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The Journal of the Operational Research Society, Volume 41, Issue 12 (Dec., 1990),
1161-1167.

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The Journal of the Operational Research Society
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Simultaneous Optimization in Process Quality Control via Prediction-interval Constrained Programming

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A challenging problem in process control is the selection of input levels which will produce desirable output quality. This problem is complicated by the unsure relationships of cause and effect and by the trade-offs between meeting conflicting output specifications. This paper proposes a new approach, which incorporates prediction-interval constraints into a goal-programming model. A process-control problem, originally solved by the desirability-function approach, is solved using this new model. Comparisons between the two approaches are discussed.

Key words: chance-constrained programming, multi-objective optimization, process control, quality control

INTRODUCTION

Output quality is usually measured by predetermined quality specifications in different dimensions. One difficulty in selecting input levels is the problem of trade-offs among different dimensions of the quality specifications. Quality in one dimension may be improved at the cost of quality in another. Another problem in process quality control is to find the functional (cause-effect) relationship between input variables and output quality (response) variables. When the functional relationship is known and deterministic, the levels of input variables can be precisely specified in order to produce outputs with desirable quality. Deterministic optimization techniques can be used to obtain optimal levels for the input variables. Hartmann and Beaumont¹ and Nicholson and Pullen² used linear programming (LP) to optimize one quality variable subject to constraints on the remaining quality variables.

However, quite often the functional relationship between input and quality variables can only be estimated by statistical approaches, such as sampling or regression analysis, because the exact relationship is not known. In these cases, owing to random variation, deterministic optimization techniques are not valid. Optimization, by its nature, yields extreme solutions which are likely to result in a high degree of risk of not meeting quality specifications.

Chance-constrained programming (CCP) was developed to optimize linear systems with uncertain coefficient values. Stochastic elements in the functional relationship, such as the variances and covariances caused by sampling, are incorporated into the chance (or probability) constraints, to control the risks of violating the specifications.^{3,4} CCP allows the decision-maker to specify a desired probability of satisfying specifications while seeking optimal objective-function values subject to that probability. However, when regression is used to estimate the functional relationship, the CCP model is not directly applicable. The additional variabilities introduced by the estimation of the least-squares line and the prediction of the response variables need to be considered. Olson *et al.*⁵ developed the prediction-interval constrained programming (PCP) model by replacing the variance term in the CCP model with the variance of the predicted value of the response variable in regression. An example using one quality variable was given in their paper.

To extend the prediction-interval constrained programming model from solving models with single response variables to solving models with multiple response variables, the present study incorporates prediction-interval constraints into a goal programming (GP) model. The next section reviews two conventional approaches that deal with the optimization of multiple-quality properties. A process-control problem, originally solved by the desirability-function approach, is solved using the proposed PCP-GP model. Finally, solutions of the two approaches are compared.

MULTIPLE-QUALITY PROPERTIES

Some complex quality-control problems require that multiple-quality specifications be satisfied simultaneously. These problems involve the balance of relative importance and possible conflicts among quality properties. Two approaches that have been used in process quality control concerning multiple-quality properties are reviewed in this section.

Desirability function approach

Harrington⁶ addressed the problem of optimizing the overall product quality among multiple-quality properties. He proposed the 'desirability' scale to reflect the decision-maker's utility about each quality property. Through appropriate transformation, every quality property can be converted to a unit-free desirability scale (d_i) ranging between 0 and 1. A $d_i = 0$ corresponds to a totally undesirable level of quality; hence, the product is not acceptable. On the other hand, a $d_i = 1$ represents a completely acceptable level of quality, so that any further improvement would not be necessary. The overall desirability (D) is defined to be the geometric mean of the component 'd's, as indicated by the following form:

$$D = (d_1 \times d_2 \times d_3 \times \dots \times d_k)^{1/k}.$$

If any of the quality properties are completely unacceptable ($d_i = 0$), then the overall desirability is unacceptable ($D = 0$). The impact of the desirability function is to emphasize the function that has the worst relative attainment. Derringer and Suich⁷ modified the functions used to transform quality properties to a desirability scale, and optimized the overall desirability function using a pattern search method. They applied the approach to a problem concerning the development of a rubber compound for tyre treads.

Goal-programming approach

Goal programming (GP) allows the decision-maker to specify a target for each objective function and rank the goals by priority level (Charnes *et al.*⁸). GP can be applied to solve quality-control problems with multiple-quality specifications. For example, Sengupta⁹ reported an application of GP in a paper-manufacturing factory. The input and output variables of the production process were modelled using regression, but the stochastic elements were ignored in model formulation. Failing to reflect the existence of these stochastic elements in a model would result in inadequate, misleading process-control limits. In this paper, we solve this problem by incorporating prediction-interval constraints into a GP model. For a problem that seeks the optimal input levels of n decision variables (X_j) in order simultaneously to satisfy m response variables (Y_i) with upper/lower specifications, the general model is given below:

$$\text{Minimize } Z = \sum_{i=1}^m P_i(w_i^+ d_i^+ + w_i^- d_i^-),$$

subject to

$$E[Y_i] + \Psi_b \{MSE(1 + X_p'(X'X)^{-1}X'_p)\}^{1/2} + d_{i1}^- - d_{i1}^+ = R_{i1} \quad (\text{upper limit}), \tag{1}$$

$$E[Y_i] - \Psi_b \{MSE(1 + X_p'(X'X)^{-1}X'_p)\}^{1/2} + d_{i2}^- - d_{i2}^+ = R_{i2} \quad (\text{lower limit}), \tag{2}$$

where $i = 1, \dots, m$, plus any constraints on X_j , and $X_j, d_i^+, d_i^- \geq 0$, where

- P_i = the pre-emptive priority level;
- w_i = the weight associated within priority level i to the variable being minimized;
- d_i^+, d_i^- = the deviational variable selected for response variable Y_i ;
- $E[Y_i] = \hat{\beta}'_i X_p$, the expected value of response variables through regression;
- $\hat{\beta}'_i$ = the transposed vector of estimated beta coefficients from regression for variable Y_i (this vector must include the estimated intercept);
- X_p = the vector of the optimal levels of input variables $X_j, j = 1, \dots, n$ (this vector must include a '1');
- Ψ_b = the normal or t variate penalty value associated with a predetermined probability b ;
- X = the matrix of input variables used in fitting the regression model (this matrix must include a column of '1's for the intercept term of the regression);

- X' = the transpose of X ;
- $X'X$ = X' multiplied by X ;
- $(X'X)^{-1}$ = the inverse of the $X'X$ matrix;
- X'_p = the transpose of X_p ;
- MSE = the mean square error;
- R_i = the upper or lower bounds for quality variables.

Constraint sets (1) and (2) in the above model are the deterministic equivalents converted from the original chance-constraint sets

$$\text{Prob}(Y_i + d_k^- - d_k^+ = R_{i1}) \geq b, \quad i = 1, \dots, m \tag{3}$$

and

$$\text{Prob}(Y_i + d_k^- - d_k^+ = R_{i2}) \geq b, \quad i = 1, \dots, m \tag{4}$$

respectively.

EXAMPLE

A real-world problem concerning simultaneous optimization of multiple-response variables reported by Derringer and Suich⁷ is solved here to demonstrate the new PCP-GP model. The problem studied was to develop a tyre-tread compound with desired property specifications. The response (output) variables and the specifications are as follows:

Quality property	Notation	Specifications	Ideal level	Practical range	Weights
PICO abrasion index	Y_1	$120 < Y_1$	170	100	6
200% modulus	Y_2	$1000 < Y_2$	1300	600	1
Elongation at break	Y_3	$400 < Y_3 < 600$	500	200	3
Hardness	Y_4	$60 < Y_4 < 75$	67.5	15	40

For variables Y_1 and Y_2 , Derringer and Suich set ideal levels at 170 and 1300. For variables Y_3 and Y_4 , the most desirable values are 500 and 67.5, the midpoint between the upper and the lower limits in each variable. The practical range for Y_3 and Y_4 is defined as the distance between the upper and lower quality specifications. For variables Y_1 and Y_2 , this range is defined as twice the distance between the ideal level and the lower specification. As these ranges are widely divergent, weights are used to adjust the relative scales of these ranges before a goal-programming model is applied. The optimal combination of the following three ingredient (independent) variables was sought:

- X_1 = parts per hundred of hydrated silica level;
- X_2 = parts per hundred of silane coupling level;
- X_3 = parts per hundred of sulphur level.

The desirability-function solution

Derringer and Suich used a central composite design, i.e. a 2^3 -factorial augmented by star points and five replications at the centre, to generate the data (Table 1). These data were then fitted to polynomial regression models. Calculated from the regression models, the predicted values of each response variable (Y_i) were then transformed into a desirability index (d_i). The four d_i s were combined into a single overall desirability scale (D). A pattern search algorithm was then applied through various levels of X_i s to find the optimum value for D . The optimum combination of the three ingredients and the resulting levels of the quality properties are as follows:

$$\begin{aligned} X_1 &= 1.175 & Y_1 \text{ (PICO)} &= 129.5 \\ X_2 &= 51.45 & Y_2 \text{ (modulus)} &= 1300 \\ X_3 &= 1.866 & Y_3 \text{ (elongation)} &= 465.7 \\ & & Y_4 \text{ (hardness)} &= 68.0 \end{aligned}$$

TABLE 1. The data

Sample	X_1	X_2	X_3	Y_1	Y_2	Y_3	Y_4
1	0.7	40	2.8	102	900	470	67.5
2	1.7	40	1.8	120	860	410	65
3	0.7	60	1.8	117	800	570	77.5
4	1.7	60	2.8	198	2294	240	74.5
5	0.7	40	1.8	103	490	640	62.5
6	1.7	40	2.8	132	1289	270	67
7	0.7	60	2.8	132	1270	410	78
8	1.7	60	1.8	139	1090	380	70
9	0.38335	50	2.3	102	770	590	76
10	2.0165	50	2.3	154	1690	260	70
11	1.2	33.667	2.3	96	700	520	63
12	1.2	66.333	2.3	163	1540	380	75
13	1.2	50	1.4833	116	2184	520	65
14	1.2	50	3.1167	153	1784	290	71
15	1.2	50	2.3	133	1300	380	70
16	1.2	50	2.3	133	1300	380	68.5
17	1.2	50	2.3	140	1145	430	68
18	1.2	50	2.3	142	1090	430	68
19	1.2	50	2.3	145	1260	390	69
20	1.2	50	2.3	142	1344	390	70

The PCP-GP solution

Given the data in Table 1, the PCP-GP approach starts by running a linear regression model for each response variable against the independent variables. The results of these regressions are given in Table 2. The regression coefficients, together with the specifications, were then used to formulate the prediction-interval constraints for the response variables. Subject to the natural constraints that keep the decision (input) variables within their sampling ranges, a PCP-GP model is formulated as shown in Table 3. The pre-emptive priorities for the three objective functions are as follows:

- priority 1: attain prescribed probability of satisfying output specifications;
- priority 2: minimize a cost function; and
- priority 3: get as close to Derringer and Suich targets as possible.

TABLE 2. Regression results

$Y_1 = -46.05717 + 32.98626 X_1 + 1.78808 X_2 + 21.81308 X_3$
(t) (-2.19) (5.70) (6.18) (3.77)
$r^2 = 0.8413$ DW = 1.016 n = 20 MSE = 111.721
$Y_2 = -1262.68224 + 536.28462 X_1 + 24.65032 X_2 + 278.96907 X_3$
(t) (-1.73) (2.66) (2.45) (1.39)
$r^2 = 0.4841$ DW = 1.730 n = 20 MSE = 135124/09
$Y_3 = 1153.69903 - 199.32595 X_1 - 3.13964 X_2 - 147.83800 X_3$
(t) (23.56) (-14.76) (-4.65) (-10.94)
$r^2 = 0.9573$ DW = 1.217 n = 20 MSE = 608.233
$Y_4 = 44.03998 - 2.81976 X_1 + 0.43197 X_2 + 3.26969 X_3$
(t) (10.43) (-2.42) (7.42) (2.81)
$r^2 = 0.8113$ DW = 1.363 n = 20 MSE = 4.519

Note that the decision-maker is allowed to specify a probability level (target probability), b , of attaining each individual output specification. The higher the probability level, the smaller the feasible solution region. Priority 3 uses the weights (6, 1, 3, 40) in order to equalize the different scales of the practical ranges associated with each response variable.

The PCP-GP model was run at various probability levels to demonstrate the trade-off effects on cost of changing the risk of not meeting one or more of the quality specifications. Results of these runs are shown in Table 4. The target probability, ranging from 0.5 to 0.8768, is the specified maximum acceptable risk of violating each of the individual quality specifications. For each of these target probabilities, the solution was found, giving the optimal X values and the resulting

TABLE 3. PCP-GP model for the example

$$\begin{aligned}
 &\text{Min. } P_1(d_1^- + d_2^- + d_3^- + d_4^+ + d_5^- + d_6^+) \\
 &P_2(d_7^+) \\
 &P_3(6d_8^- + 1d_9^- + 3d_{10}^- + 3d_{10}^+ + 40d_{11}^- + 40d_{11}^+) \\
 &\text{s.t.} \\
 &E[Y_1] - \Psi_b\{111.721(1 + X'_p(X'X)^{-1}x'_p)\}^{1/2} + d_1^- - d_1^+ = 120. \\
 &E[Y_2] - \Psi_b\{135124.09(1 + X'_p(X'X)^{-1}x'_p)\}^{1/2} + d_2^- - d_2^+ = 1000. \\
 &E[Y_3] - \Psi_b\{608.233(1 + X'_p(X'X)^{-1}x'_p)\}^{1/2} + d_3^- - d_3^+ = 400. \\
 &E[Y_3] + \Psi_b\{608.233(1 + X'_p(X'X)^{-1}x'_p)\}^{1/2} + d_4^- - d_4^+ = 600. \\
 &E[Y_4] - \Psi_b\{4.519(1 + X'_p(X'X)^{-1}x'_p)\}^{1/2} + d_5^- - d_5^+ = 60. \\
 &E[Y_4] + \Psi_b\{4.519(1 + X'_p(X'X)^{-1}x'_p)\}^{1/2} + d_6^- - d_6^+ = 75. \\
 &X_1 + X_2 + X_3 + d_7^- - d_7^+ = 0 \quad (\text{cost}) \\
 &E[Y_1] + d_8^- - d_8^+ = 170 \quad (\text{desired } Y_1) \\
 &E[Y_2] + d_9^- - d_9^+ = 1300 \quad (\text{desired } Y_2) \\
 &E[Y_3] + d_{10}^- - d_{10}^+ = 500 \quad (\text{desired } Y_3) \\
 &E[Y_4] + d_{11}^- - d_{11}^+ = 67.5 \quad (\text{desired } Y_4) \\
 &X_1 \geq 0.38335 \quad X_1 \leq 2.0165 \quad (\text{limits}) \\
 &X_2 \geq 33.667 \quad X_2 \leq 66.333 \quad (\text{limits}) \\
 &X_3 \geq 1.4833 \quad X_3 \leq 3.1667 \quad (\text{limits})
 \end{aligned}$$

where $E[Y_i]$ = expected value (regression coefficients) and X'_p is the solution vector; $X'X^{-1}$ is the inverse of the input data matrix; Ψ is the normal or t variate penalty value; and b is a predetermined target probability.

TABLE 4. Results

Target probability	0.50	0.65	0.80	0.85	0.8768	D&S
Solution X_1	1.915	1.973	1.735	1.581	1.499	1.175
X_2	36.232	41.204	52.182	58.729	63.786	51.450
X_3	1.746	1.483	1.483	1.512	1.532	1.866
Cost	39.893	44.660	55.401	61.821	69.309	55.066
$E[Y_1]$	120.000	125.054	136.845	144.108	144.096	125.402
$E[Y_2]$	1144.772	1224.855	1368.029	1455.024	1527.299	1156.267
$E[Y_3]$	400.000	411.786	424.687	430.529	435.372	482.091
$E[Y_4]$	60.000	61.125	66.538	69.892	72.217	69.053
Prob[$Y_1 \geq 120$]	0.5000	0.6500	0.9062	0.9670	0.9845	0.6830
Prob[$Y_2 \geq 1000$]	0.6266	0.6886	0.8000	0.8500	0.8769	0.6541
Prob[$400 \leq Y_3 \leq 600$]	0.5000	0.6500	0.8000	0.8500	0.8768	0.9968
Prob[$60 \leq Y_4 \leq 75$]	0.5000	0.6650	0.9897	0.9724	0.8558*	0.9909
Prob[all satisfied]	0.0783	0.1935	0.5740	0.6794	0.6478	0.4413

cost. These X values were then used to compute the expected values of the quality variables (the Y s) and, using the regression model, the probability of each variable exceeding its specifications at that level.

The last row gives an estimate of the probability that all quality specifications will be met given the optimal solution. This value is the product of the four probabilities of satisfying each of the quality specifications. This assumes that the probability of satisfying any one constraint is independent of the probability of satisfying other constraints. As there was no significant correlation among the error terms of the four regression lines, the assumption of independence appears reasonable for this situation.

Column 1 shows that if the stochastic elements are ignored (allowing a 50% probability of not meeting each individual specification), cost is 39.893. The probability of not meeting at least one specification is a rather sizeable 92.17% ($1 - 0.0783$). Columns 1–4 show that as the target probability is raised from 50% to 85%, cost increases to 61.821, while the probability of not meeting at least one specification drops to 32.06% ($1 - 0.6794$). This is still somewhat high, but reflects the realities of the situation. Column 5 demonstrates that if the target probability for each variable is increased beyond 85% to 87.68, an infeasible solution results since the joint probability of simultaneously satisfying both bounds of Y_4 is lower than the target probability.

The optimal solution found by Derringer and Suich is included in Table 4 as column 6 for ease

of comparison. The Derringer and Suich solution has a cost of 55.066, includes two rather low individual probabilities (68.3% and 65.41%) of meeting specifications, and has an overall probability of missing at least one specification of 55.87% ($1 - 0.4413$). At a target probability of 80% (column 3), the PCP-GP model has a cost of 55.401 and an overall probability of missing at least one specification of 42.60% ($1 - 0.5740$).

Comparisons of the solutions

Comparing the two approaches and their solutions, the following differences are observed:

- (1) No transformation is needed in the PCP-GP model. The desirability function involves transformation of each estimated response variable to a unit-free desirability scale between 0 and 1, while the PCP-GP model uses actual values of the response variables.
- (2) The PCP-GP model optimizes among multiple-output specifications and different objective functions. For the desirability-function approach, each individual desirability function is assessed independently through transformation equations. The PCP-GP model gives the decision-maker flexibility in assigning relative weights w_i for each target to reflect the preference of the decision-maker and/or to eliminate the scaling problem, as was done in d_8-d_{11} in the example. In addition, the PCP-GP model allows the decision-maker to prioritize multiple objectives, such as reducing cost versus satisfying specifications.
- (3) Both approaches provide ways of dealing with the trade-offs between the risk of violating the output specifications and the risk of getting infeasible solutions. The desirability function lets the decision-maker choose appropriate exponents (from 0.1 to 10) in the transformation equations, while the PCP-GP model uses the probability targets (from 50% to 99%) specified by the decision-maker to determine the feasible region. It may be easier and more reliable for a decision-maker to use the probability target as it is based on statistical theory.

The PCP-GP model can also be used to give greater flexibility along with greater precision in supporting the relative importance of various quality specifications. In the example, target possibilities for each quality variable were set to equal values for simplicity. It is more difficult for a quality variable simultaneously to satisfy both upper and lower bounds. One example is the case of variable Y_4 under a target probability of 0.8765 in Table 4. Therefore, it might be desirable to specify lower target probabilities for variables with double bounds.

Moreover, in a production setting, there are likely to be differences in importance, and decision-makers need to be able to specify acceptable risk levels. It is a trivial extension to employ different acceptable risk levels for the various specification limits in the PCP-GP model. Such uneven target probabilities might result in an enlargement of the feasible region and in lower-cost feasible solutions.

DISCUSSION AND CONCLUSIONS

Two difficulties that process control managers face in the selection of input levels are (1) the simultaneous optimization of multiple, possibly conflicting output specifications, and (2) the risk of violating the specifications when the functional relationship of input and output variables is modelled with regression. By incorporating prediction-interval constraints into a goal-programming model, this paper has proposed a new approach that will help process-control managers in overcoming these difficulties. The problem investigated by Derringer and Suich using the desirability function was solved again using the PCP-GP model, and the solutions were compared.

Implementing the PCP-GP model does not require that new programmes be developed. The model is a conventional goal-programming model containing chance constraints. Such chance-constrained models can be solved by a variety of available packages, such as those presented in Seppala and Orpana,¹⁰ Lee and Olson¹¹ and Weintraub and Vera.¹²

In conclusion, for process-control problems which involve multiple-quality specifications and which must be modelled with a regression approach, the proposed PCP-GP model provides a better alternative than the desirability-function approach. The PCP-GP model uses actual data of

the problem instead of transformed values. It also provides greater flexibility, allowing quality-control managers to rank priorities among conflicting objectives and to assess the relative importance of meeting various specifications.

Acknowledgement—The authors are grateful to the anonymous referees for their helpful suggestions. The authors alone are responsible for all errors.

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