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Comparing local minimizers for fitting neutron and muon data with the Mantid framework

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Overview and aim

We present a comparison of local minimizers for fitting a variety of datasets using the Mantid[1] framework. As well as mathematical test problems, tests have been performed using real neutron data. A new, flexible Trust Region[4] minimizer has been incorporated into Mantid, and is included in the test results.

The most used algorithm in Mantid is 'Fit' and the primary aim of this work is to improve this algorithm and thereby fitting in Mantid. Further, this framework for objectively comparing minimizers can be used by anyone to compare any new minimizer against the already compared minimizers. Currently, the best bet for a candidate to beat the default minimizer in Mantid is a new Trust Region minimizer. Also, as the neutron test suite is extended it may reveal certain best minimizers for sub-set of neutron fitting problems.

Background

Fitting is a core functionality in neutron, muon and x-ray data reduction and analysis software packages. It is required in tasks as diverse as instrument calibration, refinement of structures, and various data analysis methods specific to different scientific techniques.

One such software is the Mantid software[1]: an extensible framework that supports high-performance computing for data manipulation and visualisation of scientific data. It is used at several neutron and muon facilities worldwide.

The Mantid fitting system offers the flexibility to add and combine different functions, minimizers, constraints, and cost functions as plug-ins. Users can apply different combinations of these elements either via scripting or graphical user interfaces.

Minimizers

When fitting a function to experimental or simulated data, the minimizer is the method that adjusts the function parameters so that the model fits the data as closely as possible. The concept of how close a fit is to the data is defined by the cost function. Several local minimizers are supported in Mantid (as in other software packages used in the neutron, muon and x-rays community). However, there is a lack of openly available comparisons between them.

Trust region minimizer

A new Trust region minimizer has been developed at RAL[4], and preliminary results are included in the comparisons here. At each iteration, it calculates and returns the step that reduces the cost function by an acceptable amount by solving, or approximating a solution to, the trust-region subproblem.

Neutron and other datasets

As well as the NIST[5] and CUTEst[6] datasets, we present preliminary results for neutron data from different instruments at the ISIS facility. These datasets have observational errors, unlike the NIST and CUTEst problems and so, for a fair comparison, we present two sets of results:

1) Unweighted (no errors)

2) Weighted least squares, using real errors for neutron data and simulated errors (square root of y) for other datasets

Comparison

For each test problem, the best possible results are given a score of 1. The relative score of a minimizer is the ratio between its performance and the performance of the best. We compare accuracy (sum of squared fitting errors) and run time. For example, a ranking of 1.25 for a given problem means:

- (for accuracy) The minimizer produced a solution with squared residuals 25% larger than the best solution in Mantid.
- (for run time) The minimizer took 25% more time than the fastest minimizer.

The color coding used is shown on the right.

- best or within 10% (ranking < 1.1)
- within 33% over the best (1.1 < ranking < 1.33)
- within 75% over the best (1.33 < ranking < 1.75)
- within 200% over the best (1.75 < ranking < 3)
- over 200% of best (ranking > 3)

Nonlinear regression benchmarks

Unweighted data

	BFGS	Conjugate gradient (Fletcher-Reeves imp.)	Conjugate gradient (Polak-Ribiere imp.)	Damping	Levenberg-Marquardt	Levenberg-MarquardtMD	Simplex	SteepestDescent	Trust Region
NIST, "lower" difficulty	3.841	3.003	3.003	1	1	1	1.017	6.436	1
NIST, "average" difficulty	269	22.35	22.5	1	1	1	79.31	315.9	1
NIST, "higher" difficulty	63.63	10.82	8.366	1.847	1	1	18.55	114.7	1
CUTEst	146.1	17.22	18.89	1.803e+05	2.911	1.801e+05	96.61	230.3	1
Neutron data	1.478	1.459	1.538	1	1	1	2.334	3.546	1

Median accuracy, unweighted.

	BFGS	Conjugate gradient (Fletcher-Reeves imp.)	Conjugate gradient (Polak-Ribiere imp.)	Damping	Levenberg-Marquardt	Levenberg-MarquardtMD	Simplex	SteepestDescent	Trust Region
MGH09 1	7.705	25.02	25.02	1.817e+04	3.342	1	20.62	24.19	3.347
MGH09 2	1.62	1.621	1.62	259.8	1	1	1.025	1.604	1
Thurber 1	228.3	175.3	173.2	2.693	1	1	370.9	177.2	1
Thurber 2	422.3	20.02	40.38	1	1	1	4.43	388.8	1
BoxBOD 1	8.388	8.388	8.388	nan	8.388	1	8.388	1.515	8.388
BoxBOD 2	33.46	8.388	8.388	1	1	1	8.388	8.377	1
Rat42 1	13.33	13.27	13.27	4.759e+06	1	1	36.48	193.6	1
Rat42 2	1.331	1.213	1.302	1	1	1	1.429	1.449	1
MGH10 1	8.387e+05	8.382e+05	8.344e+05	2.384e+47	1	3.306e+05	8.422e+05	8.37e+05	8.271e+05
MGH10 2	7.834e+04	1275	1275	2.627e+51	1.92	79.78	8.385e+04	7.834e+04	1
Eckerle4 1	478.1	478.1	478.1	368	1	1	478.1	478.1	340.6
Eckerle4 2	31.01	1.02	1.026	1	1	1	1	1.003	1
Rat43 1	93.81	2.441	2.44	nan	2.717	2.393	122.3	52.15	1
Rat43 2	1.07	1.001	1	1	1	1	1	1.001	1
Bennett5 1	1294	848.7	1.028	1	1	1	1048	1307	1
Bennett5 2	880.3	3.347	1.165	1	1	1.065	1372	888.8	1

Accuracy (median). NIST "higher difficulty" problems. Unweighted.

	BFGS	Conjugate gradient (Fletcher-Reeves imp.)	Conjugate gradient (Polak-Ribiere imp.)	Damping	Levenberg-Marquardt	Levenberg-MarquardtMD	Simplex	SteepestDescent	Trust Region
ENGINX 193749 calibration, spectrum 651, peak 19	1.047	1.047	1.047	2.532e+09	1	1.024	1.045	1.399	1.001
ENGINX 193749 calibration, spectrum 651, peak 20	1.478	1.459	1.469	nan	1	1.48	1.457	6.097	1
ENGINX 193749 calibration, spectrum 651, peak 23	1.079	1.096	1.064	nan	1.146	1.089	1.055	11.52	1
ENGINX 193749 calibration, spectrum 651, peak 5	1.286	1.225	1.224	2.34	1	1.003	1.204	1.454	1
ENGINX 193749 calibration, spectrum 651, peak 6	1.047	1.004	1.005	nan	1.094	1.222	1	1.481	1.093
ENGINX 236516 vanadium, bank 1, 10 brk	1	1	1	1.138	1	1.138	1.023	1	1
ENGINX 236516 vanadium, bank 1, 30 brk	1	1	1	1.138	1	1.138	1.106	1	1

Accuracy (median). Some neutron data test problems. Unweighted.

Weighted with observational errors

	BFGS	Conjugate gradient (Fletcher-Reeves imp.)	Conjugate gradient (Polak-Ribiere imp.)	Damping	Levenberg-Marquardt	Levenberg-MarquardtMD	Simplex	SteepestDescent	Trust Region
NIST, "lower" difficulty	4.051	3.009	3.009	1	1	1	1.001	6.453	1
NIST, "average" difficulty	215.2	27.14	25.43	1.001	1	1	15.12	203.2	1
NIST, "higher" difficulty	26.92	11.91	5.804	1.005	1	1.006	6.393	40.18	1.001
CUTEst	36.53	10.1	9.345	1.579e+05	2.464	5315	14.31	58.03	1
Neutron data	1.667	1.566	1.643	1	1	1	2.334	3.546	1

Median accuracy, weighted with observational errors.

	BFGS	Conjugate gradient (Fletcher-Reeves imp.)	Conjugate gradient (Polak-Ribiere imp.)	Damping	Levenberg-Marquardt	Levenberg-MarquardtMD	Simplex	SteepestDescent	Trust Region
MGH09 1	16.11	52.98	52.98	330.1	2.947	1	7.01	40.53	2.948
MGH09 2	1.807	1.181	1	4.186	1.063	1.063	1.182	1.718	1.063
Thurber 1	1.359	1.49	1	18.14	6.775	6.787	5.695	1.946	6.77
Thurber 2	2.689	1.419	1.446	1	1.001	1.003	2.293	2.572	1.001
BoxBOD 1	2.968	2.968	2.968	nan	2.968	2.968	2.968	1	2.968
BoxBOD 2	22.01	8.641	8.641	1	1	1	8.641	8.302	1
Rat42 1	152.7	16.17	15.24	1	1	1	14.83	207.2	1
Rat42 2	1.301	1.289	1.044	1	1	1	1.448	1.422	1
MGH10 1	6.234e+05	6.282e+05	6.215e+05	9.058e+49	1	5.268e+05	6.482e+05	6.282e+05	6.097e+05
MGH10 2	6.219e+04	1308	1308	nan	3.109	147.2	6.406e+04	6.091e+04	1
Eckerle4 1	478	480.5	480.5	478	1	1	478	480.5	340.7
Eckerle4 2	30.92	33.83	33.83	1	1	1	1.001	33.83	1
Rat43 1	251.4	178.7	83.69	nan	1	2.938	1	242.8	1
Rat43 2	1.071	1.006	1.006	1.01	1.01	1.01	1.01	1	1.01
Bennett5 1	1334	560.4	1.028	nan	1	1	1919	1338	1
Bennett5 2	713.7	6.524	2.247	1	1	1.062	1573	706	1

Accuracy (median). NIST "higher difficulty" problems. Weighted with observational errors.

	BFGS	Conjugate gradient (Fletcher-Reeves imp.)	Conjugate gradient (Polak-Ribiere imp.)	Damping	Levenberg-Marquardt	Levenberg-MarquardtMD	Simplex	SteepestDescent	Trust Region
ENGINX 193749 calibration, spectrum 651, peak 19	1	1.015	1.058	nan	1.143	1.064	1.168	1.381	1.139
ENGINX 193749 calibration, spectrum 651, peak 20	1.813	1.735	1.725	nan	1	1.808	1.216	6.004	1.001
ENGINX 193749 calibration, spectrum 651, peak 23	3.102	2.989	2.923	nan	1	3.267	2.064	21.55	3.245
ENGINX 193749 calibration, spectrum 651, peak 5	1.057	1.077	1.077	nan	1.137	1.222	1.353	1	1.145
ENGINX 193749 calibration, spectrum 651, peak 6	1.136	1.021	1.141	nan	1.016	1.051	1	1.132	1.016
ENGINX 236516 vanadium, bank 1, 10 brk	1	1	1	1.138	1	1.138	1.038	1.02	1
ENGINX 236516 vanadium, bank 1, 30 brk	1	1	1	1.138	1	1.138	1.113	1.03	1

Accuracy (median). Some neutron data test problems. Weighted.

Run time

	BFGS	Conjugate gradient (Fletcher-Reeves imp.)	Conjugate gradient (Polak-Ribiere imp.)	Damping	Levenberg-Marquardt	Levenberg-MarquardtMD	Simplex	SteepestDescent	Trust Region
NIST, "lower" difficulty	2.124	1.433	1.394	1.012	1.122	1.033	1.341	6.688	4.887
NIST, "average" difficulty	1.86	6.458	6.555	1	1.115	1.117	1.824	8.851	1.979
NIST, "higher" difficulty	1.801	1.631	1.728	1.161	1.075	1.163	1.125	3.639	1.708
CUTEst	3.507	20.9	17.72	1	2.47	1.035	1.975	18.84	29.54
Neutron data	4.351	6.014	5.976	1	1.254	1.144	1.576	15.47	1.669

Median run-time Unweighted

Future

We plan to extend the comparison with more test problems from neutron and muon data, considering different science areas. Furthermore, on the basis of our comparisons, we intend to further develop and characterize the new, flexible Trust region minimizer, RAL-NLLS, whose aim is to improve the reliability and broaden the functionality of the Mantid fitting system.

References

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