Preprints of the 21st IFAC World Congress (Virtual)
Berlin, Germany, July 12-17, 2020

The Integration of Explicit MPC and ReLU based Neural Networks

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Abstract: Using neural networks to capture complex dynamics of highly nonlinear systems is a promising feature for advanced control applications. Recently it has been shown that ReLU based neural networks can be exactly recast in a mixed-integer linear programming formulation. This reformulation enables the incorporation of deep learning models in model predictive control strategies. To alleviate the computational burden of solving the piecewise linear optimization problem online, multiparametric programming is utilized to obtain the full, offline, explicit solution of the optimal control problem. In this work, a strategy is presented for the integration of deep learning models, specifically neural networks with rectified linear units, and explicit model predictive control. The proposed strategy is demonstrated on the advanced control of the ACUREX solar field.

Keywords: Neural Networks, Optimal Control, Piecewise linear controllers.

1. INTRODUCTION

Data-driven techniques in the process engineering community are seeing a new wave of excitement (Chiang et al. (2017)). Specifically, using artificial neural networks to capture complex relationships are proving to be robust and effective in chemical engineering processes. Applications of these data-driven models include surrogate models for optimization (Himmelblau (2008)), approximate models for reducing computational costs (Hough et al. (2017)), and model predictive control (MPC) (Himmelblau (2000)). In MPC problems, where the control action is dictated by the solution of an optimization problem, it is challenging to identify the optimal action in a timely manner. Neural networks are inherently nonconvex and nonlinear, and embedding these models in optimization formulations requires significant computational effort to determine the optimal solution. Neural networks have been incorporated in several studies as surrogate models in MPC strategies (Shokry et al. (2018); Afram et al. (2017)). However, limited analysis is provided for an efficient strategy to solve the resulting nonconvex optimal control problem. Because of the inherent nonconvexity associated with the resulting MPC formulation, determining the global optimal solution is on-going work (Schweidtmann et al. (2019)). Recently, it has been shown that neural networks with rectified linear units (ReLU) can be represented as a mixed-integer linear program (MILP) (Fischetti and Jo (2018); Grimstad and Andersson (2019)). Therefore, embedding ReLU based neural networks into model predictive control formulations is practical, because the overall structure of the MPC remains unchanged (either a quadratic or linear program). However, the resulting optimization problem involves mixed-integer decisions and is therefore a mixed-integer quadratic program (MIQP), or a MILP. By combining the MILP formulation of neural networks with ReLU activation functions with model predictive control strategies, the resulting optimal control problem can be solved using standard mixed-integer linear or quadratic techniques.

Solving a mixed-integer linear or quadratic program online to determine the optimal control action remains a computationally demanding problem in the worst case. Multiparametric programming is a methodology that alleviates the burden of solving an optimization problem online by developing an explicit optimal solution offline. The multiparametric programming literature has algorithms to determine the full solution for multiparametric linear (mpLP) (Jones and Morrari (2006)), quadratic (mpQP) (Gupta et al. (2011); Oberdieck et al. (2017)), mixed-integer linear (mpMILP) (Wittmann-Hohlbein and Pistikopoulos (2013)), mixed-integer quadratic (mpMIQP) (Oberdieck and Pistikopoulos (2015)), and quadratically constrained quadratic (mpQCQP) programs (Diangelakis et al. (2018)).

In these multiparametric model formulations, a key detail is their dependence on linear or piecewise linear constraints. Therefore, to incorporate more complex phenomena in parametric formulations surrogate modeling is required. Developing accurate surrogate models to represent nonlinear functional relationships is non-trivial, and neural networks based on ReLU activation functions bridge this gap. Incorporating neural networks and multiparametric programming is readily implementable because the resulting parametric optimization formulation is a mpMILP. Algorithmic strategies are available in the state-of-the-art Parametric Optimization (POP) software and the Multiparametric Programming Toolbox (MPT) to construct

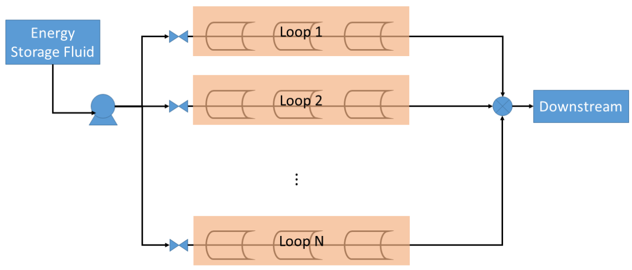

Fig. 1. A schematic diagram of the ACUREX process, adapted from Katz (2020).

the full multiparametric solution (Oberdieck et al. (2016a); Herceg et al. (2013)).

In this work, the novel contribution is the incorporation of deep neural networks in explicit MPC (Katz et al. (2020)). Current literature includes strategies to utilize ReLU neural networks with model-based control, however there is a gap in efficiently developing the optimal solution in real-time. In addition, comparisons between (i) nonlinear MPC and MPC and (ii) different nonlinear MPC formulations are available in the literature. Therefore, the intent of this research effort is to demonstrate that explicit MPC can include more advanced surrogate models in the form of deep neural networks with ReLU activation functions without sacrificing model accuracy or optimality.

To demonstrate the ability of neural networks with ReLU activation functions to capture nonlinear relationships, the proposed methodology is validated on the benchmark ACUREX process. This benchmark problem is a solar powered energy system defined by complex, nonlinear dynamics (Camacho and Berenguel (2012)). The ACUREX solar field is designed with parabolic mirrors to heat oil in a pipe to be used downstream, such as a desalination plant. The advanced control of the plant is paramount because of the intermittent and variable intensity of solar power. Fig. 1 is a schematic of the ACUREX solar field.

2. MULTIPARAMETRIC PROGRAMMING

Avoiding the online computational cost of solving an optimal control problem at each sampling time can be accomplished via multiparametric programming. The optimal control problem assumed in this work is defined by (1).

$$\begin{aligned} \min_{u} \quad & |y - y_{sp}|_{\infty} \\ \text{s.t.} \quad & y = f(x_0, u) \\ & \underline{X} \leq x_0 \leq \bar{X} \\ & \underline{Y} \leq y \leq \bar{Y} \\ & \underline{U} \leq u \leq \bar{U} \end{aligned} \tag{1}$$

where y_{sp} is the setpoint, y is the output of interest, u is the manipulated action, x_0 is the initial condition of the system, and f represents any linear or piecewise linear function.

By treating the initial conditions of the system as bounded uncertain parameters, the optimal control problem is exactly recast to its multiparametric counterpart. The developed multiparametric model predictive controller is then solved once and offline using state-of-the-art solvers. The derived explicit solution contains the optimal manipulated action as a function of the bounded uncertain parameters. In addition to the online computational savings, the map of solutions provides information of the feasible space of the explicit controller. The multiparametric problem solved in this work is a mpMILP, and the general structure is presented in (2).

$$\begin{aligned} \min_{u,y} \quad & c^T \omega + c_t^T \theta + c_c \\ \text{s.t.} \quad & [A \ E]\omega \leq d + F\theta \\ & \omega = [u^T y^T]^T \\ & u \in U, \ y \in \{0,1\}^q \\ & \theta \in \Theta \end{aligned} \tag{2}$$

where u and y are the continuous and binary variables respectively, θ is the vector of bounded, uncertain parameters, q is the total number of binary variables, and the cost matrices and vectors A, E, d, F, c, c_t, and c_c define the problem.

The multiparametric solution of (2) returns a list of critical regions, and each critical region defines affine functions relating the bounded uncertain parameters to the optimal continuous decision variables, see (3).

$$u^* = G_i \theta^* + h_i, \ \theta^* \in CR_i = \{CR_A^i \theta \leq CR_b^i\} \tag{3}$$

where u^* is the optimal solution at the parameter realization θ^*, CR_i define the ith critical region, and G_i and h_i define the affine expression for the ith critical region.

2.1 Solution Strategy

Exploring the full solution of mpMILPs in an efficient and robust way is a subject of ongoing research. Currently, approaches for the development of the multiparametric solution fall under three categories, geometrical approaches, active set approaches, and combinations of the aforementioned strategies (Oberdieck et al. (2016b)). Geometric strategies aim to explore the full explicit solution by traversing the parameter space to identify critical regions (Bemporad et al. (2002)). Active set strategies develop the explicit solution by identifying all active set combinations that yield critical regions (Gupta et al. (2011)).

2.2 Multiparametric Mixed-Integer Linear Programming

A strategy for developing the explicit solution to mpMILPs is based on an iterative procedure of solving mpLPs and generating integer cuts. The procedure is computationally demanding compared to mpLP algorithms because of the binary variables.

An overview of the solution procedure is as follows. Given the mpMILP, a deterministic optimization problem is solved where the uncertain parameters are treated as optimization variables to identify the optimal binary combination. The optimal binary combination is used to fix the binary variables and develop an explicit solution to the reduced mpLP. Because the mpLP solution is based on the original binary combination, each critical region is verified to be optimal with respect to the original mpMILP. This comparison procedure is the backbone of the mpMILP algorithm for developing the multiparametric solution. The resulting explicit map of solutions provides the optimal critical regions, the optimization variables as functions of the uncertain parameters, and the optimal integer variables. Note that improving mpMILP algorithms is accomplished via strengthening the comparison procedure, with the goal of identifying fewer candidate critical regions.

In this work, we utilize the POP toolbox to obtain the full mpMILP solution defining the optimal control law. This MATLAB based toolbox maintains the aforementioned algorithms and can readily solve mpMILP problem formulations.

3. INTEGRATING DEEP LEARNING AND MULTIPARAMETRIC MODEL PREDICTIVE CONTROL

Directly using a first-principle process model in a model predictive control formulation requires the solution of a nonlinear optimization problem at every time step. Determining the optimal solution to an NLP at every time step is computationally demanding. Therefore, the aim is to develop a surrogate model to replace the nonlinear model in the NLP formulation, at the cost of plant-model mismatch, such that obtaining the optimal solution in a real time setting is feasible. Introducing a surrogate model is not ideal, but feedback control provides a measure of robustness to mitigate the negative consequences of plant-model mismatch (Katz et al. (2018)). Typical surrogate models are linear, but in many cases they are not adequate to control the process and a nonlinear model is required (Allgower et al. (2004)).

In this work, it is assumed that the objective function is linear, the process model is nonlinear, and the states and manipulated actions of the process are bounded by upper and lower bounds. Due to the complexities of the nonlinear process model, it is necessary to develop an approximate model. The approximate model used is a feedforward neural network with ReLU activation functions to capture the nonlinearity of the process model, further details regarding neural networks can be found in Himmelblau (2000). The nonlinear model predictive control formulation is thus reduced to a mixed-integer linear model predictive control formulation via (5). The simplified control problem is then exactly recast to its multiparametric programming counterpart and is solved using existing strategies. The procedure is graphically represented by Fig. 2. Note that the arrow from "ReLU Validation" to "Input-Output Data Collection & Processing" is an optional task worth considering if the neural network is unable to identify the dynamics of the process.

3.1 Reformulation to MILP

It has been demonstrated in the literature that a neural network involving ReLU activation functions can be exactly recast as an MILP (Fischetti and Jo (2018); Grimstad and Andersson (2019)). The reformulation maintains the accuracy of the deep neural network, but results in an optimization formulation that is mixed-integer linear. Therefore, if the deep neural network is embedded in an optimization formulation, the increase in complexity results from the binary variables only. A review of the reformulation procedure is presented as follows.

For an arbitrary layer in a feedforward neural network with n nodes, the output takes the form of (4), where k is the layer, W^k is the matrix of weights for layer k, b^k is the vector of biases for layer k, $x^{k-1} \in \Re^n$ is the output of the previous layer, and $x^k \in \Re^n$ is the output of the current layer. The max operator is performed element-wise.

$$x^k = max\{0, W^k x^{k-1} + b^k\} \tag{4}$$

The importance of the ReLU activation function is its piecewise linear nature. Therefore, (4) can be exactly recast in an optimization formulation via the inclusion of binary variables. Equation (5) is the reformulation of the k^{th} hidden layer in an MILP structure.

$$W^k x^{k-1} + b^k = x^k - s^k \tag{5a}$$
$$x^k \leq My \tag{5b}$$
$$s^k \leq M(1-y) \tag{5c}$$
$$x^k \geq 0 \tag{5d}$$
$$s^k \geq 0 \tag{5e}$$
$$y \in \{0,1\}^n \tag{5f}$$

In (5), the variable y is a binary variable, $s^k \in \Re^n$ is an auxiliary variable vector, and M is a large scalar value. The total number of binary variables is equal to the total number of nodes that constitute the hidden layers. The binary variables enable the activation function to output a value of 0 or x, via the constraints (5b) and (5c). These constraints are equivalent to the max operator and are the reason the reformulation is exact. Incorporating the recasted neural network into an optimization formulation provides an effective strategy to maintain high accuracy with a surrogate model, and obtaining the global optimum does not require specialized global optimization techniques.

Following (5), the neural network is transformed to a system of equality constraints, inequality constraints, binary variables, and slack variables. To minimize the total number of variables and constraints, variable aggregation is employed to eliminate the equality constraints and intermediate optimization variables.

$$x^1 = W^1 x^0 + b^1 + s^1 \tag{6a}$$
$$x^k = \prod_{i=k}^{1} W^i x^0 + \sum_{i=1}^{k-1} \prod_{j=k}^{i+1} W^j (b^i + s^i) + b^k + s^k,\ 1 < k < K \tag{6b}$$
$$x^K = \prod_{i=K}^{1} W^i x^0 + \sum_{i=1}^{K-1} \prod_{j=K}^{i+1} W^j (b^i + s^i) + b^K \tag{6c}$$

where W^k and b^k define the weights of the k^{th} hidden layer, K is the output layer, s^k is the vector of slack variables, x^0 is the input vector to the neural network, and x^K is

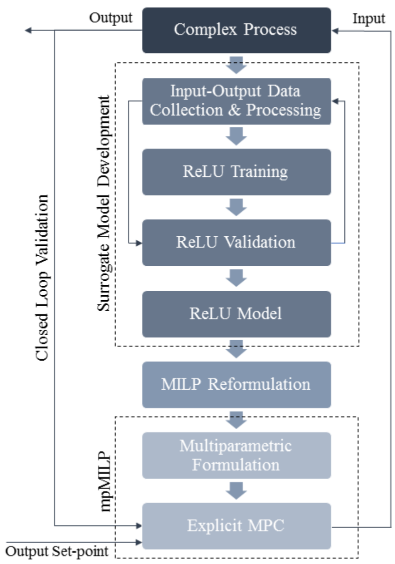

Fig. 2. The framework for integrating deep learning models with ReLU activation functions and explicit model predictive control.

the vector of outputs of the neural network. Equations (5) and (6) are combined to provide a set of constraints in the form of (2). Once the nonlinear equation representing the process is replaced with the recasted neural network, the control problem is solved using standard multiparametric techniques.

4. ACUREX PROCESS

The ACUREX solar field uses parabolic mirrors to focus the sun's rays on a pipe carrying an energy conversion fluid, typically oil. The process makes use of renewable solar energy to maintain the temperature of the energy conversion fluid at a predefined setpoint. The fluid, at the proper temperature, is then utilized further downstream to either (i) produce steam that is used to generate power in a turbine, (ii) or as a heat exchange medium in a desalination process (Camacho et al. (2007); Limon et al. (2008)). The fluid in the pipeline is assumed to be Therminol 55 (Eastman Chemical Company) because of its workable temperatures of $-28°C$ to $290°C$.

The ACUREX process is modeled by a system of partial differential equations. Following the assumptions by Camacho et al. (2007) and the additional assumption of a single loop of parametric mirrors, the system of partial differential equations is reduced to a single first order partial differential equation, (7).

$$\rho_f C_f A_f \frac{\partial T_f}{\partial t} = \eta_0 G I - h_l (T_f - T_a) - \rho_f C_f u(t) \frac{\partial T_f}{\partial x} \quad (7)$$

where T_f is the fluid temperature, x is the spatial coordinate, t is time, T_a is the ambient temperature, ρ_f is the density of the fluid, C_f is the heat capacity of the fluid, u is the fluid flowrate, η_0 is the mirror efficiency, G is the mirror aperture, I is the solar irradiance, and h_l is the coefficient of global heat losses. The partial differential system is converted to a system of ordinary differential equations that depend on time by discretizing the spacial domain via the method of lines (Sadiku and Obiozor (2000)).

The empirical relationship between the temperature of the fluid in the pipe and the density and heat capacity is defined by (8).

$$\rho_f = 903 - 0.672 T_f \quad (8a)$$
$$C_f = 1820 + 3.478 T_f \quad (8b)$$

Given the high fidelity model of the process, the control objective is to maintain the temperature of the oil at $280\ °C$. The objective function is defined by the L_1 norm between the temperature of the oil at the exit of the pipe and the setpoint. To meet the control objective, the volumetric flow rate of oil into the system is the manipulated action. There are box constraints on the manipulated action that define the limits of operation, and there is an upper bound on the temperature of the fluid in the pipe for safety and material considerations. For the development of the explicit MPC, the uncertain parameters are the temperature at the end of the pipe and the solar irradiance. These terms are the uncertain parameters because at each sampling period of the controller, these values are 'measured' and the corresponding optimal control action is determined using the explicit map of solutions. Note that these uncertain parameters are not to be confused with the neural network parameters that are determined during training and validation.

4.1 Developing the Neural Network

Given the dynamic model representing the ACUREX solar field, it is challenging to directly implement the high fidelity model in a MPC scheme. Therefore, a neural network with ReLU activation function is utilized as a surrogate model to capture the nonlinear dynamics, while minimizing model complexity when embedded in the explicit MPC.

The ACUREX plant is perturbed in open loop to properly excite the system over a range of inputs. The perturbed inputs are the solar irradiance and the fluid flow to the pipe. The measured output of the system is the temperature at the end of the pipe. Data collection accounts for $10,000$ samples and are used to train the neural network. The collected samples are split into training, validation, and testing sets following a $70\%, 15\%, 15\%$ division. Additional validation techniques such as k-fold cross validation were not incorporated in this work, but provide additional robustness on the fitting of the deep neural network on unseen datasets. Through trial and error, the size of the neural net that was found to accurately fit the open loop data has three hidden layers with sizes 8,7, and 7 respectively. The fit neural network has a mean squared error of $4 \cdot 10^{-4}$ for the test set, and the open loop response for the entire data set is presented in Fig. 3. From the figure, it is clear the trained neural network fits the data well.

4.2 Explicit Model Predictive Controller

The developed neural network with ReLU activation function is implemented in an explicit MPC. The explicit controller has an output and control horizon of one. Increasing

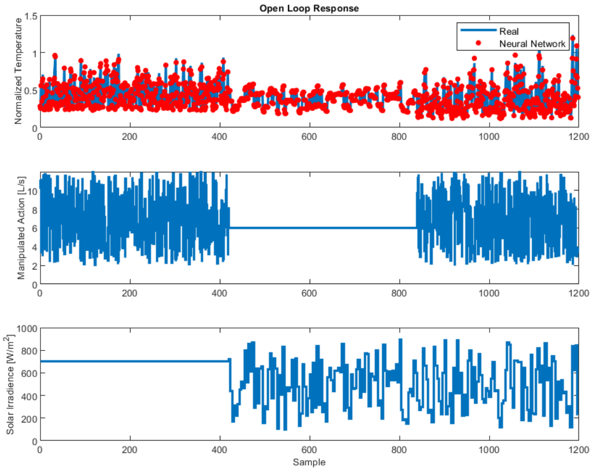

Fig. 3. Open loop response of the ACUREX solar field, adapted from Katz (2020).

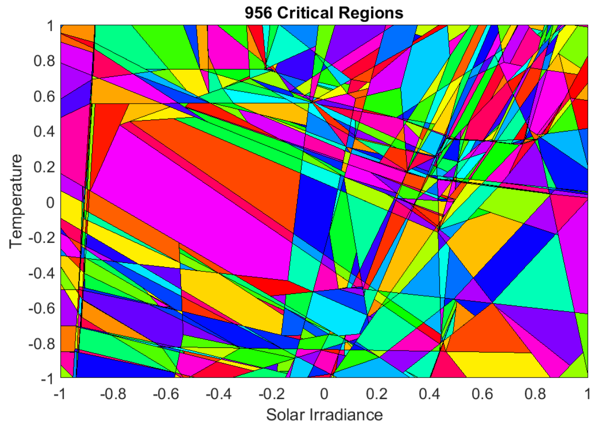

Fig. 4. The multiparametric solution for the explicit model predictive controller, adapted from Katz (2020).

the horizon length is possible by feeding the output of the neural network back into itself. For the presented process, it was found a horizon of one was sufficient for a suitable closed loop response.

The integrated neural network and explicit controller is represented by 24 continuous optimization variables, 22 binary variables, 2 uncertain parameters, and 94 constraints. The multiparametric solution is constructed using the POP toolbox with the graph algorithm. The developed multiparametric solution yields 956 critical regions and is presented in Fig. 4. Note that the time required to identify the critical region where the uncertain parameter realization exists for large explicit solutions is manageable given advanced searching techniques (Mönnigmann and Kastsian (2011)).

4.3 Closed Loop Performance

The closed loop response of the ACUREX process with an explicit model predictive controller based on a neural network with ReLU activation function is presented in Fig. 5. It is evident the explicit controller is able to maintain a set point, and recover the setpoint after a

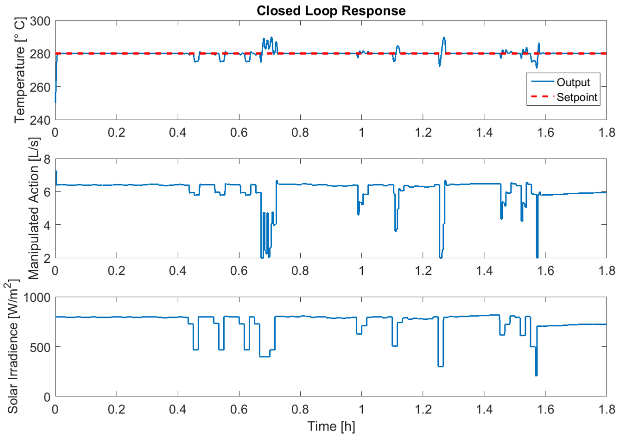

Fig. 5. The closed loop response of the ACUREX process, adapted from Katz (2020).

significant disturbance is passed to the system (Maxey (2007)). Given the ability of the controller to maintain and manage significant deviations from the setpoint, the closed loop response is considered acceptable.

5. CONCLUSION

This manuscript presented the integration of artificial neural networks with ReLU activation functions and explicit MPC. Multiparametric programming is a method to solve the advanced control formulation offline, explicitly as a function of the uncertain parameters. Developing the explicit solution reduces the online computational cost of solving the optimal control problem. Incorporating neural networks into explicit model predictive control formulations provides a suitable methodology for the advanced control of complex processes.

Integrating accurate surrogate models in optimization formulations is a critical step in many fields. Future work includes (i) using the presented methodology in various applications with real data sets to showcase the improved performance of using neural networks as surrogate models, (ii) comparisons of different surrogate modeling approaches, and (iii) reducing the time to develop the full multiparametric solution.

ACKNOWLEDGEMENTS

Financial support from the NSF SusChEM (Grant No. 1705423), NSF INFEWS (Grant no. 1739977), Texas A&M Energy Institute, and RAPID SYNOPSIS (DE-EE0007888-09-04) is gratefully acknowledged.

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