GENERATING MULTIDIMENSIONAL RESPONSE SURFACES FROM PROCESS DATA Finding Optimal Set Points for Machine Control

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1 INTRODUCTION

Technical processes, notably in the power transforming domain, continuously produce a large series of data at a given sampling rate determined by a time interval $\Delta t > 0$. At any particular time assume there are M records given, organized into a time stamp, n independent (or state) variables and m dependent (or response) variables. These fields are summarized in the n- and m-dimensional vectors xand v. For instance, when monitoring power generating systems such gas turbines, there are up to 1200 signals monitored simultaneously, comprising ambient conditions, pressures, temperatures, mass flows, guide vane angles, vibration amplitudes in various channels etc. Not all of those, of course, find their place in physical models, which are usually dominated by thermodynamics, but reveal a lot of information about the system, worthwhile to be exploited.

Therefore, whether or not there is a physical model expressing y – or, rather, its expected value – in terms of x, it is always useful and sometimes

necessary to estimate the functional dependence, using process data only.

With such a functional dependence established, a multitude of applications in system control, process optimization and experimental design come into view.

It is the goal of this paper to show that there is a class of functions, called linear combinations of Gaussian shapes below, which allow to approximate an arbitrary cloud of points precisely and can be differentiated continuously infinitely often. This property is conducive to many tasks in mathematical optimization and machine control, as shown below.

2 MODEL

Let this functional relationship be described by a function *y*, where

$$y = f(x) + \varepsilon \tag{1}$$

$$f: \mathbb{R}^n \to \mathbb{R}^m \tag{2}$$

and \mathcal{E} , for the sake of simplicity, is assumed to be a

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Mergenthaler W., Feller J., Mauersberg B. and Chevalier R.

GENERATING MULTIDIMENSIONAL RESPONSE SURFACES FROM PROCESS DATA - Finding Optimal Set Points for Machine Control. DOI: 10.5220/0003408703970404

In Proceedings of the 8th International Conference on Informatics in Control, Automation and Robotics (ICINCO-2011), pages 397-404 ISBN: 978-989-8425-74-4

random vector with

$$E[\varepsilon] = 0, Cov[\varepsilon] = I_{nxn}$$
(3)

Figure 1 shows, in the special case of n=2 and m=1, a practical example of a response surface:



Please note that the data underlying this figure as well as the following figure are arbitrarily selected from among the authors' pool of data and only serve the purpose to explain principles.

Figure 2 shows a schematic idealization:



Figure 2: Schematic Idealization.

There is one – particularly important – example for the use of response surfaces in controlling industrial processes. Assume that in a fossil power plant such as a gas turbine, two of the response variables are given by the power output and the NO_x emissions, while one particularly important independent variable is the gas inflow. It may then be of interest to find that particular input variable $x^* \in \mathbb{R}^n$ which maximizes power output given gas inflow and an upper limit on the NO_x emissions or minimizes gas inflow for given power output and - again - an upper limit on the NO_x emissions etc. In other words, one is interested in maximizing efficiency for given power output under additional conditions. This optimal value can be found in a twofold procedure, whereby the first step consists in finding the m response surfaces corresponding to the m response variables given by formula (1) and the second step is expressed as

$$Max_{x \in \mathbb{R}^n} f_1(x) \tag{4}$$

such that

$$f_2(x) \le g \tag{5}$$

and

$$f_3(x) \le f_0 \tag{6}$$

where $f_1(x)$, $f_2(x)$, $f_3(x)$, p and f_0 are power output, gas inflow, emissions, gas available and emission limit, respectively.

In a third step, whenever a process is in a state $x \in \mathbb{R}^n$ a sequence of "control variables" must be found, which drives the process towards the optimal state $x^* \in \mathbb{R}^n$.

In this paper it is shown how to find the functional relationship f, how to use this in order to find an optimal operating point under given constraints and how to use the optimal operating point in an adaptive control policy. An example concludes this research.

It is to be noted that the time dependency between signal records plays no role in this paper, because, in finding optimal operating points, as well as regression with given input variables as arguments, time is not used as a regressor. Therefore time series analysis as expressed in ARMA or ARMAX techniques (Bhattacharya, 2009) remains in the background.

3 FINDING THE RESPONSE SURFACE

This step asks for the solution of a certain type of multidimensional approximation problem, wherein - simultaneously - m real functions of n real variables are to be approximated.

3.1 The Least Squares Principle

The method suggested in this paper uses the least squares principle where the objective function is to be minimized by an appropriate selection of the function f. While classical response surface

$$Z(f) := \sum_{i=1}^{M} \left\| y_i - f(x_i) \right\|_2$$
(7)

methodology mostly works with quadratic forms of the response variable with respect to the input variables, see for instance (Myers, 2009) and (Oezer, 2004), in this paper f is to be selected from among the more general set of twice continuously differentiable functions mapping \mathbb{R}^n onto \mathbb{R}^m . From the practical point of view this requires an idea about the functional dependence of f(x) on $x \in \mathbb{R}^n$. Once this functional relationship is established and expressed in a formula with appropriate parameters, minimization over the function space is reduced to minimization over the appropriate parameter space.

3.2 Linear Combinations of Gaussian Shapes

A possible choice for the functional relationship is an element-wise linear combination of Gaussian shapes such that

$$f(x) := f(x; c, \mu, A) := \sum_{j=1}^{m} e_j f_j(x) :=$$

$$:= \sum_{i=1}^{m} e_j \sum_{k=1}^{N^{(j)}} c_k^{(j)} e^{-(x-\mu_k^{(j)})^T A_k^{(j)}(x-\mu_k^{(j)})}$$
(8)

In (8) e_i is the unit vector in *j*-direction, $N^{(j)}$ is the number of Gaussian shapes used in approximating $f_i(x), c_k^{(j)}, k \in \{1, ..., N^{(j)}\}$ is the height of the k-th shape for the corresponding element, $\mu_k^{(j)}$ is the corresponding location vector and $A_k^{(j)}$ the corresponding shape matrix. The symbols c, μ and A are abbreviations as explained in the appendix. An additional stipulation is that the matrices $A_k^{(j)}$ are required to be positively definite. Moreover, with this choice of functional representation, one works with functions that are infinitely often - not just twice - continuously differentiable. Also these functions tend towards zero with either of its arguments going to infinity, having no poles or wild erratic oscillations and therefore, being less prone to overfitting the data.

Expanding the Euclidean norm in (7) it can be seen that

$$Z(f) = \sum_{j=1}^{m} Z_{j}(f_{j}) \text{ with}$$

$$Z_{j}(f_{j}) \coloneqq \sum_{i=1}^{M} (y_{i}^{(j)} - f_{j}(x_{i}))^{2} =$$

$$\sum_{i=1}^{M} (y_{i}^{(j)} - \sum_{k=1}^{N^{(j)}} c_{k}^{(j)} e^{-(x_{i} - \mu_{k}^{(j)})^{T} A_{k}^{(j)}(x_{i} - \mu_{k}^{(j)})})^{2},$$

$$j \in \{1, ..., m\}$$

$$(9)$$

The minimization method for the objective function amounts to solving separately m individual minimization problems with the objective functions $Z_j(f_j)$. Each of these minimization problems requires finding values for the decision variables

$$N^{(j)} \in \{1, ..., M\}$$

$$c_{k}^{(j)} \in R$$

$$\mu_{k}^{(j)} \in R^{n}$$

$$A_{k}^{(j)} \in R^{n^{2}}$$

$$k \in \{1, ..., N^{(j)}\}$$

$$j \in \{1, ..., m\}$$
(10)

Since $N^{(j)}$ is a discrete parameter and all other parameters are real, the minimization problems are mixed integer real. Therefore, if derivative based, non-linear minimization techniques are to be used such as Fletcher-Reeves etc., see (Press, 2007), one must resort to a trick, whereby $N^{(j)}$ is deliberately given a sufficiently high value and it is left to the height variables $c_k^{(j)}$ to emphasize and eventually eliminate one or the other of the Gaussian shapes. Even if this trick works, there is always the risk of being trapped in a local minimum.

Both problems can be overcome simultaneously by using a local search technique such as Simulated Annealing, for instance, see (Press, 2007) and (Rayward-Smith, 1996).

It is important to note that for each input dataset

$$(x_i, y_i) \in \mathbb{R}^n \times \mathbb{R}^m, i \in \dots, M$$
(11)

there is a representation (8) which approximates the response variables to any desired degree of precision, the exact proof of which is very technical and will be omitted here. The proof follows along the following lines, however: For each response variable one begins with M shapes, each as high as the corresponding response variable and located right at the corresponding input point, with an arbitrary shape matrix. The shape matrices are then narrowed down consecutively until for each shape, the impact of remote shapes is small enough to satisfy the precision requirement.

3.3 A Note on Overfitting

Like any approximation problem on the real line, it is necessary to limit the risk of overfitting by checking the goodness of fit of the minimization routine on a validation set of points, which are not used in tuning the model parameters. This task is currently in progress between the authors.

4 FINDING THE OPTIMAL POINT ON THE RESPONSE SURFACE

In contrast to (Ribeiro, 2010) the analysis described in the present paper considers only one response variable, which determines the optimal operating point, while more than one response variable may appear in the constraints.

This step will be analyzed under the two different scenarios of unconstrained and constrained optimization.

4.1 Unconstrained Optimization

Assume that one arbitrary response variable

$$j^* \in \{1, \dots, m\}$$
 (12)

is to be maximized, i.e.

$$f_{j^*}(x^*) = Max_{x \in R^n} f_{j^*}(x)$$
(13)

Two special cases must be considered. In case 1 one assumes that $N^{(j)}=1$. Then, due to the positive definiteness of the shape matrices as required above and the monotonicity of the natural logarithm, maximizing $f_{j*}(x)$ with respect to x is equivalent to minimizing

$$\alpha(x) := (x - \mu_1^{(j^*)})^T A_1^{(j^*)} (x - \mu_1^{(j^*)})$$
(14)

which yields the simple result

$$x^* = \mu_1^{(j^*)} \tag{15}$$

In case 2, i.e. whenever $N^{(i)} > I$, one must either use a non-linear search technique with several randomized starting points or a local search technique. In view of (15), a plausible choice for the starting point may be

$$x_{0} = \frac{\sum_{k=1}^{N^{(j^{*})}} c_{k}^{(j^{*})} \mu_{k}^{(j^{*})}}{\sum_{k=1}^{N^{(j^{*})}} c_{k}^{(j^{*})}}$$
(16)

There is a variety of such search techniques, as can be seen in (Press, 2007) and (Speyer, 2010), for example. However, simple application of the first order necessary conditions of any optimal point to $f_{j*}(x)$, i.e.

$$\nabla f_{j^*}(x) = 0 \tag{17}$$

yields, along with (8), the following equation:

$$x = H_j(x)^{-1} * b_j(x)$$
(18)

with

$$H_{j}(x) \coloneqq \sum_{k=1}^{N^{(j)}} c_{k}^{(j)} e^{-(x-\mu_{k}^{(j)})^{T} A_{k}^{(j)}(x-\mu_{k}^{(j)})} A_{k}^{(j)}$$

$$b_{j}(x) \coloneqq \sum_{k=1}^{N^{(j)}} c_{k}^{(j)} e^{-(x-\mu_{k}^{(j)})^{T} A_{k}^{(j)}(x-\mu_{k}^{(j)})} A_{k}^{(j)} \mu_{k}^{(j)}$$
(19)

Observing that in (18) the right hand side depends on x as well, one may try to find an iterative expression with

$$x^{(k)} = H_j(x^{(k-1)})^{-1} * b_j(x^{(k-1)})$$

k = 1,2,3... (20)

hoping, for the time being, that $H_j(x)$ is invertible and (20) represents a contracting map. (20) may be generalized to the case of constrained optimization using the Lagrange function or a penalty term. In any case observe, that it bears a certain resemblance to the quadratic programming problem.

4.2 Constrained Optimization

As a representative of the multitude of potential constrained optimization problems assume that one must maximize a particular response variable j^* while all the other ones are to stay within a certain upper limit, which amounts to solving the following minimization problem:

$$Min_{x \in \mathbb{R}^{n}} (-f_{j^{*}}(x))$$

$$f_{j}(x) \leq f_{0,j}, j \in \{1, ..., m\} - \{j^{*}\}$$
(21)

Introducing a slack variable

$$\xi_i \in R^{m-1} \tag{22}$$

one easily sees that solving (21) is equivalent to solving a non-linear minimization problem with the following Lagrangian:

$$L(x;\lambda) = (-f_{j^*}(x)) + \sum_{\substack{j \in \{1,\dots,m\} - \{j^*\}}} \lambda_j (f_{0,j} - f_j(x) - \xi_j^{-2})$$
(23)

see (Speyer, 2010). Finding a solution to (23) with a derivative based non-linear minimization technique may be attempted by a large scale Sequential Quadratic Programming Problem such as described in (Gill, 2005), for instance.

However, in this situation local search heuristics can be used again by noting that the objective function $-f_{j*}(x)$ can be augmented by a penalty function which assumes increasingly high values, if the constraints

$$f_{j}(x) \le f_{0,j}, j \in \{1, \dots, m\} - \{j^{*}\}$$
(24)

are violated. The smallest such penalty function can then be used in the solution.

5 APPROACHING THE OPTIMAL POINT ON THE RESPONSE SURFACE

Assume that, at a certain time

$$t = l * \Delta t, l \in \{1, 2, 3, ...\}$$
(25)

throughout operation of the process under consideration, the process state is equal to

SCIENFERAND

with

$$\widetilde{x} \neq x^* \tag{27}$$

= (26)

indicating operation under sub-optimal conditions. It is then important to find a sequence of control variables

$$u_1 \in R^w, \dots, u_\tau \in R^w \tag{28}$$

for some

$$w \in \{1, 2, 3, \dots\}$$
(29)

and some

$$\tau \in \{1, 2, 3, \dots\}$$
(30)

5.1 Deterministic Case

Here one assumes that

$$x_{t} = \widetilde{x}$$

$$x_{t+1} = x_{t+1}(x_{t}, u_{1})$$
...
(31)

$$x_{t+\tau} = x_{t+\tau} (x_{t+\tau-1}, u_{\tau}) = x *$$

Assume there is a cost $\gamma(x_{t+k-1}, u_k)$ attached to the transition

$$x_{t+k-1}, u_k \to x_{t+k}, k \in \{1, ..., \tau\}$$
 (32)

The total transition cost is then given by

$$C(x_{t}, u_{1}, ..., u_{\tau}) \coloneqq \sum_{k=1}^{\tau} \gamma(x_{t+k-1}, u_{k})$$
(33)

As long as a transition law as given in (31) can be found, (33) can be - again - minimized using either non-linear minimization or local search.

5.2 Stochastic Case

Assume that the transition from x_{t+k-1} to x_{t+k} under the control u_k , $k=1,2,...,\tau$ takes place in a stochastic manner such that the distribution density of x_{t+k} is given by a density

$$g(z; x_{i+k-1}, u_k) : \mathbb{R}^{n+w} \to \mathbb{R}^n$$
(34)

The expected cost under the control policy $u_1,...,u_\tau$ is given by

$$C(x_{t}, u_{1}, ..., u_{\tau}) = \gamma(x_{t}, u_{1}) + \int_{\mathbb{R}^{n}} C(z, u_{2}, ..., u_{\tau}) g(z; x_{t}, u_{1}) dz$$
(35)

The optimal policy $u_1^*,...,u_\tau^*$ leading to the minimal expected cost $C^*(x_b,u_1^*,...,u_\tau^*)$ satisfies the Bellman equation

$$C^{*}(x_{t}, u_{1}^{*}, ..., u_{\tau}^{*}) = Min_{u_{1}^{*} \in \mathbb{R}^{w}} \{\gamma(x_{t}, u_{1}^{*}) + \int_{\mathbb{R}^{n}} C^{*}(z, u_{2}^{*}, ..., u_{\tau}^{*})g(z; x_{t}, u_{1}^{*})dz\}$$
(36)

see (Bhattacharya, 2009). The Bellman-equation can be solved by means of the classical dynamic programming approach and - again - by local search techniques such as Simulated Annealing.

6 EXAMPLE

The problem considered in this example consists in solving efficiency related optimization problems for an input file with n = 8 independent variables and m = 2 response variables. The two response variables considered are power output and NO_x emissions. M = 4560 records were available. The data correspond to a gas turbine in a French power plant. All of the signals have been normalized to values between 0.0 and 1.0 each.

As a constrained optimization problem Power output (response variable 1) will be maximized while a series of constraints, partly referring to gas inflow - one of the control variables - and partly referring to NO_x emissions (response variable 0) will be imposed. It will be shown that the data contained in the input file, when filtered with respect to those constraints, already exhibit some variance in response variable 1, without the smoothing effect brought about by response surface modelling.

6.1 Input Data

Figure 3 shows the time trajectory of the NO_x emissions throughout the time period under consideration:



Figure 3: NO_x emissions - Time Trajectory.

Figure 4 shows the time trajectory of the power output:



Figure 4: Power output - Time Trajectory.

6.2 Results

Results for this example are given for steps 1 and 2 only. Developing optimum control policies is ongoing research at this time.

6.2.1 Approximation

Figure 5 shows the goodness of fit for NO_x emissions as a result of the approximation:



Please note that - for ease of comparison - the approximated points have been ordered increasingly with respect to size and that the corresponding input values, i.e. those with equal input variables have been juxtaposed accordingly. Figure 6 shows the goodness of fit for the power output:



Figure 6: Power output - Goodness of Fit.

Figure 7 shows a three-dimensional representation of the empirical power output as contained in the input data as a function of the input variables 0 and 1 (Barometric pressure and Compressor inlet pressure, see below), whereby all the remaining input variables have been set equal to their respective midpoint between minimum and maximum:



Figure 7: Three-dimensional representation of empirical power output with respect to control variables 0 and 1.

Figure 8 is the analogous representation with the empirical power output replaced by its theoretical counterpart obtained from approximation:



Figure 8: Three-dimensional representation of theoretical power output with respect to control variables 0 and 1.

The good visual agreement between figures 7 and 8 is another view on the goodness of fit as shown in figure 6.

6.2.2 Efficiency Maximization

Optimization Problem

The problem considered was to maximize Power output under the following constraints:

- Compressor Discharge Pressure >= 97% of Maximum
- NO_x emissions $\leq 40\%$ of Maximum
- IGV guide angle >= 99,90% of Maximum
- Liquid Fuel Mass Flow <= 93% of Maximum
- Water Injection flow <= 89,4% of Maximum

Input Data Filtered with Respect to Constraints

Table 1 shows the subset of input data resulting from filtering the records with the constraints as shown above:

Table 1: Input data filtered with respect to constraints.

		Com			Com		Com-	Liquid	Water In-		
	Baro-	pressor		Ambient	pressor	IGV	Inlet	Fuel	Flow from		
	metric	Inlet	Specific	Pressure	Discharge	Angle	Thermo-	Mass	Feed-	NO _x e-	Power
Time	Pressure	Pressure	Humidity	Absolute	Pressure	In Deg	couple	Flow	back	missions	Output
09.09.2010 21:06	0,9973	0,9350	0,5960	0,9973	0,9702	0,9998	0,8076	0,9128	0,8584	0,2528	0,9177
09.09.2010 22:36	0,9969	0,9437	0,5167	0,9969	0,9721	0,9998	0,8078	0,9085	0,8807	0,2500	0,9045
09.09.2010 23:59	0,9958	0,9453	0,5377	0,9958	0,9723	0,9999	0,7967	0,9006	0,8598	0,2566	0,8997
10.09.2010 00:20	0,9971	0,9674	0,5474	0,9972	0,9794	0,9999	0,7888	0,9157	0,8893	0,2595	0,9140
10.09.2010 01:33	0,9975	0,9598	0,5531	0,9975	0,9820	1,0000	0,7971	0,9097	0,8824	0,2586	0,9191
10.09.2010 10:51	0,9943	0,9469	0,6247	0,9943	0,9708	0,9999	0,8208	0,9237	0,8686	0,2632	0,9161
10.09.2010 16:00	0,9912	0,8836	0,6122	0,9912	0,9700	0,9996	0,8395	0,9106	0,8820	0,2603	0,9004
11 09 2010 17:41	0.9897	0.8855	0.6118	0 9897	0.9696	0 0008	0.8387	0.9228	0.8861	0.2500	0.9070

Table 1 reveals that already within the filtered dataset power output shows a variance of roughly 2% with respect to the maximum value of 1.0, keeping the normalized range of values in mind, as illustrated in figure 9:



Figure 9: Variance in power output in the filtered dataset.

Optimization Results

Table 2 shows the mathematical solution to the optimization problem stated above with respect to both input variables and response variables:

Table 2: Optimization Results.

Signal	Empirical	Optimized	Sensitivity
Flow Inlet Barometric Pressure			
Transducer 96AP	0,99751004	0,99486034	0,139069565
Compressor Inlet Pressure Transducers			
96CS	0,95978566	0,94267898	-0,057540515
Specific Humidity	0,55309196	0,61269545	-0,098797211
Ambient Pressure Absolute	0,99750943	0,99415204	-0,204402616
Compressor Discharge Press Max			
Select	0,98198534	1	0,463754606
IGV angle in deg	0,99995594	0,9985449	-0,112380787
Compressor Inlet Thermocouple 1A	0,79710736	0,82604766	0,124270994
Liquid Fuel Mass Flow	0,90968848	0,92701868	1,040617104
Water Injection Flow from Feedback	0,88235664	0,89457165	-1,376676057
Power Out:	0,91913895	0,95004047	
NO _x emissions	0,25855153	0,26226289	

The following comments must be made in order to properly interpret these results:

- The column titled Empirical lists the values of all the input variables corresponding to that particular record in the filtered input file - see table 1 - with maximum overall power output.
- This goes along with an NO_x emission value of 25.85 % of the maximum as shown in the corresponding line and 91.91% of maximum power.
- The column titled **Optimized** lists the values of the input variables corresponding to the solution of the constrained optimization problem. It can

be noted that all of the constraints are satisfied to a good degree of precision:

- Compressor Discharge Pressure = 100% >= 97% of maximum
- NO_x emissions = 26,23% <= 40% of maximum
- IGV angle = 99.85% <= 99.9% required
- Liquid Fuel Mass Flow = 92.70% of maximum versus <= 93% required
- Water Injection flow = 89,45% of maximum versus 89,4% required
- Yet there is a theoretical increase in the Power output of approximately 3.09%=95.00%-91.91%. Comparison of the ratio of Power output divided by Liquid Fuel Mass Flow reveals an efficiency increase from the optimal element in the filtered dataset to the mathematical solution of the constrained optimization problem of 1.43%.
- The column titled Sensitivity is the partial derivative of the Power Output with respect to the input variable in question, averaged over the input space using the sample of input data.
- It must be noted that the solution to the optimization problem must be verified against the criteria of technological feasibility. For instance, turbine inlet temperature must not exceed a fixed value and no optimal operating point must violate this additional constraint.

7 SUMMARY

The present paper presents a technique to generate Gaussian response surfaces from high dimensional data and shows how to use them to find optimal operating points with respect to process characteristics such as Power output, NO_x -emissions, gas inflow etc.

There are two sources of optimization to be expected through an industrial application of such surfaces:

- Finding true optima by removing noise in the data and appropriate smoothing
- Consistently using those optima as set points in the context of adaptive control.

From the authors' point of view, many of the topics considered in this paper will be central to future research in the power industry around the world, such as

• Fast optimization techniques in finding the response surfaces, using a combination of non-linear and local search techniques

- Fast optimization techniques to find the optimal points on the response surfaces
- Embedding the algorithms inside machine control hardware and software to name just a few.

ACKNOWLEDGEMENTS

Our thanks go to our co-workers Sebastian Feller, Yavor Todorov and Dirk Pauli for valuable hints in numerical optimization techniques and to Tina Condon for careful proof reading.

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APPENDIX

Definition of c, μ and A:

$$c := \{c_k^{(j)}, k \in \{1, ..., N^{(j)}\}, j \in \{1, ..., m\}\}$$
$$\mu := \{\mu_k^{(j)}, k \in \{1, ..., N^{(j)}\}, j \in \{1, ..., m\}\}$$