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EAGO.jl: Next Generation Global & Robust Optimization in Julia, Revisited

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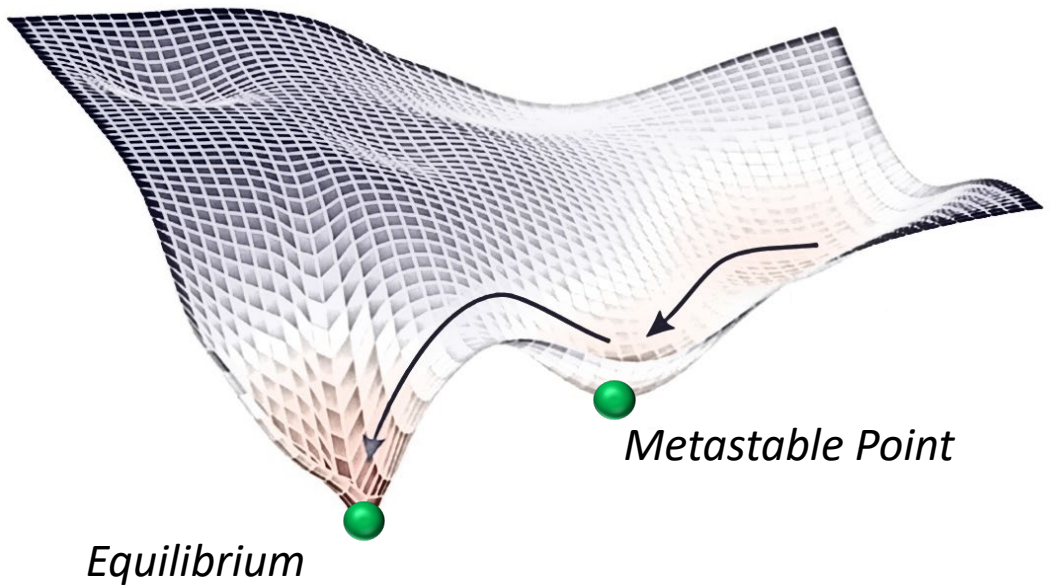
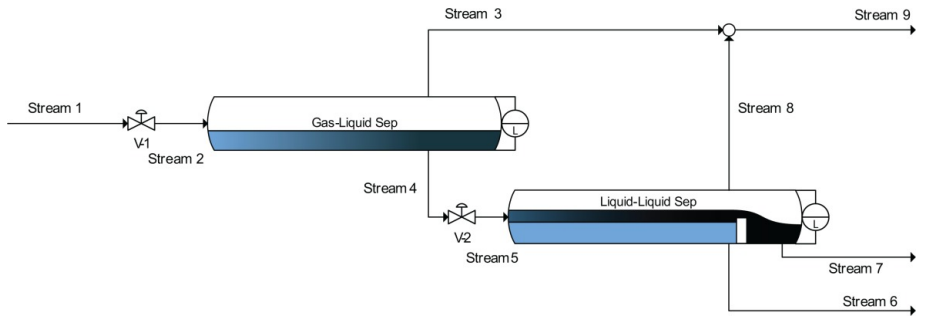
Process Systems and Operations Research Laboratory

Importance of Global Optimization

Physically Meaningful Computations[1]



Safety-Critical Systems[2]

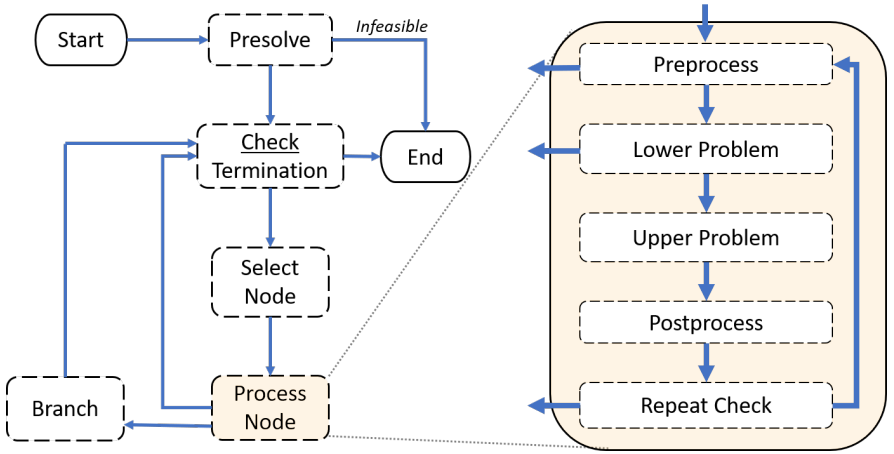


Better quality solutions than local methods…

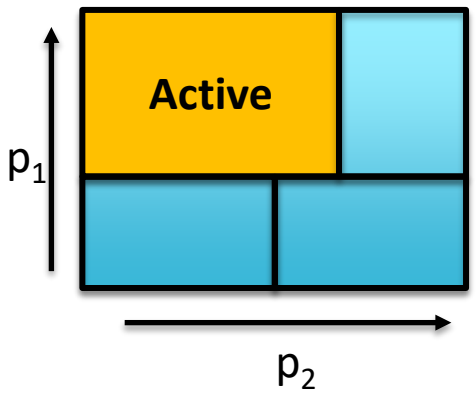
1. Grajcarova, L. **Simulations of structural phase transitions in crystals using ab initio metadynamics**. INIS-IAEA (2013)
2. Stuber, MD et al. **Worst-case design of subsea production facilities using semi-infinite programming.** *AIChE Journal* (2014): 2513-2524.

Global Optimization

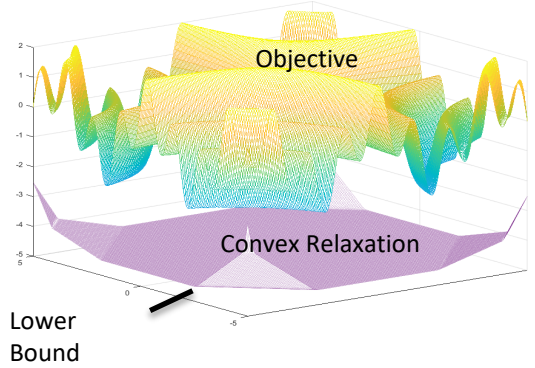
- Nonconvex MINLP formulations naturally arise in many applications.
- MINLP solvers generally rely on some variation of spatial branch-and-bound[3,4].
- Relaxed subproblems are used to compute bounds and are often derived from relaxed functions[3,4].



(Select Region)



(Relax Problem + Compute Bound)



3. Wilhelm, M.E., and Stuber, M.D.. **EAGO.jl: easy advanced global optimization in Julia.** *Optimization Methods and Software*, 1-26.
4. Horst, Reiner, and Hoang Tuy. *Global optimization: Deterministic approaches*. Springer Science & Business Media, 2013.

McCormick Relaxations of Factorable Functions

$$\mathbf{y} = \mathbf{f}(\mathbf{g}(\mathbf{x}), \dots, \mathbf{h}(\mathbf{x}))$$

Auxiliary Variable Method

$$\mathbf{z_1} = \mathbf{g}(\mathbf{x})$$

$$\vdots$$

$$\mathbf{z_n} = \mathbf{h}(\mathbf{x})$$

$$\mathbf{y} = \mathbf{f}(\mathbf{z_1}, \dots, \mathbf{z_n})$$

→ **Relaxations of *f at (x, z) in (X, Z)***

McCormick Relaxation[5,6]

Relaxations of g at x in X

⋮

Relaxations of h at x in X

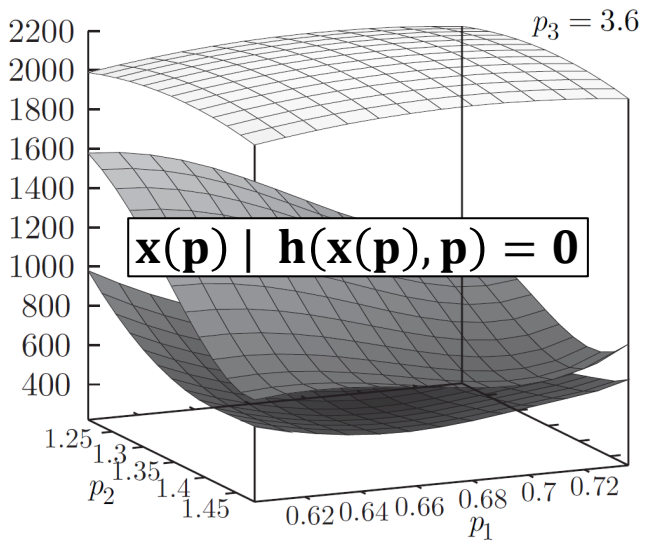
Apply **f** *composite relaxation rules* →

Relaxations of *f at x in X*

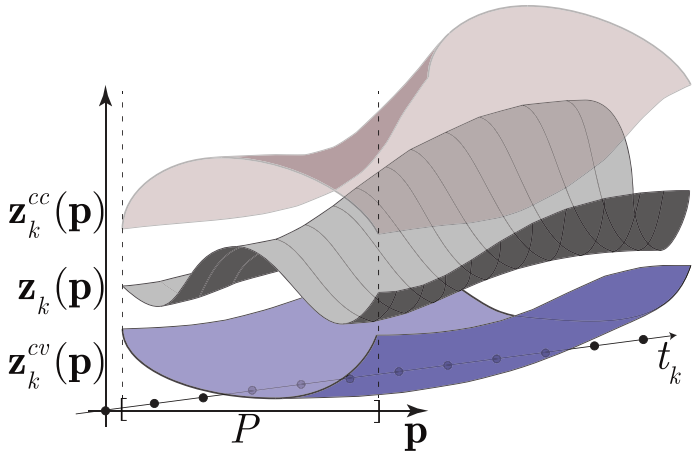
5. Mitsos, A, et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601.
6. Scott, JK, et al. **Generalized McCormick relaxations.** *Journal of Global Optimization* 51.4 (2011): 569-606.

Reduced Space Relaxations

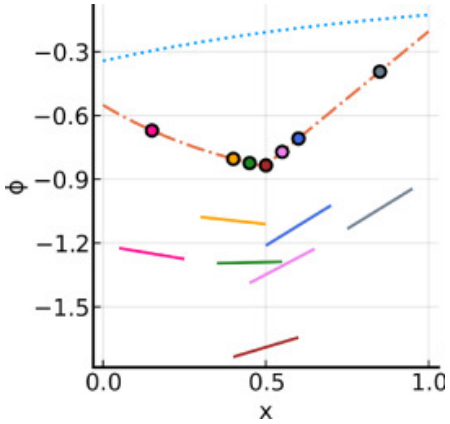
Implicit Functions[7]



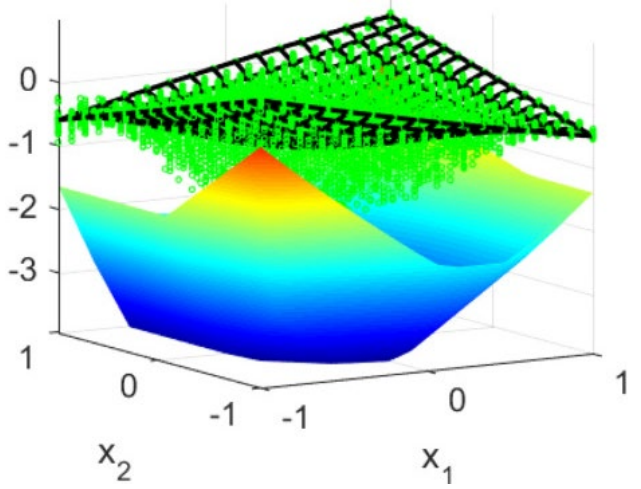
ODEs and DAEs[8]



Continuous Random Variables[9]



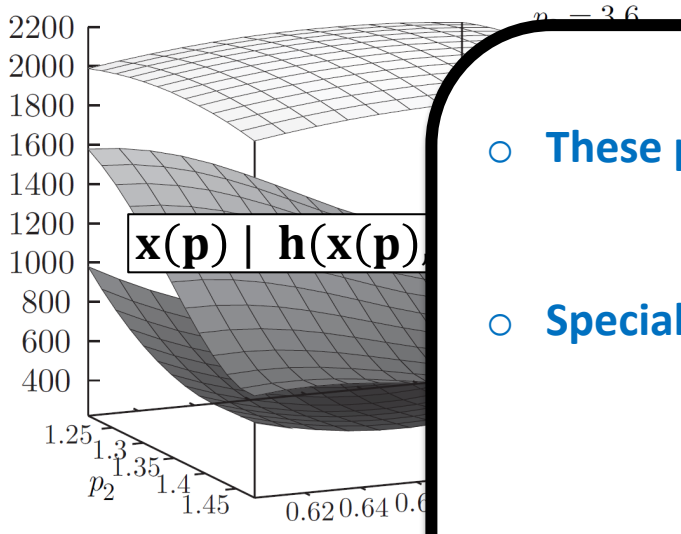
Blackbox Functions[10]



7. Stuber, MD et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* 30, (2015), 424-460
8. Wilhelm, ME; Le, AV; and Stuber. MD. **Global Optimization of Stiff Dynamical Systems.** *AIChE Journal: Futures Issue,* 65 (12), *2019*
9. Shao, Y and Scott JK. **Convex relaxations for global optimization under uncertainty described by continuous random variables**, *AIChE Journal*, (2018): 3023 – 3033.
10. Song, Y; Cao, H; Mehta, C; and Khan KA. **Bounding Convex Relaxations of Process Models from Below by Tractable Black-Box Sampling**, *Computers & Chemical Engineering*, In Press, (2021).

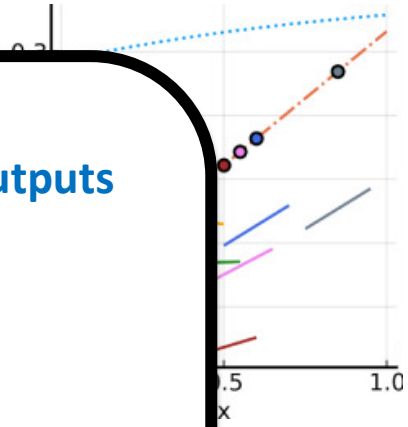
Reduced Space Relaxations

Implicit Functions[7]

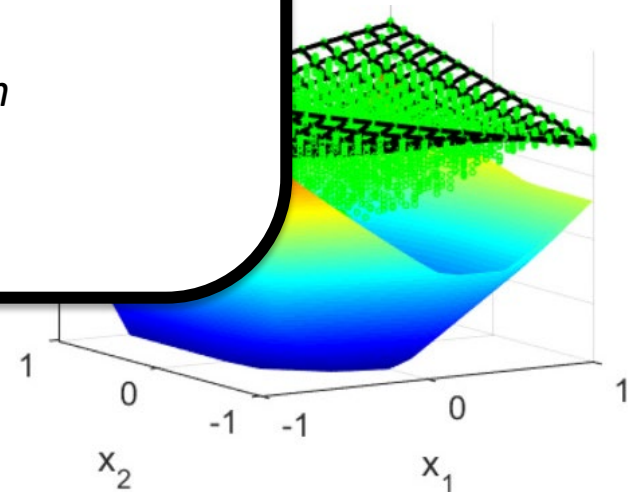


ODEs and DAEs[8]

Continuous Random Variables[9]



x Functions[10]



- **These problem types often involve vector-valued outputs**
- **Specialized relaxation routines required**
  - *Often limiting step in calculations*
  - *Need to extend problem representation*
  - *High performance is beneficial*

7. Stuber, MD et al. **Convex and** *Software* 30, (2015), 424-460
8. Wilhelm, ME; Le, AV; and Stub *Futures Issue,* 65 (12), *2019*
9. Shao, Y and Scott JK. **Convex relaxa continuous random variables**, *AIChE Journal*, (2018): 3023 – 3033.
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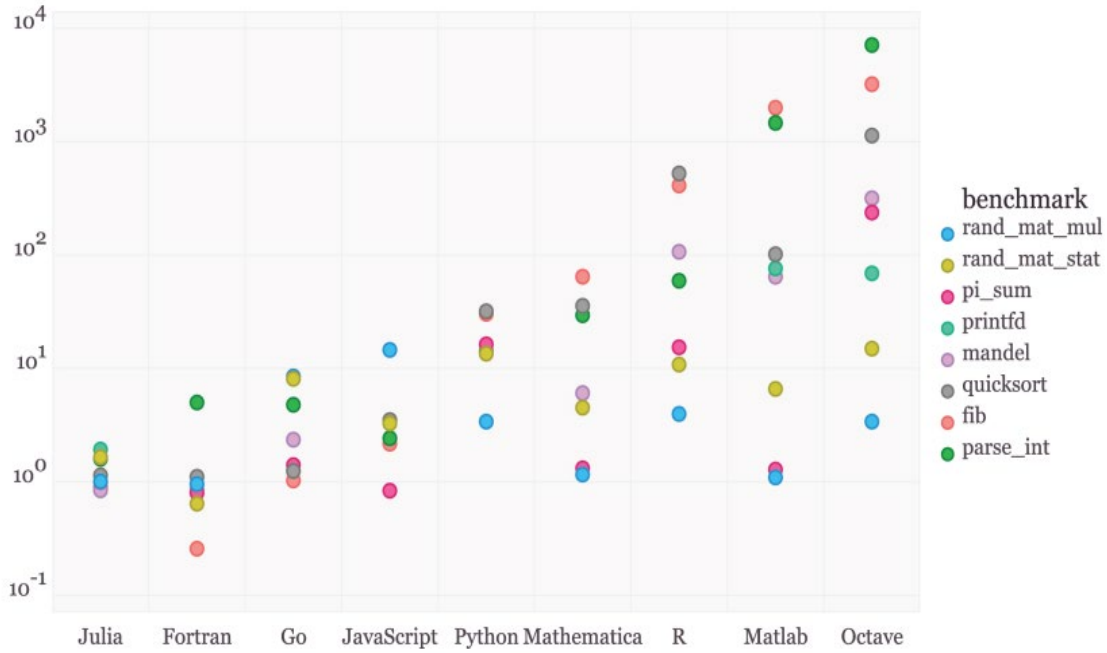
Language/Solver Capabilities

julia / JUMP

- Performance for low-level routines
- Multiple dispatch & contextual programming allow for ready extensibility (i.e., GPU, parallelism)
- Ease of setup and distribution

- Run-time benchmark comparison[11]



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

11. **Julia: A Fresh Approach to Numerical Computing**. Jeff Bezanson, Alan Edelman, Stefan Karpinski and Viral B. Shah (2017) *SIAM Review*, 59: 65–98.

Original EAGO Capabilities

Extendable Support for Script Defined Functions

Parameter Estimation for Nonideal Two-Liquid Mixture

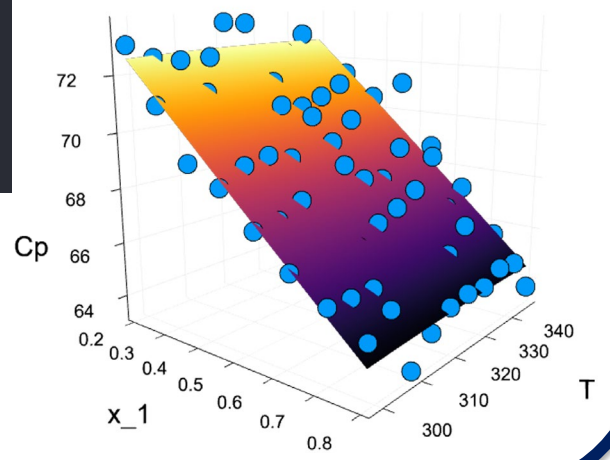
```
exGibbs(T,x1,p) = R*T*(x1*(1-x1)^2*(p[1]*T+p[2]*T^2+p[3]*log(T))+
                       (1-x1)*x1^2*(p[1]*T+p[2]*T^2+p[3]*log(T)))
GibbsA(T) = CpA*(T-T0)-T*CpA*log(T/T0)
GibbsW(T) = CpW*(T-T0)-T*CpW*log(T/T0)
Gibbs(T,x1,p) = x1*GibbsA(T)+(1-x1)*GibbsW(T)+
                R*T*(x1*log(x1)+(1-x1)*log(1-x1))+exGibbs(T,x1,p)
Cp(T,x1,p) = -T*ForwardDiff.derivative(T->ForwardDiff.derivative(T->Gibbs(T,x1,p),T),T)
```

```
function objective(T::Vector,x1::Vector,Cp_exp::Matrix,p...)
    SSE = 0.0
    for i = 1:length(T)
        for j = 1:length(x1)
            SSE += (Cp(T[i],x1[j],p)-Cp_exp[i,j])^2
        end
    end
    return SSE
end
```

```
fobj(p...) = objective(Tdata,x1data,Cp_exp,p...)
```

$$\min_{\mathbf{p}\in P} \sum_i \left(C_P^{mod}(T_i, x_i, \mathbf{p}) - C_P^{exp}(T_i, x_i)\right)$$

$$C_P^{mod}(T_i, x_i, \mathbf{p}) = -T_i \left.\frac{\partial^2 G}{\partial T^2}\right|_P (T_i, x_i, \mathbf{p})$$



Performant Subroutines

- Nonconvex MINLP & SIP solver
- Bounds Tightening Routines:
  - Optimization-based
  - Feasibility-based
- Preprocessing Routines:
  - Algebraic Rearrangements
  - Subexpression Elimination
  - Regular Problem Classification

Language/Solver Capabilities

- ❑ Extendable Graph Representation
- ❑ Dynamic Optimization
- ❑ Machine Learning in EAGO + Julia

New Nonlinear Framework

Old Framework

Evaluator

Directed Tree Structure

Compute & query value functions tied to each attribute:

- *Interval Bounds*
- *Relaxations*
- *Relaxation (Sub)gradients*

New Nonlinear Framework

Old Framework

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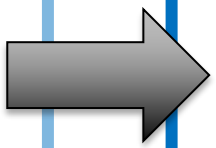
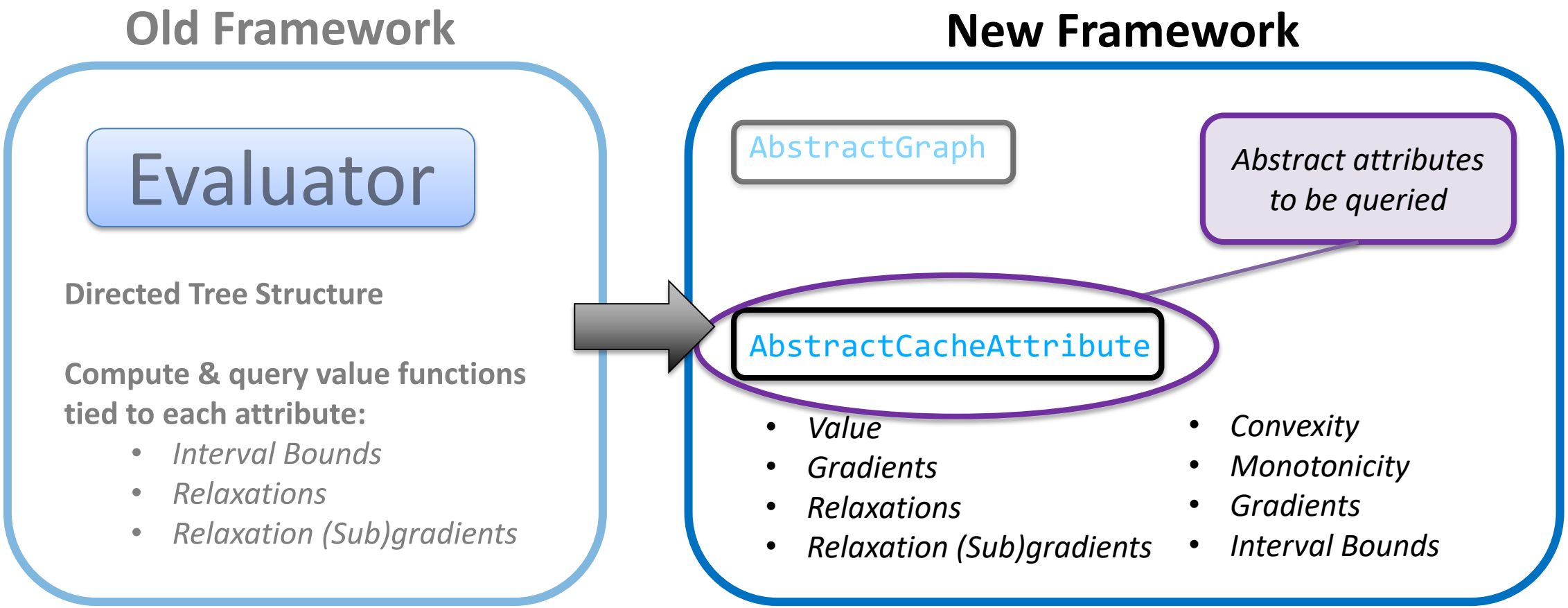


New Framework

`AbstractGraph`

Abstract graph representation of problem

New Nonlinear Framework



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Compute & query value functions tied to each attribute:

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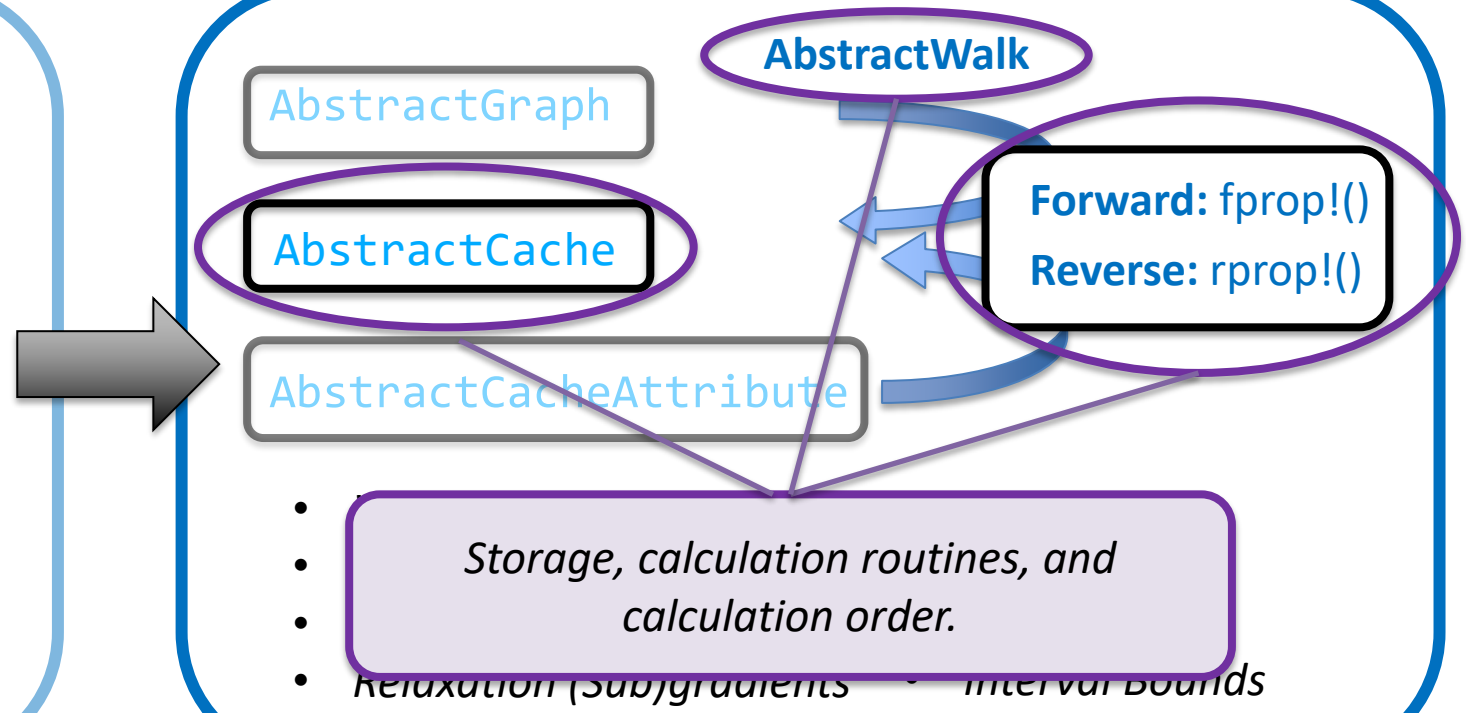
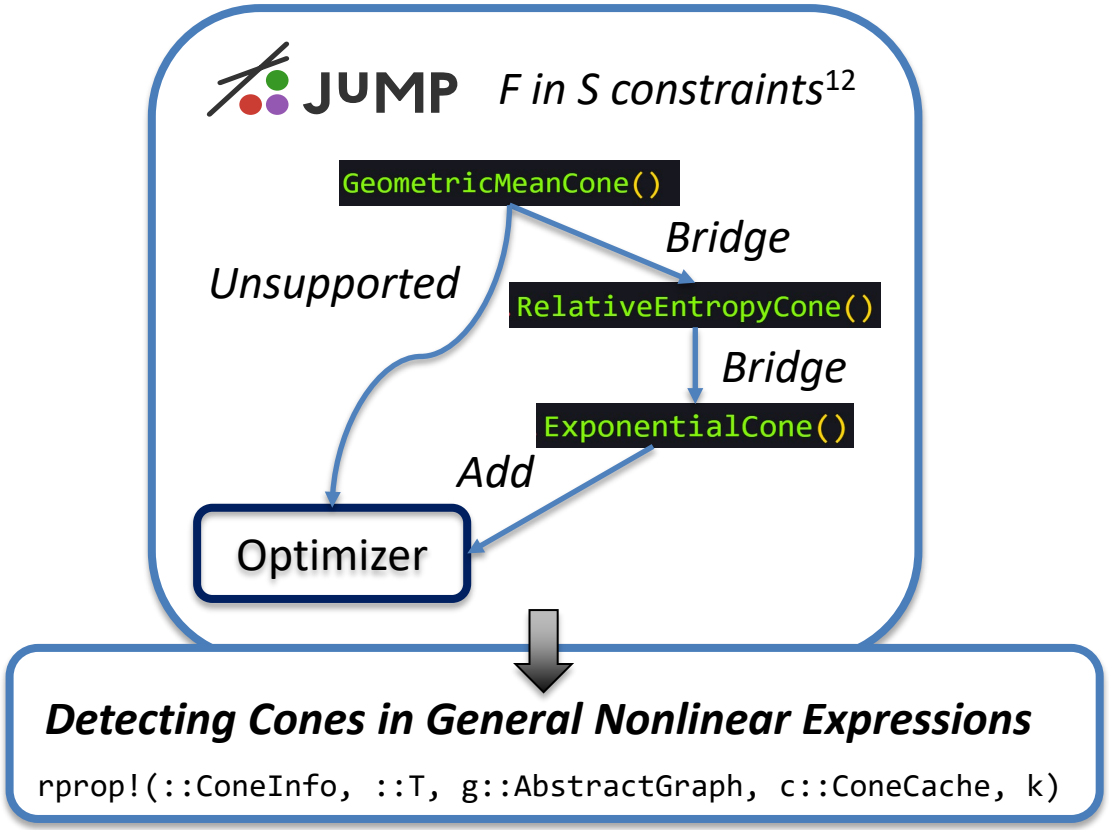
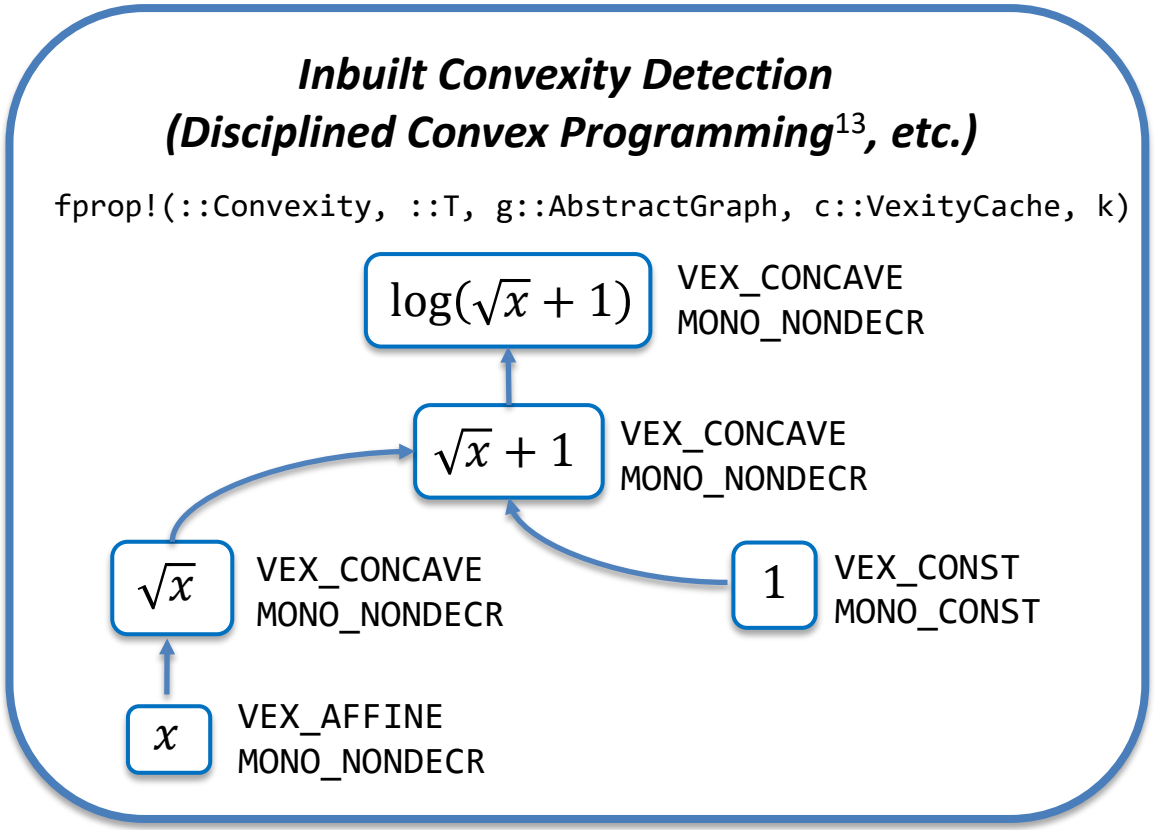
New Framework



New Graph Utilities





12. Legat, B., Dowson, O., Garcia, J. D., & Lubin, M. (2021). **MathOptInterface: a data structure for mathematical optimization problems.** *INFORMS Journal on Computing*.
13. Grant, M., Boyd, S., & Ye, Y. (2006). **Disciplined convex programming.** In *Global optimization* (pp. 155-210). Springer, Boston, MA.

ML Support + Performance

Build a MLP via UDF (Surrogates.jl)

Build Model

```
xd = sample(n, l, u, SobolSample())
yd = f.(xd)
m = Chain(Dense(2,6,tanh), Dense(6,1))
ns = NeuralSurrogate(xd, yd, l, u, model = m)
surrogate_optimize(f, SRBF(), l, u, ns, SobolSample())
```

Optimize Model

```
using JuMP, EAGO

m = Model(EAGO.Optimizer)
@variable(m, l[i] <= x[i=1:2] <= u[i])
register(m, :surrogate, 2, ns)
@NLobjective(m, surrogate(x[1],x[2]))
optimize!(m)
```

Method/Context Overloading Extension for Specialized

```
function (a::Dense)(x::AbstractVecOrMat)
    W, b, σ = a.weight, a.bias, a.σ
    return σ.(W*x .+ b)
end


function (a::Dense)(mcb::MCBox{N,T}) where {N,T}
    W, b, σ = a.weight, a.bias, a.σ
    n = length(mcb)
    yp = zeros(MC{N,T}, n)
    yn = zeros(MC{N,T}, n)
    for i = 1:n
        for j = 1:n
            Wij = @inbounds W[i,j]
            if Wij > 0.0
                yp[i] += Wij*mcb.x[j]
            else
                yn[i] += Wij*mcb.x[j]
            end
        end
        yp[i] = set_value_post(yp[i], x.v)
        yn[i] = set_value_post(yn[i], x.v)
    end
    @__dot__ yp += yn + b
    return set_value_post(σ(yp), x.v)
end
```

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Build Model

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```

```
m = Chain(Dense(2,6,tanh), Dense(6,1))
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```
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m = Model(EAGO.Optimizer)
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```

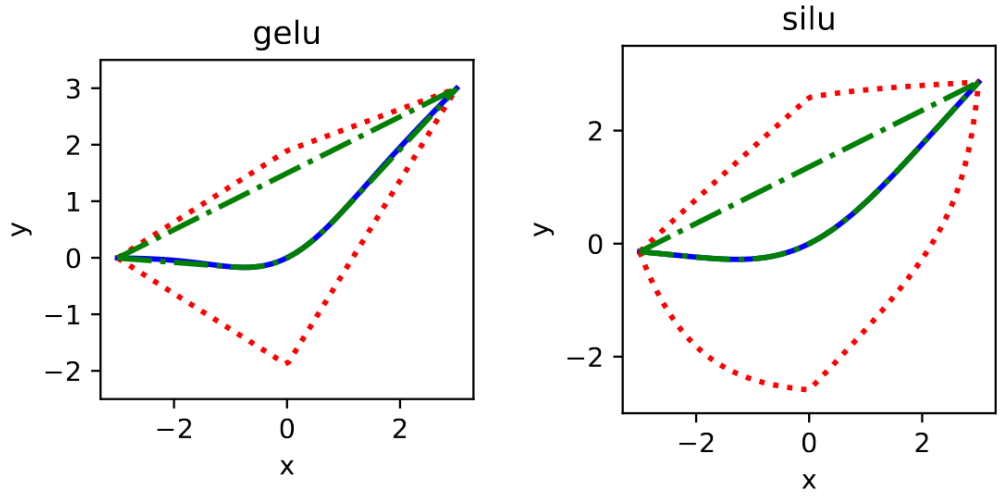
```
register(m, :surrogate, 2, ns)
@NLobjective(m, surrogate(x[1],x[2]))
```

```
optimize!(m)
```

Additional Support for ML Specific Functions

```
function (a::Dense)(x::AbstractVecOrMat)
    W, b, σ = a.weight, a.bias, a.σ
    return σ.(W*x .+ b)
end
```

Envelopes of Relaxation Functions




```
end
```

EAGO.jl and Dynamics

Abstract Layer

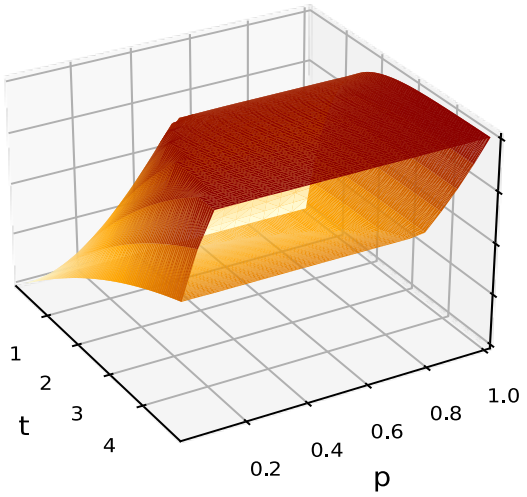
DynamicBounds.jl[14]

Extendable Global Optimizer[15]

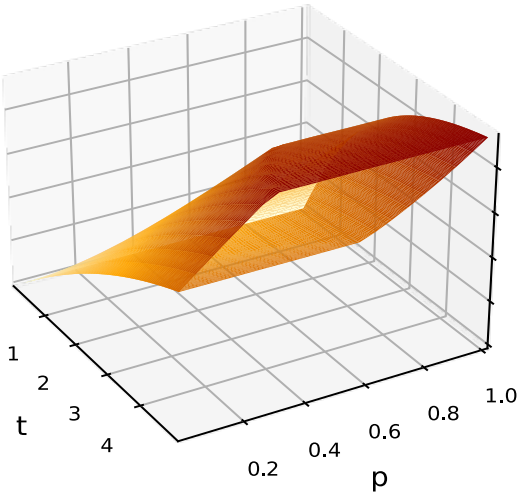
Simple ODE Relaxation

$$\frac{dx}{dt} = \exp(p)\sin(x)(2-x),$$
$$x(0) = 1, \quad p \in [0.01,1], \quad t \in [0,5]$$

Standard McCormick Relaxation



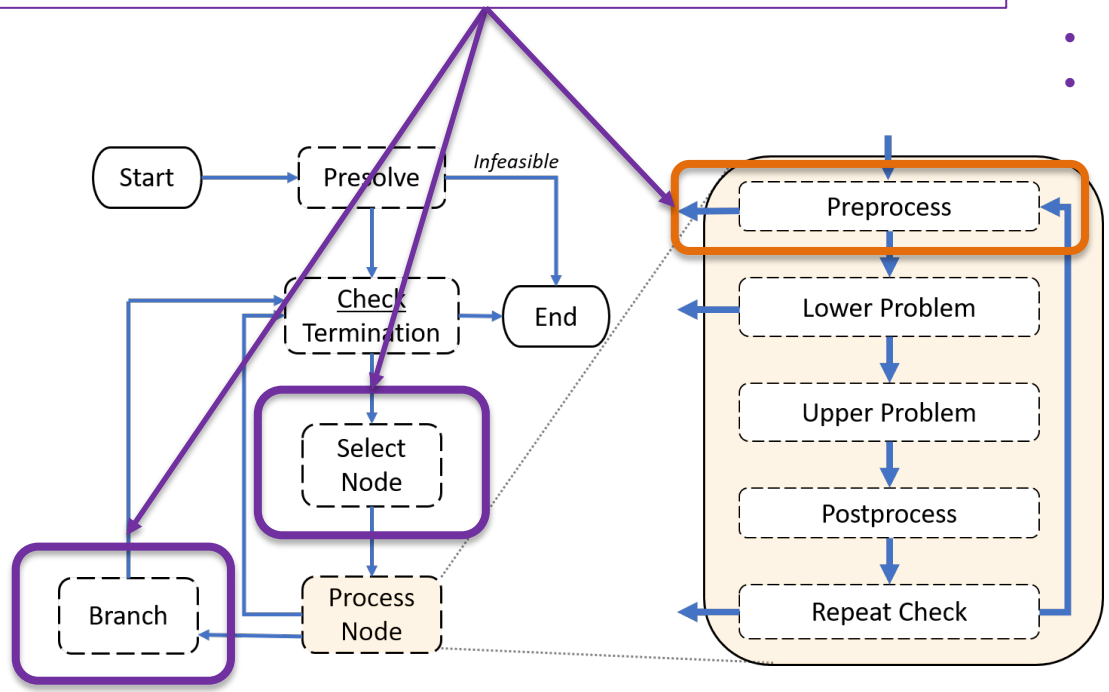
Improved Trilinear Term



14. Wilhelm, M. E., **DynamicBounds.jl**, (2020), GitHub repository, https://github.com/PSORLab/DynamicBounds.jl
15. Wilhelm, M. E., and M. D. Stuber. **EAGO.jl: easy advanced global optimization in Julia.** *Optimization Methods and Software* (2020): 1-26.

Improving EAGO with Machine Learning

Typically done by theoretically motivated heuristic



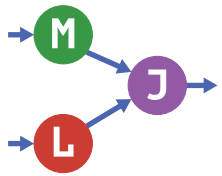
- Introduce auxiliary variable for subexpression?
- Select branch point or node?
- Use LP, SOCP, Convex relaxation?

EAGO.jl*: Extendable Low-Level Routines*

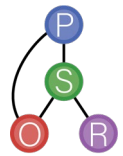
MINLPLib.jl*: Extendable Low-Level Routines*

Evolutionary.jl: *Genetic Programming*

MLJ.jl: *Random Forest Regression*
+ Interpretable Tools



3. Wilhelm, M.E., and Stuber, M.D. **EAGO.jl: easy advanced global optimization in Julia.** *Optimization Methods and Software*, 1-26.
16. Nagarajan, H. **MINLPLib.jl**, (2020), GitHub repository, https://github.com/lanl-ansi/MINLPLib.jl
17. Wild, A. **Evolutionary.jl**, (2014), GitHub repository, https://github.com/wildart/Evolutionary.jl
18. Bloam, A.D. et al. **MLJ: A Julia package for composable machine learning.** *Journal of Open Source Software*, 5 (55), p2704.



Conclusion

EAGO - an extensible deterministic global optimizer

- ❖ Architected for user-defined functions and routines
- ❖ High performance solver
- ❖ Open-source and free for non-commercial use

Future Outlook

- ❖ Parallel computing capability
- ❖ Further extension to domain specific Julia packages
- ❖ Performance improvements in core EAGO algorithms

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Questions?

Process Systems and Operations Research Laboratory

https://www.psor.uconn.edu

EAGO

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