PCP_pyglotaran

April 24, 2021

1 PCP case study

1.1 No chl prime

1.1.1 Notebook helper function for pretty output

[1]:

```python
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```")
```

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

[2]:

```python
import matplotlib.pyplot as plt
from pyglotaran_extras.plotting.plot_overview import plot_overview
from pyglotaran_extras.plotting.plot_svd import plot_svd
from pyglotaran_extras.plotting.style import PlotStyle

plot_style = PlotStyle()
plt.rc("axes", prop_cycle=plot_style.cycler)
plt.rcParams["figure.figsize"] = (21, 14)
```

1.1.3 Analysis functions

[3]:

```python
from glotaran.analysis.optimize import optimize
from glotaran.io import load_dataset, load_model, load_parameters
from glotaran.project.scheme import Scheme
```

1.1.4 Read data

[4]:

```
dataset = load_dataset("PCP490.ascii")
dataset
```

[4]:

```
<xarray.Dataset>
Dimensions:                       (left_singular_value_index: 127,
right_singular_value_index: 127, singular_value_index: 127, spectral: 127, time:
198)
Coordinates:
  * time                        (time) float64 -0.825 -0.725 … 76.7 78.7
  * spectral                    (spectral) float64 473.2 475.3 … 743.2 745.3
Dimensions without coordinates: left_singular_value_index,
right_singular_value_index, singular_value_index
Data variables:
    data                        (time, spectral) float64 0.0002336 … 0.000…
    data_left_singular_vectors  (time, left_singular_value_index) float64 -0…
    data_singular_values        (singular_value_index) float64 0.7069 … 0…
    data_right_singular_vectors (right_singular_value_index, spectral) float64
…
```

1.1.5 Load model and parameters

[5]:

```
PCP_model = load_model("models/PCP-model.yml")
PCP_parameters = load_parameters("models/PCP-parameters.yml")
print_md(PCP_model.validate(parameters=PCP_parameters))
```

Your model is valid.

[6]:

```
print_md(PCP_model)
```

2 Model

Type: kinetic-spectrum

2.1 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*: []

2.2 K Matrix

- **km1**:
  - *Label*: km1
  - *Matrix*:
    - *(‘s1’, ‘s1’)*: kinetic.9

        - *('s2', 's1')*: kinetic.1
        - *('s5', 's1')*: kinetic.2
        - *('s2', 's2')*: kinetic.9
        - *('s3', 's2')*: kinetic.3
        - *('s4', 's2')*: kinetic.4
        - *('s5', 's2')*: kinetic.8
        - *('s3', 's3')*: kinetic.9
        - *('s5', 's3')*: kinetic.5
        - *('s4', 's4')*: kinetic.9
        - *('s5', 's4')*: kinetic.6
        - *('s5', 's5')*: kinetic.7

2.3 Irf

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

2.4 Dataset

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

2.5 Megacomplex

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

2.5.1 Create scheme and optimize it

[7]:
```
PCP_scheme = Scheme(PCP_model, PCP_parameters, {"dataset1": dataset})
PCP_result = optimize(PCP_scheme)
```

```
   Iteration     Total nfev        Cost      Cost reduction    Step norm
Optimality
       0              1         2.0573e-03
3.59e-02
       1              2         1.6894e-03      3.68e-04       1.57e-02
4.09e-03
       2              3         1.6751e-03      1.43e-05       6.39e-03
8.70e-04
```

```
       3              4         1.6739e-03      1.20e-06       1.99e-03
2.53e-04
       4              5         1.6738e-03      9.04e-08       5.46e-04
6.89e-05
       5              6         1.6738e-03      6.70e-09       1.49e-04
1.87e-05
       6              7         1.6738e-03      4.94e-10       4.04e-05
5.08e-06
       7              8         1.6738e-03      3.64e-11       1.10e-05
1.38e-06
       8              9         1.6738e-03      2.68e-12       2.98e-06
3.74e-07
`ftol` termination condition is satisfied.
Function evaluations 9, initial cost 2.0573e-03, final cost 1.6738e-03, first-
order optimality 3.74e-07.
```

[8]:

```
PCP_result.data["dataset1"]
```

[8]:

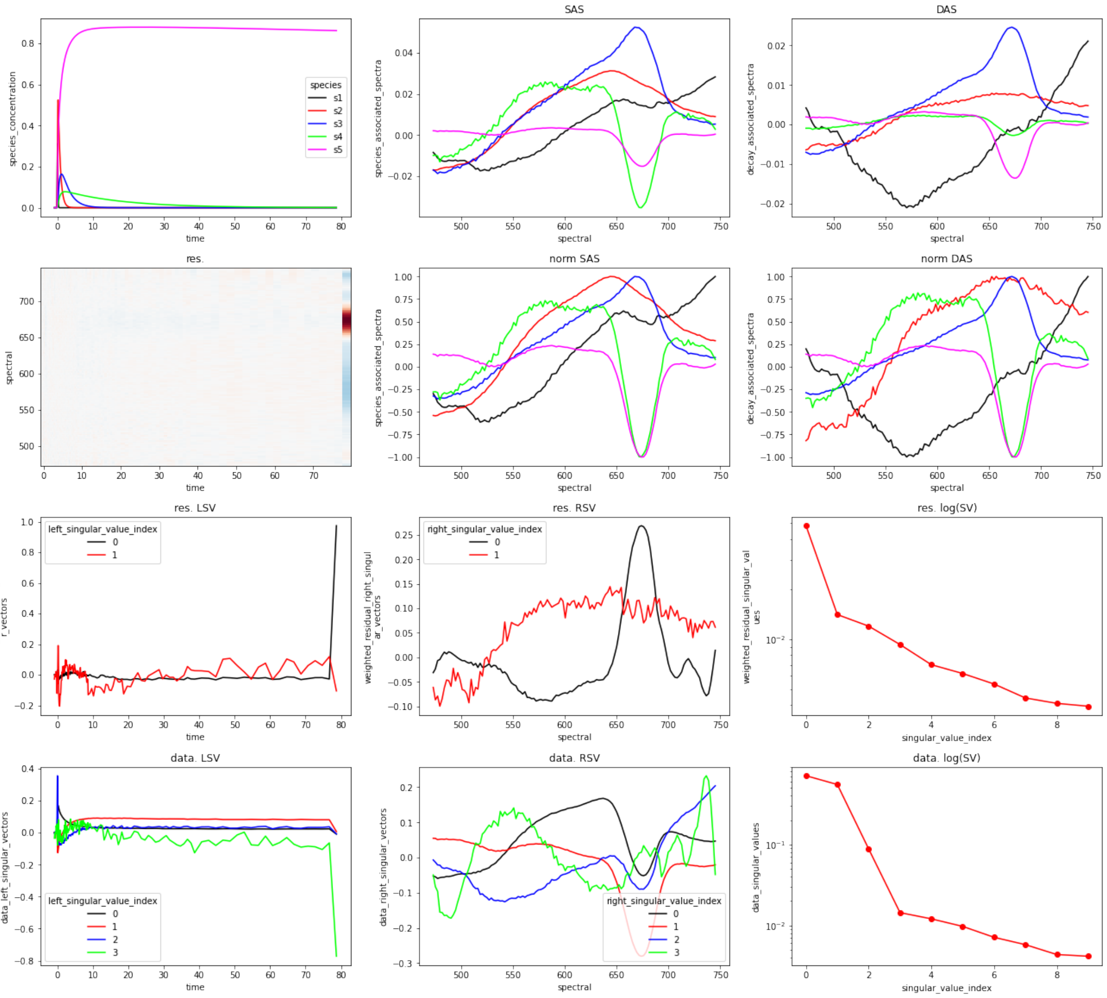
```
<xarray.Dataset>
Dimensions:                                   (clp_label: 5, component: 5,
from_species: 5, left_singular_value_index: 127, right_singular_value_index:
127, singular_value_index: 127, species: 5, spectral: 127, time: 198,
to_species: 5)
Coordinates:
  * time                                      (time) float64 -0.825 … 78.7
  * spectral                                  (spectral) float64 473.2 … 745.3
  * clp_label                                 (clp_label) <U2 's1' 's2' … 's5'
  * species                                   (species) <U2 's1' 's2' … 's5'
    rate                                      (component) float64 -15.14 … …
    lifetime                                  (component) float64 -0.06605 …
  * 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 0.0002…
    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 1.727…
    clp                                       (spectral, clp_label) float64 -…
    …                                        …
    a_matrix                                  (component, species) float64 1…
    k_matrix                                  (to_species, from_species) float64
…
```

```
    k_matrix_reduced                         (to_species, from_species) float64
…
    irf_center                               float64 0.009454
    irf_width                                float64 0.06646
    irf                                      (time) float64 5.903e-35 … 0.0
Attributes:
    root_mean_square_error:              0.0003648636062958407
    weighted_root_mean_square_error:     0.0003648636062958407
```

2.5.2 Result plots

[9]:

```python
try:
    fig = plot_overview(PCP_result.data["dataset1"], linlog=False)
except ValueError:
    # residual data aren't sorted and the plot fails
    pass
```



[10]:

```
print_md(PCP_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	0.00945429	1.31207	-inf	inf	True	False	None
width	0.0664634	0.940958	-inf	inf	True	False	None

- **kinetic**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
1	11	0	-inf	inf	False	False	None
2	4.1	0	-inf	inf	False	False	None
3	0.6	0	-inf	inf	False	False	None
4	0.2	0	-inf	inf	False	False	None
5	0.4	0	-inf	inf	False	False	None
6	0.02	0	-inf	inf	False	False	None
7	0.0005	0	-inf	inf	False	False	None
8	0.8	0	-inf	inf	False	False	None
9	0.04	0	-inf	inf	False	False	None

2.6 chl prime

2.6.1 Load model and parameters

[11]:

```
PCP_chl_prime_model = load_model("models/PCP-chl-prime-model.yml")
PCP_chl_prime_parameters = load_parameters("models/PCP-chl-prime-parameters.
 ↪yml")
print_md(PCP_model.validate(parameters=PCP_chl_prime_parameters))
```

Your model is valid.

[12]:

```
print_md(PCP_chl_prime_model)
```

3 Model

Type: kinetic-spectrum

3.1 Initial Concentration

- **input1**:
  - *Label*: input1
  - *Compartments*: [‘s1’, ‘s2’, ‘s3’, ‘s4’, ‘s5’, ‘s6’]
  - *Parameters*: [input.1, input.0, input.0, input.0, input.0, input.0]
  - *Exclude From Normalize*: []

3.2 K Matrix

- **km1**:
  - *Label*: km1
  - *Matrix*:
    - *(‘s1’, ‘s1’)*: kinetic.9
    - *(‘s2’, ‘s1’)*: kinetic.1
    - *(‘s5’, ‘s1’)*: kinetic.11
    - *(‘s6’, ‘s1’)*: kinetic.15
    - *(‘s2’, ‘s2’)*: kinetic.9
    - *(‘s3’, ‘s2’)*: kinetic.3
    - *(‘s4’, ‘s2’)*: kinetic.4
    - *(‘s5’, ‘s2’)*: kinetic.12
    - *(‘s6’, ‘s2’)*: kinetic.16
    - *(‘s3’, ‘s3’)*: kinetic.9
    - *(‘s5’, ‘s3’)*: kinetic.13
    - *(‘s6’, ‘s3’)*: kinetic.17
    - *(‘s4’, ‘s4’)*: kinetic.9
    - *(‘s5’, ‘s4’)*: kinetic.14
    - *(‘s6’, ‘s4’)*: kinetic.18
    - *(‘s5’, ‘s5’)*: kinetic.7
    - *(‘s6’, ‘s6’)*: kinetic.10

3.3 Irf

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

3.4 Dataset

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

3.5 Megacomplex

- **mc1**:
  - *Label*: mc1
  - *K Matrix*: [‘km1’]

3.6 Spectral Relations

- - *Compartment*: s5
  - *Target*: s6
  - *Parameter*: rel.r1
  - *Interval*: [[0, 1000]]

3.6.1 Create sceme and optimize it

[13]:

```
PCP_chl_prime_scheme = Scheme(
    PCP_chl_prime_model, PCP_chl_prime_parameters, {"dataset1": dataset}
)
PCP_chl_prime_result = optimize(PCP_chl_prime_scheme)
```

```
   Iteration     Total nfev        Cost      Cost reduction    Step norm
Optimality
       0              1         2.0130e-03
3.57e-02
       1              2         1.6626e-03      3.50e-04       1.51e-02
3.80e-03
       2              3         1.6506e-03      1.20e-05       5.63e-03
8.92e-04
       3              4         1.6493e-03      1.23e-06       1.93e-03
2.92e-04
       4              5         1.6492e-03      1.17e-07       5.95e-04
8.98e-05
       5              6         1.6492e-03      1.10e-08       1.82e-04
2.75e-05
       6              7         1.6492e-03      1.03e-09       5.58e-05
8.41e-06
       7              8         1.6492e-03      9.62e-11       1.71e-05
2.57e-06
       8              9         1.6492e-03      8.99e-12       5.22e-06
7.86e-07
`ftol` termination condition is satisfied.
Function evaluations 9, initial cost 2.0130e-03, final cost 1.6492e-03, first-
order optimality 7.86e-07.
```

[14]:

```
PCP_chl_prime_result.data["dataset1"]
```

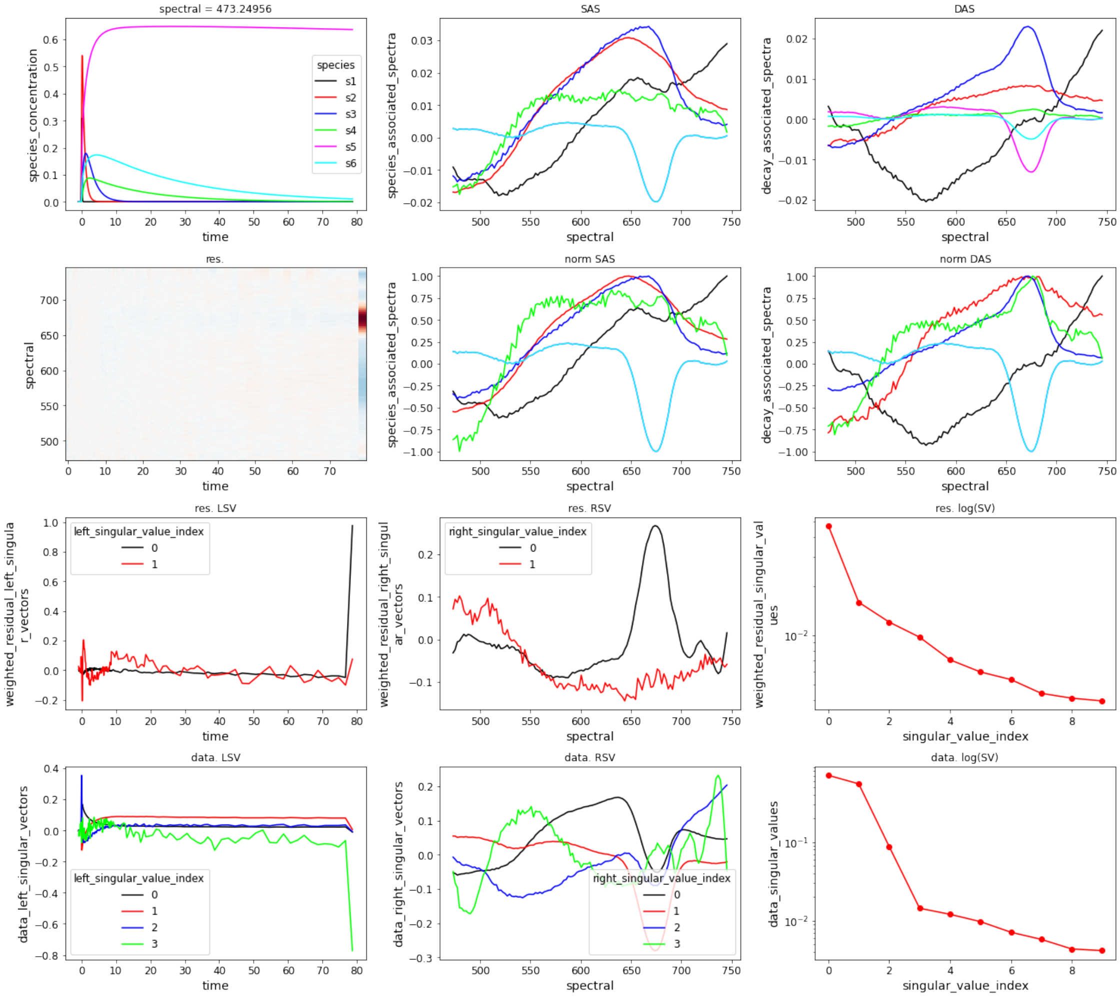
[14]:

```
<xarray.Dataset>
Dimensions:                                    (clp_label: 6, component: 6,
from_species: 6, left_singular_value_index: 127, right_singular_value_index:
```

```
127, singular_value_index: 127, species: 6, spectral: 127, time: 198,
to_species: 6)
Coordinates:
  * time                                      (time) float64 -0.825 … 78.7
  * spectral                                  (spectral) float64 473.2 … 745.3
  * clp_label                                 (clp_label) <U2 's1' 's2' … 's6'
  * species                                   (species) <U2 's1' 's2' … 's6'
    rate                                      (component) float64 -15.14 … …
    lifetime                                  (component) float64 -0.06605 …
  * to_species                                (to_species) <U2 's1' … 's6'
  * from_species                              (from_species) <U2 's1' … 's6'
Dimensions without coordinates: component, left_singular_value_index,
right_singular_value_index, singular_value_index
Data variables: (12/24)
    data                                      (time, spectral) float64 0.0002…
    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 -…
    …                                        …
    a_matrix                                  (component, species) float64 1…
    k_matrix                                  (to_species, from_species) float64
…
    k_matrix_reduced                          (to_species, from_species) float64
…
    irf_center                                float64 0.01118
    irf_width                                 float64 0.06693
    irf                                       (time) float64 1.275e-34 … 0.0
Attributes:
    root_mean_square_error:           0.0003621751818570837
    weighted_root_mean_square_error:  0.0003621751818570837
```

3.6.2 Result plots

[15]:
```python
try:
    fig = plot_overview(PCP_chl_prime_result.data["dataset1"], linlog=False)
except ValueError:
    # residual data aren't sorted and the plot fails
    pass
```



```
[16]: print_md(PCP_chl_prime_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	0.0111839	1.26513	-inf	inf	True	False	None
width	0.0669291	0.931301	-inf	inf	True	False	None

- **kinetic**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
1	11	0	-inf	inf	False	False	None
2	4.1	0	-inf	inf	False	False	None
3	0.6	0	-inf	inf	False	False	None
4	0.2	0	-inf	inf	False	False	None
5	0.4	0	-inf	inf	False	False	None
6	0.02	0	-inf	inf	False	False	None
7	0.0005	0	-inf	inf	False	False	None
8	0.6	0	-inf	inf	False	False	None
9	0.04	0	-inf	inf	False	False	None
10	0.04	0	-inf	inf	False	False	None
11	3.075	0	-inf	inf	False	False	$kinetic.2 * $scaling.1
12	0.45	0	-inf	inf	False	False	$kinetic.8 * $scaling.1
13	0.3	0	-inf	inf	False	False	$kinetic.5 * $scaling.1
14	0.015	0	-inf	inf	False	False	$kinetic.6 * $scaling.1
15	1.025	0	-inf	inf	False	False	$kinetic.2 * $scaling.2
16	0.15	0	-inf	inf	False	False	$kinetic.8 * $scaling.2
17	0.1	0	-inf	inf	False	False	$kinetic.5 * $scaling.2
18	0.005	0	-inf	inf	False	False	$kinetic.6 * $scaling.2

- **rel**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
r1	1	0	-inf	inf	False	False	None

- **scaling**:

Label	*Value*	*StdErr*	*Min*	*Max*	*Vary*	*Non-Negative*	*Expr*
1	0.75	0	-inf	inf	False	False	None
2	0.25	0	-inf	inf	False	False	None

```
[ ]:
```