```
Python 3.9.12 | packaged by conda-forge | (main, Mar 24 2022, 23:23:20)
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IPython 7.33.0 -- An enhanced Interactive Python.

Restarting kernel...
```

```
In [1]:         '/Users/fnal/Documents/Research/LWFA/LWFA 4.0/analysis
4.0/x-ray analysis/6. Python implementation/Calculate 3D Spectrum/
issue_18039_sample_code.py'      ='/Users/fnal/Documents/Research/LWFA/
LWFA 4.0/analysis 4.0/x-ray analysis/6. Python implementation/Calculate
3D Spectrum'
Sample code: Optimization starting...
Sample code: Optimization ended, printing the results next...
      fun: 1.3003448967631297e-12
 hess_inv: <5x5 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 3.29645133e-08, -1.26798629e-05,  1.17985872e-05,
-1.22448317e-05,
        5.95941114e-06])
  message: 'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 26
      nit: 24
     njev: 26
   status: 0
  success: True
        x: array([1.00000011, 1.00000021, 1.00000046, 1.00000091,
1.00000184])

In [2]:         '/Users/fnal/Documents/Research/LWFA/LWFA 4.0/analysis
4.0/x-ray analysis/6. Python implementation/Calculate 3D Spectrum/
issue_18039_sample_code.py'      ='/Users/fnal/Documents/Research/LWFA/
LWFA 4.0/analysis 4.0/x-ray analysis/6. Python implementation/Calculate
3D Spectrum'
Sample code: Optimization starting...
Sample code: Optimization ended, printing the results next...
      fun: 1.791049144913494e-11
 hess_inv: <5x5 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 5.21030684e-07, -6.41807390e-05,  4.34994048e-05,
-1.03124107e-04,
        4.49793021e-05])
  message: 'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 37
      nit: 33
     njev: 37
   status: 0
  success: True
        x: array([0.99999962, 0.99999924, 0.99999863, 0.99999722,
0.99999467])
```

```
RUNNING THE L-BFGS-B CODE

           * * *

Machine precision = 2.220D-16
 N =            5     M =           10

At X0         0 variables are exactly at the bounds

At iterate    0    f=  8.48220D+02    |proj g|=  2.08540D+03

At iterate    1    f=  3.99762D+01    |proj g|=  1.69958D+02

At iterate    2    f=  1.63703D+01    |proj g|=  1.00591D+02

At iterate    3    f=  2.73198D+00    |proj g|=  4.96538D+01

At iterate    4    f=  1.01393D+00    |proj g|=  2.20827D+01

At iterate    5    f=  1.07202D-01    |proj g|=  1.03271D+01

At iterate    6    f=  2.30119D-02    |proj g|=  8.24714D-01

At iterate    7    f=  2.22778D-02    |proj g|=  1.74719D-01

At iterate    8    f=  2.22432D-02    |proj g|=  1.18020D-01

At iterate    9    f=  2.22175D-02    |proj g|=  1.05946D-01

At iterate   10    f=  2.21319D-02    |proj g|=  2.88356D-01

At iterate   11    f=  2.19305D-02    |proj g|=  5.83854D-01

At iterate   12    f=  2.13934D-02    |proj g|=  1.06513D+00

At iterate   13    f=  2.00866D-02    |proj g|=  1.76535D+00

At iterate   14    f=  1.72122D-02    |proj g|=  2.62905D+00

At iterate   15    f=  1.25070D-02    |proj g|=  3.20973D+00

At iterate   16    f=  7.12103D-03    |proj g|=  3.34539D+00

At iterate   17    f=  4.34321D-03    |proj g|=  2.35238D+00

At iterate   18    f=  2.25392D-04    |proj g|=  4.22986D-01

At iterate   19    f=  1.96518D-05    |proj g|=  1.19854D-01

At iterate   20    f=  2.58660D-06    |proj g|=  3.79854D-02
```

```
At iterate   21    f=  1.04796D-07    |proj g|=  1.27803D-02

At iterate   22    f=  5.45817D-09    |proj g|=  2.12583D-03

At iterate   23    f=  3.45957D-10    |proj g|=  4.36388D-04

At iterate   24    f=  1.30034D-12    |proj g|=  1.26799D-05

           * * *

Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value

           * * *

   N    Tit     Tnf  Tnint  Skip  Nact     Projg        F
    5     24     26      1     0     0   1.268D-05   1.300D-12
  F =   1.3003448967631297E-012

CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
RUNNING THE L-BFGS-B CODE

           * * *

Machine precision = 2.220D-16
 N =            5     M =           10

At X0         0 variables are exactly at the bounds

At iterate    0    f=  5.28202D+03    |proj g|=  7.13940D+03

At iterate    1    f=  8.89640D+02    |proj g|=  1.40146D+03

At iterate    2    f=  3.69526D+02    |proj g|=  6.57710D+02

At iterate    3    f=  7.26261D+01    |proj g|=  2.56611D+02

At iterate    4    f=  1.26963D+01    |proj g|=  1.01802D+02

At iterate    5    f=  2.09361D+00    |proj g|=  5.69154D+01

At iterate    6    f=  6.16940D-01    |proj g|=  2.12461D+01

At iterate    7    f=  4.36429D-01    |proj g|=  1.87639D+00
```

```
At iterate    8    f=  4.34311D-01    |proj g|=  9.37364D-01

At iterate    9    f=  4.33601D-01    |proj g|=  4.30501D-01

At iterate   10    f=  4.33405D-01    |proj g|=  4.13508D-01

At iterate   11    f=  4.32901D-01    |proj g|=  5.25404D-01

At iterate   12    f=  4.31719D-01    |proj g|=  1.13234D+00

At iterate   13    f=  4.28549D-01    |proj g|=  2.13586D+00

At iterate   14    f=  4.20455D-01    |proj g|=  3.70687D+00

At iterate   15    f=  4.00663D-01    |proj g|=  6.08657D+00

At iterate   16    f=  3.61701D-01    |proj g|=  9.11429D+00

At iterate   17    f=  3.06523D-01    |proj g|=  1.12821D+01

At iterate   18    f=  2.00676D-01    |proj g|=  8.92051D+00

At iterate   19    f=  1.37282D-01    |proj g|=  8.54608D+00

At iterate   20    f=  4.80734D-02    |proj g|=  3.09705D+00

At iterate   21    f=  4.53867D-02    |proj g|=  3.65767D+00

At iterate   22    f=  2.89780D-02    |proj g|=  3.19046D+00

At iterate   23    f=  1.98914D-02    |proj g|=  2.40559D+00

At iterate   24    f=  1.24304D-02    |proj g|=  1.64984D+00

At iterate   25    f=  7.19477D-03    |proj g|=  1.46837D+00

At iterate   26    f=  2.51212D-03    |proj g|=  1.64502D+00
```

```
In [3]:         '/Users/fnal/Documents/Research/LWFA/LWFA 4.0/analysis
4.0/x-ray analysis/6. Python implementation/Calculate 3D Spectrum/
issue_18039_sample_code.py'      ='/Users/fnal/Documents/Research/LWFA/
LWFA 4.0/analysis 4.0/x-ray analysis/6. Python implementation/Calculate
3D Spectrum'
Sample code: Optimization starting...
Sample code: Optimization ended, printing the results next...
      fun: 1.791049144913494e-11
 hess_inv: <5x5 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 5.21030684e-07, -6.41807390e-05,  4.34994048e-05,
-1.03124107e-04,
```

```
        4.49793021e-05])
  message: 'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 37
      nit: 33
     njev: 37
   status: 0
  success: True
        x: array([0.99999962, 0.99999924, 0.99999863, 0.99999722,
0.99999467])

In [4]:         '/Users/fnal/Documents/Research/LWFA/LWFA 4.0/analysis
4.0/x-ray analysis/6. Python implementation/Calculate 3D Spectrum/
issue_18039_sample_code.py'      ='/Users/fnal/Documents/Research/LWFA/
LWFA 4.0/analysis 4.0/x-ray analysis/6. Python implementation/Calculate
3D Spectrum'
Sample code: Optimization starting...
Sample code: Optimization ended, printing the results next...
      fun: 1.791049144913494e-11
 hess_inv: <5x5 LbfgsInvHessProduct with dtype=float64>
      jac: array([ 5.21030684e-07, -6.41807390e-05,  4.34994048e-05,
-1.03124107e-04,
        4.49793021e-05])
  message: 'CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH'
     nfev: 37
      nit: 33
     njev: 37
   status: 0
  success: True
        x: array([0.99999962, 0.99999924, 0.99999863, 0.99999722,
0.99999467])

At iterate   27    f=  2.74070D-04    |proj g|=  4.87790D-01

At iterate   28    f=  8.66968D-05    |proj g|=  1.99382D-01

At iterate   29    f=  2.76675D-05    |proj g|=  2.23337D-01

At iterate   30    f=  6.62515D-07    |proj g|=  1.72311D-02

At iterate   31    f=  3.75344D-08    |proj g|=  2.35488D-03

At iterate   32    f=  5.49623D-10    |proj g|=  6.18132D-04

At iterate   33    f=  1.79105D-11    |proj g|=  1.03124D-04

           * * *

Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
```

```
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value

           * * *

   N    Tit     Tnf  Tnint  Skip  Nact     Projg        F
    5     33     37      1     0     0   1.031D-04   1.791D-11
  F =   1.7910491449134941E-011

CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
RUNNING THE L-BFGS-B CODE

           * * *

Machine precision = 2.220D-16
 N =            5     M =           10

At X0         0 variables are exactly at the bounds

At iterate    0    f=  5.28202D+03    |proj g|=  7.13940D+03

At iterate    1    f=  8.89640D+02    |proj g|=  1.40146D+03

At iterate    2    f=  3.69526D+02    |proj g|=  6.57710D+02

At iterate    3    f=  7.26261D+01    |proj g|=  2.56611D+02

At iterate    4    f=  1.26963D+01    |proj g|=  1.01802D+02

At iterate    5    f=  2.09361D+00    |proj g|=  5.69154D+01

At iterate    6    f=  6.16940D-01    |proj g|=  2.12461D+01

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At iterate   10    f=  4.33405D-01    |proj g|=  4.13508D-01

At iterate   11    f=  4.32901D-01    |proj g|=  5.25404D-01

At iterate   12    f=  4.31719D-01    |proj g|=  1.13234D+00

At iterate   13    f=  4.28549D-01    |proj g|=  2.13586D+00

At iterate   14    f=  4.20455D-01    |proj g|=  3.70687D+00
```

```
At iterate   15    f=  4.00663D-01    |proj g|=  6.08657D+00

At iterate   16    f=  3.61701D-01    |proj g|=  9.11429D+00

At iterate   17    f=  3.06523D-01    |proj g|=  1.12821D+01

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At iterate   20    f=  4.80734D-02    |proj g|=  3.09705D+00

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At iterate   31    f=  3.75344D-08    |proj g|=  2.35488D-03

At iterate   32    f=  5.49623D-10    |proj g|=  6.18132D-04

At iterate   33    f=  1.79105D-11    |proj g|=  1.03124D-04

           * * *

Tit   = total number of iterations
Tnf   = total number of function evaluations
Tnint = total number of segments explored during Cauchy searches
Skip  = number of BFGS updates skipped
Nact  = number of active bounds at final generalized Cauchy point
Projg = norm of the final projected gradient
F     = final function value

           * * *
```

```
   N    Tit     Tnf  Tnint  Skip  Nact     Projg        F
    5     33     37      1     0     0   1.031D-04   1.791D-11
  F =   1.7910491449134941E-011

CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
RUNNING THE L-BFGS-B CODE

           * * *

Machine precision = 2.220D-16
 N =            5     M =           10

At X0         0 variables are exactly at the bounds

At iterate    0    f=  5.28202D+03    |proj g|=  7.13940D+03

At iterate    1    f=  8.89640D+02    |proj g|=  1.40146D+03

In [5]:
```