Master's thesis

Physics-Consistent Surrogate Models with Uncertainty Quantification for Model Predictive Control

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Abstract

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Contents

Notation

Numbers and Arrays

a	A scalar (integer or real)
$\boldsymbol{a}$	A vector
$\boldsymbol{a}_{[1:N]}$	A sequence of vectors from 1 to N, such that $\boldsymbol{a}_{[1:N]} = (\boldsymbol{a}_1, \ldots, \boldsymbol{a}_N)$
$\boldsymbol{A}$	A matrix
A	A tensor
$\boldsymbol{I}_n$	Identity matrix with n rows and n columns
$\boldsymbol{I}$	Identity matrix with dimensionality implied by context
$\boldsymbol{e}^{(i)}$	Standard basis vector $[0, \ldots, 0, 1, 0, \ldots, 0]$ with a 1 at position i
$\text{diag}(\boldsymbol{a})$	A square, diagonal matrix with diagonal entries given by $\boldsymbol{a}$
a	A scalar random variable
$\mathbf{a}$	A vector-valued random variable
$\mathbf{A}$	A matrix-valued random variable

Sets and Graphs

$\mathbb{A}$	A set
$\mathbb{R}$	The set of real numbers
$\{0, 1\}$	The set containing 0 and 1
$\{0, 1, \ldots, n\}$	The set of all integers between 0 and n
$[a, b]$	The real interval including a and b
$(a, b]$	The real interval excluding a but including b

$\mathbb{A} \backslash \mathbb{B}$	Set subtraction, i.e., the set containing the elements of $\mathbb{A}$ that are not in $\mathbb{B}$
$\mathcal{G}$	A graph
$Pa_{\mathcal{G}}(\mathrm{x}_i)$	The parents of x_i in $\mathcal{G}$

Indexing

a_i	Element i of vector $\boldsymbol{a}$, with indexing starting at 1.
a_{-i}	All elements of vector $\boldsymbol{a}$ except for element i
$A_{i,j}$	Element i, j of matrix $\boldsymbol{A}$
$\boldsymbol{A}_{i,:}$	Row i of matrix $\boldsymbol{A}$
$\boldsymbol{A}_{:,i}$	Column i of matrix $\boldsymbol{A}$
$\mathsf{A}_{i,j,k}$	Element (i, j, k) of a 3-D tensor $\mathbf{A}$
$\mathbf{A}_{:,:,i}$	2-D slice of a 3-D tensor
a_i	Element i of the random vector $\mathbf{a}$

Linear Algebra Operations

$\boldsymbol{A}^\top$	Transpose of matrix $\boldsymbol{A}$
$\boldsymbol{A}^+$	Moore-Penrose pseudoinverse of $\boldsymbol{A}$
$\boldsymbol{A} \odot \boldsymbol{B}$	Element-wise (Hadamard) product of $\boldsymbol{A}$ and $\boldsymbol{B}$
$\det(\boldsymbol{A})$	Determinant of $\boldsymbol{A}$

Calculus

$\frac{dy}{dx}$	Derivative of y with respect to x
$\frac{\partial y}{\partial x}$	Partial derivative of y with respect to x
$\nabla_{\boldsymbol{x}} y$	Gradient of y with respect to $\boldsymbol{x}$
$\nabla_{\boldsymbol{X}} y$	Matrix derivatives of y with respect to $\boldsymbol{X}$
$\nabla_{\mathsf{X}} y$	Tensor containing derivatives of y with respect to $\mathbf{X}$
$\frac{\partial f}{\partial \boldsymbol{x}}$	Jacobian matrix $\boldsymbol{J} \in \mathbb{R}^{m \times n}$ of $f : \mathbb{R}^n \to \mathbb{R}^m$
$\nabla^2_{\boldsymbol{x}} f(\boldsymbol{x})$ or $\boldsymbol{H}(f)(\boldsymbol{x})$	The Hessian matrix of f at input point $\boldsymbol{x}$

$\int f(\boldsymbol{x})d\boldsymbol{x}$	Definite integral over the entire domain of $\boldsymbol{x}$
$\int_{\mathbb{S}} f(\boldsymbol{x})d\boldsymbol{x}$	Definite integral with respect to $\boldsymbol{x}$ over the set $\mathbb{S}$

Probability and Information Theory

$\mathrm{a} \perp \mathrm{b}$	The random variables a and b are independent
$\mathrm{a} \perp \mathrm{b} \mid \mathrm{c}$	They are conditionally independent given c
$P(\mathrm{a})$	A probability distribution over a discrete variable
$p(\mathrm{a})$	A probability distribution over a continuous variable, or over a variable whose type has not been specified
$\mathrm{a} \sim P$	Random variable a has distribution P
$\mathbb{E}_{\mathrm{x}\sim P}[f(x)]$	Expectation of $f(x)$ with respect to $P(\mathrm{x})$
$\mathrm{Var}(f(x))$	Variance of $f(x)$ under $P(\mathrm{x})$
$\mathrm{Cov}(f(x), g(x))$	Covariance of $f(x)$ and $g(x)$ under $P(\mathrm{x})$
$H(\mathrm{x})$	Shannon entropy of the random variable x
$D_{\mathrm{KL}}(P\|Q)$	Kullback-Leibler divergence of P and Q
$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$	Gaussian distribution over $\boldsymbol{x}$ with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$

Functions

$f : \mathbb{A} \to \mathbb{B}$	The function f with domain $\mathbb{A}$ and range $\mathbb{B}$
$f \circ g$	Composition of the functions f and g
$f(\boldsymbol{x}; \boldsymbol{\theta})$	A function of $\boldsymbol{x}$ parametrized by $\boldsymbol{\theta}$. (Sometimes we write $f(\boldsymbol{x})$ and omit the argument $\boldsymbol{\theta}$ to lighten notation)
$\log x$	Natural logarithm of x
$\sigma(x)$	Logistic sigmoid, $\dfrac{1}{1+\exp(-x)}$
$\zeta(x)$	Softplus, $\log(1+\exp(x))$
$\|\|\boldsymbol{x}\|\|_p$	L^p norm of $\boldsymbol{x}$
$\|\|\boldsymbol{x}\|\|$	L^2 norm of $\boldsymbol{x}$
x^+	Positive part of x, i.e., $\max(0, x)$

Datasets and Distributions

p_{data}	The data generating distribution
$\hat{p}_{\text{data}}$	The empirical distribution defined by the training set
$\mathbb{X}$	A set of training examples
$\boldsymbol{x}^{(i)}$	The i-th example (input) from a dataset
$y^{(i)}$ or $\boldsymbol{y}^{(i)}$	The target associated with $\boldsymbol{x}^{(i)}$ for supervised learning
$\boldsymbol{X}$	The $m \times n$ matrix with input example $\boldsymbol{x}^{(i)}$ in row $\boldsymbol{X}_{i,:}$

List of Figures

List of Tables

Chapter 1

Introduction

In the chemical process industry, system models are a fundamental tool for design and operation. Due to its techno-scientific nature, chemical engineering is about modelling physical and chemical phenomena in an accurate enough manner to realize a save and profitable conversion process. These models vary in complexity and prediction potency from single equations such as the Bernoulli equation to detailed partial differentail equation systems such as multi-phase Navier-Stokes. Physico-chemical models are at the core of optimal design or optimal control of most unit operations.
As these *first principle models* rely on intrinsic parameters such as activation energies, friction coefficients, etc. that are usually fitted by experiments, they exhibit some kind of prediction uncertainty. This uncertainty is heavily tied to the measurement uncertainty of the underlying experiments and the non-linearity in the propagation by the model. For example parametric uncertainties of ± 50 % can occur in multi-component reaction systems [1]. As most phenomena in chemical engineering exhibit strong non-lineatities, such as reaction kinetics or activity coefficients, uncertainty quantification represents a great challenge.
Model Predictive Control (MPC) is a potent optimal control algorithm that allows the optimal operation of various systems. The algorithm optimizes a custom loss or reward function under a set of constraints and the dynamics of the system model. The optimal inputs of the system are determined at every time instant as the solution of the optimization. MPC is able do deal with uncertain parameter scenarios in the form of *multi-stage* MPC, where all possible scenarios are optimized over simultaneously. This leads to tremendous computational effort especcialy for detailed system models. The computational effort growths multiplicatory with the amount of parameters and exponentially with the robust horizon [1]. These optimization tasks are impossible to solve in real time with current hardware.
Neural Networks (NNs) are able to approximate any continuous function that maps from a finite dimensional space to another up to an arbitrary small error [1]. Thus, NNs are a key component of machine learning advancements of the 2010s enabling data approximation of almost any kind such as autoregressive language generation [2], protein folding [1] or reduction of partial differential equations (PDEs). Their universal approximation ability, differentiatability and fast evaluation makes NNs greatly suitable to reduce first principle models in the context of optimal control.
For NNs to be applied successfully and savely in process engineering, another measure is of great importance – The alignment of predictions with physical conservation laws such

as mass or energy. By definition, NN predictions seek to minimize a loss function to the ground truth data. The aligment of the predictions with real balance equations is only achieved until test accuracy. Deviations accumulate especcialy in propagation scenarios where predictions are propagated through different networks or through a time horizon in autoregressive manner. This leads to bad predictions or even unstable behavior in late propagation stages and makes MPC implementations challenging.
This work investigates the usage of physics-consistent (PC) NNs in the context of robust model predictive control under parametric uncertainty. The NNs in focus shall significantly reduce the computational effort due to different parameter scenarios as well as guarantee physical correctness of the predictions over the whole prediction horizon. To account for uncertainties, quantile regression is utilized which captures a prediction confidence intervall. PC is enforced by implementing a recent type of activation function that elegantly maps a prediction into the allowed output space without altering the inference time [3].
The developed surrogate models are later evaluated regarding their simulation accuracy using a fictional plug flow tubular reactor (PFTR) model of the ethene oxide synthesis.

Chapter 2

Model Predictive Control under Uncertainty

Before diving into the application of a special model predictive (MPC) algorithm. Uncertain optimization is treated more generally. From economics, over self-driving cars to chemical plants, optimization problems are formulated in terms of uncertain variables in countless variations. These uncertainties arise in three different types – fluctuating disturbances such as wind or weather conditions, parametric offsets such as wrongly determined friction coefficients or model mismatches like unseen side reactions. As the straight maximization or minimzation of an objective often puts a problem to its boundaries, unforeseen disturbances may lead to *constraint violation* or even *instability* [4]. Therefore, *robust* optimization formulations are needed, that are proof against mentioned challenges as well as retain the *performance* with respect to the objective function.

2.1 Robust Optimization

Considering the following optimization task (2.1).

Definition 2.1. Semi-infinite program with the uncertainty $\boldsymbol{w}$.

$$\begin{aligned} \min_{\boldsymbol{u}} \max_{\boldsymbol{w}} \quad & F_0(\boldsymbol{u}, \boldsymbol{w}) \\ \text{s.t.} \quad & F_i(\boldsymbol{u}, \boldsymbol{w}) \leq 0 \quad \forall \boldsymbol{w} \in \mathbb{W} \end{aligned}$$

Here, the optimization of the objective is formulated in a bilevel form. The scalar objective function F_0 is to be minimized w.r.t the decision variables $\boldsymbol{u}$ for the worst case scenario w.r.t the disturbance vector $\boldsymbol{w}$. The inequality constraints F_i however, should be satisfied for all possible disturbances, that lie in a defined set $\mathbb{W}$. If this set is not finite, the number of possible constraints to be satisifed is infintely big. Thus, this formulation is named as *semi-infinite-program* [4]. To reduce the number of constraints, the worst-case estimate can also be applied here (2.2).

Definition 2.2. Bi-level formulation of the semi-infinite program

$$\begin{aligned} &\min_{\boldsymbol{u}} \max_{\boldsymbol{w}} \quad F_0(\boldsymbol{u}, \boldsymbol{w}) \\ \text{s.t.} \quad &\varphi_i(\boldsymbol{u}) \coloneqq \max_{\boldsymbol{w}} \quad F_i(\boldsymbol{u}, \boldsymbol{w}) \leq 0 \quad \boldsymbol{w} \in \mathbb{W} \end{aligned}$$

Now, the inequality constraints are also formulated in a bi-level manner. The maximum of F_i is constant in $\boldsymbol{w}$ and only a function of the decision variables $\boldsymbol{u}$. The function φ_i exactly describes the wost-case for F_i parametrized by $\boldsymbol{u}$. In fact, if certain assumptions hold regarding the uncertainty set $\mathbb{W}$ and the concavity of the maximization, φ_i can be exactly computed [1]. This would simplify the problem dramatically. In reality however, an analytical solution for φ_i is not possible to compute. But with the universal approximation capability of neural networks (NNs) in mind [5], a data-driven approach is promising, that delivers an approximated function $\tilde{\varphi}_i(\boldsymbol{u})$.

2.2 Robust Model Predictive Control

(A short intro to MPC) A model predictive control algorithm solves a control optimization task at each time instant. The dynamic optimization anticipates the future behavior of the controlled system through a mathematical model and determines the control inputs as the solution. Only part of the solution is applied as a control input until the next sampling instant. To yield correct inputs, the prediction quality of the underlying model is of crucial importance.

Coming from this general perspective on robust optimization, *robust MPC* specializes this concept to a dynamic closed-loop control environment. First, the continuous-time formulation is considered.

Definition 2.3. Continuous-time formulation of an MPC task under uncertainty.

$$\begin{aligned} &\min_{\boldsymbol{u}} \max_{\boldsymbol{w}} \quad J(t_0, t_{\text{end}}, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{w}) \\ \text{s.t.} \quad &\dot{\boldsymbol{x}} = f(t, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{w}) \\ &F_i(t, \boldsymbol{x}, \boldsymbol{u}, \boldsymbol{w}) \leq 0 \quad \forall t \in [t_0, t_{\text{end}}],\ \forall \boldsymbol{w} \in \mathbb{W} \\ &\boldsymbol{x}_0 = \boldsymbol{x}_{\text{init}} \end{aligned}$$

The only difference to the general problem (2.1) is that the states, denoted with $\boldsymbol{x}$, evolve along some system dynamics that are described by f, that also underlie to the uncertainty $\boldsymbol{w}$. This formulation is now infinite in time and in the uncertain parameters. To make computation feasible, the problem is discretized in the time dimension eiher using single shooting, multiple shooting or orthogonal collocation on finite elements **<empty citation>** One possibility to roughly discretize the uncertain parameter set $\mathbb{W}$ is done by *multi-stage-MPC* **<empty citation>** Which is intuitive, but leads to tremendous computational effort, especcialy with growing dimensionality of the uncertainty space.

Definition 2.4. Time-discretized multi-stage MPC

$$\min_{\boldsymbol{u}_k, \boldsymbol{x}_k} \max_{\boldsymbol{w}_k} \quad J(N_\mathrm{p}, \boldsymbol{x}_k, \boldsymbol{u}_k, \boldsymbol{w}_k)$$

2.3 Uncertainty

Model uncertainties are a main challenge in MPC. These uncertainties can occur in the form of measurement noise, unknown parameters such as activation energies or fluctuating disturbances such as wind from different directions. In the context of chemical engineering, the focus lies on parametric uncertainty of reaction kinetic parameters. Eventhough, the underlying methodlogy can be generalized to any kind of model uncertainty.
The afforementioned uncertainties can be grouped into two types (eq. 2.1).

$$\begin{aligned} \boldsymbol{x}_{k+1} &= f(\boldsymbol{x}_k, \boldsymbol{u}_k) + \boldsymbol{w}_k, \quad \boldsymbol{w}_k \in \mathbb{W} \\ \boldsymbol{x}_{k+1} &= f(\boldsymbol{x}_k, \boldsymbol{u}_k, \boldsymbol{d}_k), \quad \boldsymbol{d}_k \in \mathbb{D} \end{aligned} \tag{2.1}$$

The first one is additive disturbance and much easier to handle than the second type that propagates the disturbances non-linearly through the system [1]. The second type is more general and most parametric uncertainties occur according to this type, which is why it is investigated in this work.

Conservartiveess vs Performance

2.4 Multi-Stage MPC

Chapter 3

Surrogate Modeling

3.1 Neural Networks

Feed forward neural networks (NNs) provide a stunning capability of approximating any non-linear function from any finite dimensional space to another. According to the *Universal approximation theorem*, any finite dimensional function can be reproduced if the number of hidden layers and respective neurons is high enough, up to an arbitrarily small error [5]. Thus, NNs play a major role in recent developments in machine learning. The breakthrough of large language models such as ChatGPT heavily rely on neural networks [[2]]. NNs are applied not only in natural lanugage processing but in the chemical process industry. Use cases range from thermodynamic property prediction over unit operation design to corporate level decision making [[6]]. Their ability to approximate any non-linear function while beeing differentiable, makes NNs especcialy suitable for dynamic optimization such as MPC. In contrast to detailed first principle models, NNs have the advantage of making a prediction in a fraction of the inference time of the first principle model. As MPC operates in real time parallel to the system to be controlled, the computation duration is a key measure for a succesfull MPC implementation. Thus, surrogate models in form of NNs are a crucial tool for dynamic optimization and heavily investigated in current research. May a NN be given as a alternating series of function evaluations (eq. 3.1).

$$\begin{aligned} \mathcal{NN}(\boldsymbol{x}, \boldsymbol{\theta}) &= g_{l+1} \circ h_{l+1} \circ ... \circ g_1 \circ h_1(\boldsymbol{x}) \\ h(\boldsymbol{a}_{l-1}) &= \boldsymbol{\theta}_{Wl} \boldsymbol{a}_{l-1} + \boldsymbol{\theta}_{bl} \\ \boldsymbol{a}_l &= g_l(h(\boldsymbol{a}_{l-1})) \end{aligned} \tag{3.1}$$

In fact, a NN is a series of function combinations denoted by the $\circ$-symbol alternating between a linear function $h(\boldsymbol{a})$ and a non-linear activation function g. The linear transformation matrices $\boldsymbol{\theta}_{Wl}$ and offsets $\boldsymbol{\theta}_{bl}$, are called weights and biases respectively and are the trainable parameters of a NN. Given a set of training data $\mathbb{D}_{\text{train}}$, the optimal parameters for $\boldsymbol{\theta}$ are found by solving an optimization task that involves the minimzation of a prediction loss function (eq. 3.2).

$$\begin{aligned} \mathbb{X}_{\text{train}} &\coloneqq \{\boldsymbol{\xi}^{(0)}, \dots, \boldsymbol{\xi}^{(m)}\} \\ \mathbb{Y}_{\text{train}} &\coloneqq \{\boldsymbol{y}^{(0)}, \dots, \boldsymbol{y}^{(m)}\} \\ \mathcal{L}(\boldsymbol{\theta}, \mathbb{X}_{\text{train}}, \mathbb{Y}_{\text{train}}) &= \frac{1}{m} \sum_{i=0}^{m-1} \left|\left| \boldsymbol{y}^{(i)} - \tilde{\boldsymbol{y}}(\boldsymbol{\theta}, \boldsymbol{\xi}^{(i)}) \right|\right|_2^2 \end{aligned} \tag{3.2}$$

In *supervised learning*, the training data is separated in *features* $\mathbb{X}_{\text{train}}$, the inputs of the NN, and *labels* $\mathbb{Y}_{\text{train}}$, the outputs of the NN. During training, the parameters $\boldsymbol{\theta}$ are determined such that the NN approximates the data in best possible manner. In this example the loss function $\mathcal{L}$ portrays the mean squarred error (MSE) that is used in most regression tasks. The difference between the model prediction, denoted as $\tilde{\boldsymbol{y}}$, and the true data point $\boldsymbol{y}^{(i)}$ is penalized quadratically. The kind of loss function heavily impacts the characteristics of the NN model prediction.

Explain batching Batching allows to pass multiple data points forward through the NN.

Chapter 4

Surrogate Modelling

4.1 Physics-Constrained Neural Networks

By definition, NNs are designed to reproduce their training data in a best possible manner, defined by the characteristics of the loss function used during the training process. NN predictions minimize the loss towards the training data seen beforehand. Circumstances exist, in which the output of a NN should strictly satisfy a certain set of equations. In case of physical modeling, the prediction of a surrogate should follow the same conservation laws as a first principle model. Especcialy, when predicions are propagated through several NNs or simulated in an autoregressive manner, errors accumulate. Final predictions are untrustworthy or simulations exhibit instability [3]. As a MPC algorithm needs a reasonable approximation of the system behavior over the complete prediction horizon, the accumulation of conservation violations become an issue.

To realize physics consistent NN outputs, several strategies exists. Physics-informed neural networks (*PINN*s) for instance, embed physical balance equations into the loss function similar to a regularization term [7]. This serves as a soft constraint and comes with two downsides. The NN output does not strictly follow the constraint equation, because the physical consistency is fullfilled up to the trade off between data fit and constraint satisfaction. Every new balance equation to be included introduces a new hyperparameter worsening the ability to include network parameter regularization. To guarantee strict constraint satisfaction and thus perfect physics consistency up to machine precision, a new type of activation function is presented equivalently to the work by Chen et al. [3]. This activation function serves as a linear projection from the NN output space into the physical allowed subspace without adding neither learnable parameters nor hyperparameters. Let the output of a NN be defined as well as a set of linear equality contraints that summarize some physical conservation quantity (def. 4.1).

Definition 4.1. Crude NN output with a given set of linear equality constraints.

$$\tilde{\boldsymbol{y}}(\boldsymbol{\theta}, \boldsymbol{\xi}) \coloneqq \mathcal{NN}(\boldsymbol{\theta}, \boldsymbol{\xi})$$
$$\boldsymbol{A}(\boldsymbol{y} - \boldsymbol{z}_0) = \boldsymbol{b}$$
$$\text{with} \quad \tilde{\boldsymbol{y}}(\boldsymbol{\theta}, \boldsymbol{\xi}), \boldsymbol{z}_0 \in \mathbb{R}^{n_\text{out}} \quad \boldsymbol{A} \in \mathbb{R}^{n_\text{c} \times n_\text{out}} \quad \boldsymbol{b} \in \mathbb{R}^{n_\text{c}}$$

$\tilde{\boldsymbol{y}}$ denotes the NN output, $\boldsymbol{\xi}$ the input and the matrices $\boldsymbol{A}$ and $\boldsymbol{b}$ portray the feasible space of points. The variable $\boldsymbol{z}_0$ illustrates an external input into the constraint. This

may be a NN input, a constant, or another batched reference point. In a physical sense, $\boldsymbol{z}_0$ is often introduced as a boundary or initial condition. A feasible point $\boldsymbol{y}$ now needs to be determined that fullfills the set of linear equality constraints. For a straight forward implementation, the formulation appears in such a way that it supports batching of a certain batch size $n_\mathcal{B}$. n_out and n_c describe the number of output features and numbers of linear equality constraints respectively. The main idea is, to find a point in the feasible subspace that is closest to the NN prediction. This is forced by following quadratic programm (QP) (def. 4.2).

Definition 4.2. Minimization of the euclidian distance towards the NN output as a linear equality constrained optimization that supports batching.

$$\begin{aligned} \boldsymbol{y}^* &= \underset{\boldsymbol{y}}{\operatorname{argmin}} ||\boldsymbol{y} - \tilde{\boldsymbol{y}}||_2^2 \\ \text{s.t.} \quad & (\boldsymbol{y} - \boldsymbol{z}_0)\boldsymbol{A}^\top - \boldsymbol{b} = \boldsymbol{0} \end{aligned}$$

This means, the output of the network $\tilde{\boldsymbol{y}}$, the optimal solution $\boldsymbol{y}^*$ and $\boldsymbol{z}_0$ are matrices of dimension $n_\mathcal{B} \times n_\text{out}$. Computing frameworks that support broadcasting such as `numpy` or `pytorch` allow the implementation of $\boldsymbol{z}_0$ in the shape of $1 \times n_\text{out}$ to reduce memory usage as long as it remains constant [1]. The transposed constraint matrix $\boldsymbol{A}^\top$ must be of shape $n_\text{c} \times n_\mathcal{B}$. The vector $\boldsymbol{b}$ represents the offset of the linear equality constraints. This optimization task can be solved analytically by setting up the *Karush-Kuhn-Tucker* (KKT) conditions (th. 4.1).

Theorem 4.1. *Langrangian and KKT conditions of the QP*

$$\begin{aligned} \mathcal{L}(\boldsymbol{y}, \boldsymbol{\nu}) &= ||\boldsymbol{y} - \tilde{\boldsymbol{y}}||_2^2 + \boldsymbol{\nu}^\top (\boldsymbol{A}(\boldsymbol{y} - \boldsymbol{z}_0)^\top - \boldsymbol{b}) \\ \nabla_{\boldsymbol{y}} \mathcal{L}(\boldsymbol{y}, \boldsymbol{\nu}) &= 2(\boldsymbol{y}^* - \tilde{\boldsymbol{y}}) + \boldsymbol{\nu}^\top \boldsymbol{A} \overset{!}{=} 0 \\ \nabla_{\boldsymbol{\nu}} \mathcal{L}(\boldsymbol{y}, \boldsymbol{\nu}) &= (\boldsymbol{y}^* - \boldsymbol{z}_0)\boldsymbol{A}^\top - \boldsymbol{b} \overset{!}{=} 0 \end{aligned}$$

The Lagrangian $\mathcal{L}$ arises as the sum of the objective function and all linear equality constraints. The vector $\boldsymbol{\nu}$ contains the dual variables of the linear equality constraints. The optimality conditions lead to a linear system of equations (cor. 4.1).

Corollary 4.1. *The optimal solution in the feasible space as projection of an activation function*

$$\begin{pmatrix} \boldsymbol{y}^* & (\boldsymbol{\nu}^*)^\top \end{pmatrix} \begin{pmatrix} 2\boldsymbol{I} & \boldsymbol{A}^\top \\ \boldsymbol{A} & \boldsymbol{0} \end{pmatrix} = \begin{pmatrix} 2\tilde{\boldsymbol{y}} & \boldsymbol{z}_0\boldsymbol{A}^\top + \boldsymbol{b} \end{pmatrix}$$

$$g_{pc}(\tilde{\boldsymbol{y}}, \boldsymbol{z}_0) \coloneqq \begin{pmatrix} 2\tilde{\boldsymbol{y}} & \boldsymbol{z}_0\boldsymbol{A}^\top + \boldsymbol{b} \end{pmatrix} \begin{pmatrix} 2\boldsymbol{I} & \boldsymbol{A}^\top \\ \boldsymbol{A} & \boldsymbol{0} \end{pmatrix}^{-1} = \begin{pmatrix} \boldsymbol{y}^* & (\boldsymbol{\nu}^*)^\top \end{pmatrix}$$

The optimal solution denoted with "*" is directly yielded by projecting the NN output $\tilde{\boldsymbol{y}}$ using the additional input $\boldsymbol{z}_0$ and a projection matrix. This projection matrix only contains the constraint matrix $\boldsymbol{A}$ can be computed before runtime which drastically speeds up forward and backward passes in contrast to implicit methods [8]. The solution elegantly serves as an activation function $g_\text{pc}(\tilde{\boldsymbol{y}}, \boldsymbol{z}_0)$, that maps the crude NN

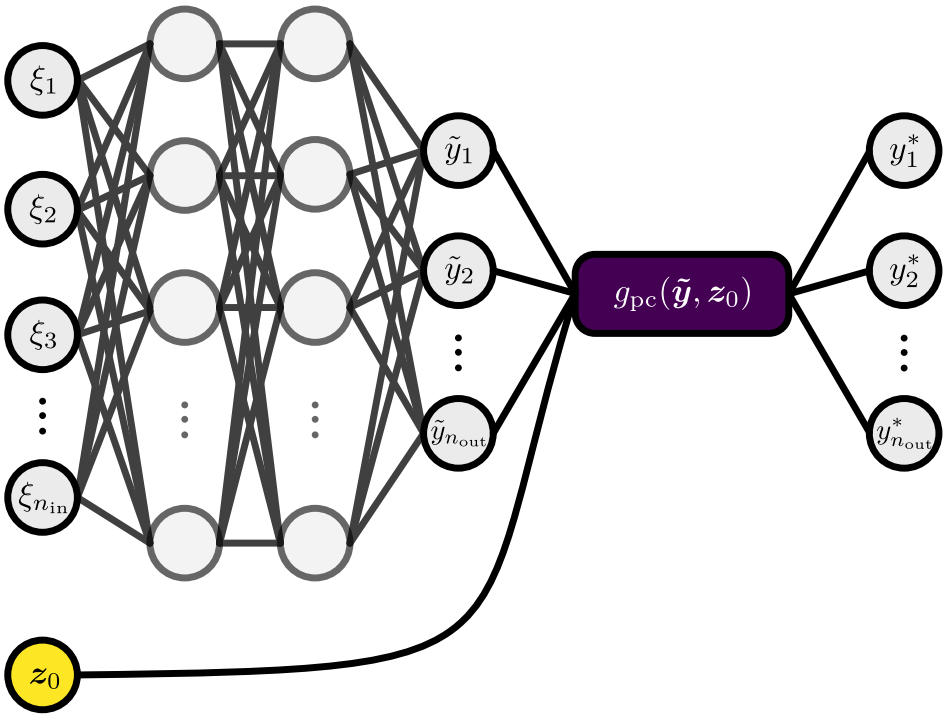

Figure 4.1: The physics constrained NN turns the input vector $\boldsymbol{\xi}$ into the crude output $\tilde{\boldsymbol{y}}$ via a feedforward NN, which is the projected by the physics constrained activation function g_{pc} into the feasible output $\boldsymbol{y}^*$. It allows to include data points such as boundary conditions as needed in the form of $\boldsymbol{z}_0$

output into a subspace defined by $\boldsymbol{A}$ and $\boldsymbol{b}$. The final output for $\boldsymbol{y}^*$ satisfies the linear equality constraints by definition, while it is located as close to the crude output $\tilde{\boldsymbol{y}}$ as possible. This is not only applicable in the field of chemical engineering but a general formulation that allows to integrate linear equality constraints into NNs. Additionally, the type of network architecture is independent of the mapping. It can be appended to any network type such as recurrent NNs, convolutional NNs or transformer-based architectures.

Due to its general applicability, the activation function could be used within a network to correct intermediate values. In most use cases howerver, it is applied as a final correction function at the output (fig. 4.1). The input $\boldsymbol{\xi}$ is propagated through a feedforward NN with the physics constrained activation function behind the last layer (purple). It takes the reference value $\boldsymbol{z}_0$ (yellow) without beeing forwarded through the network. In recent literature, NNs that utilze such a type of activation function can be found as *KKT-hPINN* [3], which is short for *Karush-Kuhn-Tucker-hard-physics-informed-neural-network*. For later reference, this activation function g_{pc} will be referred to as *physics constrained activation* (cor. 4.1) to have a short name in the context of chemical engineering. Furthermore, this procedure could be extended to support arbitrary non-linear

equality constraints by splitting the network output in frozen and unfrozen variables [9]. It enables the integration of enthalpy balances that are of non-linear nature. As this work combines the implementation of physics consistent NNs with parametric uncertainty for MPC, the focus remains on linear equality constraints.

Algorithm 1 Forward pass of the physics constrained activation function.

Require: $\boldsymbol{K} = \begin{pmatrix} 2\boldsymbol{I} & \boldsymbol{A}^\top \\ \boldsymbol{A} & \boldsymbol{0} \end{pmatrix}^{-1}$, $\tilde{\boldsymbol{y}}, \boldsymbol{z}_0, \boldsymbol{A}, \boldsymbol{b}$

$\boldsymbol{h} \leftarrow \begin{pmatrix} 2\tilde{\boldsymbol{y}} & \boldsymbol{z}_0\boldsymbol{A}^\top + \boldsymbol{b} \end{pmatrix}$

$\boldsymbol{y}^* \leftarrow \boldsymbol{h}\boldsymbol{K}$

$\boldsymbol{y}^* \leftarrow \boldsymbol{y}^*_{:,:n_{\text{out}}}$

return $\boldsymbol{y}^*$

The forward pass through the physics constrained activation involves the setup of a temporary vector $\boldsymbol{h}$ (alg. 1) and the truncation of the dual variables in the solution. The matrix inversion to yield $\boldsymbol{K}$ should be done offline and then saved as untrainable model parameter. In `pytorch` this is can be done using the `register_buffer()` method. An implementation example of the physics consistent activation can be found in the appendix (XX).

Chapter 5

Results on Surrogate Model Performance

Please choose a more expressive title for this chapter. If it makes sense for your work you can also have multiple chapters presenting your results.

5.1 Training Effectivity

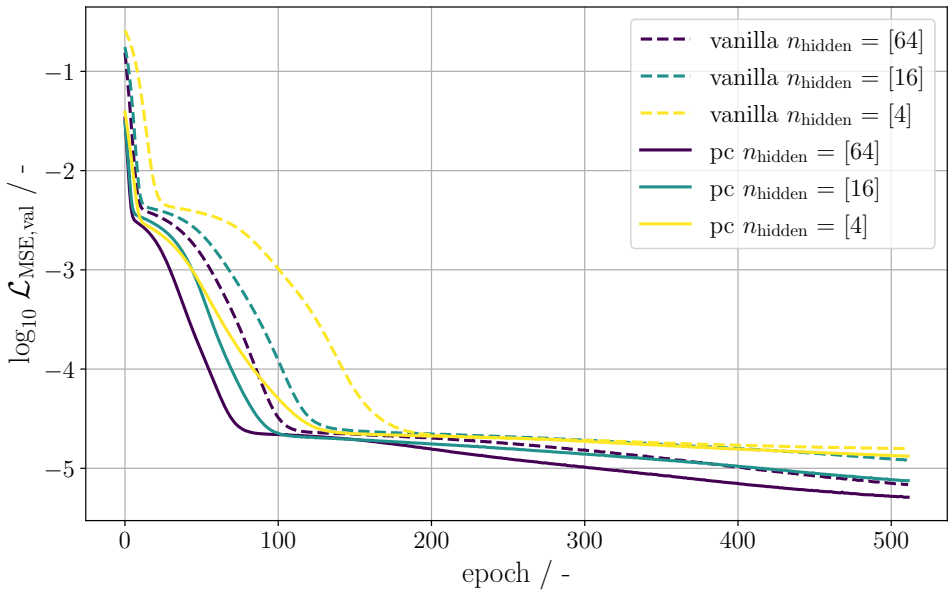

Figure 5.1: The validation loss calculated as MSE $\mathcal{L}_{\text{MSE,val}}$ during the training of the vanilla NARX (dashed line) and the physics-constrained NARX (solid line). The three data rows each indicate *one hidden layer* with $64, 16$ and 4 hidden neurons respectively. The physics-constrained NARX converges visibly faster than the vanilla NARX.

Chapter 6

Conclusions

Appendix A

Datasheets

Did your work require long tables of parameters, e.g. to configure a system model. This table would distract the main part of the thesis but including it is an important aspect of scientific work. Please attach it here.

A.1 Parameter for ...

...

Appendix B

Proofs

Did you introduce lemmas or theorems with lengthy proofs? Including them in the main part of the thesis might be distracting. You can also include them in the appendix.

B.1 Proof of Theorem X

...

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