

Package: RSEML (via r-universe)

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Type Package

Title Case-Based Least Squares Estimation of Nonlinear Structural Equation Models

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Description Estimates structural equation models by case-based least squares: the latent scores of every observation are treated as free variables of a constrained optimization problem, so that arbitrary nonlinear model equations, bounds and constraints on latent variables and inequality constraints on parameters become possible. Model equations are specified as plain text (e.g. `y == a*exp(b*eta)`). Gradients are obtained by automatic differentiation via 'RTMB', and the constrained problem is solved with 'nloptr' (SLSQP or augmented Lagrangian). Missing data are handled case-wise. The methodology is described in Oldenburg (2024) <[doi:10.19139/soic-2310-5070-1868](https://doi.org/10.19139/soic-2310-5070-1868)> and Oldenburg (2025) <[doi:10.19139/soic-2310-5070-2324](https://doi.org/10.19139/soic-2310-5070-2324)>.

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Imports RTMB, nloptr, stats

Suggests knitr, rmarkdown

NeedsCompilation no

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RSEML-package	<i>Case-Based Least Squares Estimation of Nonlinear Structural Equation Models</i>
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Description

RSEML estimates structural equation models by case-based least squares. In contrast to covariance-based SEM, the latent score of every observation is treated as a free variable of a constrained optimization problem. This makes three things possible that are difficult in classical SEM software: (i) arbitrary *nonlinear* model equations, e.g. products of latent variables or $y == a*\exp(b*\eta_a)$; (ii) *bounds and constraints on latent variables* (e.g. restriction to the unit interval, so that products of latent variables can be read as fuzzy conjunctions); and (iii) inequality constraints on parameters.

Gradients of the objective and of all constraints are obtained by automatic differentiation with **RTMB**; the constrained problem is solved with **nloptr** (SLSQP or augmented Lagrangian with an L-BFGS core). Missing data are handled case-wise per equation.

The main function is `fsem`. `sim_bollen` simulates example data.

Author(s)

Reinhard Oldenburg

References

Oldenburg, R. (2024). Least square estimation of non-linear structural models. *Statistics, Optimization & Information Computing*, 12(2), 281–297. doi:10.19139/soic231050701868

Oldenburg, R. (2025). Geometric weighted least squares estimation. *Statistics, Optimization & Information Computing*, 13(2), 611–615. doi:10.19139/soic231050702324

fsem	<i>Case-Based Least Squares Estimation of Nonlinear Structural Equation Models</i>
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Description

Estimates a structural equation model by case-based least squares: the latent score of every observation is a free variable of a constrained optimization problem. Model equations may be arbitrary nonlinear expressions in observed variables, latent variables and parameters; latent variables can be bounded or constrained. Gradients are obtained by automatic differentiation (package **RTMB**); the constrained problem is solved with **nloptr**.

Usage

```
fsem(data, observed, latent, equations, errnames = NULL,
      emean0 = TRUE, lmean0 = FALSE,
      constraints = character(), latent_bounds = NULL,
      weights = 10, with_w1 = FALSE, with_w2 = FALSE,
      le_damp = FALSE, ee_damp = FALSE,
      eee_damp = FALSE, eeee_damp = FALSE,
      damp_e_expo = 1, damp_l_expo = 1,
      damp_ee_expo = 1, damp_eee_expo = 1,
      ee_dist = 1L,
      init = list(), lat_init = 0, lat_jitter = 0.1,
      warm_start = TRUE,
      algorithm = c("auto", "slsqp", "auglag"),
      max_iter = 1000L, tol = 1e-8, verbose = 0L)
```

Arguments

data	numeric matrix or data frame with one row per case. If column names are present they are matched against observed; otherwise the columns must be in the order of observed. Missing values (NA) are allowed and are handled case-wise per equation.
observed	character vector of observed variable names.
latent	character vector of latent variable names.
equations	list or vector of model equations, each given as a string "lhs == rhs" (or a two-sided formula). The right hand side may be any arithmetic expression in observed variables, latent variables and free parameters, e.g. "y == a*exp(b*eta) + c". Every symbol that is neither an observed nor a latent variable is treated as a free parameter.
errnames	optional character vector of error-term labels (used for naming the residual matrix); defaults to e1, e2,
emean0	logical; if TRUE the residual of every equation is constrained to have mean zero.
lmean0	logical; if TRUE every latent variable is constrained to have mean zero.
constraints	character vector of constraints such as "b1 > 0", "eta <= 1" or "a + b == 1". Constraints of the simple form <i>symbol op number</i> are converted to box bounds (cheap); all others are passed to the optimizer as general nonlinear constraints. A constraint that evaluates to a vector of length <i>n</i> (because it involves a latent variable) is applied per case.
latent_bounds	optional numeric vector c(lower, upper) applied as box bounds to <i>all</i> latent scores, e.g. c(0, 1).
weights	equation weights: a positive scalar (used for all equations), a vector with one entry per equation, or a value <= 0 to use the data-driven default $10/(0.001 + sd(data))$.
with_w1	logical; if TRUE, after the first solution the model is re-estimated with weights $1/sd$ of the residuals (warm-started from the first solution).

with_w2	logical; if TRUE a further stage is run in which the weights are free variables with $w_j \geq 0.001$ and $\sum_j \log(w_j^2 \sigma_j^2) \geq 0$. The stage is accepted only if the optimizer converges and the objective is smaller than $1.05M$, where M is the number of objective blocks.
le_damp, ee_damp, eee_damp, eeee_damp	logical damping switches that add penalties on latent-error covariances, and on pairwise, triple and quadruple error-error (co)moments, respectively.
damp_e_expo, damp_l_expo, damp_ee_expo, damp_eee_expo	exponents of the sample size in the corresponding damping weights.
ee_dist	index stride used in the triple and quadruple damping sums.
init	named list of start values: scalars for parameters, scalars or length- n vectors for latent variables.
lat_init	default start value for latent scores.
lat_jitter	standard deviation of Gaussian jitter added to the latent start values. An all-constant start is a stationary point of the objective, so a small jitter (default 0.1) is recommended; set to 0 to disable (use <code>set.seed</code> for reproducibility).
warm_start	logical; if TRUE (default) and any damping option is active, the undamped problem is solved first and the damped optimization is warm-started from its solution. Damped objectives are hard to optimize from a cold start, so this should normally be left enabled.
algorithm	"slsqp" (sequential quadratic programming, reliable for small and medium problems), "auglag" (augmented Lagrangian with an L-BFGS core, scales to large problems) or "auto" (default; chooses by problem size).
max_iter	maximum number of optimizer iterations.
tol	relative convergence tolerance passed to nloptr .
verbose	0, 1 or 2 for increasing diagnostic output.

Details

For equations $f_j(\text{obs}, \text{lat}, \theta) = 0$ with residuals r_{ij} of case i in equation j , the objective is the weighted sum of residual variances

$$F = \sum_j w_j^2 \widehat{\text{Var}}(r_{\cdot j})$$

subject to the chosen mean constraints, bounds and user constraints, plus optional damping penalties that push error-error and latent-error covariances towards zero. All means and variances are computed over the cases that are complete for the respective equation, so missing data reduce the effective sample size per equation but do not remove whole cases.

Because the latent scores are explicit variables, the model equations may be nonlinear in the latent variables (products, powers, exp, log, sqrt, trigonometric functions, ...) and constraints such as `latent_bounds = c(0, 1)` give the latent variables a direct interpretation (e.g. as fuzzy truth values).

Note that `emean0 = TRUE` and `lmean0 = TRUE` are *joint* constraints: an equation such as `"x1 == eta"` without an intercept parameter then forces `mean(x1) == mean(eta) == 0`, which contradicts the

data and makes the problem infeasible (the optimizer stops immediately, often with **nloptr** status -4). Include intercept parameters (" $x1 == \eta + t1$ ") or drop one of the two mean constraints.

RMSEA is the square root of the mean unexplained residual variance per equation; RMSEAad additionally adjusts for the number of latent scores and free parameters. These indices are analogues of, but not identical to, the covariance-based RMSEA of classical SEM; see Oldenburg (2024) for details.

Value

An object of class "fsem", a list with components

coefficients	named vector of parameter estimates.
standardized	standardized coefficients (where defined, i.e. for parameters that multiply a parameter-free regressor).
scores	$n \times L$ matrix of estimated latent scores.
residuals	$n \times m$ matrix of residuals (NA for cases that are incomplete in an equation).
EVars, ECor, ECov	residual variances, correlations and covariances (pairwise complete).
LLCor	correlation matrix of the latent scores.
LECor	correlations between latent scores and residuals.
RMSEA, RMSEAad, Fmin	fit measures, see Details.
equations	fitted equations with estimates substituted.
weights	equation weights used in the final stage.
convergence, status	convergence flag and nloptr status.
time, algorithm, call	timing, algorithm and matched call.
print, summary, coef and residuals methods	are available.

Equation syntax

Each model equation is a string of the form

"<expression> == <expression>"

("=" or a two-sided formula $lhs \sim rhs$ are also accepted). Both sides are parsed with `str2lang` and must be valid R arithmetic expressions built from

- *observed variables* (names listed in `observed`; they stand for the corresponding data column),
- *latent variables* (names listed in `latent`; they stand for the case-wise vector of latent scores),
- *parameters*: every other symbol is treated as a free scalar parameter to be estimated (so misspelled variable names silently become parameters – check the parameter list of the result),
- numeric literals, parentheses, and the operators $+ \ - \ * \ / \ ^$ (unary minus included).

Supported functions are those with an automatic-differentiation method for **RTMB**'s advector class, in particular `exp`, `log`, `log1p`, `expm1`, `sqrt`, `abs`, `sin`, `cos`, `tan`, `asin`, `acos`, `atan`, `sinh`, `cosh`, `tanh`, `gamma`, `lgamma`, and the distribution functions provided by **RTMB** such as `dnorm`, `pnorm`, `plogis`. All operations are applied case-wise (vectorized over the n cases). Not allowed are control flow (`if`, loops), comparisons, indexing, assignments and functions without an advector method; smooth replacements should be used instead, e.g. $(x + \sqrt{x^2 + 1e-4})/2$ for the positive part of x . Examples of valid equations:

```
"y1 == b1*eta + c1"
"y == a*exp(b*eta)"
"A1 == b0 + b1*GEO*LOC*MUL"
"p == plogis(a + b*theta)"
```

Constraints in constraints follow the same expression syntax, combined with one relational operator `==`, `<=`, `>=`, `<` or `>`.

Author(s)

Reinhard Oldenburg

References

- Oldenburg, R. (2024). Least square estimation of non-linear structural models. *Statistics, Optimization & Information Computing*, 12(2), 281–297. doi:[10.19139/soic231050701868](https://doi.org/10.19139/soic231050701868)
- Oldenburg, R. (2025). Geometric weighted least squares estimation. *Statistics, Optimization & Information Computing*, 13(2), 611–615. doi:[10.19139/soic231050702324](https://doi.org/10.19139/soic231050702324)

See Also

[sim_bollen](#), [bollen_equations](#)

Examples

```
## a small nonlinear one-factor model: x1 = eta, x2 = c*eta,
## y = a*exp(b*eta), with the latent variable restricted to [0, 2.5]
set.seed(1)
n <- 60
eta <- abs(rnorm(n))
dat <- cbind(x1 = eta + rnorm(n, 0, 0.15),
             x2 = 0.7 * eta + rnorm(n, 0, 0.15),
             y = 0.5 * exp(0.8 * eta) + rnorm(n, 0, 0.10))
fit <- fsem(dat,
            observed = c("x1", "x2", "y"),
            latent = "eta",
            equations = c("x1 == eta",
                          "x2 == c2*eta",
                          "y == a*exp(b*eta)"),
            constraints = c("a > 0.01", "b > 0.01"),
            latent_bounds = c(0, 2.5),
            init = list(a = 0.3, b = 0.5, c2 = 0.5, eta = 0.5),
            lat_jitter = 0)
```

```

fit
cor(fit$scores[, "eta"], eta)

## Bollen-type model with three latent variables (takes a few seconds).
## The damping penalties on error-error and latent-error covariances
## with small sample-size exponents improve the estimates.
set.seed(2)
dat <- sim_bollen(50)
fit <- fsem(dat, observed = colnames(dat),
            latent = c("ind60", "dem60", "dem65"),
            equations = bollen_equations(),
            lmean0 = TRUE,
            constraints = c("b1 > 0", "b2 > 0", "b3 > 0"),
            le_damp = TRUE, ee_damp = TRUE,
            damp_e_expo = 0.1, damp_l_expo = 0.1)
summary(fit)

```

sim_bollen

*Simulate Bollen-Type Example Data and the Matching Model***Description**

sim_bollen simulates data from a three-latent-variable model in the style of Bollen's political democracy model with eleven observed indicators; bollen_equations returns the matching model equations for fsem. The structural equation for dem65 can be made nonlinear through the exponents expos:

$$DEM65 = b_2 IND60^{e_1} + b_3 DEM60^{e_2} + \epsilon.$$

Usage

```

sim_bollen(n,
            para = c(b1 = 1.2, b2 = 0.5, b3 = 0.8, c2 = 0.7, c3 = 0.9,
                     d2 = 0.3, d3 = 0.9, d4 = 1.7, d6 = 0.6, d7 = 0.4,
                     d8 = 1.3),
            sigma = c(0.1, 0.2, 0.3, 0.2, 0.1, 0.2, 0.3, 0.2, 0.1, 0.2,
                      0.3, 0.3, 0.2),
            expos = c(1, 1))

bollen_equations(expos = c(1, 1))

```

Arguments

n	number of cases to simulate.
para	named vector of true structural coefficients and loadings.
sigma	error standard deviations (11 indicators followed by the two structural disturbances).

expos exponents (e_1, e_2) of the structural equation for dem65; `c(1, 1)` gives the linear model.

Value

`sim_bollen` returns an $n \times 11$ matrix with columns `y1, ..., y8, x1, x2, x3`; the true latent scores are attached as attribute `"latent"`. `bollen_equations` returns a character vector of 13 model equations.

See Also

[fsem](#)

Examples

```
set.seed(1)
dat <- sim_bollen(40)
head(dat)
bollen_equations(expos = c(2, 1))[2]
```

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