Von Bertalanffy Tutorial

Introduction

In this Livescript, you will be shown how von Bertalanffy works and what the outputs of each sections are.

First, begin by installing all the necessary dependencies. At the time of writing this, the following were used:

Ubuntu 16.04 LTS

Python 2.7

NumPy 1.11.1

ChemAxon MarvinBeans 16.9.5.0

OpenBabel 2.3

The following commands are entered in a **terminal window (bash or similar shell)**.

Python 2

OpenBabel only works with Python 2. Most distributions should already have this installed, but if this is not the case, the following lines will do it:

sudo add-apt-repository ppa:fkrull/deadsnakes

sudo apt-get update

sudo apt-get install python2.7

NumPy

NumPy can be installed using the following commands:

sudo apt-get install python-dev

sudo apt-get install python-setuptools

sudo wget http://downloads.sourceforge.net/project/numpy/NumPy/1.11.1/numpy-1.11.1.tar.gz

sudo tar -xzvf numpy-1.11.1.tar.gz

sudo cd numpy-1.11.1

sudo python setup.py build -j 4 install

ChemAxon Calculator Plugin

ChemAxon calculator plugin requires a license. Apply for an academic license at the following link: http://www.chemaxon.com/my-chemaxon/my-academic-license/

After your license has been made available, you can download from the “My Licenses” tab on the ChemAxon website.

Download the license and place it under (replace USER by your actual user account):

/home/USER/.chemaxon

Download MarvinBeans for Linux, navigate to the directory where it was saved and make it executable (here, we downloaded version 16.9.5.0 - use the appropriate filename for your version):

sudo chmod +x marvinbeans-16.9.5.0-linux_with_jre64.sh

Execute the installer (again, use the same filename as above):

sudo ./marvinbeans-16.9.5.0-linux_with_jre64.sh

When asked for an installation directory, make it:

/opt/ChemAxon/MarvinBeans

This is important, since this is the path used by COBRA Toolbox.

Finally, add the installation path to the PATH environment variable:

PATH=$PATH:/opt/ChemAxon/MarvinBeans/bin

sudo export PATH

OpenBabel and Python bindings

Install the OpenBabel and Python 2 bindings by entering the following:

sudo apt-get install openbabel

sudo apt-get install python-openbabel

With all dependencies installed correctly, we configure our environment.

Add required fields and directories to path

```
initVonBertalanffy % Set up paths
global CBTDIR
pth=which('initCobraToolbox.m');
CBTDIR = pth(1:end-(length('initCobraToolbox.m')+1));

cd([CBTDIR filesep 'testing' filesep 'testVonBertalanffy'])
```

Configure inputs

```
load iAF1260
if model.S(952, 350)==0
    model.S(952, 350)=1; % One reaction needing mass balancing in iAF1260
end
model.metCharges(strcmp('asntrna[c]', model.mets))=0; % One reaction needing
                                                      % charge balancing

molfileDir = 'iAF1260Molfiles'; % Directory containing molfiles

cid = []; % KEGG Compound identifiers. Not required since molfile directory is
```

```
          % specified.

T = 310.15; % Temperature in Kelvin
cellCompartments = ['c'; 'e'; 'p']; % Cell compartment identifiers
ph = [7.7; 7.7; 7.7]; % Compartment specific pH
is = [0.25; 0.25; 0.25]; % Compartment specific ionic strength in mol/L
chi = [0; 90; 90]; % Compartment specific electrical potential relative to cytosol
                   % in mV

xmin = 1e-5*ones(size(model.mets)); % Lower bounds on metabolite concentrations
                                    % in mol/L
xmax = 0.02*ones(size(model.mets)); % Upper bounds on metabolite concentrations
                                    % in mol/L

confidenceLevel = 0.95; % Confidence level for estimated standard transformed
                        % reaction Gibbs energies.
                        %Used to quantitatively assign reaction directionality.
```

Call setupThermoModel

```
modelT = setupThermoModel(model,molfileDir,cid,T,cellCompartments,ph,is,chi,xmin,xmax,confider
```

```
Warning: Estimation inaccuracy may result from missing stereo in InChI for:
1. 2ddg6p
2. 2dhguln
3. fum
4. mnl1p
Mapping model metabolites to nist compounds
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C18H22O2/
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C18H24O2/
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Ag/q+1":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C20H29N1
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/AsH3O3/c2
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/AsH3O4/c2
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C10H16N2O
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Ca/q+2":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Cd/q+2":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/ClH/h1H/p
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Co/q+2":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Cu/q+2":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Cu/q+1":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C27H47N9O
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Hg/q+2":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/K/q+1": S
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C5H11NO3S
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C5H11NO3S
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C111H173N
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C114H178N
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Na/q+1":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Ni/q+2":
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/HO2/c1-2/
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/H5O10P3/c
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/H3O3P/c1-
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/C9H12NO6P
python2 /home/lemmer/work/cobratoolbox/thermo/ComponentContribution/inchi2gv.py -s -i "InChI=1/Zn/q+2":
Assuming that only metabolite species in model.metFormulas are transported across membranes.
```

```
save('iAF1260Thermo_test.mat', 'modelT', '-v7');
```

Compare test results to expected results

```
clear all;

old = load('iAF1260Thermo.mat');
new = load('iAF1260Thermo_test.mat');
```

Check for differences in estimated standard transformed Gibbs energies of formation

```
fig = figure(1);
subplot(1,3,1);
rmse1 = sqrt(mean( (new.modelT.DfGt0 - old.modelT.DfGt0).^2 ));
fprintf('RMSE difference between the old and new DfGt0: %g\n', rmse1);
```

```
RMSE difference between the old and new DfGt0: 2.19134
```

```
cdfplot(abs((new.modelT.DfGt0 - old.modelT.DfGt0)));
xhandle = xlabel('|D_f G^{\prime\circ}(new) - D_f G^{\prime\circ}(old)|');
set(xhandle,'Fontsize',9);
yhandle = title(['\Delta_f G^{\prime\circ} RMSE = ' sprintf('%g', rmse1)]);
set(yhandle,'Fontsize',9);
```

Check for differences in estimated standard transformed reaction Gibbs energies

```
subplot(1,3,2);
rmse2 = sqrt(mean( (new.modelT.DrGt0 - old.modelT.DrGt0).^2 ));
fprintf('RMSE difference between the old and new DrGt0: %g\n', rmse2);
```

```
RMSE difference between the old and new DrGt0: 1.62764
```

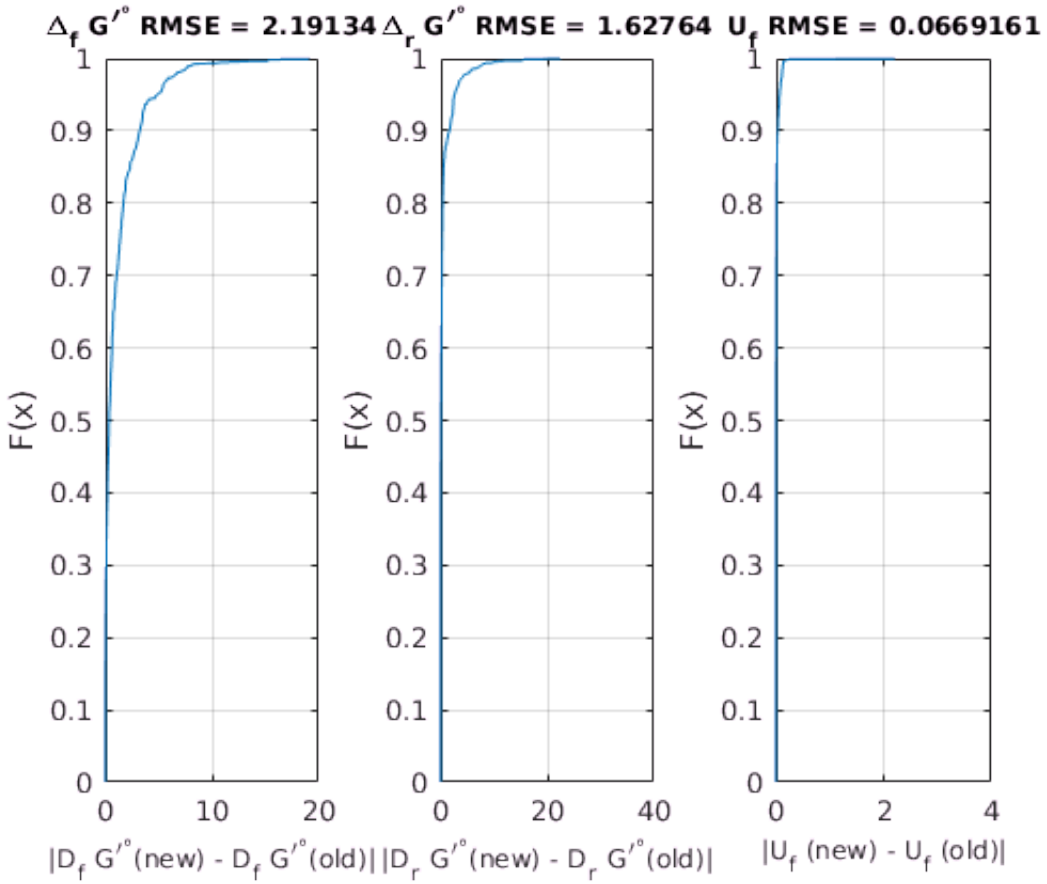
```
cdfplot(abs((new.modelT.DrGt0 - old.modelT.DrGt0)));
xhandle = xlabel('|D_r G^{\prime\circ}(new) - D_r G^{\prime\circ}(old)|');
set(xhandle, 'Fontsize', 9);
yhandle = title(['\Delta_r G^{\prime\circ} RMSE = ' sprintf('%g', rmse2)]);
set(yhandle, 'Fontsize', 9);
```

Check for differences in uncertainty levels - indicative of differences in coverage

```
subplot(1,3,3);
rmse3 = sqrt(mean( (new.modelT.uf - old.modelT.uf).^2 ));
fprintf('RMSE difference between the old and new uf: %g\n', rmse3);
```

```
RMSE difference between the old and new uf: 0.0669161
```

```
cdfplot(abs((new.modelT.uf - old.modelT.uf)));
xhandle = xlabel('|U_f (new) - U_f (old)|');
set(xhandle, 'Fontsize', 9);
yhandle = title(['U_f RMSE = ' sprintf('%g', rmse3)]);
set(yhandle, 'Fontsize', 9);
print(fig, 'iAF1260_compare.eps', '-deps');
```


$\Delta_f G'^\circ$ RMSE = 2.19134
$\Delta_r G'^\circ$ RMSE = 1.62764
U_f RMSE = 0.0669161
F(x)
$|D_f G'^\circ(new) - D_f G'^\circ(old)|$
$|D_r G'^\circ(new) - D_r G'^\circ(old)|$
$|U_f (new) - U_f (old)|$