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The toggle switch example

This toggle switch example was generated will a Hill kinetics model trained to a subset of the data provided in Lugagne et al. 201x. The example is baised in pseudo experimental-data which means that all data is generated by the model we have previously trained. This is a standard procedure that serves as means of benchmarking the algorithm.

```
clear variables;
clc;
close all;
noise_pseudo_data=0.05;
```

A number of settings is defined in the default configuration file. The assertiveness of these settings is problem dependent. Settings such as the number optimzation solver settings, the experiments considered, or number of models (sparsity cases) have default values that should be tailored to the problem.

```
SBL_config_defaults;
```

As example we modify sbl_config.exp_idx for considering only experiments 1 and 2.

```
sbl_config.exp_idx=1:3;
```

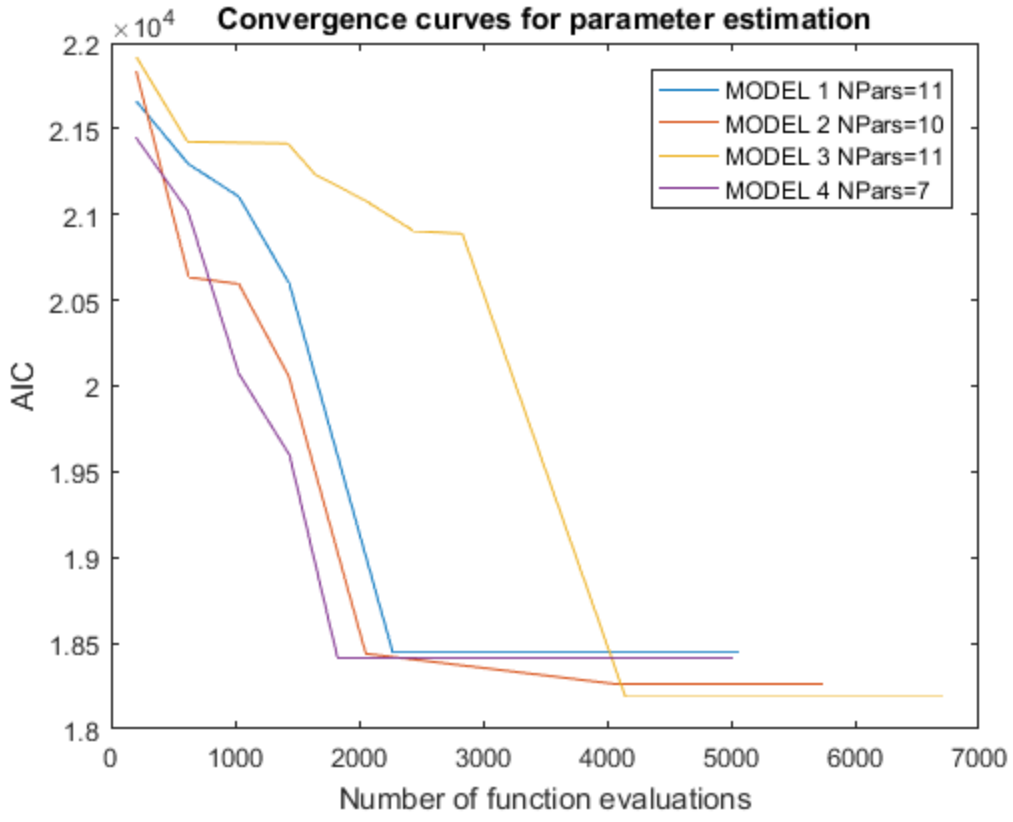
Generate and fit a family of models

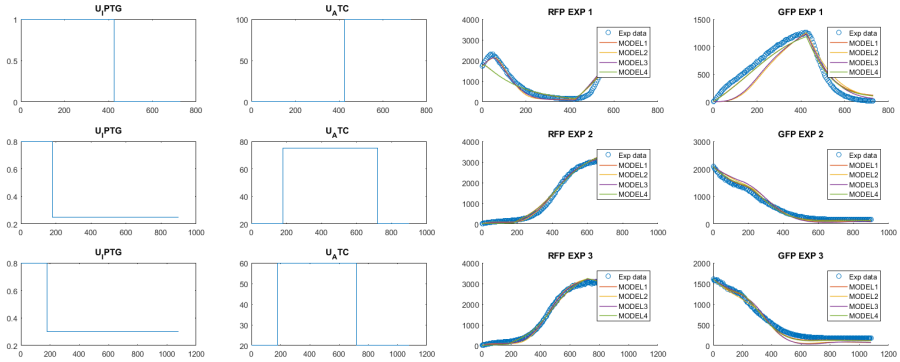
We generate a family of models with SBL and fit with AMIGO+scatter search The convergence curves are given scatter search. Time courses for each modeled observable are also ploted along with the pseudo experimental data. There is substantial progess made by the parameter estimation process.

```
MODELS=SBL_gen_model_family(sbl_config);
SBL_plotFamilyFit(MODELS);
set(gcf, 'Units', 'Normalized', 'OuterPosition', [0, 0.04, 1, 0.96]);
```

```
30-Aug-2019 13:48:48 | loop iter: 1, generating SBL data
30-Aug-2019 13:48:48 | file: experimental_data_loop_1.csv was
 successfully imported | 3  experiments was selected
30-Aug-2019 13:48:48 | loop iter: 1, running SBL
runnging sparsity case: 1/4
runnging SBL on state: 1/2
```

```
SBL iter: 1/10 took 1.88538 sec
SBL iter: 2/10 took 5.04426 sec
SBL iter: 3/10 took 3.546 sec
SBL iter: 4/10 took 9.17371 sec
SBL iter: 5/10 took 6.63062 sec
SBL iter: 6/10 took 5.20661 sec
SBL iter: 7/10 took 5.01391 sec
SBL iter: 8/10 took 3.97437 sec
SBL iter: 9/10 took 5.34479 sec
SBL iter: 10/10 took 4.02902 sec
runnging SBL on state: 2/2
SBL iter: 1/10 took 1.05419 sec
SBL iter: 2/10 took 0.894472 sec
SBL iter: 3/10 took 0.833257 sec
SBL iter: 4/10 took 0.802391 sec
SBL iter: 5/10 took 0.862429 sec
SBL iter: 6/10 took 0.823176 sec
SBL iter: 7/10 took 0.842969 sec
SBL iter: 8/10 took 0.845591 sec
SBL iter: 9/10 took 0.837469 sec
SBL iter: 10/10 took 0.816708 sec
Elapsed time is 0.855711 seconds.
state: x_1 zero_th: 9.49847e-05 dict_num: 6 (0.374298%)
state: x_2 zero_th: 9.49847e-05 dict_num: 6 (0.747198%)
ODE simulation OK
...
```





Execute OED for model discrimination

Optimal experimental design for model discrimination seeks to find the experiment that maximizes the predicted different between the models.

```
modelsAfterOED=OED4SBLdiscrimination(MODELS,sbl_config);
SBL_plotDiscriminationResult(modelsAfterOED);
set(gcf, 'Units', 'Normalized', 'OuterPosition', [0, 0.04, 1, 0.96]);
```

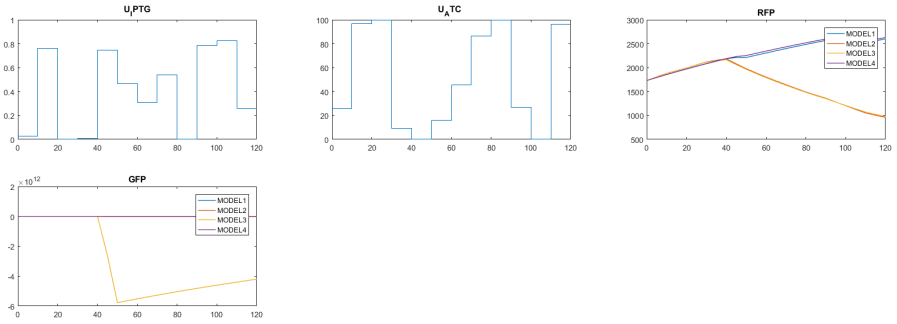
```
**********************************
     AMIGO2, Copyright @CSIC
     AMIGO2_R2017a [March 2017]
**********************************

*Date: 30-Aug-2019

------>Pre processing....this may take a few seconds.


------>Checking inputs....
n_exp
exp_type
n_obs
obs_names
obs
exp_y0
t_f
n_s
t_s
u_type
u_interp
n_steps
t_con
```

u_min
u_max
u
exp_data
...



Generate new pseudo experimental data

```
SBL_workdir;
data_file2_original=fullfile(SBL_work_dir,'Data',
['experimental_data_loop_' num2str(1) '.csv']);
data_file2_pseudo=fullfile(SBL_work_dir,'Data','experimental_data_2_pseudo.csv');
add_pseudo_data(modelsAfterOED,noise_pseudo_data,data_file2_original,data_file2_ps
```

```
**********************************
     AMIGO2, Copyright @CSIC
     AMIGO2_R2017a [March 2017]
**********************************

*Date: 30-Aug-2019

------>Pre processing....this may take a few seconds.


------>Checking inputs....
n_exp
exp_type
n_obs
obs_names
obs
t_f
n_s
t_s
```

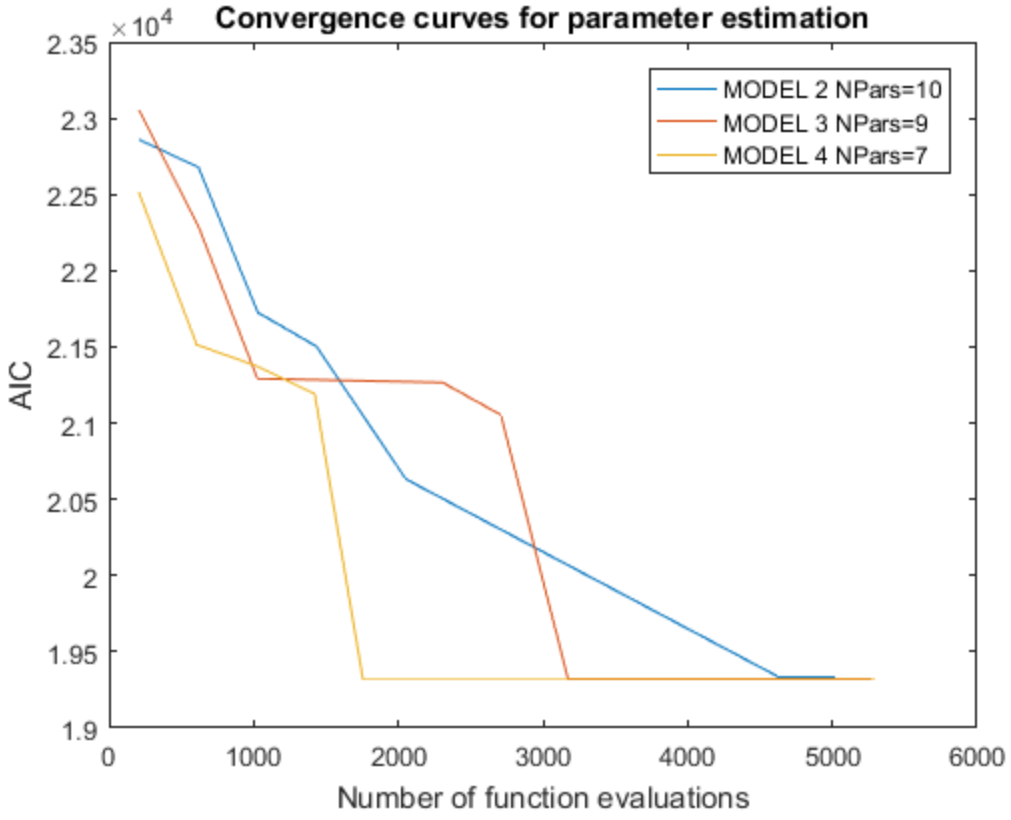
```
u_interp
t_con
n_steps
u
data_type
noise_type
exp_data
error_data
exp_y0
...
```

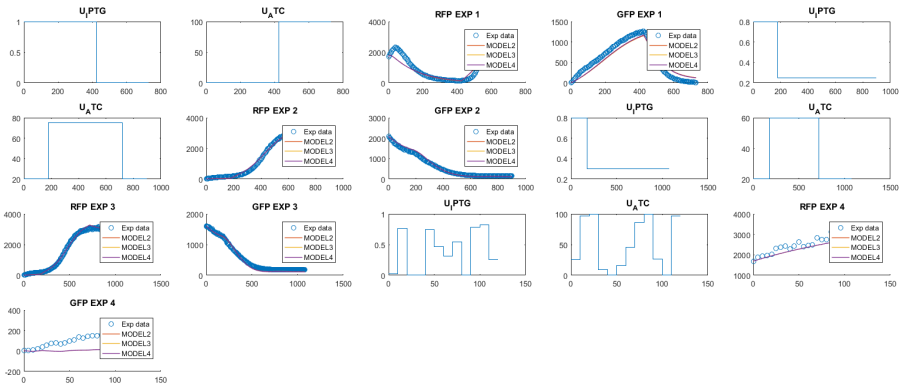
Second iteration: generate and fit a family of models

```
sbl_config.exp_idx=[1 2 3 8];
% %% Generate and fit a new family of models
sbl_config.data_dir_name = fullfile(SBL_work_dir,'Data');
sbl_config.data_file_name = 'experimental_data_2_pseudo.csv';
MODELS=SBL_gen_model_family(sbl_config);
SBL_plotFamilyFit(MODELS);
set(gcf, 'Units', 'Normalized', 'OuterPosition', [0, 0.04, 1, 0.96]);

30-Aug-2019 13:57:40 | loop iter: 1, generating SBL data
30-Aug-2019 13:57:40 | file: experimental_data_2_pseudo.csv was
 successfully imported | 4  experiments was selected
30-Aug-2019 13:57:40 | loop iter: 1, running SBL
runnging sparsity case: 1/4
runnging SBL on state: 1/2
SBL iter: 1/10 took 2.0794 sec
SBL iter: 2/10 took 1.65705 sec
SBL iter: 3/10 took 1.91759 sec
SBL iter: 4/10 took 2.00146 sec
SBL iter: 5/10 took 2.15446 sec
SBL iter: 6/10 took 5.30851 sec
SBL iter: 7/10 took 2.13166 sec
SBL iter: 8/10 took 4.43981 sec
SBL iter: 9/10 took 5.71969 sec
SBL iter: 10/10 took 3.75614 sec
runnging SBL on state: 2/2
SBL iter: 1/10 took 1.1617 sec
SBL iter: 2/10 took 1.10236 sec
SBL iter: 3/10 took 0.974459 sec
SBL iter: 4/10 took 1.03857 sec
SBL iter: 5/10 took 0.941195 sec
SBL iter: 6/10 took 0.962241 sec
SBL iter: 7/10 took 0.932872 sec
SBL iter: 8/10 took 1.20366 sec
SBL iter: 9/10 took 0.936159 sec
SBL iter: 10/10 took 0.930792 sec
Elapsed time is 0.980794 seconds.
state: x_1 zero_th: 9.49847e-05 dict_num: 5 (0.311915%)
state: x_2 zero_th: 9.49847e-05 dict_num: 5 (0.622665%)
```

```
Warning: Failure at t=5.169504e+02.  Unable to meet integration
 tolerances
...
```





Second interation of OED for model discrimination

Optimal experimental design for model discrimination seeks to find the experiment that maximizes the predicted different between the models.

```
modelsAfterOED=OED4SBLdiscrimination(MODELS,sbl_config);
SBL_plotDiscriminationResult(modelsAfterOED);
set(gcf, 'Units', 'Normalized', 'OuterPosition', [0, 0.04, 1, 0.96]);
```

```
**********************************
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     AMIGO2_R2017a [March 2017]
**********************************

*Date: 30-Aug-2019

------>Pre processing....this may take a few seconds.


------>Checking inputs....
n_exp
exp_type
n_obs
obs_names
obs
exp_y0
t_f
n_s
t_s
u_type
u_interp
n_steps
t_con
u_min
u_max
u
exp_data
...
```

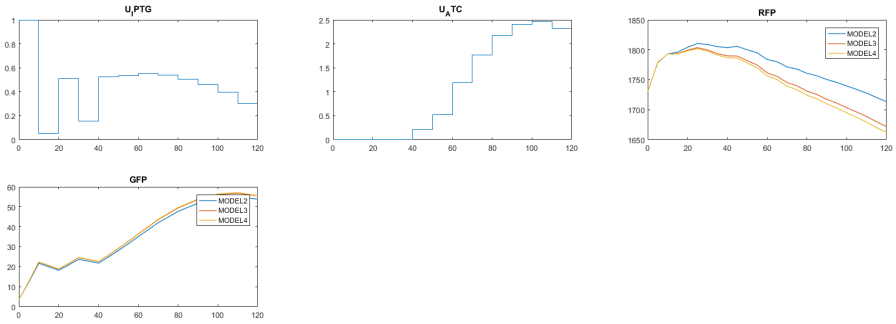

Generate new pseudo experimental data

```
SBL_workdir;
data_file2_original=fullfile(SBL_work_dir,'Data','experimental_data_2_pseudo.csv')
data_file2_pseudo=fullfile(SBL_work_dir,'Data','experimental_data_3_pseudo.csv');
add_pseudo_data(modelsAfterOED,noise_pseudo_data,data_file2_original,data_file2_ps



**********************************
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     AMIGO2_R2017a [March 2017]
**********************************

*Date: 30-Aug-2019

------>Pre processing....this may take a few seconds.


------>Checking inputs....
n_exp
exp_type
n_obs
obs_names
obs
t_f
n_s
t_s
u_interp
t_con
n_steps
u
data_type
noise_type
exp_data
```
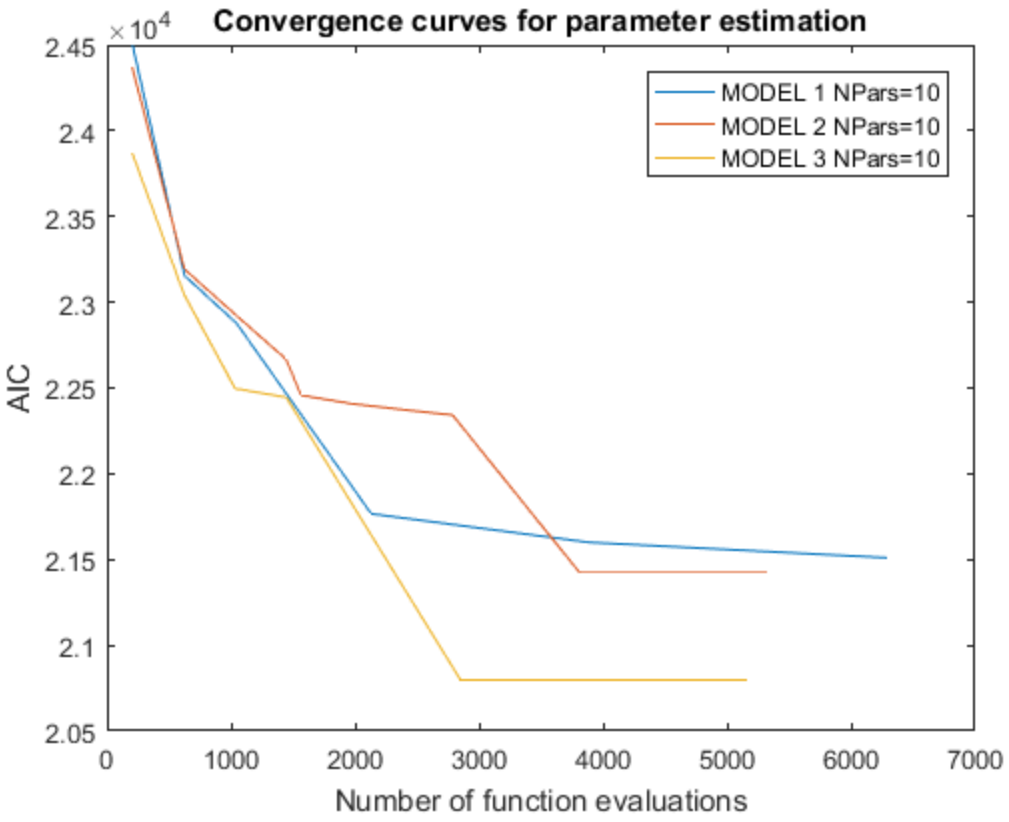
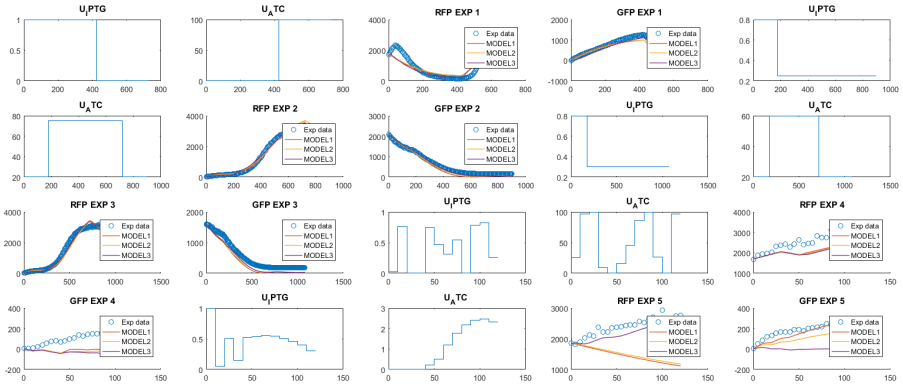

```
error_data
exp_y0
...
```

Third iteration: generate and fit a family of models

```
sbl_config.exp_idx=[1 2 3 8 9];
% %% Generate and fit a new family of models
sbl_config.data_dir_name = fullfile(SBL_work_dir,'Data');
sbl_config.data_file_name = 'experimental_data_3_pseudo.csv';
MODELS=SBL_gen_model_family(sbl_config);
SBL_plotFamilyFit(MODELS);
set(gcf, 'Units', 'Normalized', 'OuterPosition', [0, 0.04, 1, 0.96]);

30-Aug-2019 14:04:16 | loop iter: 1, generating SBL data
30-Aug-2019 14:04:17 | file: experimental_data_3_pseudo.csv was
 successfully imported | 5  experiments was selected
30-Aug-2019 14:04:17 | loop iter: 1, running SBL
runnging sparsity case: 1/4
runnging SBL on state: 1/2
SBL iter: 1/10 took 1.90564 sec
SBL iter: 2/10 took 1.7906 sec
SBL iter: 3/10 took 1.75508 sec
SBL iter: 4/10 took 1.73625 sec
SBL iter: 5/10 took 1.74325 sec
SBL iter: 6/10 took 1.99607 sec
SBL iter: 7/10 took 1.61788 sec
SBL iter: 8/10 took 1.65423 sec
SBL iter: 9/10 took 1.69231 sec
SBL iter: 10/10 took 1.85046 sec
runnging SBL on state: 2/2
SBL iter: 1/10 took 1.13093 sec
SBL iter: 2/10 took 1.0427 sec
SBL iter: 3/10 took 0.992127 sec
SBL iter: 4/10 took 0.925449 sec
SBL iter: 5/10 took 0.964139 sec
SBL iter: 6/10 took 0.972723 sec
SBL iter: 7/10 took 0.91436 sec
SBL iter: 8/10 took 0.919708 sec
SBL iter: 9/10 took 0.941921 sec
SBL iter: 10/10 took 0.950866 sec
Elapsed time is 0.996374 seconds.
state: x_1 zero_th: 9.49847e-05 dict_num: 5 (0.311915%)
state: x_2 zero_th: 9.49847e-05 dict_num: 6 (0.747198%)
ODE simulation OK
...
```

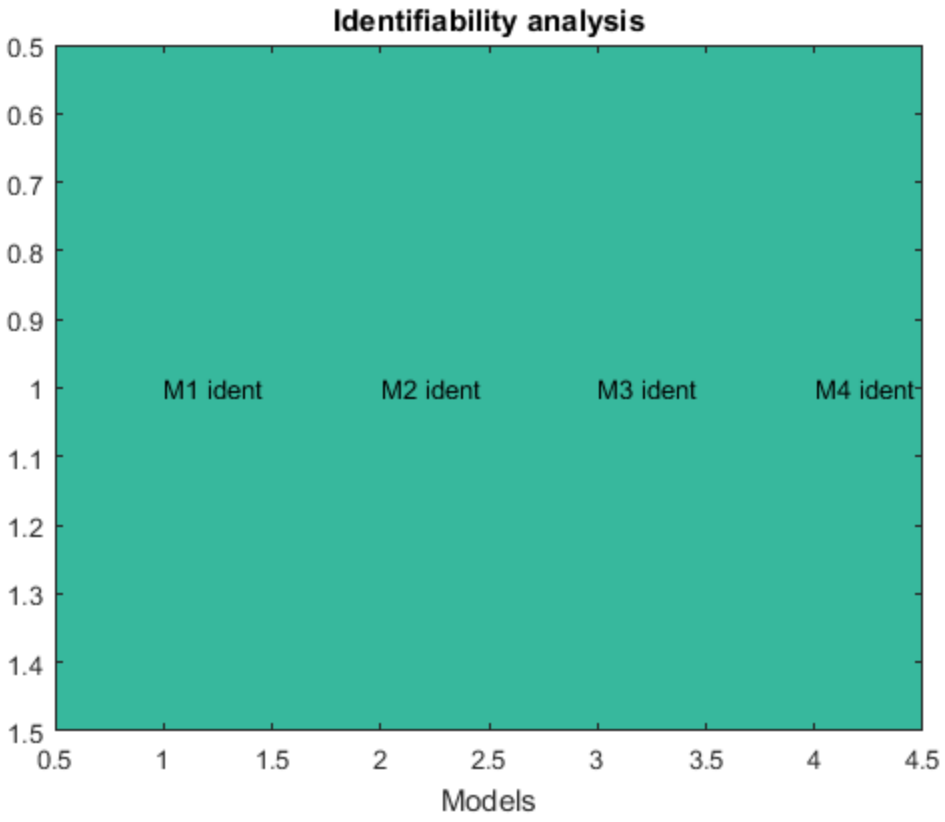




Structural identifiability of the final familly of models

```
res=SBL_structural_identifiability(sbl_config);

text()
```

```
30-Aug-2019 14:08:59 | file: experimental_data_3_pseudo.csv was
 successfully imported | 5  experiments was selected
30-Aug-2019 14:08:59 | loop iter: 1, running Strike-goldd
30-Aug-2019 14:08:59 | loop iter: 1, running SBL
runnging sparsity case: 1/4
runnging SBL on state: 1/2
SBL iter: 1/10 took 2.0076 sec
SBL iter: 2/10 took 1.75899 sec
SBL iter: 3/10 took 1.6869 sec
SBL iter: 4/10 took 1.69258 sec
SBL iter: 5/10 took 1.74748 sec
SBL iter: 6/10 took 2.0371 sec
SBL iter: 7/10 took 1.64203 sec
SBL iter: 8/10 took 1.63355 sec
SBL iter: 9/10 took 1.62268 sec
SBL iter: 10/10 took 1.6976 sec
runnging SBL on state: 2/2
SBL iter: 1/10 took 1.07356 sec
SBL iter: 2/10 took 0.970548 sec
SBL iter: 3/10 took 0.939703 sec
SBL iter: 4/10 took 0.907536 sec
SBL iter: 5/10 took 0.901307 sec
SBL iter: 6/10 took 0.92264 sec
SBL iter: 7/10 took 0.922385 sec
SBL iter: 8/10 took 0.919357 sec
SBL iter: 9/10 took 0.93169 sec
SBL iter: 10/10 took 0.94166 sec
Elapsed time is 0.978942 seconds.
state: x_1 zero_th: 9.49847e-05 dict_num: 5 (0.311915%)
state: x_2 zero_th: 9.49847e-05 dict_num: 6 (0.747198%)
ODE simulation OK
...
```



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