Nonlinear Model Predictive Control with Explicit Backoffs for Stochastic Systems under Arbitrary Uncertainty

Joel A. Paulson and Ali Mesbah

Department of Chemical and Biomolecular Engineering
University of California, Berkeley, CA 94720 USA
e-mail: {joelpaulson,mesbah}@berkeley.edu

Abstract: The majority of work on chance constrained model predictive control (MPC) for stochastic systems adopts the concept of implicit constraint backoffs for handling state chance constraints. However, implicit backoffs cannot be computed analytically in nonlinear MPC (NMPC), so that they must be approximated and, as a result, chance constraints are not guaranteed by the closed-loop system. This paper proposes a strategy for explicit computation of constraint backoffs that allows tightly guaranteeing chance constraints in NMPC for stochastic systems with arbitrary uncertainty distributions. The proposed method relies on uncertainty propagation through closed-loop system dynamics. Thus, this paper also investigates the use of stochastic surrogate models for constructing the distribution of closed-loop quantities of interest such as state constraint functions or any general performance objectives. To this end, an extension of polynomial chaos that can handle arbitrary probability measures is proposed for a class of disturbance models representing plant-model mismatch. The proposed methods are illustrated on a benchmark continuously-stirred tank reactor problem.

Keywords: Stochastic optimal control, state chance constraints, explicit backoffs, closed-loop performance verification, arbitrary polynomial chaos

1. INTRODUCTION

Model predictive control (MPC) is the most widely used approach for optimal control of constrained, multivariable systems with competing performance objectives (Rawlings and Mayne, 2009). The fact that the inherent robustness of MPC to system uncertainty may not be adequate in practice has motivated the development of numerous robust and stochastic formulations for MPC that account for uncertainty in model predictions (Bemporad and Morari; Mesbah, 1999; 2016). When probabilistic descriptions of the system uncertainty are available, they can be explicitly incorporated into the optimal control problem, so that state constraints are enforced in terms of chance constraints. Chance constraints allow for a certain percentage of state trajectories to violate constraints, enabling a systematic tradeoff between constraint satisfaction and control performance.

Chance constraints are defined as multivariate integrals over the probability distribution of the state variables. In the case of linear systems with additive uncertainty, only the mean state trajectory is a function of the inputs while the shape of the state distribution remains constant. This allows rewriting the multivariate integrals in terms of tightened – backed off – constraints on the nominal system that are fully determined offline (Kouvaritakis and Cannon, 2016). For nonlinear systems, however, the multivariable state distribution is a complex function of the initial state and control input sequence. Thus, even though a similar constraint backoff idea applies in the context of nonlinear MPC (NMPC), the backoffs cannot be directly computed offline and must instead be incorporated implicitly into the optimal control problem.

Broadly speaking, there are two main representations for implicit backoffs in stochastic NMPC: moment-based and scenario-based. The majority of moment-based NMPC strategies represent implicit backoffs as weights multiplying some function of the state covariance matrix in the state constraint equations. The weights, for example, can be selected using distributionally-robust approaches (Nemirovski and Shapiro, 2006) such as the Cantelli-Chebyshev inequality, which results in guaranteed satisfaction as long as the state mean and covariance are known exactly (Mesbah et al.; Farina et al., 2014; 2016). However, distributionally-robust approaches typically lead to overly conservative approximations, as they often provide a loose bound for continuous distributions (Heirung et al., 2018). Alternatively, the weights can be chosen by approximating the state distribution as Gaussian (Van Hessem and Bosgra; Paulson and Mesbah, 2006; 2017). This approach provides no guarantees and can perform poorly when the state distribution significantly deviates from normality. Scenario-based NMPC strategies, on the other hand, represent the system uncertainty in terms of a finite collection of scenarios, where implicit backoffs correspond to the enforcement of state constraints for each scenario (Lucia et al., 2013). It is important to note that the scenario-based approach does not provide any guarantees when the uncertainty has a continuous distribution.
This paper investigates the notion of computing backoffs explicitly in NMPC so that satisfaction of chance constraints is tightly guaranteed in a closed-loop setting. The main motivation behind explicit backoffs is to avoid the complexity of representing backoffs implicitly for all possible initial states and inputs. The idea of explicit backoffs has been demonstrated in the context of open-loop optimal control (Koller et al., 2018). This paper extends this idea to NMPC and presents an iterative strategy for determining explicit backoffs based on full distribution of the state constraints, where Monte Carlo (MC) sampling can be used to estimate, within a specified tolerance, the probability distribution of state constraints.

Although MC is the method of choice for uncertainty propagation when the number of uncertainties is large, its convergence rate can be slow (Cafélsch, 1998). This implies that a large number of samples may be needed in practice to accurately determine the explicit backoffs. For particular types of disturbance models, the uncertainty dimension can be reduced to a (relatively) small number of time-invariant uncertainties. This opens the door to more efficient uncertainty propagation methods that can achieve high accuracy with a much smaller number of samples. Thus, this work also investigates the idea of constructing stochastic surrogate models for closed-loop quantities of interest (e.g., state constraint functions or performance objectives) when disturbance models are derived from a high-fidelity model of the system, describing plant-model mismatch. To this end, an extension of polynomial chaos that can handle probabilistic disturbance models with arbitrary distributions (e.g., bimodal or time-correlated) is utilized (Paulson et al., 2017). Thus, the paper establishes how stochastic surrogate models can be used to systematically and efficiently determine explicit backoffs and shape the distribution of any general closed-loop performance objective in NMPC for stochastic systems.

**Notation.** \( \mathbb{R} \) and \( \mathbb{N} = \{1, 2, \ldots \} \) are the set of real and natural numbers, respectively. \( (a, b) = [a^T, b^T]^T \) is a shorthand for vector concatenation. Let \( z_t = (z_1, z_2, \ldots, z_j) \) denote the sequence of \( z \) from time \( i \) to \( j \). For any vector \( x \), \( [x]_i \) denotes its \( i \)-th element. The indicator function on set \( A \) is denoted by \( \mathbb{I}(A) \). \( F_X, P_X, \) and \( \mathbb{P}[X] \) denote, respectively, cumulative distribution function (cdf), probability density function (pdf), and expected value of a random variable \( X \). \( \mathbb{P}[X \in A] = \int_A dF_X(x) = \int_A P_X(x)dx \) denotes the probability of occurrence of event \( X \in A \). For any two random vectors \( X \) and \( Y \), \( X|Y \) denotes the conditional random variable \( X \) given \( Y \).

## 2. PROBLEM FORMULATION

Consider a discrete-time nonlinear system

\[
x_{t+1} = f_t(x_t, u_t) + w_t, \quad t = 0, \ldots, T - 1,
\]

where \( x_t \in \mathbb{R}^{n_x} \) is the system state, \( u_t \in \mathbb{R}^{n_u} \) is the control input, \( w_t \in \mathbb{R}^{n_w} \) is the disturbance, and the function \( f_t : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x} \) is the nominal state transition function, which can generally vary with time. The initial state \( x_0 \) is assumed to be known while the disturbance \( w_{0:T} \) is random, with a known (possibly complex) arbitrary distribution \( p_{w_{0:T}} \).

It is assumed that the state of the system (1) is measured. When the state is not accessible, it must be estimated and the estimation error introduces an additional source of uncertainty. We consider causal control policies in which \( x_{t-1} \) and \( w_{0:t-1} \) are available to the controller when the input \( u_t \) should be selected. Thus, the control input is defined by

\[
u_t = \phi_t(x_{0:t}, w_{0:t-1}), \quad t = 0, \ldots, T,
\]

where the family of functions \( \phi : \mathbb{R}^{n_x} \times \mathbb{R}^{(t-1)n_u} \to \mathbb{R}^{n_u} \) for \( t = 0, \ldots, T \) is called the control policy. For a fixed control policy, (1) and (2) can be used to express the control input trajectory \( u_{0:T} \) and the state trajectory \( x_{0:T} \) in terms of the random disturbance sequence \( w_{0:T} \). When the control policy is a function of \( x_t \) only, i.e.,

\[
\phi_t(x_{0:t}, w_{0:t-1}) = \mu_t(x_t),
\]

with \( \mu_t : \mathbb{R}^{n_x} \to \mathbb{R}^{n_u}, \) \( \phi_t \) is referred to as a state-feedback policy. When the control policy is independent of any measured state or disturbance (i.e., \( \phi_t \) is constant), it is referred to as an open-loop policy.

We assume that system performance for a given sequence of states, inputs, and disturbances is quantified in terms of a finite-horizon cost function of the form

\[
J = \sum_{t=0}^{T} \ell_t(x_t, u_t, w_t),
\]

where \( T \in \mathbb{N} \) is the time horizon and \( \ell_t : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_w} \to \mathbb{R} \) is the stage cost function at time \( t \in \{0, \ldots, T\} \). The objective \( J \) is a random variable due to the stochastic nature of (1). Without loss of generality, the control objective is to minimize the expected value of the cost function, i.e., \( \mathbb{E}[J] \). We note that penalties on higher moments (such as variance, skewness, or kurtosis) can be incorporated through proper choice of the stage cost. In addition, the dynamic evolution of (1) is considered to be subject to input and state constraints. We consider hard constraints on the control input such that

\[
u_{0:T} \in U_0 \times \cdots \times U_T = U_{0:T},
\]

for all possible disturbance realizations. Also, due to the stochastic nature of (1), state constraints can generally be posed in terms of joint chance constraints

\[
\mathbb{P}[x_t \in X_t] \geq c_t, \quad t = 1, \ldots, T,
\]

where \( c_t \in (0, 1) \) represents the confidence level of constraint satisfaction. Hard constraints can be recovered by setting \( c_t = 1 \). Note that the set of constraints (6) can also be enforced jointly in time, i.e., \( \mathbb{P}[x_{1:T} \in X_{1:T}] \geq c \), though (6) is considered here for simplicity of presentation.

The goal of stochastic optimal control for system (1) is to choose the control policy (2) that minimizes the expected cost function \( \mathbb{E}[J] \) while ensuring satisfaction of constraints (5) and (6). Thus, the stochastic optimal control problem (OCP) is formulated as

\[
\min_{\phi_{0:T}(\cdot)} \mathbb{E}\left\{ \sum_{t=0}^{T} \ell_t(x_t, u_t, w_t) \right\}
\]

s.t. \( x_{t+1} = f_t(x_t, u_t) + w_t, \quad t = 0, \ldots, T - 1, \)

\[
u_t = \phi_t(x_{0:t}, w_{0:t-1}) \in U_t, \quad t = 0, \ldots, T, \quad \mathbb{P}[x_t \in X_t] \geq c_t, \quad t = 1, \ldots, T,
\]

\[
x_0 \text{ known, } w_{0:T} \sim p_{w_{0:T}}.
\]

The decision variable in (7) is the policy \( \phi_{0:T} \), which is a collection of infinite-dimensional control laws. Note that the cost function and state constraints are in general
complex nonlinear functions of the control policy, and the probabilistic operators $\mathbb{E}\{\cdot\}$ and $\mathbb{P}\{\cdot\}$ are defined with respect to the random disturbance sequence $w_{0:T}$.

In theory, the optimal policy in (7) can be found with dynamic programming (DP) (Bertsekas and Shreve, 2004). When $w_t(x_t)$ is conditionally independent of the past disturbances $w_{0:t-1}$ for all $t = 1, \ldots, T$ and state constraints are ignored, then the optimal policy has the form (3) and must satisfy the standard Bellman recursion (Skaf et al., 2010). However, correlated disturbances and chance constraints substantially complicate the DP formulation as the state space must be formulated in terms of a much larger augmented system (Carpentier et al., 2012). These issues, along with the well-known curse of dimensionality for continuous state spaces, make the DP problem intractable for the types of systems of interest in this work. Thus, instead of attempting to solve the DP problem directly, this work considers optimal control methods that are suboptimal, but are much cheaper to solve online. In particular, we broadly adopt the notion of receding-horizon control for the uncertain, nonlinear system (1), which leads to some variant of “robust” NMPC. An important consideration in NMPC is that the performance (4) and state constraints (6) are not guaranteed by design (in a closed-loop sense) due to several approximations made in the stochastic OCP (7). Here, we are interested in simulation-based approaches that can efficiently calculate $\mathbb{E}\{J\}$ and $\mathbb{P}\{x_t \in X_t\}$ (for any fixed NMPC controller) in order to verify that closed-loop requirements are met. This allows for tuning the NMPC parameters systematically based on information gained through these closed-loop simulations.

The next section introduces a distribution-based approach for determining tightened constraints on the nominal system so that state chance constraints (6) are satisfied in closed loop. For the sake of generality, the approach applies to any form of disturbance model (e.g., disturbances correlated in time). It is shown, however, that this approach can be computationally expensive as many simulations of the closed-loop system must be executed. Therefore, in Section 4, we focus on a particular class of disturbance models that represent plant-model mismatch and can be readily derived from a high-fidelity model of the system. For this class of disturbances, which are highly correlated, we present a procedure for developing surrogate models that capture the full distribution of the closed-loop state of the system (1) under NMPC with a limited number of closed-loop simulations. Section 5 then discusses how the same procedure can be used to determine and shape the distribution of the control performance $J$.

Remark 1. The problem of interest here is a finite-time stochastic OCP (7) with a general (economic) cost function. Therefore, we do not consider stability and/or convergence to a particular equilibrium point, and instead focus on achieving the best possible performance in $T$ steps while tightly satisfying constraints.

3. NONLINEAR MODEL PREDICTIVE CONTROL UNDER UNCERTAINTY USING BACKOFFS

This section presents the so-called certainty equivalence (CE)-NMPC problem for the system (1) and discusses how state constraints can be effectively handled in the presence of uncertainty. Two of the main challenges in solving (7) result from the infinite dimension of the decision variable $\phi_{0:T}$ and the propagation of stochastic disturbances $w_{0:T}$ through the nonlinear dynamics of (1) for evaluating the cost function and chance constraints. The simplest way to address the first challenge is to convert the OCP into one with a finite number of decision variables by restricting $\phi_{0:T}$ to be an open-loop policy. That is, $\phi_{0:T} = \nu_{0:T}$, where $\nu_{0:T}$ is constant at every time; alternative finite-dimensional feedback parametrizations are discussed later. Since the open-loop policy embodies no feedback action, NMPC incorporates feedback through a receding (or shrinking) horizon implementation wherein the open-loop OCP is repeatedly solved online given the most recent state measurements.

The second challenge can be addressed by approximating the (possibly complex) disturbance distribution with one that is much easier to propagate through the nonlinear dynamics, i.e., $p_{w_{0:T}} \approx p_{\hat{w}_{0:T}}$. By far, the simplest approximation is to assume the disturbance follows a degenerate distribution, that is, the disturbance takes constant values that are known in the future. This results in the CE-NMPC formulation that utilizes the following predictions

$$z_{i+1} = f_i(z_{i:T}, v_{i:T}) + \hat{w}_{i}, \quad z_{i:T} = x_t, \quad i = t, \ldots, T,$$

where $z_{i:T} \in \mathbb{R}^n$ is the nominal state, $v_{i:T} \in \mathbb{R}^n$ is the open-loop control input, and $\hat{w}_i \in \mathbb{R}^n$ is the best estimate of the disturbance into the future. Since the disturbance may be correlated to past information, its current best estimate $\hat{w}_i = \mathbb{E}\{w_{i:T} | \hat{w}_{0:i-1}\}$ leads to a control policy of the form (2). However, this relationship can be difficult to determine. Thus, CE-NMPC often assumes $\hat{w}_i = 0$ for all $i \geq t = 0, \ldots, T$, which results in a state-feedback policy of the form (3).

Under these approximations, the stochastic OCP (7) simplifies to a deterministic nonlinear program (NLP) given the current state $x_t$

$$\min_{z_{i:T}, v_{i:T}} \sum_{t=0}^{T} \ell_i(z_{i:t}, v_{i:t}, 0)$$

s.t. $z_{i+1} = f_i(z_{i:T}, v_{i:T}), \quad z_{i:T} = x_t, \quad i = t, \ldots, T - 1,$

$z_{i+1} \in Z_{i+1:T}, \quad v_{i:t} \in V_{i:t}, \quad i = t, \ldots, T - 1,$

where the cost function equals the expectation with respect to the degenerate distribution $p_{\hat{w}_{0:T}}$ and $Z_{i+1:T}$ and $V_{i:t}$ are user-defined constraint sets. The optimal solution to (8) is denoted by $(z_{i:T}^*, v_{i:T}^*)$. Only the first element of this system is applied to the system, i.e., $v_t = v_{i:T}^*(z_t)$, implying that the OCP must be solved at every sampling time. This recursive optimal control strategy applied to (1) gives rise to closed-loop dynamics of the form $x_{t+1} = f_i(x_t, v_{i:T}^*(z_t)) + w_t$, whose properties are intimately tied to the selection of the constraint sets $Z_{i+1:T}$ and $V_{i:t}$. Since open-loop inputs are considered in (8), choosing $V_{i:t} = U_t$ ensures that $v_{i:t}^*(z_t) \in U_t$ as long as a feasible solution to the problem exists. Making a similar choice for the state constraints $Z_{i+1:T} = Z_{i+1:T}$, however, will not necessarily guarantee satisfaction of (6) due to the approximations made on the future state predictions.
Due to this neglected uncertainty in CE-NMPC, the state constraints need to be systematically tightened to ensure satisfaction of the chance constraints (6). The concept of explicit backoffs, which has been applied in the context of optimal control under uncertainty (Koller et al., 2018), can be used to find constraint sets $Z_{t+1|t}$ that guarantee (6) based on the true disturbance distribution $p_{w_0,\ldots,w_T}$. There are two different approaches for implementing explicit backoffs: (i) an online approach that updates the constraint sets based on state measurements at every sampling time $t$, and (ii) an offline approach that selects $Z_{t+1|t} = Z_{t+1}$ for all $t = 0,\ldots,T$. These two approaches are discussed next.

### 3.1 Online constraint tightening with explicit backoffs

For clarity, let the state constraint sets $X_t$ be described by a set of nonlinear inequality constraints of the form

$$X_t = \{ x \in \mathbb{R}^{n_x} : h_t(x) \leq 0 \}, \quad t = 1,\ldots,T,$$

where $h_t : \mathbb{R}^{n_x} \rightarrow \mathbb{R}^{n_h}$. Then, tightened state constraints can be expressed in terms of backoffs $b_{l|t} \in \mathbb{R}^{n_b}$:

$$Z_{l|t} = \{ z \in \mathbb{R}^{n_z} : h_l(z) + b_{l|t} \leq 0, \quad i > t = 1,\ldots,T. \}$$

Letting $H_t = h_l(x_t)$, the concept of the backoff can be stated as $h_l(z_{i|t}) + b_{i|t} = 0$ $\Rightarrow$ $\mathbb{P} \{ H_t \leq 0 \} = F_{H_t}(0) = c_t$. This implies that, when a constraint on the nominal states is active, the corresponding chance constraint on the closed-loop state is active. Using the inverse cdf, we can derive an exact expression for the backoffs $b_{i|t} = F_{H_l}^{-1}(c_t) - h_l(z_{i|t})$, which depends on the distribution of $H_t$. For $n_c > 1$, the cdf $F_{H_t}$ does not have a unique inverse, i.e., multiple backoff values can lead to exact satisfaction of the joint chance constraints. The best backoff values from this set will be the ones that lead to the smallest objective value. An approach for avoiding this complication by conservatively rewriting (6) in terms of a collection of individual chance constraints is introduced in Section 4.2.

Ideally, we could exactly represent the backoffs implicitly in terms of the state constraint distributions $F_{H_l}$, for all $x_t$ and $v_t|T|t$. This representation is not possible since the shape of the distribution is unknown and can vary drastically with $x_t$ and $v_t|T|t$ in nonlinear systems. As such, a variety of methods have been proposed to approximate implicit backoff representations, including moment-based approaches (e.g., see Paulson and Mesbah 2017 and the references therein). However, these approaches do not provide tight guarantees with respect to the original constraints. Here, we instead look to explicitly calculate the backoffs for only the current initial condition and optimal control inputs. However, the backoffs are coupled to the solution of (8) (since the optimal inputs are unknown), implying that backoffs need to be estimated based on some iterative procedure at every $t = 0,\ldots,T$.

1. Guess the initial backoffs $b_{0|T|t}$ (often equal to zero) and set iteration counter $k = 0$.
2. Compute $v_{t|T|t}(x_t)$ and $z_{t|T|t}(x_t)$ from (8) with sets $Z_{t+1|t}$ defined in terms of the current backoffs $b_{k|T|t}$.
3. Determine the distribution of the state constraint function $H_t$ for all $t = t + 1,\ldots,T$ under $v_{t|T|t}(x_t)$, for example, using Monte Carlo sampling.
4. Update backoffs according to

$$b_{i|t} = F_{H_t}^{-1}(c_t) - h_l(z_{i|t}(x_t)), \quad i = t + 1,\ldots,T, \quad (9)$$

where the inverse cdf is specified from the distribution of $H_t$ determined in the previous step.
5. Set $k = k+1$ and repeat Steps 2–4 until $b_{k|T|t}$ converges or the maximum number of iterations is reached.

This explicit backoff algorithm has not been proven to converge. However, simulation results in Section 6 show that, when this algorithm converges, it can converge quickly due to the fact that the full distribution of the state constraints are used in the update rule (9).

We propose to apply the explicit backoff strategy in the context of NMPC, meaning that the time-varying backoffs must be computed online for the most recently measured state. Not only does this strategy guarantee tight satisfaction of state chance constraints, it also avoids the need for backoffs (and their derivatives) to be evaluated at every step of the optimization procedure as in implicit backoff methods. Instead, only a nominal OCP needs to be solved at each iteration and the previous solution can be used for initialization purposes to speed-up convergence. As is true for any NMPC approach, the explicit backoff strategy can only be applied if the computations can be completed within a single sampling time of the process.

### 3.2 Offline computation of explicit backoffs

When it is expensive to determine the explicit backoffs online using the procedure in Section 3.1, the backoffs can be computed offline. Although offline computation of backoffs introduces some conservatism, the online complexity of NMPC remains the same as that of CE-NMPC. That is, “robust” constraint handling can be achieved with (8) at no additional online cost. The procedure for offline computation of explicit backoffs is summarized as:

1. Guess initial values for $b_{1:T}$.
2. Calculate $F_{H_t}(0)$ for any $i \in X_t$ from the stochastic closed-loop dynamics $x_{t+1} = f_t(x_t, v_{t|T|t}(x_t; b_{k|T|t}^T)) + w_t$.
3. If state constraints are violated, i.e., $F_{H_t}(0) < c_t$, decrease $b_t$ and repeat; otherwise stop.
Note that, in the above procedure, the backoffs do not depend on the measured state and thus are identical at every sampling time, i.e., $b_{\text{f}t} = b_t$. Since relaxing any active state constraint can only result in improved performance, it is desired that all active $F_H(0)$ are as near to $c_t$ as possible in order to avoid unnecessary conservatism. This can be thought of as a root-finding problem for the equations $F_H(0) - c_t = 0$. Any of the well-known root-finding algorithms, such as bisection and Newton’s method, can be used to solve these equations for the set of active constraints. Due to the complexity of $F_H(0) - c_t$ and the fact that its derivatives with respect to the backoff values are unknown, bisection is likely preferred in practice due to its simplicity and robustness. The problem dimension can be reduced by assuming the backoffs are constant in time, i.e., $b_t = b$. In this case, $F_H(0) - c_t$ can be replaced with the minimum deviation over time $\min_t \{F_H(0) - c_t\} = 0$.

We note that the above procedure is executed fully offline and is based on closed-loop data (as opposed to open-loop data in the online procedure in Section 3.1). Even though the offline procedure is conservative relative to the online procedure, the tightening is only done with respect to states visited in the closed-loop simulations, which depend on the specified initial conditions and objective function. Thus, the offline computed explicit backoffs are not nearly as conservative as choosing worst-case backoffs over all possible states and inputs. However, finding the distribution of $H_t$ from the closed-loop system can be an expensive prospect since $T$ separate NLPs must be solved for every sample of the uncertainty.

Depending on the type of disturbance model, alternative uncertainty propagation methods can be applied to considerably reduce the number of samples $n_u$ in comparison to Monte Carlo. For a particular class of disturbances that represent plant-model mismatch, an efficient uncertainty propagation method is presented next for constructing stochastic surrogate models for state constraint functions based on closed-loop simulations. The stochastic surrogate models can also be used to investigate the effect of any changeable (i.e., tuning) parameter in NMPC on important closed-loop properties including the distribution of the cost function $J$, as discussed in Section 5.

### 4. EFFICIENT COMPUTATION OF EXPLICIT BACKOFFS USING POLYNOMIAL CHAOS

The disturbance sequence $u_{0:T}$ typically represents several uncertainty sources such as modeling errors and exogenous disturbances. The chosen probabilistic model of the disturbance has a strong effect on the backoff computation, as it represents all randomness in the states. When $p_{w_0, \ldots, w_T} = \prod_{t=0}^{T} p_{w_t}$ is separable (i.e., disturbances are independent), then $O(n_u T)$ random variables must be propagated through the nonlinear system (1). Monte Carlo (MC) sampling is likely the best uncertainty propagation (UP) method in this case, especially for large $T$, as its convergence rate is independent of the uncertainty dimension. However, the fairly slow convergence rate of MC, $O(1/\sqrt{n_u})$, may require a large number of samples for an acceptable level of error.

Independent disturbance models assume there is no relationship between past and future disturbances. The other extreme is to assume that all randomness in the disturbances is related to some time-invariant parameters, such that the disturbances are highly correlated over time. An interesting consequence of this assumption is that the number of random variables reduces considerably. This opens the door to a variety of alternative UP methods that are able to achieve faster convergence and, therefore, require substantially fewer samples.

In this section, we present a polynomial chaos method for efficient propagation of time-invariant probabilistic uncertainties through complex closed-loop system dynamics, where the control policy is implicitly defined as the solution to some OCP. First, we establish the relationship between the disturbance sequence $u_{0:T}$ and a set of stochastic parameters $\theta \sim p_\theta$ based on a high-fidelity model of the system. The disturbances in this case represent plant-model mismatch. Then, a polynomial chaos method is presented that can readily handle arbitrary $p_\theta$.

#### 4.1 High-fidelity description of the disturbance

There are several ways to obtain a control-relevant model of the form (1) from first principles, data, or some combination of both. We consider that there exists a known high-fidelity model of the system

$$
\dot{z}(\tau; \theta) = \dot{f}(z(\tau; \theta), u(\tau), \theta, \tau), \quad \forall \tau \in (0, T_T),
$$

(10)

where $\dot{f} : \mathbb{R}^{n_z} \times \mathbb{R}^{m} \times \mathbb{R}^{n_u} \times \mathbb{R} \to \mathbb{R}^{n_z}$, $z(t; \theta) \in \mathbb{R}^{n_z}$ is the “true” state of the system with time derivative $\dot{z}$ and initial condition $z_0$, $u(\tau) \in \mathbb{R}^{n_u}$ is the continuous-time input, and $\theta \in \Theta \subseteq \mathbb{R}^{n_\theta}$ denotes the high-fidelity model parameters. It is assumed that (10) is structurally accurate with unknown parameters. In this case, we assume the posterior distribution $p_\theta$ is available from, for example, Bayesian estimation and represents the distribution of $\theta$ given available data. Hence, (10) consists of a set of stochastic ordinary differential equations (ODEs), where $\theta \sim p_\theta$ is arbitrary.

System measurements are assumed to be available at discrete time instants $\tau_t = t_0 + t_t \delta_t$ with sampling time $\delta_t$. Let $z_t = z(\tau_t; \theta)$ denote the solution to (10) at $\tau_t$, such that measurements are denoted by

$$
y_t = h(z_t), \quad t = 0, \ldots, T,
$$

(11)

where $h : \mathbb{R}^{n_z} \to \mathbb{R}^{n_z}$. Note that measurement error is neglected in (11) for simplicity, though this could be handled conceptually using the proposed framework at the cost of more uncertainties in $\theta$.

The control-relevant model (1) is generally different from the high-fidelity model (10). Often, $n_x \ll n_z$, so that the control-relevant model is amenable to online computations in NMPC. In order to relate the two models with different state spaces, we define an operator $\mathcal{P} : \mathbb{R}^{n_z} \to \mathbb{R}^{n_z}$ that projects the true state onto the state of the control-relevant model. Since full state feedback is considered in this work, $x_t$ must be uniquely determined from $y_t$. Thus, we assume $h(z_t) = \mathcal{P}(z_t) = x_t$ for simplicity. This projection operator $\mathcal{P}$ allows the disturbance in (1) to be related to the true state

```
\[ w_t = P(z_{t+1}) - f_t(P(z_t), u_t), \quad t = 0, \ldots, T - 1, \quad (12) \]

where \( w_T \) is a sequence of random variables as they are functions of \( \theta \). Expression (12) indicates that disturbances can be implicitly defined in terms of the mismatch between the high-fidelity and control-relevant models. This motivates the use of an approximate control-relevant uncertainty description for the disturbance in (1), which is explored in Section 5. Also, note that the disturbance model (12) affects the performance objective (4) and state chance constraints (6) in terms of the “true” high-fidelity states since \( x_t = P(z_t) \).

4.2 Estimating state constraint satisfaction probability using empirical distribution function

Before introducing the polynomial chaos method, we first elaborate on the estimation of the cdf \( F_{H_t}(x) \). A wide-variety of methods exist for approximating this distribution numerically. Since the structure of the distribution is unknown and likely complex in general, it is preferred to use a nonparametric inference method to avoid making unrealistic assumptions regarding the structure of the distribution. A widely used approach that meets this requirement is the empirical distribution function (Wellner, 1977). Although the empirical distribution concept can be applied to multivariate random variables, the complexity of evaluation grows quickly with dimension \( n_c \).

In the case of \( n_c > 1 \), an upper bound on the violation probability in (6) can be calculated using Boole’s inequality (Paulson and Mesbah, 2017)

\[ P\{x_t \notin X_t\} \leq \sum_{j=1}^{n_c} P\{h_t(x_t)_j > 0\} \]

\[ \iff 1 - n_c + \sum_{j=1}^{n_c} \tilde{F}_{H_t}(0) \leq F_{H_t}(0). \]

Therefore, the above expression in terms of scalar cdfs \( F_{H_t}(0) \) can be used in place of the multivariate cdf \( F_{H_t}(0) \) in the backoff strategy of Section 3. It is important to note that this bound will be exact when the support of \( p_{H_t} \) only crosses a single constraint. Take as a simple example, a scalar case with only an upper and lower bound so that the constraints have the form \( x_{\text{ub}} \leq x_t \leq x_{\text{lb}} \). The state distribution \( p_{H_t} \) would only cross both bounds if the uncertainty is very large or if the bounds are very close to one another, either of which results in a poorly posed control problem. Therefore, this strategy has the potential to provide guaranteed (yet fairly tight) estimates of the closed-loop joint chance constraint values at a low computational cost.

The empirical distribution function for each component of \( H_t \) can be defined as

\[ \tilde{F}_{H_t}(x) = \frac{1}{n_s} \sum_{k=1}^{n_s} \mathbbm{1}\{H_{t_k} \leq x\}, \quad (13) \]

where \( H_{t_k} \) is sample \( k \) of component \( j \) from a set of \( n_s \) i.i.d. samples \( \{H_{t}, \ldots, H_{t_n}\} \) of random vector \( H_t \). From the Glivenko-Cantelli theorem (Wellner, 1977), the empirical distribution function is known to converge uniformly

\[ \|\tilde{F}_{H_t} - F_{H_t}\|_{\infty} = \sup_{x \in \mathbb{R}} |\tilde{F}_{H_t}(x) - F_{H_t}(x)| \xrightarrow{n_s \to \infty} 0 \]

as \( n_s \to \infty \). Confidence intervals for the empirical distribution function can be obtained for any \( n_s \) to ensure that sufficient samples are chosen.

Standard tools can be used to efficiently construct (13), such that its main cost is generating an adequate number of samples from \( H_t \). Since \( \theta \) represents the only set of random variables under the assumed disturbance model (12), the first step is to generate i.i.d. samples \( \{\theta^1, \ldots, \theta^n\} \) from \( p_\theta \) using, e.g., Markov Chain Monte Carlo or the Rosenblatt transformation (Rosenblatt, 1952). Then, the samples \( \{H_{t_k}\} \) are determined by simulating the closed-loop system at fixed \( \theta^k \). Let \( M_{t,j} : \Theta \to \mathbb{R} \) denote the “black box” function \( [H_{t,j}] = M_{t,j}(\theta) \) that calculates the closed-loop state constraints for any given \( \theta \in \Theta \). \( M_{t,j} \) is often referred to as the quantity of interest (QoI). MC sampling requires \( M_{t,j} \) to be evaluated exactly when generating samples in (13); however, these functions are defined implicitly through a complex numerical procedure, meaning they are very computationally expensive to evaluate for each \( \theta^k \). Polynomial chaos (Xiu and Karniadakis, 2002) is an alternative to MC that builds stochastic surrogate models as approximations to the complex functions \( M_{t,j} \). In this way, samples can be cheaply generated by substituting \( \theta^k \) into the surrogate model, as described next.

4.3 Polynomial chaos expansions

This section defines the surrogate model for \( M_{t,j} \). The subscripts \( t, j \) are dropped below for notational simplicity. The polynomial chaos expansion (PCE) for function \( M \) takes the following form (Xiu and Karniadakis, 2002)

\[ M \approx P_L = \sum_{i=1}^{L} a_i \Psi_i, \quad (14) \]

where \( P_L : \Theta \to \mathbb{R} \) denotes the approximation to \( M \) truncated at \( L \in \mathbb{N} \); \( a_1, \ldots, a_L \in \mathbb{R} \) are the expansion coefficients; and \( \Psi_1, \ldots, \Psi_L \) are polynomial basis functions.

The goal is to select \( P_L \) such that it provides an “optimal” approximation to \( M \). Constructing \( P_L \) requires: (i) selecting the set of basis functions, and (ii) calculating the expansion coefficients. These two steps are discussed next, but first we define the Hilbert space of functions that are square integrable with respect to \( p_\theta \) as

\[ L_2^2 = \left\{ f : \Theta \to \mathbb{R} \mid \int_{\Theta} f^2(x) p_\theta(x) dx < \infty \right\} \]

The Hilbert space is equipped with an inner product

\[ \langle f, g \rangle_{L_2^2} = \int_{\Theta} f(x) g(x) p_\theta(x) dx \]

and corresponding norm \( ||f||_{L_2^2} = \sqrt{\langle f, f \rangle_{L_2^2}} \). The inner product of functions \( f, g \) is merely the expected value of the random variables \( f(\theta), g(\theta) \), i.e., \( \langle f, g \rangle_{L_2^2} = \mathbb{E}[f(\theta)g(\theta)] \). It is required that \( M \in L_2^2 \), so that the expansion (14) converges as \( L \to \infty \). This is a reasonable assumption, which is guaranteed to be satisfied when the random variable \( M(\theta) \) has finite variance.

4.4 Orthonormal basis for arbitrary distributions

In theory, the polynomials \( \Psi_1, \ldots, \Psi_L \) can be any basis of the space \( L_2^2 \) as long as they are complete (or dense) in that space. However, choosing the polynomials to be an orthonormal basis (ONB) of polynomials simplifies the calculation of the expansion coefficients. In order to define
a polynomial ONB, each element $\Psi_i$ must be a polynomial and for all $i, j \in \mathbb{N}$ must satisfy
\[ \langle \Psi_i, \Psi_j \rangle_{L^2_\theta} = \delta_{ij}, \]  
where $\delta_{ij}$ denotes the Kronecker delta. In practice, the ONB is constructed to satisfy the following properties: (i) the first polynomial is constant $\Psi(\theta) = 1$, which yields a convenient expression for the expectation of the polynomials $\mathbb{E}(\Psi_i(\theta)) = \delta_{1i}$; and (ii) each polynomial $\Psi_i$ contains exactly one additional monomial $\theta^a$ that is not contained in the previous polynomials $\Psi_1, \ldots, \Psi_{i-1}$. It is assumed that polynomials in (14) are an ONB that satisfy these properties. Therefore, when approximating the function $M$, the number of terms $L$ is selected such that it specifies the ansatz space $\mathcal{P}$ as
\[ \mathcal{P} = \text{span}\{\Psi_1, \ldots, \Psi_L\}. \]

If the elements of $\theta = (\theta_1, \ldots, \theta_n)$ are statistically independent, then the polynomial ONB can be constructed for each uncertain parameter $\theta_i$ separately, i.e., the multivariate polynomials are simply the product of the univariate polynomials that are orthonormal with respect to $p_\theta$. For certain well-known distributions (e.g., Gaussian and uniform), the polynomial ONB can be derived analytically (Xi and Karniadakis, 2002). For arbitrary distributions, however, the ONB of polynomials must be constructed numerically (Sinsbeek and Nowak, 2015). In the case that $\theta$ has statistically dependent elements, a more sophisticated procedure is required based on either the Gram-Schmidt process or a Cholesky decomposition of the Gram moment matrix, as discussed in detail in (Paulson et al.; Paulson and Mesbah, 2017, 2018).

**Remark 4.** There exists distributions $p_\theta$ for which $L^2_\theta$ does not admit an ONB of polynomials. In this case, the space of polynomials is not complete in $L^2_\theta$ as shown in (Ernst et al., 2012) and $\theta$ must be transformed to a new random variable (known as the germ) that is known to admit a polynomial ONB. Note, however, that this transformation can be complicated to determine and is nonlinear in general, which can slow down the rate of convergence of (14) (Paulson and Mesbah, 2018).

### 4.5 Optimization-based coefficient estimation

Since $M \in L^2_\theta$, it can be expanded with respect to the polynomial ONB $\{\Psi_i\}_{i \in \mathbb{N}}$
\[ M = \sum_{i=1}^{\infty} a_i \Psi_i, \]  
where the equality of two functions (or random variables) should be interpreted in the mean-square sense, i.e.,
\[ \lim_{L \to \infty} \mathbb{E}\{(M(\theta) - P_L(\theta))^2\} = \lim_{L \to \infty} \|M - P_L\|^2_{L^2_\theta} = 0, \]  
which follows from the completeness of $\{\Psi_i\}_{i \in \mathbb{N}}$ (Ernst et al., 2012). Note that mean-square convergence implies convergence in probability as well as convergence in distribution, i.e.,
\[ F_{M(\theta)}(x) = \lim_{L \to \infty} F_{P_L(\theta)}(x). \]

The PCE in (17) cannot be computed exactly. Thus, it is truncated in practice to a finite number of $L$ terms. Based on the Hilbert projection theorem (Soize and Ghanem, 2004), the best $\|M - P_L\|^2_{L^2_\theta}$ approximation of $M$ in the space $\mathcal{P}$ is the orthogonal projection of $M$ onto $\mathcal{P}$, i.e.,
\[ P_L = \arg\min_{P \in \mathcal{P}} \|M - P\|^2_{L^2_\theta}, \]
which implies that no other choice of coefficients $a_1, \ldots, a_L$ multiplying the polynomial ONB will result in a smaller $L^2_\theta$ norm. By taking the inner product of both sides of (17) with each of the basis functions and applying (15), the expansion coefficients can be defined exactly as
\[ a_i = \int_{\Theta} M(x)\Psi_i(x)p_\theta(x)dx, \quad i = 1, \ldots, L. \]

However, the multivariate integrals in (18) cannot be determined exactly due to the implicit definition of $M$ and, therefore, must be approximated numerically.

Here, we adopt a non-intrusive approach for approximating integrals in (18), where the coefficients are estimated using a finite number of evaluations of $M$ (Sinsbeek and Nowak, 2015). As such, $M$ can be treated as a “black-box” function. In a non-intrusive approach, a set of $n$ sample (or integration) points $\theta^{(1)}, \ldots, \theta^{(n)} \in \Theta$ is chosen and the PCE coefficients are calculated using the model response at these values, i.e., $M(\theta^{(1)}), \ldots, M(\theta^{(n)})$. This results in an integration rule that approximates (18) with a discrete expression
\[ a_i \approx \tilde{a}_i = \sum_{j=1}^{n} w_j M(\theta^{(j)})\Psi_i(\theta^{(j)}), \quad i = 1, \ldots, L, \]
where $w_1, \ldots, w_n$ are appropriately chosen weight values. Numerous methods have been proposed for approximation of multidimensional integrals using samples. Since the cost of building the expansion is essentially determined by $n$, it is desired to make $n$ as small as possible while ensuring that the approximation (19) is as accurate as possible. Thus, optimization-based techniques can be used to systematically place the points (and weights) in (19), so that the resulting error is minimized. A recently proposed approach is moment-matching optimization, which is a natural extension of Gaussian quadrature (i.e., optimal integration rule in one dimension) to the multidimensional case. In this framework, the optimization problem is formulated as an infinite-dimensional linear program (LP) that is NP-hard for $n_\theta > 1$ (Ryu and Boyd, 2015).

A simple procedure for approximately solving the moment-matching optimization is presented in (Paulson and Mesbah, 2018), which involves three steps: (i) solve a finite-dimensional LP wherein moments are matched based on a grid of $\Theta$; (ii) locate the “clusters” of sample points obtained from the LP solution, and (iii) refine this solution by locally solving a nonlinear least-squares problem with initial guess corresponding to the clustered integration rule. In this case, the number of points $n$ depends on the number of moments matched (i.e., more moments matched yields larger $n$), and higher $n$ leads to lower integration error. In practice, the error should be evaluated on a set of reasonably chosen test functions. An alternative to moment matching is the so-called optimized stochastic collocation (OSCC) method, which is based on a quasi-optimal procedure for minimizing the quadrature operator’s error norm (Sinsbeek and Nowak, 2015).

### 4.6 Truncation and aliasing error in PCE surrogate model

The discretized integration rule (19) results in the following approximate PCE surrogate model.
where the difference between $M$ and $\tilde{P}_L$ can be split into two separate terms: a truncation error and an aliasing error

$$M - \tilde{P}_L = \sum_{i=1}^{L} \tilde{a}_i \Psi_i, \quad (20)$$

where the difference between $M$ and $\tilde{P}_L$ can be split into two separate terms: a truncation error and an aliasing error

$$M - \tilde{P}_L = \sum_{i=L+1}^{\infty} a_i \Psi_i + \sum_{i=1}^{L} (a_i - \tilde{a}_i) \Psi_i.$$

Owing to the orthogonality of the polynomial ONB, these two error sources are orthogonal and their squared norm is additive, i.e.,

$$e^2 = \mathbb{E} \left\{ \left( M(\theta) - \tilde{P}_L(\theta) \right)^2 \right\} = \left\| M - \tilde{P}_L \right\|_{L^2}^2 \quad (21)$$

$$= \sum_{i=L+1}^{\infty} a_i^2 + \sum_{i=1}^{L} (a_i - \tilde{a}_i)^2.$$

For any fixed $M$, the truncation error is constant since the ansatz space $\mathcal{P}$ is selected a priori. The truncation and aliasing error sources can be controlled by increasing $L$ and $n$, respectively. A simple procedure for choosing $L$ is to increase the number of terms in (20) until the predictions of the surrogate model no longer change. Additionally, for every $L$, the number of integration points $n$ should be increased to ensure the aliasing error is low.

Remark 5. From the properties of the ONB, the mean $\mathbb{E}(M(\theta)) \approx \tilde{a}_1$ and variance $\text{Var}(M(\theta)) \approx \sum_{i=2}^{L} \tilde{a}_i^2$ can be computed directly with the coefficients.

4.7 Explicit backoff computation using PCE

The random state constraints $H = M(\theta)$, with subscripts $t,j$ dropped, can be approximated by $\tilde{P}_L(\theta)$, the expansion converges in mean-square as $L,n \to \infty$. The main advantage of the PCE surrogate model is that, while we do not have an explicit expression for function $M$, we have an explicit expression for $\tilde{P}_L$ in (20). Therefore, i.i.d. samples $\{\tilde{P}_1(\theta^1), \ldots, \tilde{P}_L(\theta^L)\}$ can be computed efficiently with $\tilde{P}_L(\theta^k) = \sum_{i=1}^{L} \tilde{a}_i \Psi_i(\theta^k)$, which can then be used to determine $F_{\tilde{P}_L}(\theta^k)$ with (13). Since the cost of generating these samples is extremely cheap, a large $n_1$ can be chosen to ensure $F_{\tilde{P}_L}(\theta^k)(x) - F_{\tilde{P}_L}(\theta^j)(x) \approx 0$ for all $x \in \mathbb{R}$. Since PCE exhibits mean-square convergence, its cdf $F_{\tilde{P}_L}(\theta)$ accurately approximates $F_H$ for reasonable $L$ and $n$.

The algorithm for constructing the PCE surrogate model for the state constraints can be summarized as follows:

1. Select $L$ and construct the polynomial ONB $\Psi_1, \ldots, \Psi_L$ using, e.g., the Cholesky decomposition based on the parameter distribution $p_\theta$.
2. Select $n$ and determine a set of “optimal” integration points $\{\theta^1, \ldots, \theta^n\}$ and weights $w_1, \ldots, w_n$ using the moment-matching or OSC method.
3. Select $n_1$ and draw a set of i.i.d. samples $\{\theta^1, \ldots, \theta^n\}$ from the parameter distribution $p_\theta$.
4. Evaluate $[H]\{\theta^k\} = M(\theta^k)$ for every $k = 1, \ldots, n_1$ by simulating the closed-loop system for each sample.
5. Determine coefficients $\tilde{a}_{t,j} = \sum_{k=1}^{n_1} w_k [H]\{\theta^k\} \Psi_i(\theta^k)$.

5. SHAPING THE DISTRIBUTION OF GENERAL PERFORMANCE OBJECTIVES

The distribution of the performance objective $J$ in (4) is strongly dependent on the structure of the control policy and the tuning parameters selected in the NMPC controller. The PCE method in Section 4 can be readily used to determine the performance distribution $p_J$ for any specified control policy under the assumed disturbance model (12). This allows for construction of a Pareto frontier between any two competing probabilistic objectives $J_1$ and $J_2$ via tracing $\lambda \in [0,1]$ for a scalar objective $\lambda J_1 + (1 - \lambda) J_2$. Note that $J_1$ and $J_2$ can be any well-defined operators applied to $p_J$. Often, we consider $J_1 = \mathbb{E}\{J\}$ and $J_2 = \text{Var}\{J\}$.

The CE-NMPC (8) problem does not account for variability in performance since the effect of $p_{w_0, \ldots, w_T}$ is neglected in the model predictions. The variance cost $J_2$ can be (approximately) penalized by replacing the constant disturbance model with some control-relevant disturbance description $p_{w_0, \ldots, w_T} \approx p_{w_0, \ldots, w_T} \approx p_{\tilde{w}_0, \ldots, \tilde{w}_T}$ at the cost of more expensive online computations. MPC strategies that account for probabilistic uncertainty are broadly termed stochastic MPC (Mesbah, 2016). The vast majority of stochastic MPC strategies (linear or nonlinear) assume the disturbances are independent in time, as this assumption simplifies analysis (especially for linear systems). In theory, correlated disturbances can always be cast in terms of an augmented system state that evolves as a Markov process. However, the size of the state space in this case can quickly become too large to handle in practice.
6. CASE STUDY: CSTR WITH STRUCTURAL AND STOCHASTIC PARAMETER UNCERTAINTY

6.1 The high-fidelity system model

The proposed methods are demonstrated on a nonlinear continuously stirred tank reactor (CSTR) benchmark problem adapted from (Subramanian et al., 2015). The following set of reactions occur in the CSTR

\[ A \rightarrow B \rightarrow C \]
\[ 2A \rightarrow D \]

The high-fidelity model of the CSTR is described by

\[
\begin{align*}
\dot{c}_A &= F(c_{A0} - c_A) - k_1 c_A - k_3 c_A^2, \\
\dot{c}_B &= -F c_B + k_1 c_A, \\
\dot{T}_R &= \frac{k_0 A \Delta H_{AB} + k_3 c_A^3 \Delta H_{AD}}{\rho c_p V_R}, \\
\dot{T}_K &= \frac{1}{m_k c_p K_T}(Q_K + k_W A (T_R - T_K)),
\end{align*}
\]

which are derived from the component balances for the concentration of A (\(c_A\)) and for the concentration of B (\(c_B\)) as well as from the energy balances for the reactor temperature (\(T_R\)) and for the coolant temperature (\(T_K\)). The control input is the feed flow \(F = V_{in}/V_R\), which is normalized by the volume of the reactor. The reaction rates follow the Arrhenius law

\[
k_1 = (1 + 0.1\beta)k_{01}(\frac{E_{A1}}{R + 273})^{-\frac{1}{\alpha}},
\]
\[
k_2 = k_{02}(\frac{E_{A2}}{R + 273})^{-\frac{1}{\beta}},
\]
\[
k_3 = k_{03}(\frac{E_{A3}}{R + 273})^{-\frac{1}{\alpha + \beta}},
\]

where the parameters \(E_{A,3}\) and \(k_{01}\) are considered to be uncertain and are modeled by random parameters \((\alpha, \beta) \in [-1, 1]^2 \sim \rho_{\alpha,\beta}\) multiplying the nominal \(E_{A,3}\) and \(k_{01}\) values. The joint distribution \(\rho_{\alpha,\beta} = \rho_{\beta|\alpha}\) is specified by two beta random variables \(\alpha \sim B(2, 2)\) and \(\beta|\alpha \sim B(\alpha + 3, -\alpha + 2)\), where a high degree of correlation exists between these two parameters since \(\beta|\alpha\) has a strong dependence on \(\alpha\). The model parameters are listed in Table 1, while the initial conditions and constraints are listed in Table 2. For the NMPC design, we consider an “economic” objective that is to maximize production of component B

\[
n_{B,T} = \int_0^{\tau_T} n_B(\tau)d\tau = V_{in} \int_0^{\tau_T} c_B(\tau) F(\tau) d\tau,
\]

at the final time \(\tau_T = 1.5\ h\).

6.2 The control-relevant model

The control-relevant model excludes the reaction \(B \rightarrow C\) and the coolant balance

\[
\begin{align*}
\dot{c}_A &= F(c_{A0} - c_A) - k_1 c_A - k_3 c_A^2, \\
\dot{c}_B &= -F c_B + k_1 c_A, \\
\dot{T}_R &= \frac{k_0 A \Delta H_{AB} + k_3 c_A^3 \Delta H_{AD}}{\rho c_p V_R} + \frac{Q_K}{\rho c_p V_R}.
\end{align*}
\]

A discrete-time model was derived from (24) using orthogonal collocation on finite elements. The sampling time was chosen as \(\Delta \tau = 0.005\ h\), which corresponds to \(T = 300\) discrete time intervals.

The control-relevant model (24) uses an additive disturbance model for simplicity, however, this can be replaced with nonlinear disturbance, i.e., \(f(x, u, w)\). Here, we let \(w_i = (\alpha, \beta)\) represent the control-relevant uncertainties in (24). Even though the same parameters are uncertain in (22) and (24), there is significant structural mismatch between the high-fidelity and control-relevant models. Additionally, we are unable to exactly utilize the true correlated distribution \(\rho_{\alpha,\beta}\) in the controller, so that this is replaced with a simpler uncertainty description in terms of a scenario tree.

6.3 Optimal control with time-varying backoffs

First, the backoff strategy in Section 3.1 is applied to this CSTR case study. Before implementing the backoff strategy online, we focus on the open-loop optimal control case with \(t = 0\). It is desired that the stochastic high-fidelity model (24) satisfies the state constraints provided in Table 2 with probability \(c_t = 0.8\). The maximum reactor temperature is the only active constraint in the OCP, so that

\[
P\{x_t \in X_t\} = P\{T_R, t \leq 150^\circ C\} \geq 0.8, \quad t = 1, \ldots, T.
\]

Thus, we aim to describe the distribution of the reactor temperature over time.

The backoff values were initialized to zero in Step 1. The nominal OCP in Step 2, corresponding to NLP (8) at \(t = 0\), is solved using CasADi (Andersson et al., 2012). The necessary Jacobians and Hessians are automatically calculated based on a symbolic implementation of the equations, and these derivatives are passed to IPOPT (Biegler and Zavala, 2009) with a tolerance of \(10^{-8}\). All computations are performed on MacBook Pro with

| Parameter | Value | Unit |
|-----------|-------|------|
| \(k_{01}\) | \(1.287 \times 10^{12}\) | h^{-1} |
| \(k_{02}\) | \(1.287 \times 10^{12}\) | h^{-1} |
| \(k_{03}\) | \(9.043 \times 10^{6}\) | L mol^{-1} h^{-1} |
| \(E_{A,1}/R\) | 9798.3 | K |
| \(E_{A,2}/R\) | 9798.3 | K |
| \(E_{A,3}/R\) | 7704.0 | K |
| \(\Delta H_{AB}\) | 4.2 | kJ mol^{-1} |
| \(\Delta H_{BC}\) | -11.0 | kJ mol^{-1} |
| \(\Delta H_{AD}\) | -41.85 | kJ mol^{-1} |
| \(\rho\) | 0.9342 | kg L^{-1} |
| \(c_p\) | 3.01 | kg kg^{-1} K^{-1} |
| \(c_{p,k}\) | 2.0 | kg kg^{-1} K^{-1} |
| \(A\) | 0.215 | m² |
| \(V_R\) | 10.01 | L |
| \(m_k\) | 5.0 | kg |
| \(T_{in}\) | 130.0 | °C |
| \(k_W\) | 4032 | kJ h^{-1} m^{-2} K^{-1} |
| \(Q_K\) | -4500 | kJ h^{-1} |

Table 1. Parameter values for CSTR.
8 GB of RAM and a 2.6 GHz Intel i5 processor. The distributions \( \{ F_{R,t} \}_{t=1} \) needed in Step 3 of the algorithm were approximated using the empirical distribution (13) with \( n_s = 10^5 \) i.i.d. samples calculated from a PCE surrogate model for (22). From these estimated cdfs, the backoff update rule (9) in Step 4 can be carried out.

As mentioned in Section 4, the size of the basis \( L \) and the number of points in the integration rule \( n \) should be systematically selected to ensure low error, as shown in (Paulson and Mesbah, 2018). This procedure is visually illustrated in Figure 1, which shows the reactor temperature pdf (estimated with standard kernel density estimation) and cdf at one time point for different PCE orders. Both the pdf and cdf converge at order \( d = 4 \), and similar results were observed throughout the simulation. Therefore, a choice of \( L = \frac{(n_s + d)!}{n_d!d!} = 15 \) is sufficient to accurately model the high-fidelity \( T_R \) in (22) over time. The PCE coefficients were estimated using the moment-matching optimization method. The number of integration points \( n \) was found to be 9, 16, 25, and 36 for moment matching orders of 5, 7, 9, and 11, respectively, and it was determined that 36 points provided sufficient accuracy for the discrete operator (19). For comparison purposes, the empirical distribution (13) determined from 100 MC samples is shown in Figure 1. Notice that there are significant estimation errors in the MC estimate as well as non-smooth behavior due to an insufficient number of samples being used, even though MC used more expensive high-fidelity model simulations than that required to construct the PCE surrogate.

The estimated time-varying backoffs and their corresponding chance constraint values \( \mathbb{P}\{T_{R,t} \leq 150^\circ \text{C}\} \) over time are presented in Figure 2 for multiple iterations of the backoff strategy. The first iteration at \( k = 0 \) results in violation probabilities much larger than the allowed 20%. After a single iteration, however, the high-fidelity system satisfies (25). After a few more iterations, the time-varying backoffs converge to the same value and (25) is active for all \( t > 5 \), implying minimal conservatism.

![Fig. 1. Reactor temperature distribution at \( t = 5 \) determined with PCE for multiple orders and Monte Carlo.](image1)

![Fig. 2. Backoff values (top) and \( \mathbb{P}\{T_{R,t} \leq 150^\circ \text{C}\} \) (bottom) over time \( t = 1, \ldots, T = 300 \) for multiple iterations of the backoff strategy in Section 3.1.](image2)

6.4 CE- and scenario NMPC with constant backoff

The offline backoff strategy in Section 3.2 is applied to three NMPC strategies: (i) CE with soft state constraints, (ii) scenario tree with open-loop inputs, and (iii) scenario tree with inputs that differ along different branches of the tree (i.e., multi-stage NMPC). The three NMPC strategies use the control-relevant model (24) with a receding-horizon prediction horizon of \( N_p = 5 \). CE-NMPC uses fixed parameter values \( \alpha = \beta = 0 \). On the other hand, open-loop scenario and multi-stage NMPC consider \( 3^2 = 9 \) possible combinations of \( \alpha, \beta \in \{-1.5, 0, 1.5\} \) based on a robust horizon \( N_r = 1 \), i.e., branching only occurs at the first stage of the OCP. Furthermore, both scenario-based NMPC strategies assume that all uncertainty realizations occur with equal probability, indicating that the objective function is an equally weighted sum of the moles of B calculated for each scenario.

A constant backoff was derived for each NMPC strategy using the closed-loop prediction method described in Section 3.2 using the PCE surrogate to efficiently estimate the cdf of the chance constraint. In this case, the bisection method was used to derive “optimal” backoffs that tightly meet the chance constraint (25) for at least one point in time. The chance constraint evolution for these three NMPC strategies with the optimally-tuned backoffs is shown in Figure 3. The backoffs that result in these profiles were found to be 3.9, −5.8, and −3.2°C for the CE, open-loop scenario, and multi-stage NMPC, respectively. Note that the backoffs are negative in the two scenario-based NMPC strategies due to the fact that the resulting implicit backoff leads to robust satisfaction of the temperature constraint with \( b = 0 \).

The average performance (23) under their respective “optimal” backoffs is equal to 166.5, 95.5, and 117.0 moles for CE-, open-loop scenario, and multi-stage NMPC, respectively. It is interesting to note that CE-NMPC results in better performance (on average) than the scenario-based NMPC strategies, while all of the NMPC strategies satisfy the desired set of constraints. This can be attributed to the fact that CE-NMPC allows the temperature change...
constraint to become active at an earlier time than the scenario-based NMPC strategies.

As discussed in Section 5, the control objective in practice may more generally be related to the full distribution of \( J \). Figure 4 shows the distribution of \( n_{B,T} \) for the three NMPC strategies. CE-NMPC yields a \( p_{B,T} \) with a long tail; however, the distribution has a large peak at a low undesirable value. Additionally, the distribution has multiple modes indicating large variability in performance depending on the specific parameter realization. Open-loop scenario and multi-stage NMPC, on the other hand, result in unimodal distributions with significantly lower variance.

**6.5 Reduced performance variability in multi-stage NMPC**

Even though CE-NMPC results in a larger \( \mathbb{E}\{n_{B,T}\} \), since uncertainty is neglected in the model predictions, there is no parameter that can be straightforwardly tuned to reduce its performance variability. This can be an issue if, for example, there is a constraint on the product standard deviation \( \sigma_{n_{B,T}} \). Since multi-stage NMPC incorporates uncertainty into the model predictions (albeit approximations of the true complex form of the uncertainty), the variability in the performance can be penalized by adding a term to the objective that calculates the difference between two neighboring scenarios in the scenario tree multiplying a weight \( k_{\text{var}} \) (see Lucia et al. 2014 for more details).

An analysis of the tradeoff between performance variability \( \sigma_{n_{B,T}} \) and the performance on average \( \mathbb{E}\{n_{B,T}\} \) for different values of \( k_{\text{var}} \) is shown in Figure 5. A different “optimal” constant backoff was tuned to tightly meet chance constraints (25) for each \( k_{\text{var}} \) value. As expected, increasing \( k_{\text{var}} \) results in decreased performance variability; however, this comes at the cost of a significant loss in the expected performance of the process. This type of analysis can be used to satisfy additional complicated performance constraints, e.g., \( \sigma_{n_{B,T}} \leq 20 \) moles can be achieved tightly with \( k_{\text{var}} = 0.4 \). Alternative statistical properties related to \( \mathbb{F}_{J} \) can also be analyzed using the PCE surrogate models. The simulation results of this case study demonstrate the usefulness of efficiently analyzing different NMPC strategies in the presence of uncertainty using surrogate models of the closed-loop quantities of interest.

**7. CONCLUSIONS AND FUTURE WORK**

For stochastic systems, this paper presents a strategy for explicit incorporation of backoffs in NMPC to guarantee state chance constraint satisfaction under closed-loop. The proposed strategy explicitly computes the backoffs for the current system state based on an iterative procedure that requires: (i) the solution to a certainty equivalence NMPC problem and (ii) the calculation of the probability distribution of the state constraint functions for the closed-loop system. It is shown that stochastic surrogate models are more efficient than Monte Carlo sampling for constructing the distribution of state constraint functions (and general performance objectives) for a class of disturbance models derived from a high-fidelity model of the system subject to arbitrary parameter uncertainty.

Future work will focus on accounting for the error between the high-fidelity and the surrogate model. Establishing
a bound on this error will allow rigorously guaranteeing chance constraint satisfaction with respect to the “true” high-fidelity model. In addition, the conditions under which NMPC with explicit backoffs guarantees closed-loop stability and convergence to desired equilibrium values will be investigated. The proposed surrogate modeling approach will also be extended to handle more general types of correlated disturbance models. For example, this can be done by using the Karhunen-Loève (KL) expansion to decompose the disturbance sequence into a set of time-invariant random variables, such that polynomial chaos can be used directly on the KL expansion.

REFERENCES

Andersson, J., Åkesson, J., and Diehl, M. (2012). CasADi: A symbolic package for automatic differentiation and optimal control. In Recent Advances in Algorithmic Differentiation, 297–307. Springer, Berlin.

Bemporad, A. and Morari, M. (1999). Robust model predictive control: A survey. In Robustness in Identification and Control, volume 245, 207–226. Springer, Berlin.

Bertsekas, D.P. and Shreve, S. (2004). Stochastic optimal control: the discrete-time case. Academic Press, New York.

Biegler, L.T. and Zavala, V.M. (2009). Large-scale nonlinear programming using IPOPT: An integrating framework for enterprise-wide dynamic optimization. Computers & Chemical Engineering, 33, 575–582.

Caflisch, R.E. (1998). Monte Carlo and Quasi-Monte Carlo methods. Acta Numerica, 7, 1–49.

Carpentier, P., Chancelier, J., Cohen, G., De Lara, M., and Girardeau, P. (2012). Dynamic consistency for stochastic optimal control problems. Annals of Operations Research, 200, 247–263.

Ernst, O., Mugler, A., Starkloff, H., and Ullmann, E. (2012). On the convergence of generalized polynomial chaos expansions. ESAIM: Mathematical Modelling and Numerical Analysis, 46, 317–339.

Farina, M., Giulioni, L., and Scattolini, R. (2016). Stochastic linear model predictive control with chance constraints—A review. Journal of Process Control, 44, 53–67.

Heirung, T.A.N., Paulson, J.A., O’Leary, J., and Mesbah, A. (2018). Stochastic model predictive control - How does it work? Computers & Chemical Engineering, 114, 158–170.

Koller, R.W., Ricardez-Sandoval, L.A., and Biegler, L.T. (2018). Stochastic back-off algorithm for simultaneous design, control and scheduling of multi-product systems under uncertainty. AIChE Journal, 64, 2379–2389.

Kouvaritakis, B. and Cannon, M. (2016). Model predictive control: Classical, robust and stochastic. Springer.

Lucia, S., Andersson, J.A.E., Brandt, H., Diehl, M., and Engell, S. (2014). Handling uncertainty in economic nonlinear model predictive control: A comparative case study. Journal of Process Control, 24, 1247–1259.

Lucia, S., Finkler, T., and Engell, S. (2013). Multi-stage nonlinear MPC applied to a semi-batch polymerization reactor under uncertainty. Journal of Process Control, 23, 1306–1319.

Mesbah, A. (2016). Stochastic model predictive control: An overview and perspectives for future research. IEEE Control Systems, 36, 30–44.

Mesbah, A., Streif, S., Findeisen, R., and Braatz, R. (2014). Stochastic nonlinear model predictive control with probabilistic constraints. In Proceedings of the European Control Conference, 2413–2419. Portland.

Nemirovski, A. and Shapiro, A. (2006). Convex approximations of chance constrained programs. SIAM Journal on Optimization, 17(4), 969–996.

Paulson, J.A., Buehler, E.A., and Mesbah, A. (2017). Arbitrary polynomial chaos for uncertainty propagation of correlated random variables in dynamic systems. IFAC-PapersOnLine, 50, 3548–3553.

Paulson, J.A. and Mesbah, A. (2017). An efficient method for stochastic optimal control with joint chance constraints for nonlinear systems. International Journal of Robust and Nonlinear Control, 1–21.

Paulson, J.A. and Mesbah, A. (2018). Arbitrary polynomial chaos for quantification of general probabilistic uncertainties: Shaping closed-loop behavior of nonlinear systems. In Proceedings of the 57th IEEE Conference on Decision and Control, Accepted. Miami.

Rawlings, J.B. and Mayne, D.Q. (2009). Model Predictive Control: Theory and Design. Nob Hill Publishing, Madison.

Rosenblatt, M. (1952). Remarks on a multivariate transformation. The Annals of Mathematical Statistics, 23, 470–472.

Ryu, E.K. and Boyd, S.P. (2015). Extensions of Gauss quadrature via linear programming. Foundations of Computational Mathematics, 15, 953–971.

Sinsbeck, M. and Nowak, W. (2015). An optimal sampling rule for nonintrusive polynomial chaos expansions of expensive models. International Journal for Uncertainty Quantification, 5, 275–295.

Skaf, J., Boyd, S., and Zeevi, A. (2010). Shrinking-horizon dynamic programming. International Journal of Robust and Nonlinear Control, 20, 1993–2002.

Soize, C. and Ghanem, R. (2004). Physical systems with random uncertainties: Chaos representations with arbitrary probability measure. SIAM Journal on Scientific Computing, 26, 395–410.

Subramaninan, S., Lucia, S., and Engell, S. (2015). Handling structural plant-model mismatch via multi-stage nonlinear model predictive control. In Proceedings of the European Control Conference, 1602–1607. Linz.

Van Hessel, D. and Bosgra, O. (2006). Stochastic closed-loop model predictive control of continuous nonlinear chemical processes. Journal of Process Control, 16, 225–241.

Wellner, J.A. (1977). A Glivenko-Cantelli theorem and strong laws of large numbers for functions of order statistics. The Annals of Statistics, 5, 473–480.

Xiu, D. and Karniadakis, G.E. (2002). The Wiener–Askey polynomial chaos for stochastic differential equations. SIAM Journal of Scientific Computing, 24, 619–644.