Optimization-based Design of Plant-Friendly Input Signals for Data-Centric Estimation and Control

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Abstract

The design of constrained, "plant-friendly" multisine input signals that optimize a geometric discrepancy criterion arising from Weyl's Theorem is examined in this paper. Such signals are meaningful for data-centric estimation methods, where uniform coverage of the output state-space is critical. The usefulness of this problem formulation is demonstrated by applying it to a linear example and to the nonlinear, highly interactive distillation column model developed by Weischedel and McAvoy (1980). The optimization problem includes a search for both the Fourier coefficients and phases in the multisine signal, resulting in an uniformly distributed output signal displaying a desirable balance between high and low gain directions. The solution involves very little user intervention (which enhances its practical usefulness) and has significant benefits compared to multisine signals that minimize crest factor. The effectiveness of data resulting from a Weyl criterion-based signal for Model-on-Demand Model Predictive Control (a data-centric multivariable control algorithm) is demonstrated for the distillation column case study.

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1   Introduction

The need for "plant-friendliness" in system identification for the process industries stems from the fundamental need for informative experiments despite practical requirements to the contrary (Rivera *et al.*, 2003). A plant-friendly identification test will produce data leading to a suitable model within an acceptable time period, while keeping the changes and variability in both input and output signals within user-defined constraints. In recent years, there has been significant interest in data-centric dynamic modeling frameworks such as Just-in-Time modeling (Cybenko, 1996) and Model-on-Demand (MoD) estimation (Stenman, 1999). The appeal of these modeling approaches is that they enable nonlinear estimation, while reducing the structural decisions made by the user and maintaining reliable numerical computations. The performance of these methods, however, is highly dependent upon the availability of quality, informative databases, and consequently, good experimental designs are an imperative. An important consideration in experimental design for these estimation methods is to achieve uniform coverage of regressors in the database. This paper examines the development of multisine input designs that meet this criterion while satisfying plant-friendliness constraints during identification testing.

The idea of uniformly distributed experimental designs for system identification relying on multisine signals has previously been examined by Duym and Schoukens (1995), who rely on minimizing an objective function quantifying the real and actual discrepancy from a user-defined grid. An iterative procedure that does not apply constraint enforcement is used in this work. A more general approach that we present in this paper is to rely on the principles of geometric discrepancy theory (Matoušek, 1999) as a means for achieving uniformity of the data in a regressor space. This is accomplished by minimizing a discrepancy function made up of trigonometric polynomials arising from Weyl's Theorem that insure that the points are equidistant on a state-space. The optimization problem calls for minimizing this discrepancy function on the anticipated outputs of the system, subject to the restrictions of an orthogonal "zippered" spectrum (used to enable multi-channel implementation) and simultaneously enforcing plant-friendliness time-domain constraints on upper and lower limits, move sizes, and rates of change in either (or both) input and output signals. The optimization problem is solved using a state-of-the-art NLP solver (KNITRO 3.1) which uses an interior point trust region method and employs SQP techniques to solve the barrier subproblems.

The paper is organized as follows: Section 2 describes the Weyl criterion that defines the geometric discrepancy objective, while Section 3 presents an example based on a simple linear highly interactive system that leads to the plant-friendly constrained optimization problem formulation that is the basis for this work. Section 4 describes the results of a more demanding case study (based on the nonlinear Weischedel-McAvoy distillation column) while Section 5 contains a Summary and Conclusions.

2   Uniform Distribution of Infinite Sequences - The Weyl Criterion

Discrepancy theory deals with the distribution of points in space (Matoušek, 1999). The Weyl criterion (Weyl, 1916) gives the necessary and sufficient conditions for a sequence to be uniformly distributed in $[0, 1)^d$, the d-dimensional unit interval. The criterion for a two-dimensional sequence can be summarized as follows:

Theorem. (H. Weyl, 1916) A sequence $\{y_1(k), y_2(k)\}$ is equidistributed in $[0,1)^2$ if and only if

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} e^{2\pi i(l_1 y_1(k) + l_2 y_2(k))} = 0 \tag{1}$$

$\forall$ sets of integers l_1, l_2 not both zero.

Decomposing (1) into real and imaginary parts we obtain that the sequence $\{y_1(k), y_2(k)\}$ is equidistributed in $[0,1)^2$ if and only if for all sets of integers l_1, l_2 (not both zero) the following conditions hold:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \cos[2\pi(l_1 y_1(k) + l_2 y_2(k))] = 0 \tag{2}$$

and

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \sin[2\pi(l_1 y_1(k) + l_2 y_2(k))] = 0 \tag{3}$$

Weyl's criterion can readily be extended to higher dimensions, as needed by the requirements of the problem under consideration.

3   An Illustrative Example

To illustrate the effectiveness of the Weyl criterion for signal design, we consider a highly interactive system based on the simplified model of a high-purity distillation column (Morari and Zafiriou, 1988). The system dynamics are described in terms of the continuous time transfer function is as follows:

$$y(s) = \frac{1}{75s+1} \begin{bmatrix} 87.8 & -86.4 \\ 108.2 & -109.6 \end{bmatrix} u(s) \tag{4}$$

where $y(s)$ and $u(s)$ are Laplace transform of the output and input signals to the system, respectively.

Our goal is to design an input signal that is uniformly distributed and as such has good directionality information in the output state space of the system; the latter goal is an important requirement when working with highly interactive multivariable systems (Morari and Zafiriou, 1988). This assumes *a priori* knowledge of the plant model as either an equation or a computer program that is available to the optimizer. We introduce two cycles of input each of length N_s and let the transients die out in the first cycle ($k = 0, \ldots, N_s - 1$) of the output. As before the input $u(k)$ and output $y(k)$ are vectors with two components. To design a plant friendly signal we impose bound constraints on both $u(k)$ and/or $y(k)$ in the second cycle. Here, z is one of y_1, y_2, u_1, u_2.

$$|z(k)| \le C_z, \qquad k = N_s, \ldots, 2N_s - 1 \tag{5}$$

The C_z are user defined constants. We would also like to have restrictions on the move size of $u(k)$ and $y(k)$, which is the difference between successive values in $u(k)$ and $y(k)$. We therefore impose the constraints,

$$|z(k+1) - z(k)| \le \Delta C_z, \quad k = N_s - 1, \ldots, 2N_s - 2 \tag{6}$$

Again ΔC_z are user defined constants. The prediction of the plant output response must be determined from a model estimated from previous identification tests, or otherwise obtained *a priori*. These relationships are:

$$y_1(k) = f_1(u_1, u_2, y_1, y_2), \ k = 0, \ldots, 2N_s - 1 \tag{7}$$

$$y_2(k) = f_2(u_1, u_2, y_1, y_2), \ k = 0, \ldots, 2N_s - 1 \tag{8}$$

Here the arguments of f_1 and f_2 indicate the dependence of y_1 and y_2 on the values of the vectors u_1, u_2, y_1 and y_2; for the Example problem these correspond to the sampled data representation for (4). The inputs $u_1(k)$ and $u_2(k)$ are chosen per the multisine structure:

$$u_j(k) = \sum_{i=1}^{(m+1)n_s} \sqrt{2\alpha_{ij}} \cos\left(\frac{2\pi i}{N_s}k + \phi_{ij}\right) \tag{9}$$

with Fourier coefficient bounds corresponding to a modified zippered spectrum as described below:

$$\alpha_{ij} = \begin{cases} \geq 0, & i = j, \ (m+1)+j, \cdots, (m+1)(n_s-1)+j \\ \geq 0, & i = m+1, \ 2(m+1), \cdots, n_s(m+1) \\ = 0, & \text{for all other } i \text{ up to } (m+1)n_s \end{cases}$$

The goal is to uniformly distribute the points $(y_1(k), y_2(k))$ in the output state space region $[-C_{y_1}, C_{y_1}) \times [-C_{y_2}, C_{y_2})$. We wish to use the Weyl Criterion described in the previous section to achieve this uniform distribution. Since the Weyl Criterion deals with uniform distributions in $[0,1)^2$, we introduce a change of variables:

$$\hat{y}_1(k) = \frac{y_1(k) + C_{y_1}}{2C_{y_1}}, \quad \hat{y}_2(k) = \frac{y_2(k) + C_{y_2}}{2C_{y_2}} \tag{10}$$

Since we only have a finite number of points in the sequences, we choose an integer L and form the set S as follows:

$$S = \{x : x \in Z \text{ and } |x| \leq L\} \tag{11}$$

where Z is the set of all integers and W corresponds to

$$W = \{(l_1, l_2) : l_1 \in S, l_2 \in S \text{ and } (l_1, l_2) \neq (0,0)\}$$

We then try to minimize the sum in equations (2) and (3) for all elements of the set W. As before we impose this "Weyl" constraint on the second cycle ($k = N_s + 1, \ldots, 2N_s - 1$) of the output. The optimization is carried out to estimate the amplitudes and phases $\alpha_{i1}, \alpha_{i2}, \phi_{i1}, \phi_{i2}, \ i = 1, \ldots, (m+1)n_s$ of the $m = 2$ multisine input channels. The complete problem statement is as follows:

$$\min_{\alpha_{i1}, \alpha_{i2}, \phi_{i1}, \phi_{i2}} t \tag{12}$$

s.t.

$$\sum_{k=N_s+1}^{2N_s-1} \cos[2\pi(l_1\hat{y}_1(k) + l_2\hat{y}_2(k))] \leq t, \forall \ (l_1, l_2) \in W$$

$$\sum_{k=N_s+1}^{2N_s-1} \sin[2\pi(l_1\hat{y}_1(k) + l_2\hat{y}_2(k))] \leq t, \forall \ (l_1, l_2) \in W$$

$$t \geq \varepsilon$$

as well as subject to constraints per Equations (5)-(10). The lower bound constraint on t is imposed to promote faster convergence. ε is chosen to be some small positive constant.

To better understand the influence of design variables L and ε on the distribution of points in the output state space we perform two experiments using the example problem per (4) with the bound and move sizes shown in Table 1.

In the first experiment, we fix ε at a value of 10^{-3} and vary L. The distribution of points in the output state space obtained for two different simulations with $L = 2$ and 6 is shown in Figure 1; Pendse (2004) contains simulations for $L = 3, 4,$ and 5. It can be seen that by increasing L, the uniformity in the output state space distribution improves dramatically. An increase in the design variable L seems to move the various clusters of points at different places in the state space to achieve an approximation to a uniform distribution.

In the second experiment, described in more detail in Pendse (2004), we fix $L = 3$ and vary ε. We know from Experiment 1 that a low value of L gives a relatively poor distribution; the effect of changing ε is then more easy to decipher on a relatively poor distribution than with a good distribution. A series of simulations with ε values ranging from 10^{-2} to 10^{-6} can be found in Figure 2. Decreasing the value of ε tends to keep the various clusters of points in more or less the same position, but leads to a redistribution of points within the same cluster. Given this information, there is not much to gain by decreasing ε beyond a certain limit; it is much more advantageous to increase L instead.

The constrained optimization problems described in this paper were solved by programming them in the modelling language AMPL which has built in automatic differentiation up to second order derivatives. The Weyl constraints are continuously differentiable and so the optimizer can make direct use of second derivative information. The optimizer used was KNITRO developed by Byrd and co-workers (Byrd *et al.*, 1999). KNITRO is an interior point trust region SQP solver and is suitable for solving both large and small problems.

4   Case Study: Nonlinear High-Purity Distillation Process

4.1   Input signal design and comparison to minimum crest factor approaches

A challenging multivariable process system that benefits from judiciously applied system identification techniques is high purity distillation; the methanol-ethanol distillation column model developed by Weischedel and McAvoy (1980) is commonly used as a benchmark problem (Sriniwas *et al.*, 1995). The highly interactive nature of high-purity distillation is reflected in the fact that dynamically the system will tend to respond in the principal gain direction (consisting of achieving greater purity in one stream at the expense of purity in the other) while the low gain direction (reflecting conditions where purities in both the distillate and bottom streams increase simultaneously) is much less evident.

To address the demands of highly interactive systems, one approach is to modify the standard multisine signal to contain correlated harmonics with high levels of power, which improve the low gain-direction content in the data and promote better coverage of the output state-space (Lee *et al.*, 2003). The optimization approach per Lee *et al.* (2003) considers minimizing crest factor (CF), the ratio of the ℓ_∞ (or Chebyshev) norm and the ℓ_2-norm of a signal x (Guillaume *et al.*, 1991). A low crest factor indicates that most of the elements in the sequence are distributed near their extremum values. An alternative rep-

resentation of signal distribution similar to crest factor is the Performance Index for Perturbation Signals (PIPS) (Godfrey *et al.*, 1999). The PIPS measure ranges between 0 and 100% (compared to 1 versus ∞ for crest factor), which gives it an intuitive, practical appeal. Design parameters for the Weischedel-McAvoy problem determined on the basis of the guidelines per Lee *et al.* (2003) using dominant time constant estimates ($\tau_{dom}^L = 5$ and $\tau_{dom}^H = 20$ min) and user choices of $\delta = 0$, $\alpha_s = 2$, and $\beta_s = 3$, lead to parameter settings of $T = 2$ minutes, $n_s = 189$, and $N_s = 378$. A value of the amplification factor $\gamma = 15$ was chosen for a min CF(y) signal with modified spectrum; the resulting input spectrum for this signal is shown in Figure 3a. Constraints applied to the problem and salient characteristics of these signals are summarized in Table 2; an output state-space plot is shown in Figure 4a.

A significant benefit of an optimization-based problem formulation for signal design is that nonlinear model forms can be readily incorporated in the design procedure, which results in an improved ability to both meet plant-friendliness requirements as well as address the directionality and uniform distribution requirements in the output for demanding applications. A polynomial Nonlinear AutoRegressive with eXternal (NARX) input model with structure as proposed by Sriniwas *et al.* (1995):

$$
\begin{aligned}
y(k) &= \theta^{(0)} + \sum_{i=1}^{n_y} \theta_i^{(1)} y(k-i) + \sum_{i=\rho}^{n_u} \theta_i^{(2)} u(k-i) + + \sum_{i=1}^{n_y} \sum_{j=1}^{i} \theta_{(i,j)}^{(3)} y(k-i) y(k-j) \\
&+ \sum_{i=\rho}^{n_u} \sum_{j=\rho}^{i} \theta_{(i,j)}^{(4)} u(k-i) u(k-j) + \sum_{i=1}^{n_y} \sum_{j=\rho}^{n_u} \theta_{(i,j)}^{(5)} y(k-i) u(k-j) + ...
\end{aligned}
\tag{13}
$$

was estimated for the Weischedel-McAvoy column and used to generate output predictions for the optimizer in both the min CF(y) and Weyl-based signal design scenarios. The benefits of the Weyl-based formulation over the minimum crest factor signal design in producing a uniform distribution in the output state-space of the data can be clearly seen by contrasting Figures 4a and 4b: the use of the Weyl-based criterion results in a much more uniformly distributed coverage of the state-space, and a much better suited dataset for data-centric estimation purposes. The uniform distribution of the output within the bounds specified in the problem results in a natural balance between the high and low gain information content in the data. From Table 2 one does notice, however, that the improvement in output state space uniformity is obtained at the cost of higher crest factor, which consequently reduces the signal-to-noise ratio of the data in a noisy data setting. As a result there is an inherent tradeoff between these objectives that needs to be recognized. One way of addressing this issue in practical input design is to include maximum crest factor bounds as inequality constraints within the Weyl problem formulation; these can be readily incorporated in the numerical optimization framework described in this paper.

An important difference between these signal designs is observed in the input spectra (Figure 3). In the min CF (y) case, only the phases and a subset of the Fourier coefficients in the high frequency range of the multisine signal are chosen by the optimizer, while for the Weyl-based design, the optimization problem includes a search for *all* Fourier coefficients and phases, including those corresponding to the correlated harmonics; this can be seen in Figure 3b. Not only do these extra degrees of freedom in the optimizer contribute to the improved performance, they reduce the number of decisions made *a priori* by the user, leading to a more practical design procedure.

4.2   Application to Model-on-Demand Estimation and Predictive Control

We noted in the Introduction about the increasing importance of data-centric (also referred to as data-driven) modeling for nonlinear problems. In recent years, data-centric estimation methods have received

significant attention in the systems literature, and signficant applications have been reported (Kulhavý, 2003). One such novel concept for nonlinear identification and control is the Model-on-Demand (MoD) framework (Stenman, 1999), which is inspired by ideas from local modeling and database systems technology (Atkeson *et al.* (1997*a*; 1997*b*)). Conceptually, MoD represents a hybrid between local and global modeling. In MoD estimation all observations are stored on a database, and the models are built "on demand" as the actual need arises. The Model on Demand predictor relies on small portions of the data relevant to the region of interest to determine a model as needed (Figure 5). The variance/bias tradeoff inherent to all modeling is optimized locally by adapting the number of data and their relative weighting. From a practical standpoint, MoD estimation allows process engineers to naturally extend insight gained from linear modeling to nonlinear identification and control. Rather than spending time in a difficult structure selection and parameter initialization, the user can focus on developing informative datasets – a common requirement for all nonlinear black-box identification approaches. The user can fully examine the uniformity of coverage the excitation signals produced in the input and output spaces (as done in the previous subsection) and better understand the impact it has on the nonlinear model validation and control problem. MoD can be formulated into a comprehensive methodology for nonlinear identification and predictive control (Braun, 2001; Braun *et al.*, 2000). A Matlab-based tool for MoD estimation and control, developed by ASU's Control Systems Engineering laboratory in collaboration with researchers from the Division of Automatic Control at Linköping University is available in the public domain (Braun *et al.*, 2002).

First, open-loop Model-on-Demand (MoD) estimation is evaluated for the Weischedel-McAvoy distillation column using for estimation purposes the data arising from the signal designs described in the Section 4.1. For validation purposes, a different data-centric signal with lower magnitude bounds was considered, which is shown in Figure 6. For all cases, an implicit second-order ARX structure with unit delays is used in the MoD estimator, with k_{min}=20, k_{max}=756, and local polynomial order = 1 as additional parameters (Braun *et al.*, 2001; Stenman, 1999).

Analysis of the results shows that data resulting from the min CF(u) signal based on the standard zippered spectrum provides the worst results of all three cases considered. Because the input-output data resulting from this signal lacks information content in the [1 -1] output direction, it results in the poorest prediction on the validation data set (Figure 7). For data resulting from the min CF(y) signal with modified spectrum, most of the output sequence is located near its minimum and maximum values, but its corresponding MoD model still seems to produce reasonable predictions in an open-loop sense with a percent unexplained variance of 0.5% (Figure 8). Nonetheless the MoD model estimated from the Weyl-based approach, because of the even state-space distribution, results in the most accurate predictions of all signals considered, with a percent unexplained variance close to 0.09% (Figure 9).

The min CF(y) and Weyl-based MoD models are subsequently evaluated in a closed-loop setting using the MoD-MPC Toolbox (Braun *et al.*, 2002); the min CF(u) MoD model was not considered in the closed-loop evaluation because a stable controller response could not be obtained. In both cases the tuning parameters are PH=35, MH=15, Ywt=[1 0; 0 1] and Uwt=[7 0; 0 7]. A series of setpoint changes that represent challenges to controller performance for a highly interactive plant such as high-purity distillation are shown in Figure 10. While stable responses are obtained in both cases, the MoD-MPC controller relying on the Weyl-based data shows faster settling time, less overshoot, and less interaction than the one resulting from the min CF(y) MoD model; these desirable performance features of the Weyl-based MoD-MPC controller point to the effectiveness of this class of signals for closed-loop control purposes in a demanding process application.

5   Summary and Conclusions

The paper describes a novel constrained optimization-based formulation of the multisine input signal problem. The objective function arises from the Weyl criterion, which seeks to minimize the geometric discrepancy of the output in the state-space. As a consequence, these signals can be used in support of data-centric estimation algorithms. A problem formulation that helped understand design variables in the Weyl objective was shown and illustrated via a numerical example, culminating in a case study demonstrating the effectiveness of the design procedure for a high purity distillation column, a challenging nonlinear, multivariable process system. Validation of the Weyl-based signal design was accomplished in the distillation column example under both open-loop and closed-loop conditions. Clearly, the power of the proposed framework lies in its flexibility, allowing the user to incorporate both linear and nonlinear models for output prediction, time-domain constraints, and information and control-theoretic frequency domain requirements. The use of state-of-the-art interior-point optimization methods enables the efficient solution of these nonlinear and nonconvex optimization problems.

6   Acknowledgments

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C_{y_1}	C_{y_2}	ΔC_{y_1}	ΔC_{y_2}	ΔC_{u_1}	ΔC_{u_2}
0.5	0.5	0.47	0.47	2.2	2.2

Table 1: Bound and move sizes used for Example Problem in Section 3.

Type	Signal (x)	CF(x)	PIPS(%)	max Δx	max x	min x
min CF (u) design; standard zippered spectrum	u_1	1.21	82.43	0.0025	0.0020	-0.0020
	u_2	1.22	81.77	0.0026	0.0020	-0.0020
	y_1	2.48	48.84	0.0037	0.0325	-0.0211
	y_2	2.19	46.12	0.0031	0.0199	-0.0204
min CF(y) design; modified zippered spectrum using NARX model prediction $|\Delta u| \leq 0.01$, $|\Delta y| \leq 0.008$ & $|y| \leq 0.0085$	u_1	3.74	31.51	0.0100	0.0365	-0.0254
	u_2	3.25	34.37	0.0100	0.0316	-0.0250
	y_1	1.30	77.45	0.0051	0.0088	-0.0086
	y_2	1.31	77.01	0.0082	0.0087	-0.0086
data-centric experiment using NARX model via a modified zippered spectrum subject to $|\Delta u| \leq 0.01$, $|\Delta y| \leq 0.08$ & $|y| \leq 0.0085$	u_1	2.78	37.52	0.0079	0.0292	-0.0268
	u_2	2.50	41.28	0.0076	0.0240	-0.0225
	y_1	1.79	56.54	0.0062	0.0084	-0.0082
	y_2	1.76	57.13	0.0053	0.0082	-0.0083

Table 2: Results summary for signals designed for the Weischedel-McAvoy distillation column Case Study.

The Weyl criterion with L=2 and ε = 1e−3
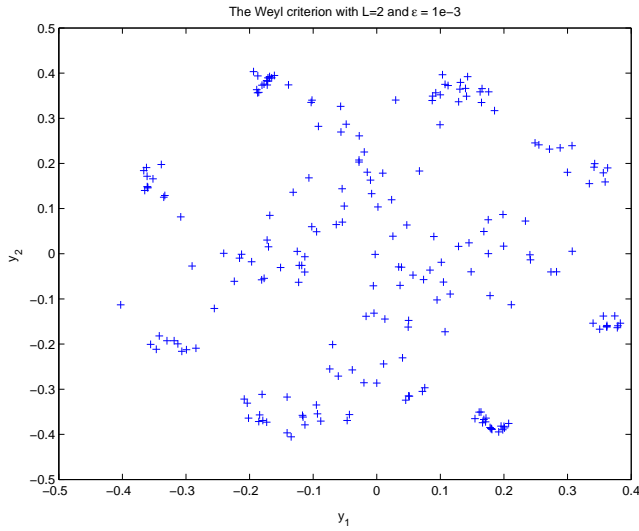
(a) $L = 2$
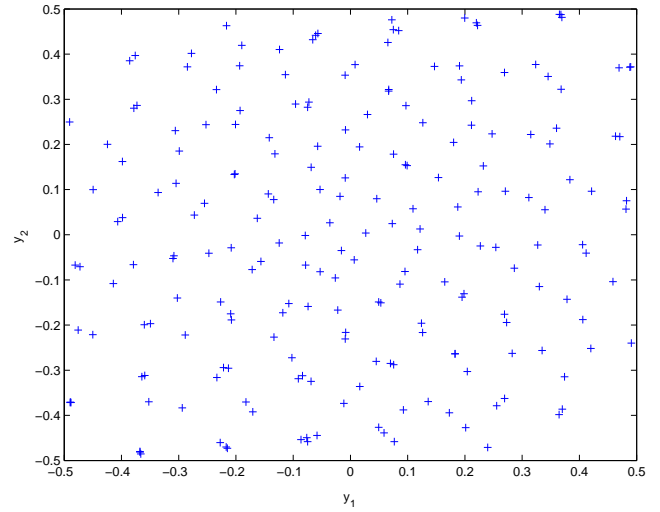
(b) $L = 6$

Figure 1: Output state space comparison for the Example problem, $L = 2$ and 6, $\varepsilon = 10^{-3}$

The Weyl criterion with L=3 and ε = 1e−2

The Weyl criterion with L=3 and ε = 1e−6
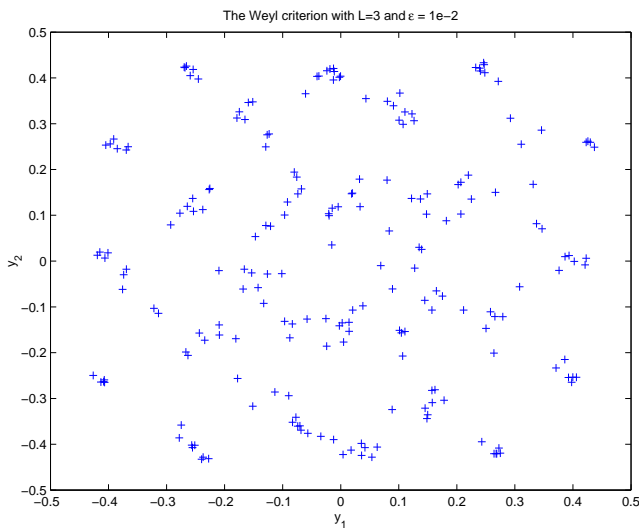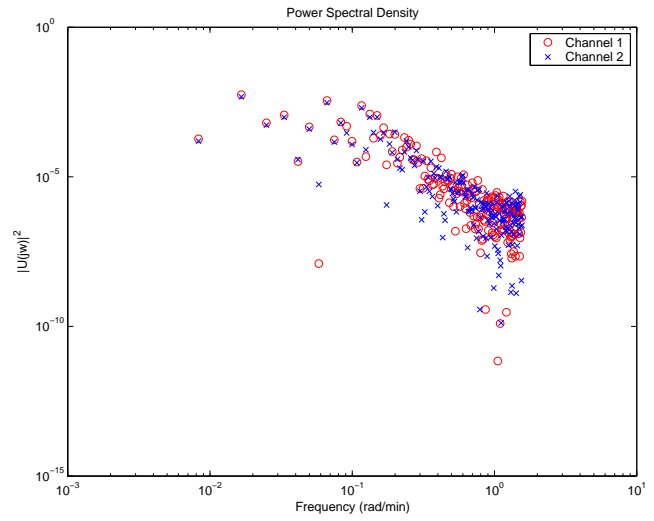
(a) $\varepsilon = 10^{-2}$
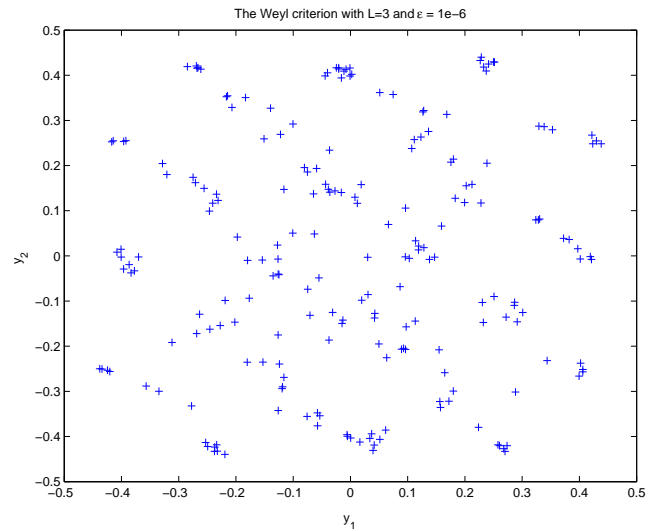
(b) $\varepsilon = 10^{-6}$

Figure 2: Output state space comparison for the Example problem, $\varepsilon = 10^{-2}$ and 10^{-6}, $L = 3$
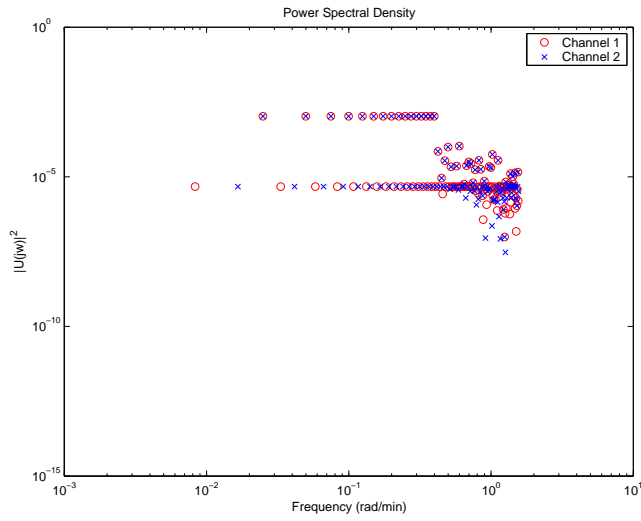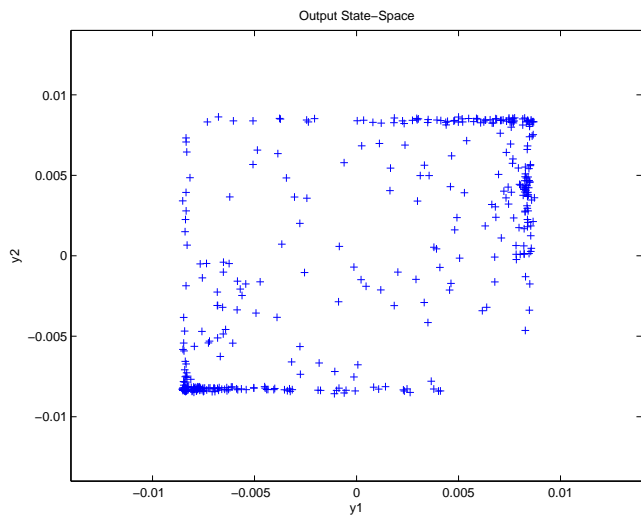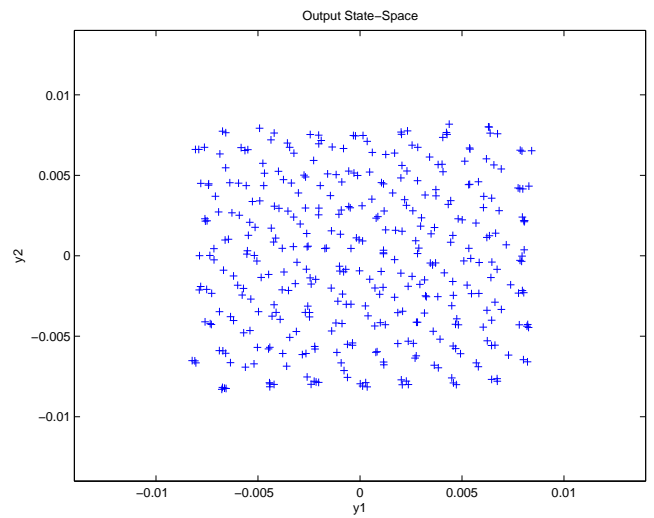
(a) min CF (y)

(b) Weyl-based Approach

Figure 3: Input power spectral densities for Weischedel-McAvoy distillation column: min CF(y) (a) versus Weyl-based design (b)

(a) min CF (y)

(b) Weyl-based Approach

Figure 4: Output state-space analysis for Weischedel-McAvoy distillation column: min CF(y) (a) versus Weyl-based design (b)
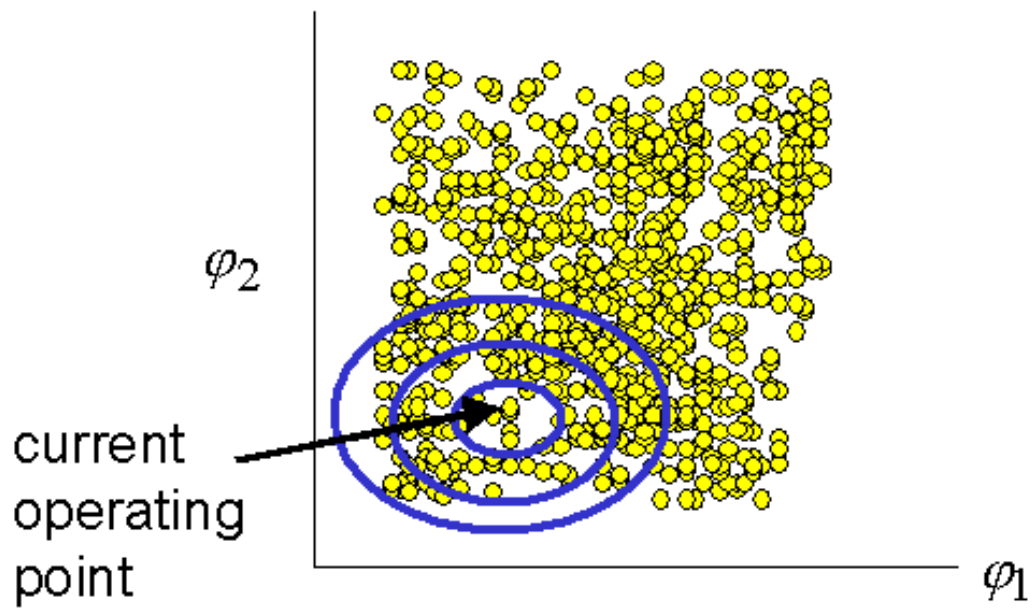
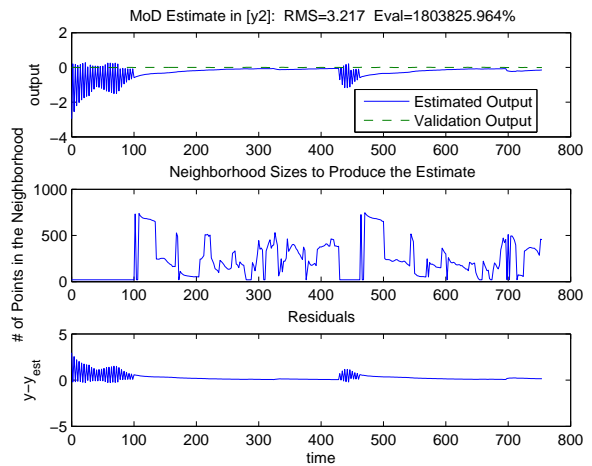Figure 5: Depiction of local regressor selection for Model-on-Demand estimation
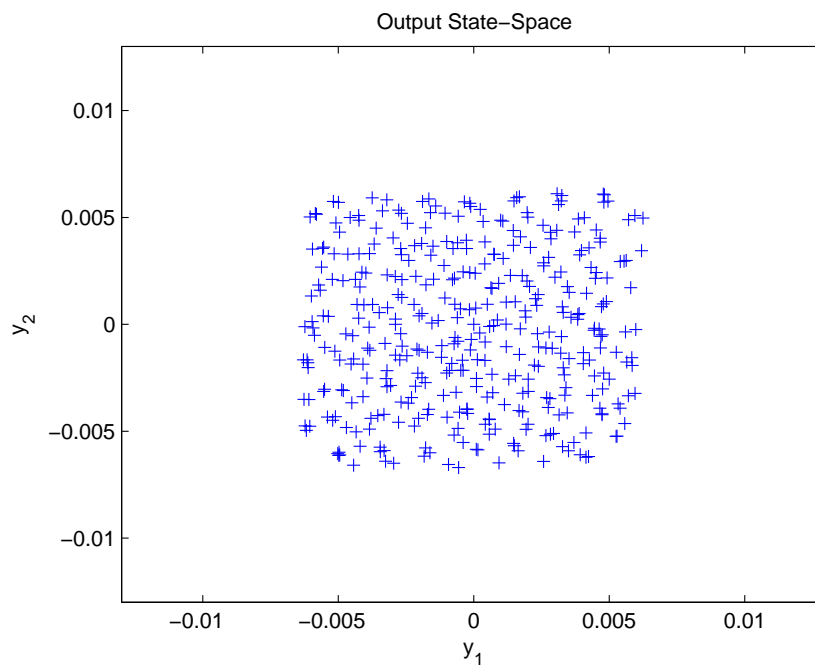
Figure 6: Validation data's output state-space for Weischedel-McAvoy distillation column
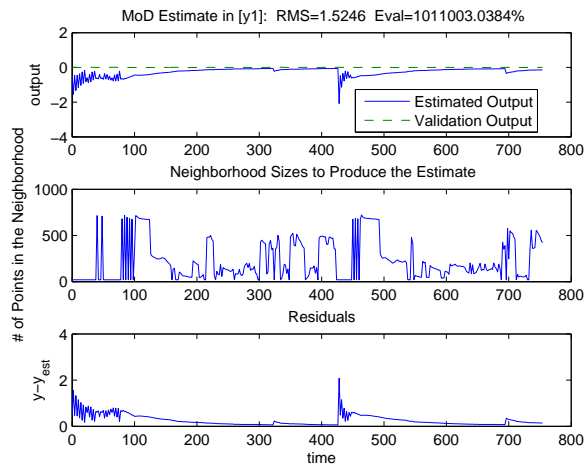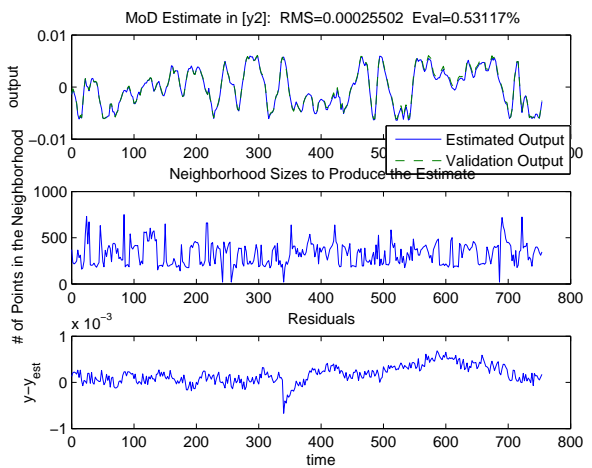
(a) Output 1 (y_1)

(b) Output 2 (y_2)

Figure 7: MoD estimation and validation results for Weischedel-McAvoy distillation column data arising from a min CF (u) signal using the standard zippered spectrum design.
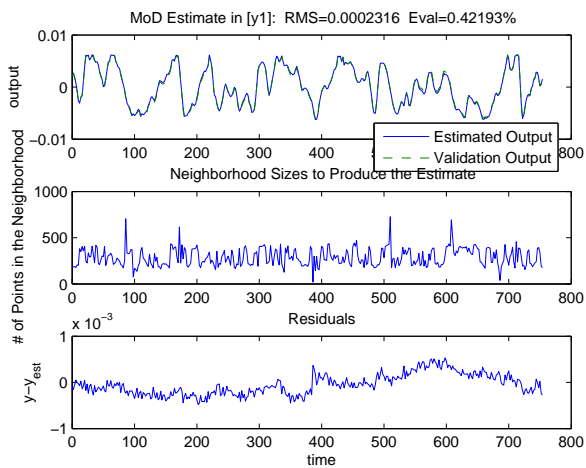
(a) Output 1 (y_1)

(b) Output 2 (y_2)

Figure 8: MoD estimation and validation results for Weischedel-McAvoy distillation column data resulting from a min CF (y) signal with modified zippered spectrum design.
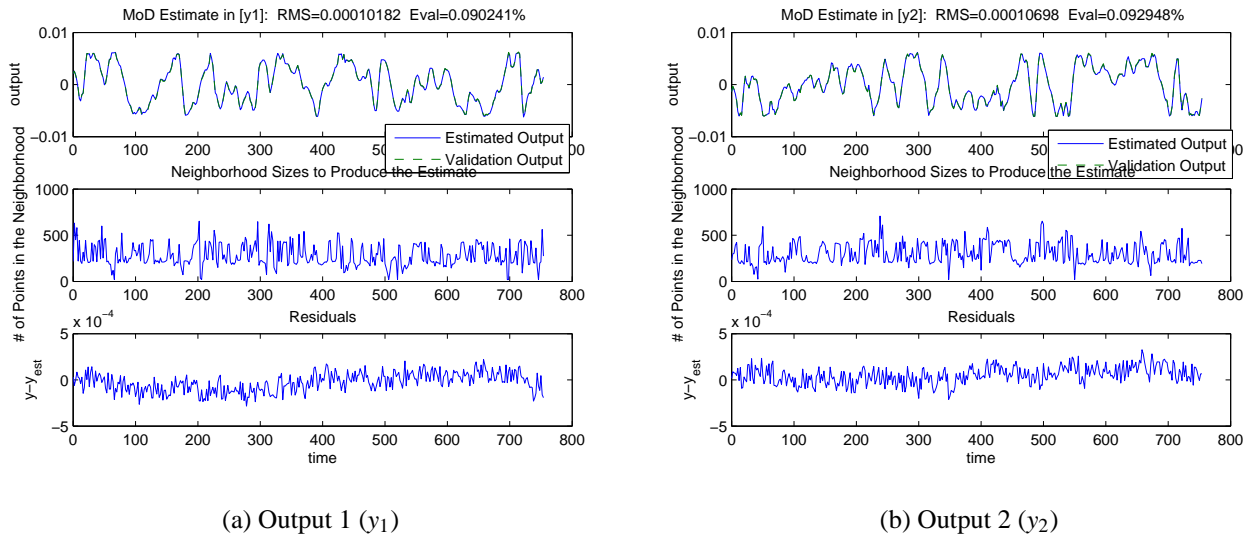
(a) Output 1 (y_1) (b) Output 2 (y_2)

Figure 9: MoD estimation and and validation results for Weischedel-McAvoy distillation column data resulting from the Weyl-based signal design.
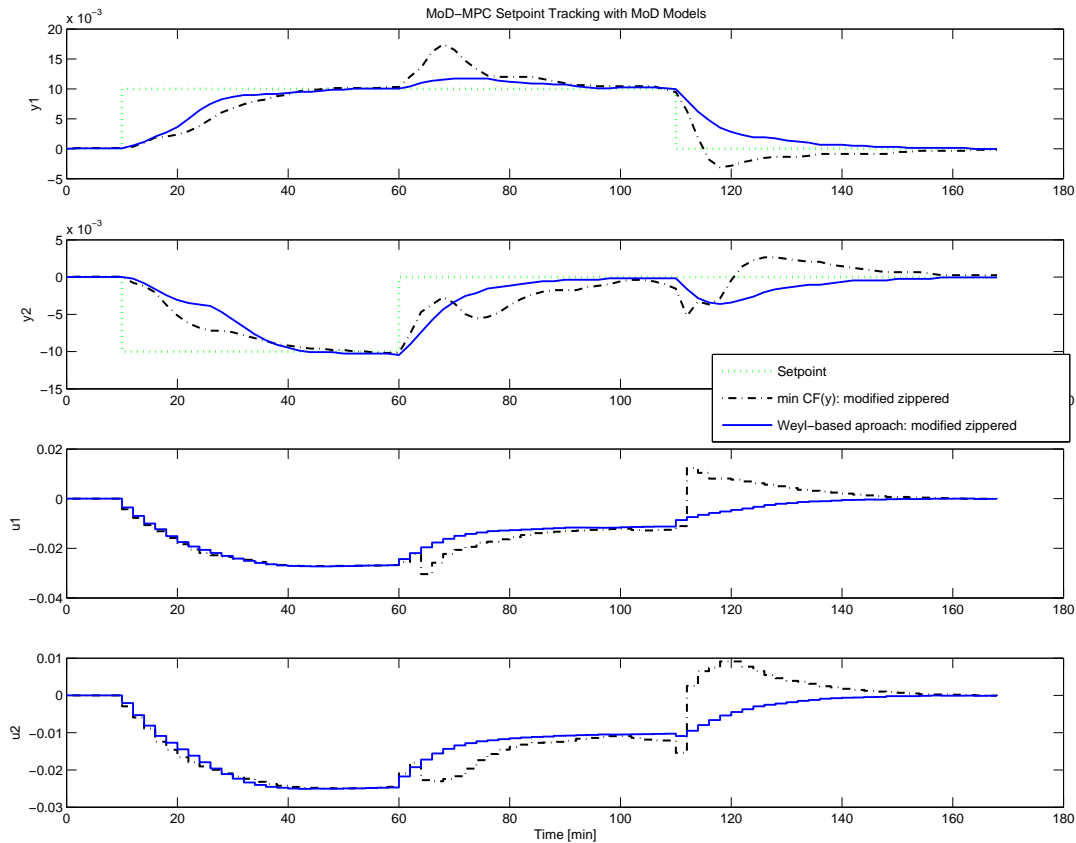

Figure 10: MoD-MPC closed-loop setpoint tracking test on the Weischedel-McAvoy distillation column using MoD Models from the min CF (y) signal (dashed) and Weyl-based (solid) signal designs. Controller parameters are PH=35, MH=15, Ywt=[1 0; 0 1] and Uwt=[7 0; 0 7]