$F(\ )$ = the perturbed feasible region resulting from the perturbation in the parenthesis
F^* = the permanently feasible region
N = number of primal variables
M = number of constraints
P = the set of all permissible perturbations in the model coefficients
R = set of indices of rows which have a dependency in the coefficients of that row
α_{ij} = the bounds on the perturbations in the a_{ij}
β_i = the bounds in the perturbations in the b_i
γ_i = a probability
μ_{ij} = coefficients of a row dependency equation
η_{ij} = coefficients of a column dependency equation
δ = a perturbation of the quantity following it

Superscripts

an element in a sequence

Subscripts

a component of a matrix

Mathematical Symbols

ϵ = a member of
$\neq$ = not equal to
ϕ = the empty set
$\cap$ = set intersection
$\cup$ = set union
$\subset$ = set inclusion
: = such that

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Flexible Solutions to Linear Programs under Uncertainty: Equality Constraints

This paper presents a framework which allows uncertainties in the matrix elements of an equality constrained linear program to be taken into account without requiring detailed knowledge of the statistical characteristics of these uncertainties. The results are derived using the model of the linear program with flexibility previously introduced for the inequality constrained case. However, because a feasible region common to all perturbed constraint sets does not exist in the equality constrained case, a flexibility set which intersects all perturbed sets individually rather than jointly is defined. The flexibility set is constructed by identifying a finite subset of all perturbed constraint sets which need to be investigated. Three cases for the equality constrained problem are considered: independent variations in the array elements, column dependent variations, and row dependent variations. In each case the problem is solved using a possibly large but decomposable linear program. In the first two cases, this program needs to be solved only once; while in the row dependent case an iterative but finite solution procedure is required.

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SCOPE

In the preceding paper (Friedman and Reklaitis, 1974) a model and solution procedure were presented which would allow uncertainties in the array and right-hand side coefficients of an inequality constrained linear program to be taken into account. The model, called the *linear program with flexibility*, was based on the assumption that the model builder will know:

1. A mean, or "best estimate," value for each matrix coefficient,
2. The intervals over which variations in each matrix coefficient are assumed to be uniformly distributed,
3. The coefficients of any linear relationships between the matrix elements which impose restrictions on the possible variations, and

4. The unit costs which must be incurred in order to provide for changes in policy in the future.

The solution strategy presented relied on the existence of a nonempty common intersection of all perturbed constraint sets. This assumption is never satisfied in the presence of equality constraints with coefficient uncertainties. Since equality constraints often occur in linear programming models and since it is desirable for the uncertainty in these constraints to be taken into account along with those in the inequality constraints, the need for further developments is clearly indicated.

CONCLUSIONS AND SIGNIFICANCE

This paper extends the notion of the linear program with flexibility, introduced in Friedman and Reklaitis (1975) for inequalities, so that equality constraints may also be accommodated. This is accomplished by formulating the concept of a region of flexibility defined by multiple correction policies. Using this concept, computational procedures paralleling the inequality constrained case are detailed for equality constrained problems in terms of three separate cases: the case with independent variations in the array elements, with column dependent variations, and with row dependent variations. In the first two cases, a solution is obtained by solving a possibly large but decomposable linear program. In the third case, the decomposable linear program must be solved iteratively using the finitely terminating cutting plane method presented in our previous paper. In applications involving large, general, linear programs all three cases may occur simultaneously; in that event, the iterative procedure will always be required. As a result of the techniques presented here, the engineer/planner will obtain a balance between the optimal policy based on current best information and the optimal amount of flexibility which will be required in the policy in order to be able to adapt it to uncertainties in his linear equality or inequality constrained model.

In a previous paper (Friedman and Reklaitis, 1974) an approach was presented for accommodating uncertainty in the matrix elements of an inequality constrained linear programming problem. Specifically, we considered the problem

$$\begin{array}{ll} \text{Minimize} & c\,x \\ \text{Subject to} & Ax \leq b \\ & x \geq 0 \end{array} \tag{1}$$

where each coefficient a_{ij} and b_i has a known range of variation,

$$\begin{array}{ll} -\alpha_{ij} \leq \delta a_{ij} \leq \alpha_{ij} & i = 1, \ldots, M \\ -\beta_i \leq \delta b_i \leq \beta_i & j = 1, \ldots, N \end{array} \tag{2}$$

and where restrictions may be imposed on these variations

$$\sum_i \eta_{ij}\, \delta a_{ij} = 0 \qquad j \in C \tag{3}$$

$$\sum_j \mu_{ij}\, \delta a_{ij} = 0 \qquad i \in R \tag{4}$$

The above problem was solved by means of the Linear Program with Flexibility,

$$\begin{array}{ll} \text{Minimize} & c\,x + c^+ z^+ + c^- z^- \\ \text{Subject to} & Ax \leq b, \quad x \geq 0 \\ \text{and} & x + z^+ - z^- \in F^* \end{array} \tag{5}$$

where c^+, c^- are costs of flexibility (see the previous work for a discussion of these coefficients).

The set F^*, called the *permanently feasible set,* was defined to be the intersection of all sets

$$F(\delta A, \delta b) = \{y \colon \Sigma(a_{ij} + \delta a_{ij}) y_j \leq b_i + \delta b_i;\ y \geq 0,\ i = 1, \ldots, M\}$$

resulting from some choice of variations $(\delta A, \delta b)$ satisfying conditions (2), (3), and/or (4). The methodology presented considered three cases which could, of course, occur jointly:

1. The independent case, in which only conditions (2) were allowed,
2. The column dependent case, in which conditions (2) and (3) were allowed, and
3. The row dependent case, in which conditions (2) and (4) were allowed.

The crucial assumption underlying these constructions was that a common intersection of the sets $F(\delta A, \delta b)$ could be in fact found, that is, that the set F^* was nonempty. Yet the case in which F^* is empty can and does occur most commonly when the linear program contains one or more equality constraints. In this paper we will present the means for dealing with uncertainty in the array coefficients of an equality constrained linear program. This will be accomplished by considering a more general form of the Linear Program with Flexibility which permits F^* to be empty.

EQUALITY AND INEQUALITY CONSTRAINTS

A conventional device for reformulating an equality constraint

$$\sum_j a_{ij}\, x_j = b_i$$

is to replace it by two inequality constraints

$$\sum_j a_{ij}\, x_j \leq b_i$$

and

$$\sum_j a_{i+1}\, x_j \leq b_{i+1}$$

where $a_{i+1,j} = -a_{ij}$ and $b_{i+1} = -b_i$. Suppose that the coefficients a_{ij} and b_i are subject to variation; then it is easily shown that the set F^* must be void. Let δa^1_{ij} and δa^2_{ij} be two perturbations in the array coefficients with $\delta a^1_{ij} > \delta a^2_{ij}$. Then, define

$$F_1 = \left\{ y: \sum_j (a_{ij} + \delta a^1_{ij}) y_j \leq b_i \quad \text{and} \quad \sum (a_{i+1,j} + \delta a^1_{i+1,j}) y_j \leq b_{i+1} \right\}$$

and let F_2 be as F_1 but with δa^2_{ij} replacing δa^1_{ij}. If w is a point belonging to both F_1 and F_2, then, since $\delta a_{ij} = -\delta a_{i+1,j}$ and $a_{ij} = -a_{i+1,j}$, it must be true that

$$\sum_j (a_{ij} + \delta a^1_{ij})\, w_j = b_i$$

and

$$\sum_j (a_{ij} + \delta a^2_{ij})\, w_j = b_i$$

But, that is not possible since $\delta a^1_{ij} > \delta a^2_{ij}$. Consequently, F_1 and F_2 must be disjoint and thus F^* which is the intersection of all such sets $(F(\delta A, \delta b))$ is void.

From the preceding it is clear that the equality constrained case cannot be solved by merely reformulating it as an inequality constrained problem and using the methodology of (Friedman and Reklaitis, 1974). Nonetheless, the result of this reformulation of the equality constraints can be identified as a case of an inequality constrained problem with column dependency in the model coefficients since the restrictions

$$\delta a_{ij} + \delta a_{i+1,j} = 0 \qquad j = 1, \ldots, N$$
$$\delta b_i + \delta b_{i+1} = 0$$

are analogous to (3). This suggests that the case in which the permanently feasible region is empty can occur not only with equality constraints but also in general with inequality constraints with column dependency.

In the previous paper it was shown that in the case of column dependency the set F^* can be described by the set of inequalities,

$$\sum_j (a_{ij} + \delta a^*_{ij})\, y_j \leq b_i - \beta_i \qquad i = 1, \ldots, M$$

$$y_j \geq 0 \qquad j = 1, \ldots, N$$

where for each i, j

$$\delta a^*_{ij} = \begin{cases} \text{MIN} \left\{ \alpha_{ij}, \sum_{\substack{k=1\\k\neq 1}}^{M} \left| \dfrac{\eta_{kj} - \alpha_{kj}}{\eta_{ij}} \right| \right\}, & \text{if} \quad \eta_{ij} \neq 0 \\ \alpha_{ij}, & \text{otherwise} \end{cases} \tag{6}$$

This selection of δa^*_{ij} can be interpreted as considering the worst case for each constraint, in the sense of choosing a perturbation of each constraint which eliminates as much of the original feasible region as possible. Solution of problem (5) thus corresponds to finding a policy x which satisfies the current best estimate of the model together with a correction policy z^+, z^- which will guarantee that regardless of the outcome, that is, actual value of $(\partial A, \partial b)$, the corrected policy $x + z^+ - z^-$ will be feasible. In addition, the policy x and the flexibility provisions z^+, z^- are chosen so as to minimize the total cost. Note, however, that because of conditions (3), the perturbations of the coefficients of any given constraint are not independent; hence, the worst case for each constraint can not occur simultaneously. Thus, a policy calculated using F^* as given above is more conservative than necessary and, consequently, even if F^* is void, it may still be possible to calculate a correction policy which will ensure feasibility.

EXAMPLE 1

The above points are readily apparent from the following simple two variable inequalities,

$$x_1 - x_2 \leq -1$$
$$-1/2\, x_1 + x_2 \leq 2$$

with

$$x_1, x_2 \geq 0$$

Suppose the coefficients of these inequalities are merely best estimates and that actually they can vary between $\pm\alpha_{ij}$, where

$$\alpha = \begin{bmatrix} 0.1 & 0.2 \\ 0.2 & 0.1 \end{bmatrix}$$

and that in addition the perturbations must satisfy

$$\delta a_{11} + 2\delta a_{21} = 0 \quad \text{and} \quad \delta a_{12} + \delta a_{22} = 0$$

Following, (Friedman and Reklaitis, 1974) the permanently feasible region, F^* will be given by

$$1.1\, x_1 - 0.9\, x_2 \leq -1 \quad \text{and} \quad -0.45\, x_1 + 1.1\, x_2 \leq 2$$

As suggested in the preceding discussion, in the column dependent case, both of the worst cases defining F^* can not occur simultaneously. Rather, if $1.1\, x_1 - 0.9\, x_2 \leq -1$, then because of dependency, the second constraint will be $-0.55\, x_1 + 0.9\, x_2 \leq 2$. Denote the common region formed by these two constraints as F_1. Similarly, if the second constraint is $-0.45\, x_1 + 1.1\, x_2 \leq 2$, then, because of dependency, the first must be $0.9\, x_1 - 1.1\, x_2 \leq 1$. Denote the common region of these constraints by F_2. All three of these regions as well as the feasible region F^0 based on the unperturbed, "best estimate" coefficients are shown in Figure 1. Note that $F^* = F_1 \cap F_2$. Now, if $x^0 = (2, 3)$ is the solution to an optimization over the feasible region F^0, then in order to ensure that F^* can be reached, the policy should have enough flexibility to reduce x_1 by 1.13 and x_2 by 0.83. However, since F_1 and F_2 can not both occur simultaneously, feasibility can be maintained if F_1 and F_2 can be reached individually. Hence, if x_1 can be reduced by 0.55, F_1 can be reached; while if x_2 can be reduced by

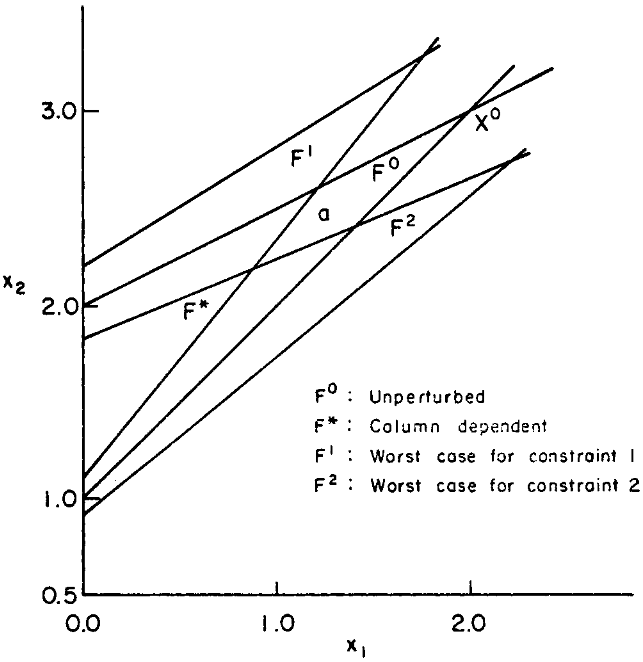

Fig. 1. Example 1.

0.36, F_2 will be reached. Clearly, the flexibility required by the F^* correction is larger, that is, this policy is more conservative than necessary.

Now, consider the above example with the additional constraints $x_1 \geqq 1.3$ and $x_2 \geqq 2.5$. In Figure 1, this means that all feasible points must lie above and beyond point (a). All of the previous constructions still apply; but now, observe that F^* is empty while F^0, F_1, F_2 are not. Clearly, a policy which has the flexibility to reach F_1 and F_2 will always be feasible even though $F^* = \phi$.

THE FLEXIBILITY SET

The above example suggests that in the column dependent case, which includes equality constraints, an optimal region of flexibility can be determined even if no permanently feasible region exists. In order to simplify the constructions required to accomplish this, we will in the subsequent discussion, consider only δA variations. The changes in the right hand sides can be incorporated in a straightforward way.

Let $\mathcal{F}$ be the family of sets $F(\delta A)$ where for each choice of δA, satisfying (2) and (3) (that is, each $\delta A \epsilon P$)

$$F(\delta A) = \{x: (A + \delta A)\, x \leqq b, \quad x \geqq 0\}$$

Assume that each set $F(\delta A)$ is nonempty and bounded. The first assumption is reasonable because if some $F(\delta A)$ is empty, then the corresponding linear programming problem has no feasible solution. The second assumption is an analytic convenience but is usually satisfied by well posed problems. As a consequence of these assumptions, the family $\mathcal{F}$ is a family of compact sets.

The problem of determining a region of flexibility for a point x satisfying the "best estimate" model corresponds to determining a neighborhood of x which will contain at least one member from every set $F(\delta A)$ in $\mathcal{F}$. If this can be achieved, then we can be sure that regardless of how F^0 is perturbed, the policy x can always be made feasible. Analytically, this corresponds to determining ρ such that for some $x \epsilon F^0$ and for every $\partial A \epsilon P$,

$$B(x) \cap F(\delta A) \neq \phi$$

where $B(x) = \{y: ||x - y|| \leqq \rho\}$ and is called the *flexibility set for x.*

Given $x \epsilon F^0$, for every $F \epsilon \mathcal{F}$, let

$$d(x, F) = \text{MIN}\, \{||x - y|| : y \epsilon F\}$$

and

$$\rho(x) = \text{MAX}\, \{d(x, F) : F \epsilon \mathcal{F}\}$$

[It can be readily verified that the MIN (MAX) operations rather than the more general infimum (supremum) are acceptable because of the properties of $d(x_1 F)$, $\mathcal{F}$, and P.]

The following elementary proposition will be useful in detailing a procedure for obtaining $\rho(x)$:

Proposition 1: Given any $x \epsilon F^0$ and any $F \epsilon \mathcal{F}$ such that $d(x_1 F) \neq \phi$, the point $y \epsilon F$ at which $d(x, F) = ||x - y||$ satisfies at least one constraint of those defining F as an equality.

Proof: Since F is closed and bounded, a $y \epsilon F$ must exist at which $d(x, F)$ is achieved. This point must be a boundary point of F since F is closed and convex. If not, then there is a neighborhood of y which is contained entirely in F. At least one point y' in this neighborhood will have $||y' - x|| < d(x, F)$, which leads to a contradiction. All boundary points of F lie on its constraint surfaces; hence, y must satisfy at least one constraint as an equality,

$$\sum_j (a_{ij} + \delta a_{ij})\, y_j = b_i.$$

Note also that since F is convex, the point y will be unique.

The following standard result, known as the Theorem of the Separating Hyperplane, is stated without proof and will be used in verifying Proposition 2.

Theorem (Rockafeller, 1970)

If two convex sets k_1 and k_2 have at most common boundary points, there exists a hyperplane $\sum_j p_j x_j = q$ which separates k_1 and k_2 in the sense that

$$\sum p_j x_j \leqq q \quad \text{for all } x \text{ in } k_1,$$

and

$$\sum p_j x_j \geqq q \quad \text{for all } x \text{ in } k_2.$$

For a point $y \epsilon F$ such that $d(x, F) = ||x - y||$, let $I(y)$ be the set of tight constraints at y,

$$I(y) = \left\{ i: \sum_j (a_{ij} + \delta a_{ij})\, y_j = b_i, \quad i = 1, \ldots, M \right\}$$

Also, let $\delta a_i^{\max}$ indicate the perturbations of the coefficients of constraint i [calculated using Equation (6)] at which each δa_{ij} is at its maximum value.

Proposition 2: Given $x \epsilon F^0$, let y^* and F^* be such that

$$\rho(x) = d(x_1 F^*) = ||x - y^*||\,.$$

Either $\delta a_i^* = \delta a_i^{\max}$ for each $i \epsilon I(y^*)$ or else there is no $F \epsilon \mathcal{F}$ which has $\delta a_i = \delta a_i^{\max}$ for each $i \epsilon I(y^*)$.

Proof: Suppose F^* does not have $\delta a_i = \delta a_i^{\max}$ for all $i \epsilon I(y^*)$ but an $F' \epsilon \mathcal{F}$ which has does exist. Define

$$B(x) = \{y : ||x - y|| \leqq \rho(x)\}\,.$$

Since $\rho(x)$ is finite, $B(x)$ is closed and bounded. Since both $B(x)$ and F^* are convex sets with only the point y^* in common, by the Separating Hyperplane Theorem there exists a hyperplane $\sum_j p_j y_j = q$ such that for all y in B,

$$\sum_j p_j y_j \geqq q$$

for all y in F^*,

$$\sum_j p_j y_j \leqq q$$

and equality holds only if $y = y^*$. Consider the sets

$$G^* = \left\{ y : \sum_j (a_{ij} + \delta a^*_{ij})\, y_j \leqq b_i, \quad i \epsilon I(y^*) \right\}$$

$$G' = \left\{ y : \sum_j (a_{ij} + \delta a_{ij}^{\max})\, y_j \leqq b_i, \quad i \epsilon I(y^*) \right\}$$

and

$$H = \left\{ y : \sum_j p_j y_j \leqq q \right\}$$

By construction, $F^* \subset G^*$ and $F' \subset G'$. Also, since F^* is convex, $G^* \subset H$. Finally, by definition of $\delta a_i^{\max}$, for any y and all i,

$$\sum_j (a_{ij} + \delta a_{ij})\, y_j \leqq \sum_j (a_{ij} + \delta a_{ij}^{\max})\, y_i$$

In particular, the inequality must be true for $i \epsilon I(y^*)$ and $\delta a_{ij} = \delta a^*_{ij}$. Consequently, $G' \subset G^*$ and it follows that

$$F' \subset G' \subset G^* \subset H$$

However, by hypothesis, there is a constraint i such that

δa_i^* is not at its maximum value. That constraint evaluated at the point y^* will yield

$$b_i = \sum_j (a_{ij} + \delta a^*_{ij})\, y^* < \sum_j (a_{ij} + \delta a_{ij}^{\max})\, y_j^*$$

Thus, y^* is in F^* but not in F'. Since y^* is the only point of H which is also in $B(x)$ and since $F' \subset H$, it follows that $B(x)$ contains no points of F'. Thus, $d(x, F') > d(x_1 F^*) = \rho(x)$, which is a contradiction of the hypothesis that $\rho(x) = \text{MAX}\,\{d(x, F) : F \in F\}$. Hence the proposition is proven.

The proposition suggests that in order to determine $\rho(x)$, those sets F ought to be investigated which have as many as possible of the coefficient perturbations set at their maximum value.

Given a set $F \in F$, let ϕ_F be the set of indices of those constraints which have δa_i set at $\delta a_i^{\max}$. A set $F' \in F$ will be called *terminal* if there is no other $F \in F$ such that $\phi_F \supset \phi_{F'}$.

All terminal sets can be obtained by means of the following conceptual partial enumeration strategy:

For each constraint, i, calculate $\delta a_i^{\max}$ using Equation (6). If the choice $\delta a_i = \delta a_i^{\max}$, for all $i \in C$ is permissible, that is, satisfies conditions (1) and (3), set $T = 1$, $\phi_1 = \{1, \ldots, M\}$ and terminate. Otherwise, set $T = 0$ and at level l where $l = 1, \ldots, M - 1$

I. Select a set L of $M - l$ different constraint indices consisting of at least one index from each J_t, $t = 1, \ldots, T$ and the remainder from among $[1, \ldots M]$. If all selections at level l have been exhausted, go to Step II. Otherwise,

a) For each $i \in L$, set $\delta a_i = \delta a_i^{\max}$

b) Compute, for each $j \in C$,

$$\sum_{i \in L} \eta_{ij}\, \delta a_{ij}^{\max} - \sum_{i \notin L} |\eta_{ij}|\, \alpha_{ij} \tag{7}$$

If the difference is nonpositive, set $T = T + 1$ and $\phi_T = L$. Let J_T be the set of those indices from $[1, \ldots, M]$ not in L and continue with (I). If the difference is positive, continue with (I).

II. Set $l = l + 1$. If $l < M - 1$ or $l = M - 1$ and $\bigcap_{t=1}^{T} J_t \neq \emptyset$ go to step I. Otherwise, terminate.

This procedure generates terminal sets by beginning with all constraints set at their maximum perturbations and then proceeds through successive levels at each of which one less constraint is at the maximum perturbation. To insure that no nonterminal sets are considered, each candidate set is required to contain at least one element from the complement of each previously generated terminal set. Step (b) of I ensures that the candidate set L, satisfies conditions (2) and (3). The procedure terminates when the level is reached at which only one constraint is set at the maximum perturbation. This level will have feasible candidates only if there are elements common to the complements of all previously generated terminal sets.

THE GENERAL LINEAR PROGRAM WITH FLEXIBILITY

In the previous section, the flexibility set $B(x)$ was defined as a hypersphere with radius $\rho(x)$. This definition is an analysis convenience which can be dispensed with by introducing any suitable distance measure. In particular, in order to maintain linearity, $B(x)$ can be obtained by retaining the correction required for each terminal set and then defining a hypercube which will envelop all these corrections.

Let δA^t, $t = 1, \ldots, T$ be the perturbations defining terminal set t. For each such perturbation, a correction can, for any $x \in F^0$, be obtained as a solution to the following inequalities:

$$(A + \delta A^t)(x + x^t(t) - x^-(t)) \leqq b$$

$$x, x^+(t), x^-(t) \quad \text{all} \geqq 0$$

and,

$$x - x^-(t) \geqq 0$$

The flexibility set $B(x)$ can thus be defined as

$$B(x) = \{y : -z^- \leqq y \leqq z^+\}$$

where

$$z^+ = \max\{x^+(t) : t = 1, \ldots, T\}$$

$$z^- = \max\{x^-(t) : t = 1, \ldots, T\}$$

Given the perturbations corresponding to each terminal set, the general *linear program with flexibility* can be defined as follows:

$$\begin{aligned} &\text{Minimize} && c\,x + c^- z^- + c^+ z^+ \\ &\text{Subject to} && Ax \leqq b \\ & && (A + \delta A^t)(x + x^+(t) - x^-(t)) \leqq b \\ & && z^+ \geqq x^+(t) \qquad t = 1, \ldots, T \\ & && z^- \geqq x^-(t) \\ & && x \geqq z^- \end{aligned} \tag{7}$$

with all variables non-negative.

Note that this is a decomposable program of the familiar bordered block-angular structure for which well known and efficient LP solution procedures exist (Dantzig, 1968).

THE LINEAR PROGRAM WITH EQUALITY CONSTRAINTS

In this section the previous constructions will be specialized to the LP with Equality Constraints. The discussion will, for convenience in presentation, be subdivided into three cases all three of which could in practice of course occur jointly.

Case I: Independent Perturbations

If there are no conditions of the form (3) or (4), then under the reformulation of the equalities as matched pairs of inequalities, the resulting program is merely a specialized case of the general inequality LP defined above. Note, however, that the requirement

$$\delta a_{2i} + \delta a_{2i-1,j} = 0$$

imposes the restriction that when $\delta a_{2i-1} = \delta a_{2i-1}^{\max}$, then $\delta a_{2i} = -\delta a_{2i}^{\max} = \delta a_{2i}^{\min}$. Thus, when viewed as an inequality constrained problem, among the $2M$ constraints only M may be allowed to undergo maximum perturbation. Hence, the terminal sets will correspond to all combinations of selecting M nonpaired inequalities set at $\delta a_i^{\max}$. Since no conditions of the type (3) or (4) are imposed, all choices $\delta a_i^{\max}$ are possible. Hence, from Proposition 2, no terminal sets with less than M constraints subject to maximum perturbation need to be investigated. In view of this, the independent case is most conveniently considered by operating directly on the equality constraints and setting each at its maximum or minimum perturbation. This leads to a total of 2^M terminal sets which may need to be employed in determining flexibility. Note, however, that 2^{M-1} of the δA^t will merely have perturbations opposite in sign to the other 2^{M-1}.

Case II: Column Dependent Perturbations

The equality constrained linear program with columnwise restrictions in the perturbations can under the inequality reformulation be viewed as a column dependent inequality constrained program with two types of perturbation restrictions:

$$\sum_i \delta a_{2i-1,j}\,\eta_{2i-1,j} = 0, \quad \sum_i \delta a_{2i,j}\,\eta_{2i,j} = 0$$

with

$$\eta_{2i} = \eta_{2i-1}$$

and

$$\delta a_{2i-1,j} = -\delta a_{2i,j}$$

Following the analysis for the inequality constrained case, the maximum perturbations for each constraint can be obtained via Equation (6). As in the independent case, $\delta a_{2i}^{\max} = -\delta a_{2i-1}^{\min}$ and the terminal sets are determined by setting as many as possible of the nonpaired constraints at their maximum perturbations. However, because of the dependency relations, some of these candidate sets may not be permissible. Consequently, the partial enumeration procedure outlined previously must be employed.

This procedure can be applied directly to the equality constraints without reformulation if account is taken of the fact that the maximum perturbation of one reformulated inequality corresponds to a minimum perturbation of its matched pair. Hence, in considering the equality constraints directly, both minimum and maximum perturbations must be examined. The modified partial enumeration scheme proceeds as follows:

For each constraint i, calculate $\delta a_i^{\max}$ using Equation (6). Set $T = 0$, let p be the smallest integer such that $p \leqq M/2$ and $\mathcal{M}$ be the set $\{\pm 1, \pm 2, \ldots, \pm M\}$.

O) Select a combination L of the M constraint indices i such that k are set at $-i$, where $k \leqq p$. If all combinations have been exhausted, go to step I. Otherwise,

a) For each $i \in L$, if $i > 0$, set $\delta a_i = \delta a_i^{\max}$
if $i < 0$, set $\delta a_i = -\delta a_i^{\max}$

b) Check whether L is permissible (as in Step Ib of the unmodified procedure). If L is not permissible, go to Step O. If it is permissible, set $\phi_{T+1} = L$, and let ϕ_{T+2} contain the negative of the indices in L. Let J_{T+1} consist of the indices $\mathcal{M} - \phi_{T+1}$ and J_{T+2} consist of $\mathcal{M} - \phi_{T+2}$. Set $T = T + 2$ and go to the beginning of Step O.

For $l = 1, 2, \ldots, M - 1$

I) Select a set L of $M - l$ different indices consisting of at least one from each J_t, $t = 1, \ldots, T$ and the remainder from the set $\mathcal{M}$. If all selections have been exhausted at level l, go to Step II. Otherwise, perform Steps Oa, Ob above but returning always to Step I.

II) Set $l = l + 1$. If $l < M - 1$ or $l = M - 1$ and $\bigcap_{t=i}^{T} J_t \neq \emptyset$, go to Step I. Otherwise terminate.

The above conceptual algorithm parallels the earlier scheme. It differs, first, in that the initial level ("Step O") must be expanded to allow for minimum and maximum perturbations. Secondly, sets ϕ_t and J_T are saved in pairs since if the set $\{i_m\}$ is permissible, then so is the set $\{-i_m\}$.

In the preceding two cases, once the family of terminal sets and their corresponding perturbations $\{\delta A^t\}$ have been determined, then the linear program with flexibility can be solved with inequalities (7) replaced by equations. The third case, the row dependent case, requires an iterative solution of the LP with flexibility.

Case 3: Row Dependent Perturbations

If the row dependent equality constrained problem with

$$\sum_j a_{ij}\, y_j = b_i$$

and

$$\sum_j \delta a_{ij}\, \mu_{ij} = 0 \qquad i \in R$$

is reformulated to two inequalities

$$\sum_j a_{2i-1,j}\, y_j \leqq b_{2i-1} \quad \text{and} \quad \sum_j a_{2i,j}\, y_j \leqq b_{2i}$$

in the usual fashion, then two row constraints on the perturbation are generated,

$$\sum_j \delta a_{2i-1,j}\,\eta_{2i-1,j} = 0 \quad \text{and} \quad \sum_j \delta a_{2i,j}\,\eta_{2i,j} = 0$$

where

$$\eta_{2i,j} = \eta_{2i-1,j}$$

and the column constraint, $\delta a_{2i-1,j} + \delta a_{2i,j} = 0$.

This corresponds to an inequality constrained problem with both column and row dependency. As in the independent case, each terminal set will correspond to a choice at which M nonpaired inequalities will be set at their maximum perturbations. Moreover, since the maximum perturbation of any given inequality can be attained independently of the perturbation of any other inequality (except its pair), it is clear that no further enumeration is necessary. However, because with row dependency the maximum perturbation of an inequality is dependent upon the choice of $x \in F^0$, the values of $a_i^{\max}$ can not be determined in advance, but rather, must be obtained using the iterative cutting plane method of Friedman and Reklaitis (1974).

Let $\delta A^t(s)$ indicate the estimate at iteration s of the perturbations corresponding to terminal set t in which, say, k constraints are allowed to achieve their minimum perturbations and the remaining $M - k$ their maximum. Based on our previous work, the following large linear program written in terms of equalities must be solved iteratively:

$$\text{Minimize} \quad c\,x + c^-\,z^- + c^+\,z^+$$

$$\text{Subject to} \quad Ax = b$$

$$\begin{array}{ll} (A + \delta A^t(s))(x + x^+(s) - x^-(s)) = b & t = 1, \ldots, T \\ z^+ \geqq x^+(s) & s = 1, \ldots, n \\ z^- \geqq x^-(s) & \\ x \geqq z^- & \end{array}$$

where all variables are non-negative and n is the current iteration number.

After each iteration the estimates $\delta A^t(s)$ are updated following the procedure of Friedman and Reklaitis, and as shown there, the iterations will terminate in a finite number of steps. However, although the above problem is amenable to decomposition techniques, it is clear that given a reasonably large LP problem to begin with the above subproblem can grow to impractical size.

Fortunately in most applications involving equality constraints, one direction of constraint violation is significantly more important than the other. For example, if a specified demand is to be met, then underproduction is usually a more important violation than overproduction. Similarly, in blending operations, a composition below specifications is often more critical than a composition above specifications (or vice versa). In these situations, the perturbation analysis in all of the above three cases is simplified since only

TABLE 1. COMPOSITION AND COST DATA

Composition of component	Blend number 1	2	3	4	5
1	10	10	40	60	30
2	10	30	50	30	30
3	80	60	10	10	40
Cost, $/lb.	4.1	4.3	5.8	6.0	7.6

one direction of perturbation (that is, max or min) needs to be examined and hence the number of terminal sets is reduced.

Example 2

As an illustration of the techniques presented above, consider the following blending problem attributed to G. B. Dantzig:

It is desired to produce a product of composition (30, 30, 40) by mixing five available blends at least cost. The composition and cost data for the blends are given in Table 1. If x_i is the pound of blend i used per pound of product, then the blending problem can be represented by the following linear program:

$$\text{Minimize} \quad 4.1\,x_1 + 4.3\,x_2 + 5.8\,x_3 + 6.0\,x_4 + 7.6\,x_5$$

Subject to

$$\begin{bmatrix}10\\10\\80\end{bmatrix} x_1 + \begin{bmatrix}10\\30\\60\end{bmatrix} x_2 + \begin{bmatrix}40\\50\\10\end{bmatrix} x_3 + \begin{bmatrix}60\\30\\10\end{bmatrix} x_4 + \begin{bmatrix}30\\30\\40\end{bmatrix} x_5 = \begin{bmatrix}30\\30\\40\end{bmatrix}$$

and all $x_i \geqq 0$

The solution to the problem is $x_1 = x_3 = x_5 = 0$, $x_2 = 0.6$, $x_4 = 0.4$ and the optimum cost is \$4.98.

Now suppose that the indicated compositions are subject to variation and that the tabulated quantities are therefore mean values. The range of variation $\pm\,\alpha_{ij}$ of each composition is given in the array,

$$\alpha = \begin{bmatrix}0 & 2 & 4 & 0 & 3\\ 0 & 6 & 5 & 3 & 3\\ 0 & 0 & 1 & 1 & 0\end{bmatrix}$$

Since, regardless of the variations, the sum of the compositions of each blend must equal 100, the linear program under uncertainty is one with column dependence. In order to determine the family of terminal perturbation sets, the partial enumeration scheme for Case II must be employed.

First, using Equation (6), $\delta A^{\max}$ is computed,

$$\delta A^{\max} = \begin{bmatrix}0 & 0 & 1 & 1 & 0\\ 0 & 2 & 4 & 0 & 3\\ 0 & 2 & 5 & 1 & 3\end{bmatrix}$$

Following Step O, with $p = 1$, the combinations

$$(+1,\ +2,\ +3),\ (+1,\ +2,\ -3),\ (+1,\ -2,\ +3),\ (+1,\ +2,\ -3)$$

are examined. Of these only the third is permissible; hence, $\phi_1 = (1,\ -2,\ 3)$ and $\phi_2 = (-1,\ 2,\ -3)$. The complements relative to $\mathcal{M} = (\pm 1, \pm 2, \pm 3)$ will be

$$J_1 = (-1,\ 2,\ -3) \quad \text{and} \quad J_2 = (+1,\ -2,\ 3).$$

Thus, $T = 2$ and Step O is completed. We continue with Step 1 with $l = 1$. The candidate sets will consist of all pairs where the first is chosen from J_1 and the second from J_2; hence $(-1, -2)$, $(-1, 3)$, $(2, 1)$, $(2, 3)$, $(-3, 1)$, $(-3, -2)$. Of these, only the second and fifth are permissible. Consequently

$$\phi_3 = (-1,\ 3) \qquad \phi_4 = (1,\ -3)$$

and the complements will be

$$J_3 = (+1,\ \pm 2,\ -3) \quad \text{and} \quad J_4 = (-1,\ \pm 2,\ +3)$$

Since, now $l = 2$ and $\bigcap_{i=1}^{4} J_i = \phi$, the process terminates with four terminal sets and the following corresponding perturbations:

$$\delta A^1 = (-\delta a_1^{\max},\ \delta a_2^{\max},\ -\delta a_3^{\max}) = -\delta A^2$$
$$\delta A^3 = (-\delta a_1^{\max},\ \delta a_2,\ \delta a_3^{\max}) = -\delta A^4$$

where δa_2 is chosen so that the column coefficient restrictions.

$$\sum_{i=1}^{3} \delta a_{ij} = 0, \quad j = 1, \ldots, 5$$

are satisfied.

Given a flexibility cost of say, 10% of the cost of each blend itself, the optimal blend will be obtained as a solution to

$$\text{Minimize} \quad c\,x + 0.1\,c\,z^+ + 0.1\,c\,z^-$$

$$\text{Subject to} \quad A\,x = b$$

$$(A + \delta A^t)(x + x^+(t) - x^-(t)) = b$$
$$z^+ \geqq x^+(t) \qquad t = 1, 2, 3, 4$$
$$z^- \geqq x^-(t)$$
$$x \geqq z^-$$

where A is the initial 3×5 array;
b is the initial right-hand side vector (30, 30, 40);
c is the cost coefficient vector

(4.1, 4.3, 5.8, 6.0, 7.6);

and δA^t are the terminal perturbations given above. The optimum cost with flexibility is 5.1735 and the optimum blend, $x^* = (0.0115, 0.5839, 0.0115, 0.3931, 0.)$ The required flexibility is

$$z^+ = (0.0603,\ 0.00793,\ 0.088,\ 0.0272,\ 0.)$$
$$z^- = (0.0115,\ 0.0760,\ 0.0115,\ 0.0844,\ 0.)$$

Hence, in order to operate feasibly and optimally within the assumed uncertainties in the model, provisions must be made to allow the blend to vary in the range

$$0 \leqq x_1 \leqq 0.0718$$
$$0.5079 \leqq x_2 \leqq 0.5918$$
$$0 \leqq x_3 \leqq 0.0995$$
$$0.3087 \leqq x_4 \leqq 0.4203$$

Note that the "best estimate" solution does not quite fall in this range.

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NOTATION

a_{ij} = coefficient of the linear constraints
b_i = constraint right-hand side
c_i = cost coefficient
c_i^+, c_i^- = costs of flexibility to operate above or below the calculated optimal policy
$d(x, F)$ = distance from x to the set F
q, p_j = coefficients of a separating hyperplane
x_j = primal variable
$x_j(t)$ = correction variable for terminal set t
y_j = dummy variable
z_j = maximum correction vector
A = matrix of constraint coefficients
$B(\ )$ = flexibility set for the point in brackets
C = set of indices of columns which have a dependency in the coefficients of that column

$F(\ )$ = perturbed feasible region resulting from the perturbation in the parenthesis
F^0 = unperturbed feasible region
F^* = permanently feasible region
$I(\ )$ = set of indices of the constraints tight at ( )
J_t = complement of ϕ_t
N = number of primal variables
M = number of constraints
P = set of permissible perturbations in the model coefficients
R = set of indices of rows which have a dependency in the coefficients of that row
T = number of terminal sets
α_{ij} = bounds on the perturbations in the a_{ij}
β_i = bounds on the perturbations in the b_i
μ_{ij} = coefficients of the row dependency equations
η_{ij} = coefficients of the column dependency equations
ϕ_t = set of indices of those constraints of terminal set t which are perturbed to their maximum values
$\rho(\ )$ = radius of the flexibility set
$\mathcal{M}$ = set of integers between $-M$ and $+M$
$\mathcal{F}$ = set of all perturbed feasible regions
Superscripts = elements in a sequence
Subscripts = component of a matrix
Prefix δ = a perturbation of the quantity following it

Mathematical Symbols

ϵ = a member of
$\neq$ = not equal to
ϕ = empty set
$\cap$ = set intersection
$\cup$ = set union
$\subset$ = set inclusion
: = such that
$\|\ \|$ = Euclidean norm

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Synthesis of Fault Tolerant Reaction Paths

The problem of synthesizing an optimal low risk reaction network from unreliable reactions is formulated. An expected cost criterion function for decision-making is derived both for the case of a continuously operating network of reactions and for the case of reaction paths that involve batch reactions. It is shown that in general the decision space has a nonserial structure and the search for the optimal path will involve use of network search methods. An example is given where the optimal reaction path is synthesized for deoxyribonucleic acid. This example demonstrates the decision-making strategy for a class of batch reaction systems.

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SCOPE

In planning the synthesis of even the simplest of molecules, the possibility of failure at each step must be carefully considered. In general, the best synthetic plan involves the conversion of the most readily available and cheapest raw materials into the desired product in the fewest number of routine steps and in the highest possible yield. The objective function which is used to measure the success of a synthetic plan will depend on the context under which the synthesis is executed. In large-scale industrial syntheses, the costs of raw materials and operations and the safety of the processing system are of major importance. In syntheses performed in the laboratory the speed and ease with which a compound can be obtained is of more interest.

In either case the reliability of the synthetic plan must be considered. In industrial syntheses a given synthetic plan may be abandoned because raw material costs have changed, because a catalyst is poisoned by an impurity, because an unforeseen impurity is difficult to separate, or because mechanical equipment required to handle the reaction mixture and products cannot be reliably designed or maintained. In the laboratory an intermediate may be too unstable to store or too insoluble to allow use of convenient laboratory apparatus. In addition, there may be no analytical technique suitable for characterization of the reaction products. Problems of this sort are difficult to anticipate and sometimes economically impossible to overcome. For this reason a synthetic plan which contains reliable reactions and alternate routes or convenient detours will be wiser and safer than one whose success is wholly dependent on one critical reaction. In this paper a strategy is presented for finding synthesis pathways which have a low risk and still maintain the desirable features