Rapid Optimization Library: A Preview



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Rapid Optimization Library





Purpose

- Optimization of differentiable simulated processes:

- partial differential equations (PDEs)
- differential algebraic equations (DAEs)
- network equations (gas networks, electrical networks)
- Inverse problems, optimal design and control problems.
- The parameter/design/control spaces can be very large, often related to the size of the computational mesh (PDEs) or the size of the device network or graph (DAEs).

⇒ Matrix-free, gradient-based, embedded methods.





History

- **ROL** started as a special-purpose effort in 2009: Delivering unconstrained optimization algorithms for PDE-constrained optimization to a few customers.
- Parallel development: **PEOpt** by Joe Young.
 - An experimental platform for a variety of optimization algorithms and utilities: unconstrained, equality-constrained, inequality-constrained optimization; checkpointing and restarting; consistency checks for derivatives, symmetry, etc.
 - Open source, not in Trilinos, available upon request.
- **ROL** is a Trilinos package for gradient-based matrix-free optimization with focus on uniform yet flexible interfaces, robustness and close-to-optimal efficiency.







- **ROL** is currently in preCopyrightTrilinos.
- Will supersede most of Aristos, MOOCHO and Optipack.
- Will include all of **PEOpt** functionality.
- Additionally focused on: inexact objective functions, inexact gradients, adaptive models, optimization under uncertainty.





Infrastructure

- User specifies linear algebra through a vector class: plus, scale, dot, norm, clone, axpy, zero, basis.
- Algorithm: Combines Step and StatusTest.
- Globalization performed at the Step level: LineSearchStep, TrustRegionStep.
- Efficient computations, restarts and checkpointing enabled through AlgorithmState and StepState.
- Minimal functional interface. For instance, Objective class: value, gradient, hessVec, invHessVec, dirDeriv.





Basic methods

• Unconstrained optimization:

Gradient descent, quasi-Newton (secant) methods, nonlinear CG, Gauss-Newton, Newton, with line-search and trust-region globalizations.

• Equality constraints:

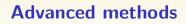
Sequential quadratic programming (SQP), with line-search and trust-region globalizations.

• Inequality constraints:

For box constraints, use projected gradient and projected Newton methods. For general inequalities, use interior-point algorithms.







- All trust-region based algorithms will take advantage of inexact objective functions and inexact gradients.
- The inexactness framework enabless (computationally feasible) large-scale *optimization under uncertainty*: Stochastic programming meets matrix-free gradient-based optimization.
- Later in 2014, subpackage for optimization under uncertainty.











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