Easy Advanced Global Optimization

A Deterministic Nonconvex Optimization Package for Julia

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

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First Things... Introductions!

I'm Matt Wilhelm!

□ I work at UCONN on robust and global nonconvex optimization

□ Started working on EAGO, I've been in response to a couple things:

No low-level routines in global optimization.

- Pyomo/JuMP: great for higher level and meta-algorithms
- Existing solvers: Not open-source or aren't meant to be extended.
- *Academic tools*: Exist as fragmented libraries across multiple languages.



- The real test is solver performance on standard benchmarks.
- Want to be able to easily distribute work.



Integrate with AML

First Things... Introductions!





Simulation Motivation



- Nonconvex models from block
 diagrams are quite common
- Typical optimization problem formulate in state-control¹

 $\min_{p \in P} f(x(p), p)$ s.t. f(x(p), p) = 0 $g(x(p), p) \le 0$

p – Control variables*x* – State variables

Offshore Liquefied Natural Gas Production²



Optimum design of chemical plants with uncertain parameters. I. E. Grossmann and R. W. H. Sargent (1978). AIChE Journal, 24(6):1021–1028.
 Differentiable McCormick relaxations. Khan, K. et al. (2017) *Journal Global Optimization*, 67(4), 687-729

McCormick Relaxations



Calculating convex bounds on bilinear term via a McCormick relaxations³

w = xy $x^{L} \le x \le x^{U}$ $y^{L} \le y \le y^{U}$

[3] Computability of global solutions to factorable nonconvex programs: Part I-Convex underestimating problems. G. P. McCormick. Mathematical Programming, 10:147–175, 1976.

[4] McCormick envelopes.

https://optimization.mccormick.northwestern.e du/index.php/McCormick_envelopes

Decomposition Method⁴



 $w \ge x^{L}y + xy^{L} - x^{L}y^{L}$ $w \ge x^{U}y + xy^{U} - x^{U}y^{U}$ $w \le x^{U}y + xy^{L} - x^{U}y^{L}$ $w \le xy^{U} + x^{L}y - x^{L}y^{U}$

Composition method



 $w^{cv}(x, y) = \max(x^{L}y + xy^{L} - x^{L}y^{L}, x^{U}y + xy^{U} - x^{U}y^{U})$ $w^{cc}(x, y) = \min(x^{U}y + xy^{L} - x^{U}y^{L}, xy^{U} + x^{L}y - x^{L}y^{U})$

McCormick Relaxations



McCormick Relaxations Via Method Overloading

```
1 # (Smooth) McCormick Object w/ Subgradient
    struct SMCg{N,V<:AbstractInterval,T<:AbstractFloat} <: Real</pre>
 2
       cc::T
 Δ
       cv::T
 5
       cc grad::SVector{N,T}
      cv grad::SVector{N,T}
 6
7
       Intv::V
8
       cnst::Bool
9
10
       function SMCg{N,V,T}(cc1::T,cv1::T,cc grad1::SVector{N,T},cv grad1::SVector{N,T},
11
                     Intv1::V,cnst1::Bool) where {N,V<:AbstractInterval,T<:AbstractFloat}</pre>
12
        new(cc1,cv1,cc_grad1,cv_grad1,Intv1,cnst1)
13
      end
14
    end
15
     # Overload Addition Operator
16
17
     function +(x::SMCg{N,V,T},y::SMCg{N,V,T}) where {N,V,T<:AbstractFloat}</pre>
18
         return SMCg{N,V,T}(x.cc+y.cc,
19
                            x.cv+y.cv,
20
                            x.cc grad+y.cc grad,
21
                            x.cv_grad+y.cv_grad,
22
                             (x.Intv+y.Intv),
23
                             (x.cnst && y.cnst))
24
    end
25
```

 [5] McCormick-based relaxations of algorithms. Mitsos et al. (2009) SIAM Journal on Optimization, SIAM, 2009, 20, 73-601
 [6] MC++: A versatile library for McCormick relaxations and Taylor models. B. Chachuat. http://www3.imperial.ac.uk/people/b.chachuat/research

McCormick Composition Rule³:

Consider the composite function $h = g \circ f$. Let $f^{cv}, f^{cc} : X \to \mathbb{R}$ be known convex and concave relaxations of f on X, respectively. Let $g^{cv}, g^{cc} : Z \to \mathbb{R}$ be known convex and concave relaxations of g on Z, respectively. Then,

$$h^{cv}(\mathbf{z}) = g^{cv}(mid(f^{cv}(\mathbf{z}), f^{cc}(\mathbf{z}), x^{min}))$$

$$h^{cc}(\mathbf{z}) = g^{cc}(mid(f^{cv}(\mathbf{z}), f^{cc}(\mathbf{z}), x^{max}))$$
(4)

Where x^{min} is a point at which g^{cv} attains its infimum on X and x^{max} is a point at which g^{cc} attains its supremum on X.

Currently Supported Operators:

- Algebraic: +, -, /, *, ^, pow
- Trigonometric: sin, cos, tan, asin, acos, atan
- Hyperbolic: sinh, cosh, tanh, asinh, acosh, atanh
- Nonsmooth: min, max, abs, step, sign
- Others: exp, exp2, exp10, log, log2, log10, sqrt

Relaxation from Macros

List of convexity properties for standard functions, dictionary structure for relaxations, and registration/generation via macros.

- :convex (exp, abs, sqr)
- :convexoconcave (tanh)
- :concave (log, sqrt)

@set cvtrait Base.sinh(x)

:concavoconvex (erfc)

:Concavoconvex :Increasing 0.0 -Inf Inf

@set_cvtrait	Base.cosh(x)
@set_cvtrait	Base.tanh(x)
@set_cvtrait	Base.sech(x)
@set_cvtrait	Base.asinh(x)
@set_cvtrait @set_cvtrait	Base.asinh(x) Base.acosh(x)

@set_cvtrait Base.asech(x)

:Convex :DecrToIncr 0.0 -Inf Inf :Convexoconcave :Increasing 0.0 -Inf Inf :Convexoconcave :IncrToDecr Inf -Inf Inf :Convexoconcave :Increasing 0.0 -Inf Inf :Convexoconcave :Increasing 0.0 -Inf Inf :Concave :Increasing Inf 1.0 Inf :Convexoconcave :Decreasing 0.5 0.0 1.0





McCormick Relaxations - Example

using EAGO

```
# create SmoothMcCormick seed object for x = 2.0 on [1.0, 4.0] for relaxing
    # a function f(x) on the interval box xIbox using mBox as a reference point
    f(x) = x^*(x-5.0)^*\sin(x)
6
                                      # value of independent variable x
8
    x = 2.0
                                      # set initial subgradient of x to [1.0]
    subx = seed g(Float64,1,1)
    Intv = Interval(1.0, 4.0)
                                     # define interval to relax over
11
    # create McCormick object
    SMC = SMCg{1,Interval{Float64},Float64}(x,x,subx,subx,Intv,false)
13
    fSMC = f(SMC)
                             # relax the function
    cv = fSMC.cv
                               # convex relaxation
    cc = fSMC.cc
                              # concave relaxation
18
    cvgrad = fSMC.cv_grad
                              # subgradient/gradient of convex relaxation
    ccgrad = fSMC.cc grad
                              # subgradient/gradient of concave relaxation
                              # retrieve interval bounds of f(x) on Intv
21
    Iv = fSMC.Intv
22
23
```



Standard McCormick Relaxation



McCormick Relaxations (Extensions)

$f(x) = -x^2 \exp(x) + max(x - 5, \sin(x))$

Subgradient Refinement **Differentiable McCormick Relaxation** Relaxations for max and min⁷ Function Convex McCormick Relaxation Differentiable (x) Concave McCormick Relaxation Convex Natural Interval ave Natural Interv Function **McCormick** Convex McCormick Relaxation Concave McCormick Relaxati f(x) Convex Natural Interval relaxations.² Concave Natural Interva Convex Affine Concave Affin **Tighter Interval Bound**

Subgradient-based interval tightening method⁸
 Reverse McCormick contractors⁹

[7] Multivariate McCormick relaxations. Tsoukalas, A. and Mitsos, A. (2014) Journal of Global Optimization, 633-662

[2] Differentiable McCormick relaxations. Khan, K. et al. (2017) Journal Global Optimization, 67(4), 687-729

[8] Tighter McCormick Relaxations through Subgradient Propagation. Najman, J. and Mitsos, A. (2017) https://arxiv.org/abs/1710.09188

[9] **Reverse propagation of McCormick relaxations**. Wechsung, Achim, et al. (2015) *Journal of Global Optimization* 63(1): 1-36.



McCormick Relaxation: Branch & Bound



McCormick Relaxations:

- Nonsmooth NLP (Bundle Solver)
- Affine Relaxation (LP Solver)

Differentiable McCormick Relaxations:

NLP solver

The standard EAGO solver

Search Routine:

- Best-first

Preprocessing:

- Interval constraint propagation¹⁰
- LP contractor¹⁰ (NS McCormick Relaxations)

Lower Bounding Problem:

- NLP solve via Ipopt¹¹
- LP solve with user selected solver

Upper Bounding Problem:

- Local NLP solve via Ipopt

Postprocessing:

- Duality-based bound tightening¹⁰.



and L. T. Biegler (2006), Mathematical Programming 106(1), 25-57.

^[10] Domain reduction techniques for global NLP and MINLP optimization Puranik, Y. and Sahinidas, N. (2017) Constraints, 22: 338-376.

^[11] On the Implementation of a Primal-Dual Interior Point Filter Line Search Algorithm for Large-Scale Nonlinear Programming A. Wächter



McCormick versus Interval Methods

Three-hump camel function via Interval Method





Three-hump camel function via McCormick Approach

Swapping in a custom lower-bound

```
m = Model(solver = EAGO NLPSolver())
    @variable(m, -5 \le x \le 5)
    @variable(m, -5 \le x \le 5)
    @NLobjective(m, Min, 2*x^2-1.05*x^4+(x^6)/6+x*y+y^2)
    JuMP.build()
8
    function custom LBD(x::Vector{Interval{Float64}},
                                                         # Box
                        k::Int.
                                                         # Iteration number
                         p::Int,
                                                         # Tree Depth
                         opt,
                                                         # Data passed from solver
                                                         # Data passed between problems
14
                        temp)
        pnt = mid.(X) # Solution point
        val = (2*x[1]^2-1.05*x[1]^4+(x[1]^6)/6+x[1]*x[2]+x[2]^2).lo # Solution value
        # Return lower bound, solution value, feasibility, and duality info
        return [val,pnt,true,[]]
    end
    set LBD!(custom LBD,m)
    solve(m)
```

Branch and Bound Implementation

Full Customizable

All blocks are functions that can be reset.

Common Heuristics are available via API:

- Search Methods: Best-First Search, etc.
- **Bisection Methods:** Relative Width, etc.

□ Typical output templates available

- Convergence plots
- CSV data for batch runs
- Solver progress output to console

Setting search to a breadth-first style

julia> EAGO.set_Branch_Scheme!(a,"breadth")

Console display with solver progress

Iteration	NodeID	Current_LBD	Global_LBD	Global_UBD	NodesLeft	Absolute_Gap	Absolute_Ratio	
60,	115,	3.0004273,	3.0000000,	3.0005493,	8,	0.0005493,	0.9998169	
61,	118,	3.0000000,	3.0000000,	3.0004883,	9,	0.0004883,	0.9998373	
62,	119,	3.0000610,	3.0000000,	3.0004883,	10,	0.0004883,	0.9998373	
63,	120,	3.0000000,	3.0000000,	3.0002747,	11,	0.0002747,	0.9999085	
64,	121,	3.0002136,	3.0000000,	3.0002747,	8,	0.0002747,	0.9999085	
65,	124,	3.0000000,	3.0000000,	3.0002747,	7,	0.0002747,	0.9999085	
66,	125,	3.0000305,	3.0000000,	3.0002747,		0.0002747,	0.9999085	
67,	122,	3.0000610,	3.0000610,	3.0002747,		0.0002136,	0.9999288	
68,	123,	3.0002747,	3.0000610,	3.0002747,	4,	0.0002136,	0.9999288	
69,	116,	3.0001221,	3.0001221,	3.0002747,	З,	0.0001526,	0.9999491	
70,	117,	3.0005493,	3.0001221,	3.0002747,	2,	0.0001526,	0.9999491	
71,	110,	3.0002441,	3.0002441,	3.0002747,	1,	0.0000305,	0.9999898	
Convergence	e Tolerano	e Reached						
First Solu	tion Found	l at Node 64						
UBD = 3.000	0274661055	3004						
Solution is								
X[1] =	-0.999969	482421875						
X[2] =	2.0000267	/028808594						
Total UBD problems solved = 62 in 0.02245968799999999 seconds.								
Total LBD problems solved = 72 in 1.2186544090000009 seconds.								

Transform MINLP to nonconvex NLP



<u>Objective:</u> min F_2

Constraints:

Mass Balances + Process Models AND the below:

Polytropic Gas

$$(\kappa - 1)\ln(P_1^s) + \kappa \ln(T_2) = (\kappa - 1)\ln(P_2^s) + \kappa \ln(T_1)$$

Pinch-Point Energy Balances

$$\begin{split} \min_{p \in P} \{ EBP_{H}^{p} - EBP_{C}^{p} \} &= -Q_{c} \\ Q_{H} + \sum_{i \in H} Fc_{p,i}(T_{i}^{in} - T_{i}^{out}) = Q_{C} + \sum_{j \in C} Fc_{p,j}(T_{j}^{in} - T_{j}^{out}) \\ EBP_{H}^{p} &= \sum_{i \in H} Fc_{p,i} \Big[\max\left\{ 0, T^{p} - T_{i}^{out} \right\} - \max\left\{ 0, T^{p} - T_{i}^{in} \right\} - \max\left\{ 0, T^{\min} - T_{i}^{p} \right\} + \max\left\{ 0, T^{p} - T_{i}^{\max} \right\} \Big] \\ EBP_{C}^{p} &= \sum_{j \in C} Fc_{p,j} \Big[\max\left\{ 0, (T^{p} - \Delta T_{\min}) - T_{j}^{in} \right\} - \max\left\{ 0, (T^{p} - \Delta T_{\min}) - T_{j}^{out} \right\} - \max\left\{ 0, (T^{p} - \Delta T_{\min}) - T_{j}^{out} \right\} - \max\left\{ 0, (T^{p} - \Delta T_{\min}) - T_{j}^{max} \right\} + \max\left\{ 0, t^{\min} - (T^{p} - \Delta T_{\min}) \right\} \Big] \\ \forall p \in P \end{split}$$

Offshore Liquidfied Natural Gas Production²



Transform MINLP to nonconvex NLP





Offshore Liquidfied Natural Gas Production¹

Branching on Implicit Functions

McCormick relaxations can bound functions via fixed-point methods:

- Theoretically, well-behaved relaxations of state variables that aren't factorable.
- Applicable to process units containing nonlinear equations that require nonlinear solve.
- Assumes the existence of an implicit function y = x(p).

Linear Parametric System:

A(p)x = b(p)

[12] Convex and concave relaxations of implicit functions. Stuber, M.D. et al. (2015) Optimization Methods and Software, 30, 424-460
[5] McCormick-based relaxations of algorithms. Mitsos et al. (2009) SIAM Journal on Optimization, SIAM, 2009, 20, 73-601
[12] Direct measurement of the fast reversible addition of everyon to a statement of the fast reversible addition.

 $\left[13\right]$ Direct measurement of the fast, reversible addition of oxygen to

cyclohexadienyl radicals in nonpolar solvents, J. W. Taylor, et al. *Phys. Chem. A*, 108 (2004), pp. 7193–7203.

GeneralNonineonSystems: $h(z, p) = \begin{cases} c_A^{i-1} - c_A^i + \Delta t \left(k_1 c_Y^i c_Z^i - C_{o_2} (k_{2f} + k_{3f}) c_A^i + \frac{k_{2f}}{k_2} c_D^i + \frac{k_{3f}}{k_3} c_B^i - k_5 c_A^{i\,2} \right) = 0\\ c_B^{i-1} - c_B^i + \Delta t \left(k_{3f} c_A^i C_{o_2} - \left(\frac{k_{3f}}{k_3} + k_4 \right) c_B^i \right) = 0\\ c_D^{i-1} - c_D^i + \Delta t \left(k_{2f} c_A^i C_{o_2} - \frac{k_{2f}}{k_2} c_D^i \right) = 0\\ c_Y^{i-1} - c_Y^i + \Delta t \left(-k_{1s} c_Y^i c_Z^i \right) = 0\\ c_Z^{i-1} - c_Z^i + \Delta t \left(-k_{1s} c_Y^i c_Z^i \right) = 0 \end{cases}$

Special Forms from General Functions

Can we formulate a global solver with as low a barrier to entry as low solvers with AD methods?

```
# Globally optimize script
#(Nonlinear Regression for Indentation)
function f(x)
A = 0.0
SSE = 0.0
for j=1:100
A = 0.0
for i=1:2
A += x[i]*exp(-x[2*i]*j)
end
SSE += (A - data[j])^2
end
return A
end
Optimize Script(f,xL,xU, g = ginput, h = hinput,
```

```
solver = EAGO_NLPSolver())
```

end



...and Mixed-Integer Forms (Coming Soon)

Reformulation Architecture



Further Software Development



^[7] Multivariate McCormick relaxations. Tsoukalas, A. and Mitsos, A. (2014) Journal of Global Optimization, 633-662

[14] Branch-locking AD techniques for nonsmooth composite functions and nonsmooth implicit functions Khan, K. et al. (2017) Optimization Methods and Software, 0, 1-29

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Fin...

SIP Solvers



• EAGOSemiInfinite implements implicit and explicit meta-algorithms

Explicit SIP $f^* = \min_{\mathbf{x} \in X} f(\mathbf{X})$

s.t.
$$g(\hat{\mathbf{y}}, \mathbf{x}, \mathbf{p}) \le 0, \forall (\mathbf{y}, \mathbf{p}) \in Y \times P$$

 $\mathbf{h}(\hat{\mathbf{y}}, \mathbf{x}, \mathbf{p}) = \mathbf{0}, \ \forall (\mathbf{y}, \mathbf{p}) \in Y \times P$

Implicit SIP

$$f^* = \min_{\mathbf{x} \in X} f(\mathbf{X})$$

s.t. $g(\mathbf{y}(\mathbf{x},\mathbf{p}),\mathbf{x},\mathbf{p}) \leq 0, \quad \forall \mathbf{p} \in P$

- $\circ~$ Solved generally via restriction of right-hand side method 9,4
 - Discretization of uncertainty set for upper/lower bounds.
 - Finite convergence (if Slater point arbitrarily near minimizer).
- Problem size and complexity dramatically increased with equality constraints^{4,9,10}

[9] Global optimization of semi-infinite programs via restriction of the right-hand side. Mitsos, A. (2011). *Optimization* 60:10-11, 1291-1308

[4] **Semi-Infinite Optimization with Implicit Functions.** Stuber, M.D., Barton, P.I. (2015) *Industrial & Engineering Chemistry Research*, 54, 307-317

[10] Evaluation of process systems operating envelopes. Stuber, M.D., (2013) Ph.D Thesis.

Flowchart for restriction of RHS method⁴

