

# RSiena

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## 1. Grand overview of RSiena

This overview of **RSiena** sometimes refers to the earlier version **Siena3** to facilitate understanding by those who have a knowledge of the code of **Siena3**. Readers who have no such knowledge can happily ignore these references.

Two special features of the **RSiena** package are that it uses C++ code for time-consuming parts, and that a wrapper is available to use the package seemingly independently of R.

The script file *sienascript* starts up R in such a way that it launches a tcl/tk graphical user interface (gui) resembling the Stocnet interface for **Siena3**, and controls all processing thereafter. This interface is accessible on Windows via the command *siena01Gui*. (Prior to R 2.12.0 the function `siena.exe` was provided as an equivalent to *sienascript*: it has been removed as it was rarely used and proved difficult to maintain.)

The high-level functions called by the gui, such as *siena07* described below, are also accessible within R with the usual R-type user interface along the lines of model-fitting functions such as `lm()`. (A formula interface is still on the wish list, but already now it is relatively straightforward to use the package without the gui.)

The R functions call C++ only where speed is critical. From my profiling of *siena07*, the estimation function, I think that only the simulation function (which simply performs one simulation of the complete model for a given

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set of parameters and returns the statistics from the simulated networks) needs to be in C++. The bulk of the time is spent in calculating the contributions to the effects when simulating.

In **Siena3**, this simulation function is **FRAN** which, for method of moments estimation, simply calls **simstats**: in **RSiena**, it is the C++ function *model* called by one of the R functions *simstats0c* or *maxlikec*, which are the two candidates currently available for the element of the **RSiena** model object named *FRAN*. In this document I have used the name **FRAN** to refer to the simulation routine.

*siena07* is intended to be written in such a way that different simulation functions could be used within the same Robbins Monro algorithm. In practice the separation is not quite complete, but it is nearly so.

It would be feasible within a C++ **FRAN** to call R functions for some effects or functions if desired, to facilitate adding new ones, although they would be slow to run!

We use functions from the C part of R, to provide random numbers within the C++.1 *simstats0c* and *maxlikec* have three types of calls: a initial one which calls various C++ routines to setup the data, a final one which sets the C++ data pointers to null to clean up the C++ memory, and multiple “normal” ones which call the function *model* to perform one complete simulation. (In this it does not correspond exactly to **simstats** in **Siena3**!)

With this design, we have introduced parallel processing by using multiple R processes. In *simstats0c* we run some of the simulations in each process: this was trivial to introduce into Phase 1 and Phase 3, but to use it in Phase2 we have altered the algorithm to use the average of more than one simulation at a time.

For *maxlikec* we use different processes for each wave. This is because the chains are carried from one simulation to the next, and organizing the parallel processes by simulations (update steps of the Robbins Monro algorithm) would require too much passing of information.

We use the R package **parallel** to create and control the multiple processes, and to provide multiple random number streams. The term ‘cluster’ below refers to the cluster of multiple processors. (I vary between using *processors* and *processes* as it is possible to run **RSiena** with multiple *processes* on a machine with only one processor.)

## 2. Data types

RSiena provides various classes of data objects, designed to interface with the functions *robmon* and *simstats*. A brief list:

**siena** Data for a single project

**sienaGroup** A list of *siena* objects, with global attributes, used for multi-group projects

**sienaEffects** Data frame of effects.

**sienaGroupEffects** Data frame of effects for a group object.

**sienaModel** Contains the fitting options.

**sienaNodeSet** Actor set, used to distinguish nodes in data sets with multiple or two-mode networks.

**sienaDependent** A single dependent variable, (i.e. network or behavior variable, all waves)

**coCovar** Constant covariate

**coDyadCovar** Constant dyadic covariate

**varCovar** Varying covariate

**varDyadCovar** Varying dyadic covariate

**sienaCompositionChange** List of changes, entry for each node.

**sienaFit** Currently contains (almost) everything from the estimation.

The structure of each is documented in the corresponding R help file: `?classname`.

Data objects of class *siena* are created by the function *sienaDataCreate*.

Effect objects of class *sienaEffects* are created by the function *getEffects*.

The creation functions can be called directly by the user or from the Gui or via *sienaDataCreateFromSession*, depending on whether the data is already in R objects or still on files.

The function *robmon* requires a *sienaModel* object as an argument. One element of this object is named `FRAN` and contains the name of the required simulation function.

The functions *simstats0c* or *maxlikec*, used as an instance of `FRAN`, require a *siena* (or *sienaGroup*) object and a *sienaEffects* (or *sienaGroupEffects*) object as arguments.

### 3. *sienaDataCreate*

This function has only one named argument: a list of actor (node) sets. The default is a single set of the required size named **Actors**. All other arguments are unnamed and correspond to networks, covariates or composition change files. The objects are validated and have various attributes added. For covariates the attributes are added using a *method* for their class.

Check that objects have names, using the object name if none is given in the function call.

**if** no objects **then**

stop

**if** any duplicate names **then**

stop

create a list of each type of object, checking that all dependent variables have the same number of observations. (Stop if not).

**if** no dependent variables **then**

stop

**if** no node set argument **then**

create a list of nodesets containing a single nodeset named **Actors**, with the number of nodes equal to the number of senders of the first dependent variable

**for all** covariates **do**

Appropriate validation and processing (see below).

Process any composition change objects (see section 3.2)

Process the dependent variables (see section 3.4)

Check constraints if there are multiple networks. (section 3.8).

Calculate similarity means for alters for each covariate and dependent network (see section 3.9): dropped in version 1.1-285.

### 3.1 Covariates

#### 3.1.1 *Constant Covariate*

Check the nodeset (section 3.3)

Create attributes: (a class method)

*mean* ignore missings

*range* Extent of range, ignore missings. Make sure is a double.

*range2* Ends of range, ignore missings

*moreThan2* TRUE if more than 2 distinct values, ignoring missings

*vartotal* sum of non-missing values

*poszvar* TRUE if more than 1 distinct value in the centered values or any missing

*simMean* See section 3.5

*nonMissingCount* count of non missing values

*name* name of object

Subtract the mean from the values

#### 3.1.2 *Changing covariate*

**if** less than 3 waves **then**

Stop: changing covariate inappropriate (to reduce confusion among users!)

Check the nodeset (section 3.3)

**if** less than (number of waves - 1) columns **then**

Stop: not enough values

**if** more than (number of waves - 1) columns **then**

remove the excess, carefully preserving the attributes apart from the dimensions.

Create attributes: (a class method)

*mean* ignore missings

*meanp* mean for each wave, ignore missings

*range* Extent of range, ignore missings. Make sure a double.

*rangep* Extent of range for each wave, ignore missings. Make sure is a double.

*range2* Ends of range, ignore missings

*moreThan2* TRUE if more than 2 distinct values, ignoring missings

*vartotal* sum of non-missing values

*poszvar* TRUE if more than 1 distinct value in the centered values or any missing

*simMean* See section 3.5

*nonMissingCount* count of non missing values

*name* name of object  
Subtract the mean from the values

### 3.1.3 *Constant dyadic covariate*

Check the nodesets (section 3.3)  
**if** attribute type is oneMode **then**  
    set diagonal to *missing* so is ignored in mean and range  
Create attributes: (a class method)  
    *mean* ignore missings  
    *range* Extent of range, ignore missings. Make sure a double.  
    *range2* Ends of range, ignore missings  
    *name* name of object  
**if** attribute type is oneMode **then**  
    set diagonal to *zero*

### 3.1.4 *Changing dyadic covariate*

**if** less than 3 waves **then**  
    Stop: changing covariate inappropriate (to reduce confusion among users!)

Check the nodesets (section 3.3)  
**if** less than (number of waves - 1) columns **then**  
    Stop: not enough values

**if** more than (number of waves - 1) columns **then**  
    remove the excess, carefully preserving the attributes apart from the dimensions.

**if** attribute type is oneMode **then**  
    set all diagonals to *missing* so are ignored in mean and range

Create attributes: (a class method)  
    *mean* ignore missings  
    *range* Extent of range, ignore missings. Make sure a double.  
    *name* name of object  
**if** attribute type is oneMode **then**  
    set all diagonals to *zero*

## 3.2 Composition change objects

Check there are no duplicates in the nodesets: only one change object per nodeset is allowed.  
**for all** composition change objects **do**  
    Check the nodeset (section 3.3)

Check that the ends of each interval in each object are not less than 1 or greater than the number of waves and that each line has an even number of digits.

Generate a data frame of events(section 3.2.1), a matrix of activeStart flags(section 3.2.2) and a matrix of actions(section 3.2.3)  
Add these to the object as attributes

### 3.2.1 *Events*

Data frame with columns:

*event* “join” or “leave” (a factor)

*period*

*actor*

*time* between 0 and 1

### 3.2.2 *ActiveStart Flags*

activeStart matrix has a row per actor and a column per period

TRUE if the actor is active at the start of the period, otherwise FALSE

### 3.2.3 *Action*

Action matrix is same shape as Active flag matrix, with entries

0 Active at start

1 Inactive at start, never previously active

2 Inactive at start, previously active but never active again

3 Inactive at start, previously active and active again

## 3.3 Check NodeSet

**if** Nodeset name in the list and lengths match **then**

Valid

**else**

Invalid

## 3.4 Dependent variables

NB The attributes list tends to change rather quickly and some items may no longer be required. Some should be used in the C, but are not...

Validate the nodeset(s)

Create an attribute *name* with name of the object

**if** behavior variable **then**

Create attributes:

*distance* sum of absolute differences by period, ignoring missings

*vals* table of values by period, NA included as a value

*nval* vector of non-missing counts by period

*noMissing* vector of missing counts by period

*range* overall range

*range2* overall min and max

*moreThan2* TRUE if number of distinct values more than 2

(includes missings as a value) ??? inconsistent with covariates?

*poszvar* TRUE if more than one distinct value or any missing

values.

*modes* vector of modes of rounded values per period. Might give multiple results?

*missing* TRUE if any missing

*simMean* value of similarity mean (see section 3.5)

*structural* FALSE Not allowed!

*balmean* NA

*structMean* NA

*uponly* TRUE if all changes increase, ignoring missings

*downonly* TRUE if all changes decrease, ignoring missings

**else** {bipartite or onemode}

create attributes:

*distance* count of changes, ignoring missing and structural values and diagonals if not bipartite.

*uponly* TRUE if ties are only ever created, never lost

*downonly* TRUE if ties are only ever lost, never created

**if** one-mode **then**

Create attributes:

*balMean* see section(3.6)

*structMean* see section(3.7)

*symmetric* TRUE if all waves are symmetric

*missing* TRUE if any missing values (except on diagonal)

*structural* TRUE if any 10 or 11

*vals* table of counts of values by period

*nval* Counts of non-missing values by period, excluding diagonal

*range2* Min and max of non-structural values

*noMissing* Number of missing values by period

*noMissingEither* Number of missing values at start or finish of period (excludes final).

*nonMissingEither* Number of non missing values at start or



finish of period (excludes final).  
*simMean* NA  
*ones* Count of values equal to 1 by period  
*density* Density of network by period  
*degree* Average degree by period  
*averageOutDegree* overall average degree  
*averageInDegree* overall average degree  
*maxObsOutDegree* Maximum observed outdegree by period  
*missings* count of missings by period  
**else if** bipartite **then**  
 Create attributes:  
*balMean* NA  
*structMean* NA  
*symmetric* FALSE  
*missing* TRUE if any missing values  
*structural* TRUE if any 10 or 11  
*vals* table of counts of values by period  
*nval* Counts of non-missing values by period  
*range2* Min and max of non-structural values  
*noMissing* Number of missing values by period  
*noMissingEither* Number of missing values at start or finish of  
 period (excludes final).  
*nonMissingEither* Number of non missing values at start or  
 finish of period (excludes final).  
*simMean* NA  
*ones* Count of values equal to 1 by period  
*density* Density of network by period  
*degree* Average degree by period  
*averageOutDegree* overall average degree  
*averageInDegree* overall average degree  
*missings* count of missings by period

### 3.5 Similarity mean

**for all** columns of matrix **do** {waves}  
**for all** entries in column **do** {actors}  
 in a copy of the column set this entry to NA  
 Calculate  $1 - \text{abs}(\text{this entry} - \text{copy column}) / \text{range}$   
 Sum this over the nonmissing entries in this vector  
 Count the nonmissing entries in this vector  
 Sum nonmissing entries and counts over the columns

Calculate the similarity mean as this total sum divided by total count.  
 For possible later use, also return the total sum and total count.

### 3.6 Balance mean

In calculations, remove diagonal and replace structural values by the values represented.

Numerator = sum over all columns of

$2 * \text{count of non-zero entries} * \text{count of non-missing non-nonzero entries}$

Denominator = sum over all columns of

count of non-missing entries times one less than this.

Mean is numerator divided by denominator.

### 3.7 Structural mean

In calculations, remove diagonal and replace structural values by the values represented.

Numerator = sum over all rows of

$2 * \text{count of non-zero entries} * \text{count of non-missing non-nonzero entries}$

Denominator = sum over all rows of

count of non-missing entries times one less than this.

Mean is numerator divided by denominator.

### 3.8 Constraints between networks

Make a two column matrix containing the names of all possible pairs of dependent variables, including pairs with themselves.

Identify any dependent variables that can relate: same type and have the same node sets.

Create a list of these possibly relating dependent variables for each of access later.

**for all** row in the matrix of pairs where the two columns are not the same **do**

**if** nodeset(s) match and type matches and not behavior and either both networks are symmetric or neither is **then**

In checks, replaces structurals by 0/1 first, and ignore missings

Check *higher*: first network always greater than or equal to second network.

Check *disjoint*: sum of product of two networks not greater than 0.

Check *atLeastOne*: sum of two networks never equal 0.

### 3.9 Similarity means at distance 2

```
for all constant covariates, varying covariates do  
  for all dependent networks which have the node set of the constant  
  covariate as their receivers (not behavior variables) do  
    Calculate the corresponding similarity mean: see section 3.9.1).  
for all behavior variables do  
  for all dependent networks which have the node set of the constant  
  covariate as their receivers (not behavior variables) do  
    Subtract the mean from the behavior variable  
    Find the range of the behavior variable  
    Calculate the corresponding similarity mean using the centered  
    behavior variable values (omitting final column) and the  
    calculated range: see section 3.9.1). (i.e. centering and range are  
    done on complete variable)
```

#### 3.9.1 *Alter similarity calculation*

```
for all observations except the last do  
  Replace structurals by 0/1  
  for all rows of network matrix do  
    if sum of nonmissing entries is 0 then  
      Set vi for row to 0  
    else if all covariate values corresponding to non zero network  
    entries are missing then  
      Set vi for row to NA  
    else  
      Set vi for row to sum of covariate times network row  
      divided by the sum of the network row, ignoring missings in  
      both cases.  
  Call rangeAndSimilarity using vi and the range if passed in  
  (behavior variables) to obtain the values simTotal and simCnt for  
  this overvation.  
  Accumulate these two values  
Divide sum of simTotal by sum of simCnt over observations (excluding  
the final one).
```

## 4. `getEffects`

This function generates an effects data object corresponding to a Siena Data object or a Siena Group Object.

In general, effects are driven by selecting rows in the `allEffects` data frame for some effect group and then substituting variable names into the spaces marked by `xxxxxx` and similar.

For a group object, the effects are created using the first data object plus the total number of observations. Attributes are first copied from the group level to the first data object. The only changes required are to fill in the starting values for the rate effects for the later objects and to adjust the starting values for density, reciprocity, linear effects.

The function `networkRateEffects` creates the required number of rate effects for networks. `createEffects` extracts the rows from the effects data frame for an effect group and calls the function `substituteNames` to replace the variable fields by the current variable name. It now creates the complete effect rows including endowment effect copies.

#### 4.1 Siena Data Object

```
for all dependent variables do
  Create appropriate effects
```

#### 4.2 OneMode Network Effects

Call `networkRateEffects` to get the rate effects

Use `symmetricObjective` or `nonSymmetricObjective` effect groups to create the basic objective function effects.

```
for all dyadic covariates with first node set matching do
```

```
  Use dyadObjective effect group to add appropriate objective
  function effects
```

```
for all constant covariates, behavior variables, changing covariates with
the same node set do
```

```
  Call function covarOneModeEff to add the appropriate effects.
```

```
  Note poszvar is always TRUE for behavior variables.
```

```
if any covariates or behavior variables then
```

```
  Add nintn rows for user specified interaction effects
```

```
for all distinct dependent network variables with the same node set do
```

```
  if oneMode then
```

```
    Use nonSymmetricSymmetricObjective or
    nonSymmetricNonSymmetricObjective effect groups to add
    appropriate effects
```

```
    Use tripleNetworkObjective effect group to add appropriate
    effects for pairs of other dependent networks ('other' meaning
    that they have the role of explanatory variables) that either are
```

both one-mode, or both are bipartite with the same second node sets

**else if** bipartite which matches on nodeset 1 **then**  
 Use `nonSymmetricBipartiteObjective` effect group to add appropriate effects

**for all** actor covariates or behavior variables with the same node set **do**  
 Use `covarNetNetObjective` effect group to add appropriate effects.

**if** more than one network **then**  
 paste the network name at the front of all the objective function effects

Alter the text for endowment effects to start "Lost ties:"

Calculate the starting values for the default effects (see section 4.14)

Select the default rate effects by setting *include* to TRUE for the **basic rate** effects.

Add the starting value for the rate to the *initialValue* column of the basic rate effects

**if** symmetric **then**  
 Set *include* to TRUE for the degree (density) evaluation effect and transitive triads evaluation effect.

**else**  
**if** no period is uponly or downonly **then**  
 Set *include* to TRUE for the degree (density) evaluation effect  
 Add the starting values for the degree(density) evaluation effect calculated by `getNetworkStartingVals` to the *initialValue*.

**else**  
 Remove both degree (density) effects from the data frame.  
 Set *include* to TRUE for the reciprocity evaluation effect.

### 4.3 Behavior Variable Effects

Use `behaviorRate` effect group to get the rate effects. Either remove the second one or duplicate the second and remove the first to match the number of observations.

Use `behaviorObjective` effect group to create the basic objective function effects.

**for all** other dependent variables which match on first node set **do**  
 Use `behaviorOneModeObjective` or `behaviorBipartiteObjective` to add the objective function effects with respect to this network.  
 Use `behaviorOneModeRate` or `behaviorBipartiteRate` to add the

rate effects with respect to this network.

**for all** constant covariates, other behavior variables or changing covariates **do**

    Call `covBehEff` and `covBBehEff` to add the interaction effects

**for all** networks with same node set (first for bipartite) **do**

    Use `behaviorOneModeObjective2` or `behaviorBipartiteObjective2` effect group to create a second set of objective function effects.

Add *behNintn* unspecified behavior interaction effects

Create the effects data frame by calling `createObjEffectList` and `createRateEffectList`. This creates e.g. the evaluation and endowment effect copies.

Select the default effects by setting *include* to TRUE for `basic` `rate` and `linear` `shape` (if not any period uponly or downonly) and `quadratic` `shape` (if the range of the variable is greater than or equal to 2) evaluation effects.

**if** any period uponly or downonly **then**

    remove the linear effects (evaluation and endowment) from the data frame.

Add the starting values for the default effects calculated by `getBehaviorStartingVals` (see section 4.13) to the *initialValue* column of the data frame.

Alter the text for endowment effects to start with "dec. beh."

#### 4.4 Bipartite Network Effects

Call `networkRateEffects` to get the rate effects

Use `bipartiteObjective` effect group to create the objective function effects.

**for all** dyadic covariates with both node sets matching **do**

    Use `dyadObjective` effect group to create the appropriate effects

**for all** constant covariates, behavior variables, changing covariates **do**

    Call function `covarBipartiteEff` to add the appropriate effects

    poszvar is always TRUE for behavior variables.

**if** any covariates or behavior variables **then**

    Add *nintn* rows for user specified interaction effects

**for all** distinct dependent network variables with the same node set **do**

**if** oneMode **then**

        Use `bipartiteSymmetricObjective` or `bipartiteNonSymmetricObjective` effect groups to add the appropriate the effects

**else if** bipartite and matches first node set) **then**  
 Use `bipartiteBipartiteObjective` effect group to add the appropriate effects  
 NB no `covarNetNetObjective` here?  
**if** more than one network **then**  
 paste the network name at the front of all the objective function effects  
 Create the effects data frame by calling `createObjEffectList` and `createRateEffectList`. This creates e.g. the evaluation and endowment effect copies.  
 Alter the text for endowment effects to start "Lost ties:"  
 Calculate the starting values for the default effects (see section 4.15)  
 Select the default rate effects by setting *include* to TRUE for the **basic rate** effects.  
 Add the starting value for the rate to the *initialValue* column of the basic rate effects  
**if** no period is uponly or downonly **then**  
 Set *include* to TRUE for the degree (density) evaluation effect  
 Add the starting values for the degree(density) evaluation effect calculated by `getBipartiteStartingVals` to the *initialValue*.  
**else**  
 Remove both degree (density) effects from the data frame.

#### 4.5 covarOneModeEff

Use `covarSymmetricObjective` or `covarNonSymmetricObjective` effect group to create the objective function effects  
 Use `covarSymmetricRate` or `covarNonSymmetricRate` to create the rate effects  
**if** not poszvar **then**  
 Reduce the new objective function effects to just "altX" and "altSqX" (symmetric) or "egoX" (non symmetric)  
**if** not morethan2 **then**  
 Remove the "altSqX" effect.

#### 4.6 covarBipartiteEff

**if** first node set matches **then**  
 Use `covarBipartiteRate` effect group to create the rate effects  
 Use `covarBipartiteObjective` effect group to create the objective function effects  
**if** first node set matches **then**

reduce the objective function effects to “egoX”, “altDist2”, and  
“totDist2”  
**else if** *poszvar* **then**  
reduce the new objective function effects to the rows “altX” and  
“altSqX”  
**if** not *morethan2* **then**  
remove the “altSqX” effect  
**else**  
no objective function effects

#### 4.7 covBehEff

Use *covarBehaviorObjective* effect group to create a potential set of  
objective function effects  
**if** covariate and behavior variable are different **then**  
Create objective function effects as the first row of potential set  
**for all** oneMode dependent variables with the same node set **do**  
Add an objective function effect from the second row of the potential  
set.  
**if** any objective function effects **then**  
Set *shortName* to *effFrom*  
Use *covarBehaviorRate* effect group to create the rate effects  
Use *covarABehaviorBipartiteObjective* effect group to create  
objective function effects for bipartite dependent networks combined with  
covariates on the first node set

#### 4.8 covBBehEff

Use *covarBBehaviorBipartiteObjective* effect group to create  
objective function effects for bipartite dependent networks combined with  
covariates on the second node set

#### 4.9 covarNetNetEff

**if** *poszvar* **then**  
Use *covarNetNetObjective* effect group to create additional  
objective function effects if the second network is one-mode;  
Use *covarABNetNetObjective* effect group to create additional  
objective function effects if the second network is one-mode or  
two-mode;  
Use *covarANetNetObjective* effect group to create additional  
objective function effects if the second network is one-mode or



{two-mode while the covariate is defined for the first mode};  
 Use `covarBNetNetObjective` effect group to create additional  
 objective function effects if the second network is one-mode or  
 {two-mode while the covariate is defined for the second mode}.

#### 4.10 CreateRateEffectList

Add the *name* column by duplicating the dependent variable name, and  
*effectFn* and *statisticFn* as empty lists.

#### 4.11 CreateObjectEffectList

Add the *name* column by duplicating the dependent variable name, and  
*effectFn* and *statisticFn* as empty lists.

Add an endowment effect row if required for each objective function  
 effect.

#### 4.12 SienaGroupObject

First create the effects for the first data object, but inserting the correct  
 number of basic rate effects for the whole group.

**for all** other data objects **do**

**for all** dependent variables **do**

Create the starting values for this dependent variable

Insert the rate starting values in the *initialValue* field of the  
 correct effects

Combine the starting values to create an overall one for the  
 objective function effects:

**if** behavior **then**

Add new  $d_i, i = 1, \dots, n - 1$  to make one long vector of  
 difference vectors between  $n$  observations

**if** rounded range of variable (max-min) is 2 (what happens  
 with range 1) **then**

Add to  $n_{min+} = \sum_i n_{i,min+}$  and the others

Tendency is

$$\log\left(\frac{(n_{min+} + 2) * (n_{max+} + n_{max0} + 4))}{(n_{max-} + 2) * (n_{min+} + n_{min0} + 4))}\right)$$

**if** abs(tendency) > 2 **then**

trim to  $\pm 2$

**else** {range less than 2 or greater than 2}

Let  $\bar{d} = \text{mean}(d_i)$ , ignoring missing values  
 Let  $\sigma_d^2 = \text{var}(d_i)$ , ignoring missing values  
**if**  $\bar{d} < 0.9 * \sigma_d^2$  **then**  
     tendency =  $0.5 * \log((\bar{d} + \sigma_d^2)/(\bar{d} - \sigma_d^2))$   
**else**  
     tendency =  $\bar{d}/(\sigma_d^2 + 1)$   
**if** abs(tendency) greater than 3) **then**  
     Trim to  $\pm 3$   
**else if** onemode **then**  
  
**else** {bipartite}

#### 4.13 Behavior Starting Values

Calculate  $d_i, i = 1, \dots, n - 1$  difference vectors between  $n$  observations  
**if** rounded range of variable (max-min) is 2 (what happens with range 1)  
**then**

**for all** intervals  $i$  **do**

Let  $n_{i,min+}$  = number who start at minimum and go up  
 Let  $n_{i,min0}$  = number who start at minimum and stay there  
 Let  $n_{i,max-}$  = number who start at maximum and go down  
 Let  $n_{i,max0}$  = number who start at maximum and stay there  
 Calculate

$$v = \frac{n_{i,min+} + 1}{n_{i,min+} + n_{i,min0} + 2} + \frac{n_{i,max-} + 1}{n_{i,max0} + n_{i,max-} + 2}$$

**if**  $v > 0.9$  **then**

$$v = 0.5$$

Starting rate is  $-\log(1 - v)$

Let  $n_{min+} = \sum_i n_{i,min+}$  total number who start at minimum and go up

Let  $n_{min0} = \sum_i n_{i,min0}$  total number who start at minimum and stay there

Let  $n_{max-} = \sum_i n_{i,max-}$  total number who start at maximum and go down

Let  $n_{max0} = \sum_i n_{i,max0}$  total number who start at maximum and stay there

Tendency is

$$\log\left(\frac{(n_{min+} + 2) * (n_{max+} + n_{max0} + 4))}{(n_{max-} + 2) * (n_{min+} + n_{min0} + 4))}\right)$$

```

    if abs(tendency) > 2 then
        trim to  $\pm 2$ 
else {range less than 2 or greater than 2}
    for all intervals  $i$  do
        starting rate is  $\max(\text{var}(d_i), 0.1 * \sum_i \text{abs}(d_i) / \text{nactors})$ 
        Let  $\bar{d} = \text{mean}(d_i)$ , ignoring missing values
        Let  $\sigma_d^2 = \text{var}(d_i)$ , ignoring missing values
        if  $\bar{d} < 0.9 * \sigma_d^2$  then
            tendency =  $0.5 * \log((\bar{d} + \sigma_d^2) / (\bar{d} - \sigma_d^2))$ 
        else
            tendency =  $\bar{d} / (\sigma_d^2 + 1)$ 
        if abs(tendency) greater than 3 then
            Trim to  $\pm 3$ 

```

#### 4.14 One mode network Starting Values

Temporarily subtract 10 from structural values

Let  $\text{dif}_i$  be the number of differences between start and end of interval  $i$ , ignoring missings

Let  $n_{ijk}, j, k = 0, 1$  be counts of cells with value  $j$  at start and  $k$  at end of interval  $i$ , ignoring missings

Let  $n_i$  be the number of cells which are not missing at both start and end of interval  $i$ .

Let  $d_i$  be the sum of absolute differences by period, ignoring missings (already calculated and stored in the attribute *distance*).

Let  $\lambda_i$  be the starting value of basic rate parameter for interval  $i$

**if** symmetric **then**

$$\lambda_i = \text{nactors} * (0.2 + d_i) / (n_i \% \% 2 + 1)$$

**else**

$$\lambda_i = \text{nactors} * (0.2 + 2 * d_i) / (n_i + 1)$$

Trim  $\lambda_i$  to be between 0.1 and 100.

**if** symmetric **then**

Divide  $n_{ijk}$  by 2

starting value for degree parameter:

$$\begin{aligned}
 \text{Define } p_{i01} &= \begin{cases} n_{i01}/(n_{i01} + n_{i00}) & n_{i01} + n_{i00} \geq 1 \\ 0.5 & \text{otherwise} \end{cases} \\
 p_{i10} &= \begin{cases} n_{i10}/(n_{i10} + n_{i11}) & n_{i10} + n_{i11} \geq 1 \\ 0.5 & \text{otherwise} \end{cases} \\
 p_{i00} &= \begin{cases} n_{i00}/(n_{i01} + n_{i00}) & n_{i01} + n_{i00} \geq 1 \\ 0.5 & \text{otherwise} \end{cases} \\
 p_{i11} &= \begin{cases} n_{i11}/(n_{i10} + n_{i11}) & n_{i10} + n_{i11} \geq 1 \\ 0.5 & \text{otherwise} \end{cases}
 \end{aligned}$$

Trim  $p_{ijk}$  to lie between 0.02 and 0.98

Calculate  $p_i$

$$p_i = \begin{cases} 4/(p_{i00}/n_{i01} + p_{i11}/n_{i10}) & n_{i10} * n_{i01} \geq 1 \\ 1e - 6 & \text{otherwise} \end{cases}$$

Starting value for degree parameter is

$$\sum_i 0.5 * \log(p_{i01}/p_{i10}) * p_i / \sum_i p_i$$

#### 4.15 Bipartite Starting Values

Temporarily subtract 10 from structural values

Let  $diff_i$  be the number of differences between start and end of interval  $i$ , ignoring missings

Let  $n_{ijk}, j, k = 0, 1$  be counts of cells with value  $j$  at start and  $k$  at end of interval  $i$ , ignoring missings

Let  $n_i$  be the number of cells which are not missing at both start and end of interval  $i$ . (Diagonal included here.)

Let  $d_i$  be the sum of absolute differences by period, ignoring missings (already calculated and stored in the attribute ***distance***).

Let  $\lambda_i$  be the starting value of basic rate parameter for interval  $i$

$$\lambda_i = \text{nsenders} * (0.2 + 2 * d_i) / (n_i + 1)$$

Trim  $\lambda_i$  to be between 0.1 and 100.

starting value for degree parameter:

$$\begin{aligned}
 \text{Define } p_{i01} &= \begin{cases} n_{i01}/(n_{i01} + n_{i00}) & n_{i01} + n_{i00} \geq 1 \\ 0.5 & \text{otherwise} \end{cases} \\
 p_{i10} &= \begin{cases} n_{i10}/(n_{i10} + n_{i11}) & n_{i10} + n_{i11} \geq 1 \\ 0.5 & \text{otherwise} \end{cases} \\
 p_{i00} &= \begin{cases} n_{i00}/(n_{i01} + n_{i00}) & n_{i01} + n_{i00} \geq 1 \\ 0.5 & \text{otherwise} \end{cases} \\
 p_{i11} &= \begin{cases} n_{i11}/(n_{i10} + n_{i11}) & n_{i10} + n_{i11} \geq 1 \\ 0.5 & \text{otherwise} \end{cases}
 \end{aligned}$$

Trim  $p_{ijk}$  to lie between 0.02 and 0.98

Calculate  $p_i$

$$p_i = \begin{cases} 4/(p_{i00}/n_{i01} + p_{i11}/n_{i10}) & n_{i10} * n_{i01} \geq 1 \\ 1e-6 & \text{otherwise} \end{cases}$$

Starting value for degree parameter is

$$\sum_i 0.5 * \log(p_{i01}/p_{i10}) * p_i / \sum_i p_i$$

## 5. `sienaGroupCreate`

This function combines a list of `siena` data objects for common processing. It is also used in `initializeFRAN` to convert a single data object to a group one so that all later processing can have a common argument.

Some validation is performed to check that all the data objects match in terms of the dependent variables (name, type, nodesets) and covariates (names and nodesets).

If there is more than one data object, the constant covariates and constant dyadic covariates must be changed into changing ones. New covariates are created and the old ones removed from the lists. The attributes are copied over rather than recalculated (although they are mostly changed later).

Overall values are calculated for the balance mean, and network ranges. For behavior variables and covariates overall ranges, means and similarity mean values are calculated.

The following overall values are copied down to the individual objects:

**dependent variables** symmetric, missing, structural, poszvar, range, moreThan2 (some only if behavior)

**changing covariates** range, poszvar, moreThan2

**changing dyadic covariates** range, range2

## 5.1 Group attributes

The group object has various attributes, copied from or combinations of the attributes on the individual objects.

**netnames** the names of the dependent variables (these must be the same in each data object)

**symmetric** logical vector indicating whether the corresponding independent variable is symmetric (set to FALSE for behavior variables and bipartite networks).

**structural** logical vector indicating presence or absence of any structural values

**numberNonMissingNetwork** vector of count of non missing values for non behavior variables

**numberMissingNetwork** vector of count of missing values for non behavior variables

**numberNonMissingBehavior** vector of count of non missing values for behavior variables

**numberMissingBehavior** vector of count of missing values for behavior variables

**allUpOnly** logical vector indicating that the values for this independent variable never decrease over time

**allDownOnly** logical vector indicating that the values for this independent variable never increase over time

**anyUpOnly** logical vector indicating that for one or more of the intervals the values for this independent variable do not decrease

**anyDownOnly** logical vector indicating that for one or more of the intervals the values for this independent variable do not increase.

**allHigher** Table of logicals indicating whether *higher* attribute is true for each pair of networks in every data object

**allDisjoint** Table of logicals indicating whether *disjoint* attribute is true for each pair of networks in every data object

**allAtLeastOne** Table of logicals indicating whether *atLeastOne* attribute is true for each pair of networks in every data object

**anyHigher** Table of logicals indicating whether *higher* attribute is true for each pair of networks in any data object

**anyDisjoint** Table of logicals indicating whether *disjoint* attribute is true for each pair of networks in any data object

**anyAtLeastOne** Table of logicals indicating whether *atLeastOne* attribute is true for each pair of networks in any data object

**types** types of the independent variables

**observations** A single integer with the total number of periods to process.

**periodNos** A list of the period numbers (misses out the final one for each data object)

**groupPeriods** Vector of the number of total number of periods for each data object.

**netnodesets** A list containing the nodeset(s) for each dependent variable

**cCovars** Vector of names of constant covariates

**vCovars** Vector of names of changing covariates

**dycCovars** Vector of names of constant dyadic covariates

**dyvCovars** Vector of names of changing dyadic covariates

**ccnodesets** A vector containing the nodeset(s) for each constant covariate

**cvnodesets** A vector containing the nodeset(s) for each changing covariate

**dycnodesets** A list containing the nodeset(s) for each constant dyadic covariate

**dyvnodesets** A list containing the nodeset(s) for each changing dyadic covariate

**compositionChange** Logical vector indicating the presence of composition change data for any of the data objects

**exooptions** Named vector of composition change file options for the named node sets. Read from the first data object: assumed all the same

**names** Vector of names of the data objects

**class** ("sienaGroup", "siena")

**balmean** Vector of overall balance means, one for each dependent variable, NA for behavior variables and bipartites.

**structmean** Vector of overall structural means, one for each dependent variable, NA for behavior variables and bipartites.

**averageOutDegree** Vector of overall average outdegrees. NA for behavior variables.

**averageInDegree** Vector of overall average indegrees. NA for behavior variables and bipartites.

**bRange** Vector of overall ranges for behavior variables: entries corresponding to networks are NA

**behRange** Matrix with two rows, and column for each independent variable. Set to the overall min and max for behavior variables, NA for others

**bSim** Overall similarity mean for behavior variables, NA for networks

**bPoszvar** logical vector, NA for networks. For behavior variables TRUE if more than 1 distinct value in the overall values or any missing (always?)

**bMorethan2** logical vector. NA for networks. For behavior variables TRUE if more than 2 distinct values in overall variable, ignoring missings

**cCovarPoszvar** logical vector for constant covariates indicating presence if more than one distinct value or any missing (overall). NB only exist if there is only one data object.

**cCovarMoreThan2** logical vector for constant covariates indicating presence of more than 2 distinct values (missing is counted as a value)



**cCovarRange** vector of ranges for constant covariates

**cCovarRange2** matrix of min and max for constant covariates

**cCovarSim** vector of overall similarity means for constant covariates

**cCovarMean** vector of means for constant covariates

**vCovarPoszvar** logical vector for changing covariates indicating presence if more than one distinct value or any missing (overall).

**vCovarMoreThan2** logical vector for changing covariates indicating presence of more than 2 distinct values (missing is counted as a value)

**vCovarRange** vector of ranges for changing covariates

**vCovarSim** vector of overall similarity means for changing covariates

**vCovarMean** vector of means for changing covariates

**dycCovarRange** vector of ranges for constant dyadic covariates

**dycCovarRange2** matrix of min and max for constant dyadic covariates

**dycCovarMean** vector of means for constant dyadic covariates

**dyvCovarRange** vector of ranges for changing dyadic covariates

**dyvCovarRange2** matrix of min and max for constant dyadic covariates

**dyvCovarMean** vector of means for changing dyadic covariates

**anyMissing** logical vector indicating any missing values in the each dependent variable

**netRanges** Matrix with two rows and a column for each dependent variable. Overall min and max for networks, NA for behavior variables

## 6. *siena07*

This is a wrapper for the function *robmon* which performs the processing that used to be in *polrup* in *Siena3*. An optional tck/tk gui is provided, or progress messages are provided on the console. The choice between these is made by using `batch=FALSE` or `batch=TRUE` respectively.

Details of input and output are on the R help page. Required input is an object containing control information for the Robbins-Monro algorithm, and

any extra parameters required by the `FRAN` to be used. As the distinction between the two parts is not complete, flags `maxlike` and `cconditional` are on the input object, although not logically relevant to the algorithm.

There is user output written to a file (.txt), together with optional additional output to the console (suppressed unless `verbose=TRUE`), which can be redirected using the `sink()` command.

*robmon* attempts to duplicate the output of the `Siena3` procedure `polrup`. It uses a special function, *Report* for all output. This function knows about four files: `outf`, `lf`, `cf`, `bof`, and can also write to the console. Currently, all files except `outf` are null, with any other output suppressed or written to the console. Only *Report* would need altering to alter this behaviour. No file connections need to be passed around as parameters.

The object returned from *siena07* is an object containing everything of interest from the run, including the estimates of the parameters and the covariance matrix. Details of the more useful parts are in the R documentation.

## 7. User Interrupts

These are set in callbacks from the *siena07* tcl/tk gui. When they are read, a parallel set of flags is used to store the states, so that interrupts can be processed reliably. All is done using functions, to avoid global variables, or passing variables around. There are 3 interrupts:

**UserInterrupt** Stop everything, but return the values so far, with (I hope) some flag to indicate we did not finish.

**UserRestart** Go back to the beginning of phase 1 with the current parameters

**EarlyEndPhase2** Stop the estimation routine and proceed to phase 3 using the current parameters.

All six functions, if called with an argument, store the argument as the current value and if called with no argument, return the value. All values are booleans. The functions are not exported from the namespace, to avoid burdening the user with the details of their existence.

## 8. Robbins Monro Algorithm—*robmon*

The routine *robmon* contains the Robbins Monro (stochastic approximation) algorithm. It is the replacement for the *Siena3* procedure *polrup*. It is not designed to be called directly by the user, so there will not be an R help page for it.

The outline of the algorithm is given in the text *Siena algorithms*, and to understand the description of the code given here it may be helpful to have read that outline.

## 9. *robmon*

### 9.1 Input (from *siena07*)

**z** Model fitting object.

**x** Input model object, as described in the help page for *sienaModelCreate*.

... Extra parameters for **FRAN** (including the data!).

It may seem surprising that the data is simply a parameter passed unchanged to **FRAN**. But this is the point of the separation of the simulation and estimation routines: *robmon* could be used to solve the moment equation for any data: it does not matter whether the data is a network or something else entirely, as long as a matching **FRAN** is used.

### 9.2 Output

**z** . More or less everything used in the processing. Details in the help page for *siena07*.

### 9.3 Details

#### 9.3.1 *Initialize*

Copy from **x** everything that we may change during the run. Initialize number of iterations, restarted flag, force finite difference flag, etc.

### 9.3.2 *Initial call to FRAN*

This call is used to set up the parameters for conditional estimation, and to set up data in a call to C. The values of the statistics in the observed data (targets) are returned, along with the addresses of the data objects in C. The processed data and selected effects is written to a hidden data object within the function *FRANstore* from where it can be accessed on later calls, or passed to other processes.

### 9.3.3 *Initialise cluster of processes, if required*

This needs to access (but not understand!) the data object created in the call to *FRAN*. It sets up the processes and random number streams and passes the data object across. It then does a special call to *FRAN* to create the data objects in C++ for each process. Later calls to the processes only need minimal communication, done using cut-down versions of *x* and *z*.

### 9.3.4 *Calculate epsilon*

Used only for MoM estimation in the finite differences option. Currently 0.1, except for parameters which must be positive, where it is 0.1 times the parameter starting values.

TS: Here I would prefer  $\min\{0.1, 0.1 \times \text{starting value}\}$ .

Ruth: Easily changed, but we are using typically much bigger values than this: will it work? Are you sure you don't want max?

To be improved, to use prior information on standard error of parameter if available.

### 9.3.5 Main loop

Note R has no GOTO statement. I use the term *break* to indicate exit from the current loop only. Interrupts are checked after every iteration except the first few of phase 3. This documentation does not include all the details, or it would duplicate the code.

```
repeat
  repeat {this one is just to jump out of, only executed once}
    if all parameters now fixed (2 opportunities to do this in previous
    loop!) then
      set a flag to just do Phase 3.
    initialize interrupts
    announce phase 0 (set up progress bar, calculate iteration min and
    max for phase 2 subphases.)
    reset fixed flags
    if not just-phase-3 flag set then
      if need to do phase 1 then
        initialize phase 1
        run phase 1 iterations 1 to 10
        if using finite diffs then
          check number of changes and change epsilon if
          necessary
        if user stop or user restart or error or (using finite
        difference and need to repeat with new epsilon) then
          break
        if using finite diffs then
          fix PARAMETERS with 0 or 1 changes, if any exist
        run rest of phase 1 iterations
        if user stop or user restart or error then
          break
        calculate derivative matrix
        if necessary then
          change the length of phase 1 or force the use of finite
          differences
        if user stop or error or user restart then
          break
        if necessary then
          fix some parameters.
      Initialise phase 2
      run phase 2 subphase 1
      if error or user stop or user restart then
        break
```

```

        run phase 2 subphase 2
        if error or user stop or user restart or we have restarted because
        of epsilon change in phase 1 and not restarted from here before!
        then
            break
        run rest of phase 2 subphases
        if error or user stop or user restart then
            break
    run phase3
    if not user restart then
        break
until for ever
if do not need to restart because of epsilon or user restart then
    break
until for ever

```

### 9.3.6 Final processing

- Do a final call to **FRAN**. In conditional estimation, the rescaling of basic rate parameters will be done here.
- reset the covariance matrix to 33, 999 as in phase3.

## 10. Phase 1

### 10.1 Input

As for *robmon*.

### 10.2 Output

As for *robmon*.

### 10.3 Details

#### 10.3.1 Initialise

- Reset *SomeFixed* flag (have we fixed any parameters in this run).
- Announce phase 1
- Create arrays to store simulated statistics, scores and contributions to the derivative matrix from either the finite difference or maximum

likelihood routines. These arrays are currently redefined in Phase 3, so lost.

### 10.3.2 *Timing*

Timings are calculated between the start of the 2nd iteration and the start of the 6th iteration. This is just for determining the frequency of writing information to the gui. Write frequency is set to a prettified version of  $20/\text{time}$  for 5 iterations, or 5 if elapsed time is very small. For batch mode this is multiplied by 10, which seems unnecessary in phase 1. If using multiple clusters the total number of iterations are adjusted to be a multiple of the number of processes, and the 6th is replaced by the first one greater than or equal to 6 in the iteration sequence advancing in steps of the number of processes. I think this is wrong: it should be from 2 to 6 steps... but not very important! (I have made some adjustments for those users who have more than 9 processors: we do at least 10 simulations in the first part, and ignore timing if we do them in too few steps. If there are enough steps in the second part the timing is done there.)

### 10.3.3 *An iteration*

- call FRAN. If not OK, return
- store simulated statistics, scores if present, derivatives if present, simulated networks (part!) if present.
- if required, call finite differences routine and store result
- check for user interrupts and return if requested
- Report progress via progress bar or to console

### 10.3.4 *Check epsilons (only for finite differences option)*

- If derivatives are being calculated by finite differences, check after 10 iterations that enough different values of the statistics have occurred. Ideally 5 or more. (The check may not be done immediately after 10 iterations if we have 4 processors, say, but I do only look at 10 of the results.)
- If there are less than 3, `epsilon` is multiplied by 3 for parameters which must be positive, and by 10 otherwise.
- If there are 3 or 4, the multipliers are 2 and  $\sqrt{10}$ .

- If any new values are less than 0.1 times the scale factor, or more than 100 times it, replace by the bound.
- If any are less than 5, we will restart with the new epsilons, unless we have already done so 4 times.
- If we have already restarted 4 times then we continue, after fixing the last parameter with only 0 or 1 changes, if there are any such.

### 10.3.5 End of phase processing

- Calculate derivative estimate.
  - For finite differences or maximum likelihood: the mean of the arrays returned at each iteration.
  - For the score based method, we need a little notation:  
Let  $\mathbf{f}_i$  be the simulated deviations from the targets in iteration  $i$ , and  $\mathbf{s}_i$  the score function in iteration  $i$ ,  $N$  be the number of iterations. Then the estimated derivative matrix  $d_{ij}$  is given by:

$$D = \sum_i \text{outer}(\mathbf{f}_i, \mathbf{s}_i) / N - \text{outer}(\bar{\mathbf{f}}, \bar{\mathbf{s}}) / N^2$$

- For the score based method, if any of the diagonal values is non-positive, we do not continue. First we double the number of iterations in phase 1 and start again. Once this number exceeds 200, we stop increasing it and force the use of Finite differences. Then we don't come through this check!
  - For either method, if still processing, set the rows and columns related to fixed parameters to 0's with 1 on the diagonal.
  - If any diagonal values for non-fixed parameters are not positive, make them fixed, and set *newfixed* flags to record which ones have been fixed.
  - Calculate the standard deviations of the deviations.
- Invert the derivative matrix:
  - Set the rows and columns related to fixed parameters to 0's with 1 on the diagonal.
  - Replace any diagonal values less than 1e-8 by 1e-3.
  - Do the inversion



- If it fails, add 1 to the diagonal and try again
- Quasi-Newton step
  - If inversion of matrix was successful, set **fchange** to 0.5 times the gain parameter times the matrix product of inverse with the mean deviations from targets, otherwise to zero.
  - Zero the change for any fixed parameters.
  - Check the jump is not too large: if the maximum absolute value of the change divided by the corresponding input gain parameter is greater than 10, divide the changes by this value and multiply them by 10. This caps the maximum ratio to the scale at 10.
  - Check that positive parameters will stay positive. If not, replace the change for that parameter by half the current value of the parameter.
  - If the requested number of subphases in phase 2 is greater than 0, make the change by subtracting the changes from the current value of the parameters.

## 11. Phase2

### 11.1 Input

as for *robmon*

### 11.2 Output

as for *robmon*

### 11.3 Details

#### 11.3.1 Initialize Phase

Turn off calculation of derivatives. Multiply the gain parameter by 2.

#### 11.3.2 Process subphase

- Initialize
  - Announce subphase

- Extract max and min number of iterations from values stored from start. (They are calculated at the start to find the length of the progress bar, and it seemed better not to repeat it here!).
- Divide the gain parameter by 2
- Initialize the sum (which will become the mean) of thetas with the current value.
- Create arrays to store products of successive thetas.
- Perform iterations
  - Timing is calculated over the ten iterations 2 to 11. Write frequency is set to  $20/(\text{time for these 10 iterations})$  or 20 if time is too small. It is then prettified. Reporting using progress bar or console is done for each of the first 10 iterations and then at write frequency.
  - Call `FRAN` and store the deviations returned.
  - The update:
    - \* if only the diagonal of the derivative matrix is to be used in the update step (flag `x$diag`), calculate `maxrat`, the maximum ratio of the absolute deviations to their standard deviation (as estimated in Phase 1). If this is greater than the parameter `maxmaxrat`, set `maxrat` to `maxmaxrat/maxrat`, and record that the values were truncated.
    - \* if `x$diag`, update is `current gain * current deviations * maxrat / diagonal of derivative`
    - \* otherwise, update is `current gain * matrix product of current deviations with inverse of derivative matrix`.
    - \* For parameters which must be positive and would not remain so, replace change by 0.5 times current value of parameter,
    - \* Zero the change for any fixed parameters.
    - \* update theta by subtracting the change.
    - \* Add new value of theta to sum of thetas.
  - After each pair of iterations, add the product of the two deviations and the square of the most recent to accumulators, and calculate the ratio of the former to the latter, `ac`.
  - Check for user interrupts

- Stop the subphase when either the minimum number of iterations has been reached, and the maximum of `ac` is less than  $1e-10$  or the maximum number of iterations has been reached; or (the next condition is a rare occurrence but helps a lot when it occurs) at least 50 iterations have been done and the minimum `ac` is  $< -0.8$  and we have not done the maximum number of subphase repeats already (or user interrupt or error)
- Repeat the subphase if we stopped because of the minimum value of `ac`, unless we have already done the maximum number (set to 4).
- End of subphase. Replace parameters by the average in the subphase. Report details.

## 12. Phase3

### 12.1 Input

as for *robmon*

### 12.2 Output

as for *robmon*

### 12.3 Details

#### 12.3.1 *Initialize*

- Initialize arrays for deviations, scores, derivatives.
- Divide write frequency by the number of parameters for finite differences, 2 for score derivatives. Leave unchanged for maximum likelihood. Then re-prettify.
- Announce Phase

#### 12.3.2 *Iterations*

- Update progress via console or progress bar for each of first 5 iterations, then at the 10th and then at the write frequency.
- Call `FRAN` and store the deviations, scores, derivative contributions, and simulation values returned.

- If using finite differences (we revert to the method requested by the user here, even if we altered it in phase 1 because the score method did not work), call FiniteDifferences routine and store the resulting differences.
- After the 10th iteration check for user interrupts each time.

### 12.3.3 *End of Phase 3*

- Calculate derivative matrix `dfra`. Formulae as in Phase 1.
- Create a flag `diver` for each parameter, set to true if all the parameter values are fixed and the absolute value of the corresponding diagonal of the derivative matrix is less than 1e-6. .
- Calculate the covariance matrix of the simulated deviations, and the autocorrelations between them. (Done in the CalculateDerivative3 routine).
- Report. . .
- Calculate  $t$ -values for deviations from targets, as mean deviation divided by sqrt of diagonal entry of covariance matrix. Use 0 for small values of deviations and 999 for small values of variance.
- Report  $t$ -values, and comments on their values.
- For maximum likelihood, report autocorrelations
- Calculate `cov`, the covariance matrix of the estimates:
  - For maximum likelihood, inverse of `[dfra]` - variance matrix of deviations (here=scores!). (0 the rows and columns corresponding to fixed parameters, and put 1 on the diagonal, first.)
  - For others, matrix product of `dinv`, the adjusted covariance matrix of the deviations and the transpose of `dinv`.
  - Try to invert `cov`. Report. . .
  - Update the flag `diver` to mean: Not all parameters are fixed and this one is fixed or `diver` was true before (section 12.3.3) or the corresponding entry in the diagonal of the covariance matrix of the estimates is less than 1e-9.
  - set entries in `cov` to 33\* sqrt(diagonal) off diagonal and 999 on diagonal for parameters with `diver` true.
- Do ScoreTests if any have been requested.

## 13. FiniteDifferences

### 13.1 Input

as for *robmon* plus *fra*, the simulated value of the targets.

### 13.2 Output

as for *robmon*

### 13.3 Details

For each parameter,

- Call `FRAN` with epsilon added to this parameter only
- Calculate the deviations from the simulated statistics with no epsilon.
- In first 10 iterations of phase 1: Record if difference is greater than 1e-06
- Store and return these deviations divided by epsilon.

.

## 14. Score Tests

### 14.1 Control

- Do general test: call `EvaluateTestStatistic` with the complete arrays *dfra*, *msf*, the covariance matrix of the deviations, and *fra* the mean deviations.
- The values returned are a chi-squared test and, if the degrees of freedom are 1, a one-sided test.
- If only one test was requested, the two values returned correspond to the results required.
- If more than one test was requested, call `EvaluateTestStatistic` with data from which all but one of the parameters for which tests are required have been removed. Repeat for each parameter for which tests were requested.

## 14.2 EvaluateTestStatistic

- Partition `dfra` into four: R code is clear enough, I hope ( `drop=FALSE` just retains the matrix class even if one of the dimensions is 1)

```
d11 <- dfra[!test,!test,drop=FALSE]
d22 <- dfra[test,test,drop=FALSE]
d21 <- dfra[test,!test,drop=FALSE]
d12 <- t(d21)
```

- Similarly create  $\Sigma_{11}$ ,  $\Sigma_{22}$ ,  $\Sigma_{12}$  and  $\Sigma_{21}$  from `msf`, and `z1` and `z2` from `fra`. Then

For maximum likelihood

$$\begin{aligned} \text{ov} &= -\mathbf{z}_2 \\ \mathbf{vav} &= (\mathbf{d}_{22} - \mathbf{d}_{21} \mathbf{d}_{11}^{-1} \mathbf{d}_{12})^{-1} \end{aligned}$$

Otherwise

$$\begin{aligned} \text{ov} &= \mathbf{z}_2 - \mathbf{d}_{21} \mathbf{d}_{11}^{-1} \mathbf{z}_1 \\ \mathbf{vav} &= (\Sigma_{22} - \mathbf{d}_{21} \mathbf{d}_{11}^{-1} \Sigma_{12} - (\Sigma_{21} - \mathbf{d}_{21} \mathbf{d}_{11}^{-1} \Sigma_{11}) \mathbf{d}_{11}^{-T} \mathbf{d}_{21}^T)^{-1} \end{aligned}$$

then

$$\text{test statistic} = \text{ov}^T \mathbf{vav} \text{ov}$$

and the one-sided one, if appropriate,

$$\text{ov} \sqrt{\mathbf{vav}}$$

as  $\mathbf{vav}$  is then a scalar.