Notes for libEMMI_MGFD

Pengliang Yang
Harbin Institute of Technology, China
E-mail: ypl.2100@gmail.com

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1 Input parameters

- `mode`: `mode=0`, forward modelling; `mode=1`, 3D CSEM inversion;
- `freqs:` the frequencies used for CSEM modelling and inversion, a number of frequencies can be given by comma separated values;
- `chsrc:` source channels (i.e. Ex, Ey, Ez, Hx, Hy, Hz)
- `chrec:` receiver channels (i.e. Ex, Ey, Ez, Hx, Hy, Hz)
- `nx,ny,nz`: number of intervals in x, y and z axes for input resistivity model on equispaced FD grid;
- `dx,dy,dz`: grid spacing of input resistivity model on equispaced FD grid;
- `ox,oy,oz`: origin of the 3D coordinates in x, y and z directions;
- `fbathy`: a binary input file of size `nx*ny` to specify bathymetry information;
- `frho11,frho22,frho33`: binary file of size `nx*ny*nz` to specify resistivities;
- `fsrc`: an ASCII file to specify source locations and orientations;
- `frec`: an ASCII file to specify receiver locations and orientations;
- `fsrcrec`: an ASCII file to specify the connection between source and receivers;
- `niter`: number of iterations for nonlinear optimization;
- `npar`: number of parameters used for inversion, default value=2;
- `bound`: `bound=1` uses bounded LBFGS; `bound=0` does not apply bound constraint;
- `idxpar`: index of the inversion parameter, default value=1,2 indicating horizontal and vertical resistivities;
- `minpar`: the minimum values for the physical parameters;

- `maxpar`: the maximum values for the physical parameters;
- `gamma1`: strength of 1st order Tikhonov regularization;
- `gamma2`: strength of Total Variational (TV) regularization;

An example job script `run.sh` using the above parameters is listed in the following.

```
#!/bin/bash

export OMP_NUM_THREADS=2
mpirun -n 25 ../bin/main mode=1 \
       freqs=0.25,1,2.75 \
       chsrc=Ex \
       chrec=Ex ,Ey,Hx,Hy \
       nx=100 \
       ny=100 \
       nz=100 \
       dx=200 \
       dy=200 \
       dz=40 \
       ox=-10000 \
       oy=-10000 \
       oz=0 \
       fbathy=fbathy \
       frho11=frho_init \
       frho22=frho_init \
       frho33=frho_init \
       fsrc=sources.txt \
       frec=receivers.txt \
       fsrcrec=src_rec_table.txt \
       niter=30 \
       npar=2 \
       bound=1 \
       idxpar=1,2 \
       minpar=1.0,1.0 \
       maxpar=100.0,100.0 \
       gamma1=100 \
       gamma2=0
```

2 Source-receiver configuration

The locations and orientations for every source/transmitter and receiver are written in a 6-column table. The following is an example of source table `sources.txt` where `x,y,z` are coordinates, `azimuth,dip` are orientations, `iTx` is the index of the transmitter.

```
     x             y             z          azimuth       dip   iTx
-2196.15234   -8196.15234    903.652222   30.0000000      0      1
 401.923828   -6696.15234    870.258484   30.0000000      0      2
```

```
 3000.00000   -5196.15234   834.029785   30.0000000    0      3
 5598.07617   -3696.15234   810.434204   30.0000000    0      4
 8196.15234   -2196.15234   809.226013   30.0000000    0      5
-3696.15234   -5598.07617   865.961426   30.0000000    0      6
-1098.07617   -4098.07617   832.172302   30.0000000    0      7
 1500.00000   -2598.07617   807.180298   30.0000000    0      8
 4098.07617   -1098.07617   802.881104   30.0000000    0      9
 6696.15234    401.923828   821.753967   30.0000000    0     10
 ......
```

The following is an example of receiver table `receivers.txt` where `x,y,z` are coordinates, `azimuth,dip` are orientations, `iRx` is the index of the receiver.

```
     x              y              z        azimuth  dip  iRx
-10000.0000     0.00000000     1000.00000      0      0     1
-9800.00000     0.00000000     1000.00000      0      0     2
-9600.00000     0.00000000     1000.00000      0      0     3
-9400.00000     0.00000000     1000.00000      0      0     4
-9200.00000     0.00000000     1000.00000      0      0     5
-9000.00000     0.00000000     1000.00000      0      0     6
-8800.00000     0.00000000     1000.00000      0      0     7
-8600.00000     0.00000000     1000.00000      0      0     8
-8400.00000     0.00000000     1000.00000      0      0     9
-8200.00000     0.00000000     1000.00000      0      0    10
-8000.00000     0.00000000     1000.00000      0      0    11
-7800.00000     0.00000000     1000.00000      0      0    12
-7600.00000     0.00000000     1000.00000      0      0    13
-7400.00000     0.00000000     1000.00000      0      0    14
-7200.00000     0.00000000     1000.00000      0      0    15
-7000.00000     0.00000000     1000.00000      0      0    16
......
```

The connections between sources and receivers (which receivers record data from which source) must be specified by a source-receiver connection table `src_rec_table.txt` according to the index of the source and receivers.

```
 isrc        irec
   1           1
   1           2
   1           3
   1           4
   1           5
   1           6
   1           7
   1           8
   1           9
   1          10
   ...
   2           1
   2           2
   2           3
```

```
2           4
2           5
2           6
2           7
2           8
2           9
2          10
...
```

3 Output EMF files

The simulated CSEM data are stored in ASCII files. An example EM data file `emf_0001.txt` from source index `0001` includes index of source and receivers (`iTx`, `iRx`), the recording channels of the receiver `chrec`, frequencies in Hz, real and imaginary part of the frequency domain data. They form a 6-column table in the following.

```
iTx  iRx   chrec frequency/Hz    Real{E/H}     Imag{E/H}
1     1      Ex     0.25       -8.794095e-15 2.336085e-14
1     2      Ex     0.25       -8.236141e-15 2.632050e-14
1     3      Ex     0.25       -7.451898e-15 2.954083e-14
1     4      Ex     0.25       -6.390576e-15 3.306965e-14
1     5      Ex     0.25       -4.998464e-15 3.694922e-14
1     6      Ex     0.25       -3.228805e-15 4.118009e-14
1     7      Ex     0.25       -1.026235e-15 4.577336e-14
1     8      Ex     0.25       1.681961e-15 5.075206e-14
1     9      Ex     0.25       4.974577e-15 5.613805e-14
1     10     Ex     0.25       8.933074e-15 6.194364e-14
......
1     1      Ex      1     -1.045790e-12   9.924710e-13
1     2      Ex      1     -1.119678e-12   1.968149e-12
1     3      Ex      1     -8.904390e-13   3.433207e-12
1     4      Ex      1     -1.103422e-13   6.096019e-12
1     5      Ex      1     1.431065e-12   1.066018e-11
1     6      Ex      1     6.458673e-12   2.313294e-11
1     7      Ex      1     2.208377e-11   5.329251e-11
1     8      Ex      1     1.162063e-10   1.498437e-10
1     9      Ex      1     3.530520e-10   3.849713e-10
1     10     Ex      1     -1.178124e-09   6.435691e-10
......
```

4 Convergence information on CSEM inversion

After the 3D inversion, the convergence history of the nonlinear optimization will be stored in an ASCII file named `iterate.txt`.

```
 ============================================================
l-BFGS memory length: 5
Maximum number of iterations: 30
```

```
Convergence tolerance: 1.00e-06
maximum number of line search: 5
initial step length: alpha=1
==========================================================
iter    fk        fk/f0      ||gk||     alpha    nls   ngrad
  0   1.08e+03  1.00e+00  5.30e+00  1.00e+00   0      0
  1   9.16e+02  8.49e-01  4.50e+00  4.00e+00   2      3
  2   6.48e+02  6.01e-01  5.15e+00  2.50e-01   2      6
  3   5.96e+02  5.52e-01  8.72e+00  1.00e+00   0      7
  4   4.35e+02  4.03e-01  4.40e+00  1.00e+00   0      8
  5   3.35e+02  3.11e-01  3.20e+00  1.00e+00   0      9
  6   2.58e+02  2.39e-01  5.29e+00  5.00e-01   1     11
  7   2.09e+02  1.94e-01  3.69e+00  1.00e+00   0     12
  8   1.71e+02  1.58e-01  2.00e+00  1.00e+00   0     13
  9   1.44e+02  1.34e-01  1.53e+00  1.00e+00   0     14
 10   1.23e+02  1.14e-01  2.09e+00  1.00e+00   0     15
 11   1.16e+02  1.07e-01  2.28e+00  1.00e+00   0     16
 12   8.96e+01  8.31e-02  2.02e+00  1.00e+00   0     17
 13   7.71e+01  7.15e-02  1.77e+00  1.00e+00   0     18
 14   6.27e+01  5.82e-02  8.97e-01  1.00e+00   0     19
 15   5.48e+01  5.08e-02  1.11e+00  1.00e+00   0     20
 16   4.93e+01  4.57e-02  7.89e-01  1.00e+00   0     21
 17   4.45e+01  4.13e-02  6.47e-01  1.00e+00   0     22
 18   4.06e+01  3.76e-02  7.92e-01  1.00e+00   0     23
 19   3.69e+01  3.42e-02  6.41e-01  1.00e+00   0     24
 20   3.42e+01  3.17e-02  7.62e-01  1.00e+00   0     25
 21   3.30e+01  3.06e-02  9.15e-01  1.00e+00   0     26
 22   3.01e+01  2.79e-02  6.26e-01  1.00e+00   0     27
 23   2.80e+01  2.60e-02  6.31e-01  1.00e+00   0     28
 24   2.66e+01  2.47e-02  6.19e-01  1.00e+00   0     29
 25   2.60e+01  2.41e-02  7.20e-01  1.00e+00   0     30
 26   2.58e+01  2.40e-02  1.13e+00  1.00e+00   0     31
 27   2.50e+01  2.31e-02  8.96e-01  2.00e+00   1     38
 28   2.44e+01  2.26e-02  8.16e-01  1.00e+00   0     39
 29   2.35e+01  2.18e-02  4.30e-01  1.00e+00   0     40
==>Maximum iteration number reached!
```

In the above example, each columns has clear meaning:

- `iter`: the iteration index k;
- `fk`: the misfit at the k-th iteration;
- `fk/f0`: the normalized misfit at the k-th iteration;
- `||gk||`: the norm of the gradient;
- `alpha`: step length used in line search;
- `nls`: number of line search at the k-th iteration;
- `ngrad`: number of gradient evaluations

5 The Green's function and the reciprocity

Assume only electrical current $J_j(x_s,\omega)=\delta(x-x_s)e_j$ where e_j is the j-directed unit vector. We have

$$\begin{cases}\nabla\times G_{ij}^{E|E}-\mathrm{i}\omega\mu G_{ij}^{H|E} & =0\\ \nabla\times G_{ij}^{H|E}-\sigma G_{ij}^{E|E} & =\delta(x-x_s)e_j\end{cases}, \tag{1}$$

which defines two Green's function $G_{ij}^{E|E}$ and $G_{ij}^{H|E}$: $G_{ij}^{E|E}$ is the ith electrical (E) component of Green's function induced by jth component of electrical (E) source; $G_{ij}^{H|E}$ is the ith magnetic (H) component of Green's function induced by jth component of electrical (E) source. The representation theorem gives

$$E_i=G_{ij}^{E|E}J_j, H_i=G_{ij}^{H|E}J_j. \tag{2}$$

We can do the same assuming only a magnetic source $M_j=\delta(x-x_s)e_j$: $G_{ij}^{E|H}$ is the ith electrical (E) component of Green's function induced by jth component of magnetic (H) source; $G_{ij}^{H|H}$ is the ith magnetic (H) component of Green's function induced by jth component of magnetic (H) source.

$$\begin{cases}\nabla\times G_{ij}^{E|H}-\mathrm{i}\omega\mu G_{ij}^{H|H} & =\delta(x-x_s)e_j\\ \nabla\times G_{ij}^{H|H}-\sigma G_{ij}^{E|H} & =0\end{cases}, \tag{3}$$

which defines another two Green's function $G_{ij}^{E|H}$ and $G_{ij}^{H|H}$. Similar to equation (2), the representation theorem gives

$$E_i=G_{ij}^{E|H}M_j, H_i=G_{ij}^{H|H}M_j. \tag{4}$$

The total electrical and magnetic fields in the coupled system is then the superposition of two contributions:

$$E_i=\sum_j G_{ij}^{E|E}J_j+G_{ij}^{E|H}M_j,\quad H_i=\sum_j G_{ij}^{H|E}J_j+G_{ij}^{H|H}M_j. \tag{5}$$

It is shown that the reciprocity for EM system holds in the following form

$$\begin{cases}G_{ij}^{E|E}(x_s|x_r)=G_{ji}^{E|E}(x_r|x_s),\\ G_{ij}^{H|H}(x_s|x_r)=G_{ji}^{H|H}(x_r|x_s),\\ G_{ij}^{H|E}(x_s|x_r)=-G_{ji}^{E|H}(x_r|x_s).\end{cases} \tag{6}$$

Without magnetic source, we have

$$\underbrace{\begin{bmatrix}E_x\\E_y\\E_z\end{bmatrix}}_{E}=\underbrace{\begin{bmatrix}G_{xx}^{E|E} & G_{xy}^{E|E} & G_{xz}^{E|E}\\ G_{yx}^{E|E} & G_{yy}^{E|E} & G_{yz}^{E|E}\\ G_{zx}^{E|E} & G_{zy}^{E|E} & G_{zz}^{E|E}\end{bmatrix}}_{G^{E|E}}\underbrace{\begin{bmatrix}J_x\\J_y\\J_z\end{bmatrix}}_{J_s},\ \underbrace{\begin{bmatrix}H_x\\H_y\\H_z\end{bmatrix}}_{H}=\underbrace{\begin{bmatrix}G_{xx}^{H|E} & G_{xy}^{H|E} & G_{xz}^{H|E}\\ G_{yx}^{H|E} & G_{yy}^{H|E} & G_{yz}^{H|E}\\ G_{zx}^{H|E} & G_{zy}^{H|E} & G_{zz}^{H|E}\end{bmatrix}}_{G^{H|E}}\underbrace{\begin{bmatrix}J_x\\J_y\\J_z\end{bmatrix}}_{J_s}. \tag{7}$$

If $J_s|_{x=x_s} = (1,0,0)^{\mathrm{T}}$, we have the 1st column of the matrix $G^{E|E}$ and $G^{H|E}$ extracted from vector fields E and H

$$\begin{bmatrix} E_x(x_r) \\ E_y(x_r) \\ E_z(x_r) \end{bmatrix} = \begin{bmatrix} G^{E|E}_{xx}(x_r|x_s) \\ G^{E|E}_{yx}(x_r|x_s) \\ G^{E|E}_{zx}(x_r|x_s) \end{bmatrix} = \begin{bmatrix} G^{E|E}_{xx}(x_s|x_r) \\ G^{E|E}_{xy}(x_s|x_r) \\ G^{E|E}_{xz}(x_s|x_r) \end{bmatrix}, \tag{8a}$$

$$\begin{bmatrix} H_x(x_r) \\ H_y(x_r) \\ H_z(x_r) \end{bmatrix} = \begin{bmatrix} G^{H|E}_{xx}(x_r|x_s) \\ G^{H|E}_{yx}(x_r|x_s) \\ G^{H|E}_{zx}(x_r|x_s) \end{bmatrix} = -\begin{bmatrix} G^{E|H}_{xx}(x_s|x_r) \\ G^{E|H}_{xy}(x_s|x_r) \\ G^{E|H}_{xz}(x_s|x_r) \end{bmatrix}, \tag{8b}$$

where the last equality comes from the reciprocity in (6). It implies that by switching the source and receiver position, we can reproduce the E_x, E_y and E_z response from the E_x-channel of the receiver at source position by repeating the modeling using the electrical sources at receiver location, i.e., $J_s|_{x=x_r} = (1,0,0)^{\mathrm{T}}$, $J_s|_{x=x_r} = (0,1,0)^{\mathrm{T}}$ and $J_s|_{x=x_r} = (0,0,1)^{\mathrm{T}}$. Similarly, we should reproduce $-H_x$, $-H_y$ and $-H_z$ response from the E_x-channel of the receiver at source position by repeating the modeling using the magnetic sources at receiver location, i.e., $M_s|_{x=x_r} = (1,0,0)^{\mathrm{T}}$, $M_s|_{x=x_r} = (0,1,0)^{\mathrm{T}}$ and $M_s|_{x=x_r} = (0,0,1)^{\mathrm{T}}$.

If $J_s|_{x=x_s} = (0,1,0)^{\mathrm{T}}$, we have the 2nd column of the matrix $G^{E|E}$ and $G^{H|E}$ extracted from vector fields E and H

$$\begin{bmatrix} E_x(x_r) \\ E_y(x_r) \\ E_z(x_r) \end{bmatrix} = \begin{bmatrix} G^{E|E}_{xy}(x_r|x_s) \\ G^{E|E}_{yy}(x_r|x_s) \\ G^{E|E}_{zy}(x_r|x_s) \end{bmatrix} = \begin{bmatrix} G^{E|E}_{yx}(x_s|x_r) \\ G^{E|E}_{yy}(x_s|x_r) \\ G^{E|E}_{yz}(x_s|x_r) \end{bmatrix}, \tag{9a}$$

$$\begin{bmatrix} H_x(x_r) \\ H_y(x_r) \\ H_z(x_r) \end{bmatrix} = \begin{bmatrix} G^{H|E}_{xy}(x_r|x_s) \\ G^{H|E}_{yy}(x_r|x_s) \\ G^{H|E}_{zy}(x_r|x_s) \end{bmatrix} = -\begin{bmatrix} G^{E|H}_{yx}(x_s|x_r) \\ G^{E|H}_{yy}(x_s|x_r) \\ G^{E|H}_{yz}(x_s|x_r) \end{bmatrix}. \tag{9b}$$

By switching the source and receiver position, we obtain the E_x, E_y and E_z response from the E_y-channel of the receiver at source position by repeating the modeling placing the sources at receiver location, i.e., $J_s|_{x=x_r} = (1,0,0)^{\mathrm{T}}$, $J_s|_{x=x_r} = (0,1,0)^{\mathrm{T}}$ and $J_s|_{x=x_r} = (0,0,1)^{\mathrm{T}}$. Also, we obtain $-H_x$, $-H_y$ and $-H_z$ response from the E_y-channel of the receiver at source position by repeating the modeling placing the magnetic sources at receiver location, i.e., $M_s|_{x=x_r} = (1,0,0)^{\mathrm{T}}$, $M_s|_{x=x_r} = (0,1,0)^{\mathrm{T}}$ and $M_s|_{x=x_r} = (0,0,1)^{\mathrm{T}}$.