FORTRAN IMPLEMENTATION OF QNSTOP FOR GLOBAL AND STOCHASTIC OPTIMIZATION.

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INTRO: REAL-WORLD MODELING

- Computers are used to model complex systems in domains such as biology, physics, and neuroscience.
- Real-world phenomena may have random, or **stochastic**, elements that need to be included in the model.
- Finding optimal parameters to these models provides further insight into the problems.
- For example, when designing an airplane, there are many design alternatives resulting in different performances and costs, and **design process optimization** helps minimize cost and maximize performance.

STOCHASTIC OPTIMIZATION

- These models can be represented as a mathematical **function** with which a **minimum or maximum** value needs to be found.
- These functions can contain hundreds or thousands of input values and take minutes to reach a final outcome, a single value, and therefore, solving these functions **analytically** can be infeasible.
- Random sampling to find the optimal value is infeasible because the set of feasible values can take years to exhaust.
- **Optimization** algorithms are used to approximate a function's minimum value.
- **QNSTOP** (quasi-Newton Methods for Stochastic Optimization) is a new algorithm under development to help optimize functions with stochastic elements.

QUASI-NEWTON METHODS

quasi-Newton Methods

- **Newton** methods find zeros of a function using derivative information.
- **quasi-Newton** methods estimate derivative information rather than requiring the user to provide derivative information.
- Complex computer models and simulations are difficult to obtain derivative information from, and quasi-Newton methods provide a reasonable estimate.

QNSTOP MOTIVATION

- There are many existing approaches to stochastic optimization. 2 iterative methods are:
  - **Stochastic approximation (SA).** Large numbers of crude, inexpensive iterations. Linear approximations of the function constructed by coarse finite differencing.
  - **Response surface methodology (RSM).** Small numbers of carefully planned, expensive iterations. Linear and quadratic approximations of the function constructed by regression experiments.
- QNSTOP is proposed in Brent Castle's PhD dissertation at Indiana University in 2012 and combines ideas from SA and RSM.

THE QNSTOP ALGORITHM

- Provides **global** and **stochastic** modes.

Global optimization in each iteration k.

- Update design and trust region radius τ_k
- In each iteration $k \geq 0$, QNSTOP samples N points from an experimental design region (ellipsoid) E_k in $\mathbb{R}^p$ centered at ξ_k with radius τ_k.
- Obtain a semilocal quadratic approximation

$$\hat{m}_k(X-\xi_k) = \hat{f}_k + \hat{g}_k^T(X-\xi_k) + (1/2)(X-\xi_k)^T\hat{H}_k(X-\xi_k)$$

of the objective function $f : \mathbb{R}^p \to \mathbb{R}$, where $\hat{g}$ and $\hat{H}$ are the approximations to the gradient and Hessian. $\hat{H}$ is obtained using the BFGS method

$$\hat{H}_k = \hat{H}_{k-1} + \frac{\nu_k\nu_k^T}{\nu_k^T s_k} - \frac{\hat{H}_{k-1}s_k s_k^T H_{k-1}}{s_k^T\hat{H}_{k-1}s_k},$$

where $\nu_k = \hat{g}_k - \hat{g}_{k-1}$ and $s_k = \xi_k - \xi_{k-1}$.
- Calculate the Lagrange multiplier of the trust region subproblem μ_k by solving $[\hat{H}_k + \mu_k W_k]s_k = -\hat{g}_k$, where W_k is the scaling matrix.
- Update the ellipsoid center

$$\xi_{k+1} = \left(\xi_k - \left[\hat{H}_k + \mu_k W_k\right]^{-1}\hat{g}_k\right)_{\Theta},$$

where $\Theta \subset \mathbb{R}^p$ is the feasible set.
- Update the scaling matrix

$$W_{k+1} = \left(\hat{H}_k + \mu_k W_k\right)^T \tilde{V}_k^{-1}\left(\hat{H}_k + \mu_k W_k\right)$$

and design ellipsoid with

$$E_{k+1}(\chi_{p,1-\alpha}) = \{X \in \mathbb{R}^p : (X-\xi_{k+1})^T W_{k+1}(X-\xi_{k+1}) \leq \chi^2_{p,1-\alpha}\}$$

Stochastic optimization.

- Similar structure to global optimization.
- Use different updates for τ_k, $\hat{H}_k$, and μ_k better suited to stochastic optimization.

CONTRIBUTIONS

Fortran implementation.

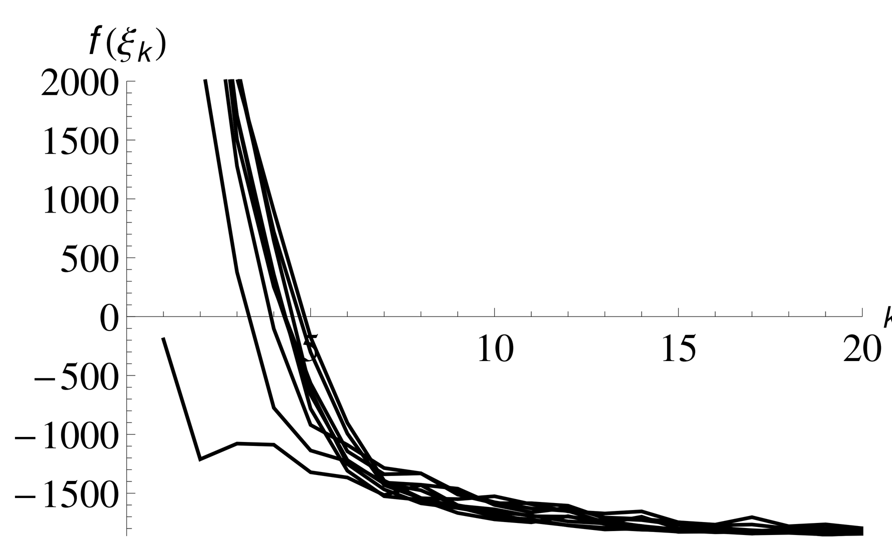
- Matlab was well-suited for prototyping, but is not as suitable for high-end computing as Fortran.
- Modern state of the art mathematical software and real-world models are still implemented in Fortran.
- Fortran is faster and uses less resources than Matlab.
- Fortran provides robust parallelization environments: OpenMP and MPI.

QUADRATIC DUAL FUNCTION

- Nonconvex and nonsmooth 57-dimensional unconstrained minimization problem.
- Exact solution of -1866.01.
- Objective function has the form

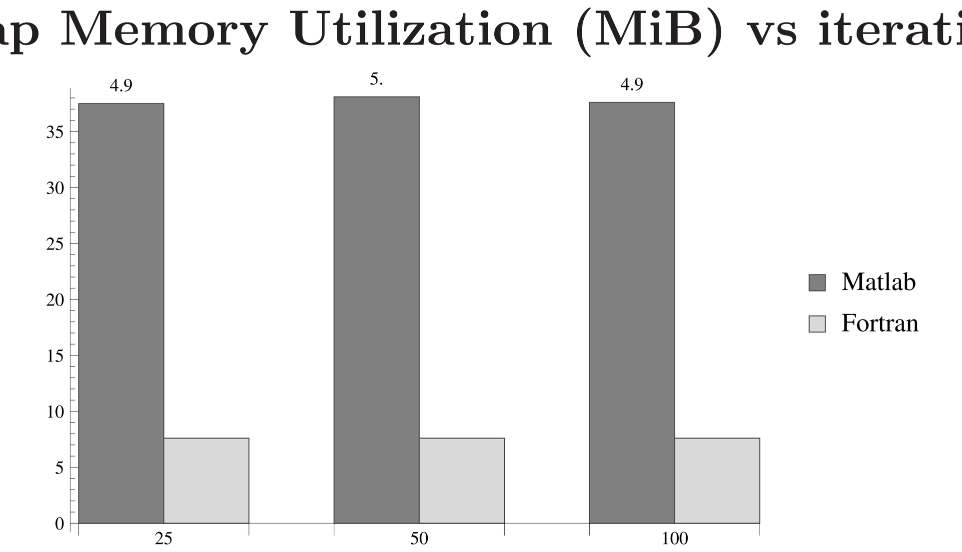
$$\mathcal{Q}(\sigma) = \frac{1}{2}\sigma^T\sigma - \sum_{i=1}^{n}|f_i + (B^T\sigma)_i|,$$

where σ, B, and f are defined in [1].
- Plot shows the best value QNSTOP finds $f(\xi_k)$ in each iteration k.

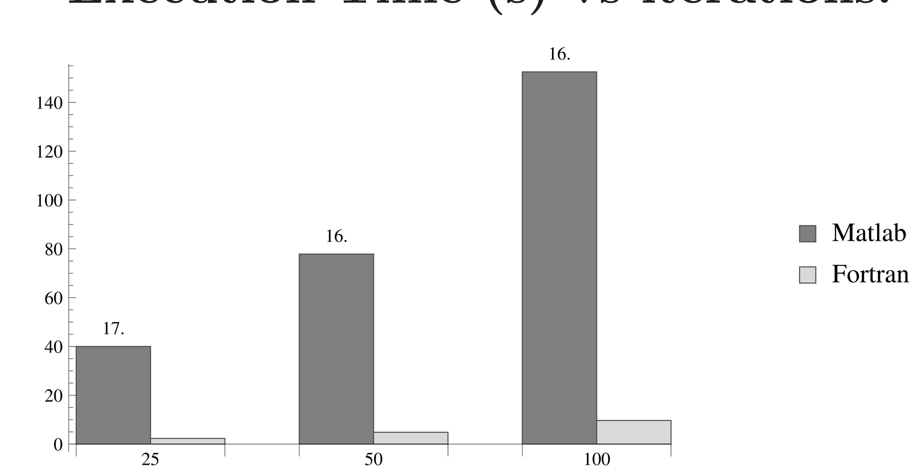


PERFORMANCE SPEEDUPS

Heap Memory Utilization (MiB) vs iterations.



Execution Time (s) vs iterations.

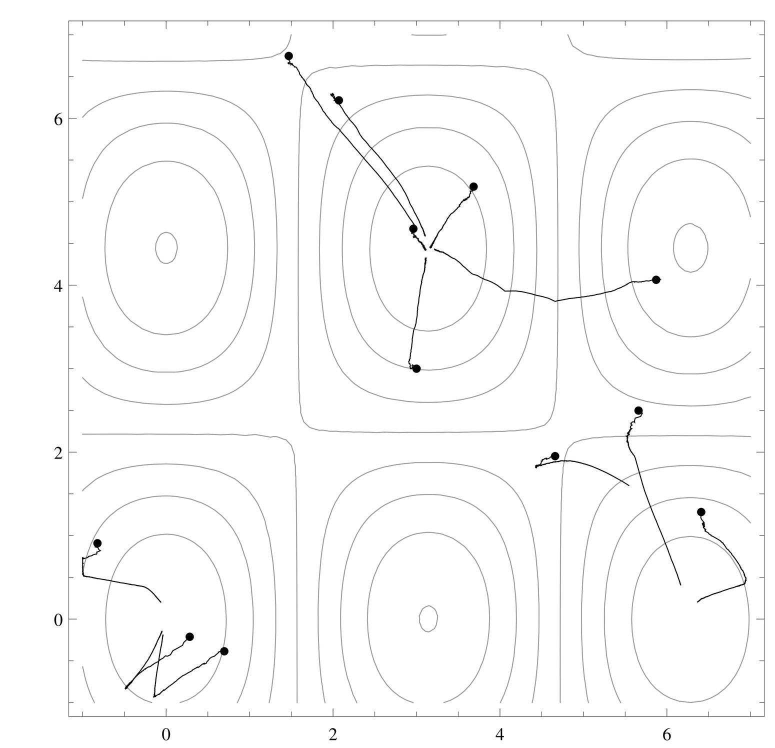


GRIEWANK TEST FUNCTION

- The Griewank function is used to test optimization algorithms and is defined by

$$f(c) = 1 + \sum_{i=1}^{p}\frac{c_i^2}{d} - \prod_{i=1}^{p}\cos\left(\frac{c_i}{\sqrt{i}}\right),$$

for $d > 0$. A contour plot is shown below.
- Global minimum: $f(0) = 0$.
- Plot shows the points sampled by QNSTOP from a Latin hypercube as dots and the lines show QNSTOP progression in each iteration.



PUBLICATIONS

1. "*Fortran 95 implementation of QNSTOP for global and stochastic optimization.*"
   B. Amos, D. Easterling, L. Watson, B. Castle, M. Trosset, W. Thacker.
   SpringSim'14 High Performance Computing Symposium. Tampa, Florida, USA, April 2014.
2. "*Global Parameter Estimation for a Eukaryotic Cell Cycle Model in Systems Biology.*"
   T. Andrew, **B. Amos**, D. Easterling, C. Oguz, W. Baumann, J. Tyson, L. Watson. Submitted.
3. "*Estimating parameters for spatial pooling within the WalnutiQ neocortex model.*"
   B. Amos, Q. Liu. In preparation.