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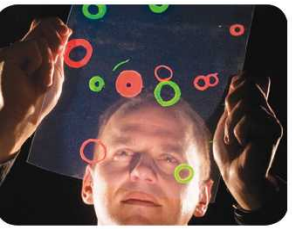

Recent developments in Pyomo

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Discrete Math & Optimization (1464)
Center for Computing Research
Sandia National Laboratories
Albuquerque, NM USA

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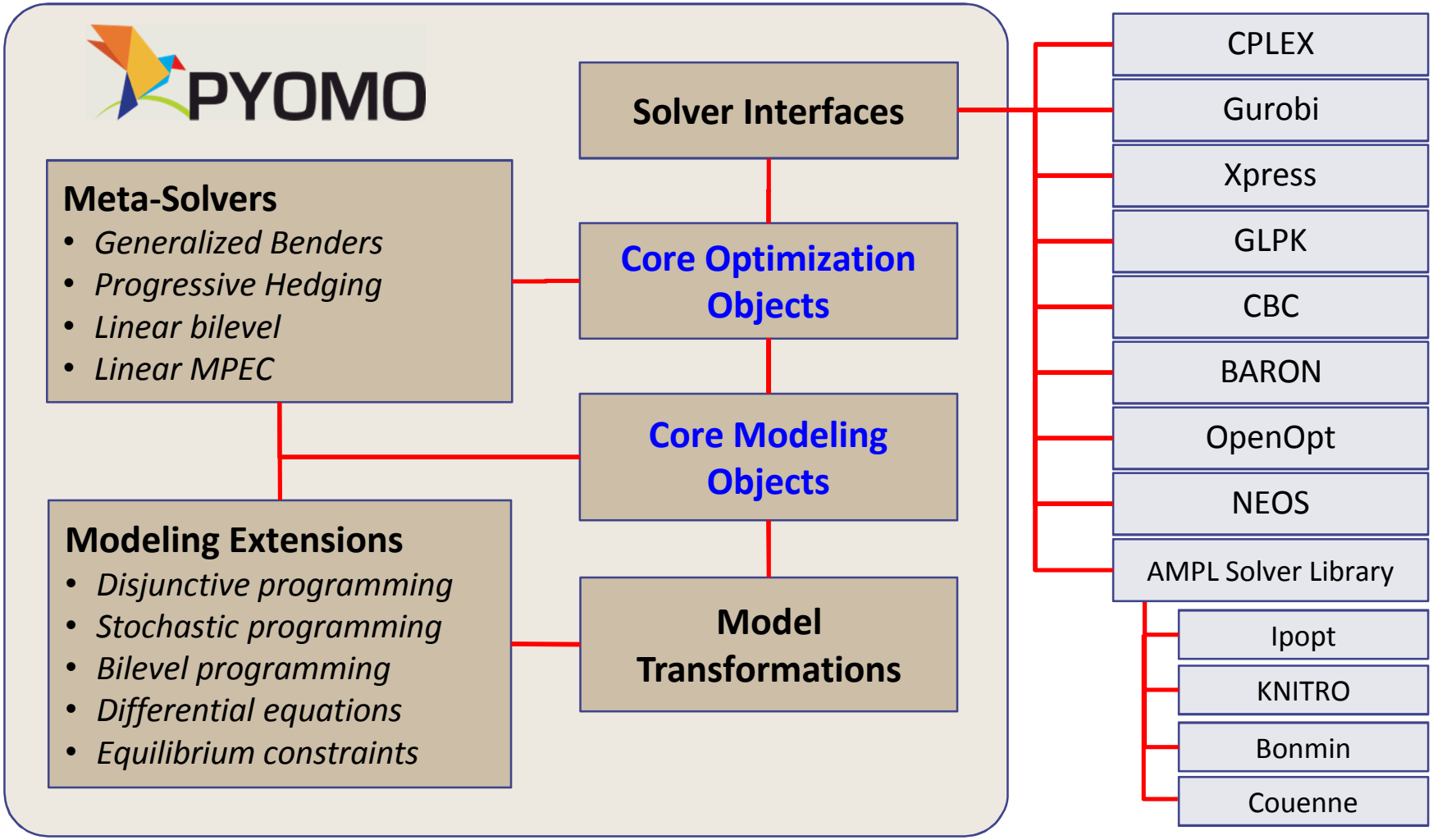
Pyomo: *Python Optimization Modeling Objects*



A Quick Tour of Pyomo

PYOMO

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Idea: a Pythonic framework for formulating optimization models

- Provides a natural syntax to describe mathematical models
- Leverages an extensible optimization object model
- Formulates large models with a concise syntax
- Separates modeling and data declarations
- Enables data import and export in commonly used formats

Highlights:

- Python provides a clean, readable syntax
- Python scripts provide a flexible context for exploring the structure of Pyomo models

```
from pyomo.environ import *

model = ConcreteModel()

model.x1 = Var()
model.x2 = Var(bounds=(-1,1))
model.x3 = Var(bounds=(1,2))

model.obj = Objective(
    expr= m.x1**2 + (m.x2*m.x3)**4 +
          m.x2*sin(m.x1+m.x3) + m.x2,
    sense= minimize)
```

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More than *just* mathematical modeling

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Scripting

- Construct models using native Python data
- Iterative analysis of models leveraging Python functionality
- Data analysis and visualization of optimization results

Model transformations (a.k.a. reformulations)

- Automate generation of one model from another
- Leverage Pyomo's object model to apply transformations sequentially
- E.g.: relax integrality, GDP -> Big M

Meta-solvers

- Integrate scripting and/or transformations into optimization solver
- Leverage power of Python to build "generic" capabilities
- E.g.: progressive hedging, SP extensive form -> MIP

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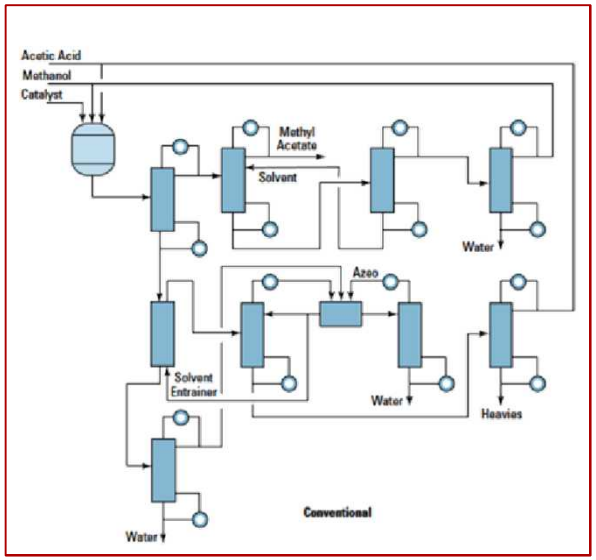
Motivation

- Institute for the Design of Advanced Energy Systems (IDAES)
  - Multi-year National Lab + University collaboration
    - Develop and utilize multi-scale, simulation-based computational tools and models to support the design, analysis, optimization, scale-up and troubleshooting of innovative, advanced fossil energy systems with carbon capture.
  - Next generation modeling and optimization platform
    - Flexible and open model
    - Complete provenance information
    - Supports advanced solvers and computer architecture
    - Intrusive UQ
    - Process Synthesis, Integration, and Intensification
    - Process Control and Dynamics
  - Built on Pyomo
    - IDAES has driven 2016 core Pyomo development



What are the “big” developments

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- Updated modeling
  - Improved Connector modeling component
  - Explicit unit annotation and verification
  - “Template” expressions
  - Support for efficiently slicing / iterating over hierarchical models
- New analysis
  - Ties to ODE simulators
- New algorithm / transformation support
  - Symbolic differentiation
  - Acceleration strategies for Progressive Hedging
- General
  - Improved installation support (pip)
  - “conda” channel for getting pyomo + solvers

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What are the “big” developments

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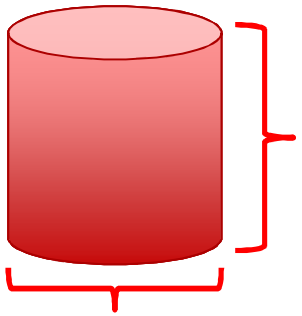
A trivial "Soda Can Example"

Problem: minimize the metal used in a soda can

minimize $2 \pi r (r + h)$ *# Surface Area*

with $\pi h r^2 = 355$ *# Volume*

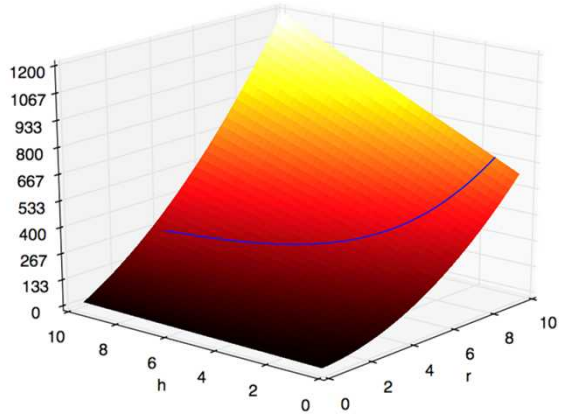



```
# sodacan.py
from pyomo.environ import *
from math import pi

M = ConcreteModel()
M.r = Var(bounds=(0,None), initialize=5.0)
M.h = Var(bounds=(0,None), initialize=15.0)

M.surf_area = Objective(expr=  2*pi*M.r*(M.r + M.h))
M.volume = Constraint(expr= pi*M.h*M.r**2 == 355)

SolverFactory('ipopt').solve(model)
print('-- optimal solution --\nradius: %0.2f\nheight: %0.2f\narea: %0.2f'
      % (value(model.r), value(model.h), value(model.surf_area)))
```



“Soda Can” with units

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```
# sodacan.py
from pyomo.environ import *
from math import pi
um = UnitsManager()

M = ConcreteModel()
M.r = Var(bounds=(0,None), initialize=5.0, units=um.cm)
M.h = Var(bounds=(0,None), initialize=15.0, units=um.cm)

M.surf_area = Objective(expr=  2*pi*M.r*(M.r + M.h))
M.volume = Constraint(expr= pi*M.h*M.r**2 == 355)

SolverFactory('ipopt').solve(model)
print('-- optimal solution --\nradius: %0.2f\nheight: %0.2f\narea: %0.2f'
      % (value(model.r), value(model.h), value(model.surf_area)))
```

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Check the "Soda Can" units

```
# sodacan.py
from pyomo.environ import *
from math import pi
um = UnitsManager(enable_units_checking=True)

M = ConcreteModel()
M.r = Var(bounds=(0,None), initialize=5.0, units=um.cm)
M.h = Var(bounds=(0,None), initialize=15.0, units=um.cm)

M.surf_area = Objective(expr=  2*pi*M.r*(M.r + M.h))
M.volume = Constraint(expr= pi*M.h*M.r**2 == 355)

um.check_units(model)

SolverFactory('ipopt').solve(model)
print('-- optimal solution --\nradius: %0.2f\nheight: %0.2f\narea: %0.2f'
      % (value(model.r), value(model.h), value(model.surf_area)))
```

Fix the "Soda Can" units

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```
# sodacan.py
from pyomo.environ import *
from math import pi
um = UnitsManager(enable_units_checking=True)

M = ConcreteModel()
M.r = Var(bounds=(0,None), initialize=5.0, units=um.cm)
M.h = Var(bounds=(0,None), initialize=15.0, units=um.cm)

M.surf_area = Objective(expr=  2*pi*M.r*(M.r + M.h))
M.volume = Constraint(expr= pi*M.h*M.r**2 == 355*um.cm**3)

um.check_units(model)

SolverFactory('ipopt').solve(model)
print('-- optimal solution --\nradius: %0.2f\nheight: %0.2f\narea: %0.2f'
      % (value(model.r), value(model.h), value(model.surf_area)))
```

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We *do not* do automatic conversion

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```
# sodacan.py
from pyomo.environ import *
from math import pi
um = UnitsManager(enable_units_checking=True)

M = ConcreteModel()
M.r = Var(bounds=(0,None), initialize=5.0, units=um.cm)
M.h = Var(bounds=(0,None), initialize=15.0, units=um.cm)

M.surf_area = Objective(expr=  2*pi*M.r*(M.r + M.h))
M.volume = Constraint(expr= pi*M.h*M.r**2 == 12*um.fluid_ounce)

um.check_units(model)

SolverFactory('ipopt').solve(model)
print('-- optimal solution --\nradius: %0.2f\nheight: %0.2f\narea: %0.2f'
      % (value(model.r), value(model.h), value(model.surf_area)))
```

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…but allow explicit conversion

```
# sodacan.py
from pyomo.environ import *
from math import pi
um = UnitsManager(enable_units_checking=True)

M = ConcreteModel()
M.r = Var(bounds=(0,None), initialize=5.0, units=um.cm)
M.h = Var(bounds=(0,None), initialize=15.0, units=um.cm)

M.surf_area = Objective(expr=  2*pi*M.r*(M.r + M.h))
M.volume = Constraint(expr= um.convert(pi*M.h*M.r**2, um.fluid_ounce)
                            == 12*um.fluid_ounce)
um.check_units(model)

SolverFactory('ipopt').solve(model)
print('-- optimal solution --\nradius: %0.2f\nheight: %0.2f\narea: %0.2f'
      % (value(model.r), value(model.h), value(model.surf_area)))
```

…and support custom units

```
# sodacan.py
from pyomo.environ import *
from math import pi
um = UnitsManager(enable_units_checking=True)
um.create_new_unit('can_of_coke', 'fluid_ounces', 101)

M = ConcreteModel()
M.r = Var(bounds=(0,None), initialize=5.0, units=um.cm)
M.h = Var(bounds=(0,None), initialize=15.0, units=um.cm)

M.surf_area = Objective(expr=  2*pi*M.r*(M.r + M.h))
M.volume = Constraint(expr= um.convert(pi*M.h*M.r**2, um.can_of_coke)
                                == 1*um.can_of_coke)
um.check_units(model)

SolverFactory('ipopt').solve(model)
print('-- optimal solution --\nradius: %0.2f\nheight: %0.2f\narea: %0.2f'
  % (value(model.r), value(model.h), value(model.surf_area)))
```

Checking offset units is … *nuanced*

- Offset units (units without a common origin) are challenging:
  - $27°\mathrm{C} + 27°\mathrm{C} = 54°\mathrm{C}$

Checking offset units is … *nuanced*

- Offset units (units without a common origin) are challenging:
  - $27°\mathrm{C} + 27°\mathrm{C} = 54°\mathrm{C}$
- Addition of two offset units does not make sense!
  - "Proof": converting terms to other units shouldn't change truth
    - $300\mathrm{K} + 300\mathrm{K} = 600\mathrm{K}, \quad 600\mathrm{K} \neq 54°\mathrm{C}$
  - Corrected: "delta units"
    - $27°\mathrm{C} + 27\Delta°\mathrm{C} = 54°\mathrm{C}$
- Subtraction of offset units yields delta units
  - $50°C - 30°C = 20\Delta°\mathrm{C}$
- This does not "play well" with non-units aware model manipulation.
  - For the time being, offset units are not allowed in expressions
    - But explicit conversion is OK.

pyomo.dae recent developments

- Interface to ODE integrators in Scipy for:
  - Simulating systems of ODEs
  - Initializing discretized dynamic optimization problems
  - Verifying dynamic optimization solutions

- Demonstrated compatibility with other Pyomo extensions like PySP for stochastic programming
  - Dynamic systems under uncertainty
    - Parameter estimation
    - Optimal control

Interfacing with Scipy integrators

$$\frac{d\theta}{dt} = \omega$$

$$\frac{d\omega}{dt} = -b * \omega - c * \sin\theta$$

$$\theta(0) = \pi - 0.1, \quad \omega(0) = 0$$

```
from pyomo.environ import *
from pyomo.dae import *

model = ConcreteModel()

model.t = ContinuousSet(bounds=(0.0, 10.0))

model.b = Param(initialize=0.25)
model.c = Param(initialize=5.0)

model.omega = Var(model.t)
model.theta = Var(model.t)

model.domegadt = DerivativeVar(model.omega, wrt=model.t)
model.dthetadt = DerivativeVar(model.theta, wrt=model.t)

model.omega[0] = 0.0
model.theta[0] = 3.14 - 0.1

def _diffeq1(m,t):
    return m.dthetadt[t] == m.omega[t]
model.diffeq1 = Constraint(model.t, rule=_diffeq1)

def _diffeq2(m,t):
    return m.domegadt[t] == -m.b*m.omega[t] \
        - m.c*sin(m.theta[t])
model.diffeq2 = Constraint(model.t, rule=_diffeq2)
```

- ODE model simulation

```
mysim = Simulator(model, package='scipy')
mysim.simulate()
```

- Model initialization

```
discretizer = TransformationFactory('dae.collocation')
discretizer.apply_to(model, nfe=8, ncp=5)

mysim.initialize_model()
```

Interface with Scipy integrators

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System of ODEs

$$\frac{d\theta}{dt} = \omega$$
$$\frac{d\omega}{dt} = -b * \omega - c * \sin\theta$$
$$\theta(0) = \pi - 0.1, \quad \omega(0) = 0$$

Pyomo Model

```
from pyomo.environ import *
from pyomo.dae import *

m = ConcreteModel()

m.t = ContinuousSet(bounds=(0.0, 10.0))

m.b = Param(initialize=0.25)
m.c = Param(initialize=5.0)

m.omega = Var(m.t)
m.theta = Var(m.t)

m.domegadt = DerivativeVar(m.omega, wrt=m.t)
m.dthetadt = DerivativeVar(m.theta, wrt=m.t)

m.omega[0] = 0.0
m.theta[0] = 3.14 - 0.1

def _diffeq1(m,t):
    return m.dthetadt[t] == m.omega[t]
m.diffeq1 = Constraint(m.t, rule=_diffeq1)

def _diffeq2(m,t):
    return m.domegadt[t] == -m.b*m.omega[t] \
        - m.c*sin(m.theta[t])
m.diffeq2 = Constraint(m.t, rule=_diffeq2)
```

Simulate and/or initialize optimization model

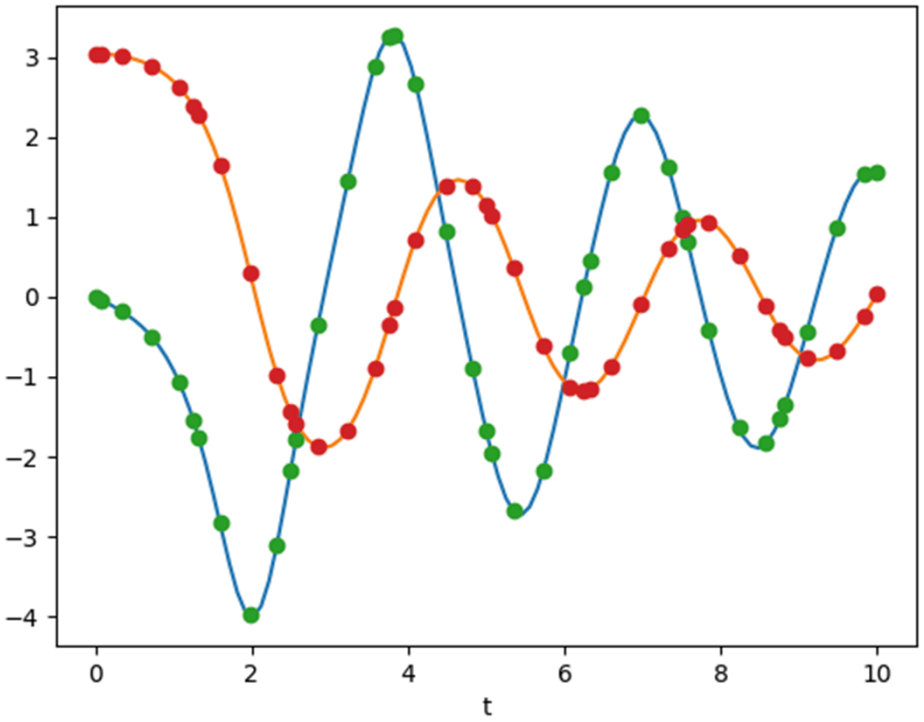
- ODE model simulation

```
mysim = Simulator(m, package='scipy')
mysim.simulate()
```

- Model initialization

```
discretizer = TransformationFactory('dae.collocation')
discretizer.apply_to(m, nfe=8, ncp=5)

mysim.initialize_model()
```



Omega simulated

Theta simulated

Omega initialized at discretization points

Theta initialized at discretization points

Use the same Pyomo model for simulation and optimization!

Stochastic programming in PySP

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- PySP provides a convenient framework for describing and generating stochastic programming problems in Pyomo
- Our workhorse algorithm is Progressive Hedging
  - Scenario-based decomposition
    - "No" master problem
    - One subproblem per scenario
    - Relax nonanticipativity constraints
  - Iteratively converge the stage nonanticipativity constraints
    - Penalize decision variable value by weight $w^T x$
    - Penalize deviation from average, $\rho \, \|x - \bar{x}\|^2$
    - Update w using ρ

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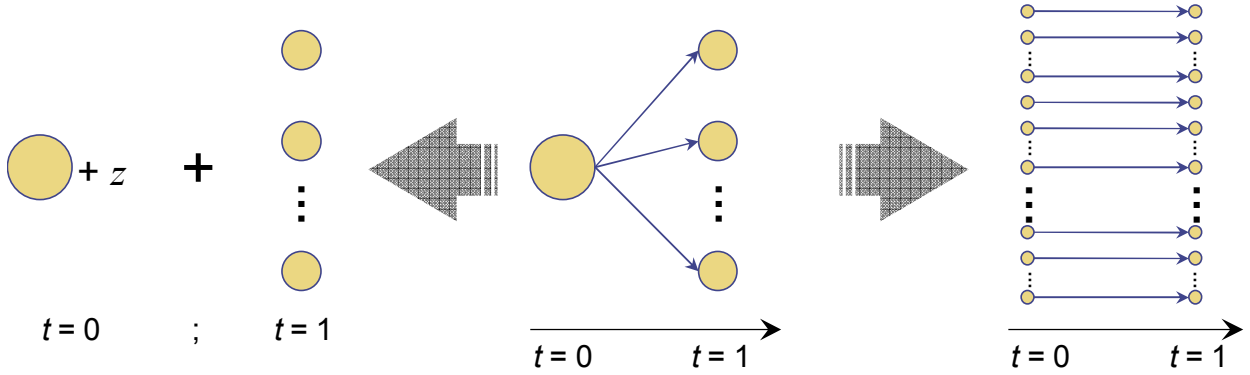
PH: Benefits and open challenges

- PH avoids many of the challenges experienced by Benders
  - No restriction on stage variable domains (discrete 2nd stage OK)
  - "Trivially" extends to multistage problems
  - No master problem, no cuts generated: no problem "bloat"

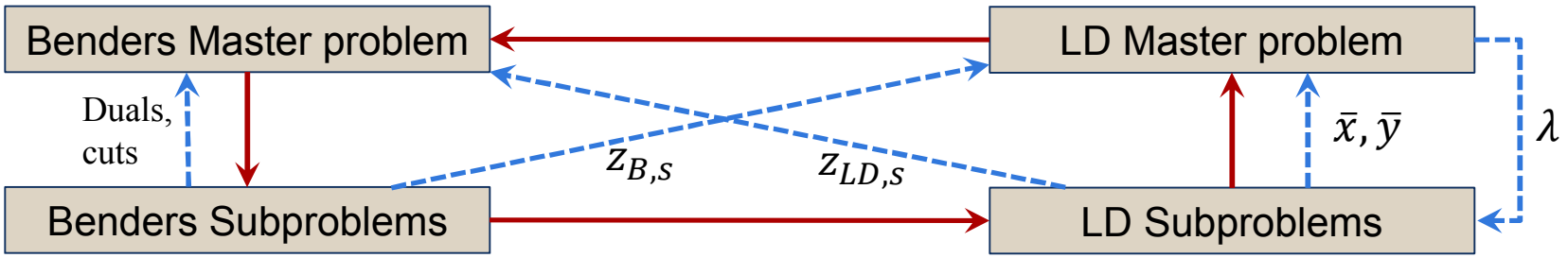
- BUT…
  - Not provably convergent for the discrete case
    - …although bounds exist on the quality of solution you get
  - "Infeasible path" algorithm
  - Discrete variable cycling
  - Slow convergence due to "holdout" scenarios
  - How to choose ρ???

We will attempt to address these challenges

PH + Benders: orthogonal decompositions

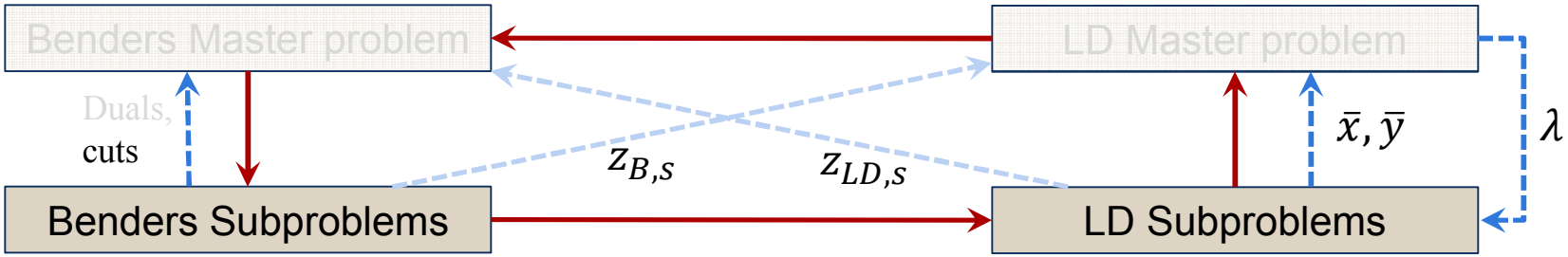


- Can we leverage ideas from each to accelerate the other?
  - Related: Cross Decomposition (Lagrangean Decomposition + Benders)
    - [Van Roy 1983; Holmberg, 1990; Mitra,et al. 2016]

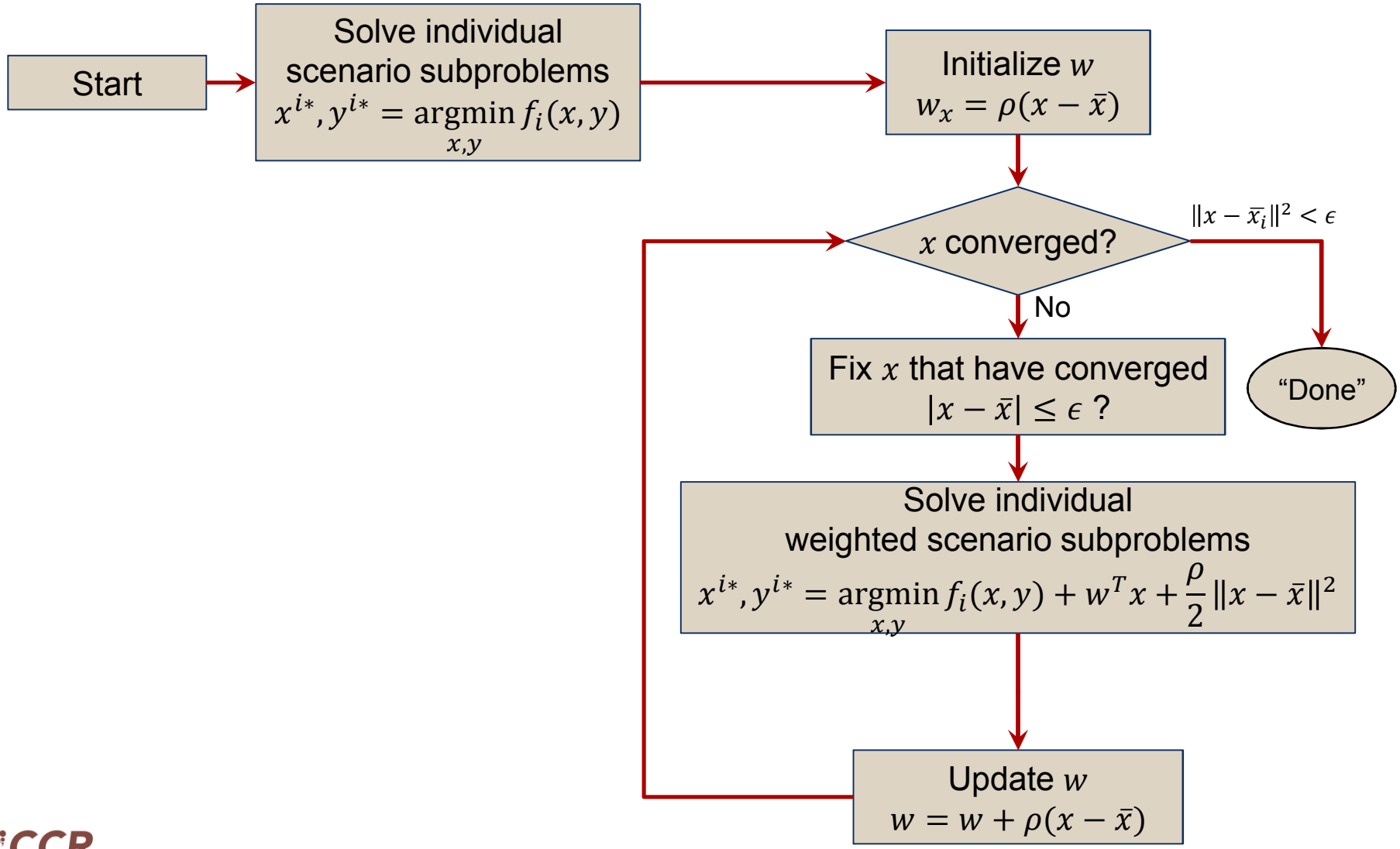


Cross Decomposition for PH?

- Challenges with naïve Cross Decomposition for PH
  - No LD Master problem
  - Discrete second stage variables
  - PH subproblems do not provide proper Lagrangean bounds
    - Except at *iteration 0*



Progressive Hedging: the algorithm



Improving PH: borrowing from Benders

- Consider the Benders "feasibility" cut:
  - Given x^* computed by the RMP, if (dual) subproblem is unbounded, add a cut determined by an extreme ray in the dual space to the RMP
- In PH, a similar operation would be fix the values of x in subproblem f_j to the values computed by subproblem f_i:

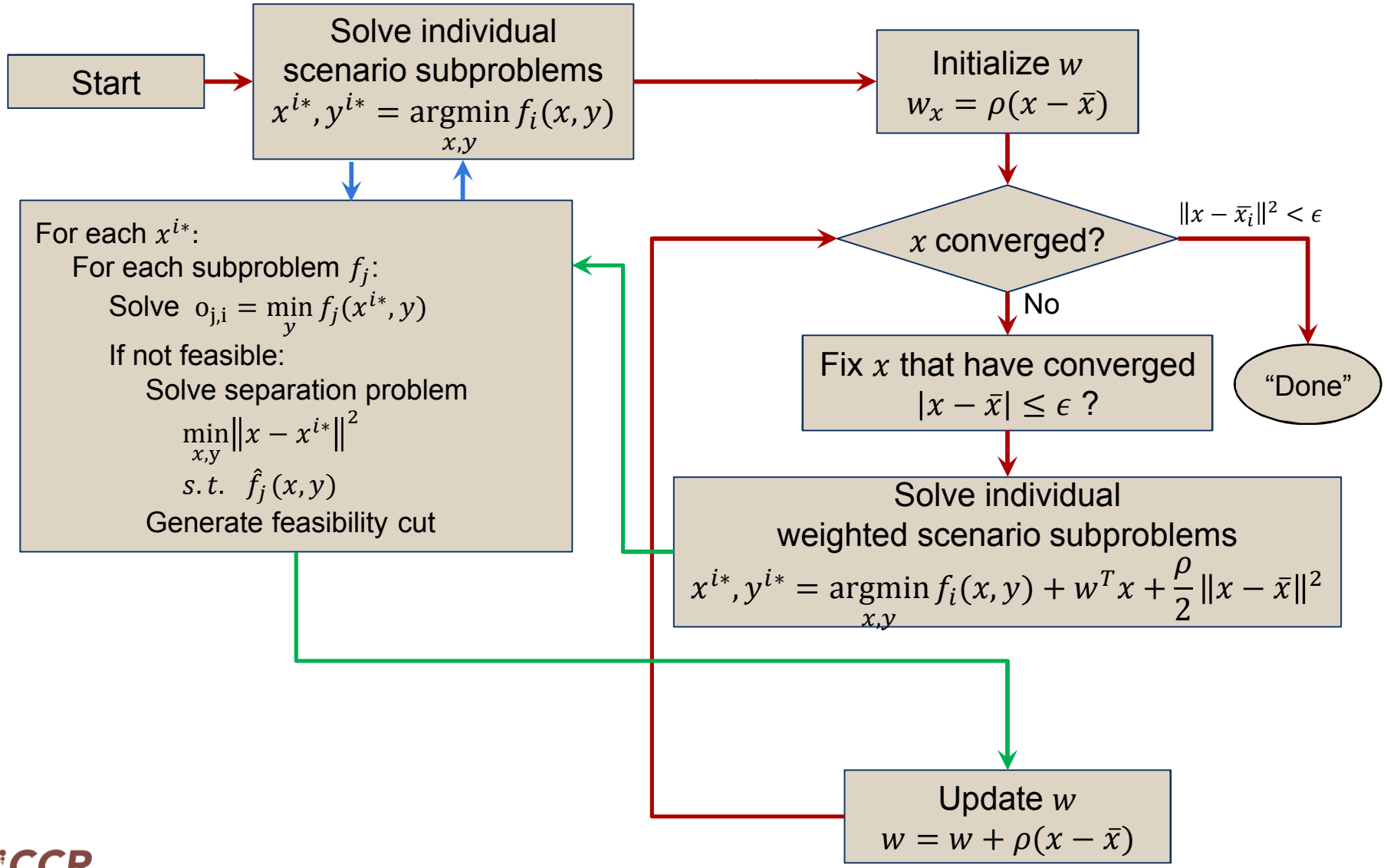
$$\min_y f_j(x^{i*}, y)$$

  - If the problem is infeasible, then we can solve a separation problem (in the primal space) to determine a valid cut in the 1st-stage variables:

$$\min_{x,y} \|x - x^{i*}\|^2$$
$$s.t. \quad \hat{f}_j(x, y)$$

  - Notes:
    - $\hat{f}_j$ is the continuous relaxation of f_j → not guaranteed to generate a cut
    - The resulting cut is valid for *all* scenario subproblems
    - $\sum p_i f_i(x^{i*}, y^{i*})$ for initial scenario solves ($w = 0$) gives Lagrangian bound

PH + feasibility



Case study: stochastic network flow

- 2-stage stochastic network flow from [Watson & Woodruff, 2011]:
  - 1st stage variables:
    - $x_a \; \forall \; a \in Arcs; \; \{x_a |\; x_a \in R, 0 \leq x_a \leq x_a^{UB}\}$ Capacity of Arc a
    - $b_a^0 \; \forall \; a \in Arcs; \quad \mathrm{b_a^0} \in \{0,1\}$ Arc a is available
  - 2nd stage variables:
    - $y_a^s \; \forall \; a \in Arcs, s \in Scenarios; \; \{y_a^s \mid y_a^s \in R, 0 \leq y_a^s \leq x_a\}$ Flow across Arc a in scenario s
    - $b_a^s \; \forall \; a \in Arcs, s \in Scenarios; \quad \mathrm{b_a^s} \in \{0, b_a^s\}$ Arc a is in use for scenario s
- PH ($\rho = 100$, with "Watson-Woodruff" extensions)
  - Significant cycling (no convergence after 1000 iterations)
- PH ($\rho = 100$, with WW extensions, with feasibility cuts)
  - Converges in 42 iterations (objective: 164426, 2726 seconds)
  - 6 preliminary cut passes: raises Lagrangian LB 135085 → 148656

Case study: UC + *N-1* + switching

- 2-stage unit commitment model for the electric power grid
  - 24-hour horizon, 1-hour commitment intervals
  - Explicitly include *N-1* analysis (loss of any 1 generator / non-radial line)
    - Each contingency modeled as a no-cost recourse scenario
    - Line switching (opening /closing a line) in 1st and 2nd stages

- Case 1: 5 busses, 7 generators (13 scenarios):
  - Optimal solution (extensive form): 19.9756
  - Default PH ($\rho = 1$):
    - 17 iterations, objective = 22.9997, total time 123 seconds
  - PH ($\rho = 1$) + Feasibility cuts:
    - 3 feasibility cut iterations at PH iteration 0
      - Improved Lagrangean bound from 19.7 to 19.88
    - 12 iterations, objective = 20.11, total time 568 seconds

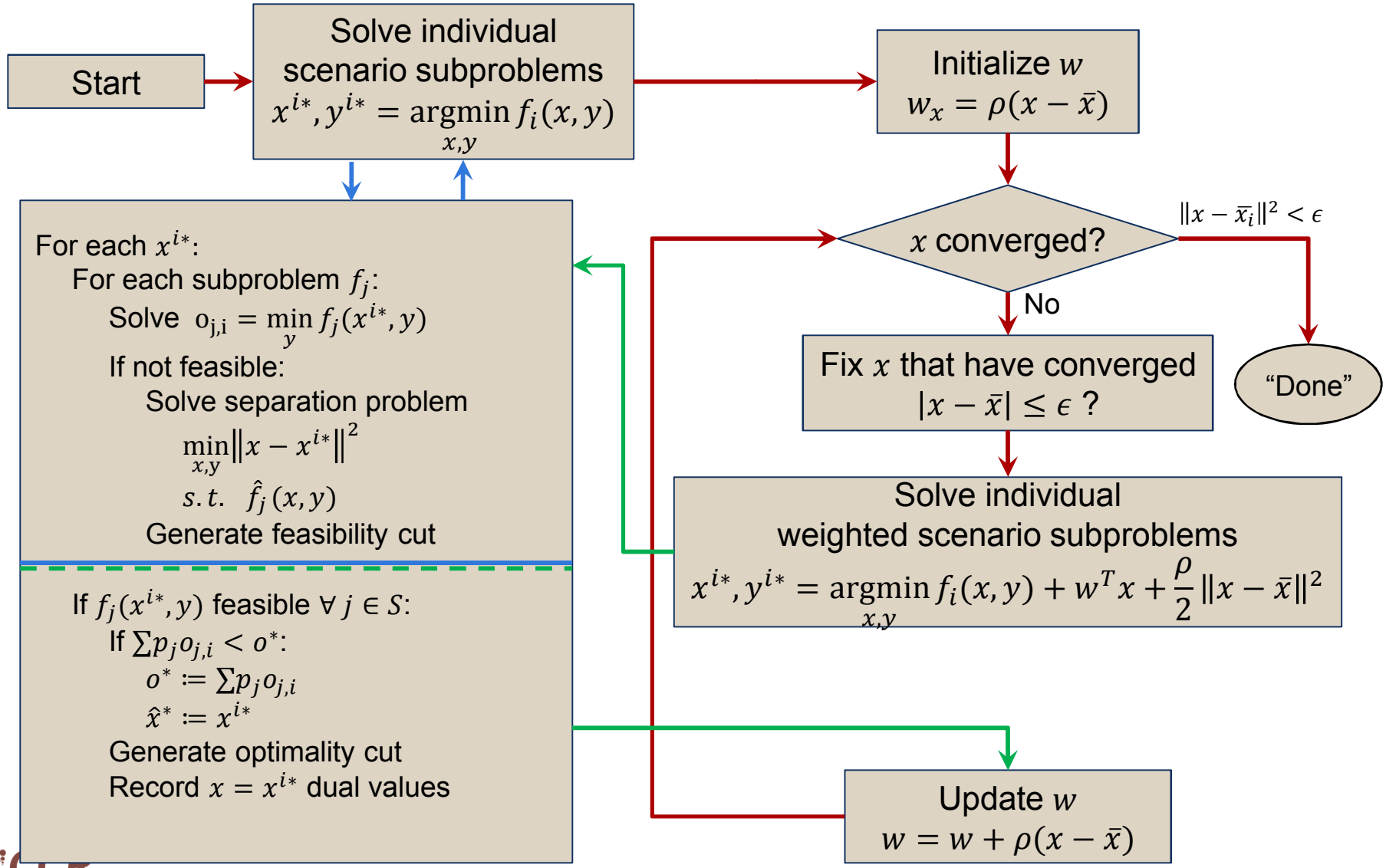
Improving PH: borrowing from Benders

- What happens if the subproblem $\min_y f_i(x^{j*}, y)$ is feasible?
  - The 1st stage decisions are valid in this scenario
  - If x^{j*} is valid in ALL scenarios, then x^{j*} satisfies nonanticipativity and the expectation of the subproblems forms a valid upper bound

$$E[f(x^*, y)] \leq E\left[f\left(x^{j*}, y\right)\right]$$

- If the first stage variables are all discrete
  - Repeating this process for all x^{i*} and identify additional nonanticipative solutions, then the upper bound can be used to generate *optimality cuts* to exclude sub-optimal solutions
  - These cuts are also valid on all scenario subproblems

PH + feasibility + optimality cuts



Case Studies: *farmer*

- 3-scenario farmer problem [Birge & Louveaux]
  - Integer acreage allocations
  - Cplex 12.5
    - PH ($\rho = 1$): 297 iterations, 21.55 seconds: objective = -108390
    - PH + optimality: 47 iterations, 8.75 seconds: objective = -108390

Case Studies: *farmer*

- 3-scenario farmer problem [Birge & Louveaux]
  - Integer acreage allocations
  - Cplex 12.5
    - PH ($\rho = 1$): 297 iterations, 21.55 seconds: objective = -108390
    - PH + optimality: 47 iterations, 8.75 seconds: objective = -108390
- Very sensitive to the solver!
  - Gurobi 6.0.4
    - PH ($\rho = 1$): 39 iterations, 1.09 seconds: objective = -108390
    - PH + optimality: 154 iterations, 16.4 seconds: objective = -108390

Case Studies: *farmer*

- 3-scenario farmer problem [Birge & Louveaux]
  - Integer acreage allocations
  - Cplex 12.5
    - PH ($\rho = 1$): 297 iterations, 21.55 seconds: objective = -108390
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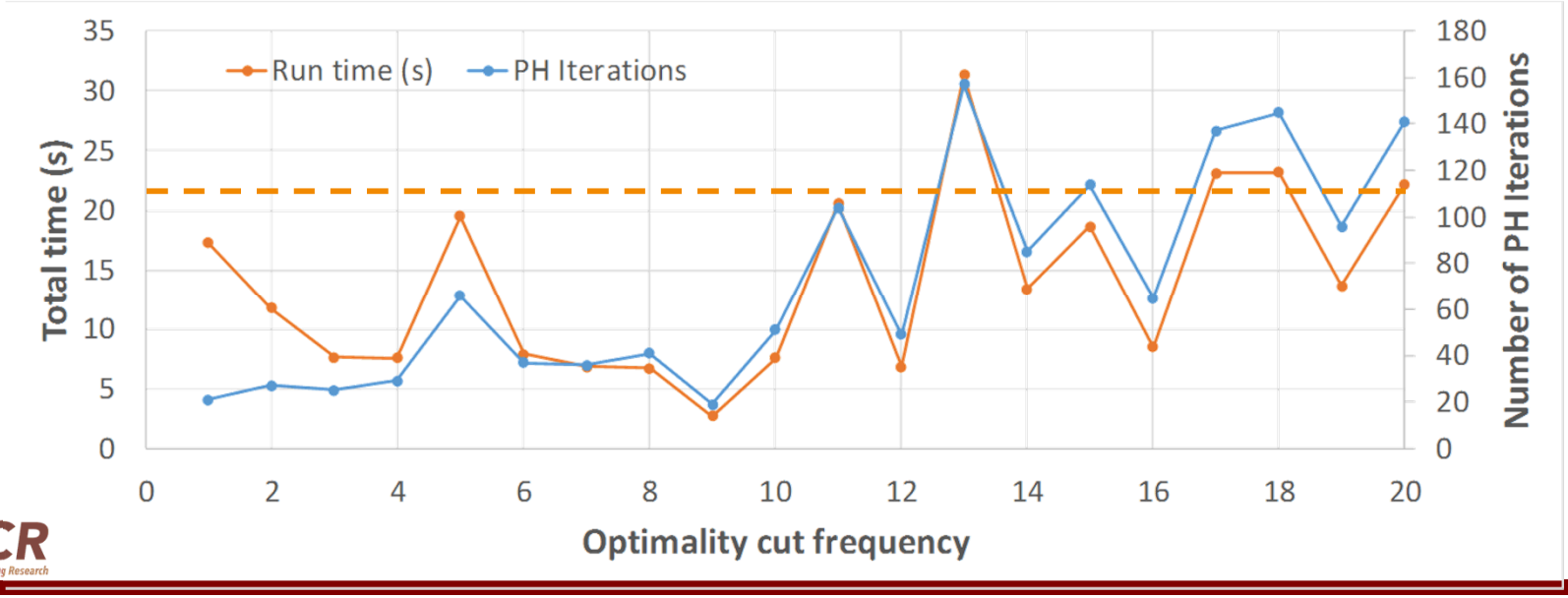
- Very sensitive to the strategy!



Case study: Stochastic Unit Commitment

- Unit commitment under demand uncertainty
  - 24 hour horizon, 1-hour intervals

- Case 1: 5 busses, 7 generators, 3 load scenarios
  - Optimal solution (extensive form): 348.98
  - Default PH ($\rho = 10$):
    - Significant cycling (no convergence after 100 iterations)
  - PH ($\rho = 10$) + Optimality cuts:
    - 20 iterations, objective = 348.9835

Improving PH: setting ρ

- How do we get "good" values of ρ?
  - Currently: experimentation
  - Challenge: ρ is problem dependent
    - Too low and PH never converges
    - Too high and PH rapidly converges to suboptimal solution
  - Hint: scale relative to cost of each variable [Watson & Woodruff, 2011]

$$\rho_i \propto \frac{C_i}{\left|x_i^{min} - x_i^{max} + 1\right|}$$

- We can get good cost estimates from the subproblem duals
  - When we evaluate $f_j(x^{i*}, y)$, record the duals for $x = x^{i*}$
  - Compute average duals weighted relative to scenario probability

Case Studies: *farmer*

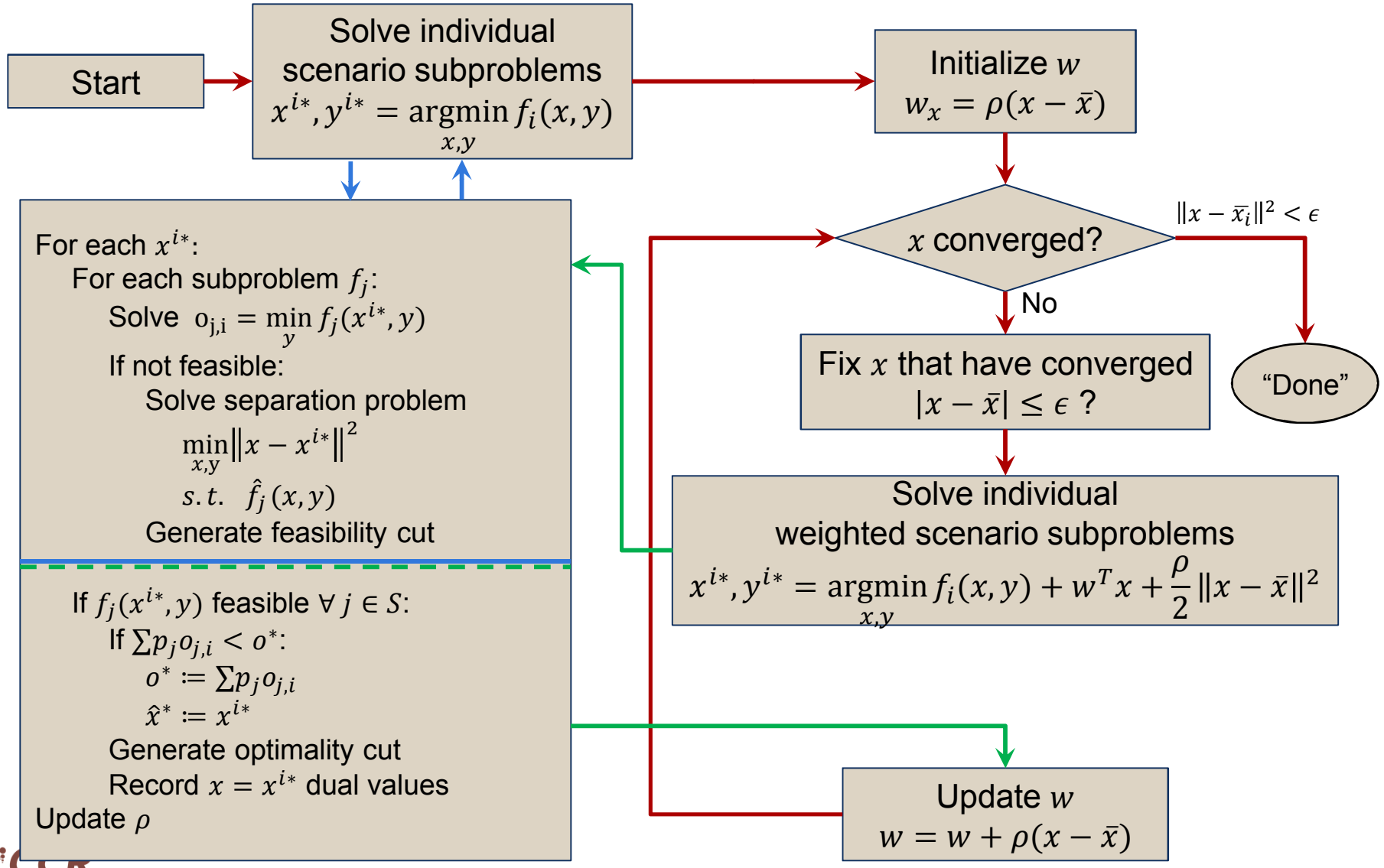
- 3-scenario farmer problem [Birge & Louveaux]
  - Continuous acreage allocations
    - PH ($\rho = 1$):
      - 33 iterations, 1.06 seconds: objective = -108388.7726
    - PH + ρ setter:
      - 34 iterations, 1.34 seconds: objective = -108389.7811
  - Discrete acreage allocations
    - PH ($\rho = 1$):
      - 39 iterations, 1.09 seconds: objective = -108390
    - PH + optimality cuts:
      - 154 iterations, 16.4 seconds: objective = -108390
    - PH + optimality cuts + ρ setter:
      - 40 iterations, 4.42 seconds: objective = -108390

Case studies: UC + *N-1* analysis

- Recall:
  - Optimal solution (extensive form): 19.9756
  - Default PH ($\rho = 1$):
    - 17 iterations, objective = 22.9997, total time 123 seconds
  - PH ($\rho = 1$) + Feasibility cuts:
    - 3 feasibility cut iterations at PH iteration 0
      - Improved Lagrangian bound from 19.7 to 19.88
    - 12 iterations, objective = 20.11, total time 568 seconds

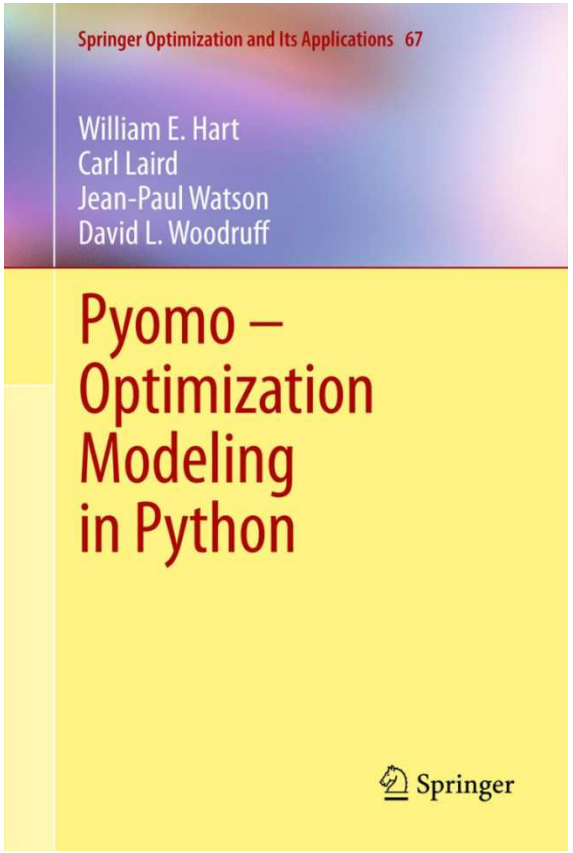
- Now:
  - PH + Feasibility cuts + ρ setter
    - 20 iterations, objective = 19.9808, total time 494 seconds

PH + feasibility + optimality cuts+ ρ



For more information…

- Project homepage
  - http://www.pyomo.org
  - https://github.com/Pyomo/pyomo
- Mailing lists
  - "pyomo-forum" Google Group
  - "pyomo-developers" Google Group
- "The Book"
  - Second edition going to press in O(days)



- Mathematical Programming Computation paper:
  - Pyomo: Modeling and Solving Mathematical Programs in Python (3(3), 2011)

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