind(SP_EM_G_res$mu, SP_EM_G_res$sigma, SP_EM_G_res$mix_ratio))
print(cbind(true_mu, true_sigma, true_mix_ratio))
```

`show_lmm_curve` *Visualization of the result of spect_em_lmm*

Description

Visualization of the result of spect_em_lmm().

Usage

```
show_lmm_curve(spect_em_lmm_res, x, y, mix_ratio_init, mu_init, gam_init)
```

Arguments

spect_em_lmm_res	data set obtained by spect_em_lmm()
x	measurement steps
y	intensity
mix_ratio_init	initial values of the mixture ratio of the components
mu_init	initial values of the mean of the components
gam_init	initial values of the scale parameter of the components

Details

Perform a visualization of fitting curve estimated by Lorentz mixture model.

Value

Show the fitting curve and variation of the parameters.

References

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019). Spectrum adapted expectation-maximization algorithm for high-throughput peak shift analysis. Science and technology of advanced materials, 20(1), 733-745.

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2021). Spectrum adapted expectation-conditional maximization algorithm for extending high–throughput peak separation method in XPS analysis. Science and Technology of Advanced Materials: Methods, 1(1), 45-55.

Examples

```
#generating the synthetic spectral data based on three component Lorentz mixture model.
x               <- seq(0, 100, by = 0.5)
true_mu         <- c(35, 50, 65)
true_gam        <- c(3, 3, 3)
true_mix_ratio  <- rep(1/3, 3)
degree          <- 4

#Normalized Lorentz distribution
dCauchy <- function(x, mu, gam) {
    (dcauchy(x, mu, gam)) / sum(dcauchy(x, mu, gam))
  }

y <- c(true_mix_ratio[1] * dCauchy(x = x, mu = true_mu[1], gam = true_gam[1])*10^degree +
       true_mix_ratio[2] * dCauchy(x = x, mu = true_mu[2], gam = true_gam[2])*10^degree +
       true_mix_ratio[3] * dCauchy(x = x, mu = true_mu[3], gam = true_gam[3])*10^degree)

plot(y~x, main = "genrated synthetic spectral data")

#Peak fitting by EMpeaksR
#Initial values
K <- 3

mix_ratio_init  <- c(0.2, 0.4, 0.4)
mu_init         <- c(20, 40, 70)
gam_init        <- c(2, 5, 4)

#Coducting calculation
SP_ECM_L_res <- spect_em_lmm(x, y, mu = mu_init, gam = gam_init, mix_ratio = mix_ratio_init,
                             conv.cri = 1e-6, maxit = 100000)

#Plot fitting curve and trace plot of parameters
show_lmm_curve(SP_ECM_L_res, x, y, mix_ratio_init, mu_init, gam_init)

#Showing the result of spect_em_lmm()
print(cbind(c(mu_init), c(gam_init), c(mix_ratio_init)))
print(cbind(SP_ECM_L_res$mu, SP_ECM_L_res$gam, SP_ECM_L_res$mix_ratio))
print(cbind(true_mu, true_gam, true_mix_ratio))
```

---

show_pvmm_curve   *Visualization of the result of spect_em_pvmm*

Description

Visualization of the result of spect_em_pvmm().

Usage

```
show_pvmm_curve(spect_em_pvmm_res, x, y, mix_ratio_init, mu_init, sigma_init, eta_init)
```

Arguments

spect_em_pvmm_res
: data set obtained by spect_em_pvmm()

x
: measurement steps

y
: intensity

mix_ratio_init
: initial values of the mixture ratio of the components

mu_init
: initial values of the mean of the components

sigma_init
: initial values of the standard deviation of the components

eta_init
: initial values of the mixing ratio of Gauss and Lorentz distribution

Details

Perform a visualization of fitting curve estimated by Pseudo-Voigt mixture model.

Value

Show the fitting curve and variation of the parameters.

References

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019). Spectrum adapted expectation-maximization algorithm for high-throughput peak shift analysis. Science and technology of advanced materials, 20(1), 733-745.

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2021). Spectrum adapted expectation-conditional maximization algorithm for extending high–throughput peak separation method in XPS analysis. Science and Technology of Advanced Materials: Methods, 1(1), 45-55.

Examples

```
#generating the synthetic spectral data based on three component Pseudo-Voigt mixture model.
x               <- seq(0, 100, by = 0.5)
true_mu         <- c(35, 50, 65)
true_sigma      <- c(3, 3, 3)
true_eta        <- c(0.3, 0.8, 0.5)
true_mix_ratio  <- rep(1/3, 3)
degree          <- 4

#Normalized Pseudo-Voigt distribution
  truncated_pv <- function(x, mu, sigma, eta) {
    (eta*dcauchy(x, mu, sqrt(2*log(2))*sigma) + (1-eta)*dnorm(x, mu, sigma)) /
      sum(eta*dcauchy(x, mu, sqrt(2*log(2))*sigma) + (1-eta)*dnorm(x, mu, sigma))
  }

y <- c(true_mix_ratio[1]*truncated_pv(x = x,
                                      mu = true_mu[1],
                                      sigma = true_sigma[1],
                                      eta = true_eta[1])*10^degree +
       true_mix_ratio[2]*truncated_pv(x = x,
```

```
                                      mu = true_mu[2],
                                      sigma = true_sigma[2],
                                      eta = true_eta[2])*10^degree +
       true_mix_ratio[3]*truncated_pv(x = x,
                                      mu = true_mu[3],
                                      sigma = true_sigma[3],
                                      eta = true_eta[3])*10^degree)

plot(y~x, main = "genrated synthetic spectral data")

#Peak fitting by EMpeaksR
#Initial values
K <- 3

mix_ratio_init  <- c(0.2, 0.4, 0.4)
mu_init         <- c(20, 40, 70)
sigma_init      <- c(2, 5, 4)
eta_init        <- c(0.5, 0.4, 0.3)

#Coducting calculation
SP_ECM_PV_res <- spect_em_pvmm(x = x,
                               y = y,
                               mu = mu_init,
                               sigma = sigma_init,
                               eta = eta_init,
                               mix_ratio = mix_ratio_init,
                               conv.cri = 1e-6,
                               maxit = 100000)

#Plot fitting curve and trace plot of parameters
show_pvmm_curve(SP_ECM_PV_res, x, y, mix_ratio_init, mu_init, sigma_init, eta_init)

#Showing the result of spect_em_pvmm()
print(cbind(c(mu_init), c(sigma_init), c(eta_init), c(mix_ratio_init)))
print(cbind(SP_ECM_PV_res$mu, SP_ECM_PV_res$sigma, SP_ECM_PV_res$eta, SP_ECM_PV_res$mix_ratio))
print(cbind(true_mu, true_sigma, true_eta, true_mix_ratio))
```

---

spect_em_dsgmm *Spectrum adapted ECM algorithm by DSGMM*

Description

Perform a peak fitting based on the spectrum adapted ECM algorithm by Doniach-Sunjic-Gauss mixture model.

Usage

```
spect_em_dsgmm(x, y, mu, sigma, alpha, eta, mix_ratio, conv.cri, maxit)
```

Arguments

`x`	measurement steps
`y`	intensity
`mu`	mean of the components
`sigma`	standard deviation of the components
`alpha`	asymmetric parameter of the component
`eta`	mixing ratio of Gauss and Lorentz distribution
`mix_ratio`	mixture ratio of the components
`conv.cri`	criterion of the convergence
`maxit`	maximum number of the iteration

Details

Peak fitting is conducted by spectrum adapted ECM algorithm.

Value

`mu`	estimated mean of the components
`sigma`	estimated standard deviation of the components
`alpha`	estimated asymmetric parameter of the components
`eta`	estimated mixing ratio of Gauss and Lorentz distribution
`mix_ratio`	estimated mixture ratio of the components
`it`	number of the iteration to reach the convergence
`LL`	variation of the weighted log likelihood values
`MU`	variation of mu
`SIGMA`	variation of sigma
`ALPHA`	variation of alpha
`ETA`	variation of beta
`MIX_RATIO`	variation of mix_ratio
`W_K`	decomposed component of the spectral data
`convergence`	message for the convergence in the calculation
`cal_time`	calculation time to complete the peak fitting. Unit is seconds

References

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019). Spectrum adapted expectation-maximization algorithm for high-throughput peak shift analysis. Science and technology of advanced materials, 20(1), 733-745.

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2021). Spectrum adapted expectation-conditional maximization algorithm for extending high–throughput peak separation method in XPS analysis. Science and Technology of Advanced Materials: Methods, 1(1), 45-55.

Examples

```
#generating the synthetic spectral data based on three component Doniach-Sunjic-Gauss mixture model.
x               <- seq(0, 100, by = 0.5)
true_mu         <- c(20, 50, 80)
true_sigma      <- c(3, 3, 3)
true_alpha      <- c(0.1, 0.3, 0.1)
true_eta        <- c(0.4, 0.6, 0.1)
true_mix_ratio  <- rep(1/3, 3)
degree          <- 4

#trancated Doniach-Sunjic-Gauss
truncated_dsg <- function(x, mu, sigma, alpha, eta) {
                 ((eta*(((gamma(1-alpha)) /
                 ((x-mu)^2+(sqrt(2*log(2))*sigma)^2)^((1-alpha)/2)) *
                 cos((pi*alpha/2)+(1-alpha)*atan((x-mu) /
                 (sqrt(2*log(2))*sigma))))) + (1-eta)*dnorm(x, mu, sigma)) /
                 sum( ((eta*(((gamma(1-alpha)) /
                 ((x-mu)^2+(sqrt(2*log(2))*sigma)^2)^((1-alpha)/2)) *
                 cos((pi*alpha/2)+(1-alpha)*atan((x-mu) /
                 (sqrt(2*log(2))*sigma))))) + (1-eta)*dnorm(x, mu, sigma)))
}

y <- c(true_mix_ratio[1]*truncated_dsg(x = x,
                                       mu = true_mu[1],
                                       sigma = true_sigma[1],
                                       alpha = true_alpha[1],
                                       eta = true_eta[1])*10^degree +
       true_mix_ratio[2]*truncated_dsg(x = x,
                                       mu = true_mu[2],
                                       sigma = true_sigma[2],
                                       alpha = true_alpha[2],
                                       eta = true_eta[2])*10^degree +
       true_mix_ratio[3]*truncated_dsg(x = x,
                                       mu = true_mu[3],
                                       sigma = true_sigma[3],
                                       alpha = true_alpha[3],
                                       eta = true_eta[3])*10^degree)

plot(y~x, main = "genrated synthetic spectral data")

#Peak fitting by EMpeaksR
#Initial values
K <- 3
mix_ratio_init <- c(0.2, 0.4, 0.4)
mu_init        <- c(20, 40, 70)
sigma_init     <- c(4, 3, 2)
alpha_init     <- c(0.3, 0.2, 0.4)
eta_init       <- c(0.5, 0.4, 0.3)

#Coducting calculation
SP_ECM_DSG_res <- spect_em_dsgmm(x = x,
                                 y = y,
```

```
                                  mu = mu_init,
                                  sigma = sigma_init,
                                  alpha = alpha_init,
                                  eta = eta_init,
                                  mix_ratio = mix_ratio_init,
                                  conv.cri = 1e-6,
                                  maxit = 100)

#Plot fitting curve and trace plot of parameters
show_dsgmm_curve(SP_ECM_DSG_res,
                 x,
                 y,
                 mix_ratio_init,
                 mu_init,
                 sigma_init,
                 alpha_init,
                 eta_init)

#Showing the result of spect_em_dsgmm()
print(cbind(c(mu_init),
            c(sigma_init),
            c(alpha_init),
            c(eta_init),
            c(mix_ratio_init)))

print(cbind(SP_ECM_DSG_res$mu,
            SP_ECM_DSG_res$sigma,
            SP_ECM_DSG_res$alpha,
            SP_ECM_DSG_res$eta,
            SP_ECM_DSG_res$mix_ratio))

print(cbind(true_mu,
            true_sigma,
            true_alpha,
            true_eta,
            true_mix_ratio))
```

`spect_em_gmm` *Spectrum adapted EM algorithm by GMM*

Description

Perform a peak fitting based on the spectrum adapted EM algorithm by Gaussian mixture model.

Usage

```
spect_em_gmm(x, y, mu, sigma, mix_ratio, conv.cri, maxit)
```

Arguments

x	measurement steps
y	intensity
mu	mean of the components
sigma	standard deviation of the components
mix_ratio	mixture ratio of the components
conv.cri	criterion of the convergence
maxit	maximum number of the iteration

Details

Peak fitting is conducted by spectrum adapted EM algorithm.

Value

mu	estimated mean of the components
sigma	estimated standard deviation of the components
mix_ratio	estimated mixture ratio of the components
it	number of the iteration to reach the convergence
LL	variation of the weighted log likelihood values
MU	variation of mu
SIGMA	variation of sigma
MIX_RATIO	variation of mix_ratio
W_K	decomposed component of the spectral data
convergence	message for the convergence in the calculation
cal_time	calculation time to complete the peak fitting. Unit is seconds

References

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019). Spectrum adapted expectation-maximization algorithm for high-throughput peak shift analysis. Science and technology of advanced materials, 20(1), 733-745.

Examples

```
#generating the synthetic spectral data based on three component Gausian mixture model.
x               <- seq(0, 100, by = 0.5)
true_mu         <- c(35, 50, 65)
true_sigma      <- c(3, 3, 3)
true_mix_ratio  <- rep(1/3, 3)
degree          <- 4

y <- c(true_mix_ratio[1] * dnorm(x = x, mean = true_mu[1], sd = true_sigma[1])*10^degree +
      true_mix_ratio[2] * dnorm(x = x, mean = true_mu[2], sd = true_sigma[2])*10^degree +
      true_mix_ratio[3] * dnorm(x = x, mean = true_mu[3], sd = true_sigma[3])*10^degree)
```

```
plot(y~x, main = "genrated synthetic spectral data")

#Peak fitting by EMpeaksR
#Initial values
K <- 3

mix_ratio_init  <- c(0.2, 0.4, 0.4)
mu_init         <- c(20, 40, 70)
sigma_init      <- c(2, 5, 4)

#Coducting calculation
SP_EM_G_res <- spect_em_gmm(x, y, mu = mu_init, sigma = sigma_init, mix_ratio = mix_ratio_init,
                            conv.cri = 1e-8, maxit = 100000)

#Plot fitting curve and trace plot of parameters
show_gmm_curve(SP_EM_G_res, x, y, mix_ratio_init, mu_init, sigma_init)

#Showing the result of spect_em_gmm()
print(cbind(c(mu_init), c(sigma_init), c(mix_ratio_init)))
print(cbind(SP_EM_G_res$mu, SP_EM_G_res$sigma, SP_EM_G_res$mix_ratio))
print(cbind(true_mu, true_sigma, true_mix_ratio))
```

---

spect_em_lmm *Spectrum adapted ECM algorithm by LMM*

Description

Perform a peak fitting based on the spectrum adapted ECM algorithm by Lorentz mixture model.

Usage

```
spect_em_lmm(x, y, mu, gam, mix_ratio, conv.cri, maxit)
```

Arguments

x	measurement steps
y	intensity
mu	mean of the components
gam	scale parameter of the components
mix_ratio	mixture ratio of the components
conv.cri	criterion of the convergence
maxit	maximum number of the iteration

Details

Peak fitting is conducted by spectrum adapted ECM algorithm.

Value

mu	estimated mean of the components
gam	estimated scale parameter of the components
mix_ratio	estimated mixture ratio of the components
it	number of the iteration to reach the convergence
LL	variation of the weighted log likelihood values
MU	variation of mu
GAM	variation of gam
MIX_RATIO	variation of mix_ratio
W_K	decomposed component of the spectral data
convergence	message for the convergence in the calculation
cal_time	calculation time to complete the peak fitting. Unit is seconds

References

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019). Spectrum adapted expectation-maximization algorithm for high-throughput peak shift analysis. Science and technology of advanced materials, 20(1), 733-745.

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2021). Spectrum adapted expectation-conditional maximization algorithm for extending high–throughput peak separation method in XPS analysis. Science and Technology of Advanced Materials: Methods, 1(1), 45-55.

Examples

```
#generating the synthetic spectral data based on three component Lorentz mixture model.
x               <- seq(0, 100, by = 0.5)
true_mu         <- c(35, 50, 65)
true_gam        <- c(3, 3, 3)
true_mix_ratio  <- rep(1/3, 3)
degree          <- 4

#Normalized Lorentz distribution
dCauchy <- function(x, mu, gam) {
    (dcauchy(x, mu, gam)) / sum(dcauchy(x, mu, gam))
  }

y <- c(true_mix_ratio[1] * dCauchy(x = x, mu = true_mu[1], gam = true_gam[1])*10^degree +
       true_mix_ratio[2] * dCauchy(x = x, mu = true_mu[2], gam = true_gam[2])*10^degree +
       true_mix_ratio[3] * dCauchy(x = x, mu = true_mu[3], gam = true_gam[3])*10^degree)

plot(y~x, main = "genrated synthetic spectral data")

#Peak fitting by EMpeaksR
#Initial values
K <- 3

mix_ratio_init  <- c(0.2, 0.4, 0.4)
```

```
mu_init         <- c(20, 40, 70)
gam_init        <- c(2, 5, 4)

#Coducting calculation
SP_ECM_L_res <- spect_em_lmm(x, y, mu = mu_init, gam = gam_init, mix_ratio = mix_ratio_init,
                             conv.cri = 1e-6, maxit = 100000)

#Plot fitting curve and trace plot of parameters
show_lmm_curve(SP_ECM_L_res, x, y, mix_ratio_init, mu_init, gam_init)

#Showing the result of spect_em_lmm()
print(cbind(c(mu_init), c(gam_init), c(mix_ratio_init)))
print(cbind(SP_ECM_L_res$mu, SP_ECM_L_res$gam, SP_ECM_L_res$mix_ratio))
print(cbind(true_mu, true_gam, true_mix_ratio))
```

`spect_em_pvmm` *Spectrum adapted ECM algorithm by PVMM*

Description

Perform a peak fitting based on the spectrum adapted ECM algorithm by Pseudo-Voigt mixture model.

Usage

```
spect_em_pvmm(x, y, mu, sigma, eta, mix_ratio, conv.cri, maxit)
```

Arguments

x	measurement steps
y	intensity
mu	mean of the components
sigma	standard deviation of the components
eta	mixing ratio of Gauss and Lorentz distribution
mix_ratio	mixture ratio of the components
conv.cri	criterion of the convergence
maxit	maximum number of the iteration

Details

Peak fitting is conducted by spectrum adapted ECM algorithm.

Value

mu	estimated mean of the components
sigma	estimated standard deviation of the components
eta	estimated mixing ratio of Gauss and Lorentz distribution
mix_ratio	estimated mixture ratio of the components
it	number of the iteration to reach the convergence
LL	variation of the weighted log likelihood values
MU	variation of mu
SIGMA	variation of sigma
ETA	variation of beta
MIX_RATIO	variation of mix_ratio
W_K	decomposed component of the spectral data
convergence	message for the convergence in the calculation
cal_time	calculation time to complete the peak fitting. Unit is seconds

References

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2019). Spectrum adapted expectation-maximization algorithm for high-throughput peak shift analysis. Science and technology of advanced materials, 20(1), 733-745.

Matsumura, T., Nagamura, N., Akaho, S., Nagata, K., & Ando, Y. (2021). Spectrum adapted expectation-conditional maximization algorithm for extending high–throughput peak separation method in XPS analysis. Science and Technology of Advanced Materials: Methods, 1(1), 45-55.

Examples

```
#generating the synthetic spectral data based on three component Pseudo-Voigt mixture model.
x               <- seq(0, 100, by = 0.5)
true_mu         <- c(35, 50, 65)
true_sigma      <- c(3, 3, 3)
true_eta        <- c(0.3, 0.8, 0.5)
true_mix_ratio  <- rep(1/3, 3)
degree          <- 4

#Normalized Pseudo-Voigt distribution
  truncated_pv <- function(x, mu, sigma, eta) {
    (eta*dcauchy(x, mu, sqrt(2*log(2))*sigma) + (1-eta)*dnorm(x, mu, sigma)) /
      sum(eta*dcauchy(x, mu, sqrt(2*log(2))*sigma) + (1-eta)*dnorm(x, mu, sigma))
  }

y <- c(true_mix_ratio[1]*truncated_pv(x = x,
                                      mu = true_mu[1],
                                      sigma = true_sigma[1],
                                      eta = true_eta[1])*10^degree +
       true_mix_ratio[2]*truncated_pv(x = x,
                                      mu = true_mu[2],
```

```
                                    sigma = true_sigma[2],
                                    eta = true_eta[2])*10^degree +
       true_mix_ratio[3]*truncated_pv(x = x,
                                    mu = true_mu[3],
                                    sigma = true_sigma[3],
                                    eta = true_eta[3])*10^degree)

plot(y~x, main = "genrated synthetic spectral data")

#Peak fitting by EMpeaksR
#Initial values
K <- 3

mix_ratio_init  <- c(0.2, 0.4, 0.4)
mu_init         <- c(20, 40, 70)
sigma_init      <- c(2, 5, 4)
eta_init        <- c(0.5, 0.4, 0.3)

#Coducting calculation
SP_ECM_PV_res <- spect_em_pvmm(x = x,
                               y = y,
                               mu = mu_init,
                               sigma = sigma_init,
                               eta = eta_init,
                               mix_ratio = mix_ratio_init,
                               conv.cri = 1e-6,
                               maxit = 100000)

#Plot fitting curve and trace plot of parameters
show_pvmm_curve(SP_ECM_PV_res, x, y, mix_ratio_init, mu_init, sigma_init, eta_init)

#Showing the result of spect_em_pvmm()
print(cbind(c(mu_init), c(sigma_init), c(eta_init), c(mix_ratio_init)))
print(cbind(SP_ECM_PV_res$mu, SP_ECM_PV_res$sigma, SP_ECM_PV_res$eta, SP_ECM_PV_res$mix_ratio))
print(cbind(true_mu, true_sigma, true_eta, true_mix_ratio))
```

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