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# State-of-the-art in the Solution of Control-Related Nonlinear Optimisation Problems

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**Abstract:** In current research nonlinear optimization problems arise that are challenging for existing, even state-of-the-art, software. In this paper we take a comprehensive look at this. First, we describe three related services provided for free to the community, guides on optimization software and its performance as well as web-based optimization solvers. Then, two representative problems are given in detail, both are from recent research in control. It is reported how these problems can be solved with the best available software tools. This connects back to the first part of the paper into which these problems and their solution have been integrated.

Pls provide AMS Subject Classification and Keywords

**AMS Subject Classification:**
**Keywords:**

## 1. Introduction

This paper refers back to the contributions made by Mittelmann and Tröltzsch [1], as well as Mittelmann and Pendse [2]. The common theme is that of optimal control problems being solved as large nonlinear and constrained optimisation problems. In addition to the earlier and current research, this paper reports on certain related service components of the author's work.

The work of Mittelmann and Tröltzsch [1] represents the last in a series of papers [3-7] on PDE constrained optimisation problems. These problems, for elliptic and parabolic PDEs, are solved after discretisation, with what is known as the one-shot approach, i.e. the reduction of a problem with control as well as state constraints and typical objective functionals to a single large nonlinear optimisation problem. The solution of such problems presents challenges to the best available optimisation codes.

As a free service to the community, information about available optimisation software has been made available on two webpages. The first webpage [8] lists, systematically, software available in various areas and related material, such as literature. The second webpage [9] provides detailed information on the performance of some of the available software. Naturally, the problems from the

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author's PDE-constrained optimisation research has been integrated into the latter, 'benchmarking' effort. In particular, it has facilitated not only the research by others in the field, but also the development of methods and software for such problems.

Mittelmann and Pendse [2] made an important contribution to other works on control-related problems, starting with those on system identification [10, 11] and, now, extending to model-on-demand model predictive control. In fact, their work [2] formed the basis for some of the latest results. The optimisation problems arising in [2] were integrated into [9].

This paper, begins with an overview of the two key webpages concerned with optimisation software. Then it describes another component of the "service to the community", which is the installation and maintenance of a substantial portion of the web-based interactive optimisation solvers accessible through the NEOS gateway (*neos.mcs.anl.gov*). It is followed by the description of an exemplary PDE-constrained optimisation problem, both in mathematical terms and in the modelling language AMPL [12]. Thereafter, the corresponding part of the author's benchmarks are cited for this optimisation problem as well as for the system identification and control problems, along with latest research results.

## 2. Decision Tree, Benchmarks and NEOS Solvers

A Google search for 'optimization software' lists, among the first few links, two webpages [8, 9]. An overview is given for readers who have not consulted these frequently-visited websites. The first webpage [8] facilitates the search for a suitable optimisation program by having a hierarchical structure from a coarse to a finer classification of the problems that can be solved by different programs. A user can browse through the given hierarchy to look for a particular piece of software or other item of interest such as online and printed information etc. Another way is to search through a link given on the entry page, which is marked "Decision Tree for Optimisation Software" and has links to the next level pages, viz., "Problems/Software, Benchmarks, Testcases, Books/ Tutorials, Tools, Websubmission, Other Sources". In fact, a navigation menu unfolds to show the entire substructuring and permits direct access to all levels.

There are more than 600 links to the optimisation software given under 'Problems/Software'. This page is further split into:

- Global optimisation
- LP/NLP-linear and nonlinear optimisation
  - Unconstrained
  - Constrained
  - ¿ Least squares (other norms -¿ approximation)
- Zero
- MCP-complementarity problem
- Multi-objective optimisation
- Discrete optimisation
- Approximation

The most extensive sub-area is the one on constrained optimisation, which is further split into:

- The LP-problem, also mixed integer and stochastic

- The QP-problem, also mixed integer
- Semidefinite and second-order cone programming
- Geometric programming
- The general nonlinear problem (dense, sparse, nonsmooth, SIP)
- Mixed integer nonlinear programming
- Network constraints
- Special/constraint solvers
- Control problems
- Other collections/problems

In addition to the local search engine the entry page contains a link to an extensive statistic on accesses to these webpages, which are updated daily. Every user can check, at any time, which pages were accessed and from where accesses were made. For example, a reverse domain lookup for sites ending in '.com' for the month of March 2007 revealed that, among others, the industrial sites, which accessed our pages included Boeing, CalPOP, CONNX, Cosmixcorp, CrispyCritter, Fidelity, Freescale, Harris Corporation, Honeywell, IBM Watson, ILOG, Land O'Lakes, lmco.external, Microsoft, mmm, Philips Research, Raytheon, Royalbank, sas.unx, Siemens, Statoil, Synopsys, Trading Technologies International Inc., VNI Houston, Volvo etc.

The first-level subpage 'Benchmarks' links to a collection of software comparisons done by others and to other related information. Mainly, it links to a second major webpage "Benchmarks of Optimisation Software" [9]. These benchmarks are comprehensive as they give links to all the problem and result files used, as well as to the software tested. They are frequently updated. The current list of benchmarks includes:

- Serial vs. parallel optimisation
  - Parallel CSDP on SDP problems
  - Parallel CPLEX on MIP problems
- Combinatorial optimisation
  - Concorde-TSP with different LP solvers
- Linear programming
  - Benchmark of commercial LP solvers
  - Benchmark of free LP solvers
  - MILP Benchmark-free codes
  - CPLEX vs. XPRESS-MP on LP and MILP problems
- Semidefinite/SQL programming
  - Several SDP-codes on SDP problems with free variables
  - Several SDP codes on problems from SDPLIB
  - Newer SDP/SOCP-codes on the $7^{th}$ DIMACS challenge problems
  - Several SDP codes on sparse and other SDP problems
  - SOCP (second-order cone programming) benchmark
- Nonlinear programming
  - Benchmark of commercial and other (QC)QP solvers
  - AMPL-NLP benchmark
- Mixed integer nonlinear programming

- MIQP benchmark
- Problems with equilibrium constraints
  - MPEC benchmark

Finally, the first-level subpage 'Websubmission' links to a number of interactive web-based solvers, including all those accessible through the NEOS gateway as well as those that are installed and maintained locally. The current list includes BNBS, BPMPD, Concorde, CONDOR, CSDP, DDSIP, ICOS, FEASPUMP, NSIPS, PENBMI, PENSDP, QSOPT-EX, SCIP, SDPA, SDPA-C, SDPLR, SDPT3, and SeDuMi.

Many solvers have three or more different input formats available in which users can submit problems, thereby, greatly enhancing the usefulness of these solvers. The most frequented solvers are SCIP, BPMPD, FEASPUMP, QSOPT-EX, Concorde and NSIPS. The first two are powerful solvers in categories wherein several commercial solvers are also available. The next four, however, are the only ones of their kind available at NEOS. Together with the informative webpages, this service component facilitates research and instruction worldwide.

## 3. PDE-constrained Optimisation

A typical PDE-constrained optimisation problem taken from earlier research [1, 3-7] is described. It will serve as an example to demonstrate the state-of-the-art in solving such problems with existing software.

Consider the following boundary control problem

$$F(y,u) = \int_{\Omega} f(x,y)dx + \int_{\Gamma_1} g(x,y,u)dx + \int_{\Gamma_2} k(x,u)dx$$

subject to the elliptic state equation

$$-\Delta y(x) + d(x, y(x)) = 0, \text{ for } x \in \Omega$$

boundary conditions of Neumann or Dirichlet type

$$\partial_\nu y(x) = b(x, y(x), u(x)) \qquad \text{for } x \in \Gamma_1$$

$$y(x) = a(x, u(x)) \qquad \text{for } x \in \Gamma_2$$

as well as control and state inequality constraints

$$C(x, u(x)) \le 0 \qquad \text{for } x \in \Gamma$$

$$S(x, y(x)) \le 0 \qquad \text{for } x \in \Omega$$

The necessary optimality conditions for this problem are

$$-\Delta\bar{q} + \bar{q}(x)d_y(x,\bar{y}) + f_y(x,\bar{y}) + S_y(x,\bar{y})\bar{\mu} = 0 \text{ on } \Omega$$

$$\partial_\nu\bar{q} - \bar{q}(x)b_y(x,\bar{y},\bar{u}) + g_y(x,\bar{y},\bar{u}) = 0 \text{ on } \Gamma_1$$

$$\bar{q} = 0 \text{ on } \Gamma_2$$

minimum condition for $x \in \Gamma_1$

$$g_u(x,\bar{y},\bar{u}) - \bar{q}b_u(x,\bar{y},\bar{u}) + \bar{\lambda}C_u(x,\bar{u}) = 0$$

minimum condition for $x \in \Gamma_2$

$$k_u(x,\bar{u}) + \partial_\nu \bar{q}a_u(x,\bar{u}) + \bar{\lambda}C_u(x,\bar{u}) = 0$$

complementarity conditions ($J$ active sets)

$$\bar{\lambda}(x) \geq 0 \text{ on } J(C), \qquad \bar{\lambda}(x) = 0 \text{ on } \Gamma \setminus J(C)$$

$$d\bar{\mu} \geq 0 \text{ in } J(S), \qquad d\bar{\mu} = 0 \text{ in } \Omega \setminus J(S)$$

In many applications, the cost functional is of *tracking* type

$$F(y,u) = \frac{1}{2}\int_\Omega (y(x) - y_d(x))^2\,dx + \frac{\alpha}{2}\int_\Gamma (u(x) - u_d(x))^2\,dx$$

with given functions $y_d \in C(\bar{\Omega})$, $u_d \in L^\infty(\Gamma)$ and non-negative weight $\alpha \geq 0$. The control and state constraints are taken to be box constraints of the simple type

$$y(x) \leq \psi(x) \text{ in } \Omega \qquad u_1(x) \leq u(x) \leq u_2(x) \text{ on } \Gamma$$

with functions $\psi \in C(\bar{\Omega})$ and $u_1, u_2 \in L^\infty(\Gamma)$.

Let $\Omega = [0, 1]^2$, $\Gamma_2 = \{(x_1, 1) \mid 0 \leq x_1 \leq 1\}$ and $\Omega_0 = [0.25, 0.75]^2$, therefore, the control problem considered here is to determine a function $u \in L^\infty(\Gamma_2)$ which minimises

$$F(y,u) = \frac{1}{2}\int_{\Omega_0} (y(x) - 1)^2\,dx + \frac{\alpha}{2}\int_{\Gamma_2} \left(u(x)^2\right) dx \tag{1}$$

subject to the state equation, Neumann and Dirichlet boundary conditions as well as control and state inequality constraints

$$\begin{array}{rlll}
-\Delta y(x) = 0 & \text{in } \Omega & & \\
\partial_\nu y(x) = 0 & \text{for} & x_2 = 0 & 0 \leq x_1 \leq 1 \\
\partial_\nu y(x) = y(x) - 5 & \text{for} & x_1 \in \{0, 1\} & 0 \leq x_2 \leq 1 \\
y(x) = u(x) & \text{for} & x_2 = 1 & 0 \leq x_1 \leq 1 \\
y(x) \leq 3.15 & \text{in} & \Omega_0 & \\
y(x) \leq 10 & \text{in} & \Omega \setminus \Omega_0 & \\
0 \leq u(x) \leq 10 & \text{for} & x_2 = 1 & 0 \leq x_1 \leq 1
\end{array}$$

Applying a standard finite difference discretisation, this problem can be phrased in the modelling language AMPL [12] as

```
param z{i in 1..n, j in 1..n}: = 1;
var x{0..n – 1, 0..n – 1};

minimise f:
.5*h2*sum{i in n1/4..3*n1/4, j in n1/4..3*n1/4}
(x[i, j] – z[i, j])^2 + .5*h*a*sum{i in 1..n} x[i, n1]^2;

s.t. pde{i in 1..n, j in 1..n}:
4*x[i, j] – sum{k in {– 1, 1}}(x[i + k, j] + x[i, j + k]) = g*h2;
```

```
s.t. bc1{i in 1..n}: x[i, 0] = x[i, 1];
s.t. bc2{i in 1..n}: x[0, i] – x[1, i] = h*(x[0, i] – t);
s.t. bc3{i in 1..n}: x[n1, i] – x[n, i] = h*(x[n1, i] – t);
s.t. sc{i in 0..n1, j in 0..n}: 0 < = x[i, j] < = if n1/4
< = i < = 3*n1/4 && n1/4 < = j < = 3*n1/4 then 3.15 else 10;
s.t. cc{i in 1..n}: 0 < = x[i, n1] < = 10;
```

The computed solutions were graphed. Figure 1 shows the case of bangbang control, $\alpha = 0$, solution and adjoint variable.

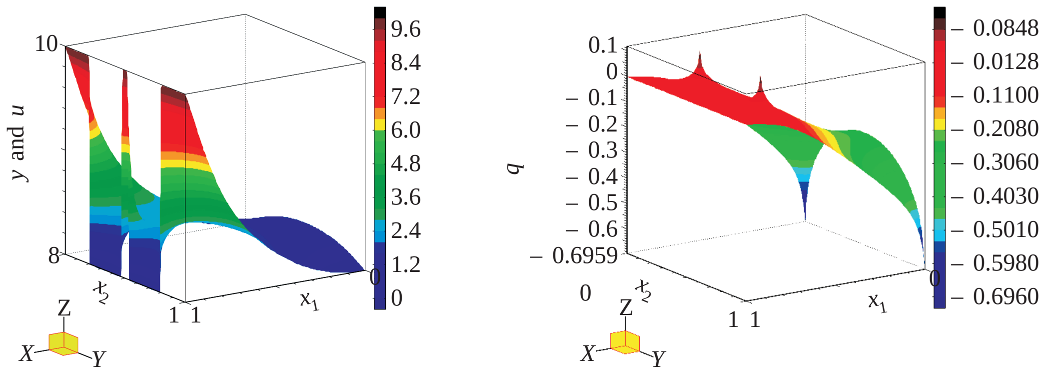



**Fig. 1. State and control resp adjoint variable of boundary control problem.** resp?

The AMPL model as well as those for other test cases have been considered in the works on PDE-constrained optimisation, which can be accessed together with additional information at [13], where it is cited on the 'Testcases' subpage of the 'Decision Tree'. The above example has also been included in the AMPL-NLP benchmark [14], which can be referred to for further details.

In the meantime, several researchers have used these problems [15-17]. In particular, Schenk, Waechter and Hagemann [17] used rather large dimensions. The authors could solve the boundary control problem shown above with 6.25 million variables and constraints in four hours on one node of an IBM SP2 parallel computer, while one of the author's distributed control examples, in which the number of variables was 12.5 million, took the same time when solved on two nodes.

## 4. System Identification and Control

Researchers [2, 18] have shown that a geometric equidistribution approach to system identification does produce signals that are significantly better spatially distributed than those found in other ways without substantial deterioration of other quality measures. The main reason for this approach is the application of a special control technique called Model-on-Demand (MoD). The numerical solution of the resultant nonlinear optimisation problems is somewhat more challenging, as discussed later. Therefore, following Lee et al. [19], the verification of the expected improvement in the signals obtained for the MoD control is presented here.

In recent years, there has been significant interest in data-centric dynamic modelling frameworks such as just-in-time modelling [20], MoD estimation [21] and, more recently, direct weight optimisation

(DWO) [22]. The appeal of these modelling 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 this class of estimation methods is to achieve uniform coverage of regressors in the database. Here we examine the development of multisine input designs that meet this criterion while satisfying plant-friendliness constraints during identification testing. 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 [11].

The approach described below for achieving uniformly distributed experimental designs for system identification relies on geometric discrepancy theory [23]. This is accomplished by minimising a discrepancy function made up of trigonometric polynomials arising from Weyl's Theorem [24] that ensure that the points are equidistant on a state-space. The optimisation problem calls for minimising this discrepancy function on the anticipated outputs of the system, subject to the requirements of an orthogonal 'zippered' spectrum (used to enable multi-channel implementation) and while enforcing time-domain constraints on upper and lower limits, move sizes, and rates of change in either (or both) input and output signals. The optimisation problem is solved using a state-of-the-art NLP solver (KNITRO) which uses an interior point trust region method and employs SQP techniques to solve the barrier subproblems.

The effectiveness of data resulting from an optimisation-based signal design using the proposed Weyl criteria is demonstrated in a binary high-purity distillation column case study by Weischedel and McAvoy [25], a demanding nonlinear and strongly interactive process application. A MoD Model Predictive Control (MoD-MPC) algorithm [21, 26, 27] is evaluated using a Weyl-based data-centric experiment vs. a multisine input design with equivalent harmonics, but minimising crest factor. Improvements in closed-loop performance are achieved in the Weyl-based data set, without the need to compromise plant-friendliness in the experimental design.

### 4.1 Model-on-Demand Modelling Methodology

Model-on-Demand is a data-centric, nonlinear black-box estimation method, which enhances the classical local modelling problem. In MoD, an adaptive bandwidth selector determines the size of data to be used for the local regression. The data is weighted using a kernel or weighting function. A local regression is performed using a linear or quadratic model to estimate the plant output at each time step. All observations are stored on a database and the models are built 'on demand' as the actual need arises. Local modelling techniques such as the MoD predictor use only small portions of data, relevant to the region of interest, to determine a model as needed. The variance/bias tradeoff inherent to all modelling is optimised locally by adapting the number of data and their relative weighting. As a consequence, the non-convex optimisation problem associated with most global nonlinear modeling techniques is avoided. Moreover, the user is presented with fewer decisions regarding model structure and can use intuition developed from linear model identification as the basis for obtaining an accurate nonlinear model.

#### *Model on Demand Estimation*

The MoD modelling formulation is described with a SISO process based on the approach of

Stenman [21]. Consider a SISO process with nonlinear ARX structure, i.e.

$$y(k) = m(\varphi(k)) + e(k) \quad k = 1, \ldots, N \tag{2}$$

where $m(\cdot)$ is an unknown nonlinear mapping and $e(k)$ is an error term modelled as random variables with zero mean and variance $\sigma_k^2$. The MoD predictor attempts to estimate output predictions based on a local neighbourhood of the regressor space $\varphi(t)$. The regressor vector is of the form

$$\varphi(t) = [\, y(t-1) \ldots y(t-n_a)\ u(t-n_k) \ldots u(t-n_b-n_k)]^T \tag{3}$$

where $n_a$, $n_b$ and $n_k$ denote the number of previous outputs and inputs as well as the degree of delays in the model.

A local estimate $\hat{y}$ can be obtained from the solution of the weighted regression problem

$$\hat{\beta} = \arg\min_{\hat{\beta}} \sum_{k=1}^{N} \ell(y(k) - \hat{m}(\varphi(k), \beta)) \times W\left(\frac{\| \varphi(k) - \varphi(t) \|_M}{h}\right) \tag{4}$$

where $\ell(\cdot)$ is a quadratic norm function, $\| u \|_M \triangleq \sqrt{u^T M u}$ is a scaled distance function on the regressor space, $h$ is a bandwidth parameter controlling the size of the local neighborhood and $W(\cdot)$ is a window function – usually, referred to as the kernel – assigning weights to each remote data point according to its distance from $\varphi(t)$ [28]. The window is, typically, a bell-shaped function with bounded support. These weights can be chosen to minimise the point-wise mean square error of the estimate. Assuming a local model structure

$$m(\varphi(t), \beta) = \beta_0 + \beta_1^T (\varphi(k) - \varphi(t)) \tag{5}$$

which is linear in the unknown parameters; an estimate can easily be computed using least squares methods. If $\beta_0$ and $\beta_1$ denote the minimisers of Eq. (4) using the model from Eq. (5). A one-step ahead prediction is given by

$$\hat{y}(t) = m(\varphi(t), \hat{\beta}) = \hat{\beta}_0 \tag{6}$$

Each local regression problem produces a single prediction $\hat{y}(t)$ corresponding to the current regression vector $\varphi(t)$. To obtain prediction at other locations in the regressor space, the weights change and new optimisation problems must be solved. This is in contrast to the global modelling approach where the model is fitted to data only once and then discarded. The bandwidth $h$ controls the neighborhood size and has a critical impact on the resulting estimate since it governs a trade-off between the bias and variance errors of the estimate. Traditional bandwidth selectors produce a single global bandwidth. In MoD estimation, a bandwidth is computed adaptively at each prediction.

***Model-on-Demand Model Predictive Control***

Model predictions from MoD estimates can be incorporated into a MPC framework [21, 26, 27]. The objective function

$$\min_{\Delta u(k|k) \ldots \Delta u(k+m-1|k)} \sum_{\ell=1}^{p_h} Q_e(\ell)(\hat{y}(k+\ell \mid k) - r(k+\ell))^2 + \sum_{\ell=1}^{m_h} Q_{\Delta u}(\ell)(\Delta u(k+\ell-1 \mid k))^2 \tag{7}$$

is subject to constraints on outputs ($0 \le y(k) \le y_{\max}$), inputs ($0 \le u(k) \le u_{\max}$), and their rate-of-change ($\Delta u_{\min} \le \Delta u_k \le \Delta u_{\max}$). The weight functions $Q_e(\ell)$ and $Q_{\Delta u}(\ell)$ are adjusted to obtain desired levels of robustness and performance.

**4.2 Uniform Distribution of Infinite Sequences: The Weyl Criterion**

Discrepancy theory deals with the distribution of points in space [23]. The Weyl's criterion [24] 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 summarised as follows:

*Theorem* [24]: A sequence $\{y_1(k), y_2(k)\}$ is equidistributed in $[0, 1)^2$ if and only if

$$\lim_{N\to\infty} \frac{1}{N}\sum_{k=1}^{N} e^{2\pi i(l_1 y_1(k)+l_2 y_2(k))} = 0 \tag{8}$$

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

Decomposing Eq. (8) 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 $l_1$, $l_2$ (both not zero) the following conditions hold

$$\lim_{N\to\infty} \frac{1}{N}\sum_{k=1}^{N} \cos[2\pi(l_1 y_1(k) + l_2 y_2(k))] = 0 \tag{9}$$

and

$$\lim_{N\to\infty} \frac{1}{N}\sum_{k=1}^{N} \sin[2\pi(l_1 y_1(k) + l_2 y_2(k))] = 0 \tag{10}$$

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

**4.3 Optimisation Problem Formulation**

The goal is to design an input signal, which 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 strongly interactive multivariable systems [29]. This assumes *a priori* knowledge of the plant model either as an equation or a computer program that is available to the optimiser. For simplicity of presentation, we consider that input $u(k)$ and output $y(k)$ as vectors with two components; this corresponds to the dimensions of a case study presented later.

To meet the objectives of plant friendliness we need to impose bound constraints on both $u(k)$ and/or $y(k)$. Here, $z$ is one of $y_1$, $y_2$, $u_1$, $u_2$.

$$|z(k)| \le C_z \qquad k = 0, \ldots, N_s - 1 \tag{11}$$

where $C_z$ are user defined constants. Since a multisine is a periodic signal it needs to be applied over one cycle length $N_s$. Also, there should be restrictions on the move size of $u(k)$ and $y(k)$, which is the difference between successive values in $u(k)$ and $y(k)$. Therefore, the following constraints are imposed

$$|z(k+1) - z(k)| \le \Delta C_z \quad k = 0, \dots, N_s - 1 \tag{12}$$

Again, $\Delta C_z$ 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 represented as

$$y_1(k) = f_1(u_1, u_2, y_1, y_2) \qquad k = 0, \dots, N_s - 1 \tag{13}$$

$$y_2(k) = f_2(u_1, u_2, y_1, y_2) \qquad k = 0, \dots, N_s - 1 \tag{14}$$

where 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 $y_2$. The inputs $u_1(k)$ and $u_2(k)$ are chosen per the multisine structure

$$u_j(k) = \sum_{i=1}^{(m+1)n_s} \sqrt{2\alpha_{ij}} \cos\left(\frac{2\pi i}{N_s} k + \phi_{ij}\right) \tag{15}$$

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

$$\alpha_{ij} = \begin{cases} \ge 0, \; i = j, (m+1)+j, \dots, (m+1)(n_s - 1) + j \\ \ge 0, \; i = m+1, 2(m+1), \dots, n_s(m+1) \\ = 0, \text{ for all other } i \text{ upto } (m+1)n_s \end{cases}$$

The goal is to uniformly distribute the points $(y_1(k), y_2(k))$ in the output state space region $\left[-C_{y_1}, C_{y_1}\right) \times \left[-C_{y_2}, C_{y_2}\right)$. The Weyl's criterion is used to achieve this uniform distribution. Since the Weyl's criterion deals with uniform distributions in $[0, 1)^2$, a change of variables is introduced

$$\hat{y}_1(k) = \frac{y_1(k) + C_{y_1}}{2C_{y_1}}, \quad \hat{y}_2(k) = \frac{y_2(k) + C_{y_2}}{2C_{y_2}} \tag{16}$$

Since there are only a finite number of points in the sequences, an integer $L$ is chosen and the set S is formed as

$$S = \{x : x \in Z \text{ and } |x| \le L\} \tag{17}$$

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

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

Then we try to minimise the sum in Eqs. (9) and (10) for all elements of the set $W$. The optimisation is carried out to estimate the amplitudes and phases $\alpha_{i1}$, $\alpha_{i2}$, $\phi_{i1}$, $\phi_{i2}$, $i = 1, \dots, (m+1)n_s$ of the $m = 2$ multisine input channels. The complete problem statement is

$$\min_{\alpha_{i1}, \alpha_{i2}, \phi_{i1}, \phi_{i2}} t \tag{18}$$

such that

$$\sum_{k=0}^{N_s - 1} \cos[2\pi(l_1 \hat{y}_1(k) + l_2 \hat{y}_2(k))] \le t, \forall (l_1, l_2) \in W$$

$$\sum_{k=0}^{N_s-1} \sin[2\pi(l_1\hat{y}_1(k) + l_2\hat{y}_2(k))] \le t, \forall(l_1, l_2) \in W$$

$$t \ge \varepsilon$$

as well as subject to constraints as per Eqs. (11) to (16). The lower-bound constraint on $t$ is imposed to promote faster convergence and ε is chosen to be some small positive constant.

Pendse [18] and Rivera et al. [30] have presented experiments that show the influence of design variables $L$ and ε on the distribution of points in the output state space.

The constrained optimisation problems described in this paper were solved by programming them in the modelling language AMPL, which has built-in automatic differentiation upto second order derivatives. The Weyl equations are continuously differentiable and, therefore, the optimiser can make direct use of second derivative information. The optimiser used was KNITRO, which has been developed by Byrd et al. [31]. KNITRO is an interior point trust region SQP solver and is suitable for solving both large and small problems.

### 4.4 Case Study: Nonlinear High-Purity Distillation Process

***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 [25] is commonly used as a benchmark problem for this type of application [32]. 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. Such an approach has been presented by Lee, Rivera and Mittelmann [33] and lee [34], who have applied an optimisation approach that minimises the crest factor (CF), the ratio of the $\ell_\infty$ (or Chebyshev) norm and the $\ell_2$-norm of a signal $x$ [35]. A low CF indicates that most of the elements in the sequence are distributed near their extremum values. Design parameters for the Weischedel-McAvoy problem that are determined on the basis of the guidelines as per Lee, Rivera and Mittelmann [33], using dominant time constant estimates ($\tau^L_{\mathrm{dom}} = 5$ and $\tau^H_{\mathrm{dom}} = 20$ min) and user choices of $\delta = 0$, $\alpha_s = 2$ and $\beta_s = 3$, lead to parameter settings of $T = 2$ min, $n_s = 189$ and $N_s = 378$. Table 1 summarises the constraints applied to the problem and salient characteristics of the signals considered (min CF($u$), min CF($y$) and Weyl data-centric). The value of the amplification factor for the correlated harmonics $\gamma = 15$ was chosen for a min CF($y$) signal with modified spectrum. The resultant input spectrum for this signal is shown in Fig. 2(a). The output state-space plot is shown in Fig. 3(a).

A significant benefit of an optimisation-based problem formulation for input 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 Auto-Regressive with eXternal (NARX) input model with the structure proposed by Srinivas et al. [32] is

$$y(k)=\theta^{(0)}+\sum_{i=1}^{n_y}\theta_i^{(1)}y(k-i)+\sum_{i=\rho}^{n_u}\theta_i^{(2)}u(k-i)+\sum_{i=1}^{n_y}\sum_{j=1}^{i}\theta_{(i,j)}^{(3)}y(k-i)y(k-j)$$

$$+\sum_{i=\rho}^{n_u}\sum_{j=\rho}^{i}\theta_{(i,j)}^{(4)}u(k-i)u(k-j)+\sum_{i=1}^{n_y}\sum_{j=\rho}^{n_u}\theta_{(i,j)}^{(5)}y(k-i)u(k-j)+\ldots \qquad (19)$$

It was obtained 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.

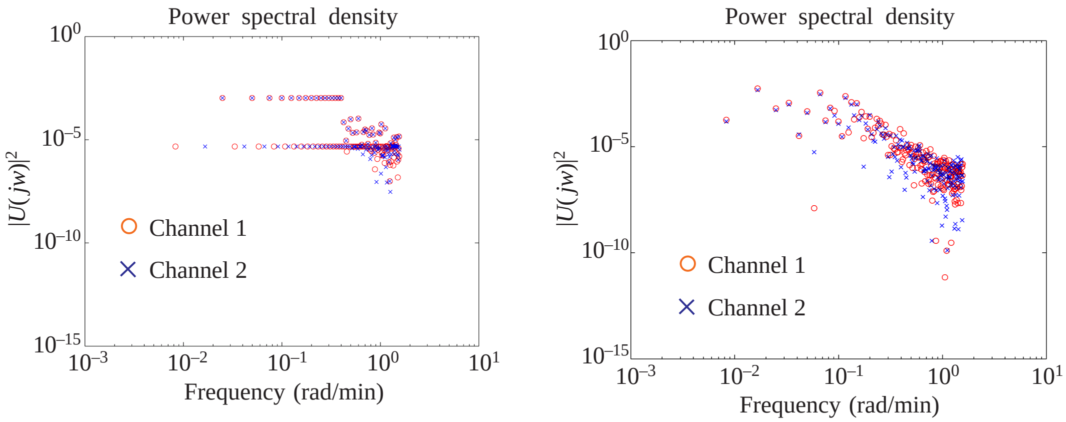
The benefits of the Weyl-based formulation over the minimum crest factor signal design in producing a uniform distribution in the output state-space of the data can be clearly seen in Figs. 3a and 3b. The use of Weyl's criterion results in a much more uniformly distributed coverage of the state-space, 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. Table 1, however, shows that the improvement in output state-space uniformity is obtained at the cost of higher crest factor that, 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 recognised. 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 optimisation framework described in this paper.

An important difference between these signal designs is observed in the input spectra (Fig. 2). 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 optimiser, while for the Weyl-based design, the optimisation problem includes a search for *all* Fourier coefficients and phases, including those corresponding to the correlated harmonics (Fig. 2(b)). These extra degrees of freedom in the

**Table 1. Description and results of multisine signals designed for the Weischedel-McAvoy distillation column case study**

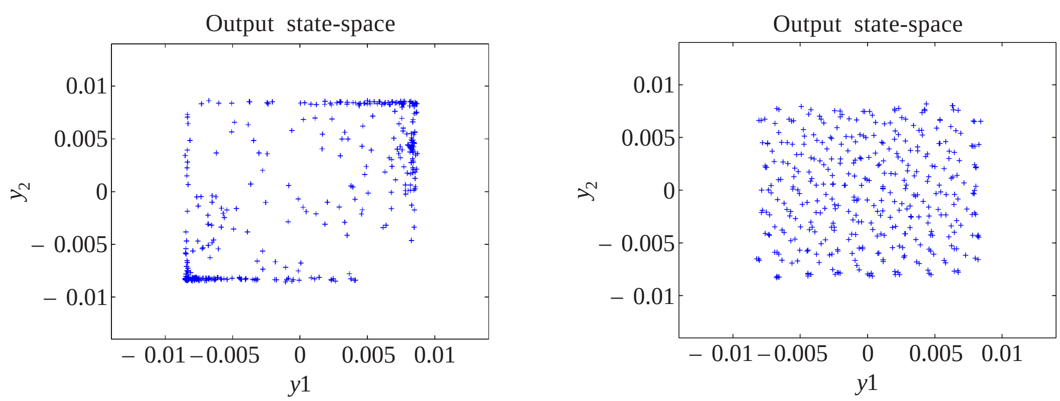
| Type | Signal ($x$) | CF ($x$) | PIPS (%) | max $\Delta x$ | max $x$ | min $x$ |
|---|---|---|---|---|---|---|
| min CF ($u$) design; standard zippered spectrum | $u_1$ | 1.21 | 82.43 | 0.0025 | 0.0020 | – 0.0020 |
| | $u_2$ | 1.22 | 81.77 | 0.0026 | 0.0020 | – 0.0020 |
| | $y_1$ | 2.48 | 48.84 | 0.0037 | 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 $\|\Delta u\| \le 0.01$, $\|\Delta y\| \le 0.008$ and $\|y\| \le 0.0085$ | $u_1$ | 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 Weyl design using NARX model via a modified zippered spectrum subject to $\|\Delta u\| \le 0.01$, $\|\Delta y\| \le 0.08$ and $\|y\| \le 0.0085$ | $u_1$ | 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 |

optimiser not only contribute to the improved performance, but also reduce the number of decisions made *a priori* by the user, leading to a more practical design procedure.




(a) min CF($y$) (b) Weyl-based approach

**Fig. 2. Power spectral densities for input signals for the Weischedel-McAvoy distillation column: (a) min CF($y$) vs. (b) Weyl-based design.**




(a) min CF ($y$) (b) Weyl-based approach

**Fig. 3. Output state-space plots for Weischedel-McAvoy distillation column: (a) min CF($y$) vs. (b) Weyl-based design.**

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

Firstly, open-loop MoD estimation is evaluated for the Weischedel-McAvoy distillation column using the data arising from the signal designs (Table 1) for estimation purposes. For validation purposes, a different data-centric signal with lower magnitude bounds was considered, which has been given by Lee [34]. For all cases, an implicit NARX structure with [$n_a = 1$, $n_b = 1$, $n_k = 1$] is used in the MoD estimator. A local polynomial order, as per Eq. (5) and limits on the database size $k_{min}$ = 20 and $k_{max}$ = 756 serve as additional parameters [36].

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 low gain direction, it results in the poorest prediction on the validation data set (Table 2). 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 percentage unexplained variance of 0.5% (Table 2). 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 percentage unexplained variance close to 0.09% (Table 2).

**Table 2. Summary of open-loop cross validation results for the Weischedel-McAvoy distillation column case study**

| Type | Signal ($y$) | RMS | Eval. (%) |
|---|---|---|---|
| min CF ($u$) design; standard zippered spectrum | $y_1$ | 1.5246 | 1011003.038 |
| | $y_2$ | 3.2170 | 1803825.964 |
| min CF($y$) design; modified zippered spectrum | $y_1$ | 0.0002316 | 0.422 |
| | $y_2$ | 0.0002550 | 0.531 |
| Data-centric Weyl design | $y_1$ | 0.0001018 | 0.090 |
| | $y_2$ | 0.0001070 | 0.093 |

The min CF($y$) and Weyl-based MoD models are, subsequently, evaluated in a closed-loop setting using the MoD-MPC toolbox [37]. Results for the min CF($u$) MoD model are not shown because a stable controller response could not be obtained. In both cases the tuning parameters are $p_h$ = 35, $m_h$ = 15, $Q_e$ = [1 0; 0 1] and $Q_{\Delta u}$ = [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 Fig. 4. 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.

### 4.5 Solving the Optimisation Problems

Since the control problems, described earlier, mainly serve as a source for difficult nonlinear optimisation problems (NLPs), some details on their computational solution are given. Just as in an earlier section on PDE-constrained problems, the resulting NLPs were integrated into the benchmarking effort [8] and, consequently, the AMPL files for these problems were also made available. The models used for the minimum crestfactor and Weyl-based NARX formulations of the system identification problems are accessible [14], but they are too lengthy to be quoted here. It is clear, however, that there is no principal difficulty. In both cases, a scalar variable is minimised

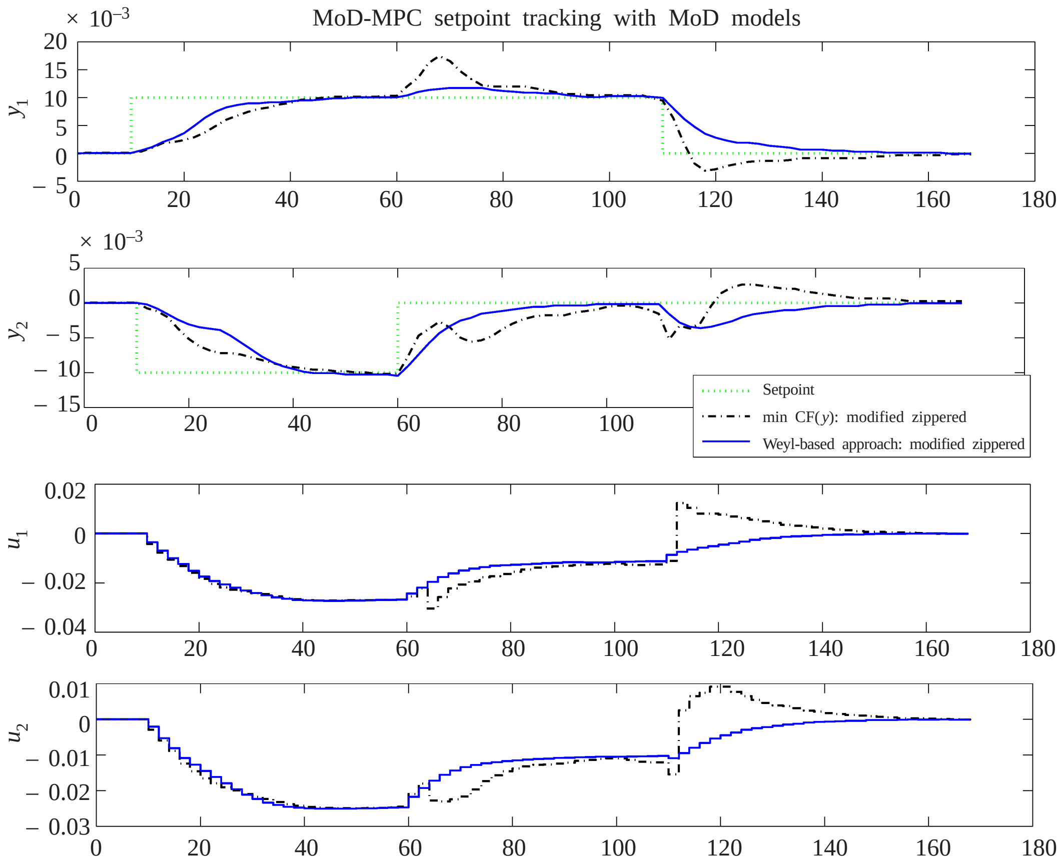



**Fig. 4. MoD-MPC closed-loop setpoint tracking test on the Weischedel-McAvoy distillation column using MoD models from the min CF ( *y*) signal (dashed) and Weyl-based (solid) signal designs. Controller parameters are $p_h$ = 35, $m_h$ = 15, $Q_e$ = [1 0; 0 1] and $Q_{\Delta u}$ = [7 0; 0 7].**

and everything is moved into the constraints. An excerpt from the benchmark tables [14] is given as follows:

| Problem | nv/nc | IPOPT | KNITRO | LOQO | SNOPT |
|---|---|---|---|---|---|
| NARX_CFy | 43973/46744 | 624 | 235 | fail | t |
| NARX_Weyl | 44244/45568 | fail | 3893 | fail | t |

nv/nc: number of variables/constants; t: time exceeded (2 h)

Here, IPOPT [38] and LOQO [39] are two other well-known interior point methods, while SNOPT [40] is a SQP method. The user seconds on a 3.2 GHz P4 are also given. It can be seen that the dimensions of the solved NLPs are substantial, but not large by today's standards. KNITRO is the only code solving both problems in a few minutes respectively in less than two hours.

## 5. Conclusion

This paper gives an overview of three services provide for free to the community: (i) a guide for optimisation software, (ii) a performance comparison of such software, and (iii) interactive, web-based solvers for a variety of optimisation problems. Two classes of control-related problems were also described, one from the control of partial differential equations and the other from system identification. The latter was accomplished in two different ways by: (i) minimising the CF of the signals and (ii) applying a geometric equidistribution criterion. The latter is found to be advantageous for MoD control purposes. Details and references from literature are given on the numerical realisation in the PDE-constrained case, as well as on the performance of state-of-the-art software for the examples from system identification. All the results are also integrated into the service efforts described at the beginning of the paper. While several codes failed on the two system identification problems, at least one code solved both reliably and in reasonable time.

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