

# smol\_case

April 1, 2019

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In [1]: import ingestor, modeller, fitter
import numpy as np
import matplotlib.pyplot as plt

In [2]: plt.style.use('seaborn-notebook')
plt.rc('text', usetex=True)
plt.rc('font', family='serif')
plt.rcParams['figure.figsize'] = [15, 10]

In [3]: from cycler import cycler

new_color = cycler(color=["k"])
plt.rcParams['axes.prop_cycle'] = plt.rcParams['axes.prop_cycle'].concat(new_color)

In [4]: from importlib import reload

reload(fitter)
reload(modeller)
reload(ingestor)

Out[4]: <module 'ingestor' from '/media/dwu402/Data/wrap-mad/ingestor.py'>

In [5]: context = ingestor.Context("runs/minimal3.3.run")

In [6]: model = modeller.Model(context)

In [7]: solver = fitter.Fitter()
solver.construct_objectives(context, model)

In [8]: solver.construct_problems()

In [9]: for rhoi in np.logspace(-7, 4.5, num=51):
    solver.solve(rhoi)
    solver.problems[0].initial_guess = solver.solutions[str(rhoi)][-1].x

In [10]: solver.solutions

Out[10]: {'1e-07': [      fun: 0.009769724762800525
    hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
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        jac: array([ 7.83767880e-14, -3.29762767e-13,  4.14931009e-13, -6.71932110e-13,
        -1.38075815e-11,  5.21768544e-11,  2.26872019e-11,  1.41893791e-11,
        -2.66128147e-11,  1.53658600e-13,  2.55399452e-11])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 3
nit: 2
status: 0
success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'1.6982436524617461e-07': [      fun: 0.009769724762800525
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
        jac: array([ 1.28492624e-12,  2.14334655e-13,  5.49323424e-13, -6.43176529e-13,
        -1.35747308e-11,  5.10750656e-11,  1.75809963e-11,  2.80658575e-11,
        -3.03025061e-11,  3.52709468e-12,  2.61407238e-11])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 1
nit: 0
status: 0
success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'2.8840315031266057e-07': [      fun: 0.009769724762800525
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
        jac: array([ 3.33393303e-12,  1.13833933e-12,  7.77558605e-13, -5.94353137e-13,
        -1.31792782e-11,  4.92039288e-11,  8.90942837e-12,  5.16315440e-11,
        -3.65684596e-11,  9.25598431e-12,  2.71610074e-11])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 1
nit: 0
status: 0
success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'4.897788193684466e-07': [      fun: 0.009769724762800525
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
        jac: array([ 6.81362223e-12,  2.70750906e-12,  1.16516943e-12, -5.11469668e-13,
        -1.25076592e-11,  4.60261930e-11, -5.81696832e-12,  9.16519515e-11,
        -4.72094554e-11,  1.89849576e-11,  2.88937415e-11])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 1
nit: 0
status: 0
success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'8.317637711026709e-07': [      fun: 0.009769724762800525
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
        jac: array([ 1.27229144e-11,  5.37229737e-12,  1.82346128e-12, -3.70801438e-13,
        -1.13669596e-11,  4.06293655e-11, -3.08258670e-11,  1.59616729e-10,
        -6.52801130e-11,  3.55069020e-11,  3.18364728e-11])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'

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nfev: 1
nit: 0
status: 0
success: True
x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'1.4125375446227554e-06': [      fun: 0.009769724762800525
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 2.27581362e-11,  9.89762962e-12,  2.94149997e-12, -1.32166564e-13,
-9.42940693e-12,  3.14634934e-11, -7.32967501e-11,  2.75038563e-10,
-9.59674948e-11,  6.35645472e-11,  3.68343129e-11])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL '
nfev: 1
nit: 0
status: 0
success: True
x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'2.3988329190194897e-06': [      fun: 0.009769724762800525
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 3.97998227e-11,  1.75823785e-11,  4.84048684e-12,  2.72360942e-13,
-6.13791326e-12,  1.58954633e-11, -1.45421734e-10,  4.71056076e-10,
-1.48079269e-10,  1.11211413e-10,  4.53229168e-11])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL '
nfev: 1
nit: 0
status: 0
success: True
x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'4.073802778041131e-06': [      fun: 0.009769724762800525
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 6.87391283e-11,  3.06318935e-11,  8.06625033e-12,  9.57234465e-13,
-5.45106200e-13, -1.05490331e-11, -2.67904867e-10,  8.03950564e-10,
-2.36569462e-10,  1.92122062e-10,  5.97416728e-11])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL '
nfev: 1
nit: 0
status: 0
success: True
x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'6.9183097091893625e-06': [      fun: 0.009769702934991702
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([-1.53288196e-10,  3.09946076e-10, -1.04639853e-10,  2.99012766e-10,
2.85078773e-11, -5.28739384e-11, -1.51197456e-10, -1.77703409e-10,
1.55057197e-12,  3.58612280e-10, -1.00903551e-10])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL '
nfev: 1
nit: 0
status: 0
success: True

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        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'1.1748975549395302e-05': [      fun: 0.009769718426512846
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 1.21096215e-10,  3.93027497e-11,  1.23806033e-10, -1.62146701e-10,
    -4.15533759e-10,  7.42427673e-10, -6.20284788e-11, -2.66644065e-09,
    -4.22183711e-10,  3.76755915e-10, -1.07867815e-09])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
    nfev: 1
    nit: 0
    status: 0
    success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'1.995262314968883e-05': [      fun: 0.009769718426512846
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 2.06799943e-10,  6.74912094e-11,  2.10126474e-10, -2.74941554e-10,
    -6.95782138e-10,  1.22326828e-09, -1.26073349e-10, -4.52427391e-09,
    -7.01840005e-10,  6.42984732e-10, -1.84897987e-09])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
    nfev: 1
    nit: 0
    status: 0
    success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'3.3884415613920276e-05': [      fun: 0.009769718426512846
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 3.52340565e-10,  1.15307871e-10,  3.56774199e-10, -4.66635659e-10,
    -1.17167169e-09,  2.03981361e-09, -2.34435159e-10, -7.67928392e-09,
    -1.17631605e-09,  1.09490897e-09, -3.15693134e-09])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
    nfev: 1
    nit: 0
    status: 0
    success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'5.7543993733715664e-05': [      fun: 0.009769692319177625
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 6.41108920e-10, -8.76657573e-10,  1.56216770e-09, -3.10949928e-09,
    -4.41834733e-10,  6.78839625e-10,  1.24137796e-09, -2.75640339e-09,
    1.28389903e-09, -3.42626666e-10, -2.28655158e-09])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
    nfev: 1
    nit: 0
    status: 0
    success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'9.772372209558111e-05': [      fun: 0.009769748287232812
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 1.32108294e-09,  4.30496585e-10,  5.33666386e-09, -9.36875510e-09,

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-1.82907998e-09, 5.02978351e-09, 3.54115028e-09, -8.63250419e-09,
-1.18828567e-10, 4.35488988e-09, -8.15816915e-09])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 1
nit: 0
status: 0
success: True
x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.00016595869074375615': [ fun: 0.009769762001061055
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([-4.71053407e-10, 9.58539189e-10, 1.53693301e-08, -2.87497568e-08,
6.23295085e-09, -5.09581782e-09, -7.48746717e-09, -5.85212438e-09,
-8.16511883e-09, 6.30023740e-09, -2.45726630e-08])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 1
nit: 0
status: 0
success: True
x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.0002818382931264455': [ fun: 0.009769786001576658
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 8.54760923e-09, -1.00798779e-08, 3.08786709e-08, -6.00859512e-08,
-1.23665495e-08, 3.02993100e-08, 3.05317801e-08, -1.73010597e-08,
-2.28457014e-09, 1.48579839e-08, -4.19675895e-08])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 1
nit: 0
status: 0
success: True
x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.00047863009232263854': [ fun: 0.009770313128894616
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 1.65750189e-08, 2.03934236e-09, 1.09842449e-07, -2.02680478e-07,
-8.77603475e-09, 4.59520950e-08, 3.40977217e-08, -1.22603558e-07,
9.28711720e-09, 3.89131699e-08, -2.21008443e-07])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 1
nit: 0
status: 0
success: True
x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.0008128305161640995': [ fun: 0.009771373428985684
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 4.92207026e-08, -4.23867849e-09, 3.41546521e-07, -6.37778329e-07,
-3.62362621e-08, 1.48683209e-07, 1.25906068e-07, -3.12590432e-07,
-2.46165417e-09, 1.19183050e-07, -5.88368501e-07])
message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
nfev: 1

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        nit: 0
        status: 0
        success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.0013803842646028866': [      fun: 0.009773602840200846
        hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
        jac: array([ 1.37662408e-07, -5.14861058e-08,  9.60600883e-07, -1.80870459e-06,
        -3.19892621e-07,  6.72152920e-07,  7.43542433e-07, -7.11356559e-07,
        1.28801399e-08,  3.42995534e-07, -1.55250619e-06])
        message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
        nfev: 1
        nit: 0
        status: 0
        success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.0023442288153199225': [      fun: 0.009780300109039977
        hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
        jac: array([ 3.60078370e-07, -6.49249971e-08,  2.78428243e-06, -5.22846076e-06,
        -1.03443413e-06,  2.20181827e-06,  2.46540983e-06, -1.99416165e-06,
        1.63918196e-07,  8.34987392e-07, -4.13435512e-06])
        message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
        nfev: 1
        nit: 0
        status: 0
        success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.003981071705534978': [      fun: 0.009798153218724853
        hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
        jac: array([ 9.58235829e-07, -3.63530475e-07,  7.71902979e-06, -1.45670271e-05,
        -3.28848712e-06,  6.90249810e-06,  7.94460822e-06, -5.04457911e-06,
        8.36212994e-07,  2.41804663e-06, -1.03615943e-05])
        message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
        nfev: 20
        nit: 1
        status: 0
        success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.006760829753919818': [      fun: 0.009843694258870618
        hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
        jac: array([ 2.22967121e-06, -9.72575122e-07,  2.16141750e-05, -4.09623164e-05,
        -1.21762272e-05,  2.41377774e-05,  2.84615090e-05, -1.29068680e-05,
        3.70352240e-06,  5.92989194e-06, -2.50033359e-05])
        message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
        nfev: 16
        nit: 1
        status: 0
        success: True
        x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),

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'0.01148153621496884': [      fun: 0.00995285914503156
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 4.56558321e-06, -2.93180249e-06,  5.83794751e-05, -1.11241705e-04,
    -4.09475216e-05,  7.96526032e-05,  9.50837837e-05, -3.13105457e-05,
    1.39978754e-05,  1.28739468e-05, -5.61308871e-05])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 21
    nit: 1
    status: 0
    success: True
    x: array([1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]),
'0.019498445997580455': [      fun: 0.01019156187969454
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([-1.65399893e-06,  1.26334730e-06, -1.52270683e-06,  3.40234349e-06,
    -1.61213990e-06,  2.93578861e-06,  7.02940364e-06,  3.57792074e-06,
    1.86048410e-06,  3.31248560e-06,  9.73885606e-07])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
    nfev: 9
    nit: 3
    status: 0
    success: True
    x: array([0.99947965, 1.00057208, 0.99320214, 1.01275681, 1.00563947,
    0.98895727, 0.98730816, 1.00317441, 0.99843378, 0.99909509,
    1.00558945])),
'0.03311311214825914': [      fun: 0.01068117062059188
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 5.70212986e-07, -7.69863064e-07, -2.77158213e-07,  6.29715111e-07,
    -3.11379303e-07, -3.55181411e-08, -1.55816056e-06,  1.42321750e-06,
    -1.24378664e-06, -1.10395808e-06,  7.33941010e-07])
  message: b'CONVERGENCE: NORM_OF_PROJECTED_GRADIENT_<=_PGTOL'
    nfev: 4
    nit: 3
    status: 0
    success: True
    x: array([0.99945986, 1.00162072, 0.98593862, 1.02593216, 1.01470503,
    0.97055785, 0.96716071, 1.00448169, 0.99706707, 0.9988513 ,
    1.00967823])),
'0.05623413251903491': [      fun: 0.011573749655347548
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 1.17877888e-05, -1.94896949e-05, -1.76862247e-05,  3.33850906e-05,
    -1.46997347e-06, -3.77466512e-06, -3.41669507e-05,  3.74944984e-05,
    -2.63373862e-05, -2.32096708e-05,  1.54548119e-05])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 24
    nit: 3
    status: 0
    success: True
    x: array([1.00017247, 1.00420156, 0.97538257, 1.04436114, 1.03232405,

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0.93297841, 0.93008712, 1.00405997, 0.9979624 , 0.99983258,
1.01532679]]],
'0.09549925860214369': [      fun: 0.01302734646333351
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 3.62266571e-07,  3.72314048e-06, -1.36383586e-06, -3.95185567e-06,
-6.91192504e-06,  1.69259779e-05,  7.48089291e-06, -5.35104557e-06,
 7.08473222e-07,  1.69764434e-06,  3.44252991e-06])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
nfev: 64
nit: 5
status: 0
success: True
x: array([1.00116933, 1.01363722, 0.97026629, 1.05208167, 1.06095262,
0.87164519, 0.88335407, 0.99260418, 1.00889409, 1.0091027 ,
1.02128022]]],
'0.16218100973589297': [      fun: 0.015183780054537348
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 1.67845014e-06,  3.73491474e-06, -3.16765033e-06,  4.72082479e-06,
-4.84549124e-06,  1.33910334e-05,  1.28199886e-06, -1.67391329e-06,
-3.90536360e-06,  2.71523478e-06,  9.27942677e-06])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
nfev: 88
nit: 6
status: 0
success: True
x: array([1.00331589, 1.03185874, 0.97498837, 1.03858628, 1.0889445 ,
0.80869426, 0.83637059, 0.98369711, 1.02005751, 1.02445408,
1.03865796]]],
'0.2754228703338169': [      fun: 0.018350546681340844
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 4.40866406e-06, -4.44372000e-05, -3.44924544e-06,  3.73323758e-05,
-6.23369213e-05,  1.13010157e-04,  1.27649758e-04,  2.66862025e-05,
-1.89999516e-05, -2.63481310e-05, -3.12380576e-05])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
nfev: 77
nit: 11
status: 0
success: True
x: array([1.00685479, 1.06366838, 0.96864421, 1.02431929, 1.10132501,
0.774632 , 0.79795668, 0.98818059, 1.02377163, 1.04758622,
1.06086587]]],
'0.4677351412871981': [      fun: 0.023118124512305178
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 2.69274731e-04, -4.01938496e-04, -3.09905819e-05,  3.59296364e-05,
1.29080267e-04, -3.65461635e-04, -2.68760007e-04,  3.70511369e-04,
-2.63652522e-04,  1.58915602e-06,  4.32158467e-05])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
nfev: 48

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        nit: 5
        status: 0
        success: True
            x: array([1.02294126, 1.11523241, 0.9115699 , 1.06549471, 1.10504448,
                    0.75798978, 0.76734684, 0.99198168, 1.0196779 , 1.09338739,
                    1.07563186])),
'0.7943282347242822': [        fun: 0.02959196763936291
        hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
            jac: array([ 4.05400169e-05,  1.99369384e-04, -4.03243126e-05, -1.50040783e-04,
                    -8.62649887e-05,  3.45695852e-04, -5.89924318e-05, -1.10486497e-04,
                    1.45214492e-05,  2.00231256e-04, -8.95037192e-05])
        message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
            nfev: 34
            nit: 11
            status: 0
            success: True
                x: array([1.10948292, 1.19158311, 0.82552249, 1.18395229, 1.09408313,
                        0.7091117 , 0.83783094, 0.90036267, 1.0325825 , 1.19659369,
                        1.06579514])),
'1.3489628825916533': [        fun: 0.03713665748364884
        hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
            jac: array([-1.85532832e-05,  1.49506629e-04, -8.49120202e-05, -2.34639276e-05,
                    -7.11797778e-05,  1.25664259e-04,  5.27560741e-05, -8.70581987e-05,
                    8.05365157e-05,  9.53580661e-05, -3.76756897e-05])
        message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
            nfev: 79
            nit: 11
            status: 0
            success: True
                x: array([1.18812974, 1.27083959, 0.81249272, 1.26585077, 1.09033113,
                        0.64381209, 0.94095119, 0.81128402, 1.03105444, 1.3018432 ,
                        1.12068567])),
'2.290867652767775': [        fun: 0.04544078614907872
        hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
            jac: array([ 9.59135792e-05, -1.01131264e-05, -5.27015097e-05, -1.64321652e-05,
                    -9.08124653e-05,  7.69947199e-05,  4.21351263e-05,  6.45303640e-05,
                    -1.07996996e-04,  5.42540499e-05, -2.95033214e-05])
        message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
            nfev: 99
            nit: 16
            status: 0
            success: True
                x: array([1.24800827, 1.37290484, 0.89535654, 1.28360723, 1.08523259,
                        0.60598041, 1.00883749, 0.74688554, 1.0287479 , 1.43750381,
                        1.18438876])),
'3.890451449942813': [        fun: 0.0540546370648527
        hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
            jac: array([ 4.18568669e-04, -1.41220392e-04, -1.13235861e-04,  1.13570326e-04,

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-4.90347208e-05, 1.94346146e-04, -1.32862774e-06, 3.42586618e-04,
-5.43922276e-04, 2.12104865e-04, 2.17638107e-04])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
nfev: 83
nit: 15
status: 0
success: True
x: array([1.32349702, 1.47025149, 1.04072873, 1.2426781 , 1.10034303,
0.59338908, 1.05562467, 0.69668487, 1.05838673, 1.60197334,
1.22664563])),
'6.606934480075965': [ fun: 0.06322347214663938
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([-3.41073869e-04, 3.71845112e-04, -8.93907879e-05, 1.32538918e-05,
2.28493283e-05, 4.10772764e-04, -2.40909609e-04, -1.23503045e-04,
4.49423368e-05, -1.23103192e-04, 1.68656245e-04])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
nfev: 68
nit: 15
status: 0
success: True
x: array([1.40082532, 1.57337971, 1.15905829, 1.19997535, 1.13986703,
0.59807762, 1.09483462, 0.68330576, 1.09306943, 1.72219983,
1.23544337])),
'11.220184543019652': [ fun: 0.0739658480589599
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([ 1.80568112e-04, 1.64633454e-04, -1.98437024e-04, 7.63125616e-05,
-7.45654455e-05, -1.43277486e-03, -1.31258374e-04, -7.28248622e-04,
6.10997444e-04, -5.52415527e-05, -1.44740218e-05])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
nfev: 81
nit: 15
status: 0
success: True
x: array([1.52179975, 1.6988351 , 1.26675339, 1.15226762, 1.20116422,
0.61465911, 1.13722286, 0.67150642, 1.1192861 , 1.82077119,
1.21506589])),
'19.054607179632523': [ fun: 0.08643937437288961
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
jac: array([-3.77834843e-05, 2.29271595e-04, -2.41508380e-04, 3.29981369e-05,
-1.16599126e-04, 1.66719764e-05, 2.29591762e-05, -1.48834893e-04,
-3.65866499e-04, 3.08966698e-05, -2.38992298e-05])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
nfev: 47
nit: 17
status: 0
success: True
x: array([1.66580611, 1.81786853, 1.36607892, 1.10519253, 1.30566154,
0.64925444, 1.18143849, 0.64433281, 1.12964653, 1.90240947,

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1.15459672]]],
'32.35936569296281': [      fun: 0.09369662396531224
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([-6.02034317e-04, -2.27950836e-04, -4.13134921e-04,  2.17576696e-04,
      -3.30112610e-04, -2.45262256e-04,  6.16025110e-04,  3.26837772e-05,
      6.84655392e-05, -3.51513804e-04,  1.38313893e-04])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 98
    nit: 22
    status: 0
    success: True
      x: array([1.58044603, 1.65531024, 1.3444025 , 1.24831246, 1.34867443,
        0.64113452, 1.11662896, 0.44053019, 1.04359856, 2.13435868,
        1.11379447]))],
'54.954087385762485': [      fun: 0.09756900339420053
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([-4.83156417e-04,  3.90070710e-04,  2.90563041e-07, -2.67879918e-05,
      -3.50139342e-05, -1.31017455e-04,  4.34936896e-04, -1.16259081e-03,
      8.54376106e-04, -1.91197481e-04, -4.32492087e-04])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 88
    nit: 16
    status: 0
    success: True
      x: array([1.61949883, 1.63062624, 1.34334672, 1.23343762, 1.37411929,
        0.67702062, 1.0765624 , 0.34026975, 0.9547427 , 2.19642353,
        1.03079557]))],
'93.32543007969925': [      fun: 0.1001918226157554
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 1.13032959e-04, -4.65362246e-05, -1.25821419e-04, -5.73810212e-05,
      8.40770367e-05,  3.14636821e-05, -1.88077149e-04,  1.00070279e-03,
      -6.05367663e-04,  4.03836482e-05,  1.09930469e-04])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 86
    nit: 30
    status: 0
    success: True
      x: array([1.6725086 , 1.5765243 , 1.27887253, 1.16591702, 1.33716126,
        0.732705 , 0.96569362, 0.17193503, 0.7541414 , 2.24350398,
        0.89465985]))],
'158.48931924611173': [      fun: 0.10185363203245928
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([ 6.83507203e-04, -1.23433657e-04,  1.80624908e-04, -3.08988503e-04,
      7.65397706e-05,  1.23150866e-04, -7.81722094e-04, -5.80134089e-04,
      8.40739219e-04,  1.17103794e-03,  2.16386999e-05])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 98
    nit: 23

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status: 0
success: True
      x: array([1.70364752, 1.60865592, 1.225663 , 1.1151601 , 1.31008872,
0.82382752, 0.85877559, 0.06108475, 0.5641047 , 2.24297946,
0.74368819])),
'269.1534803926914': [      fun: 0.1019215638014199
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
      jac: array([-5.54814784e-04, 1.68197709e-04, 1.54927525e-05, 6.79369934e-05,
-4.72122667e-04, -2.63227373e-05, -2.77319678e-04, 1.01368028e-04,
1.56311677e-04, -1.15867857e-04, 1.27678882e-04])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
      nfev: 96
      nit: 32
status: 0
success: True
      x: array([1.54177216, 1.65138993, 1.22417697, 1.17468074, 1.40156717,
0.82355597, 0.92782251, 0.0663759 , 0.51604528, 2.21297538,
0.64393038])),
'457.0881896148752': [      fun: 0.10249759759041074
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 5.18237507e-04, 2.52809443e-04, 1.74181202e-04, -5.10735611e-06,
-3.95118471e-04, -1.31481011e-04, -3.20999273e-04, 1.18409765e-04,
-2.29736444e-04, 8.46928571e-05, 1.24302681e-04])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
      nfev: 101
      nit: 22
status: 0
success: True
      x: array([1.57647054, 1.67566693, 1.2255468 , 1.14767916, 1.44013955,
0.82566607, 0.95178158, 0.07173707, 0.51747204, 2.19480309,
0.63560525])),
'776.2471166286928': [      fun: 0.1761986534750552
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
      jac: array([-0.04219883, 0.30812668, 0.17924368, -0.0713948 , 0.3445268 ,
-0.4724434 , -0.48925113, -1.34693958, 0.72663166, 0.04340999,
-0.17148676])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
      nfev: 49
      nit: 1
status: 0
success: True
      x: array([1.57647054, 1.67566693, 1.2255468 , 1.14767916, 1.44013955,
0.82566607, 0.95178158, 0.07173707, 0.51747204, 2.19480309,
0.63560525])),
'1318.25673855641': [      fun: 0.2723248763796188
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 0.02494338, 0.00480497, -0.03529772, 0.17565735, 0.000644 ,
0.00516487, -0.02350584, -0.02428059, -0.03224987, 0.01075532,

```

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0.00400572]))
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
  nfev: 13
  nit: 3
  status: 0
  success: True
    x: array([0.78210434, 1.20708328, 1.28463633, 0.57082071, 1.04779136,
1.2182526 , 0.          , 1.6073751 , 0.          , 1.50846555,
1.33692978])),
'2238.7211385683377': [      fun: 1.3520126996355728
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
  jac: array([ 0.54158832, -0.00801342,  0.11813477, -0.17369636,  0.06701562,
-0.3115425 , -0.55597386,  0.00289201,  0.31371013, -0.11337851,
-0.02161638])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
  nfev: 18
  nit: 7
  status: 0
  success: True
    x: array([0.          , 0.67880898, 1.09927552, 1.53288587, 1.17318363,
1.00657777, 0.          , 1.64596578, 0.78589434, 1.5264725 ,
0.          ]]),
'3801.8939632056126': [      fun: 0.8994975686078084
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
  jac: array([ 0.3340622 , -0.63164044, -0.04640475, -0.11790373,  0.13519675,
-0.53257491, -0.71573026,  0.04459905,  0.30653784, -0.17645342,
0.0482719 ]])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
  nfev: 10
  nit: 2
  status: 0
  success: True
    x: array([0.          , 0.92753971, 1.02821776, 1.62098748, 1.06400915,
1.37364174, 0.          , 1.61817935, 0.68815824, 1.58598473,
0.          ]]),
'6456.542290346562': [      fun: 0.6719868487679822
hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
  jac: array([ 1.23596654, -0.40591063, -3.10084725,  2.73346514, -0.49013296,
0.15072429,  0.55432514,  0.03574438,  0.43651438,  0.75056121,
0.10840786])
message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
  nfev: 64
  nit: 3
  status: 0
  success: True
    x: array([0.04491126, 1.42016531, 0.84070062, 1.92180777, 0.97040892,
1.83535812, 0.64405538, 1.4790569 , 0.44054605, 1.76517922,
0.          ]]),

```

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'10964.781961431874': [      fun: 0.9052527138728723
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([-0.87432833,  0.45345148, -0.2600789 ,  0.29709803, -0.58378445,
    0.40801301, -0.08378355, -0.08170062,  1.4587171 ,  0.04144252,
    0.10468135])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 7
    nit: 1
    status: 0
    success: True
      x: array([0.04491126, 1.42016531, 0.84070062, 1.92180777, 0.97040892,
    1.83535812, 0.64405538, 1.4790569 , 0.44054605, 1.76517922,
    0.      ])],
'18620.871366628733': [      fun: 1.108586833953849
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([-0.45846963,  0.24880145,  0.02524249, -0.19604348,  0.1309178 ,
    -0.05306981,  0.34146084, -0.21541254,  0.83463852, -0.27085591,
    0.12811275])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 23
    nit: 12
    status: 0
    success: True
      x: array([0.38217896, 2.656752 , 1.02537715, 0.78118327, 1.95557347,
    1.68196915, 1.04208317, 1.15695358, 0.34868613, 1.20985985,
    0.      ])],
'31622.776601683792': [      fun: 1.062795493087772
  hess_inv: <11x11 LbfgsInvHessProduct with dtype=float64>
    jac: array([-0.78445465,  0.41993724, -0.19463718,  0.51285212,  0.24964896,
    -0.01945827,  0.133645 , -0.15712145,  0.56423545, -0.36799996,
    -0.15937153])
  message: b'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
    nfev: 22
    nit: 3
    status: 0
    success: True
      x: array([0.78512637, 2.57341551, 0.95187004, 1.01897977, 1.93024834,
    1.70376731, 1.41787113, 1.1678113 , 1.14192916, 1.25898213,
    0.03660564])]]}

```

```

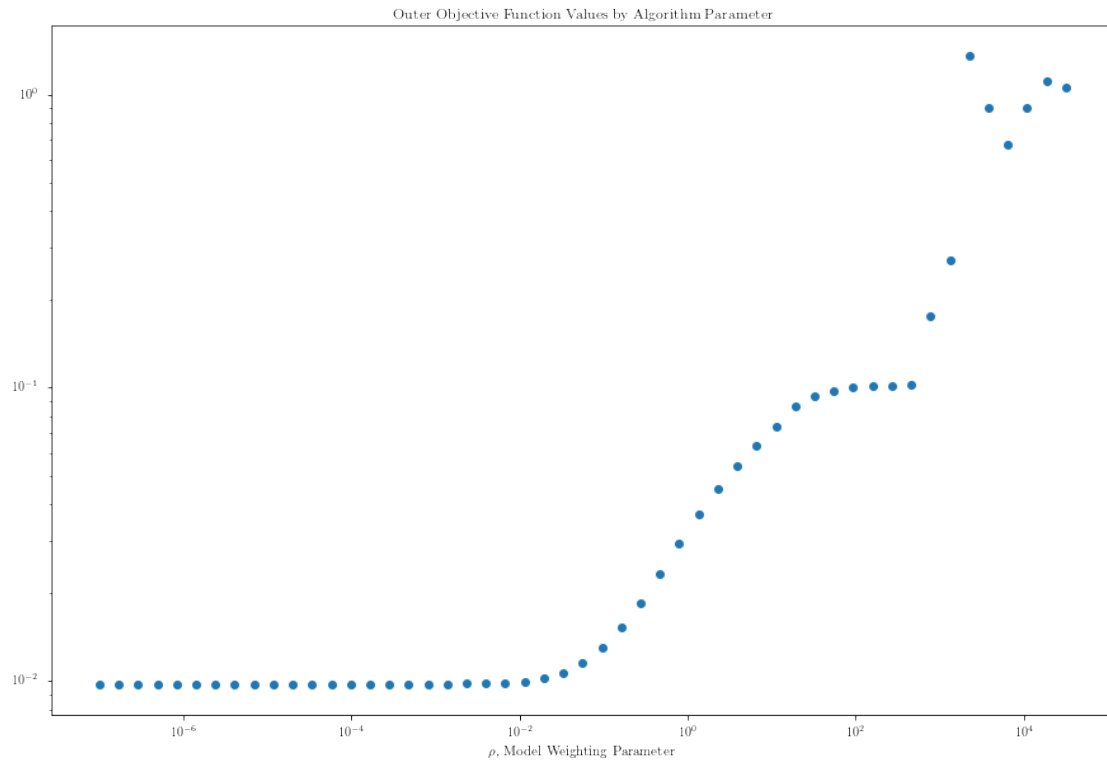
In [11]: outer_objective_values = np.array([[float(rho), val[0].fun] for rho, val in solver.solu
plt.loglog(*outer_objective_values.T, 'o')
plt.title("Outer Objective Function Values by Algorithm Parameter")
plt.xlabel(r"$\rho$, Model Weighting Parameter")

```

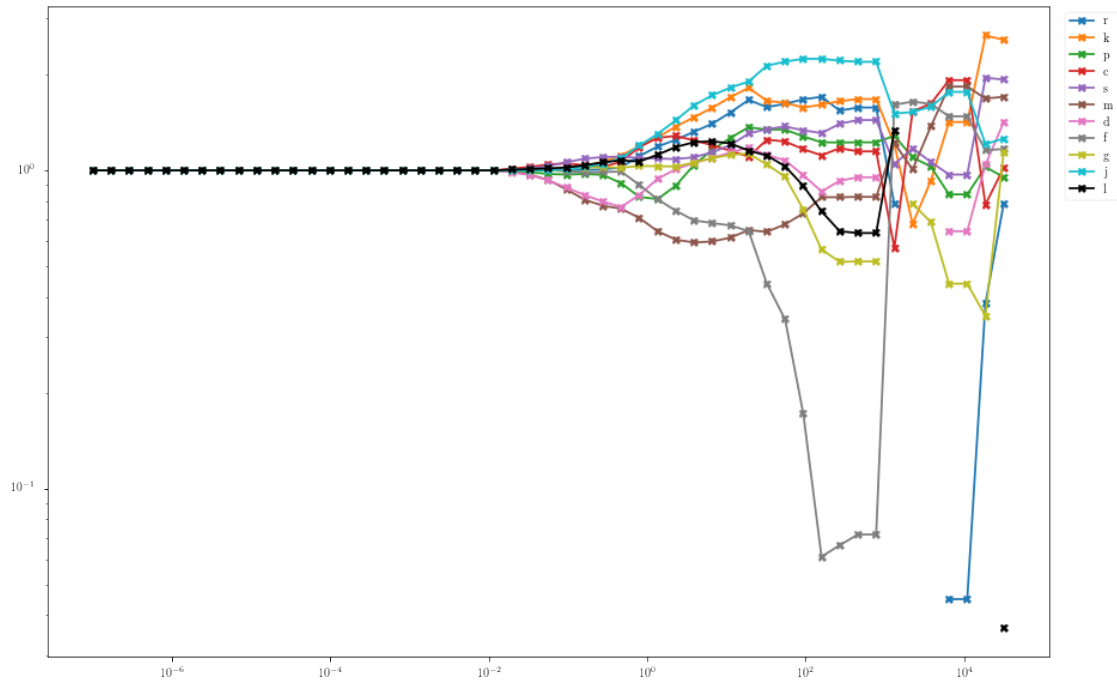
```

Out[11]: Text(0.5, 0, '$\rho$, Model Weighting Parameter')

```



```
In [12]: rhos = [float(rho) for rho in solver.solutions.keys()]
          vals = [val[0].x for val in solver.solutions.values()]
          plt.plot(rhos, vals, 'X-')
          plt.legend("rkpcsmdfgjl", loc="best", bbox_to_anchor=(1.01, 1))
          plt.xscale("log")
          plt.yscale("log", nonposy="mask")
```



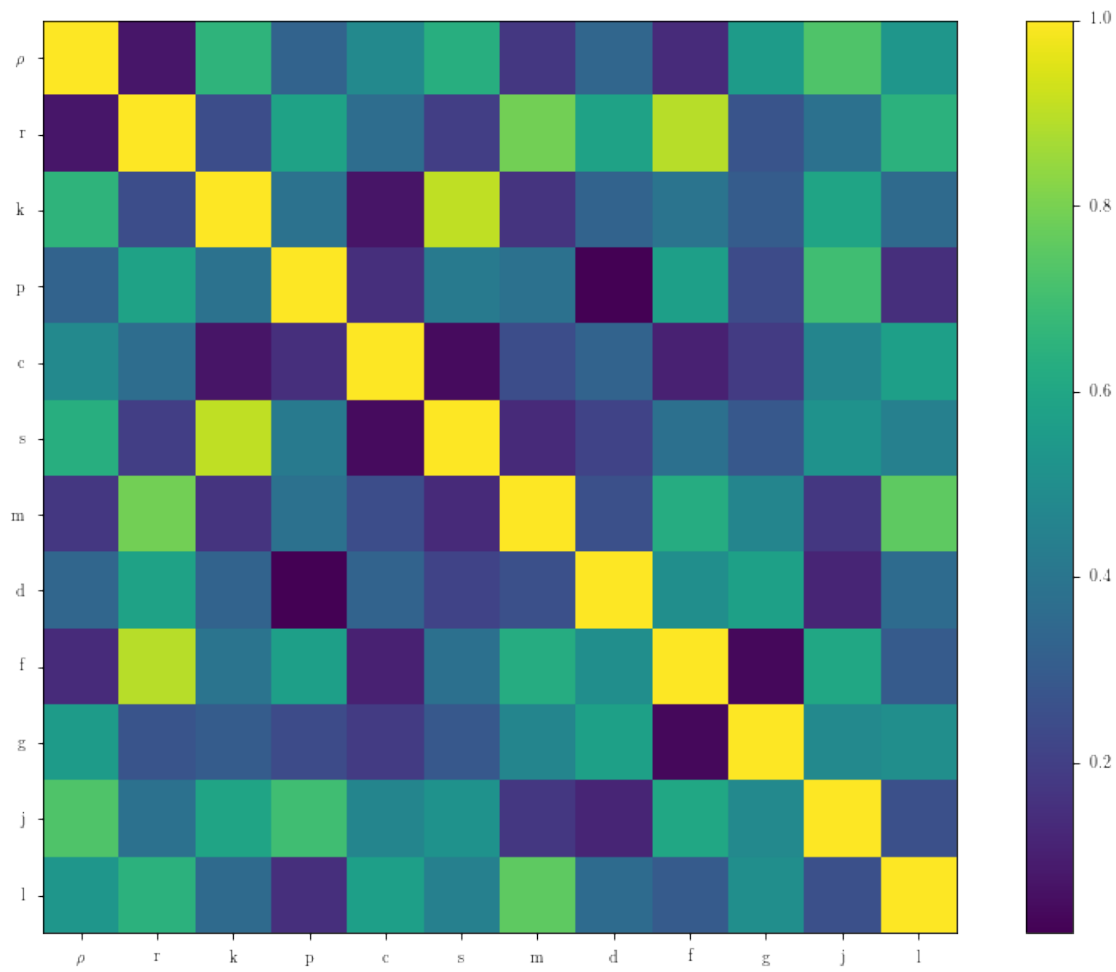
In [13]: # generate a crude correlation plot

```
import pandas as pd
```

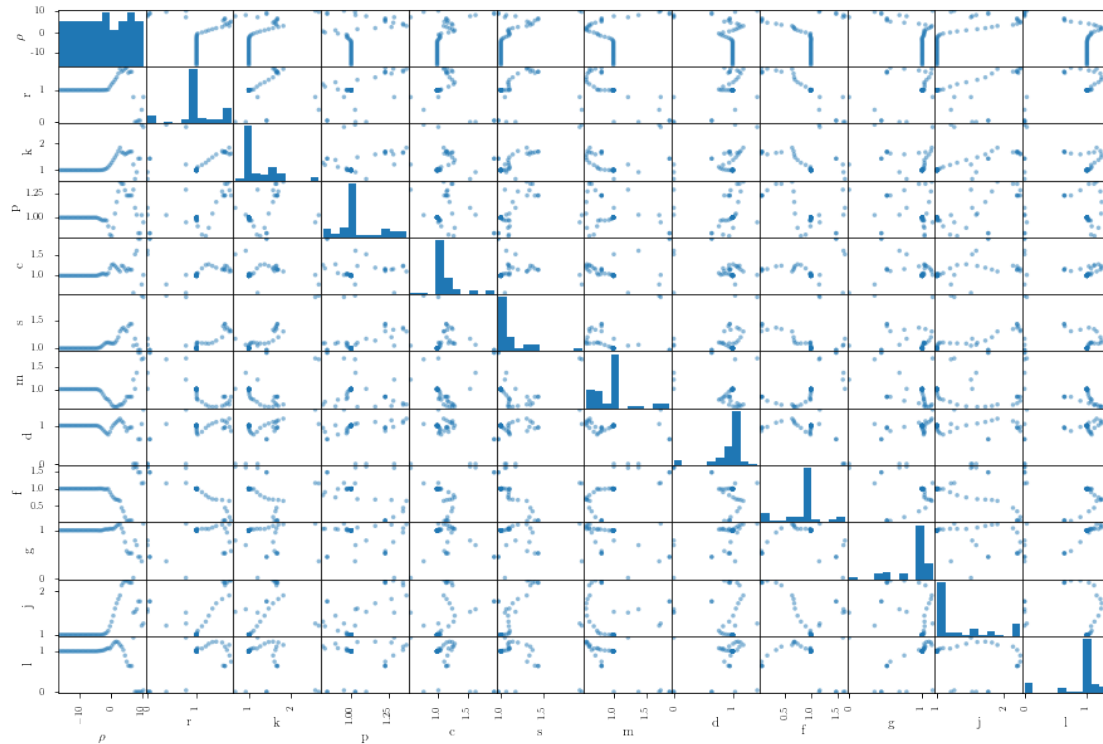
```
results = pd.DataFrame({r"$\rho$": np.log(rhos)})
for idx, name in enumerate("rkpcsmdfgjl"):
    results[name] = [v[idx] for v in vals]
```

```
In [14]: plt.imshow(np.abs(results.corr()))
plt.colorbar()
plt.xticks(range(12), [r"$\rho$"] + list("rkpcsmdfgjl"))
plt.yticks(range(12), [r"$\rho$"] + list("rkpcsmdfgjl"))
plt.grid(False)
```





```
In [15]: ax = pd.plotting.scatter_matrix(results)
         for a in ax.flatten():
             a.grid(False)
```

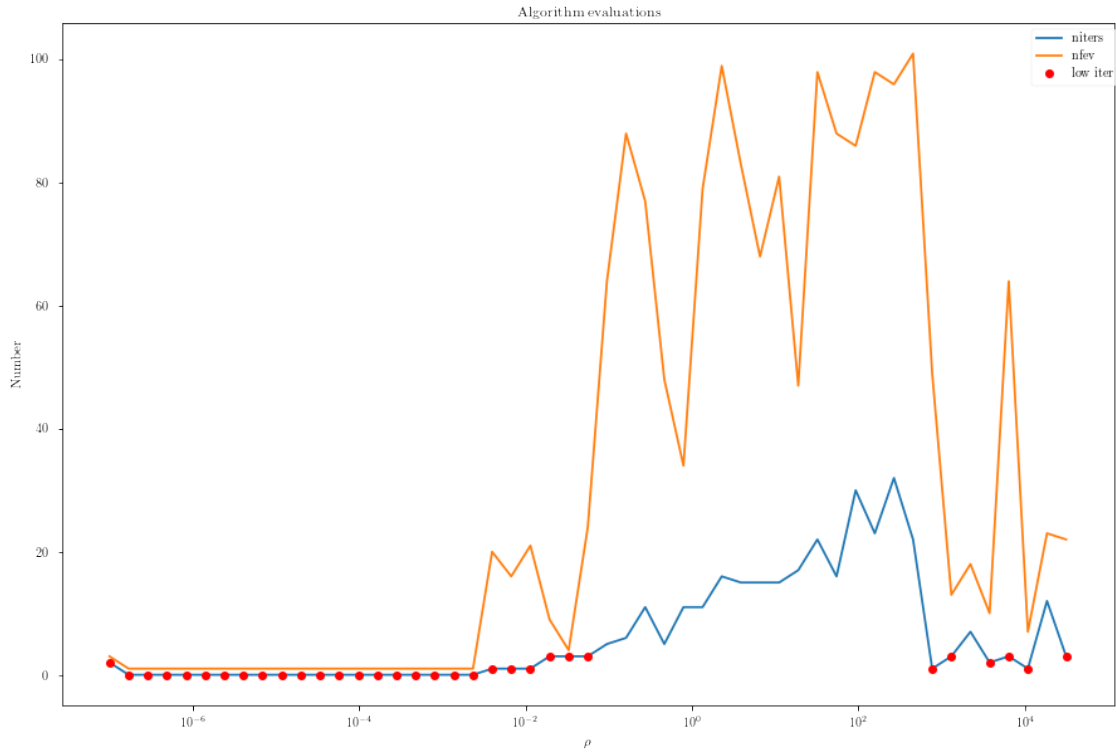


```
In [16]: iters_list = np.array([[float(key), value[0].nit] for key, value in solver.solutions.it
fevs_list = np.array([[float(key), value[0].nfev] for key, value in solver.solutions.it
plt.semilogx(*iters_list.T, *fevs_list.T)

low_iters = np.array([[k,v] for k,v in iters_list if v < 5])
plt.plot(*low_iters.T, 'ro')

plt.legend(["niters", "nfev", "low iter"],
           loc="best", bbox_to_anchor=(1.01, 1))
plt.title("Algorithm evaluations")
plt.xlabel(r"$\rho$")
plt.ylabel("Number")

Out[16]: Text(0, 0.5, 'Number')
```



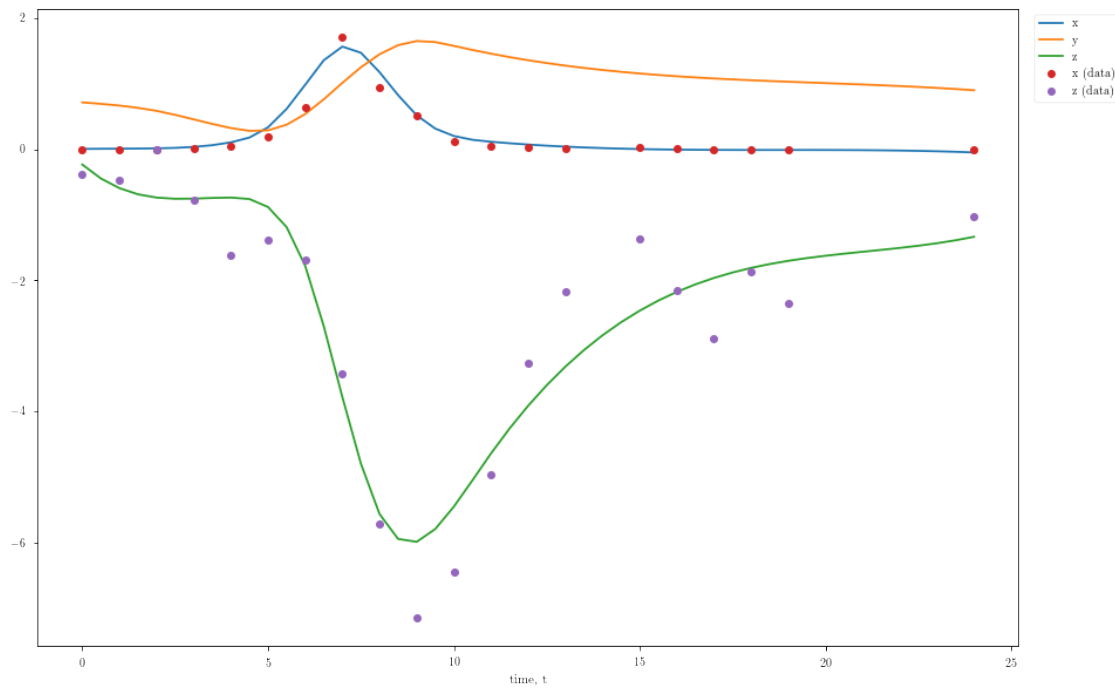
```
In [17]: def tokey(rho, ps):
          return f"{'y'.join(map(str,ps))}r{rho}"
          getx = fitter.ca.Function("getx", [model.ts, *model.cs], model.xs)

In [33]: target_rho = 93.32543007969925
          c_end = solver.problems[0].cache.results[tokey(target_rho, solver.solutions[str(target_rho)])[0].x)
          print(solver.solutions[str(target_rho)][0].x)
          xs_end = np.array([np.array(i) for i in getx(model.observation_times,
                                                         *fitter.argsplit(c_end,
                                                         3)
                                                         )])

          print(xs_end[:,0].T)
          plt.plot(model.observation_times, np.hstack([xs_end[0], xs_end[1], xs_end[2]]),
                    context.datasets[0]['t'], context.datasets[0]['x'], 'o',
                    context.datasets[0]['t'], context.datasets[0]['z'], 'o')
          plt.legend(list("xyz") + ["x (data)", "z (data)"], loc="best", bbox_to_anchor=(1.01, 1))
          plt.xlabel("time, t")

[1.6725086  1.5765243  1.27887253 1.16591702 1.33716126 0.732705
 0.96569362 0.17193503 0.7541414  2.24350398 0.89465985]
[[ 0.0045466  0.714481 -0.233282 ]]
```

Out [33]: Text(0.5, 0, 'time, t')

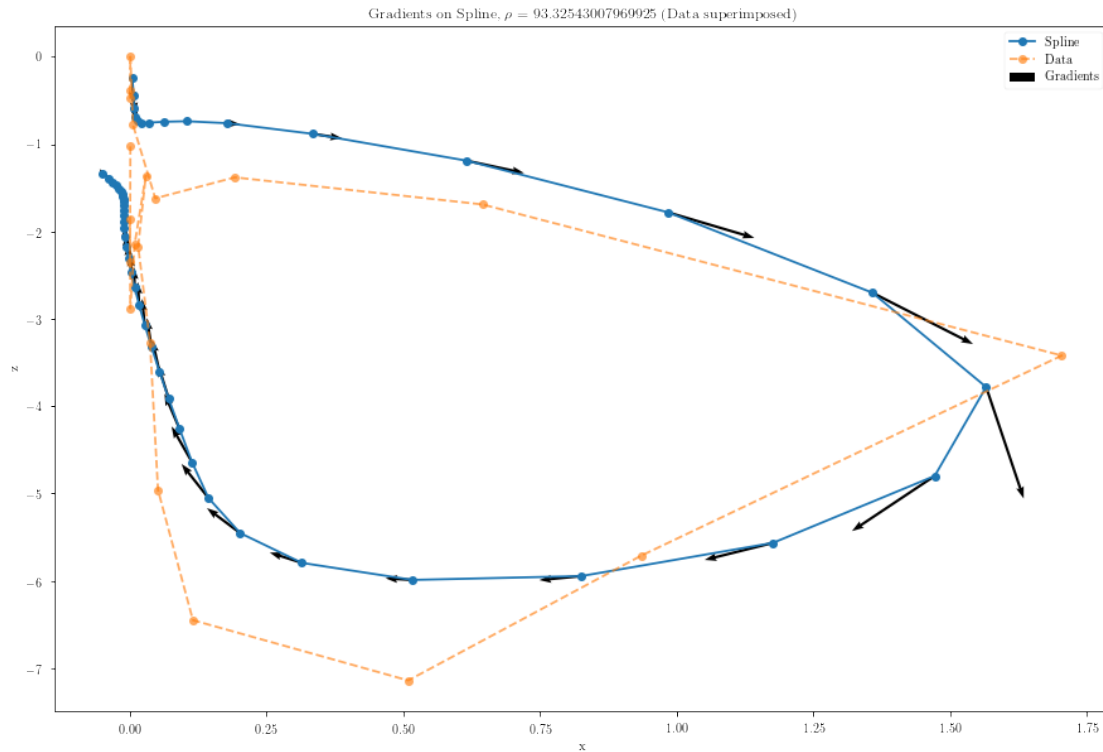


```
In [29]: spline_dfield = np.array([context.model(t, xs_end[:,i], solver.solutions[str(target_rho)
                                             for i,t in enumerate(model.observation_times)])

spline_dfield = spline_dfield.reshape(spline_dfield.shape[:2])

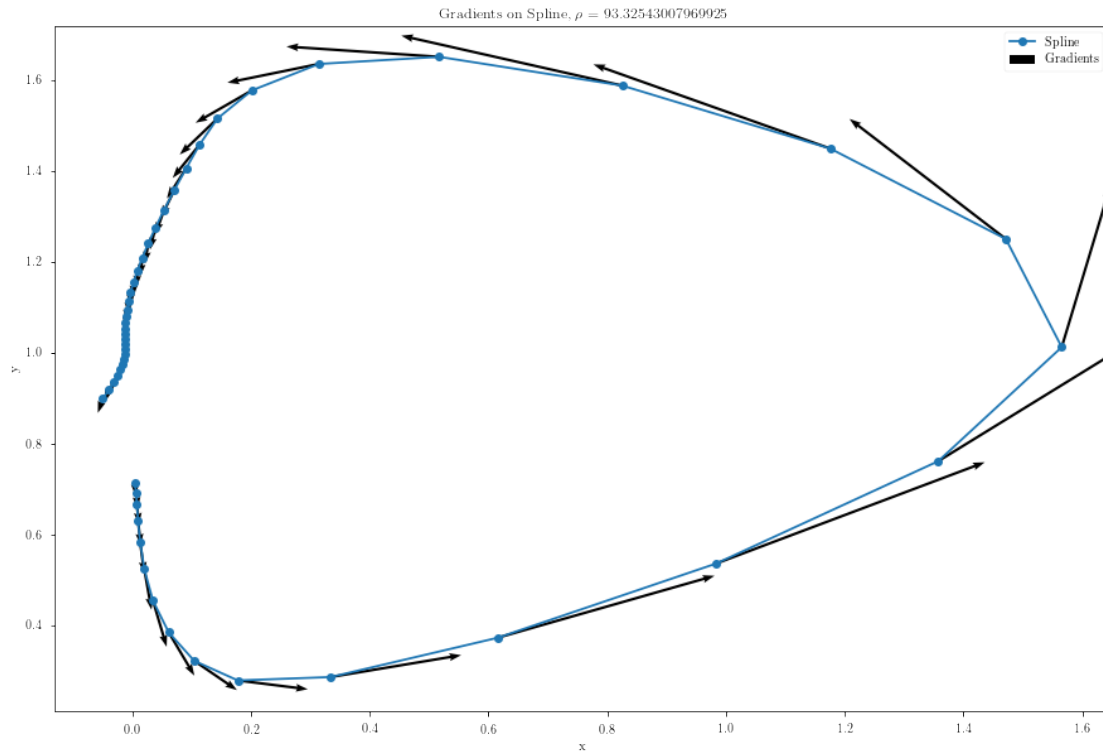
plt.plot(xs_end[0], xs_end[2], 'o-')
plt.plot(context.datasets[0]['x'], context.datasets[0]['z'], 'o--', alpha=0.65)
plt.quiver(xs_end[0], xs_end[2], spline_dfield[:,0], spline_dfield[:,2],
           scale=v220, angles='xy', headwidth=3, headlength=4.5, headaxislength=4, width=0.001)
plt.title(f"Gradients on Spline,  $\rho = \{target\_rho\}$  (Data superimposed)")
plt.xlabel("x")
plt.ylabel("z")
plt.legend(["Spline", "Data", "Gradients"])
```

Out [29]: <matplotlib.legend.Legend at 0x7f7b4d122940>



```
In [30]: plt.plot(xs_end[0], xs_end[1], 'o-')
plt.quiver(xs_end[0], xs_end[1], spline_dfield[:,0], spline_dfield[:,1],
           scale=None, angles='xy', headwidth=3, headlength=4.5, headaxislength=4, width=0.005)
plt.title(f"Gradients on Spline,  $\rho = \{target\_rho\}$ ")
plt.xlabel("x")
plt.ylabel("y")
plt.legend(["Spline", "Gradients"])
```

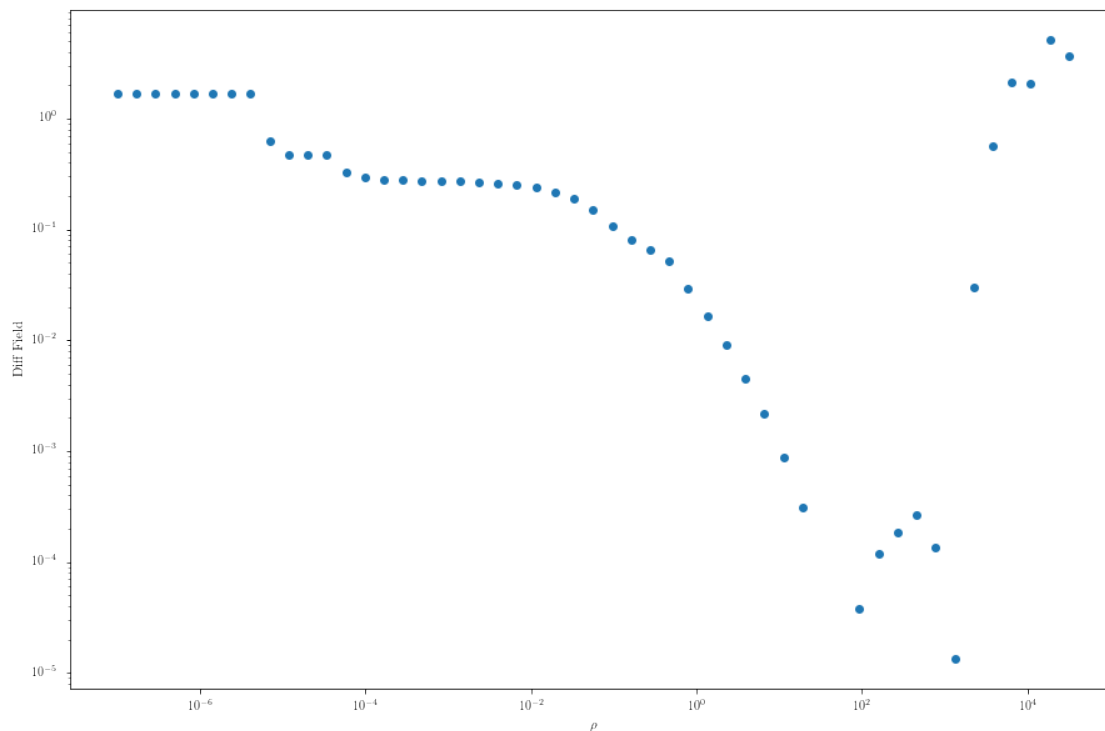
```
Out[30]: <matplotlib.legend.Legend at 0x7f7b4d0a9898>
```



```
In [21]: inner_objective_values = np.array([[r, solver.problems[0].cache.results[tokey(r, v)].fu
      dfield = np.hstack([np.array(rhos).reshape(-1,1),
      ((inner_objective_values - outer_objective_values)[:,1] / rhos).res
```

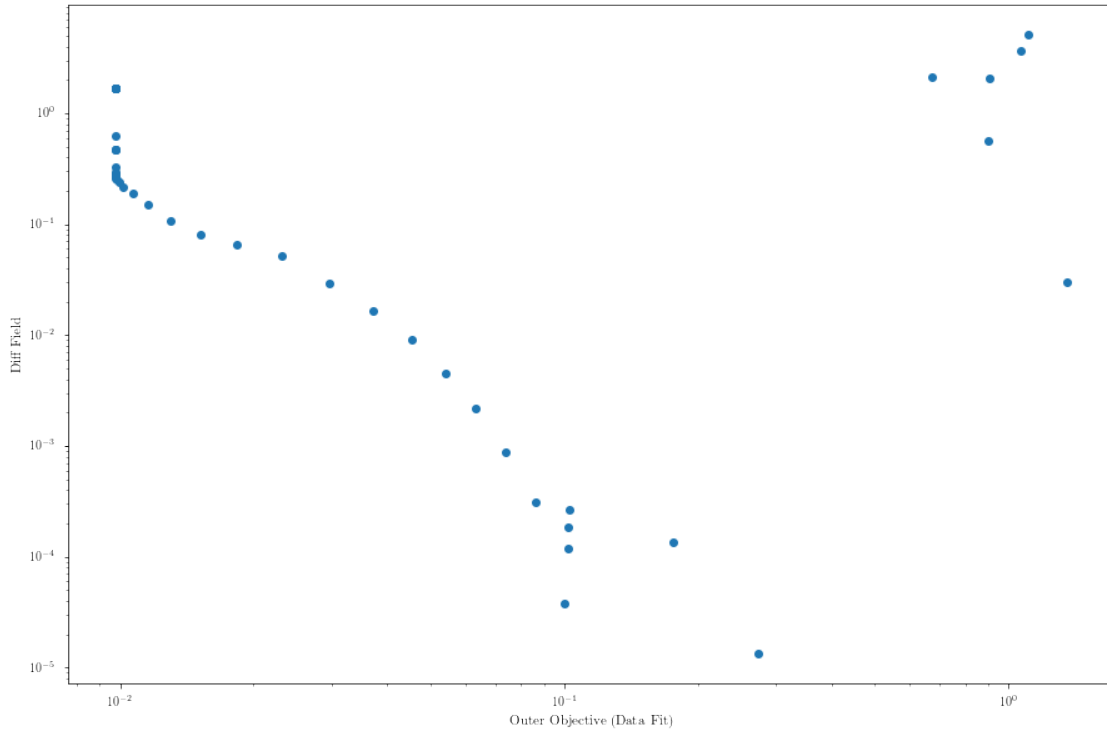
```
In [22]: plt.loglog(*dfield.T, 'o')
      plt.xlabel(r"$\rho$")
      plt.ylabel("Diff Field")
```

```
Out[22]: Text(0, 0.5, 'Diff Field')
```



```
In [23]: plt.loglog(outer_objective_values[:,1], dfield[:,1], 'o')
          plt.xlabel("Outer Objective (Data Fit)")
          plt.ylabel("Diff Field")
```

```
Out[23]: Text(0, 0.5, 'Diff Field')
```



```
In [24]: curv_dx = np.gradient(np.log(outer_objective_values[:,1]))
         curv_dy = np.gradient(np.log(dfied[:,1]))
         curv_dx2 = np.gradient(curv_dx)
         curv_dy2 = np.gradient(curv_dy)

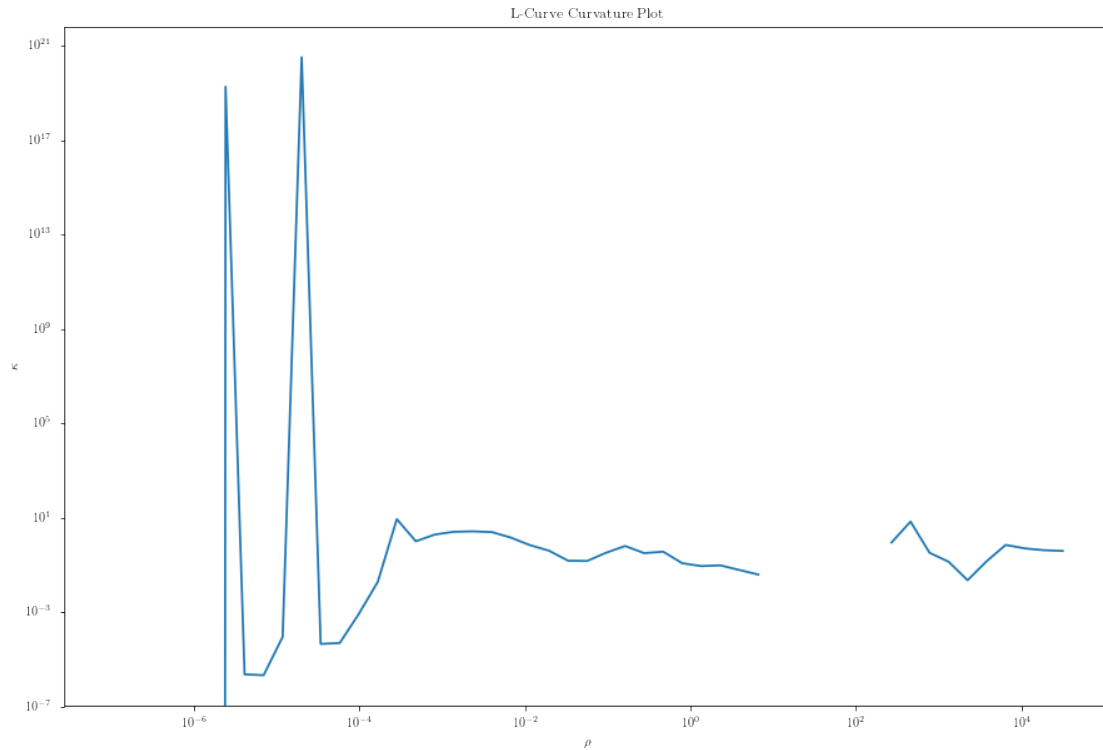
         kappa = np.abs(curv_dx*curv_dy2 - curv_dy*curv_dx2)/(curv_dx**2 + curv_dy**2)**(3/2)

         plt.loglog(rhos, kappa)
         plt.title("L-Curve Curvature Plot")
         plt.xlabel(r"$\rho$")
         plt.ylabel(r"$\kappa$")

/home/dwu402/.virtualenvs/scider/lib/python3.6/site-packages/ipykernel_launcher.py:2: RuntimeWarning:

Out[24]: Text(0, 0.5, '$\kappa$')
```





In [25]: rhos

Out [25]: [1e-07,  
1.6982436524617461e-07,  
2.8840315031266057e-07,  
4.897788193684466e-07,  
8.317637711026709e-07,  
1.4125375446227554e-06,  
2.3988329190194897e-06,  
4.073802778041131e-06,  
6.9183097091893625e-06,  
1.1748975549395302e-05,  
1.995262314968883e-05,  
3.3884415613920276e-05,  
5.7543993733715664e-05,  
9.772372209558111e-05,  
0.00016595869074375615,  
0.0002818382931264455,  
0.00047863009232263854,  
0.0008128305161640995,  
0.0013803842646028866,  
0.0023442288153199225,  
0.003981071705534978,

```

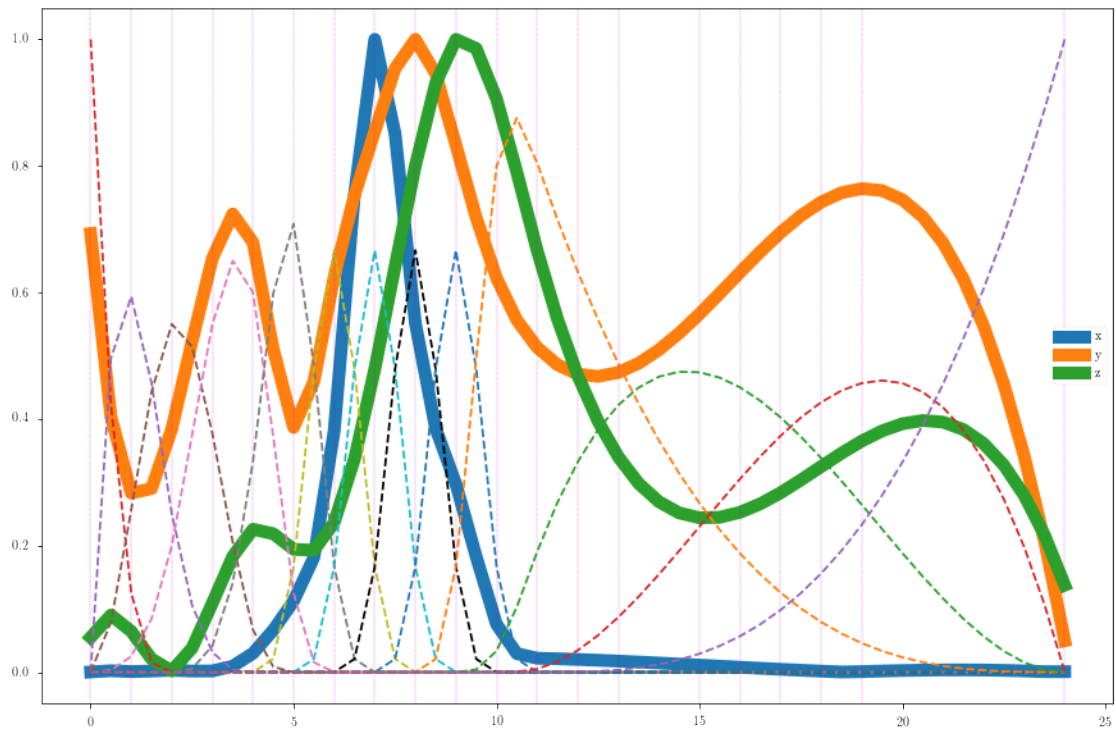
0.006760829753919818,
0.01148153621496884,
0.019498445997580455,
0.03311311214825914,
0.05623413251903491,
0.09549925860214369,
0.16218100973589297,
0.2754228703338169,
0.4677351412871981,
0.7943282347242822,
1.3489628825916533,
2.290867652767775,
3.890451449942813,
6.606934480075965,
11.220184543019652,
19.054607179632523,
32.35936569296281,
54.954087385762485,
93.32543007969925,
158.48931924611173,
269.1534803926914,
457.0881896148752,
776.2471166286928,
1318.25673855641,
2238.7211385683377,
3801.8939632056126,
6456.542290346562,
10964.781961431874,
18620.871366628733,
31622.776601683792]

```

```

In [26]: bfn = modeller.ca.Function('basis_fns', [model.ts], [model.basis])
plt.plot(model.observation_times, np.abs(np.hstack([xs_end[0]/max(abs(xs_end[0])),
                                                    xs_end[1]/max(abs(xs_end[1])),
                                                    xs_end[2]/max(abs(xs_end[2]))])),
          linewidth=10)
plt.plot(model.observation_times, bfn(model.observation_times), '--')
plt.legend('xyz')
[plt.axvline(x=i, color='m', linewidth=0.25, linestyle='--') for i in context.datasets]
print("")

```



```
In [27]: plt.plot(range(model.K), np.array(fitter.argsplit(c_end, 3)).T, 'o')
plt.legend('xyz')
```

```
Out[27]: <matplotlib.legend.Legend at 0x7f7b4d2c5080>
```

