The stoichBondGraph module: From Stoichiometry to Bond Graph

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Note: this is the stoichBondGraph.ipynb notebook. The PDF version "The stoichBondGraph 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 multiport transformer 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 compex 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 stoichimetric 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 stoichometric matrices Nf and Nr 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

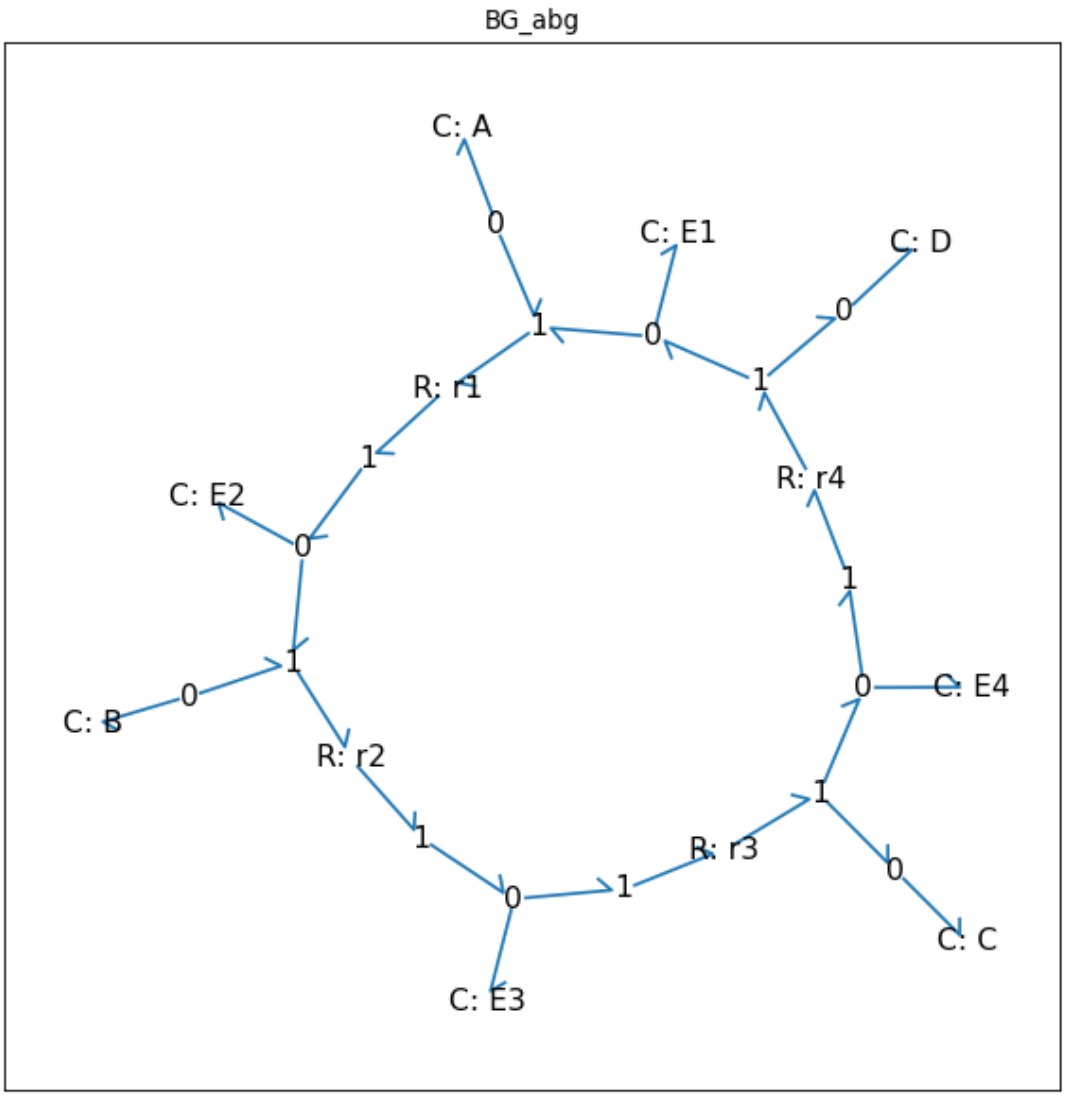
This example corresponds to ABCD_abg.svg in Tutorial svgBondGraph.

[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)

## And import
import BG_abg
```

2.2 Draw the BG

[3]:
```
## Draw the BG
bgt.draw(BG_abg.model())
```



[ ]:

References

P. J. Gawthrop and E. J. Crampin. Modular bond-graph modelling and analysis of biomolecular systems. *IET Systems Biology*, 10(5):187–201, October 2016. ISSN 1751-8849. doi: 10.1049/iet-syb.2015.0083. Available at arXiv:1511.06482.

Peter J. Gawthrop and Edmund J. Crampin. Energy-based analysis of biochemical cycles using bond graphs. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science*, 470(2171):1–25, 2014. doi: 10.1098/rspa.2014.0459. Available at arXiv:1406.2447.

Peter J. Gawthrop and Edmund J. Crampin. Energy-based analysis of biomolecular pathways. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 473(2202), 2017. ISSN 1364-5021. doi: 10.1098/rspa.2016.0825. Available at arXiv:1611.02332.

Peter J. Gawthrop, Joseph Cursons, and Edmund J. Crampin. Hierarchical bond graph modelling of biochemical networks. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 471(2184):1–23, 2015. ISSN 1364-5021. doi: 10.1098/rspa.2015.0642. Available at arXiv:1503.01814.

J. Orth, R. Fleming, and B. Palsson. Reconstruction and use of microbial metabolic networks: the core escherichia coli metabolic model as an educational guide. *EcoSal Plus*, pages 1–47, 2010. doi: 10.1128/ecosalplus.10.2.1.

George Oster, Alan Perelson, and Aharon Katchalsky. Network thermodynamics. *Nature*, 234: 393–399, December 1971. doi: 10.1038/234393a0.

George F. Oster, Alan S. Perelson, and Aharon Katchalsky. Network thermodynamics: dynamic modelling of biophysical systems. *Quarterly Reviews of Biophysics*, 6(01):1–134, 1973. doi: 10.1017/S0033583500000081.

Bernhard Palsson. *Systems biology: properties of reconstructed networks*. Cambridge University Press, 2006. ISBN 0521859034.

Bernhard Palsson. *Systems Biology: Simulation of Dynamic Network States*. Cambridge University Press, 2011.

Bernhard Palsson. *Systems Biology: Constraint-Based Reconstruction and Analysis*. Cambridge University Press, Cambridge, 2015.