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;
- `istretch`: `istretch=1`, nonuniform grid stretching; `istretch=0`, no grid stretching;
- `addair`: `addair=1`, add air layers on top of input model; `addair=0`, extending the model using topmost value without adding air layers;
- `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*z` 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 \
       istretch=0 \
       addair=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

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

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

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

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

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

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 $M_s|_{x=x_r} = (0,0,1)^{\mathrm{T}}$.