Stanford University, Management Science and Engineering (and ICME)

CME 338 Large-Scale Numerical Optimization

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Homework 1, Due Wednesday April 17

`http://stanford.edu/class/cme338/homework.html`

NEOS (`https://neos-server.org/neos/`) is a free service developed originally at Argonne National Laboratory and now hosted by the University of Wisconsin, Madison. It allows us to submit optimization problems in various formats (AMPL, GAMS, CPLEX, MPS, C, Fortran, ...) to be solved remotely on geographically distributed machines by a range of solvers.

It will be worthwhile for everyone to learn about submitting an optimization problem to NEOS. Homework 1 involves one of the multiscale systems biology LP problems stored here in MPS format as zip files: `http://stanford.edu/group/SOL/multiscale/models/quadLP/MPS/`.

1. Download data file `TMA_ME.zip` (a model of *Thermotoga maritima Metabolism and macromolecular Expression*). From [1], the optimal objective value should be 8.7036315385e-07 (but double-precision solvers are unlikely to obtain this value).

2. Submit `TMA_ME` to NEOS specifying the SoPlex80bit solver with default parameters. Use `TMA_ME.zip` itself (no need to unzip) and no parameters file. Summarize the results you obtain.

3. One parameter has default value `bool:lifting = false`. Run the same problem and solver with a parameter file specifying `bool:lifting = true`. Describe any difference you see in solver performance.

Notes

SoPlex80bit is run on a server at Arizona State University. Apparently certain default parameter values are specified here:

`http://plato.asu.edu/soplex/default.set`

although that's different from the official set of parameters here:

`http://soplex.zib.de/doc/html/PARSLIST.php`

For SoPlex80bit, the NEOS submission form chooses Parsing mode "rational/integer" and Solving mode "exact with rational factorization", which probably correspond to options

```
int:readmode = 1
int:solvemode = 1
```

Please specify `0` in your parameter file to get floating-point for both options.

There are rather many parameters! Don't worry about their meaning at this stage; just know that typical optimization solvers allow users to specify certain options that might be helpful for any particular problem. Most parameters have sensible values by default, and it's best to experiment with them just one at a time.

Multiscale problems cause difficulty for solvers because of large entries in the constraint matrix. Solvers are likely to scale the data and solve the scaled problem reasonably well, but when they unscale the solution, certain residuals are magnified and the solution may no longer satisfy the feasibility and optimality tests.

Reference [2] applies the concept of "lifting" to the biology problems. Extra variables and constraints are added to obtain an equivalent problem that has fewer large entries in the constraint matrix. Ideally, less damage will be done to the solution when it is unscaled.

Reference [1] describes a more reliable procedure for solving the biology models (and other challenging problems) using both double-precision and quadruple-precision versions of MINOS.

References

[1] D. Ma, L. Yang, R. M. T. Fleming, I. Thiele, B. O. Palsson, and M. A. Saunders. Reliable and efficient solution of genome-scale models of Metabolism and macromolecular Expression. *Sci. Rep.*, 7, Article number: 40863, http://rdcu.be/oCpn, 2017.

[2] Y. Sun, R. M. T. Fleming, I. Thiele, and M. A. Saunders. Robust flux balance analysis of multiscale biochemical reaction networks. *BMC Bioinformatics*, 14(240), 2013.