

final

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1 final

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1.1.1 3

loading data

```
[1]: import cvxpy as cp
import json
import numpy as np
with open("Recon3D.json", "r") as file_handle:
    dictionary = json.load(file_handle);
    data = dictionary["reactions"];
    temp_name = [(data[i])["name"] for i in range(len(data))];
    b = [i for i in range(len(data)) if temp_name[i] == "Generic Human Biomass_
    ↳Reaction"];
    b = b[0];
    order = [i for j in (range(b), range(b+1, len(data)), range(b,b+1)) for i_
    ↳in j];
    name = [(data[i])["name"] for i in order];
    lower_bound = [(data[i])["lower_bound"] for i in order];
    upper_bound = [(data[i])["upper_bound"] for i in order];
    subsystem = [(data[i])["subsystem"] for i in order];
    metabolites = [(data[i])["metabolites"] for i in order];
    id = [((dictionary["metabolites"])[i])["id"] for i in_
    ↳range(len(dictionary["metabolites"]))];
    S = np.zeros((len(id), len(metabolites)));
    for i in range(len(metabolites)):
        for j in range(len(id)):
            if id[j] in metabolites[i].keys():
                S[j, i] = metabolites[i][id[j]];
```

a)

```
[2]: v = cp.Variable(len(upper_bound))
constraints = [upper_bound>=v, lower_bound<=v, S*v==0]
```

```

objective = cp.Maximize(v[-1])
problem = cp.Problem(objective,constraints)
problem.solve()
w = problem.value
print("wild v is:",round(w,2))

```

wild v is: 753.34

b)

```

[3]: knockout_indx1 = []
for i in range(len(subsystem)):
    if("Transport, nuclear" in subsystem[i]):
        knockout_indx1.append(i)
knockout_indx1 = np.array(knockout_indx1)

knockout_problem1 = cp.Problem(objective,constraints+[v[knockout_indx1]==0])
knockout_problem1.solve()
print("change after knocking out Transport, nuclear:",(w-knockout_problem1.
    ↳value)/w)
print("difference is near 1 so these reactions were very important")

```

change after knocking out Transport, nuclear: 0.9999999999997521

difference is near 1 so these reactions were very important

```

[4]: knockout_indx2 = []
for i in range(len(subsystem)):
    if("Fatty acid oxidation" in subsystem[i]):
        knockout_indx2.append(i)
knockout_indx2 = np.array(knockout_indx2)

knockout_problem2 = cp.Problem(objective,constraints+[v[knockout_indx2]==0])
knockout_problem2.solve()
print("change after knocking out Fatty acid oxidation:",(w-knockout_problem2.
    ↳value)/w)
print("difference is near 0 so these reactions were not important")

```

change after knocking out Fatty acid oxidation: -1.8715845223013645e-11

difference is near 0 so these reactions were not important

c)

```

[5]: for indx in knockout_indx1:
    knockout_problem = cp.Problem(objective,constraints+[v[indx]==0])
    knockout_problem.solve()
    if((problem.value-knockout_problem.value)/problem.value>=0.02):
        print(name[indx])

```

DATP diffusion in nucleus
DGTP diffusion in nucleus

1.1.2 5

```
[6]: w = cp.Variable(pos=True)
l = cp.Variable(pos=True)
objective_fn = 2*w*l+2*np.pi*w+2*l
constraints = [l<=2*w,w<=1,300*cp.inv_pos(l)<=w,10<=w,w<=20,20<=l,l<=30]
problem = cp.Problem(cp.Minimize(objective_fn), constraints)
problem.solve(gp=True)
print("mask is:",round(l.value,2),"in",round(w.value,2))
```

mask is: 24.49 in 12.25

1.1.3 6

```
[7]: n=3
gamma = 2
u = 2
d = cp.Variable(n,pos=True)
k = cp.Variable(n,pos=True)
v = cp.Variable(n,pos=True)
landa = cp.Variable(1,pos=True)
G = np.ones((3,3))-np.identity(3)
D = cp.diag(d)
K = cp.diag(k)
A = D+K*G
constraints = [gamma*cp.sum(cp.inv_pos(d))+cp.sum(cp.inv_pos(k))<=u]
constraints += [cp.hstack([d[0],k[1]/2,k[2]/2])*v*cp.inv_pos(landa*v[0])<=1]
constraints += [cp.hstack([k[0]/2,d[1],k[2]/2])*v*cp.inv_pos(landa*v[1])<=1]
constraints += [cp.hstack([k[0]/2,k[2]/2,d[2]])*v*cp.inv_pos(landa*v[2])<=1]
objective = cp.Minimize(landa)
problem = cp.Problem(objective,constraints)
problem.solve(gp=True)
print("D is:\n",D.value)
print("K is:\n",K.value)
print("A is:\n", (D+K*G).value)
```

D is:

```
[[4.95195719 0.          0.          ]
 [0.          4.99531724 0.          ]
 [0.          0.          5.2830707 ]]
```

K is:

```
[[3.38863977 0.          0.          ]
 [0.          5.37683063 0.          ]
```

```
[0.          0.          2.97539551]]  
A is:  
[[4.95195719 3.38863977 3.38863977]  
 [5.37683063 4.99531724 5.37683063]  
 [2.97539551 2.97539551 5.2830707 ]]
```