

# Sample of Nelder-Mead method (minsearch) with sxrd solver

## Optimization by minsearch algorithm with sxrd solver

In this sample we will show how to perform the optimization by Nelder-Mead method (minsearch) with sxrd solver like using [sim-trhepd-rheed](#) solver. The specific calculation procedure is as follows.

### 1. Preparation of the reference file for sxrd solver

The reference file should match the format of `sxrdcalc`, detail is described below in **Reference file** section.

### 2. Preparation of the input file for sxrd solver

The `[algorithm]` section should be change to satisfy the minsearch algorithm, detail is described below in **Input file** section.

### 3. Execute 2DMAT

After preparing the reference file and input file, we can easily call 2DMAT and submit the input file:

```
python3 2dmat input.toml
```

And we will get the output file, you can find the reference output files in this sample, and detail is described below in **Output file** section.

## Reference file

The reference file containing the data to be targeted to fit. The path is specified by `f_in_file` in the `[solver.reference]` section of input file. For each line `h k l F sigma` is given. Here, `h k l` are the wavenumbers, `F` is the intensity, and `sigma` is the uncertainty of `F`. An example file is shown below.

```
0.000000 0.000000 0.050000 572.805262 0.1
0.000000 0.000000 0.150000 190.712559 0.1
0.000000 0.000000 0.250000 114.163340 0.1
0.000000 0.000000 0.350000 81.267319 0.1
0.000000 0.000000 0.450000 62.927325 0.1
0.000000 0.000000 0.550000 51.209358 0.1
```

...

## Input file

The parameters in `[base]`, `[solver]` sections will keep the same as the sample of using mapper algorithm. We need to change the parameter in `[algorithm]` section.

- `[algorithm]`  
`name = "minsearch"` Name should be change to minsearch  
`label_list = ["z1", "z2"]` The list number should equal to `dimension` in `[base]` section and number of `type_vector` in `[solver.config]` section.
- `[algorithm.param]`

```
min_list = [-0.2, -0.2]
```

```
max_list = [0.2, 0.2]
```

The `min_list` and `max_list` specify the minimum and maximum values of the search range, respectively.

```
initial_list = [0.0, 0.0]
```

 The `initial_list` specifies the initial values.

## Output

The standard output is the same as tutorial **Optimization by Nelder-Mead method**, The final estimated parameters will be output to `res.dat`.

```
fx = 0.000106
```

```
z1 = -2.351035891479114e-05
```

```
z2 = 0.025129315870799473
```

Here is the reference result of 2DMAT calculation.