PS1_pyglotaran

April 21, 2021

1 Notes K-matrix

- $K_{ij} \iff$ energy flow from state j to state i

1.1 parallel (DAS)

Energy leaves system directly

Full matrix $\iff$ Reduced maxtrix:

- $K_{ij} = 0 \; \forall i \neq j$

1.2 sequntial (EAS)

Energy flows from one compartment i to the next $i+1$ until it leaves the system (K_{nn})

Assume $\mathbf{K}$ is $n \times n$ and sequence is in order

Full matrix:

- $K_{i+1i} = -K_{ii} \; \forall i < n \wedge K_{nn} \neq 0$

Reduced matrix:

- $K_{i+1i}^{Reduced} = K_{i+1i}^{Full} \wedge K_{ii} = 0 \; \forall i < n \wedge K_{nn} \neq 0$

1.3 General

Full matrix:

- $K_{ii} \iff -$ sum flows out of the compartment i (to other compartments or out of the system)
- $K_{ij} \; \forall i \neq j \iff$ flow from compartment j to comparment i

Reduced matrix:

- $\left(\sum_{k \neq i}^{n} K_{ki}\right) - K_{ii}^{Full} \iff$ flow of the compartment i out of the system
- $K_{ij}^{Reduced} = K_{ij}^{Full} \; \forall i \neq j \iff$ flow from compartment j to comparment i

2 cyano-PS1 case study

As in the lecture note we first try a global analysis

2.1 Global analysis

Assumpotion the process can ne described by a simple sequential model.

2.1.1 K-matrix sequential

The full K-matrix for a 4 compartment sequential scheme has the form of $\mathbf{K}^{Full}$

$$\mathbf{K}^{Full} = \begin{bmatrix} -k_{21} & & & \\ k_{21} & -k_{32} & & \\ & k_{32} & -k_{43} & \\ & & k_{43} & k_{4Out} \end{bmatrix}$$

Since both glotaran and pyglotaran use a reduced form of the K-matrix, it need to be transformed

$$\mathbf{K}^{Reduced} = \begin{bmatrix} k_{21} & & & \\ & k_{32} & & \\ & & k_{43} & k_{4Out} \end{bmatrix}$$

2.1.2 Notebook helper function for pretty output

[1]:
```
from IPython.display import Markdown, display


def print_md(markdown_printable):
    """Pretty render Markdown."""
    display(Markdown(str(markdown_printable)))


def print_yaml_file(file_path):
    """Pretty render yaml file."""
    with open(file_path) as f:
        print_md(f"```yaml\n{f.read()}\n```")
```

2.1.3 Plotting functions (`pyglotaran_extras` + `matplotlib`)

[2]:
```
import matplotlib.pyplot as plt
from pyglotaran_extras.plotting.plot_overview import plot_overview
from pyglotaran_extras.plotting.plot_svd import plot_svd

plt.rcParams["figure.figsize"] = (21, 14)
```

2.1.4 Analysis functions

[3]:
```
from glotaran.analysis.optimize import optimize
from glotaran.io import load_dataset, load_model, load_parameters
from glotaran.project.scheme import Scheme
```

2.1.5 Read data

[4]:
```
dataset = load_dataset("streakdata.ascii")
dataset
```

[4]:
```
<xarray.Dataset>
Dimensions:                       (left_singular_value_index: 49,
right_singular_value_index: 49, singular_value_index: 49, spectral: 49, time:
923)
Coordinates:
  * time                          (time) float64 -101.0 -100.8 … 99.24 99.46
  * spectral                      (spectral) float64 626.1 629.5 … 785.3 788.7
Dimensions without coordinates: left_singular_value_index,
right_singular_value_index, singular_value_index
Data variables:
    data                          (time, spectral) float64 50.75 59.21 … 113.1
    data_left_singular_vectors    (time, left_singular_value_index) float64 -0…
    data_singular_values          (singular_value_index) float64 2.802e+05 …
    data_right_singular_vectors   (right_singular_value_index, spectral) float64
…
```

2.1.6 Load model and parameters

[5]:
```
global_model = load_model("models/global-model.yml")
global_parameters = load_parameters("models/global-parameters.yml")
print_md(global_model.validate(parameters=global_parameters))
```

Your model is valid.

[6]:
```
print_md(global_model)
```

3 Model

Type: kinetic-spectrum

3.1 Initial Concentration

- **input1**:
  - *Label*: input1
  - *Compartments*: [‘s1’, ‘s2’, ‘s3’, ‘s4’]
  - *Parameters*: [input.1, input.0, input.0, input.0]
  - *Exclude From Normalize*: []

3.2 K Matrix

- **km1**:
  - *Label*: km1
  - *Matrix*:
    - *('s2', 's1')*: kinetic.1
    - *('s3', 's2')*: kinetic.2
    - *('s4', 's3')*: kinetic.3
    - *('s4', 's4')*: kinetic.4

3.3 Irf

- **irf1** (gaussian):
  - *Label*: irf1
  - *Type*: gaussian
  - *Center*: irf.center
  - *Width*: irf.width
  - *Normalize*: True
  - *Backsweep*: True
  - *Backsweep Period*: irf.backsweep

3.4 Dataset

- **dataset1**:
  - *Label*: dataset1
  - *Megacomplex*: ['mc1']
  - *Initial Concentration*: input1
  - *Irf*: irf1

3.5 Megacomplex

- **mc1**:
  - *Label*: mc1
  - *K Matrix*: ['km1']

3.5.1 Create scheme and optimize it

[7]:
```
global_scheme = Scheme(
    global_model,
    global_parameters,
    {"dataset1": dataset},
    non_negative_least_squares=True,
)
global_result = optimize(global_scheme)
```

```
   Iteration     Total nfev        Cost      Cost reduction    Step norm
Optimality
       0              1         4.7450e+07
2.84e+10
```

```
       1              2         4.3767e+07      3.68e+06       1.55e-01
5.88e+08
       2              3         4.3750e+07      1.73e+04       1.16e-02
1.63e+08
       3              4         4.3750e+07      6.34e+01       3.25e-04
2.50e+07
       4              5         4.3750e+07      6.14e-01       2.41e-05
2.84e+06
       5              6         4.3750e+07      8.45e-03       2.04e-06
4.06e+05
`ftol` termination condition is satisfied.
Function evaluations 6, initial cost 4.7450e+07, final cost 4.3750e+07, first-
order optimality 4.06e+05.
```

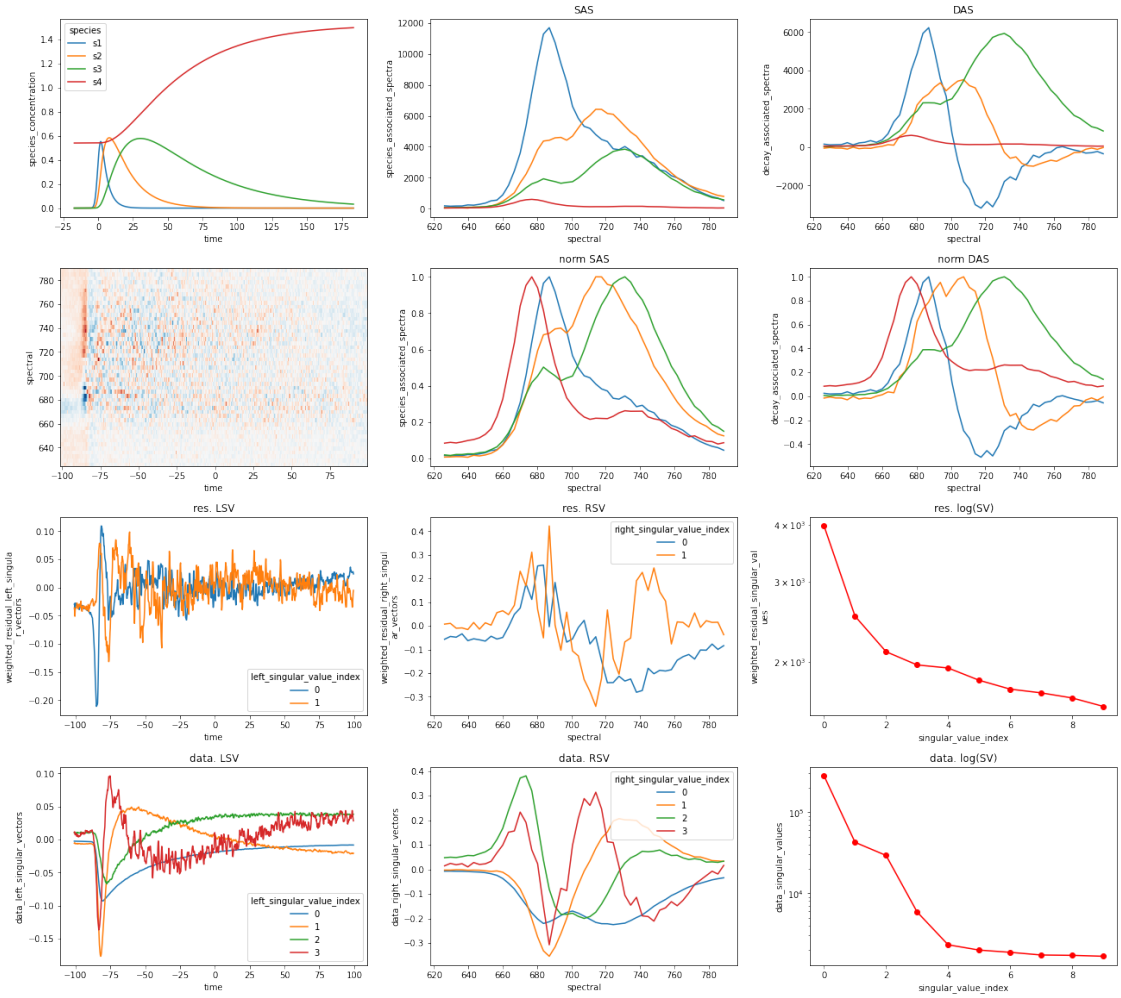
[8]:
```
global_result.data["dataset1"]
```

[8]:
```
<xarray.Dataset>
Dimensions:                                     (clp_label: 4, component: 4,
from_species: 4, left_singular_value_index: 49, right_singular_value_index: 49,
singular_value_index: 49, species: 4, spectral: 49, time: 923, to_species: 4)
Coordinates:
  * time                                        (time) float64 -101.0 … 99.46
  * spectral                                    (spectral) float64 626.1 … 788.7
  * clp_label                                   (clp_label) <U2 's1' 's2' … 's4'
  * species                                     (species) <U2 's1' 's2' 's3' 's4'
    rate                                        (component) float64 -0.225 … …
    lifetime                                    (component) float64 -4.445 … …
  * to_species                                  (to_species) <U2 's1' … 's4'
  * from_species                                (from_species) <U2 's1' … 's4'
Dimensions without coordinates: component, left_singular_value_index,
right_singular_value_index, singular_value_index
Data variables: (12/24)
    data                                        (time, spectral) float64 50.75 …
    data_left_singular_vectors                  (time, left_singular_value_index)
float64 …
    data_singular_values                        (singular_value_index) float64 …
    data_right_singular_vectors                 (right_singular_value_index,
spectral) float64 …
    matrix                                      (time, clp_label) float64 9.683…
    clp                                         (spectral, clp_label) float64 1…
    …                                          …
    a_matrix                                    (component, species) float64 1…
    k_matrix                                    (to_species, from_species) float64
…
    k_matrix_reduced                            (to_species, from_species) float64
…
    irf_center                                  float64 -83.85
```

```
    irf_width                                   float64 1.61
    irf                                         (time) float64 2.691e-25 … 0.0
Attributes:
    root_mean_square_error:            43.98496106181416
    weighted_root_mean_square_error:   43.98496106181416
```

3.5.2 Result plots

[9]:
```
fig = plot_overview(global_result.data["dataset1"], linlog=False)
```



[10]:
```
print_md(global_result.optimized_parameters)
```

- **input**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
1	1	0	-inf	inf	False	False	None

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
0	0	0	-inf	inf	False	False	None

- **irf**:

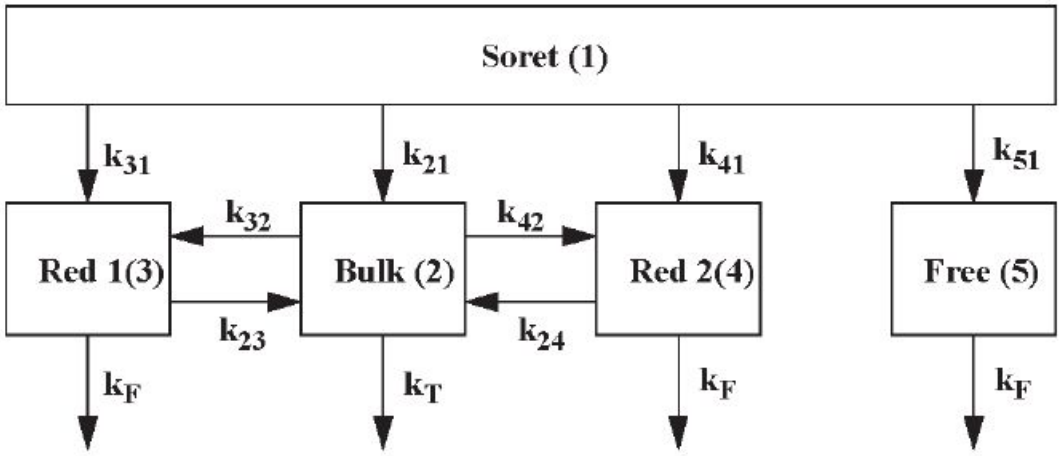
Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
center	-83.8533	6.73391e-05	-inf	inf	True	False	None
width	1.60986	6.95281e-05	-inf	inf	True	False	None
backsweep	13200	0	-inf	inf	False	False	None

- **kinetic**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
1	0.224983	3.32612e-05	-inf	inf	True	False	None
2	0.0680691	1.19792e-05	-inf	inf	True	False	None
3	0.0212251	1.18649e-06	-inf	inf	True	False	None
4	0.000159693	2.24382e-08	-inf	inf	True	False	None

3.6 Target analysis

Theoretical background from `compartmental_models.pdf`



Compartmental model describing the kinetics of cyanobacterial PS I core particles upon excitation at 400 nm.

Concentration vector

$$c(t) = \begin{bmatrix} S(t) & B(t) & R_1(t) & R_2(t) & F(t) \end{bmatrix}^T$$

The concentration function correspond to

Function name	***S(t)***	***B(t)***	***R_1(t)***	***R_2(t)***	***F(t)***
Name in the schema	Soret	Bulk	Red1	Red2	Free

Differential equation

$$\frac{\mathrm{d}}{\mathrm{dt}}c(t) = \mathbf{K}c(t) + j(t)$$

Input function

$$j(t) = i(t)\begin{bmatrix}1 & 0 & 0 & 0 & 0\end{bmatrix}^T$$

Transfer maxtrix **K**

$$\mathbf{K} = \begin{bmatrix} -(k_{21}+k_{31}+k_{41}+k_{51}) & & & & \\ k_{21} & -(k_T+k_{32}+k_{42}) & k_{23} & k_{24} & \\ k_{31} & k_{32} & -(k_F+k_{23}) & & \\ k_{41} & k_{42} & & -(k_F+k_{24}) & \\ k_{51} & & & & k_F \end{bmatrix}$$

- k_T: effective rate constantof Chl, T stands for photochemical Trapping of the excitation energy
- k_F: natural decay rate of free Chl, F stands for Fluorescence

[11]:
```
# Just a little helper to quickly make a pretty table
from tabulate import tabulate

headers = list(
    map(
        lambda x: f"***{x}***",
        ["Function name", "S(t)", "B(t)", "R_1(t)", "R_2(t)", "F(t)"],
    )
)
print(
    tabulate(
        [["**Name in the schema**", "Soret", "Bulk", "Red1", "Red2", "Free"]],
        headers=headers,
        tablefmt="github",
    )
)
```

```
| ***Function name***    | ***S(t)***   | ***B(t)***   | ***R_1(t)***   |
***R_2(t)***   | ***F(t)***   |
|------------------------|--------------|--------------|----------------|-------
---------|--------------|
```

| **Name in the schema** | Soret | Bulk | Red1 | Red2 | Free |

3.6.1 Reduced K-matrix

$$\mathbf{K} = \begin{bmatrix} & & & & \\ k_{21} & k_T & k_{23} & k_{24} & \\ k_{31} & k_{32} & k_F & & \\ k_{41} & k_{42} & & k_F & \\ k_{51} & & & & k_F \end{bmatrix}$$

3.6.2 Reduced K-matrix ignoring input to Red1 and Red2

$$\mathbf{K} = \begin{bmatrix} & & & & \\ k_{21} & k_T & k_{23} & k_{24} & \\ & k_{32} & k_F & & \\ & k_{42} & & k_F & \\ k_{51} & & & & k_F \end{bmatrix}$$

With the rate relations:

- $k_{23} = a_1\ k_{32}$
- $k_{24} = a_2\ k_{42}$

3.6.3 target-model.yml

[12]:
```
print_yaml_file("models/target-model.yml")
```

```
type: kinetic-spectrum

megacomplex:
  mc1:
    k_matrix: [km1]

k_matrix:
  km1:
    matrix:
      (s2, s1): kinetic.1
      (s5, s1): kinetic.2
      (s2, s2): kinetic.3
      (s3, s2): kinetic.4
      (s4, s2): kinetic.5
#       (s2, s3): {expr:scaling.a1*kinetic.4}
#       (s2, s3): $scaling.1 * $kinetic.4
      (s2, s3): kinetic.7
      (s3, s3): kinetic.6
#       (s2, s4): {expr:scaling.a2*kinetic.5}
#       (s2, s4): $scaling.2 * $kinetic.5
      (s2, s4): kinetic.8
      (s4, s4): kinetic.6
```

```
      (s5, s5): kinetic.6

spectral_constraints:
  - type: zero
    compartment: s1
    interval:
      - [100, 1000]
  - type: zero
    compartment: s3
    interval:
      - [100, 680]
  - type: zero
    compartment: s4
    interval:
      - [100, 690]


irf:
  irf1:
    type: gaussian
    center: irf.center
    width: irf.width
    backsweep: True
    backsweep_period: irf.backsweep


initial_concentration:
  input1:
    compartments: [s1, s2, s3, s4, s5]
    parameters: [
      input.1,
      input.0,
      input.0,
      input.0,
      input.0]


dataset:
  dataset1:
    initial_concentration: input1
    megacomplex: [mc1]
    irf: irf1
```

3.6.4 target-parameters.yml

[13]:
```
print_yaml_file("models/target-parameters.yml")
```

```
input:
```

```
  - ["1", 1]
  - ["0", 0]
  - {vary: false}

irf:
  - ["center", -84.0]
  - ["width", 1.6]
  - ["backsweep", 13800.0, {vary: false}]

kinetic:
  - [2, {vary: false}]
  - [0.1, {vary: false}]
  - 0.05
  - 0.1
  - 0.03
  - 0.00016
  - ["7", {expr: '$kinetic.4 * $scaling.1'}]
  - ["8", {expr: '$kinetic.5 * $scaling.2'}]
#   - {non-negative: true}


scaling:
  - [1.87, {vary: false}]
  - [1.37, {vary: false}]
```

[14]:
```
target_model = load_model("models/target-model.yml")
target_parameters = load_parameters("models/target-parameters.yml")
print_md(target_model.validate(parameters=target_parameters))
```

Your model is valid.

[15]:
```
print_md(target_model)
```

4 Model

Type: kinetic-spectrum

4.1 Initial Concentration

- **input1**:
  - *Label*: input1
  - *Compartments*: ['s1', 's2', 's3', 's4', 's5']
  - *Parameters*: [input.1, input.0, input.0, input.0, input.0]
  - *Exclude From Normalize*: []

4.2 K Matrix

- **km1**:
  - *Label*: km1

- *Matrix*:
  - *('s2', 's1')*: kinetic.1
  - *('s5', 's1')*: kinetic.2
  - *('s2', 's2')*: kinetic.3
  - *('s3', 's2')*: kinetic.4
  - *('s4', 's2')*: kinetic.5
  - *('s2', 's3')*: kinetic.7
  - *('s3', 's3')*: kinetic.6
  - *('s2', 's4')*: kinetic.8
  - *('s4', 's4')*: kinetic.6
  - *('s5', 's5')*: kinetic.6

4.3 Irf

- **irf1** (gaussian):
  - *Label*: irf1
  - *Type*: gaussian
  - *Center*: irf.center
  - *Width*: irf.width
  - *Normalize*: True
  - *Backsweep*: True
  - *Backsweep Period*: irf.backsweep

4.4 Dataset

- **dataset1**:
  - *Label*: dataset1
  - *Megacomplex*: ['mc1']
  - *Initial Concentration*: input1
  - *Irf*: irf1

4.5 Megacomplex

- **mc1**:
  - *Label*: mc1
  - *K Matrix*: ['km1']

4.6 Spectral Constraints

- **zero**:
  - *Type*: zero
  - *Compartment*: s1
  - *Interval*: [[100, 1000]]
- **zero**:
  - *Type*: zero
  - *Compartment*: s3
  - *Interval*: [[100, 680]]
- **zero**:
  - *Type*: zero

- *Compartment*: s4
- *Interval*: [[100, 690]]

4.6.1 Create scheme and optimize it

[16]:
```
target_scheme = Scheme(
    target_model,
    target_parameters,
    {"dataset1": dataset},
    non_negative_least_squares=True,
)
target_result = optimize(target_scheme)
```

```
   Iteration     Total nfev        Cost      Cost reduction    Step norm
Optimality
       0              1         1.3863e+08
1.20e+11
       1              2         4.8613e+07      9.00e+07       2.65e-01
2.49e+10
       2              3         4.6291e+07      2.32e+06       2.78e-02
5.90e+09
       3              4         4.6058e+07      2.33e+05       1.30e-02
2.13e+09
       4              5         4.6049e+07      8.58e+03       2.76e-03
2.53e+08
       5              6         4.6049e+07      5.01e+02       7.49e-04
1.09e+08
       6              7         4.6049e+07      3.21e+01       1.90e-04
2.18e+07
       7              8         4.6049e+07      2.07e+00       5.00e-05
6.48e+06
       8              9         4.6049e+07      1.34e-01       1.26e-05
1.52e+06
`ftol` termination condition is satisfied.
Function evaluations 9, initial cost 1.3863e+08, final cost 4.6049e+07, first-
order optimality 1.52e+06.
```

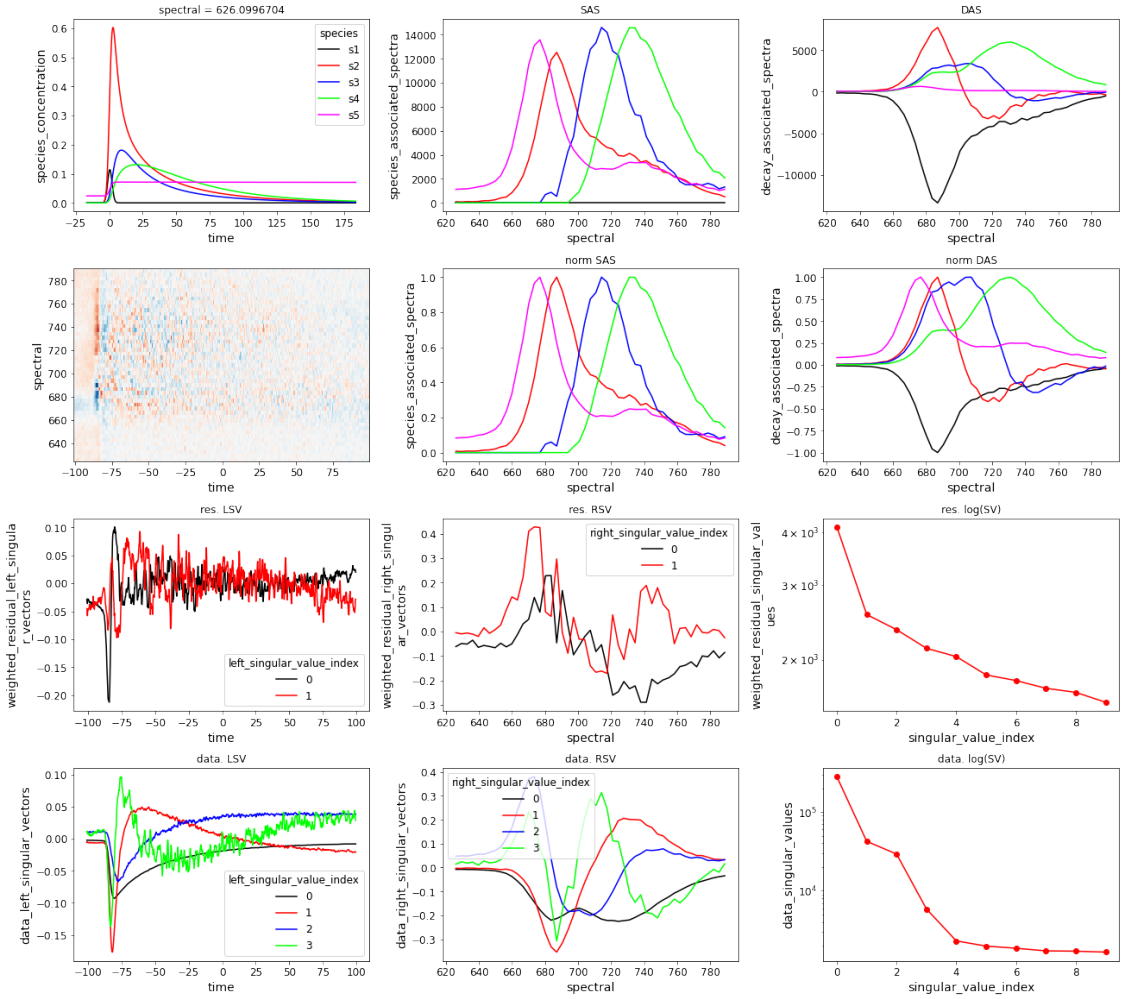
[17]:
```
target_result.data["dataset1"]
```

[17]:
```
<xarray.Dataset>
Dimensions:                                    (clp_label: 5, component: 5,
from_species: 5, left_singular_value_index: 49, right_singular_value_index: 49,
singular_value_index: 49, species: 5, spectral: 49, time: 923, to_species: 5)
Coordinates:
  * time                                       (time) float64 -101.0 … 99.46
  * spectral                                   (spectral) float64 626.1 … 788.7
  * clp_label                                  (clp_label) <U2 's1' 's2' … 's5'
  * species                                    (species) <U2 's1' 's2' … 's5'
```

```
    rate                                        (component) float64 -2.1 … -0…
    lifetime                                    (component) float64 -0.4762 …
  * to_species                                  (to_species) <U2 's1' … 's5'
  * from_species                                (from_species) <U2 's1' … 's5'
Dimensions without coordinates: component, left_singular_value_index,
right_singular_value_index, singular_value_index
Data variables: (12/24)
    data                                        (time, spectral) float64 50.75 …
    data_left_singular_vectors                  (time, left_singular_value_index)
float64 …
    data_singular_values                        (singular_value_index) float64 …
    data_right_singular_vectors                 (right_singular_value_index,
spectral) float64 …
    matrix                                      (spectral, time, clp_label)
float64 …
    clp                                         (spectral, clp_label) float64 0…
    …                                          …
    a_matrix                                    (component, species) float64 1…
    k_matrix                                    (to_species, from_species) float64
…
    k_matrix_reduced                            (to_species, from_species) float64
…
    irf_center                                  float64 -84.26
    irf_width                                   float64 1.602
    irf                                         (time) float64 2.23e-24 … 0.0
Attributes:
    root_mean_square_error:           45.125714328556704
    weighted_root_mean_square_error:  45.125714328556704
```

4.6.2 Result plots

[18]:
```
fig = plot_overview(target_result.data["dataset1"], linlog=False)
```



[19]:
```
print_md(target_result.optimized_parameters)
```

- **input**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
1	1	0	-inf	inf	False	False	None
0	0	0	-inf	inf	False	False	None

- **irf**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
center	-84.2618	6.00839e-05	-inf	inf	True	False	None
width	1.60168	6.52861e-05	-inf	inf	True	False	None
backsweep	13800	0	-inf	inf	False	False	None

- **kinetic**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
1	2	0	-inf	inf	False	False	None
2	0.1	0	-inf	inf	False	False	None
3	0.0680715	3.36631e-06	-inf	inf	True	False	None
4	0.072446	1.19977e-05	-inf	inf	True	False	None
5	0.0281201	2.88594e-06	-inf	inf	True	False	None
6	0.000159065	2.17346e-08	-inf	inf	True	False	None
7	0.135474	0	-inf	inf	False	False	$kinetic.4 * $scaling.1
8	0.0385246	0	-inf	inf	False	False	$kinetic.5 * $scaling.2

- **scaling**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
1	1.87	0	-inf	inf	False	False	None
2	1.37	0	-inf	inf	False	False	None

[ ]: