Imperial College London

Carnegie Mellon University

Sandia National Laboratories

OMLT: Optimization & Machine Learning Toolkit

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*These authors contributed equally, †These authors contributed equally

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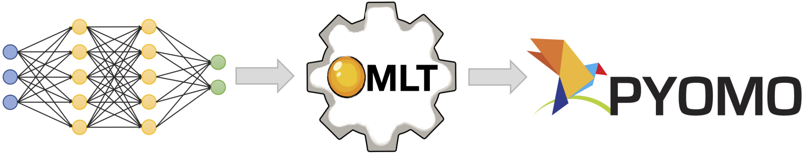
You?
Join us on GitHub!

OMLT: Optimization & Machine Learning Toolkit

`https://github.com/cog-imperial/OMLT`

CI passing | codecov 94% | docs passing



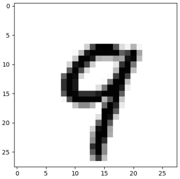
Why represent trained machine learning models as Pyomo [Bynum et al., 2021] formulations?

- **Adversarial examples** Verification [Lomuscio and Maganti, 2017], optimal adversary [Anderson et al., 2020], minimally-distorted adversary [Croce and Hein, 2020], lossless compression [Serra et al., 2020]
- **Machine learning** Maximize a neural acquisition function [Volpp et al., 2019], Bayesian optimization [Thebelt et al., 2021]
- **Engineering** Machine learning models may replace complicated constraints or serve as surrogates in larger design & operations problems.

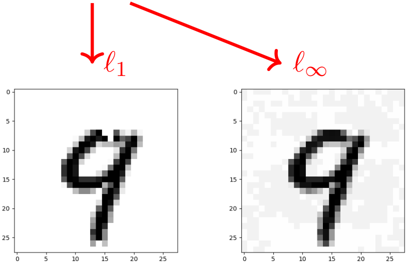
Optimization challenges to analyze trained neural networks

Example: Classification of MNIST digits

[Tsay et al., 2021]



Given	
Trained NN	
Image	$\bar{\boldsymbol{x}}$
Label	$j = 9$
Adversary?	$k = 4$



$\|\boldsymbol{x} - \bar{\boldsymbol{x}}\|_1 = 4$ $\qquad$ $\|\boldsymbol{x} - \bar{\boldsymbol{x}}\|_\infty = 0.05$

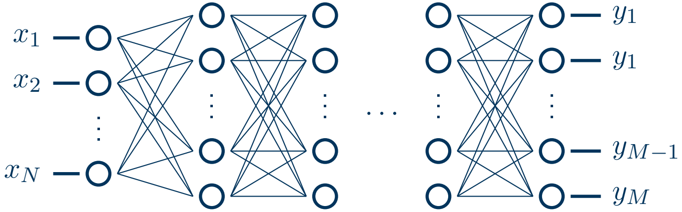
- **Verification** *[Feasibility]* Is there an adversary labeled k within a given perturbation (e.g., by ℓ_1- or ℓ_∞-norm)?
- **Optimal adversary** [Anderson et al., 2020] What image within a perturbation radius maximizes the prediction difference?
- **Minimally distorted adversary** [Croce and Hein, 2020] Smallest perturbation over which the NN can predict adversarial label k?
- **Lossless compression** [Serra et al., 2020] Can I safely remove NN nodes or layers?

What type of optimization problem do we want to solve?

Hybridize mechanistic, model-based optimization with surrogate models learned from data

$$\min_{\boldsymbol{x},\boldsymbol{y}} \quad f_0(\boldsymbol{x},\boldsymbol{y})$$

$$f_i(\boldsymbol{x},\boldsymbol{y}) \leq 0 \quad \forall i \in \{1,2,\ldots,C\}$$



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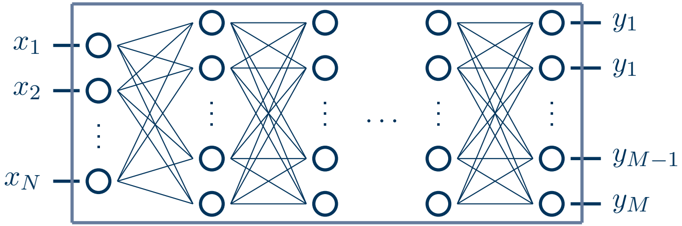


What type of optimization problem do we want to solve?

Hybridize mechanistic, model-based optimization with surrogate models learned from data

$$\min_{\boldsymbol{x},\boldsymbol{y}} \quad f_0(\boldsymbol{x},\boldsymbol{y})$$
$$f_i(\boldsymbol{x},\boldsymbol{y}) \leq 0 \quad \forall i \in \{1,2,\ldots,C\}$$

What are the expressions f_i?

Affine • Have discrete variables (may want ReLU NN or GBT surrogates) • Nonlinear (may want smooth NN activations)

In OMLT v 1.0, what can the `OmltBlock` abstraction encapsulate?

Dense neural networks • Convolutional neural networks (CNN) • Gradient boosted trees (GBT)

Interface with ONNX for interoperability

PyTorch

scikit learn

TensorFlow

Keras

ONNX

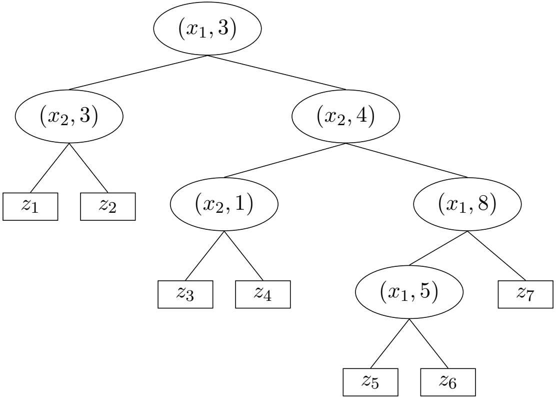
OMLT

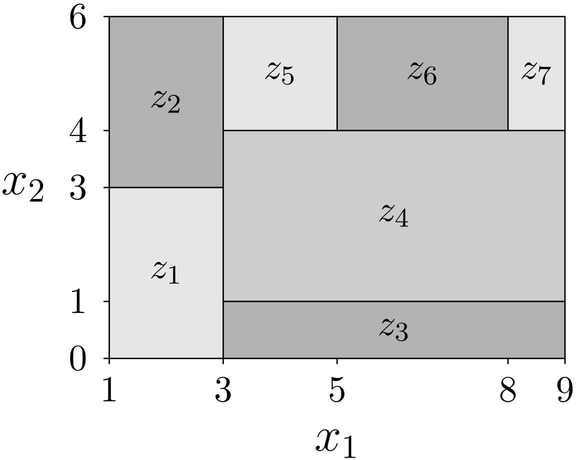
OMLT 1.0 Keras interface supports NN only (not GBT)

Want to join us?
OMLT 1.0 needs another GBT interface, e.g., LightGBM. ONNX doesn't support categorical variables

Most software *evaluates* a trained model . . . [Mistry et al., 2021]

Consider gradient boosted trees (GBTs). *Evaluating* a single tree is easy!





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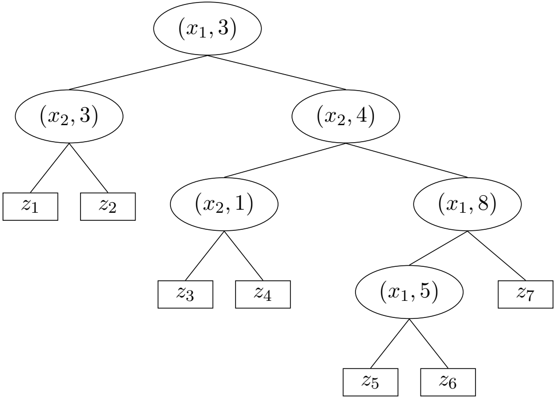
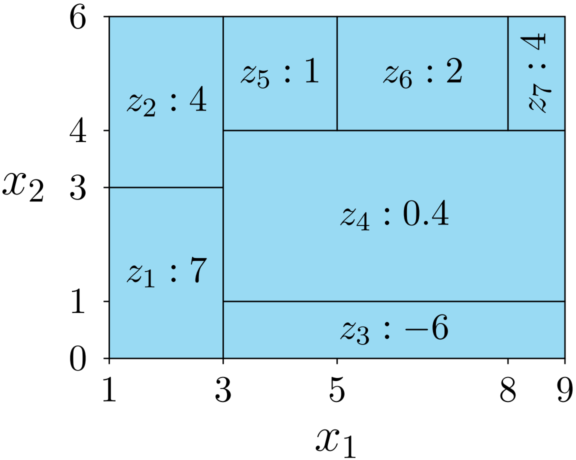
Consider gradient boosted trees (GBTs). *Evaluating* a single tree is easy!

- Calculate for $\boldsymbol{x} = (4, 2)$





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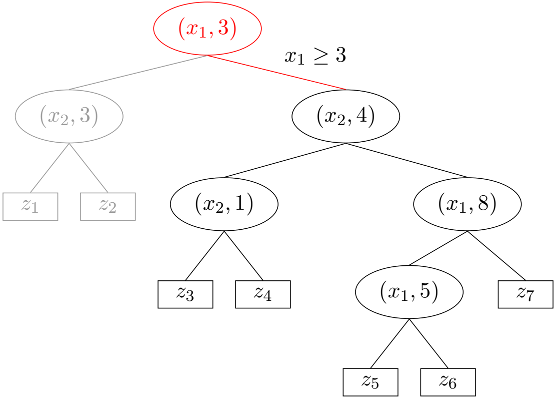

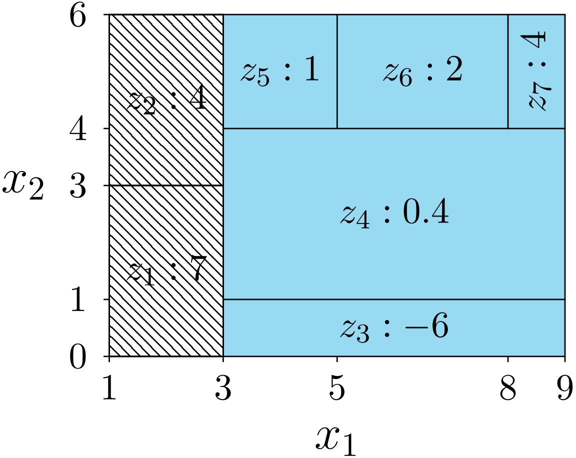

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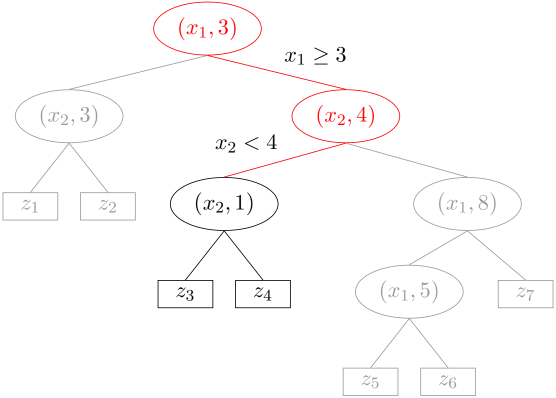
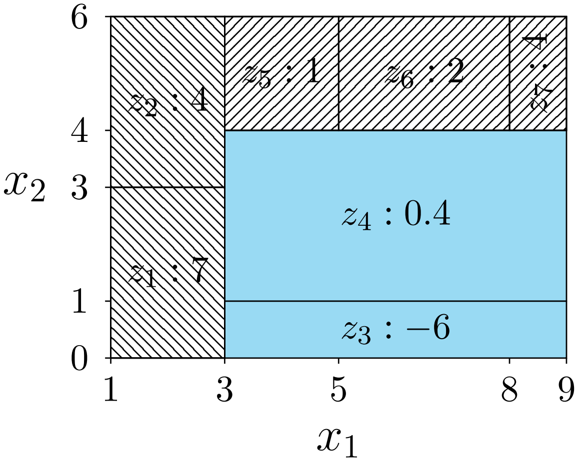
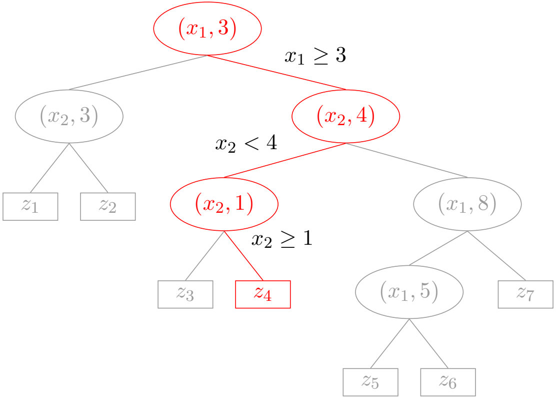


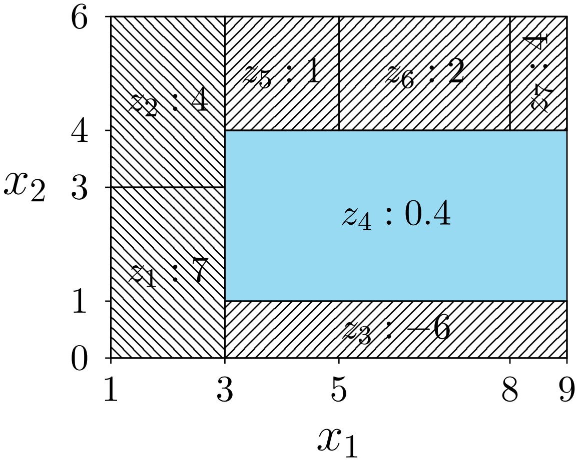


Most software *evaluates* a trained model . . . [Mistry et al., 2021]

Consider gradient boosted trees (GBTs). *Evaluating* a single tree is easy!

- Calculate for $\boldsymbol{x} = (4, 2)$
  - $t(\boldsymbol{x}) = 0.4$

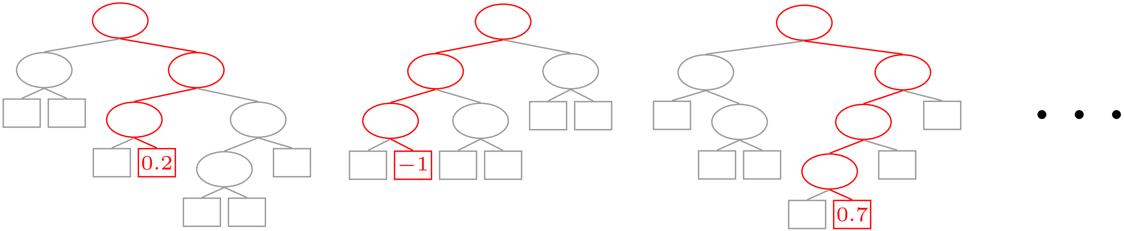




Most software *evaluates* a trained model . . . [Mistry et al., 2021]

Continuing the gradient boosted tree (GBT) example, it's also straightforward to *evaluate* the entire ensemble!

- GBT function defined by a set of trees, $\mathcal{T}$, and a constant, C
- To evaluate at $\boldsymbol{x} \in [\boldsymbol{L}, \boldsymbol{U}] \subset \mathbb{R}^n \longrightarrow y = \mathrm{GBT}(\boldsymbol{x}) = C + \sum_{t \in \mathcal{T}} t(\boldsymbol{x})$

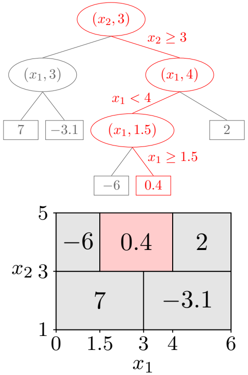


What if $\mathrm{GBT}(\boldsymbol{x})$ is in an optimization problem where $\boldsymbol{x}$ are decision variables, i.e., not fixed?

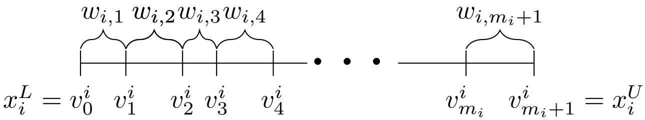
There are mathematical programming formulations incorporating function $y = \mathrm{GBT}(\boldsymbol{x})$ with decision variables $\boldsymbol{x}$ into a larger optimization problem [Mišić, 2020, Mistry et al., 2021, Thebelt et al., 2021]. OMLT automates the translation from ML model to optimization model!

Here's what OMLT allows users to ignore . . .

The `OMLTBlock` abstraction holds optimization formulations, e.g., by Mišić [2020] and Mistry et al. [2021]



$$
\begin{aligned}
y = \quad & \mathrm{GBT}(\boldsymbol{x}) = \sum_{t \in \mathcal{T}} \sum_{l \in \mathcal{L}_t} F_{t,l} z_{t,l} && \\
& \sum_{l \in \mathcal{L}_t} z_{t,l} = 1, && \forall t \in \mathcal{T}, \\
& \sum_{l \in \mathrm{Left}_{t,s}} z_{t,l} \leq \quad w_{i(s),j(s)}, && \forall t \in \mathcal{T},\ s \in \mathcal{V}_t, \\
& \sum_{l \in \mathrm{Right}_{t,s}} z_{t,l} \leq 1 - w_{i(s),j(s)}, && \forall t \in \mathcal{T},\ s \in \mathcal{V}_t, \\
& w_{i,j} \leq w_{i,j+1}, && \forall i \in [n], j \in [m_i - 1], \\
& w_{i,j} \in \{0, 1\}, && \forall i \in [n],\ j \in [m_i], \\
& z_{t,l} \geq 0, && \forall t \in \mathcal{T},\ l \in \mathcal{L}_t,
\end{aligned}
$$



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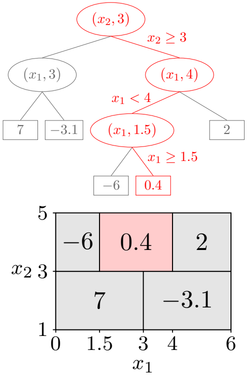
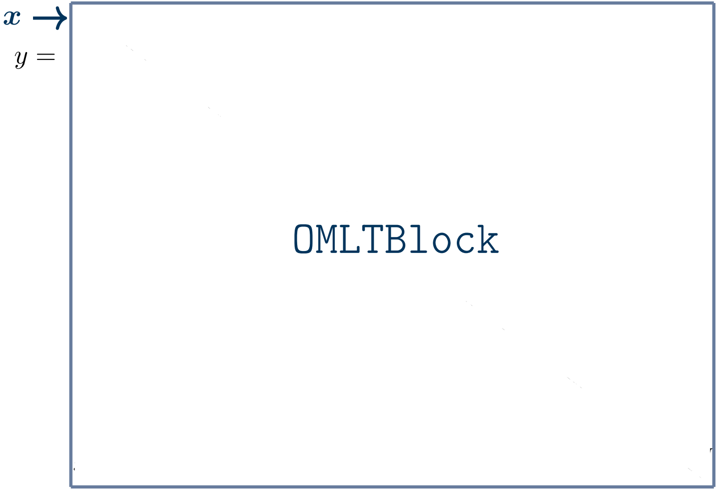
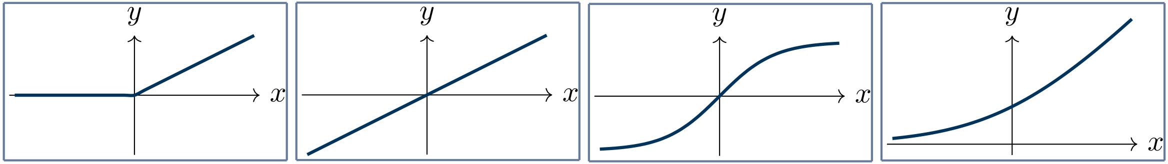




How NN activation functions map onto OMLT formulations . . .



ReLU

linear

tanh

softplus

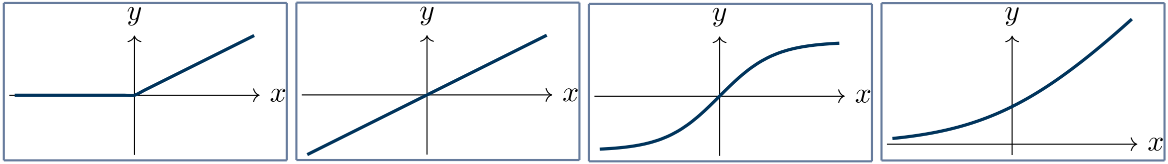
`ReluBigMFormulation`
`ReluComplementarityFormulation`
`ReluPartitionFormulation`

`FullSpaceSmoothNNFormulation`
`ReducedSpaceSmoothNNFormulation`

Formulations of activations [Schweidtmann and Mitsos, 2019, Anderson et al., 2020, Tsay et al., 2021]

Non-smooth [`ReluBigMFormulation`, `ReluComplementarityFormulation`, `Relu PartitionFormulation`] ReLU • **Smooth** [`{Full, Reduced}SpaceSmoothNNFormulation`] Linear • Tanh • Sigmoid • Softplus • Smooth monotonic

How NN activation functions map onto OMLT formulations . . .



ReLU linear tanh softplus

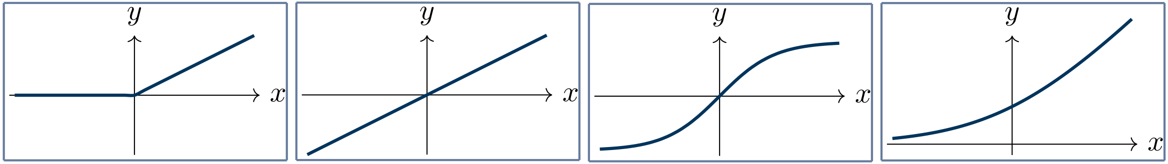
ReluBigMFormulation
`ReluComplementarityFormulation`
ReluPartitionFormulation

`FullSpaceSmoothNNFormulation`
`ReducedSpaceSmoothNNFormulation`

Optimization solver software EPL $\equiv$ Eclipse Public License; Prop $\equiv$ Proprietary

Mixed-integer linear [`Relu{BigM,Partition}Formulation`] CBC [EPL] • Gurobi [Prop] • Xpress [Prop] • CPLEX [Prop] **Nonlinear** [`{Full, Reduced}SpaceSmoothNNFormulation`, `ReluComplementarityFormulation`] Ipopt [EPL] • SNOPT [Prop] • MINOS [Prop]

How NN activation functions map onto OMLT formulations . . .



ReLU linear tanh softplus

`ReluBigMFormulation`
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`FullSpaceSmoothNNFormulation`
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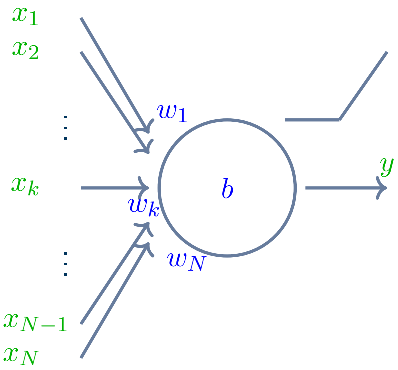
OMLT puts *optimization formulations* in competition

Key idea One optimization formulation may be more effective than another

- Algebraic modelling languages, e.g., Pyomo, make switching optimization *solvers* easy
- OMLT makes switching formulations as easy as changing a couple lines of code



Big-M formulation [Anderson et al., 2020]

```
formulation = ReluBigMFormulation(net_relu)
```

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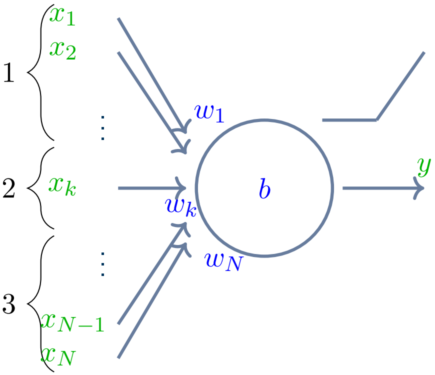


Big-M formulation [Anderson et al., 2020]

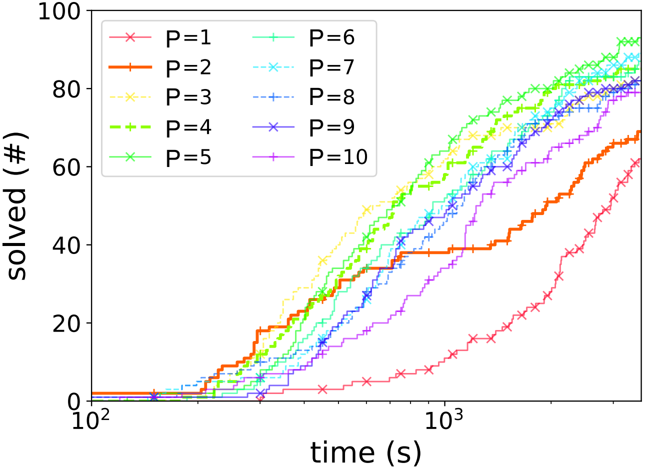
```
formulation = ReluBigMFormulation(net_relu)
```

Partition-based formulation [Tsay et al., 2021]

```
P = 3
split_func = lambda w: partition_split_func(w, P)
formulation = ReluPartitionFormulation(
    net_relu, split_func=split_func)
```

Importance of parameter P: Number solved vs. run time $\left(\|\boldsymbol{x} - \bar{\boldsymbol{x}}\|_1 = 5\right)$

Optimal adversary CIFAR-10; NN with $n_{\text{Layers}} = 2$ & $n_{\text{Hidden}} = 100$; Each line averages 100 examples $\bar{\boldsymbol{x}}$

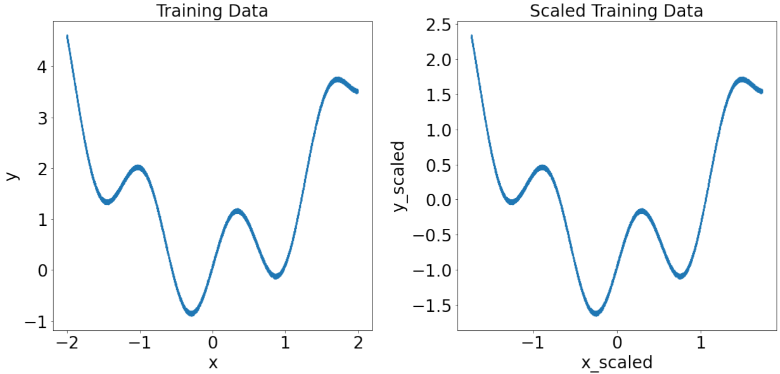


Observations [Tsay et al., 2021]

- $P = 1$ (equivalent to big-M) performs worst;
- $P = 2$ good for easy problems;
- Intermediate P balances model size vs. tightness;
- Performance declines $P \geq 7$

Neural Network Formulation Example: Data

neural_network_formulations.ipynb

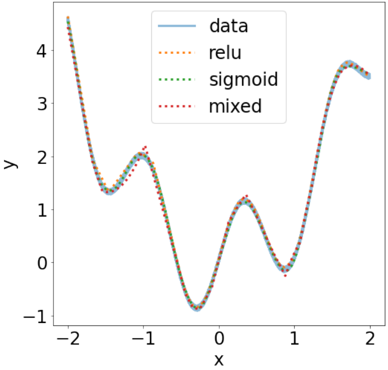


Read in the data 1 input x, 1 output y, 10^4 samples, Scaled has mean 0 & stdev 1

```
df = pd.read_csv("../data/sin_quadratic.csv",index_col=[0]);
```

Neural Network Formulation Example: Trained Neural Networks

`neural_network_formulations.ipynb`

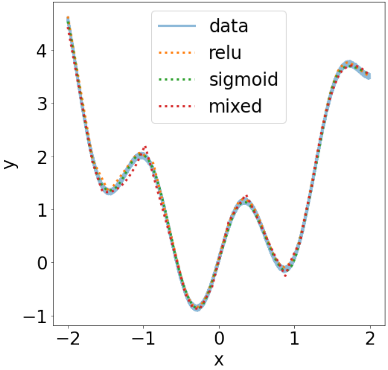


Build a Keras NN with ReLU activation

```
nn = Sequential(name='sin_wave_relu')
nn.add(Input(1))
nn.add(Dense(30, activation='relu'))
nn.add(Dense(30, activation='relu'))
nn.add(Dense(1))
nn.compile(optimizer=Adam(), loss='mse')
history = nn.fit(x=df['x_scaled'], y=df['y_scaled'],
    verbose=1, epochs=75)
```

Neural Network Formulation Example: Trained Neural Networks

neural_network_formulations.ipynb

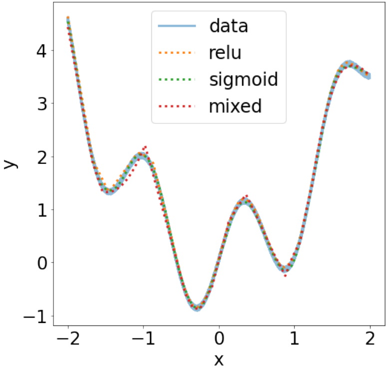


Build a Keras NN with sigmoid activation

```
nn = Sequential(name='sin_wave_sigmoid')
nn.add(Input(1))
nn.add(Dense(50, activation='sigmoid'))
nn.add(Dense(50, activation='sigmoid'))
nn.add(Dense(1))
nn.compile(optimizer=Adam(), loss='mse')
history = nn.fit(x=df['x_scaled'], y=df['y_scaled'],
    verbose=1, epochs=75)
```

Neural Network Formulation Example: Trained Neural Networks

`neural_network_formulations.ipynb`



Build a Keras NN with mixed (sigmoid/ReLU) activation

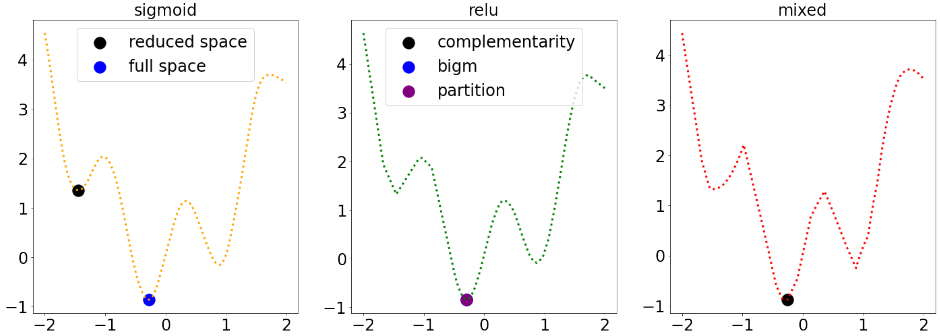
```
nn = Sequential(name='sin_wave_mixed')
nn.add(Input(1))
nn.add(Dense(50, activation='sigmoid'))
nn.add(Dense(50, activation='relu'))
nn.add(Dense(1))
nn.compile(optimizer=Adam(), loss='mse')
history = nn.fit(x=df['x_scaled'], y=df['y_scaled'],
    verbose=1, epochs=150)
```

Neural Network Formulation Example: Set up the optimization problem

```
net_sigmoid = keras_reader.load_keras_sequential(nn,scaler,input_bounds)
model = pyo.ConcreteModel()
model.x = pyo.Var(initialize = 0)
model.y = pyo.Var(initialize = 0)
model.obj = pyo.Objective(expr=(model.y))
model.nn = OmltBlock()
formulation = FullSpaceSmoothNNFormulation(net_sigmoid) #or ReducedSpaceSmoothNNFormulation
model.nn.build_formulation(formulation)

@model.Constraint()
def connect_inputs(mdl):
    return mdl.x == mdl.nn.inputs[0]

@model.Constraint()
def connect_outputs(mdl):
    return mdl.y == mdl.nn.outputs[0]

status = pyo.SolverFactory('ipopt').solve(model, tee=True)
solution = (pyo.value(model.x),pyo.value(model.y))
```

Neural Network Formulation Example: Optimization results

`neural_network_formulations.ipynb`



FullSpaceSmoothNNFormulation [Ipopt]

variables: 209, # constraints: 208

$x = -0.28, y = -0.86$

Solve Time: 0.14s

ReducedSpaceSmoothNNFormulation [Ipopt]

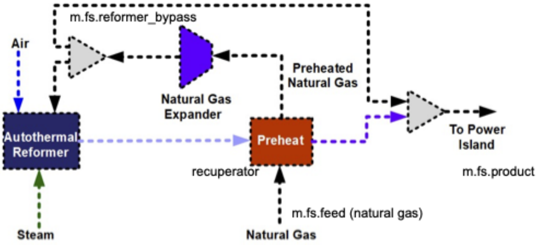
variables: 6, # constraints: 5

$x = -1.44, y = 1.36$

Solve Time: 0.08s

Other notebook examples . . .

https://github.com/cog-imperial/OMLT/tree/main/docs/notebooks



auto-thermal-reformer{-relu}.ipynb

develops an NN surrogate with data from a process model built using IDAES-PSE [Lee et al., 2021]

Even more notebook examples . . .

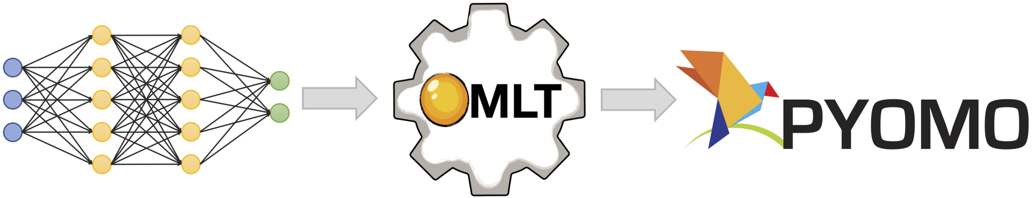
- `import_network.ipynb` imports NN models directly from Keras & ONNX. Using ONNX interoperability, it imports a NN model from PyTorch.
- `build_network.ipynb` builds a `NetworkDefinition` manually.
- `mnist_example_{dense, cnn}.ipynb` train fully dense and convolutional NNs on MNIST [LeCun et al., 2010] and find adversarial examples [Tjeng et al., 2017].
- `bo_with_trees.ipynb` optimizes the Rosenbrock function.

OMLT v 1.0 Summary

https://github.com/cog-imperial/OMLT

Key Contributions

- Automatically translate a trained machine learning model (neural network or gradient boosted tree) into Pyomo optimization constraints
- Achieve interoperability via the ONNX interface
- Easily switch and compare optimization formulations



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