validation_runs

March 25, 2019

```
In [1]: import ingestor, modeller, fitter
        import numpy as np
        from matplotlib import pyplot as plt
In [2]: plt.rc('text', usetex=True)
       plt.rc('font', family='serif')
In [3]: from importlib import reload
        reload(ingestor)
        reload(modeller)
        reload(fitter)
Out[3]: <module 'fitter' from '/media/dwu402/Data/wrap-mad/fitter.py'>
In [4]: context = ingestor.initialise_context()
        ingestor.read_run_file(context, "runs/mouse4.3.run")
In [5]: model = modeller.Model(context)
In [6]: solver = fitter.Fitter()
        solver.construct_objectives(context, model)
In [7]: solver.construct_problems()
        print(solver.solutions)
{}
In [8]: for rhoi in np.logspace(-3, 9, num=31):
            solver.solve(rhoi)
In [9]: solver solutions
Out[9]: {'0.001': [
                         fun: 0.024380412583615972
           hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
                jac: array([-9.95473641e-07, 4.60171174e-07, -3.78563317e-06, 4.40194962e-06,
                 -8.24609856e-06, -2.09672015e-05, 1.26333076e-05, 2.65451365e-06,
                 -1.48823914e-05])
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message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 22
      nit: 1
   status: 0
  success: True
        x: array([3.00000000e-01, 1.00000000e+00, 7.00000000e-01, 2.00000000e+00,
       1.00000000e+00, 1.00000000e+00, 1.00000000e+00, 1.00000000e+00,
       1.00000003e-03])],
'0.0025118864315095794': [
                               fun: 0.0244033721634419
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
       jac: array([-1.49201066e-06, 1.81047405e-06, -9.91341043e-07, 1.97517753e-06,
       -5.58708456e-06, -1.04167441e-05, 7.39205580e-06, 3.94426658e-07,
       -2.26169737e-06])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 16
      nit: 1
   status: 0
  success: True
        x: array([3.00000000e-01, 1.00000000e+00, 7.00000000e-01, 2.00000000e+00,
       1.00000000e+00, 1.00000000e+00, 1.00000000e+00, 1.00000000e+00,
       1.00000002e-03])],
'0.00630957344480193': [
                            fun: 0.0244247079881888
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-9.29475141e-06, 1.21656298e-05, -5.22883281e-07, 1.35112463e-06,
       -5.22188405e-06, -2.03330204e-05, 1.47308827e-05, -4.01198808e-06,
       -2.94901056e-07])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 19
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])],
'0.01584893192461114': [
                             fun: 0.024438026497777647
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([7.00010044e-08, 5.75651149e-06, 3.61222353e-06, 2.88925346e-06,
       -7.73055501e-06, -4.76442013e-06, 1.74136127e-06, 4.43652209e-06,
        3.27501125e-05])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'</pre>
     nfev: 21
      nit: 14
   status: 0
  success: True
        x: array([0. , 0. , 2.07308963, 2.25116766, 0.96817756,
       6.02625311, 4.33460562, 2.52747574, 0.
                                                    ])],
'0.039810717055349734': [
                             fun: 0.024548367734489013
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 9.63979661e-06, 4.35841744e-06, -6.79015579e-06, 3.91520298e-06,
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-2.28668849e-06, -2.45304813e-06, 2.64105156e-07, 7.58923836e-06,
        1.01787869e-04])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
     nfev: 19
      nit: 17
   status: 0
  success: True
        x: array([ 0.02265607,  0. ,  2.02846154,  0.35223308,  0.17276806,
       13.12096767, 6.51070315, 2.19781235, 0.
                                                        ])],
'0.1': [
             fun: 0.025031436423910564
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-2.20667913e-07, 4.05111576e-06, -6.92275078e-06, 9.17821777e-08,
        8.37410025e-06, -1.59803317e-07, 2.83448135e-07, -6.41772269e-06,
        7.19431689e-05])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
      nit: 28
   status: 0
  success: True
        x: array([ 0. , 0. , 2.04337038, 13.17449798, 0.48717461, 100. , 11.85032935, 2.0107947 ,
         0.
                   ])],
'0.25118864315095824': [
                          fun: 0.027633066622827964
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 1.02755095e-05,  3.92602473e-04, -4.34810985e-04,  3.35769341e-04,
       -1.89578801e-03, -3.07391129e-03, 6.31590132e-03, 6.76740953e-05,
       -4.52855378e-04])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 37
      nit: 26
   status: 0
  success: True
        x: array([1.59017917e-03, 0.00000000e+00, 2.42271411e+00, 6.59662029e+00,
       1.70600575e+00, 2.62019894e+00, 1.51002629e+00, 3.13481749e+00,
       0.00000000e+00])],
'0.6309573444801936': [
                           fun: 0.032395461859291166
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-3.13610452e-04, 7.43665100e-05, -1.86816055e-03, 1.59555027e-03,
       -3.87528453e-03, -9.59200534e-03, 1.34406447e-02, 1.34150205e-03,
         1.62465197e-03])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 108
      nit: 28
   status: 0
  success: True
        x: array([0.02571322, 0.12912826, 2.78579744, 9.8243031, 2.87487168,
       2.69940481, 1.73011609, 3.80626908, 0.
                                                      ])],
'1.584893192461114': [ fun: 0.033383260719877045
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hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-2.45863356e-04, 1.54556066e-04, 1.00704311e-05, 6.15573673e-05,
       -1.59284155e-05, -1.69670734e-04, 2.17428587e-04, -3.84920581e-05,
        7.36590815e-03])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 121
      nit: 56
   status: 0
  success: True
        x: array([4.8415793 , 7.62318745, 0.6500189 , 6.44660889, 3.16343382,
       7.12750178, 6.59853544, 7.94891932, 0.
                                                    ])],
'3.981071705534973': [
                          fun: 0.081383886606366
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-8.04091461e-05, 2.36089406e-03, 2.89799943e-03, -1.44940438e-03,
        2.48092421e-03, -1.04647279e-04, 3.89541356e-03, -9.62113342e-05,
        1.93791341e-04])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 28
      nit: 22
   status: 0
  success: True
        x: array([0. , 0. , 0. , 3.93782917, 3.7058558 ,
       6.53469153, 0.1639838, 2.64820963, 0.
                                                    ])],
              fun: 0.11659551773675354
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 0.0015577 , 0.00052261, 0.00431102, 0.00309955, -0.00589516,
       -0.00393452, 0.00335105, -0.0001108, 0.05017417])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 205
      nit: 114
   status: 0
  success: True
        x: array([ 0. , 0. , 0. , 92.03676676, 48.49627956,
       11.53778792, 13.80508639, 2.88788409, 0.
                                                       ])],
                         fun: 0.23734009481259952
'25.11886431509582': [
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 0.0383218 , -0.04448113, -0.06276841, -0.06629281, 0.17414605,
       -0.0336714 , 0.03870851, 0.001113 , 0.02215383])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 75
      nit: 10
   status: 0
  success: True
        x: array([0.73459336, 0.49029393, 1.42036535, 0.8716332, 1.10257999,
       2.34152542, 2.0340173 , 1.18657005, 0.48931455])],
'63.09573444801943': [
                         fun: 0.5419226184222689
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-0.01428789, 0.00825008, -0.06291067, 0.34376497, -0.67530851,
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0.15810603, -0.35183333, -0.00957186, -0.35570014)
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 13
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])].
'158.48931924611142': [
                            fun: 1.7126266980971563
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-1.11697339, 0.62366906, -3.75796828, 0.75690658, -0.39539502,
        0.98534532, -3.06166197, 0.3001869, -0.60997705
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 9
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])],
'398.1071705534977': [
                           fun: 0.2202633563728994
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
       jac: array([ 1.02005065e-01, 9.53122827e-04, 4.31390138e-02, 6.65237762e-06,
       -8.81999149e-06, -1.05943149e-04, 3.03746052e-03, 2.01529137e-06,
        8.11125246e-04])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
     nfev: 100
      nit: 74
   status: 0
  success: True
        x: array([ 0. , 0. , 0. 
0.60818631, 100. , 0. , 4
                                                     , 1.19043596,
                                              , 4.79602492.
         0.
                   ])],
                fun: 0.5331571639261616
'1000.0': Γ
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-0.44011411, 0.40329745, -0.31896729, -0.32023578, 1.01484215,
        -0.33972759, 0.03724525, 0.0178111, 0.03004021])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 46
      nit: 15
   status: 0
  success: True
        x: array([0.48378271, 0.75239156, 1.00495573, 1.65720397, 0.99250495,
       1.31471113, 1.49956997, 1.0159564, 0.7826698])],
'2511.886431509582': [
                           fun: 0.2908837113544197
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 0.01423672, -0.01914859, -0.00460876, -0.08281285,  0.16988423,
       -0.00137508, 0.00232168, -0.00068715, -0.01426714])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
```

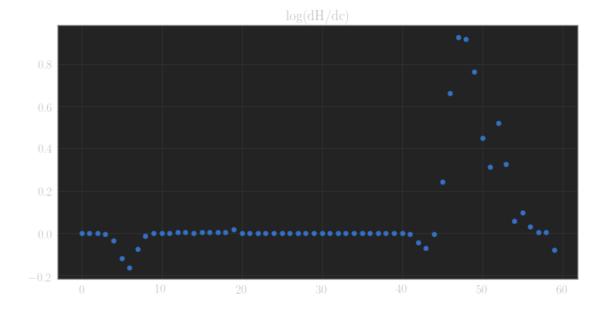
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nfev: 101
      nit: 35
   status: 0
  success: True
        x: array([0.5786771 , 0. , 4.91400721, 0.
                                                                , 0.12361767,
       6.92949322, 5.7710018 , 1.0713397 , 0.77617093])],
'6309.573444801943': [
                           fun: 4.52133116356414
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ -0.89421277, 0.96932528, -1.10060303, 20.19796726,
       -38.83529455, -15.46193238, 13.61360514, 0.27630133,
        -5.44070997])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 13
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])],
'15848.93192461114': [
                           fun: 0.34886905124273543
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-9.58153328e-07, -8.64108007e-08, 7.36584400e-06, -1.17787042e-06,
       -6.06698440e-04, 1.12443215e-03, -3.65570280e-02, -7.51061416e-06,
       -5.39469153e-041)
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 107
      nit: 29
   status: 0
  success: True
        x: array([1.46496696e+00, 4.60845632e+01, 1.00000000e+02, 7.65750425e-02,
       0.00000000e+00, 4.27150488e+01, 4.98221867e-01, 9.91312727e+01,
       9.43482361e+01])],
'39810.71705534977': [
                           fun: 5.525819985314521
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ -0.97660071, 1.07884269, -0.71781098, 36.03149592,
       -72.31328858, -38.27314602, 37.79983024, 0.2742951,
       -11.72768176])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 18
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])],
'100000.0': Γ
                  fun: 4.310199619298702
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-13.80684136, 5.93633831, -6.10338952, -2.24870079,
         8.65720575, -3.05413245, 6.46774325, -2.0015123,
        -0.84304102])
```

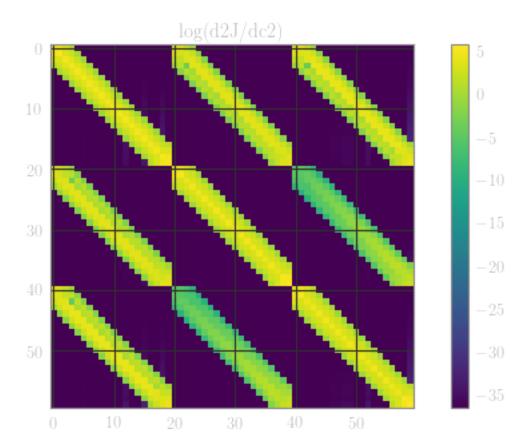
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message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 60
      nit: 3
   status: 0
  success: True
        x: array([0.36611713, 0.99241885, 0.73582688, 1.99209613, 1.08615299,
       1.07554898, 0.91742604, 1.04899766, 0.03630869])],
'251188.6431509582': [
                           fun: 5.608842781717838
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
       jac: array([ -0.63146147,  0.69393503, -0.33941175, 34.55931334,
       -68.67190378, -35.2512121, 34.6990354, 0.16378955,
       -11.69300362])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 92
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])],
'630957.3444801943': [
                           fun: 4.317897235777234
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-14.26469746, 6.27314671, -10.03393611, -2.67866133,
        11.6133819 , -4.265811 , 8.43170499, -2.33794762,
        -1.25522228])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 51
      nit: 3
   status: 0
  success: True
        x: array([0.36603371, 0.99183793, 0.7378561 , 1.9920578 , 1.08884712,
       1.07629622, 0.91664076, 1.04933126, 0.03681048])],
'1584893.1924611174': [
                            fun: 0.8047103792315696
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 4.21360046e-06, 5.17085215e-08, 1.15455451e-06, -1.47051658e-07,
       -8.56158937e-06, 6.74350970e-07, 9.92915347e-03, 1.95952504e-07,
        9.47467212e-07])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'</pre>
     nfev: 68
      nit: 44
   status: 0
  success: True
        x: array([ 0.77082245, 73.99076609, 99.99982058, 3.19188483, 0.72390078,
        2.16717774, 0.
                               , 63.63267887, 99.99984873])],
'3981071.7055349858': [ fun: 9.413737464235533
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ -0.15471806,  0.14411707,  0.03558107,  -3.1839143 ,
        16.12740315, 20.97360717, -24.89283959, -0.1926991,
        13.382032 ])
```

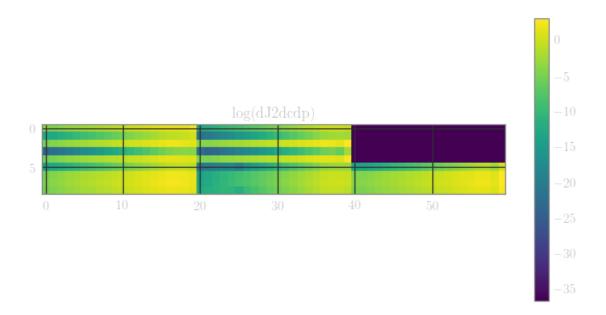
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message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 48
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
'10000000.0': Γ
                    fun: 6.573853781865785
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 2.49775499e-07, -1.07783992e-13, -1.32801179e-06, -8.25173657e-18,
        1.87674814e-05, -2.96521051e-05, 4.89283233e+00, -8.28881589e-07,
       -1.15004600e-05])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 10
      nit: 2
   status: 0
  success: True
        x: array([1.17864472e+01, 0.00000000e+00, 1.38016230e-07, 1.71504936e+00,
       4.55082281e+00, 2.13600789e+00, 0.00000000e+00, 3.51180395e+00,
       1.84574275e+001)1.
'25118864.315095823': [
                            fun: 9.324599193666817
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-12.02970959, 1.3984476, 42.01315212, 8.21363729,
       -39.72854683, 3.4668683, -4.09479275, 2.28368274,
         1.80383979])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 40
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])],
'63095734.44801943': [
                           fun: 6.573904474391823
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 3.81420100e-08, -2.59926039e-15, -2.03027835e-07, -3.21946723e-20,
        2.92661136e-06, -4.68266550e-06, 4.89310587e+00, -1.28437371e-07,
       -1.81615905e-06])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
     nfev: 2
      nit: 1
   status: 0
  success: True
        x: array([11.88171101, 0. , 0. , 1.7389175 , 4.50780486,
        2.08906509, 0. , 3.48861411, 1.80136528])],
'158489319.24611175': [
                          fun: 9.834154074458391
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([ -5.53938601, -0.88095399, 43.71260352, 8.7684714,
       -43.67107666, 4.97374453, -8.12779747, 3.56602544,
```

```
1.98117714])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'</pre>
     nfev: 88
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])],
'398107170.55349857': [
                            fun: 6.573912338030069
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
       jac: array([ 5.88882617e-09, -6.37014897e-17, -3.14970144e-08, -1.28492010e-22,
        4.62596204e-07, -7.43313333e-07, 4.89314830e+00, -2.00205158e-08,
       -2.88292158e-07])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
     nfev: 2
      nit: 1
   status: 0
  success: True
        x: array([11.96641858, 0. , 0. , 1.75182946, 4.48036017,
        2.0670886 , 0.
                              , 3.47993429, 1.78128027])],
'1000000000.0': [
                     fun: 11.175582550484712
 hess_inv: <9x9 LbfgsInvHessProduct with dtype=float64>
      jac: array([-24.47149082, 7.92764309, 34.40111149, 3.56260487,
       -30.12775371,
                       3.00971271, -8.00196421,
                                                   5.01279634,
         1.005763931)
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 81
      nit: 1
   status: 0
  success: True
        x: array([3.e-01, 1.e+00, 7.e-01, 2.e+00, 1.e+00, 1.e+00, 1.e+00, 1.e+00,
       1.e-03])]}
```

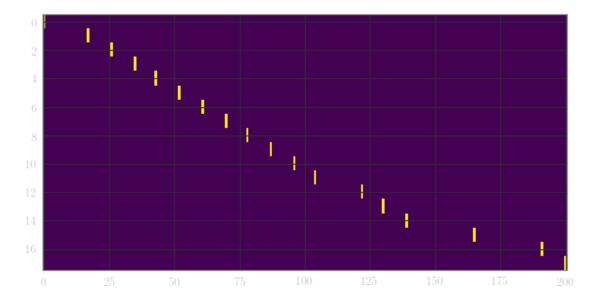
0.1 Validation







Out[18]: <matplotlib.image.AxesImage at 0x7fb97f5d56a0>

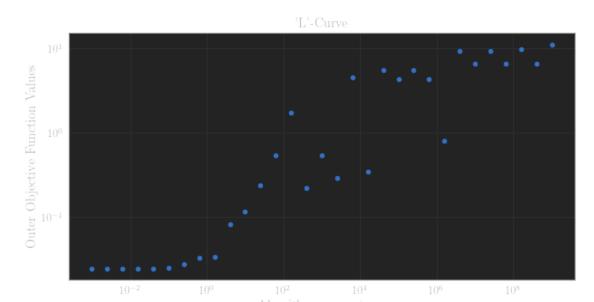


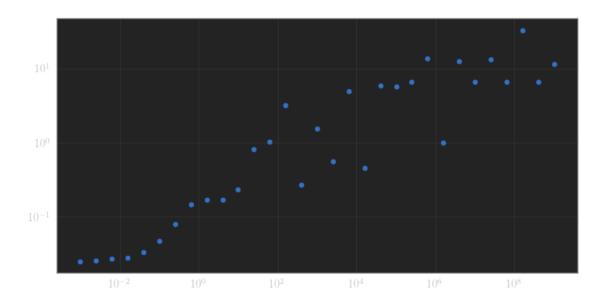
In [19]: # create and profile calls

obj_fn, obj_jac = solver._inner_objective.create_objective_functions(model, context['da

-5.36165767e+00, -3.99792748e+01, -5.16282656e+02, -5.75382747e+03, -4.08190501e+04, -1.93135665e+05, -8.71960662e+05, -4.87640830e+06,

-5.78240064e+06])





In [28]: diff_field_value = [[okey, (ivalue-ovalue)/(ikey)] for (ikey, ivalue), (okey, ovalue) i
In [29]: plt.loglog(*np.array(diff_field_value).T, 'o')
Out[29]: [<matplotlib.lines.Line2D at 0x7fb97f39e5c0>]

