Recent Advances in EAGO: Global and Robust Optimization in Julia

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Process Systems and Operations Research Laboratory

UCONN SCHOOL OF ENGINEERING

Outline

Introduction to EAGO

- Motivation
- EAGO Optimization
- EAGO Toolkit

Algorithm Development

- Main Algorithm
- Relaxations
- Domain Reduction

Motivation

- We often model systems in terms of simulations.
- The resulting optimization problems are complex (nonsmooth, nonconvex).
- In development, we want to do things other than optimize.

Simulation

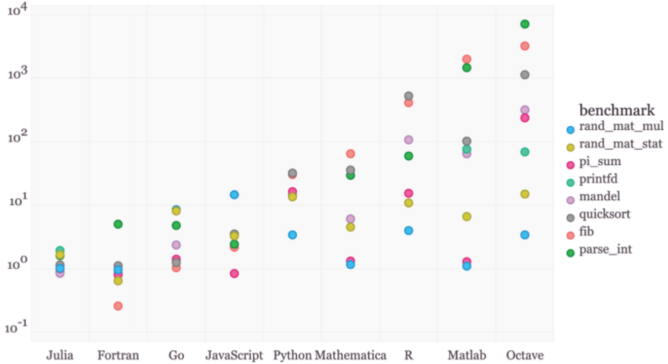
A large literature has developed around optimizing simulations. Can we provide enough flexibility to address these specialized forms?

No Barrier to Entry

Can we make a fast global solver that works like fmincon but provides strong guarantees?

The Julia Language

- Speed of C/Fortran
- Distributed Computing & Parallelism
- Extensive Compile Time Optimization



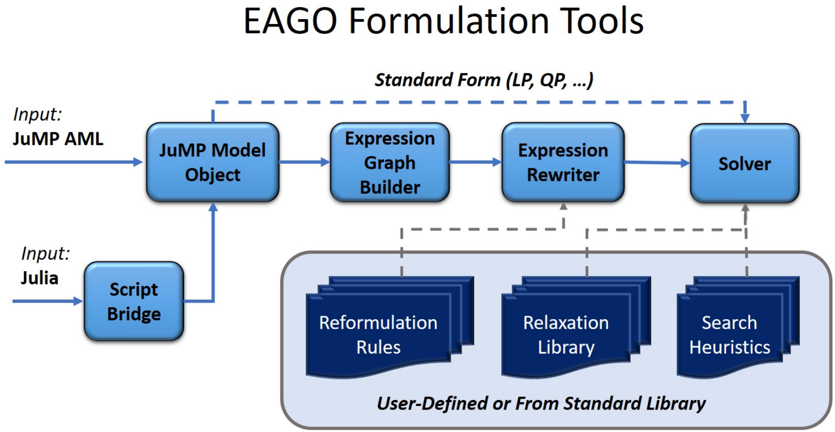
Performance comparison of various languages performing simple microbenchmarks. Benchmark execution time relative to C. (Smaller is better; C performance = 1.0.)

1 Bezanson, J, et al. SIAM Review, 59, (2017), p65-98

EAGO Optimization

```julia
struct Storage
    val::Float64
end

+(x::Storage,y::Storage) = x.val + y.val

function objective(x::Float64)
    # Type assertions in definition and storage
    y = zeros(Float64,2)
    # Operators nested in structures
    sto = Storage(x[1])
    sto += sto
    # Collection operators
    a = []
    push!(a,y[1]^2)
    # Control flow elements
    if (x > 0)
        y[1] = x^2 + x
    else
        y[1] = sin(x)
    end
    # Access from array structure
    y[1] + y[2] + sto.val + pop!(a)
end
```

- **Original Scope:** A general script-based solver that constructs McCormick relaxations by method overloading.
- **Issue:** "General" overloading approaches aren't adequately general.
- **Issue:** Introducing auxiliary variables, rearranging expressions, and presolving can be quite beneficial.


EAGO Formulation Tools
Standard Form (LP, QP, ...)
Input:
JuMP AML
JuMP Model Object
Expression Graph Builder
Expression Rewriter
Solver
Input:
Julia
Script Bridge
Reformulation Rules
Relaxation Library
Search Heuristics
User-Defined or From Standard Library

Interface - Script

Consider the kinetic parameter estimation problem given in [1]. Parameters are desired that minimize the sum-square error.

$$\min_{\mathbf{p}\in P} \sum_{i=1}^{n} \left((x_A^i + \frac{2}{21} x_B^i + \frac{2}{21} x_D^i) - I_i^d \right)^2$$

Decision parameters are the reaction rate constants

$$\mathbf{p} = (k_{2f}, k_{3f}, k_4) \in [100, 1200] \times [100, 1200] \times [0.001, 40]$$

The explicit Euler discretization of the kinetic mechanism is given by:

$$
\begin{aligned}
x_A^{i+1} &= x_A^i + \Delta t \left(k_1 x_Y^i x_Z^i - C_{O2}(k_{2f} + k_{3f}) x_A^i + \frac{k_{2f}}{K_2} x_D^i + \frac{k_{3f}}{K_3} x_B^i - k_5 (x_A^i)^2 \right) \\
x_B^{i+1} &= x_B^i + \Delta t \left(k_{3f} C_{O2} x_A^i - \left(\frac{k_{3f}}{K_3} + k_4 \right) x_B^i \right) \\
x_D^{i+1} &= x_D^i + \Delta t \left(k_{2f} C_{O2} x_A^i - \frac{k_{2f}}{K_2} x_D^i \right) \\
x_Y^{i+1} &= x_Y^i + \Delta t \left(-k_{1s} x_Y^i x_Z^i \right) \\
x_Z^{i+1} &= x_Z^i + \Delta t \left(k_1 x_Y^i x_Z^i \right)
\end{aligned}
$$

2 Mitsos A. et al. SIAM Journal on Optimization, SIAM, 20, (2009), 573-601

Interface - Script

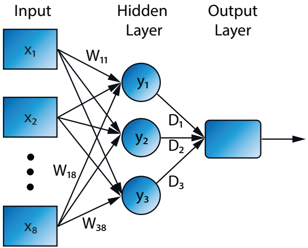
```julia
function fd(p,data)

    x = zeros(1000,typeof(p)); SSE = 0    # data storage array
    x[4] = 0.4; x[5] = 140                # sets initial condition

    # sets known parameter values
    T = 273; delT = 0.01; cO2 = 2e-3; k1 = 53; k1s = k1*1e-6
    K2 = 46exp(-6500/T-18); K3 = 2*K2;
    for i=1:200

        # Advances one time-step
        temp1 = delT*(k1s*x[5i-1]*x[5i]-cO2*(p[1]+p[2])*x[5i-4])
        temp2 = delT*(p[1]*x[5i-4]/K2+p[2]*x[5i-3]/K3-k5*x[5i-4]^2)
        x[5i+1] = x[5i-4] + temp1 + temp2
        x[5i+2] = x[5i-3] + delT*(p[2]*cO2*x[5i-4]-(p[2]/K3+p[4])x[5i-3])
        x[5i+3] = x[5i-2] + delT*(p[1]*cO2*x[5i-4]-p[1]/K2)
        x[5i+4] = x[5i-1] + delT*(-k1s*x[5i-1]*x[5i])
        x[5i+5] = x[5i] + delT*(k1*x[5i-1]*x[5i])

        # Updates the SSE value
        SSE += ((x[i+1] + (2/21)*x[i+2] + (2/21)*x[i+5]) - data[i])^2

    end

    return SSE
end

# load data from file to variable d
using JLD2, FileIO
@load "KineticData.jld2" d

# makes function with data fixed to file contents
f(x) -> fd(x,d)

# solve optimality problem
objective, solution, feasibility = ScriptSolve(f,lb,ub)
```

- The global optimal solution, within a 5 difference between lower and upper bounds, is found within 3 seconds.
- Times comparable to C++ implementation in literature.

$$\max_{\mathbf{x}\in X} B_2 + \sum_{i=1}^{3} \frac{2D_i}{1+\exp(-2Y_i)}$$

$$Y_i = B_i + \sum_{i=1}^{3}\sum_{j=1}^{8} W_{ij}x_j$$

- Consider the flooded bed bioreactor process optimization problem in [3].
- x_j input variables. The weight between variables j and hidden layer node i are W_{ij} and the weight for the hidden node i's output D_i.



3 Cheema, J. et al. Biotechnology progress 18(6), 2002 p1356-1365.

4 Schweidtmann, AM., Mitsos Journal of Optimization Theory and Applications, 2018, p1-24.

Interface - JuMP

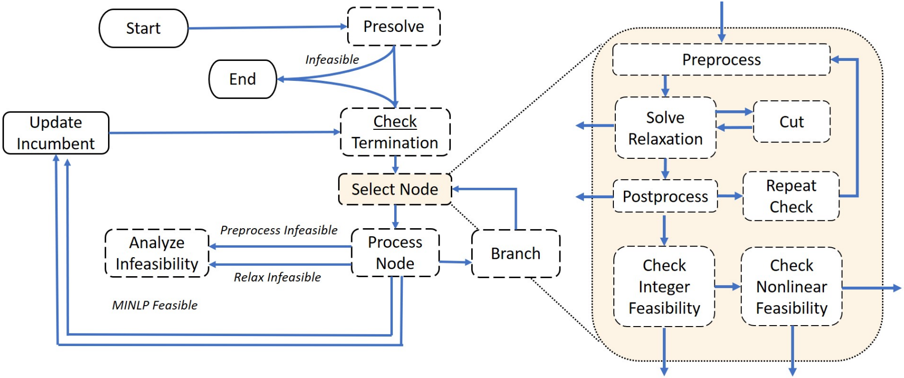
```julia
using JuMP
using EAGO

# Box constraints for input variables
xLBD = [0.623, 0.093, 0.259, 6.56, 1114,  0.013, 0.127, 0.004]
xUBD = [5.89,  0.5,   1,     90,   25000, 0.149, 0.889, 0.049]

# Weights associated with the hidden layer
W = [ 0.54, -1.97,  0.09, -2.14,  1.01, -0.58,  0.45, 0.26;
     -0.81, -0.74,  0.63, -1.60, -0.56, -1.05,  1.23, 0.93;
     -0.11, -0.38, -1.19,  0.43,  1.21,  2.78, -0.06, 0.40]

# Weights associated with the output layer
D = [-0.91 0.11 0.52]

# Bias associated with the hidden layer
B1 = [-2.698 0.012 2.926]

# Bias associated with the output layer
B2 = -0.46

# Model construction
model = Model(with_optimizer(EAGO.Optimizer()))
@variable(model, xLBD[i] <= x[i=1:8] <= xUBD[i])
@NLexpression(m, prop[i], B1[i] + sum(W[i,j]*x[i] for i=1:3,j=1:8))
@NLobjective(model, Max, B2 + sum(D[i]*(2/(1+exp(-2*prop[i])) for i=1:3))

# Solves the model
optimize!(model)

# Access functions for the solution
ObjectiveValue = getobjectivevalue(model)
Feasibility = getfeasibility(model)
Solution = getvalue(x)
```

- EAGO provides native support for the JuMP AML [4].
- JuMP provides automatic differentiation utilities and expression input via syntactic macros.
- Similiar complexity to Pyomo [5].
- Example is solved in under less than one second.

4 Dunning, I. et al. SIAM Review, 59, 2017, 295-320
5 Hart, W. et al. Mathematical Programming Computation, 3, 2011, 219

Outline

Solver Routine



- EAGO now supports a Branch-and-Cut [6] framework.
- Individual subroutines can be set using a simple API.

```
#Sets preprocessing rule of s to function f
@SetPreprocessingRule(s,f)
```


6 Rustem, B. et al. Optimization Methods and Software, 2001, 16, 21-47

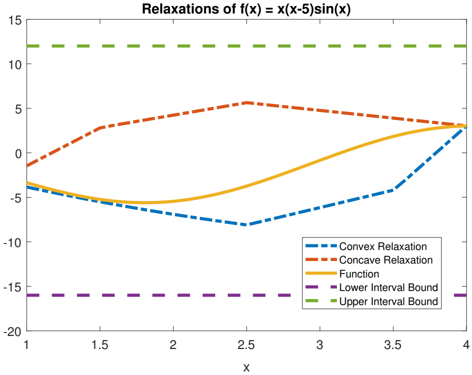
Relaxations - Framework

New framework for organizing relaxations

- All relaxations now generated from tape and parsed into expression graph via source-code transformation.
- Relaxations are registered with properties
  - Differentiable
  - MILP, etc.
- Schemes contain rules for composing relaxations using directed acyclic graph
  - **FullAVM**: Generate relaxation at each node.
  - **SetValue**: Propagate from user input.
  - User-defined schemes supported.

Relaxations - Currently Supported

- Outer-Approximations(LP/MIP) [8]
- αBB-Type Relaxations [9]
- Interval Arithmetic [7]
- Convex/Concave Envelopes



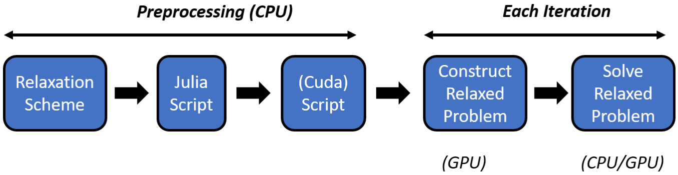
7 Moore, R. Methods and Application of Interval Analysis, SIAM, 1979

8 Tawarmalani, M. et al. Mathematical Programming, 99, 2004, 563-591

9 Adjiman, C.S et al. Computers & Chemical Engineering, 20, 1996, 419-424

Relaxations - GPU Programming

- Source-code transformation approach builds functions that additional Julia code can manipulate.
- Integrates with Cassette.jl, Intel's Parallel Accelerator or Cuda (CudaNative.jl [10]) utilities to generate relaxation functions into code that can be run on a GPU.

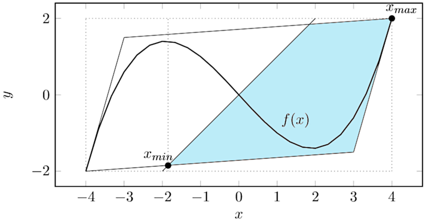


10 Besard, T. et al. IEEE Transactions on Parallel and Distributed Systems, 2018

Domain Reduction - OBBT

- Optimization-based bound tightening with filtering and greedy-ordering [11].
- Additional algorithms for: Poor Man's LP/NLP [12], Newton/Krawczyk methods [13], and more.
- Integrates with new relaxation framework.

$$\min_{x,y} x - y$$
$$y = 0.1x^3 - 1.1x$$
$$-4 \leq x \leq 4$$
$$-2 \leq y \leq 2$$



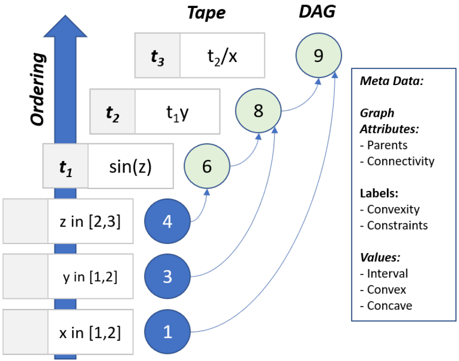
11 Gleixner, A. et al. J. Global Optim, 67, 2017, 731-757

12 Puranik, Y. et al. Constraints, 22, 2017, 338-376

13 Stuber, M. et al. Optimization Methods & Software, 30, 2015, 424-460

Domain Reduction - Constraint Walking

- Wengert tape storage for structures
- Adaptive methods or function built from DAG for constraint propagation (CP) [14]
- Supports for validated interval arithmetic CP [15]



14 Vu, X. et al. J. Global Optim, 45, 2008, 499

15 Moore, R. et al. Intro to Interval Analysis, SIAM 2009, 110

Future Work

- JuMP extension for DAE models: Enabled by new MathOptInterface Bridge feature.
- Automatic recognition of implicit functions in explicit forms.
- Incorporation of fixed-point routines for relaxing implicitly-defined functions for forming relaxations and domain reduction [13].

13 Stuber, M. et al. Optimization Methods & Software, 30, 2015, 424-460

Acknowledgements

EAGO

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Process Systems and Operations Research Laboratory

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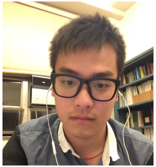

Chenyu Wang

William Hale

Connor Dion

Jacob Chicano

Abiha Jafri

Shameless Promotion...

Other EAGO Talks at AIChE

Session: **Advances in Determininstic Global Optimization**
Date: **Tuesday, October 30, 2018**
Session Time: 8:00 AM - 10:30 AM

Presentation Title: Quadratic Underestimators of Differentiable Mccormick Relaxations for Deterministic Global Optimization
Presentation Time: **9:35 AM - 9:54 AM**
Location: David L. Lawrence Convention Center, 409

Session: **Advances in Computational Methods and Numerical Analysis**
Date: **Tuesday, October 30, 2018**
Session Time: 12:30 PM - 3:00 PM

Presentation Title: Tightening Mccormick Relaxations Via Reformulation of Intermediate Functions into Schema
Presentation Time: **2:05 PM - 2:24 PM**
Location: David L. Lawrence Convention Center, 410

Fin...

- The EAGO suite is a registered Julia 1.0 package and can be installed as follows:

```julia
Pkg.add("EAGO")
```

- Development versions, examples, and documentation may be accessed from the Processing System and Engineering Lab's Github website:

https://github.com/PSORLab/EAGO.jl

Questions?