Derivative-free optimization (DFO)

Final Report, May 2024

The project started June 16, 2021 and ended December 31, 2023.

The project web page at the URL
$$\texttt{https://arnold-neumaier.at/DFO.html}$$
contains the results obtained during the project, together with links to the papers, preprints and software created.

Researchers supported. Supported by the budget were:

• Dr. Morteza Kimiaei from June 2021 until June 2023 (full time),

• The master students Roman Kostal and Maximilian Stollmayer from August 2021 until February 2022 (both 15 hours/week).

• Mag. Romana Ježek from June 2022 until June 2023 (20 hours/week).

Changes compared to the project application. Compared to the original plans in the project application, the project moved in a slightly different direction. The strategy language approach for combining solvers has been discarded due to the difficulty of bringing all solvers into a compatible module structure. Instead, we opted

• for incorporating the key functionality of other solvers into our own solvers (which we achieved except for the case of nonlinear constraints, which remains as future work),

• and for working towards a flexible tuning environment that allows to tune each solver separately (where we ran out of time and currently only have a preliminary version not yet ready for distribution).

Algorithms designed. We designed several new algorithms for noisy derivative-free optimization under various conditions:
• noiseless unconstrained [14],
• noisy unconstrained [1, 3, 8],
• unconstrained matrix evolution strategy for problems with very large noise [10],
• linearly constrained [12],
• integer bound-constrained [9],
• mixed integer bound-constrained [11],
• subspace methods for nonlinear systems [4] and nonlinear least squares [7].

We also upgraded several of our other optimization algorithms [2, 13, 15, 17, 18].

Software designed. We designed

• a software package `TTSopt` for testing and tuning optimization software [6]. The package has several consistently interacting parts whose details and interplay are still under development:

• `TEsolv`, a package with wrappers for 53 derivative-free solvers for unconstrained, bound-constrained, and general constrained optimization problems, with or without discrete constraints. This includes our own solvers VRBBO, VRDFON, SSDFO, IMATRS, MATRS, MADFO developed or upgraded during the project, and described below.

• `TEprob`, a package with interfaces for 18 well-known collections of optimization problems with continuous, integer, and mixed-integer variables and various kinds of constraints.

• `TEnvOpt` [5], a testing environment for comparing a configurable set of solvers on a configurable set of test problems, producing automatically a graphical and tabular result analysis.

• `TUopt`, a tuning environment for the optimal selection of tuning parameters of a solver, using a new machine learning based tuning strategy [16].

• In the final stage, the tuning environment will allow for a fairly complex structure of the tuning parameters, including categorical parameters and case-dependent dimensionality.

All our solvers were tested and tuned to ensure being competitive with the best noncommercial solvers available, or even better. Some of our solvers exist in a reentrant version that allows the solution of optimization problems where function values may be computed by software on different platforms or measured by performing experiments or external simulations, with communication through file updates.

Improving the `TTSopt` package (which is the union of the above four packages) and the tuning and benchmarking of competitive solvers will continue after the end of the project.

• We also designed a much improved Goldstein line search [17] and applied it first to a new conjugate gradient method [18] and a bound-constrained solver [15] for noiseless optimization.

Software available. The following derivative-free solvers for various kinds of optimization problems were finished or upgraded during the project, and are publicly available.

VRBBO: Vienna Randomized Black Box Optimization (unconstrained)
`https://zenodo.org/records/5648165#.YaZKRCYo_xg`

VRDFON: Vienna Randomized Noisy Derivative-Free Optimization (unconstrained)
`https://github.com/GS1400/VRDFON`

SSDFO: Subspace Derivative-Free Optimization (unconstrained)
`https://github.com/GS1400/SSDFO`

IMATRS: Matrix Adaptation Trust Region Derivative-Free Optimization (pure-integer bound-constrained)
`https://github.com/GS1400/IMATRS`

MATRS: Matrix Adaptation Trust Region Derivative-Free Optimization (mixed-integer bound-constrained)
`https://github.com/GS1400/MATRS`

MADFO: Matrix Adaptation Derivative-Free Optimization (unconstrained)
`https://github.com/GS1400/MADFO`

In addition, we made the software package

TEnvOpt: Test Environment for Optimization
`https://github.com/Computational-Mathematics-Vienna/TEnvOpt`

available, which contains our test environment together with the solver collection `TEsolv` and the problem collection `TEprob`. This release, however, does not yet contain the automatic tuning facilities that are still under development.

References

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