

The stoichBondGraph module: From Stoichiometry to Bond Graph

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Note: this is the stoichBondGraph.ipynb notebook. The PDF version “The stoich-BondGraph module: From Stoichiometry to Bond Graph” is available [here](#).

1 Introduction

The bond graph approach [Gawthrop and Crampin \(2016, 2014, 2017\)](#); [Gawthrop et al. \(2015\)](#); [Oster et al. \(1971, 1973\)](#) to modelling biomolecular systems of interest to systems biologists developed independently from the stoichiometric approach [Palsson \(2006, 2011, 2015\)](#).

However, the conceptual point of intersection of the two approaches is the fact that the stoichiometric matrix is the modulus of the conceptual multiplier linking reactions to species. This means that the two approaches are complementary and each can build on the strengths of the other.

This tutorial illustrates how a stoichiometric system description can be used to automatically create the corresponding bond graph. However, more complex systems such as the ecoli core model [Orth et al. \(2010\)](#) can also be translated in the same way.

1.1 Import some python code

The bond graph analysis uses a number of Python modules:

```
[1]: ## Some useful imports
import BondGraphTools as bgt
import numpy as np

## Stoichiometry to BG
import stoichBondGraph as stbg
```

2 Create a stoichiometric representation

In this context a stoichiometric representation is a python dictionary with the following fields

- name (string): the name of the bg to be created
- N (numpy integer array): the stoichiometric matrix
- species (list of strings): the names of the species
- reaction (list of strings): the names of the reaction

Optionally, the forward and reverse stoichiometric matrices N_f and N_r can be included instead of N

Note that there is one species per row, and one reaction per column, of N

A file name.py is written containing the function model() which returns the bg in bgt form

2.1 Example

This example corresponds to ABCD_abg.svg in Tutorial svgBondGraph.

```
[2]: ## Stoichiometric matrix N
N = np.array(
    [
        [-1, 0, 0, 0],
        [ 0, -1, 0, 0],
```

```

        [ 0, 0, 1, 0],
        [ 0, 0, 0, 1],
        [-1, 0, 0, 1],
        [ 1,-1, 0, 0],
        [ 0, 1,-1, 0],
        [ 0, 0, 1,-1]
    ]
)

## Species and reactions
species = ['A', 'B', 'C', 'D', 'E1', 'E2', 'E3', 'E4']
reaction = ['r1', 'r2', 'r3', 'r4']

## Pack into a dict with name 'ABCDE_abg'
s = {
    'name': 'BG_abg',
    'N': N,
    'species': species,
    'reaction': reaction
}

## Convert to a bondgraph
stbg.model(s)

```

```
[3]: import BG_abg; BG = BG_abg.model(); help(BG_abg)
```

Help on module BG_abg:

NAME

BG_abg

FUNCTIONS

model()

Acausal bond graph BG_abg.py

Created by stoichBondGraph at Wed May 22 09:59:40 2024

Usage:

import BG_abg; model = BG_abg.model()

FILE

/home/peterg/WORK/Research/SystemsBiology/Notes/2024/Tutorial/stoichBondGraph/BG_abg.py

Various properties of the BGT model can now be extracted.

```
[4]: BG.state_vars
```

```
[4]: {'x_0': (C: A, 'q_0'),
      'x_1': (C: B, 'q_0'),
```

```
'x_2': (C: C, 'q_0'),
'x_3': (C: D, 'q_0'),
'x_4': (C: E1, 'q_0'),
'x_5': (C: E2, 'q_0'),
'x_6': (C: E3, 'q_0'),
'x_7': (C: E4, 'q_0')}
```

```
[5]: BG.constitutive_relations
```

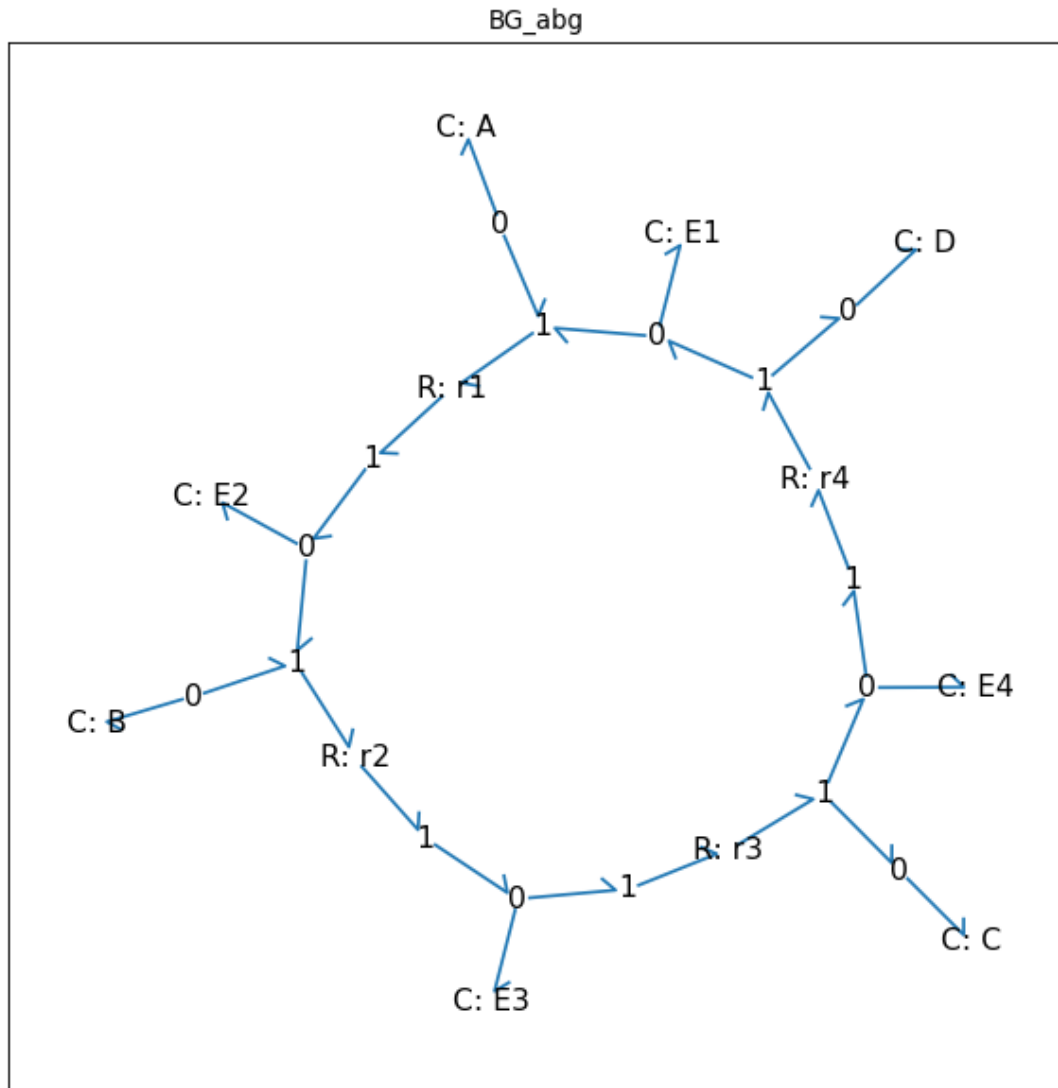
```
[5]: [K_A*K_E1*kappa_r1*x_0*x_4 - K_E2*kappa_r1*x_5 + dx_0,
      K_B*K_E2*kappa_r2*x_1*x_5 - K_E3*kappa_r2*x_6 + dx_1,
      K_C*K_E4*kappa_r3*x_2*x_7 - K_E3*kappa_r3*x_6 + dx_2,
      K_D*K_E1*kappa_r4*x_3*x_4 - K_E4*kappa_r4*x_7 + dx_3,
      K_A*K_E1*kappa_r1*x_0*x_4 + K_D*K_E1*kappa_r4*x_3*x_4 - K_E2*kappa_r1*x_5 -
      K_E4*kappa_r4*x_7 + dx_4,
      -K_A*K_E1*kappa_r1*x_0*x_4 + K_B*K_E2*kappa_r2*x_1*x_5 + K_E2*kappa_r1*x_5 -
      K_E3*kappa_r2*x_6 + dx_5,
      -K_B*K_E2*kappa_r2*x_1*x_5 - K_C*K_E4*kappa_r3*x_2*x_7 + K_E3*kappa_r2*x_6 +
      K_E3*kappa_r3*x_6 + dx_6,
      K_C*K_E4*kappa_r3*x_2*x_7 - K_D*K_E1*kappa_r4*x_3*x_4 - K_E3*kappa_r3*x_6 +
      K_E4*kappa_r4*x_7 + dx_7]
```

```
[6]: BG.control_vars
```

```
[6]: {}
```

2.2 Draw the BG

```
[7]: ## Draw the BG
      bgt.draw(BG_abg.model())
```



[]:

References

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