Bridging Machine Learning and Optimization with JuMP

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Highlights

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- AI & Optimization: Friends and Foes.
- JuMP and Deep Learning: How to Train Optimization Surrogates?
- Julia’s Multiple Dispatch: It is Great when Things Just Work.
- JuMP and Reinforcement Learning: How to Train Policies?
- Hopes and Plans for the Future!

AI & Optimization: Friends and Foes

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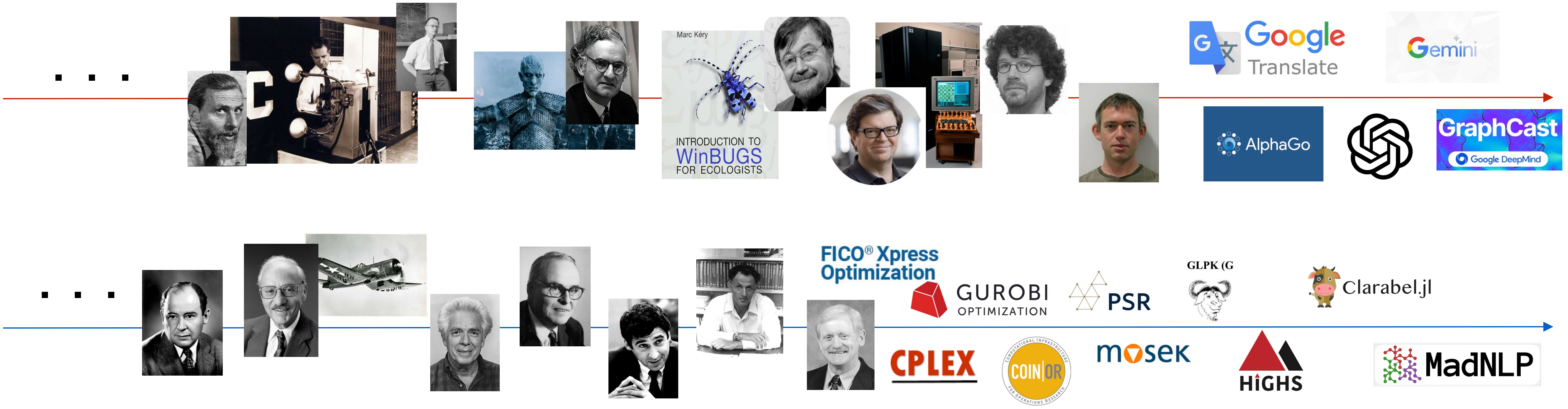

- AI & ML mostly concerned with Descriptive / Predictive Problems
  - RL: Failures to then positive results
- Optimization focused on Prescriptions
  - Uncertainty: Stochastic / Robust Optimization

AI & Optimization: Finally, Friends?

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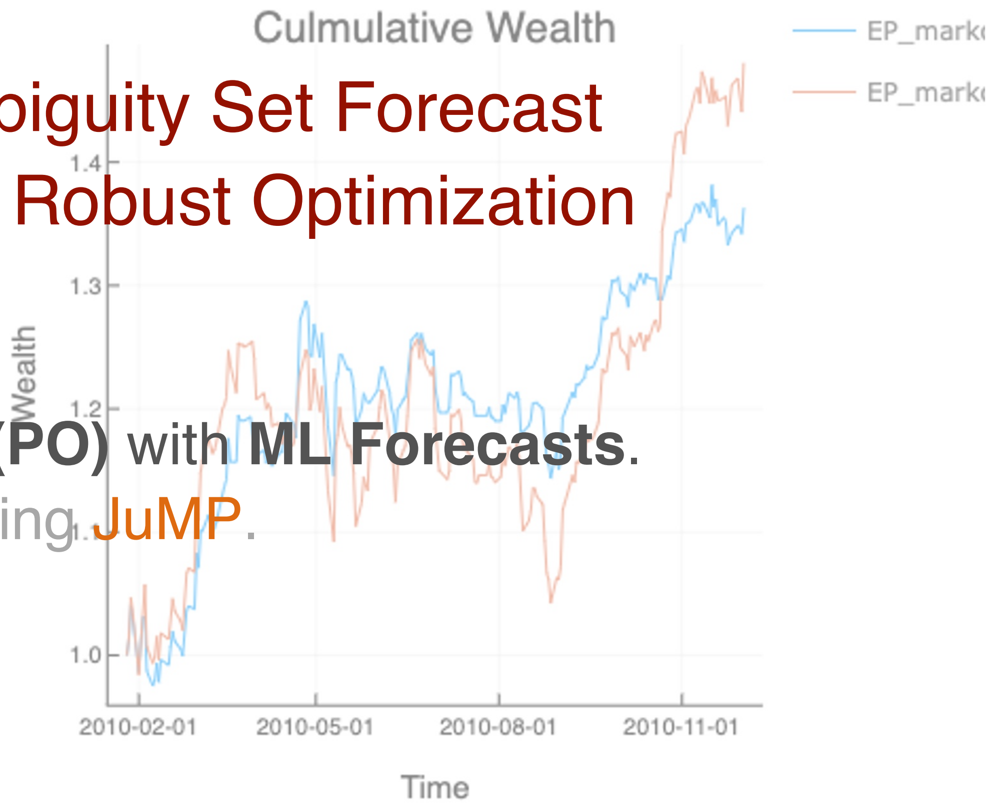
- Predict than Optimize
  - Point Prediction / Scenario Selection / Ambiguity Set Forecast
  - Deterministic / Stochastic / Distributionally Robust Optimization

At [redacted],
JuMP allowed complicated **Portfolio Optimization (PO)** with **ML Forecasts**.
» PortfolioOpt.jl: Portfolio Optimization (PO) using JuMP.



- Predict than Optimize – than loop
  - Application's aware objective for ML models

DiffOpt (Differential Optimization) allowed us to feedback financial PO performance to ML-Models.

AI & Optimization: Teammates!

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- Parametric - Optimization Problems
  - Repetitive (Learnable) structure – What can we do?

$$
\begin{aligned}
\min_{\mathbf{x}} \quad & \mathbf{c}_\beta^\top \mathbf{x} \\
\text{s.t.} \quad & \mathbf{A}_\beta \mathbf{x} = \mathbf{b}_\beta \\
& \mathbf{x} > 0
\end{aligned}
$$

Proxy

$$\beta \rightarrow f(x)$$

$$\beta \rightarrow x$$

$$\beta \rightarrow \mathbf{c}_\beta^\top \mathbf{x}$$

Old News: Learning Value Functions

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$$\mathbf{x} \to \mathbb{E}[\mathcal{Q}(\mathbf{x}, \omega)]$$

$$1^{\text{st}} \text{ Stage} \begin{cases} \min\limits_{\mathbf{x}} & c^T\mathbf{x} + \mathbb{E}[\mathcal{Q}(\mathbf{x}, \omega)] \\ \text{s.t.} & \mathbf{x} \in \mathcal{X} \end{cases}$$

Convexity for Tractability

$$2^{\text{nd}} \text{ Stage} \left\{ \mathcal{Q}(\mathbf{x}, \omega) = \left\{ \begin{array}{ll} \min\limits_{y} & g^T y \\ \text{s.t.} & Ay = b(\omega) - H\mathbf{x} \\ & y \in \mathcal{Y} \end{array} \right\} . \right.$$

Using Value Functions Approximations

- Cutting Planes

$$\begin{aligned} \min_{\mathbf{x}} \quad & c^T\mathbf{x} + \Theta \\ \text{s.t.} \quad & \Theta \geq \bar{g}_k + \bar{\pi}_k^T H(-\mathbf{x}) \qquad \forall k = 1..K \end{aligned}$$

$\bar{\pi}$ $\bar{g}$

$\mathbf{x}$

$$\begin{aligned} \min_{y} \quad & g^T y \\ \text{s.t.} \quad & Ay = b(\omega) - H \ldots \pi(\omega) \\ & y \in \mathcal{Y} \end{aligned}$$

Expensive

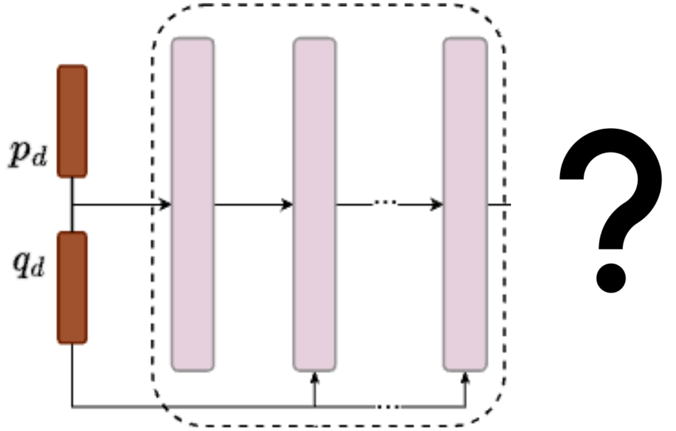
Using Value Functions Approximations

- Cutting Planes

$$\begin{aligned} \min_{\mathbf{x}} \quad & c^T\mathbf{x} + \Theta \\ \text{s.t.} \quad & \Theta \geq \bar{g}_k + \bar{\pi}_k^T H(-\mathbf{x}) \qquad \forall k = 1..K \end{aligned}$$

$\bar{\pi}$ $\bar{g}$

$\mathbf{x}$



$\mathbf{x} \rightarrow \mathbb{E}[\mathcal{Q}(\mathbf{x}, \omega)]$

Input-Convex Neural Network (ICNN)

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$$\mathbf{x}^k = h^k(\mathbf{x}^{k-1}) = \mathrm{ReLU}(W^k\mathbf{x}^{k-1} + H^k\mathbf{x}^0 + d^k), \qquad (9)$$

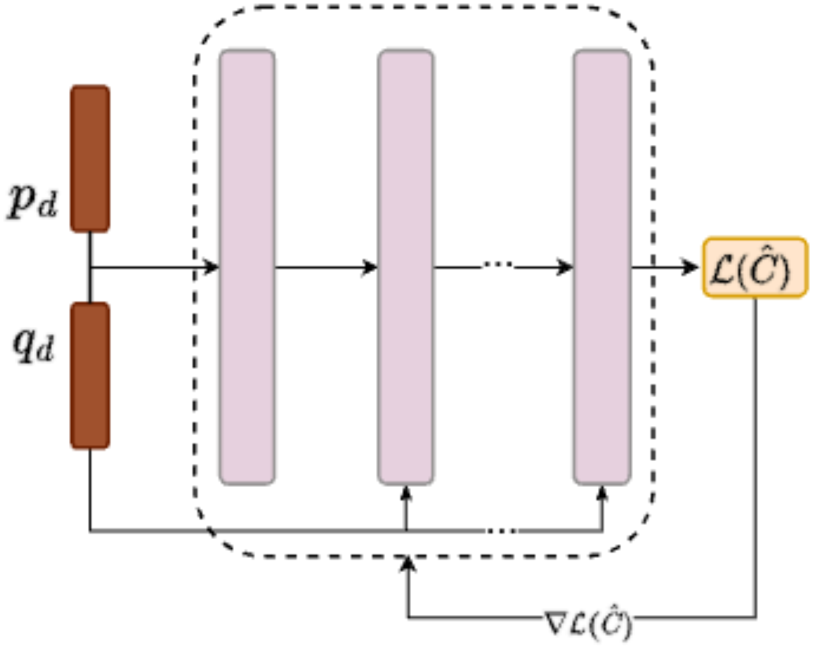
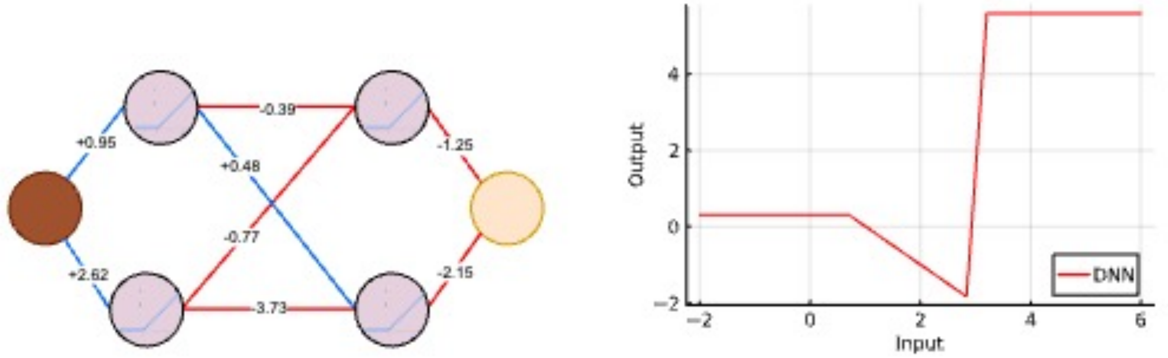
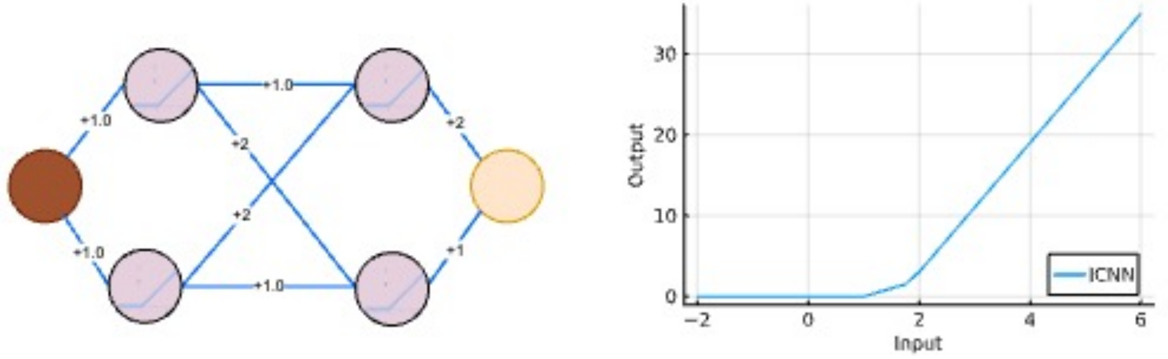


Fig. 2. Fully Connected ICNN



(a) Example DNN (left) and its Output (right). The DNN defines a non-convex function.



(b) Example ICNN (left) and its Output (right). All ICNN weights are positive and it defines a convex function.

Fig. 1. Illustration of Input-Convex Neural Networks.

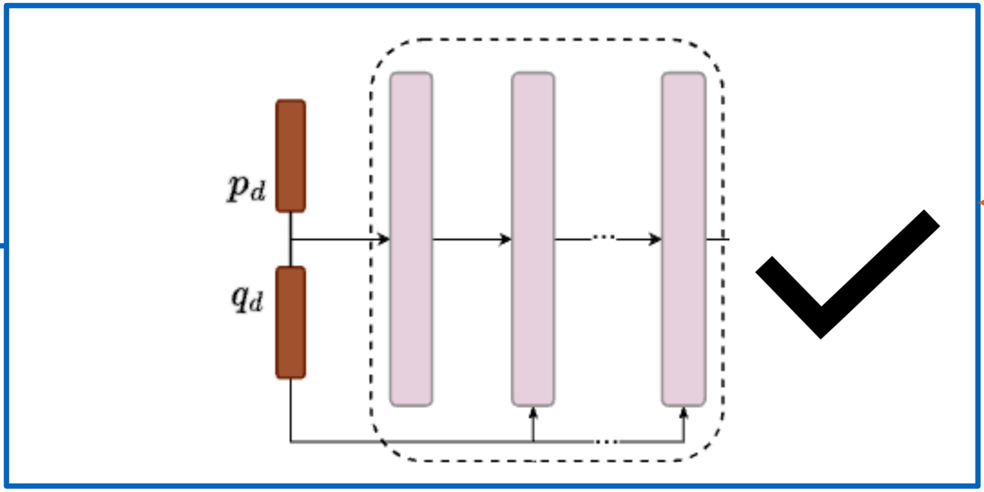
Using Value Functions Approximations

- Cutting Planes

$$
\begin{aligned}
\min_{\mathbf{x}} \quad & c^T\mathbf{x} + \Theta \\
\text{s.t.} \quad & \Theta \geq \bar{g}_k + \bar{\pi}_k^T H(-\mathbf{x}) \qquad\qquad \forall k = 1..K
\end{aligned}
$$

$\bar{\pi}$ $\bar{g}$

$\mathbf{x}$



Can ICNNs approximate OPF value functions?

$$1^{\text{st}}\ \text{Stage}\begin{cases}\min\limits_{\mathbf{x}} & c^T\mathbf{x} + \mathbb{E}[\mathcal{Q}(\mathbf{x},\omega)] \\ \text{s.t.} & \mathbf{x} \in \mathcal{X}\end{cases}$$

$$2^{\text{nd}}\ \text{Stage}\left\{\ \mathcal{Q}(\mathbf{x},\omega) = \right.$$

Model 1 The AC-OPF Model

$$
\begin{aligned}
\min \quad & \sum_{i \in \mathcal{N}} c_i \mathbf{p}_i^{\text{g}} & \\
\text{s.t.} \quad & \mathbf{S}_i^{\text{g}} - \text{S}_i^{\text{d}} - (Y_i^s)^\star |\mathbf{V}_i|^2 = \sum_{ij \in \mathcal{E} \cup \mathcal{E}^R} \mathbf{S}_{ij}^{\text{f}} & \forall i \in \mathcal{N} \\
& \mathbf{S}_{ij}^{\text{f}} = (Y_{ij} + Y_{ij}^c)^\star |\mathbf{V}_i|^2 - Y_{ij}^\star \mathbf{V}_i \mathbf{V}_j^\star & \forall ij \in \mathcal{E} \\
& \mathbf{S}_{ji}^{\text{f}} = (Y_{ij} + Y_{ji}^c)^\star |\mathbf{V}_j|^2 - Y_{ij}^\star \mathbf{V}_i^\star \mathbf{V}_j & \forall ij \in \mathcal{E} \\
& |\mathbf{S}_{ij}^{\text{f}}|, |\mathbf{S}_{ji}^{\text{f}}| \leq \bar{s}_{ij} & \forall ij \in \mathcal{E} \\
& \underline{\text{v}}_i \leq |\mathbf{V}_i| \leq \bar{\text{v}}_i & \forall i \in \mathcal{N} \\
& \underline{\text{p}}_i^{\text{g}} \leq \mathbf{p}_i^{\text{g}} \leq \bar{\text{p}}_i^{\text{g}} & \forall i \in \mathcal{N} \\
& \underline{\text{q}}_i^{\text{g}} \leq \mathbf{q}_i^{\text{g}} \leq \bar{\text{q}}_i^{\text{g}} & \forall i \in \mathcal{N}
\end{aligned}
$$

Yes, they can!

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- Demonstrated ICNN efficacy on **large-scale systems**, showing they match DNNs with most optimality gaps below 0.5%.

- For **AC-OPF**, **SOC** relaxation, and **DC-OPF** formulations.

- **Bounds** on ICNN generalization error based on training data performance.

New tool to help efficiently solve larger OPF applications!

Yes, we can!

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$$\text{gap} = \frac{|\tilde{z} - z^*|}{|z^*|}.$$

TABLE II
ICNN PERFORMANCE RESULTS.

		Mean gap (%)				Worst gap (%)			
System	OPF	ICNN	DNN	DC	SOC	ICNN	DNN	DC	SOC
ieee300	DC	0.15	0.19	0.00	-	1.58	1.90	0.00	-
	SOC	0.31	0.37	5.43	0.00	5.77	4.96	10.79	0.00
	AC	0.39	0.39	7.35	1.98	15.81	14.56	21.95	16.47
pegase1k	DC	0.28	0.33	0.00	-	2.35	1.83	0.00	-
	SOC	0.33	0.82	1.60	0.00	2.22	2.15	1.88	0.00
	AC	0.33	0.68	2.91	1.32	2.37	1.95	3.49	1.89
pegase2k	DC	0.22	0.30	0.00	-	3.45	3.21	0.00	-
	SOC	1.03	0.32	2.15	0.00	3.15	2.36	2.35	0.00
	AC	0.24	0.27	3.02	0.80	8.59	8.89	8.887	9.13
rte6k	DC	0.27	0.38	0.00	-	1.76	1.15	0.00	-
	SOC	0.29	0.57	2.67	0.00	1.69	5.52	3.17	0.00
	AC	0.25	0.33	3.05	0.33	2.71	3.08	3.67	0.36

L2O: JuMP + POI + Flux = ♥

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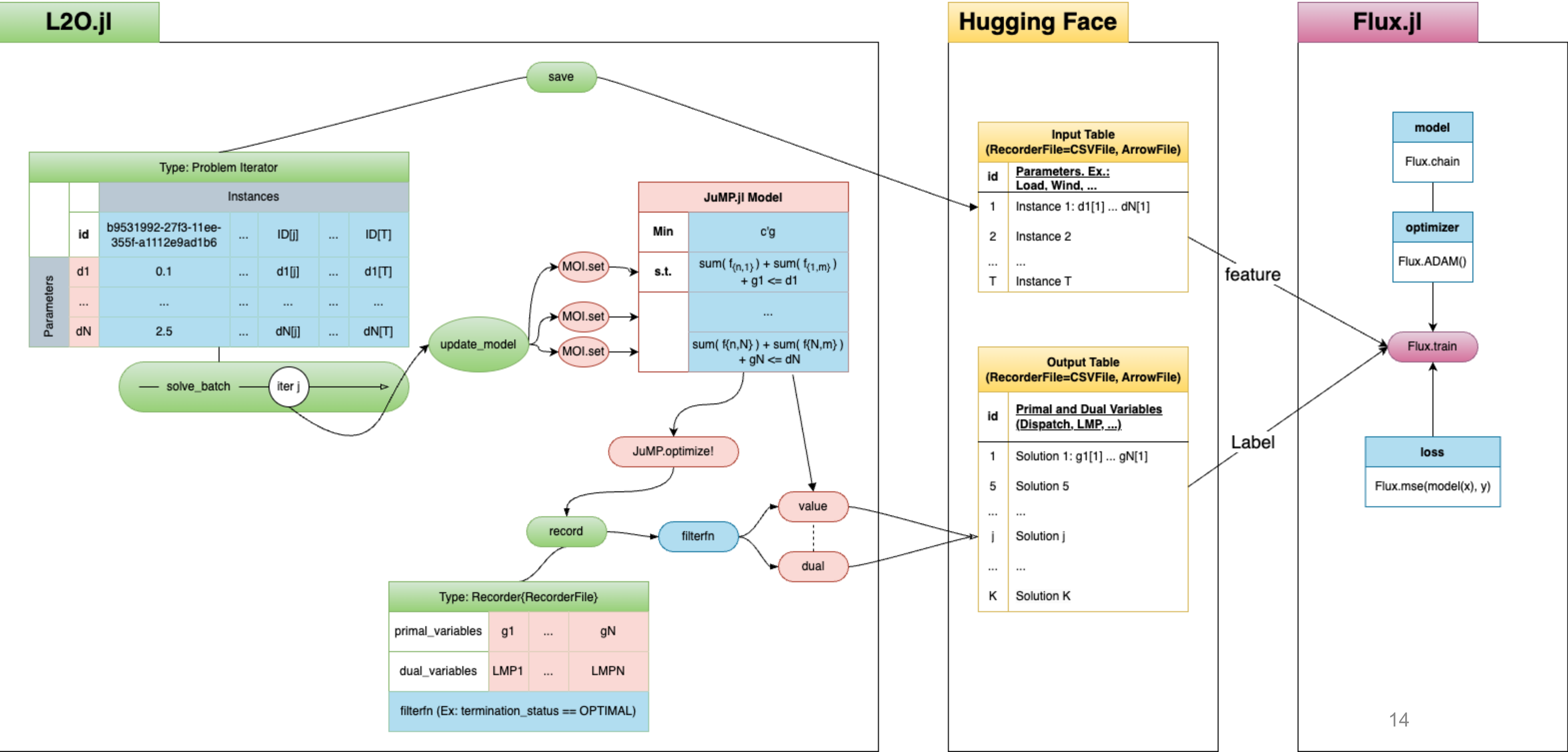

It’s Great when Things Just Work

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- What if I want to represent my entire NN in JuMP?

```
function NNlib.relu(ex::AffExpr)
    model = owner_model(ex)
    relu_out = @variable(model, lower_bound = 0.0)
    @constraint(model, relu_out >= ex)
    return relu_out
end
```

```
icnn = Chain(Dense(1000, 10, relu), Dense(10, 10, relu), Dense(10, 1))
train_icnn(icnn)

model = Model(Highs.Optimizer)
@variable(model, x[1:1000] >= 0)
@constraint(model, sum(x) == 1.0)
@objective(model, Min, icnn(x))

JuMP.optimize!(model)
```

```
function NNlib.relu(ex::AffExpr)
    tol = 0.00001
    model = owner_model(ex)
    aux = @variable(model, binary = true)
    relu_out = @variable(model, lower_bound = 0.0)
    @constraint(model, relu_out >= ex * (1-tol))
    @constraint(model, relu_out <= ex * (1+tol) + big_M * (1 - aux))
    @constraint(model, relu_out <= big_M * aux)
    return relu_out
end
```

Learning OPF Value Functions with ICNN

Andrew Rosemberg , Mathieu Tanneau, Bruno Fanzeres, Joaquim Garcia‡ and Pascal Van Hentenryck

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What else? Proxies as Direct Policies!

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- Multistage Stochastic Programing

$$\min_{(\mathbf{y}_1,\mathbf{x}_1)\in\mathcal{X}_1(\mathbf{x}_0)} f(\mathbf{x}_1,\mathbf{y}_1) + \mathbf{E}[\min_{(\mathbf{y}_2,\mathbf{x}_2)\in\mathcal{X}_2(\mathbf{x}_1,w_2)} f(\mathbf{x}_2,\mathbf{y}_2) + \mathbf{E}[\cdots +$$
$$\mathbf{E}[\min_{(\mathbf{y}_t,\mathbf{x}_t)\in\mathcal{X}_t(\mathbf{x}_{t-1},w_t)} f(\mathbf{x}_t,\mathbf{y}_t) + \mathbf{E}[\cdots]]]$$

$$\begin{aligned} V_t(\mathbf{x}_{t-1},w_t) = \min_{\mathbf{x}_t,\mathbf{y}_t} \quad & f(\mathbf{x}_t,\mathbf{y}_t) + \mathbf{E}[V_{t+1}(\mathbf{x}_t,w_{t+1})] \\ \text{s.t.} \quad & \mathbf{x}_t = \mathcal{T}(\mathbf{x}_{t-1},w_t,\mathbf{y}_t) \\ & h(\mathbf{x}_t,\mathbf{y}_t) \geq 0 \end{aligned}$$

What else? Proxies as Direct Policies!

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- Multistage Stochastic Programing

$$\min_{(\mathbf{y}_1,\mathbf{x}_1)\in\mathcal{X}_1(\mathbf{x}_0)} f(\mathbf{x}_1,\mathbf{y}_1) + \mathbf{E}[\min_{(\mathbf{y}_2,\mathbf{x}_2)\in\mathcal{X}_2(\mathbf{x}_1,w_2)} f(\mathbf{x}_2,\mathbf{y}_2) + \mathbf{E}[\cdots + \mathbf{E}[\min_{(\mathbf{y}_t,\mathbf{x}_t)\in\mathcal{X}_t(\mathbf{x}_{t-1},w_t)} f(\mathbf{x}_t,\mathbf{y}_t) + \mathbf{E}[\cdots]]]$$

$$\begin{aligned} \pi_t^*(\{w_j\}_{j=2..t},\mathbf{x}_0) \in \arg\min_{\mathbf{x}_t,\mathbf{y}_t} \quad & f(\mathbf{x}_t,\mathbf{y}_t) + \mathcal{V}_{t+1}(\mathbf{x}_t) \\ \text{s.t.} \quad & \mathbf{x}_t = \mathcal{T}(\mathbf{x}_{t-1},w_t,\mathbf{y}_t) \\ & h(\mathbf{x}_t,\mathbf{y}_t) \geq 0 \end{aligned}$$

Two-stage general decision rules (TS-GDR)

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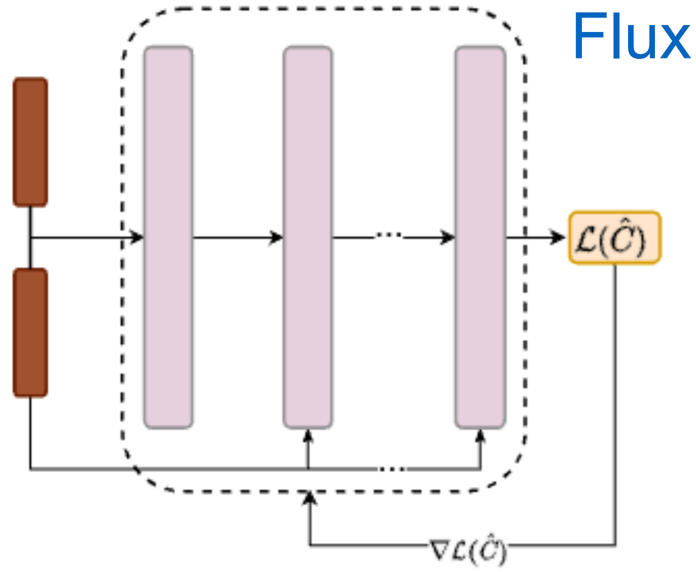
JuMP

$$
\begin{aligned}
\mathcal{Q}(w;\theta) = \min_{\mathbf{x},\mathbf{y},\delta} \quad & \sum_t f(\mathbf{x}_t,\mathbf{y}_t) + C_t^{\delta}||\delta_t|| & \\
\text{s.t.} \quad & \mathbf{x}_t = \mathcal{T}(\mathbf{x}_{t-1}, w_t, \mathbf{y}_t) & \forall t \\
& \mathbf{x}_t + \delta_t = \boxed{\pi_t(\{w_j\}_{j=2..t}, \mathbf{x}_0; \theta_t)} : \lambda_t & \forall t \\
& h(\mathbf{x}_t,\mathbf{y}_t) \geq 0 & \forall t
\end{aligned}
$$

s1

Flux



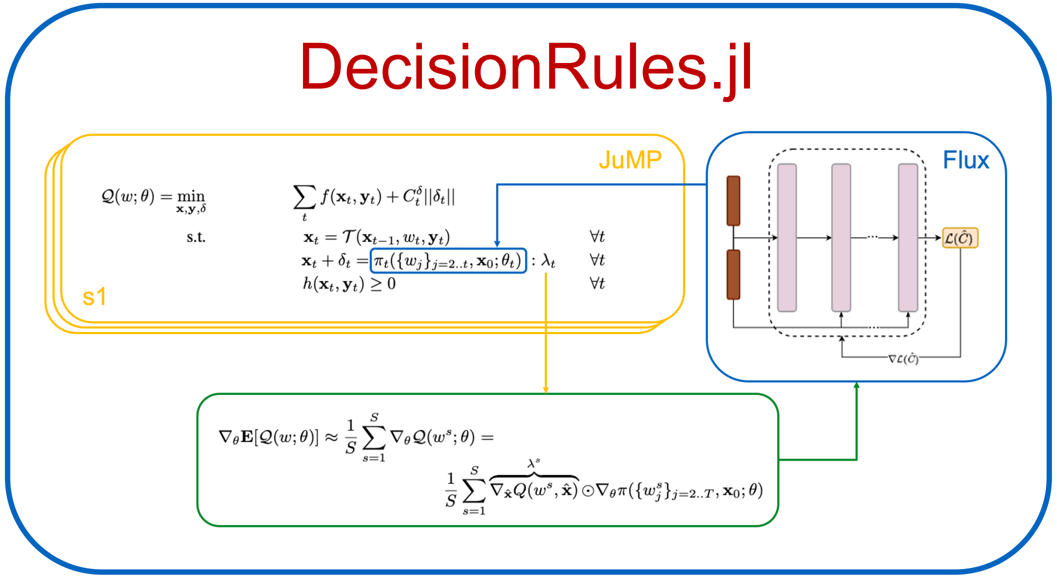
$$
\nabla_\theta \mathbf{E}[\mathcal{Q}(w;\theta)] \approx \frac{1}{S}\sum_{s=1}^{S} \nabla_\theta \mathcal{Q}(w^s;\theta) =
$$

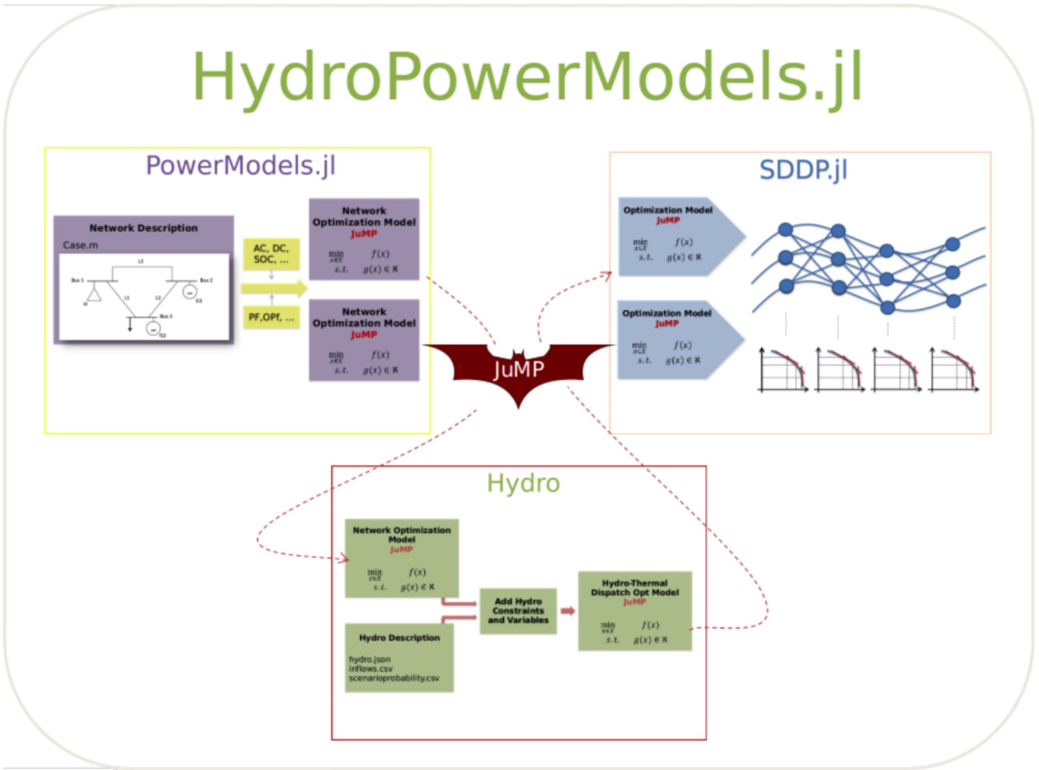
$$
\frac{1}{S}\sum_{s=1}^{S} \overbrace{\nabla_{\hat{\mathbf{x}}} Q(w^s, \hat{\mathbf{x}})}^{\lambda^s} \odot \nabla_\theta \pi(\{w_j^s\}_{j=2..T}, \mathbf{x}_0; \theta)
$$

TS-GDR vs SDDP

Table 3: Comparison of SDDP and ML Decision Rule for Bolivia with AC Implementation.

Model	Plan	Imp Cost (USD)	GAP (%)	Training (Min)	Execution (Min)
TS-DDR	AC	301851(±4876)	-	60	0.067
SDDP	SOC	302816(±5431)	0.32(±2.34)	-	480
TS-LDR	AC	319326(±4715)	5.79(±1.30)	226.01	0.067
SDDP	DCLL	323895(±3944)	7.30(±2.27)	-	320





What about Control Problems?

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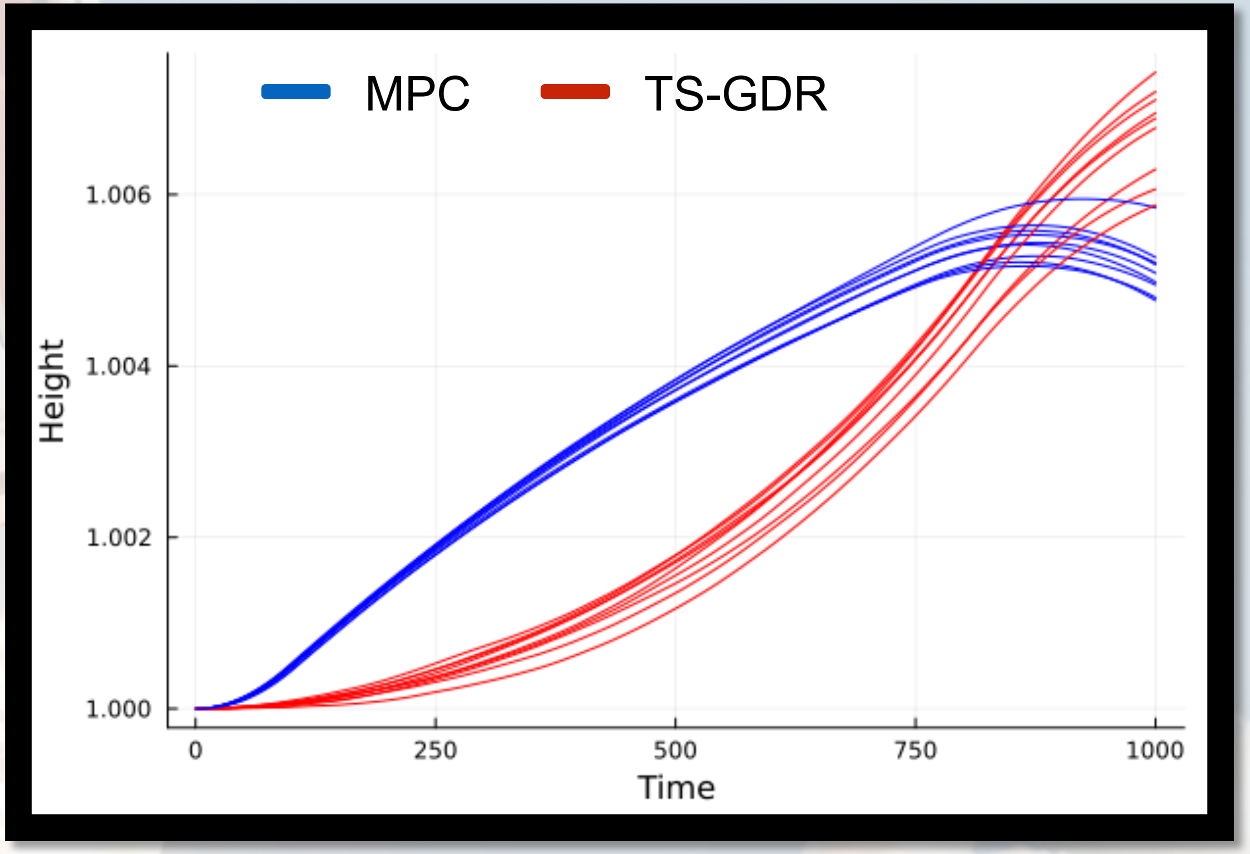
- Stochastic Goddard Rocket

$$
\begin{aligned}
\max_{h,v,m,u} \quad & h_T \\
\text{s.t.} \quad & \frac{h_t - h_{t-1}}{\Delta t} = v_{t-1} \quad \text{for } t = 2, \ldots, T, \\
& \frac{v_t - v_{t-1}}{\Delta t} = \frac{u_{t-1} - D(h_{t-1}, v_{t-1})}{m_{t-1}} - g(h_{t-1}) \boxed{- w_{t-1}} \quad \text{for } t = 2, \ldots, T, \\
& \frac{m_t - m_{t-1}}{\Delta t} = -\frac{u_{t-1}}{c} \quad \text{for } t = 2, \ldots, T, \\
& D(h, v) = D_c v^2 \exp\left(-\frac{h_c(h - h_0)}{h_0}\right), \\
& g(h) = g_0 \left(\frac{h_0}{h}\right)^2 \\
& v_1 = v_0,\ h_1 = h_0,\ m_1 = m_0,\ u_T = 0.0, \\
& v_t \geq 0,\ m_t \geq m_T,\ 0 \leq u_t \leq u_t^{\max} \quad \text{for } t = 1, \ldots, T.
\end{aligned}
$$

$$\boxed{w_t \in \mathcal{N}(0, 1)}$$



Godspeed!

Two-stage general decision rules (TS-GDR)

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Georgia Institute of Technology

PUC RIO

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