

# Package ‘SoilHyP’

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**Type** Package

**Title** Soil Hydraulic Properties

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**Description** Provides functions for (1) soil water retention (SWC) and unsaturated hydraulic conductivity (Ku) (van Genuchten-Mualem (vGM or vG) [1, 2], Peters-Durner-Iden (PDI) [3, 4, 5]), (2) fitting of parameter for SWC and/or Ku using Shuffled Complex Evolution (SCE) optimisation and (3) calculation of soil hydraulic properties (Ku and soil water contents) based on the simplified evaporation method (SEM) [6, 7].

Main references:

[1] van Genuchten (1980) <doi:10.2136/sssaj1980.03615995004400050002x>,

[2] Mualem (1976) <doi:10.1029/WR012i003p00513>,

[3] Peters (2013) <doi:10.1002/wrcr.20548>,

[4] Iden and Durner (2013) <doi:10.1002/2014WR015937>,

[5] Peters (2014) <doi:10.1002/2014WR015937>,

[6] Wind G. P. (1966) and

[7] Peters and Durner (2008) <doi:10.1016/j.jhydrol.2008.04.016>.

**BugReports** <https://bitbucket.org/UlliD/soilhyp/issues>

**Encoding** UTF-8

**License** GPL (>= 2)

**Depends** R (>= 3.4.0)

**RoxygenNote** 6.1.1

**NeedsCompilation** no

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Felix Andrews [ctb] (For the code copied from the hydromad::SCEoptim function (Version: 0.9-15) which is not on r-cran

(<https://github.com/floybix/hydromad>). The SCEoptim function is

adapted, and substantially revised from Brecht Donckels MATLAB code which is in turn adopted from Qingyun Duans MATLAB code),

Brecht Donckels [ctb] (For the Matlab code which was adapted and revised in the hydromad::SCEoptim function.),

Qingyun Duan [ctb] (For the MATLAB code adapted from Brecht Donckels.)

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AIC_HY	<i>Akaike Information Criterion (AIC)</i>
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### Description

Akaike Information Criterion with or without correction term. Expression from Ye et al. (2008). Correction term by Hurvich and Tsai (1989).

### Usage

```
AIC_HY(Phi, n.data, n.par, corr = TRUE)
```

### Arguments

Phi	objective function value
n.data	number of measured data
n.par	number of adjustable parameters
corr	correction term TRUE or FALSE (see details)

**Details**

corr:

If number of measurements is small compared to the number of parameters, AIC can be extended by a correction term.

**References**

Ye, M., P.D. Meyer, and S.P. Neuman (2008): On model selection criteria in multimodel analysis. *Water Resources Research* 44 (3) W03428, doi:10.1029/2008WR006803.

Hurvich, C., and C. Tsai (1989): Regression and time series model selection in small samples. *Biometrika* 76 (2), 297–307, doi:10.1093/biomet/76.2.297.

Peters and Durner (2015): SHYPFIT 2.0 User's Manual.

Akaike, H. (1974): A new look at statistical model identification, *IEEE Trans. Autom. Control*, AC-19, 716–723.

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BIC\_HY

*Bayesian Information Criterion (BIC)*

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**Description**

Bayesian Information Criterion (Schwarz, 1978) for least square estimations.

**Usage**

BIC\_HY(Phi, n.data, n.par)

**Arguments**

Phi	objective function value
n.data	number of measured data
n.par	number of adjustable parameters

**References**

Ye, M., P.D. Meyer, and S.P. Neuman (2008): On model selection criteria in multimodel analysis. *Water Resources Research* 44 (3) W03428, doi:10.1029/2008WR006803.

Schwarz, G. (1978): Estimating the dimension of a model. *The Annals of Statistics* 6 (2), 461–464. URL: <http://dx.doi.org/10.1214/aos/1176344136>.

Peters and Durner (2015): SHYPFIT 2.0 User's Manual.

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dataSEM	<i>Evaporation experiment data</i>
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**Description**

Example data of an Evaporation experiment

**Usage**

```
data(dataSEM)
```

**Format**

An object of class `data.frame` with 332 rows and 4 columns.

**Details****Columns:**

hour: time [hour]

weight: total weight of soil sample [g]

tens.up: measurements of upper tensiometer [cm]

tens.bot: measurements of lower tensiometer [cm]

---

dataSHP	<i>Soil hydraulic property data</i>
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**Description**

Soil hydraulic property data including soil water contents (th), unsaturated hydraulic conductivities (Ku) and the corresponding suctions/pressure heads.

**Usage**

```
data(dataSHP)
```

**Format**

An object of class `data.frame` with 331 rows and 3 columns.

**Details****Columns:**

Ku: unsaturated hydraulic conductivity

th: volumetric water content

suc: suction

fitSHP

*Fit soil hydraulic properties***Description**

Estimate parameter for soil water retention (SWC) and/or unsaturated hydraulic conductivity function (Ku) using Shuffled Complex Evolution (SCE) optimisation. Parameter can be estimated for van Genuchten-Mualem (vg or vgm) or Peters-Durner-Iden (PDI) parameterisation of the soil hydraulic properties.

**Usage**

```
fitSHP(obs = list(th = NULL, K = NULL), suc = list(th = NULL, K =
  NULL), par = NULL, lower = NULL, upper = NULL, FUN.shp = "vg",
  modality = "uni", par.shp = NULL, fit = "both",
  weighting = "var", log = c("alfa", "n", "ks"),
  control = list(ncomplex = 15, reltol = 1e-07, tolsteps = 7),
  suc.negativ = TRUE, integral = FALSE, L = NULL,
  print.info = TRUE)
```

**Arguments**

obs	list with named observations (th for water content and K for unsaturated hydraulic conductivity data)
suc	list of named suctions corresponding to th and/or K
par	a numeric vector of initial parameter values (see also <a href="#">SCEoptim</a> ). If missing default values are set.
lower	lower bounds on the parameters. Should be the same length as par and as upper, or length 1 if a bound applies to all parameters. If missing default values are set.
upper	upper bounds on the parameters. Should be the same length as par and as lower, or length 1 if a bound applies to all parameters. If missing default values are set.
FUN.shp	Funktion for soil hydraulic properties (vG or PDI) (see <a href="#">SWC</a> or <a href="#">Ku</a> )
modality	pore size distribution ('uni' or 'bi')
par.shp	fixed parameter value named in list or vector
fit	fit parameter for 'SWC', 'Ku' or 'both' simultaneous.
weighting	weighting between SWC and Ku. Used if fit == both ('var', 'norm' or '2step').
log	names of parameter in list or vector which should be logarithmized during optimization
control	a list of options as in <code>optim()</code> , see <a href="#">SCEoptim</a>
suc.negativ	set TRUE if suction/pressure heads are negative and FALSE if positive
integral	th as point value vs. <code>suc(h)</code> (FALSE) or th as mean water content over the column divided by the height (L) vs. <code>suc(h)</code> (TRUE) (see details).
L	sample height [cm]. Only needed for <code>integral == TRUE</code>
print.info	print information about default values for par, lower, and upper if missing or fitting accuracy (TRUE or FALSE)

## Details

- weighting:** var: th and K are weighted in the objective function by the measurement variance  
 norm: th and K are normed in objective function  
 2step: the parameter for th are fitted first and the remaining parameter for K afterwards
- log:** The use of log is suggested for parameter 'alfa', 'n' and 'ks' for modality == 'uni'. For modality 'bi' additional 'alfa2' and 'n2' and for Fun.shp == 'pdi' additional 'omega'. Parameter in output (\$par) are not returned logarithmized.  
 Default parameter values for par, lower and upper are logarithmized automatically  
 If not the default values for par, lower and upper are taken, parameter which are named in 'log' must be scaled by the user in par, lower and upper.
- integral:** The "integral" method is suggested from Peters and Durner (2008, 2015) to fit parameter on data from experiments where water contents are measured as mean water contents (e.g. simplified evaporation method or multi-step outflow experiments). Under the assumption that the water content is distributed linear over the column, the measured mean water content of the column is the integral over the whole column divided by the column length (L). Under hydraulic equilibrium this is equal to the integral of the retention function over the matric heads from the lower boundary to the upper boundary of the column divided by the height of the column (Peters 2008, 2015).
- integral == TRUE can be very slow.

## Value

"fitSHP" class

## Author(s)

Ullrich Dettmann

## References

- Peters, A., & Durner, W. (2008). Simplified evaporation method for determining soil hydraulic properties. *Journal of Hydrology*, 356(1), 147-162.
- Peters and Durner (2015). SHYPPFIT 2.0 User's Manual
- Peters, A., Iden, S. C., & Durner, W. (2015). Revisiting the simplified evaporation method: Identification of hydraulic functions considering vapor, film and corner flow. *Journal of Hydrology*, 527, 531-542.

## See Also

[SCEoptim](#), [SWC](#), [Ku](#)

## Examples

```
## Not run:
data('dataSHP')
# -----
```

```

# fit Soil Hydraulic Properties (SHP)
# -----
ans <- fitSHP(obs      = list(th = dataSHP$th, K = dataSHP$Ku),
             suc      = list(th = dataSHP$suc, K = dataSHP$suc),
             FUN.shp  = 'vg',
             modality = 'uni',
             par.shp  = NULL,
             fit      = 'both',
             weighting = 'var',
             log      = c('alfa', 'n', 'ks'),
             control  = list(ncomplex = 15, reltol = 1e-07, tolsteps = 7),
             suc.negativ = TRUE,
             integral = FALSE,
             L        = 0,
             print.info = TRUE
           )
ans$par
plot(ans)
# -----
# bimodal van Genuchten-Mualem
ans <- fitSHP(obs      = list(th = dataSHP$th, K = dataSHP$Ku),
             suc      = list(th = dataSHP$suc, K = dataSHP$suc),
             FUN.shp  = 'vg',
             modality = 'bi',
             par.shp  = c(),
             fit      = 'both',
             weighting = 'var',
             log      = c('alfa', 'n', 'ks', 'alfa2', 'n2'),
             suc.negativ = TRUE,
             integral = FALSE,
             L        = 0,
             print.info = TRUE,
             control  = list(ncomplex = 15, reltol = 1e-07, tolsteps = 7)
           )
ans$par
plot(ans)

## End(Not run)

```

---

Kcap

*Relative capillary conductivity*


---

### Description

Relative capillary conductivity based on Mualem's conductivity model for unimodal or bimodal van Genuchten-Mualem.

### Usage

Kcap(suc, par.shp, suc.negativ = TRUE, modality = "uni")

**Arguments**

suc	Suction/pressure heads. Negative if suc.negative = TRUE
par.shp	named parameter in list or vector
suc.negative	set TRUE if suction/pressure heads are negative and FALSE if positive
modality	pore size distributions ('uni' or 'bi')

**Details**

**par.shp:** alfa [1/L]: van Genuchten shape parameter  
 n [-]: van Genuchten shape parameter  
 m [-]: shape parameter ( $m = 1 - (1/n)$  if missing)  
 tau [-]: tortuosity and connectivity parameter (minimum -1 or -2 for the PDI model; for details see Peters (2014))  
 h0 [L]: suction at water content of 0 (i.e. oven dryness) ( $h_0 = 10^{6.8}$  if missing, corresponding to oven dryness at 105°C (Schneider and Goss, 2012))

additional for bimodal (modality == 'bi')

w2 [-]: weighting between pore space distribution  
 alfa2 [1/L]: van Genuchten parameter alfa for second pore space distribution  
 n2 [-]: van Genuchten parameter n for second pore space distribution

**References**

- Peters, A. (2014). Reply to comment by S. Iden and W. Durner on Simple consistent models for water retention and hydraulic conductivity in the complete moisture range. *Water Resour. Res.* 50, 7535–7539.
- Van Genuchten, M. T. (1980). A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil science society of America journal*, 44(5), 892-898.
- Mualem, Y. (1976). A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water resources research*, 12(3), 513-522.
- Schneider, M., & Goss, K. U. (2012). Prediction of the water sorption isotherm in air dry soils. *Geoderma*, 170, 64-69.

**See Also**

[Ku](#)

---

Kfilm

*Relative film conductivity*

---

**Description**

Relative film conductivity described by Peters (2013).



**Usage**

```
Kfilm(suc, par.shp, modality = "uni", suc.negativ = TRUE)
```

**Arguments**

suc	Suction/pressure heads. Negative if suc.negativ = TRUE
par.shp	named parameter in list or vector
modality	pore size distribution ('uni' or 'bi')
suc.negativ	set TRUE if suction/pressure heads are negative and FALSE if positive

**Details**

**par.shp:** ths [-]: saturated water content  
 thr [-]: residual water content  
 alfa [1/L]: van Genuchten shape parameter  
 n [-]: van Genuchten shape parameter  
 h0 [L]: suction at water content of 0 (i.e. oven dryness) (h0 = 10<sup>6.8</sup> if missing, corresponding to oven dryness at 105°C (Schneider and Goss, 2012))  
 a: slope at the log scale (a = -1.5 if missing as suggested by Tokunaga (2009) and Peters (2013))

additional for bimodal (modality == 'bi'):  
 alfa2 [1/L]: van Genuchten parameter alfa for second pore space distribution  
 n2 [-]: van Genuchten parameter n for second pore space distribution

**References**

- Peters, A. (2013). Simple consistent models for water retention and hydraulic conductivity in the complete moisture range. *Water Resour. Res.* 49, 6765–6780. physics-a review. *Vadose Zone J.* <http://dx.doi.org/10.2136/vzj2012.0163>.
- Tokunaga, T. K. (2009). Hydraulic properties of adsorbed water films in unsaturated porous media. *Water resources research*, 45(6).
- Schneider, M., & Goss, K. U. (2012). Prediction of the water sorption isotherm in air dry soils. *Geoderma*, 170, 64-69.

**See Also**

[Ku](#)

---

Ku *Unsaturated hydraulic conductivity*

---

### Description

Calculates unsaturated hydraulic conductivity for a given suction for unimodal or bimodal van Genuchten-Mualem (vg/vgm) or Peters-Durner-Iden (PDI) parameterisation.

### Usage

```
Ku(suc, FUN.shp = "vG", par.shp, modality = "uni",
   suc.negativ = TRUE)
```

### Arguments

suc	Suction/pressure heads. Negative if suc.negativ = TRUE
FUN.shp	Funktion for soil hydraulic properties (vGM or PDI) (see details)
par.shp	named parameter in list or vector
modality	pore size distribution ('uni' or 'bi')
suc.negativ	set TRUE if suction/pressure heads are negative and FALSE if positive

### Details

**FUN.shp:** vGM: van Genuchten-Mualem (uni or bimodal) ('vg' works aswell)  
PDI: Peters-Durner-Iden with van Genuchtens saturation function (uni or bimodal)

**par.shp:** ths [-]: saturated water content  
thr [-]: residual water content  
alfa [1/L]: van Genuchten shape parameter  
n [-]: van Genuchten shape parameter  
m [-]: shape parameter (m = 1-(1/n) if missing)  
Ks [L/time]: saturated hydraulic conductivity  
tau [-]: tortuosity and connectivity parameter (minimum -1 or -2 for the PDI model; see Peters (2014) for details)

additional for 'PDI':

omega: weighting between relative capillary and film conductivity  
h0 [L]: suction at water content of 0 (i.e. oven dryness) (h0 = 10<sup>6.8</sup> if missing, corresponding to oven dryness at 105°C (Schneider and Goss, 2012))  
a: slope at the log scale (a = -1.5 if missing as suggested by Tokunaga (2009) and Peters (2013))

additional for bimodal (modality == 'bi'):

w2 [-]: weigthing between pore space distributions  
alfa2 [1/L]: van Genuchten parameter alfa for second pore space distribution  
n2 [-]: van Genuchten parameter n for second pore space distribution

most input works for upper- and lowercase letters

**Value**

unsaturated hydraulic conductivity (ku)

**Author(s)**

Ullrich Dettmann

**References**

- Van Genuchten, M. T. (1980). A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil science society of America journal*, 44(5), 892-898.
- Mualem, Y. (1976). A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water resources research*, 12(3), 513-522.
- Peters, A. (2013). Simple consistent models for water retention and hydraulic conductivity in the complete moisture range. *Water Resour. Res.* 49, 6765–6780. physics-a review. *Vadose Zone J.* <http://dx.doi.org/10.2136/vzj2012.0163>.
- Iden, S., Durner, W. (2014). Comment to Simple consistent models for water retention and hydraulic conductivity in the complete moisture range by A. Peters. *Water Resour. Res.* 50, 7530–7534.
- Peters, A. (2014). Reply to comment by S. Iden and W. Durner on Simple consistent models for water retention and hydraulic conductivity in the complete moisture range. *Water Resour. Res.* 50, 7535–7539.
- Tokunaga, T. K. (2009), Hydraulic properties of adsorbed water films in unsaturated porous media, *Water Resour. Res.*, 45, W06415, doi: 10.1029/2009WR007734.
- Priesack, E., Durner, W., 2006. Closed-form expression for the multi-modal unsaturated conductivity function. *Vadose Zone J.* 5, 121–124.
- Durner, W. (1994). Hydraulic conductivity estimation for soils with heterogeneous pore structure. *Water Resources Research*, 30(2), 211-223.
- Schneider, M., & Goss, K. U. (2012). Prediction of the water sorption isotherm in air dry soils. *Geoderma*, 170, 64-69.

**See Also**

[SWC and Sat](#)

**Examples**

```
# -----
# Unimodal van Genuchten
# -----
Ku(suc = seq(1, 1000, by = 1), FUN.shp = 'vGM',
  par.shp = list(Ks = 10, ths = 0.5, thr = 0, alfa = 0.02, n = 1.5, tau = 0.5),
  modality = 'uni', suc.negative = FALSE)
# -----
# Bimodal van Genuchten
# -----
Ku(suc = seq(1, 1000, by = 1), FUN.shp = 'vGM',
  par.shp = list(Ks = 10, ths = 0.5, thr = 0, alfa = 0.02,
```

```

n = 1.5, tau = 0.5, w2 = 0.1, alfa2 = 0.1, n2 = 3),
modality = 'bi', suc.negativ = FALSE)
# -----
# Unimodal Peters-Durner-Iden (PDI)
# -----
Ku(suc = seq(1, 1000, by = 1), FUN.shp = 'PDI', modality = 'uni',
par.shp = list(Ks = 10, ths = 0.5, thr = 0, alfa = 0.02, n = 1.5, tau = 0.5, omega = 0.001),
suc.negativ = FALSE)

```

---

NSE	<i>Nash-Sutcliffe efficiency (NSE)</i>
-----	--

---

### Description

Nash-Sutcliffe efficiency (NSE)

### Usage

```
NSE(obs, sim)
```

### Arguments

obs	measured values
sim	predicted values

### References

Nash, J. E., and J.V. Sutcliffe (1970): River flow forecasting through conceptual models. 1. a discussion of principles. *Journal of Hydrology* 10, 282–290.

---

plot.fitSHP	<i>Plot fitSHP object</i>
-------------	---------------------------

---

### Description

Creates plot of fitSHP object with measured and fitted SWC, KU or both depending on fitSHP object

### Usage

```
## S3 method for class 'fitSHP'
plot(x, ...)
```

### Arguments

x	object of class fitSHP
...	arguments for plot

---

predict.fitSHP	<i>Predict values using fitSHP object</i>
----------------	---

---

**Description**

Predicts values using fitSHP object with calibrated parameter of SWC, KU or both depending on the fitSHP object

**Usage**

```
## S3 method for class 'fitSHP'
predict(object, suc = NULL, length.out = 100,
        suc.negativ = FALSE, ...)
```

**Arguments**

object	object of class fitSHP
suc	Suction/pressure heads for the prediction of the soil hydraulic properties
length.out	output length if suc == NULL
suc.negativ	set TRUE if suction/pressure heads are negative and FALSE if positive
...	arguments for predict

---

RMSE	<i>Root mean square error (RMSE)</i>
------	--------------------------------------

---

**Description**

Calculate Root mean square error (RMSE)

**Usage**

```
RMSE(obs, sim)
```

**Arguments**

obs	measured values
sim	predicted values

Sad

*Relative saturation function***Description**

Relative saturation function for adsorptive water storage described by a piecewise linear function (Iden and Durner, 2014).

**Usage**

```
Sad(suc, par.shp, modality = c("uni"), suc.negativ = TRUE)
```

**Arguments**

suc	Suction/pressure heads. Negative if suc.negativ = TRUE
par.shp	named parameter of soil hydraulic properties in list or vector (see details)
modality	pore size distribution ('uni' or 'bi')
suc.negativ	set TRUE if suction/pressure heads are negative and FALSE if positive

**Details**

**par.shp:** ths [-]: saturated water content  
 thr [-]: residual water content  
 alfa [1/L]: van Genuchten shape parameter  
 n [-]: van Genuchten shape parameter  
 h0 [L]: suction at water content of 0 (i.e. oven dryness) (h0 = 10<sup>6.8</sup> if missing, corresponding to oven dryness at 105°C (Schneider and Goss, 2012))

additional for bimodal (modality == 'bi'):  
 alfa2 [1/L]: van Genuchten parameter alfa for second pore space distribution  
 n2 [-]: van Genuchten parameter n for second pore space distribution

**Author(s)**

Ullrich Dettmann

**References**

Iden, S., Durner, W. (2014). Comment to Simple consistent models for water retention and hydraulic conductivity in the complete moisture range by A. Peters. *Water Resour. Res.* 50, 7530–7534.

Schneider, M., & Goss, K. U. (2012). Prediction of the water sorption isotherm in air dry soils. *Geoderma*, 170, 64-69.

---

Sat *Capillary saturation function*

---

**Description**

Capillary saturation function of van Genuchten for unimodal or bimodal pore space distributions.

**Usage**

```
Sat(suc, par.shp, modality = c("uni"), suc.negativ = TRUE)
```

**Arguments**

suc                    Suction/pressure heads. Negative if suc.negativ = TRUE  
 par.shp                named parameter in list or vector  
 modality               pore size distribution ('uni' or 'bi')  
 suc.negativ            set TRUE if suction/pressure heads are negative and FALSE if positive

**Details**

**par.shp:** alfa [1/L]: van Genuchten shape parameter  
 n [-]: van Genuchten shape parameter  
 m [-]: shape parameter ( $m = 1 - (1/n)$  if missing)  
 additional for bimodal (modality == 'bi'):  
 w2 [-]: weighing between pore space distribution  
 alfa2 [1/L]: van Genuchten parameter alfa for second pore space distribution  
 n2 [-]: van Genuchten parameter n for second pore space distribution

**References**

Van Genuchten, M. T. (1980). A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil science society of America journal*, 44(5), 892-898.  
 Durner, W. (1994). Hydraulic conductivity estimation for soils with heterogeneous pore structure. *Water Resources Research*, 30(2), 211-223.

---

Scap *Rescaled capillary saturation function*

---

**Description**

Rescaled capillary saturation function by Iden and Durner (2014)

**Usage**

```
Scap(suc, par.shp, modality = c("uni"), suc.negativ = FALSE)
```

**Arguments**

suc	Suction/pressure heads. Negative if suc.negativ = TRUE
par.shp	named parameter in list or vector
modality	pore size distribution ('uni' or 'bi')
suc.negativ	set TRUE if suction/pressure heads are negative and FALSE if positive

**Details**

**par.shp:** alfa [1/L]: van Genuchten shape parameter  
 n [-]: van Genuchten shape parameter  
 m [-]: shape parameter ( $m = 1 - (1/n)$  if missing)  
 h0 [L]: suction at water content of 0 (i.e. oven dryness) ( $h_0 = 10^{6.8}$  if missing, corresponding to oven dryness at 105°C (Schneider and Goss, 2012))

additional for bimodal ('bi') pore size distribution:  
 w2 [-]: weighing between pore space distribution  
 alfa2 [1/L]: van Genuchten parameter alfa for second pore space distribution  
 n2 [-]: van Genuchten parameter n for second pore space distribution  
 m2 [-]: shape parameter ( $m = 1 - (1/n_2)$  if missing)

$$\text{Scap}(h) = (\text{Gamma}(h) - \text{Gamma}(h_0)) / (1 - \text{Gamma}(h_0))$$

Gamma describes the capillary saturation function. Here the saturation function of van Genuchten is used:

$$\text{gamma}(h) = (1 / (1 + \text{suc} * \text{alfa}^n))^m \text{ (see also [Sat](#))}$$
**References**

Iden, S., Durner, W. (2014). Comment to Simple consistent models for water retention and hydraulic conductivity in the complete moisture range by A. Peters. *Water Resour. Res.* 50, 7530–7534.

Schneider, M., & Goss, K. U. (2012). Prediction of the water sorption isotherm in air dry soils. *Geoderma*, 170, 64-69.

**Description**

Shuffled Complex Evolution (SCE) optimisation. Designed to have a similar interface to the standard [optim](#) function.

The function is copied from the hydromad package (<https://github.com/floybix/hydromad/>)



**Usage**

```
SCEoptim(FUN, par, lower = -Inf, upper = Inf, control = list(), ...)
```

**Arguments**

<code>FUN</code>	function to optimise (to minimise by default), or the name of one. This should return a scalar numeric value.
<code>par</code>	a numeric vector of initial parameter values.
<code>lower</code>	lower bounds on the parameters. Should be the same length as <code>par</code> and as <code>upper</code> , or length 1 if a bound applies to all parameters.
<code>upper</code>	upper bounds on the parameters. Should be the same length as <code>par</code> and as <code>lower</code> , or length 1 if a bound applies to all parameters.
<code>control</code>	a list of options as in <code>optim()</code> , see Details.
<code>...</code>	further arguments passed to <code>FUN</code>

**Details**

This is an evolutionary algorithm combined with a simplex algorithm.

Options can be given in the list `control`, in the same way as with `optim`:

**ncomplex** number of complexes. Defaults to 5.

**cce.iter** number of iteration in inner loop (CCE algorithm). Defaults to NA, in which case it is taken as  $2 * \text{NDIM} + 1$ , as recommended by Duan et al (1994).

**fnscale** function scaling factor (set to -1 for a maximisation problem). By default it is a minimisation problem.

**elitism** influences sampling of parents from each complex. Duan et al (1992) describe a 'trapezoidal' (i.e. linear weighting) scheme, which corresponds to `elitism` = 1. Higher values give more weight towards the better parameter sets. Defaults to 1.

**initsample** sampling scheme for initial values: "latin" (hypercube) or "random". Defaults to "latin".

**reltol** `reltol` is the convergence threshold: relative improvement factor required in an SCE iteration (in same sense as `optim`), and defaults to  $1e-5$ .

`tolsteps` is the number of iterations where the improvement is within `reltol` required to confirm convergence. This defaults to 7.

**tolsteps** `reltol` is the convergence threshold: relative improvement factor required in an SCE iteration (in same sense as `optim`), and defaults to  $1e-5$ .

`tolsteps` is the number of iterations where the improvement is within `reltol` required to confirm convergence. This defaults to 7.

**maxit** maximum number of iterations. Defaults to 10000.

**maxeval** maximum number of function evaluations. Defaults to Inf.

**maxtime** maximum duration of optimization in seconds. Defaults to Inf.

**returnpop** whether to return populations (parameter sets) from all iterations. Defaults to FALSE.

**trace** an integer specifying the level of user feedback. Defaults to 0.

**REPORT** number of iterations between reports when `trace`  $\geq$  1. Defaults to 1.

**Value**

a list of class "SCEoptim".

par	optimal parameter set.
value	value of objective function at optimal point.
convergence	code, where 0 indicates successful coverage.
message	(non-)convergence message.
counts	number of function evaluations.
iterations	number of iterations of the CCE algorithm.
time	number of seconds taken.
POP.FIT.ALL	objective function values from each iteration in a matrix.
BESTMEM.ALL	best parameter set from each iteration in a matrix.
POP.ALL	if (control\$returnpop = TRUE), the parameter sets from each iteration are returned in a three dimensional array.
control	the list of options settings in effect.

**Author(s)**

This code is copied from the hydromad package

<https://github.com/floybix/hydromad/>  
<http://hydromad.catchment.org/>

and written from Felix Andrews <felix@nfrac.org>

who adapted, and substantially revised it, from Brecht Donckels' MATLAB code, which was in turn adapted from Qingyun Duan's MATLAB code:

**References**

Qingyun Duan, Soroosh Sorooshian and Vijai Gupta (1992). Effective and Efficient Global Optimization for Conceptual Rainfall-Runoff Models *Water Resources Research* 28(4), pp. 1015-1031.

Qingyun Duan, Soroosh Sorooshian and Vijai Gupta (1994). Optimal use of the SCE-UA global optimization method for calibrating watershed models, *Journal of Hydrology* 158, pp. 265-284.

**See Also**

[optim](#), [DEoptim](#) package, [rgenoud](#) package

## Examples

```
## reproduced from help("optim")

## Rosenbrock Banana function
Rosenbrock <- function(x){
  x1 <- x[1]
  x2 <- x[2]
  100 * (x2 - x1 * x1)^2 + (1 - x1)^2
}
#lower <- c(-10,-10)
#upper <- -lower
ans <- SCEoptim(Rosenbrock, c(-1.2,1), control = list(trace = 1))
str(ans)

## 'Wild' function, global minimum at about -15.81515
Wild <- function(x)
  10*sin(0.3*x)*sin(1.3*x^2) + 0.00001*x^4 + 0.2*x+80
ans <- SCEoptim(Wild, 0, lower = -50, upper = 50,
  control = list(trace = 1))
ans$par
```

---

SEM

*Simplified evaporation method (SEM)*


---

## Description

Determines unsaturated hydraulic conductivity and water retention characteristics from laboratory evaporation experiments.

## Usage

```
SEM(suc.up, suc.low, weight = NULL, t, ths = NULL, r = 3.6, L = 6,
  z1 = 1.5, z2 = 4.5, sd.tens = 0.2, suc.negative = TRUE,
  suc.out = "weighted")
```

## Arguments

suc.up	a numeric vector containing the measured suctions [cm] of the upper tensiometer
suc.low	a numeric vector containing the measured suctions [cm] of the lower tensiometer
weight	a numeric vector containing the measured weights [g]
t	time in seconds [s]
ths	saturated water content (optional) for the calculation of the soil water contents (th)
r	sample radius [cm]
L	sample height [cm]

z1	depth of upper tensiometer [cm]
z2	depth of lower tensiometer [cm]
sd.tens	measurement accuracy of tensiometer [cm]
suc.negative	set TRUE if suction/tensiometer values are negative and FALSE if positive
suc.out	'weighted' (default), arithmetic ('ari') or geometric ('geo') mean of the tensiometer readings (see Peters (2015) for details)

### Details

**sd.tens:** At the beginning of the experiment when gradients of the hydraulic head are small, hydraulic conductivities cannot be calculated. Following Peters and Durner (2008) hydraulic conductivities calculated from gradients smaller than  $(6 * \text{sd.tens}) / (z2 - z1)$  are set to NA.

### Value

#### data.frame

Ki: unsaturated hydraulic conductivity [cm/day]

th: water content (th) is returned if ths is provided as input

suc: suction, either (1) weighted between arithmetic and geometric mean (default), (2) the arithmetic mean or (3) the geometric mean (see Peters 2015)

### Author(s)

Ullrich Dettmann

### References

Wind, G. P. (1966). Capillary conductivity data estimated by a simple method (No. 80). [sn].

Peters, A., Iden, S. C., & Durner, W. (2015). Revisiting the simplified evaporation method: Identification of hydraulic functions considering vapor, film and corner flow. *Journal of Hydrology*, 527, 531-542.

Peters, A., & Durner, W. (2008). Simplified evaporation method for determining soil hydraulic properties. *Journal of Hydrology*, 356(1), 147-162.

Schindler, U., 1980. Ein Schnellverfahren zur Messung der Wasserleitfähigkeit im teilgesättigten Boden an Stechzylinderproben. *Arch. Acker- Pflanzenbau Bodenkd.* 24, 1-7.

### Examples

```
# -----
# Calculate hydraulic properties with the 'Simplified Evaporation Method' (SEM)
# -----
data('dataSEM')
ths <- 0.7 # define saturated water content (ths) (optional)
shp <- SEM(suc.up      = dataSEM$tens.up,
           suc.low     = dataSEM$tens.low,
           weight      = dataSEM$weight,
           t           = dataSEM$hour*60*60,
```

```

r          = 3.6, # radius of sample
L          = 6,   # height of sample
z1         = 1.5, # depth of upper tensiometer [cm]
z2         = 4.5, # depth of lower tensiometer [cm]
sd.tens    = 0.1, # tensiometer accuracy (see ?SEM)
ths        = ths,
suc.negativ = TRUE,
suc.out     = 'weighted'
)

```

SWC

*Soil water content*

### Description

Calculates the volumetric soil water content for a corresponding suction/pressure head ( $th(suc)$ ) for unimodal or bimodal van Genuchten (vG) or Peters-Durner-Iden (PDI) parameterisation.

### Usage

```

SWC(suc, par.shp = c(th = 0.9, thr = 0, alfa = 0.02, n = 2),
    FUN.shp = "vg", modality = "uni", suc.negativ = TRUE)

```

### Arguments

suc	Suction/pressure heads. Negative if suc.negativ = TRUE
par.shp	named parameter in list or vector
FUN.shp	Funktion for soil hydraulic properties (vG or PDI) (see details)
modality	pore size distribution ('uni' or 'bi')
suc.negativ	set TRUE if suction/pressure heads are negative and FALSE if positive

### Details

**FUN.shp:** vG: van Genuchten (uni or bimodal) (vGM is working aswell)  
PDI: Peters-Durner-Iden with saturation function van Genuchten (uni or bimodal)

**par.shp (vG and PDI):** ths [-]: saturated water content  
thr [-]: residual water content  
alfa [1/L]: van Genuchten shape parameter  
n [-]: van Genuchten shape parameter  
m [-]: shape parameter ( $m = 1 - (1/n)$  if missing)

additional for 'PDI':

h0 [L]: suction at water content of 0 (i.e. oven dryness) ( $h0 = 10^{6.8}$  if missing, corresponding to oven dryness at 105°C (Schneider and Goss, 2012))

additional for bimodal (modality == 'bi'):

w2 [-]: weighing between pore space distributions

alfa2 [1/L]: van Genuchten parameter alfa for second pore space distribution

n2 [-]: van Genuchten parameter n for second pore space distribution

m2 [-]: shape parameter ( $m2 = 1 - (1/n2)$  if missing)

PDI:

$\theta(h) = (\theta_s - \theta_r) * Scap(h) + \theta_r * Sad(h)$

**Scap**: Rescaled capillary saturation function

**Sad**: Relative saturation function for adsorbed water

input for FUN.shp and modality works for upper- and lowercase letters

### Value

volumetric water content theta (th) [ $L^3/L^3$ ]

### Author(s)

Ullrich Dettmann

### References

Van Genuchten, M. T. (1980). A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil science society of America journal*, 44(5), 892-898.

Durner, W. (1994). Hydraulic conductivity estimation for soils with heterogeneous pore structure. *Water Resources Research*, 30(2), 211-223.

Peters, A. (2013). Simple consistent models for water retention and hydraulic conductivity in the complete moisture range. *Water Resour. Res.* 49, 6765–6780. physics-a review. *Vadose Zone J.* <http://dx.doi.org/10.2136/vzj2012.0163>.

Iden, S., Durner, W. (2014). Comment to Simple consistent models for water retention and hydraulic conductivity in the complete moisture range by A. Peters. *Water Resour. Res.* 50, 7530–7534.

Peters, A. (2014). Reply to comment by S. Iden and W. Durner on Simple consistent models for water retention and hydraulic conductivity in the complete moisture range. *Water Resour. Res.* 50, 7535–7539.

Schneider, M., & Goss, K. U. (2012). Prediction of the water sorption isotherm in air dry soils. *Geoderma*, 170, 64-69.

### See Also

[Ku Sat](#)

### Examples

```
# -----
# Unimodal van Genuchten
# -----
SWC(suc = seq(1, 1000, by = 1), par.shp = c(th_s = 0.4, thr = 0, alfa = 0.02, n = 1.5),
```

```
FUN.shp = c('vG'), modality = 'uni', suc.negativ = FALSE)
# -----
# Bimodal van Genuchten
# -----
SWC(suc = seq(1, 1000, by = 1),
par.shp = c(thb = 0.4, thr = 0, alfa = 0.02, n = 2, w2 = 0.2, alfa2 = 1, n2 = 10),
FUN.shp = c('vG'), modality = c('bi'), suc.negativ = FALSE)
# -----
# Unimodal PDI
# -----
SWC(suc = seq(1, 1000, by = 1), par.shp = list(thb = 0.4, thr = 0, n = 1.6, alfa = 0.02),
FUN.shp = c('pdi'), modality = c('uni'), suc.negativ = FALSE)
# -----
```

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