Using SBML Control

Preliminaries

In [1]:
```
import controlSBML.control_sbml as ctl
import pandas as pd
```

In [2]:
```
ctlsb = ctl.ControlSBML("https://www.ebi.ac.uk/biomodels/model/download/BIOMD
```

In [3]:
```
# Print the first few lines of the antimony representation of this model
print(ctlsb.antimony[:380])
```

```
// Created by libAntimony v2.12.0
function Constant_flux__irreversible(v)
  v;
end

Constant_flux__irreversible is "Constant flux (irreversible)"

function Henri_Michaelis_Menten__irreversible(substrate, Km, V)
  V*substrate/(Km + substrate);
end

Henri_Michaelis_Menten__irreversible is "Henri-Michaelis-Menten (irreversibl
e)"

function HMM_Mod(V, s, m, Km)
  V*s*m/(Km + s);
end
```

In [4]:
```
ctlsb.species_names
```

Out[4]:
```
['IR',
 'pIR',
 'IRS',
 'pIRS',
 'iIRS',
 'Akt',
 'pAkt',
 'mTORC1',
 'pmTORC1',
 'mTORC2',
 'pmTORC2',
 'imTORC2',
 'mTORC1_DEPTOR',
 'mTORC2_DEPTOR',
 'DEPTOR',
 'pDEPTOR']
```

In [5]:
```
ctlsb.jacobian
```

Out[5]:

	IR	pIR	IRS	pIRS	iIRS	Akt	pAkt	mTORC1	pmTORC1
IR	-0.004518	0.028571	0.0	0.000000	0.00	0.0	0.000000	0.00	0.000000
pIR	0.004518	-0.028571	0.0	0.000000	0.00	0.0	0.000000	0.00	0.000000
IRS	0.000000	-0.066667	0.0	0.020000	0.02	0.0	0.000000	0.00	-0.066667
pIRS	0.000000	0.066667	0.0	-0.020000	0.00	0.0	0.000000	0.00	0.000000
iIRS	0.000000	0.000000	0.0	0.000000	-0.02	0.0	0.000000	0.00	0.066667
Akt	0.000000	0.000000	0.0	-0.046729	0.00	0.0	0.058824	0.00	0.000000
pAkt	0.000000	0.000000	0.0	0.046729	0.00	0.0	-0.058824	0.00	0.000000
mTORC1	0.000000	0.000000	0.0	0.000000	0.00	0.0	-0.099206	-0.35	5.999848
pmTORC1	0.000000	0.000000	0.0	0.000000	0.00	0.0	0.099206	0.00	-5.999848
mTORC2	0.000000	-0.166667	0.0	0.000000	0.00	0.0	0.000000	0.00	0.000000
pmTORC2	0.000000	0.166667	0.0	0.000000	0.00	0.0	0.000000	0.00	0.000000
imTORC2	0.000000	0.000000	0.0	0.000000	0.00	0.0	0.000000	0.00	0.000000
mTORC1_DEPTOR	0.000000	0.000000	0.0	0.000000	0.00	0.0	0.000000	0.35	0.000000
mTORC2_DEPTOR	0.000000	0.000000	0.0	0.000000	0.00	0.0	0.000000	0.00	0.000000
DEPTOR	0.000000	0.000000	0.0	0.000000	0.00	0.0	0.000000	-0.35	-0.291667
pDEPTOR	0.000000	0.000000	0.0	0.000000	0.00	0.0	0.000000	0.00	0.291667

In [6]:

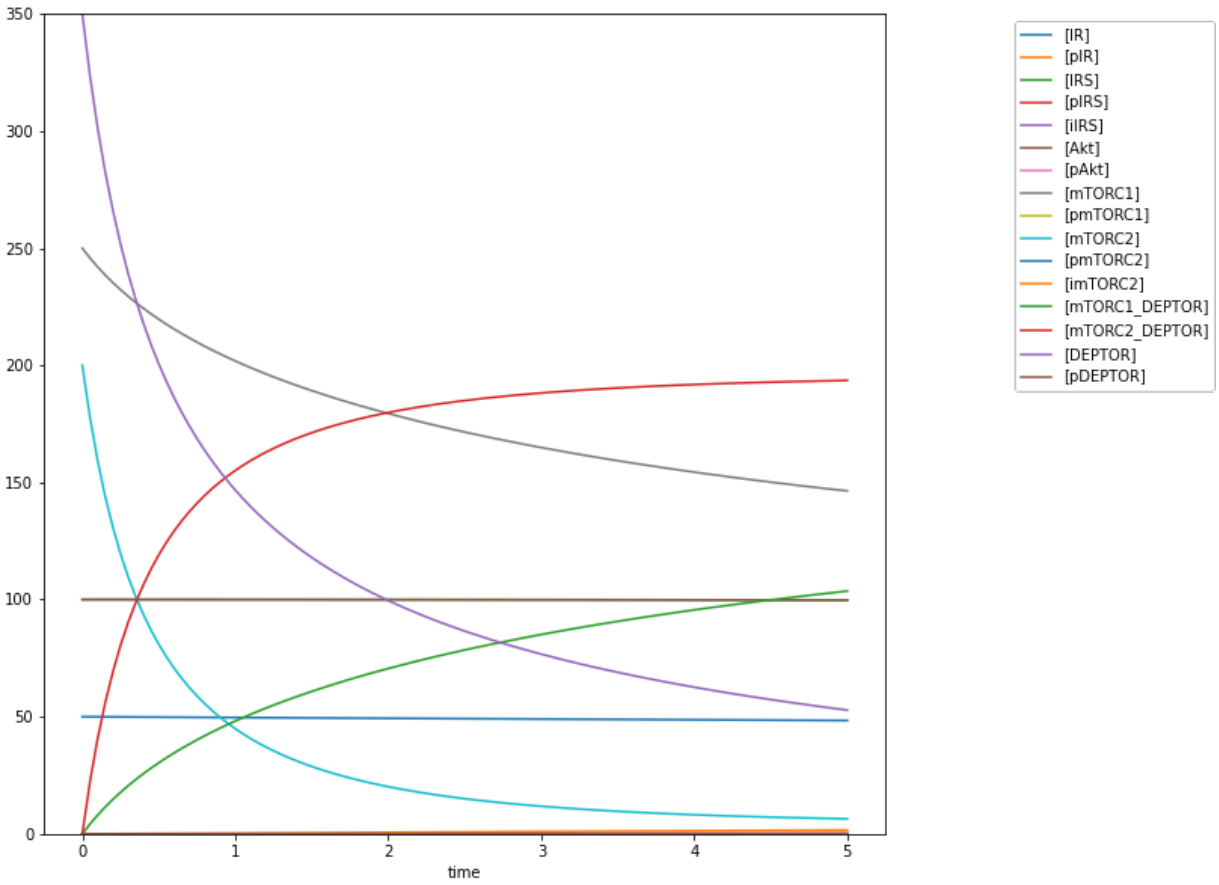
```
# Create a state space representation of the model using the Jacobian at time
ctlsb.setTime(1)
sys = ctlsb.makeStateSpace()
pd.DataFrame(sys.A)
```

Out[6]:

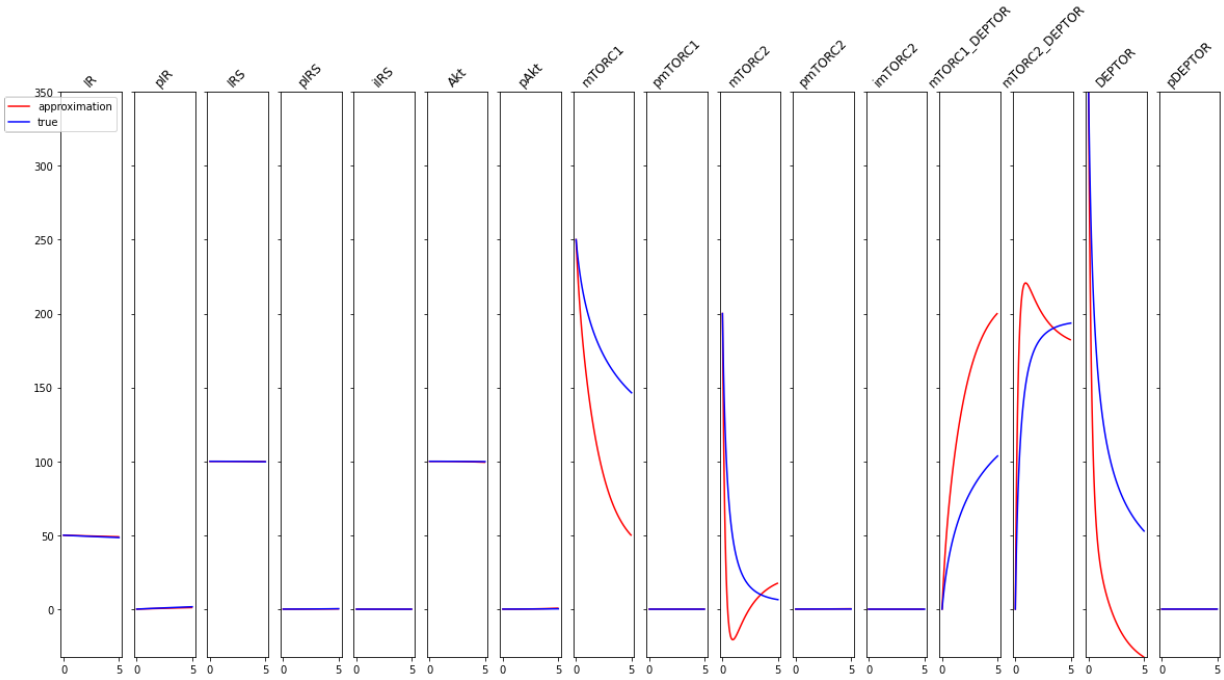
	0	1	2	3	4	5	6	7	
0	-0.00454	0.028026	0.000000e+00	0.000000	0.00	0.000000	0.000000	0.000000e+00	0.0000
1	0.00454	-0.028026	0.000000e+00	0.000000	0.00	0.000000	0.000000	0.000000e+00	0.0000
2	0.00000	-0.066664	-7.541108e-05	0.019991	0.02	0.000000	0.000000	0.000000e+00	-0.0666
3	0.00000	0.066664	7.539203e-05	-0.019991	0.00	0.000000	0.000000	0.000000e+00	0.0000
4	0.00000	0.000000	1.904712e-08	0.000000	-0.02	0.000000	0.000000	0.000000e+00	0.0666
5	0.00000	0.000000	0.000000e+00	-0.046729	0.00	-0.000008	0.058797	0.000000e+00	0.0000
6	0.00000	0.000000	0.000000e+00	0.046729	0.00	0.000008	-0.058797	0.000000e+00	0.0000
7	0.00000	0.000000	0.000000e+00	0.000000	0.00	0.000000	-0.099019	-1.467335e-01	5.9989
8	0.00000	0.000000	0.000000e+00	0.000000	0.00	0.000000	0.099019	3.691504e-08	-5.9989
9	0.00000	-0.065718	0.000000e+00	0.000000	0.00	0.000000	0.000000	0.000000e+00	0.0000
10	0.00000	0.065718	0.000000e+00	0.000000	0.00	0.000000	0.000000	0.000000e+00	0.0000
11	0.00000	0.000000	0.000000e+00	0.000000	0.00	0.000000	0.000000	0.000000e+00	0.0000
12	0.00000	0.000000	0.000000e+00	0.000000	0.00	0.000000	0.000000	1.467334e-01	0.0000
13	0.00000	0.000000	0.000000e+00	0.000000	0.00	0.000000	0.000000	0.000000e+00	0.0000

	0	1	2	3	4	5	6	7	
14	0.00000	0.000000	0.000000e+00	0.000000	0.00	0.000000	0.000000	-1.467334e-01	-0.1222

In [7]:
```
# Plot roadrunner simulation, with better placement of the legend.
ctlsb.plotTrueModel()
```



In [9]:
```
# Compare the linear approximation using the Jacobian at time 0 with the true
ctlsb.setTime(1)
ctlsb.plotLinearApproximation(figsize=(20, 10))
```


IR
pIR
IRS
pIRS
iIRS
Akt
pAkt
mTORC1
pmTORC1
rmTORC2
pmTORC2
imTORC2
mTORC1_DEPTOR
mTORC2_DEPTOR
DEPTOR
pDEPTOR
approximation
true
350
300
250
200
150
100
50
0
0
5