fig_toc

February 9, 2022

[13]:
```
import numpy as np
import pandas as pd
import scipy.stats as stats
import scipy.optimize as optimize
import pymc3 as pm
import arviz as az
import theano.tensor as tt

import networkx as nx

import matplotlib.pyplot as plt
import matplotlib.gridspec as gridspec
import seaborn as sns; sns.set_theme(style='ticks', context='paper',␣
 ↪font_scale=0.8);

%reload_ext watermark
%watermark -a "Mathieu Baltussen" -d -t -u -v -iv
```

```
Author: Mathieu Baltussen

Last updated: 2022-02-08 15:04:51

Python implementation: CPython
Python version       : 3.9.5
IPython version      : 7.28.0

arviz     : 0.11.4
numpy     : 1.20.3
networkx  : 2.6.3
sys       : 3.9.5 | packaged by conda-forge | (default, Jun 19 2021, 00:32:32)
[GCC 9.3.0]
theano    : 1.1.2
scipy     : 1.6.2
matplotlib: 3.4.2
pandas    : 1.2.4
seaborn   : 0.11.1
pymc3     : 3.11.4
```

[2]:

```python
data = pd.read_csv("../data/CEKS33.csv")
kf = 0.125  # minute^-1
E = 0.012
data = data.assign(kf=kf, Tr=E)
data_1 = data[data.AAA == 0]
data_2 = data[data.AAA != 0]
```

[3]:

```python
with pm.Model() as model_1:
    k_cat = pm.Uniform("k_cat", 0, 500)
    K_M = pm.Uniform("K_M", 0, 500)
    K_I = pm.Uniform("K_I", 1000, 10000)
    sigma = pm.Exponential("sigma", 10)

    S_in = data_1["R"].values
    I_in = data_1["AAA"].values
    P_obs = data_1["AMC"].values
    S_obs = (
        S_in - P_obs
    )  # Substrate concentration inside reactor determined via stoichiometric␣
↪conservation at steady-state
    E = data_1["Tr"].values
    kf = data_1["kf"].values

    # Inference of probabilistic model at steady-state conditions
    P = pm.Normal(
        "obs",
        mu=k_cat * E * S_obs / (kf * (K_M + S_obs * (1 + I_in / K_I))),
        sigma=sigma,
        observed=P_obs,
    )
    idata_1 = pm.sample(
        1000,
        tune=1000,
        cores=4,
        step=pm.NUTS(target_accept=0.95),
        return_inferencedata=True,
    )

with pm.Model() as model_2:
    k_cat = pm.Uniform("k_cat", 0, 500)
    K_M = pm.Uniform("K_M", 0, 500)
    K_I = pm.Uniform("K_I", 1000, 10000)
    sigma = pm.Exponential("sigma", 10)

    S_in = data_2["R"].values
    I_in = data_2["AAA"].values
    P_obs = data_2["AMC"].values
```

```
    S_obs = (
        S_in - P_obs
    )  # Substrate concentration inside reactor determined via stoichiometric␣
 ↪conservation at steady-state
    E = data_2["Tr"].values
    kf = data_2["kf"].values

    # Inference of probabilistic model at steady-state conditions
    P = pm.Normal(
        "obs",
        mu=k_cat * E * S_obs / (kf * (K_M + S_obs * (1 + I_in / K_I))),
        sigma=sigma,
        observed=P_obs,
    )
    idata_2 = pm.sample(
        1000,
        tune=1000,
        cores=4,
        step=pm.NUTS(target_accept=0.95),
        return_inferencedata=True,
    )

with pm.Model() as model:
    k_cat = pm.Uniform("k_cat", 0, 500)
    K_M = pm.Uniform("K_M", 0, 500)
    K_I = pm.Uniform("K_I", 1000, 10000)
    sigma = pm.Exponential("sigma", 10)

    S_in = data["R"].values
    I_in = data["AAA"].values
    P_obs = data["AMC"].values
    S_obs = (
        S_in - P_obs
    )  # Substrate concentration inside reactor determined via stoichiometric␣
 ↪conservation at steady-state
    E = data["Tr"].values
    kf = data["kf"].values

    # Inference of probabilistic model at steady-state conditions
    P = pm.Normal(
        "obs",
        mu=k_cat * E * S_obs / (kf * (K_M + S_obs * (1 + I_in / K_I))),
        sigma=sigma,
        observed=P_obs,
    )
    idata = pm.sample(
        1000,
```

```
        tune=1000,
        cores=4,
        step=pm.NUTS(target_accept=0.95),
        return_inferencedata=True,
    )
```

```
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [sigma, K_I, K_M, k_cat]

<IPython.core.display.HTML object>

Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws
total) took 6 seconds.
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [sigma, K_I, K_M, k_cat]

<IPython.core.display.HTML object>

Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws
total) took 13 seconds.
There were 2 divergences after tuning. Increase `target_accept` or
reparameterize.
There were 2 divergences after tuning. Increase `target_accept` or
reparameterize.
There was 1 divergence after tuning. Increase `target_accept` or reparameterize.
The number of effective samples is smaller than 25% for some parameters.
Multiprocess sampling (4 chains in 4 jobs)
NUTS: [sigma, K_I, K_M, k_cat]

<IPython.core.display.HTML object>

Sampling 4 chains for 1_000 tune and 1_000 draw iterations (4_000 + 4_000 draws
total) took 4 seconds.
```

[4]:

```
posterior_df_1 = idata_1.to_dataframe(["posterior"])
posterior_df_2 = idata_2.to_dataframe(["posterior"])
posterior_df = idata.to_dataframe(["posterior"])

with model_1:
    post_pred_1 = pm.sample_posterior_predictive(
        idata_1, var_names=["obs", "k_cat", "K_M", "K_I", "sigma"]
    )
posterior_df_1 = pd.DataFrame(
    {
        "k_cat": post_pred_1["k_cat"],
        "K_M": post_pred_1["K_M"],
        "K_I": post_pred_1["K_I"],
        "sigma": post_pred_1["sigma"],
    }
)
```

```python
with model_2:
    post_pred_2 = pm.sample_posterior_predictive(
        idata_2, var_names=["obs", "k_cat", "K_M", "K_I", "sigma"]
    )
posterior_df_2 = pd.DataFrame(
    {
        "k_cat": post_pred_2["k_cat"],
        "K_M": post_pred_2["K_M"],
        "K_I": post_pred_2["K_I"],
        "sigma": post_pred_2["sigma"],
    }
)
with model:
    post_pred = pm.sample_posterior_predictive(
        idata, var_names=["obs", "k_cat", "K_M", "K_I", "sigma"]
    )
posterior_df = pd.DataFrame(
    {
        "k_cat": post_pred["k_cat"],
        "K_M": post_pred["K_M"],
        "K_I": post_pred["K_I"],
        "sigma": post_pred["sigma"],
    }
)
```

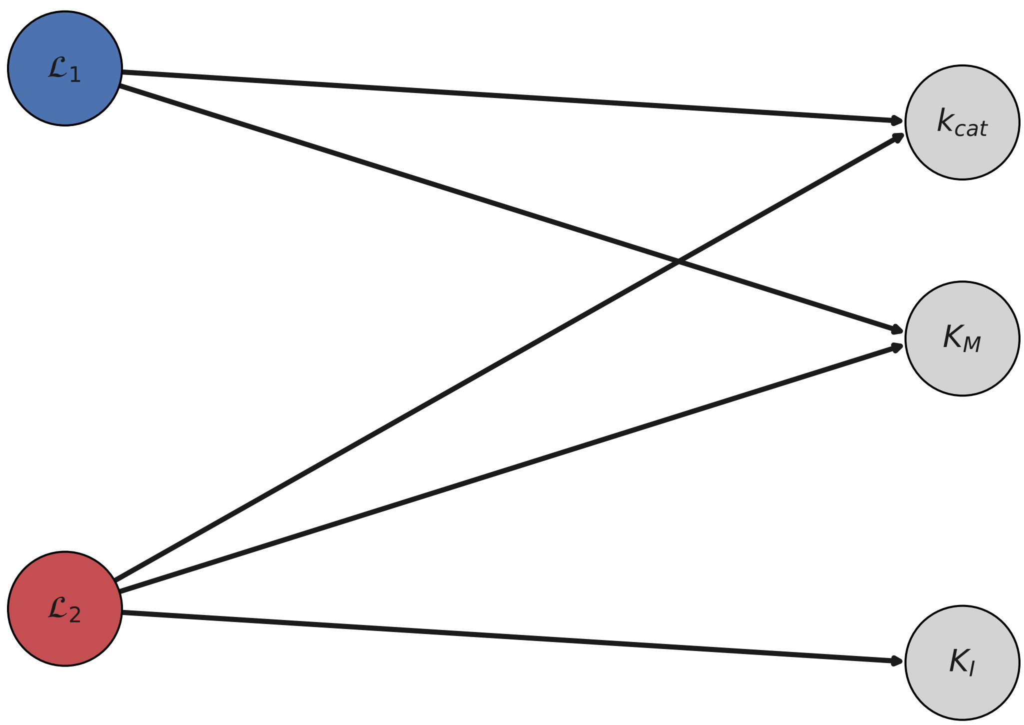
```
<IPython.core.display.HTML object>

<IPython.core.display.HTML object>

<IPython.core.display.HTML object>
```

[25]:

```python
left = nx.bipartite.sets(model_graph)[0]
pos = nx.bipartite_layout(model_graph, list(left)[::-1], scale=0.8)
print(pos)

pos = {
    "$\\mathcal{L}_{2}$": np.array([0.25, 0.25]),
    "$\\mathcal{L}_{1}$": np.array([0.25, 0.75]),
    "$k_{cat}$": np.array([0.75, 0.7]),
    "$K_M$": np.array([0.75, 0.5]),
    "$K_I$": np.array([0.75, 0.2]),
}

fig, ax = plt.subplots(constrained_layout=True)

with sns.color_palette("deep"):
    nx.draw(
        model_graph,
```

```
        pos=pos,
        ax=ax,
        with_labels=True,
        node_size=2000,
        node_color=["C0", "lightgrey", "lightgrey", "C3", "lightgrey"],
        width=2,
        edgecolors="black",
        arrowstyle="-|>",
        arrowsize=6,
        connectionstyle="arc,armB=-15",
    )
```

```
{'$\\mathcal{L}_{2}$': array([-0.8, -0.5]), '$\\mathcal{L}_{1}$': array([-0.8,
0.5]), '$k_{cat}$': array([ 0.53333333, -0.5       ]), '$K_M$':
array([0.53333333, 0.        ]), '$K_I$': array([0.53333333, 0.5       ])}
```



[85]:
```
def plot_ridgeplots(fig, gs, n_plots, data, start_color=0):
    pal = sns.cubehelix_palette(n_plots, start=start_color, rot=-.2, dark=0.4,␣
↪light=0.9)
    axes = [fig.add_subplot(gs[i,0]) for i in range(n_plots)]

    for i in range(n_plots):
```

```
        sns.kdeplot(data[i], ax=axes[i], fill=True, clip_on=True, alpha=0.6,␣
↪color=pal[i])
        sns.kdeplot(data[i], ax=axes[i], fill=False, clip_on=True,␣
↪color="black", lw=.2)

    # y_max = max(max(ax.get_yticks()) for ax in axes)*1.1
    x_min, x_max = min(axes[-1].get_xticks()),  max(axes[-1].get_xticks())
    for i, ax in enumerate(axes):
        # ax.set_ylim(0, y_max)
        ymax = max(ax.get_yticks())*(n_plots - i)
        ax.set_ylim(0)
        ax.set_xlim(x_min, x_max)
        ax.patch.set_alpha(0)

    for ax in axes[:-1]:
        ax.axis("off")
        sns.despine(ax=ax, left=True, bottom=True)

    axes[-1].set_yticks([])
    axes[-1].set_ylabel("")
    sns.despine(ax=axes[-1], left=True)

    return axes, pal
```

[114]:
```
palette = sns.cubehelix_palette(3, start=0.4, rot=-.2, dark=0.4, light=0.9)
palette
```

[114]:
```
[[0.8785578419340125, 0.9014144832192498, 0.9687173115546507],
 [0.6406706030956623, 0.622799643084166, 0.8302502287527784],
 [0.4428111826648146, 0.3448837880001888, 0.5788669999260483]]
```

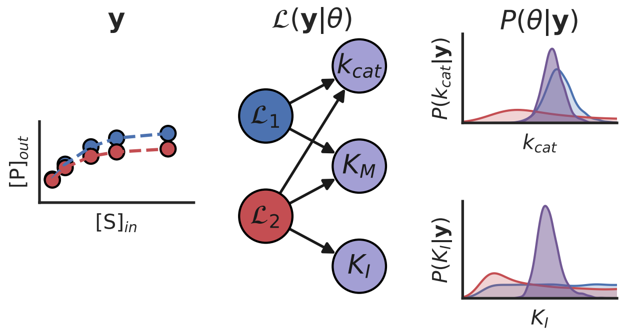
[218]:
```
model_graph = nx.DiGraph()
model_graph.add_edge(r"$\mathcal{L}_{1}$", r"$k_{cat}$")
model_graph.add_edge(r"$\mathcal{L}_{1}$", r"$K_M$")
model_graph.add_edge(r"$\mathcal{L}_{2}$", r"$k_{cat}$")
model_graph.add_edge(r"$\mathcal{L}_{2}$", r"$K_M$")
model_graph.add_edge(r"$\mathcal{L}_{2}$", r"$K_I$")
pos = {
    "$\\mathcal{L}_{2}$": np.array([0.33, 0.425]),
    "$\\mathcal{L}_{1}$": np.array([0.33, 0.575]),
    "$k_{cat}$": np.array([0.66, 0.65]),
    "$K_M$": np.array([0.66, 0.5]),
    "$K_I$": np.array([0.66, 0.35]),
}



fig = plt.figure(figsize=(3.25, 1.75), constrained_layout=True)
```

```
gs = fig.add_gridspec(4, 3, wspace=0.2, hspace=0.0)

# gs.subplots()


ax_1 = fig.add_subplot(gs[1:3, 0])
ax_1.scatter(data_1.R, data_1.AMC, ec="black", fc="C0", label=r"[I]=0 $\mu M$",
↪s=32)
ax_1.scatter(data_2.R, data_2.AMC, ec="black", fc="C3", label=r"[I]=1500 $\mu
↪M$", s=32)
ax_1.plot(data_1.R, data_1.AMC, "--", c="C0")
ax_1.plot(data_2.R, data_2.AMC, "--", c="C3")
# ax_1.legend()
ax_1.set_xlim(0, 600)
ax_1.set_ylim(0, 9)
# ax_1.text(-0.18, 0.95, 'A', transform=ax_1.transAxes, weight="bold", size=10)
ax_1.set_xlabel(r"$[$S$]_{in}$")
ax_1.set_ylabel(r"$[$P$]_{out}$")
ax_1.set_xticks([])
ax_1.set_yticks([])
sns.despine(ax=ax_1)
ax_1.margins(y=-0.3)

ax_2 = fig.add_subplot(gs[:, 1])

with sns.color_palette("deep"):
    nx.draw(
        model_graph,
        pos=pos,
        ax=ax_2,
        with_labels=True,
        node_size=400,
        node_color=["C0", palette[1], palette[1], "C3", palette[1]],
        width=1,
        edgecolors="black",
        arrowstyle="-|>",
        arrowsize=9,
        connectionstyle="arc",
        font_size=10
    )
    ax_2.margins(x=0.25, y=0.1)

    ax_3 = fig.add_subplot(gs[0:2, 2:])

    sns.kdeplot(posterior_df_1["k_cat"], ax=ax_3, fill=True, color="C0")
    sns.kdeplot(posterior_df_2["k_cat"], ax=ax_3, fill=True, color="C3")
```

```
    sns.kdeplot(posterior_df["k_cat"], ax=ax_3, fill=True, color=palette[2],␣
 ↪alpha=0.5)
    sns.despine(ax=ax_3)
    ax_3.set_xlim(75, 120)
    ax_3.set_ylabel(r"$P(k_{cat}|\mathbf{y})$")
    ax_3.set_xlabel(r"$k_{cat}$")
    ax_3.set_xticks([])
    ax_3.set_yticks([])


    # gs_rp = gs[2:, 2].subgridspec(3,1, hspace=-0.1)
    # axes, pal = plot_ridgeplots(fig, gs_rp, 3, [
    #                                             posterior_df_1['K_I'],
    #                                             posterior_df_2['K_I'],
    #                                             posterior_df['K_I']],
    #                             start_color=0.4
    #                             )

    ax_4 = fig.add_subplot(gs[2:, 2])

    sns.kdeplot(posterior_df_1["K_I"], ax=ax_4, fill=True, color="C0")
    sns.kdeplot(posterior_df_2["K_I"], ax=ax_4, fill=True, color="C3")
    sns.kdeplot(posterior_df["K_I"], ax=ax_4, fill=True, color=palette[2],␣
 ↪alpha=0.5)
    sns.despine(ax=ax_4)
    ax_4.set_xlim(0, 8000)
    ax_4.set_ylabel(r"$P(K_{I}|\mathbf{y})$")
    ax_4.set_xlabel(r"$K_{I}$")
    ax_4.set_xticks([])
    ax_4.set_yticks([])

# ax_0 = fig.add_subplot(gs[0, 0])
# sns.despine(ax=ax_0, left=True, bottom=True)
ax_1.text(0.5, 2.25, r"$\mathbf{y}$", transform=ax_1.transAxes, ha='center',␣
 ↪fontsize=10, va='center', weight='bold', in_layout=False)
ax_2.text(0.5, 1.05, r"$\mathcal{L}(\mathbf{y}|\theta)$", transform=ax_2.
 ↪transAxes, fontsize=10, ha='center', va='center', weight='bold',␣
 ↪in_layout=False)
ax_3.margins(y=0.2)
ax_3.text(0.5, 1.13, r"$P(\theta|\mathbf{y})$", transform=ax_3.transAxes,␣
 ↪ha='center', fontsize=10,  va='center', weight='bold', in_layout=True)

plt.savefig("../figures/fig_toc.svg", dpi=300)
plt.show()
```

```
/home/mathieu/anaconda3/envs/phd/lib/python3.9/site-
packages/numpy/core/_asarray.py:171: VisibleDeprecationWarning: Creating an
```

```
ndarray from ragged nested sequences (which is a list-or-tuple of lists-or-
tuples-or ndarrays with different lengths or shapes) is deprecated. If you meant
to do this, you must specify 'dtype=object' when creating the ndarray.
  return array(a, dtype, copy=False, order=order, subok=True)
```




```
[ ]:
```