STATE OF THE ART CONSTRAINED OPTIMIZATION TECHNIQUES

by

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Optimization plays a major part in industrial chemistry and process engineering. Here current methods for solving constrained optimization problems are discussed, analyzed and compared.

We begin by describing with simple analogies the behavior of constrained problems and optimality conditions. Three examples familiar to industrial chemists and process engineers are then described and formulated as constrained optimization problems, or nonlinear programs. Next we survey state-of-the-art strategies for solving smooth optimization problems. These are divided into three broad classes:

1) Active set strategies which optimize reduced problems in the space of "free" variables.

2) Penalty function methods which add penalties due to violated constraints to the objective function and perform unconstrained minimizations.

3) Successive approximation programming which approximates the nonlinear program by linear or quadratic programs that are easily solved.

Advantages and disadvantages of these methods and current computer programs that use these strategies are discussed.

Finally, some general guidelines for formulating the nonlinear programming problem and obtaining appropriate results from available optimization methods are presented.

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Introduction

Optimization plays an important part in many areas of chemistry and chemical engineering. To help motivate this talk we will consider three simple yet typical problems of interest to industrial chemists and chemical engineers. First, however, some concepts of optimization of smooth functions will be reviewed.

Very often the optimization problem can be formulated as the minimization of a smooth (i.e., differentiable) objective function subject to smooth inequality and equality constraints. This problem is termed a differentiable nonlinear program (NLP) with the following mathematical form [1]:

$$\begin{aligned} &\text{Min } f(x) \\ &\text{Subject to: } g(x) \leq 0 \\ &\qquad\qquad\quad h(x) = 0 \end{aligned}$$

Here f is a scalar function, x is an n-dimensional vector of decision variables, g is an m-vector of inequality constraint function, and h is a k-vector of equality constraint functions.

In two dimensions the problem has a very simple physical analogy. Consider a smooth valley enclosed by fences. Now a sphere in this valley will roll to the lowest (minimum) point and stop. At this stationary point the surface will either be flat or the sphere will be restrained by one or more of the fences (inequality constraints). If, in addition, the sphere is forced to roll on a smooth rail (equality constraint) the sphere will seek the lowest point on the rail if either the surface parallel to the rail is flat or the sphere is again pinned by one or more fences. This concept can be summarized in very elegant, mathematical terms by the necessary Kuhn-Tucker conditions for optimality [2]:

$$\nabla f(x) + \nabla g(x)u + \nabla h(x)v = 0 \qquad (1)$$

$$g(x) \leq 0 \qquad (2)$$

$$h(x) = 0 \qquad (3)$$

$$u \geq 0 \qquad (4)$$

$$u^T g(x) = 0 \qquad (5)$$

Equation (1) merely states that the gradient of the surface and the normal directions of the fences or rails (in which force is exerted) need to be balanced with an m + k vector of weights (u, v) as shown in Figure 1. Note that the surface is not necessarily flat at this optimum. Only if the weights are zero and $\nabla f(x)=0$ can the surface be flat. Equations (2) and (3) state that the optimum must be in the feasible region. Equation (4) states that force exerted by the fences can only be in one direction while equation (5) states that the weight u_i may be positive when the sphere is at the fence ($g_i=0$), but zero otherwise ($g_i<0$).

With the analogy of the smooth valley one can easily see the possibility of several local minima. Sufficient but very restrictive conditions for having only one minimum are the following:

1. The valley surface (the function f(x)) must be convex.

2. If inequality constraints (the fences, $g \leq 0$) are present, these must be convex also.

3. If equality constraints are present, the functions h(x) •ust be linear.

The above conditions guarantee [1] that only one minimum is present although there is an infinite number of single minimum problems that do not satisfy these conditions. Among these are many problems routinely considered by industrial chemists and engineers.

Example Problems

Now that some concepts of optimization have been reviewed let us consider some typical chemical and engineering problems and discuss their formulation and solution as nonlinear programs.

1. Chemical equilibrium

Consider the following sequence of gas-phase reactions:

$CH4 + H_20 \wedge CO + 3H_2$ (r^

$CO + H_20 \wedge \wedge C0_2 + H_2$ (r_2)

present in steam reforming[3,4]. We let both reactions be in equilibrium and need to compute compositions at T=1067K and P=1.235 HPa. To solve this problem we must first realize that:

a. mass is conserved and moles can be calculated from extents of reaction.

b. Gibb's free energy of the system is minimized.

Moles of each compound can be written as:

CH_4: $n_1 = n_1^o - \xi_1$

H_2O: $n_2 = n_2^o - (\xi_1 + \xi_2)$

CO: $n_3 = n_3^o - (\xi_1 - \xi_2)$

$C0_2$: $n_4 = n_4^o + \xi_2$

H_2: $n_5 = n_5^o + 3\xi_1 + \xi_2$

where §i and ξ_2 are the extents of reactions ri and *ri* , and i^ and n£ are final and initial moles of species i. The total free energy of the system is given by:

$$G = \sum_{1-1}^{5} n_i G_i$$

where

$$Q_i - G_i^o + RT\, In\, (\frac{n_i p}{n})$$

$$5\ 'hi^{n}.i$$

It can easily be seen that the corresponding nonlinear program is:

$$\text{Min} \sum_{i=1}^{5} n_i (G_i + RT\, in(\frac{\wedge i P}{n}))$$

$$h_i = n_i^o + \sum_{j=1}^{2} \upsilon_{ij}\xi_j - n_i = 0 \quad i = 1,5$$

s.t.

$$h_6 = \bar{n} - \sum_{i} n_i = 0$$

$$g_i = n_i \geq 0 \quad i = 1,5$$

$$g_6 = \xi_1 \geq 0$$

$$g_7 = \xi_2 \geq 0$$

where υ_{ij} are the stoichiometric coefficients of species i in reaction j. The problem has eight variables (n_i, $\bar{n}$, ξ_1, ξ_2), six equality constraints and seven inequality constraints for nonnegativity. Only two degrees of freedom are present and it is easily seen by manipulating the variables n_i and ξ_2 and solving for the other variables, the problem is a minimization in only two dimensions, bounded by nonnegativity of n_i.

Although this simple problem cam easily be solved by introducing equilibrium constants, the nonlinear programming formulation (modified by using atom baaances instead of extents of of reaction) allows straightforward generaaizations of the equilibrium problem to large multiphase, multiple reaction cases and even situations where not all reactions may be at equilibrium.

2. Nonlinear Regression of Reactor Data

Consider the stirred tank reactor in Figure 2, and the consecutive reaction:

$$A \xrightarrow{r_1} B \xrightarrow{r_2} C$$

with unknown kinetics. We postulate a general power law rate expression for both reactions and an Arrhenius temperature dependence on the rate constant. If the density of reactant and effluent streams remains the same, we can write the modeling equations as:

$$C_A - C_{A0} + \tau r_1 = 0$$

$$C_B - C_{B0} + \tau(r_2 - r_1) = 0$$

$$C_C - C_{C0} + \tau r_2 = 0$$

$$r_1 = k_{10} e^{-E_1/RT} C_A^m$$

$$r_2 = k_{20} e^{-E_2/RT} C_A^p C_B^q C_C^r$$

where $\tau = V/F$, the residence time. By varying temperature and residence time of the species we can measure steady-state concentration of the three species and fit these data to find unknown power law exponents, activation energies and preexponential coefficients. A crude but conceptually easy formulation of the regression problem is to minimize the weighted sum of squares of the error between the measured data and the model prediction for experiment all experiments j:

$$\text{Min} \sum w_{ij}(C_{ir} - C_{Ai})^2 +$$

$$+\sum w_{2j}(c_B - c_{B0} - T(V\ r_1))_j^2$$
$$+\sum w_{3j}(V\ c_{CO} + r_2)_j^2$$

where ri and 12 are given above and we minimize with respect to m, n, p, q, s, k_{10}, fc^ and E^ and E_2 . This problem may be formulated as an unconstrained minimization or with bounds on the decision variables posed as inequality constraints. Alternatively, all of the predicted concentrations could be represented with modeling equations as equality constraints.

A large part of nonlinear regression and parameter estimation lies in formulating the problem as a nonlinear program and applying an efficient algorithm to solve it.

3. Process Flowsheet Optimization

The above applications represent localized applications of optimization, in that a particular system is modeled and solved. Process optimization frequently involves the integration of several systems and consideration of the interactions of these systems when formulating the nonlinear program. As an example we will consider the classic process problem of Williams and Otto[5]«

Figure 3 gives the flowsheet of a fairly simple chemical process. Two feed streams of pure A and pure B are mixed with a recycle stream and react xn a stirred tank reactor. The following reactions take place:

A + B-* C	r^
C + B-* P + E	r_2
P + C-* G	r_3

Each reaction rate observes an elementary second order rate law with an Arrhenius temperature dependence, i.e.,

$$r_i = k_{oi} e^{-E_{ai}/RT} F_{Ri} F_{R2}$$

where FRii^nd F_{Ri2} are flowrates for reactants 1 and 2 of reaction i. The reactor effluent is cooled by a heat exchanger. After an oily waste product, G, is removed, the mixture is transferred to a distillation column where the valuable product P forms the overhead. The bottoms product consisting of 10% P in E (an azeotrope) and C is split into two streams; one is recycled to the reactor, the other is burned as fuel.

The objective is to maximize the annual rate of return on plant investment, so we can pose the objective function as:

$$\text{Min} - 100\ |8400[(0.3F_P + 0.0068F_D>(0.876)$$

(* sales; overhead factor)

$$- (0.02F_A - 0.03F - - 0.0U-_)]$$

(raw materials & waste)

$$- 60V_P - 2.22F_{O1}/\ 600V_P$$

(plant fixed charge (10% of investment); utility cost; plant investment)

The equality constraints for the optimization are the mass balances, reactor modeling equations and unit operations relationships for the process. An overall mass balance gives:

$$h_1 = F_A + F_B - F_G - F_P - F_D = 0$$

The composition of the azeotrope in the bottoms provides a P balance over the distillation column.

$$h_2 = F_{RP} - 0.1F_{RE} - F_P = 0$$

P in feed — P in bottom — P in overhead

An overall mass balance on E gives:

$$h_3 = (M_E/M_B) - \left({}_{F}Z_{R} \qquad D\ F_R F_p\ F_G \right) = 0$$

E formed in reactor — E lost in F_D

The nass balance for P is:

$$h_4 = C^k 2^F RB^F RC - \langle YV^k 3^F RC^F Rp \} {}^V p/{}^F R^2$$

P formed in reactor

$$- {}^F P - {}^F D\ t \langle {}^F RP - V' \langle {}^F R - F_G - F_P)] = 0$$

P in overhead — P in F_D

Remaining equations are:
Mass balance on A:

$$h_5 = \langle -{}^k F^F RA^F RB \rangle {}^V p/{}^F R^2 - W < V\ {}^F G - V\wedge\ {}^+ F A$$

formed — fuel — feed

Mass balance on B:

$$h_6 - F_B + (-\wedge\wedge - VRB^F RC \rangle {}^V p/{}^F R^2 - 'D\wedge BB\wedge R - {}^F P - {}^F G\rangle = 0$$

feed — formed — fuel

Mass balance on C:

$$h_7 = K\ V\ V\ {}^k l^F RA^F RB - \wedge/{}^M B > {}^k 2^F RB^F RC$$

$$- k_3 F_{RC} F_{RD}]V_p/F_R^2 - F_D F_{RC}/(F_R - {}^F P - {}^F G\rangle$$

formed — fuel

Mass Balance on G:

$$h_8 = \underset{\text{formed}}{V V k_3 F_{RC} F_{RP} V_p / F_R^2} - \underset{\text{waste}}{F_6} = 0$$

Definition of total reactor effluent, F

$$h_9 * F_R - F_{RA} - F_{RB} - F_{RC} - F_{RE} - F_G - F_{RP} - 0$$

The inequality constraints are limits on the reactor temperature:

$$580 * T * 680°R$$

the production rate

$$0 \leq F_p \leq 4763 \text{ lbs/hr}$$

and nonnegativity of all the flow rates: $F_i \geq 0$

and the reactor volume: $V \geq 0$

Overall, the problem has 13 variables, nine equality constraints, and 15 inequality constraints. This problem has been solved by many investigators using a number of methods [5-8].

Although the Williams-Otto model takes some work to derive, the problem is very simple compared to process optimization models routinely encountered in industry. Because of complicated modeling equations, complex physical property correlations, large numbers of components, and entangled recycle streams leading to many mass balance relationships, industrial processes are often modeled by many thousands of equations.

Solving these problems is very difficult and time-consuming. To aid in calculation, most companies use process simulators which greatly simplify the modeling but not the optimization. Only recently have techniques been applied which simplify the optimization step as well[9,10].

Having reviewed some detailed applications of constrained optimization, let us now consider some state-of-the-art tools that allow their solution.

Constrained Optimization Techniques

Methods for constrained optimization can be divided into three broad categories. These are:

1. active set strategies - where inequality constraints are added or dropped from the set of equality constraints. An unconstrained minimization then takes place in the reduced space of the remaining degrees of freedom.

2. penalty function methods - where the violated constraints form a penalty term in an extended or augmented objective function, on which unconstrained minimization can be applied.

3. successive approximation methods - where the nonlinear programming problem is approximated repeatedly by either a linear program (SLP methods) or a quadratic program (SQP methods).

Categories 1 and 2 use unconstrained minimization algorithms such as Newton's method, quasi-Newton methods or conjugate gradient methods. Excellent reviews of these methods are given in [11,12]. The last category uses standard linear or quadratic programming packages that are available in almost every computer installations library (e.g., MPS, simplex, QPSOL)•

Active Set Strategies

These algorithms choose a set of active constraints and then optimize a problem with fewer degrees of freedom. If the Kuhn-Tucker conditions are satisfied at this solution, the algorithm terminates. Otherwise the set of active constraints is changed and another unconstrained problem is solved.

The problem

$$\begin{aligned} &\text{Min } f(x) \\ &\text{s.t. } g(x) \leq 0 \\ &\quad\; h(x) = 0 \\ &L \leq x \leq U \end{aligned}$$

is modified by adding slack variables ($s \geq 0$) to inequality constraints. The set of variables is then partitioned into basic (dependent) variables, y, and nonbasic (independent) variables, z.

This problem.

$$\begin{aligned} &\text{Min } f(x) \\ &\quad g(x) + s = 0 \\ &\quad h(x) = 0 \\ &\quad L \leq x \leq U \\ &\quad s \geq 0 \end{aligned} \Bigg\rangle \begin{aligned} &h(z,y) = 0 \\ &(x,s) = (z,y) \end{aligned}$$

is then converted into a problem with simple bounds of the form:

$$\begin{aligned} &\text{Min } F(z,y(z)) \\ &\quad \text{s.t. } L \leq z \leq U \end{aligned}$$

Since the eliminated constraints, g and h, can be nonlinear and not directly reducible to form F, a reduced gradient is calculated and used to compute search directions for the unconstrained minimization.

Writing the gradient of F in terms of y and z gives

$$\frac{dF}{dz} = \frac{\partial f}{\partial z} + bz\,by$$

dy/dz is obtained by enforcing feasibility of the constraints and writing:

$$dh = 0 = \frac{\partial h}{\partial y}\,dy + \frac{\partial h}{\partial z}\,dz$$

$$\frac{dy}{dz} = -\left[\frac{\partial h}{\partial y}\right]^{-1}\frac{\partial h}{\partial z}$$

The reduced gradient is therefore

$$\frac{df_m}{dz} = \frac{\partial f_m}{\partial z} - \frac{\partial h}{\partial z}\left[\frac{\partial h}{\partial y}\right]^{-1}\frac{\partial f}{\partial y}$$

with (n-k) nonbasic variables, z_r and (m+fc) basic variables, y.

Several types of search directions are incorporated into active set strategies. Probably the most efficient is given in [13,14]. Here the nonbasic set is partitioned into the superbasic set, those variables between upper and lower bounds, and remaining variables which are at their bounds. The reduced gradient is then examined for each remaining non-basic variable to see if it should join the superbasic set. This occurs if the reduced gradient is negative (positive) and the variable is at its lower (upper) bound. The search direction is then set to zero for the remaining nonbasic variables and the unconstrained algorithm generates search directions for the superbasic set.

The earliest active set strategy is the simplex method of linear programming. If the problem is linear, the search direction for the variable z_j [15] is:

$$d_j = \begin{cases} 0 \text{ if } \left|\frac{dF}{dz_j}\right| \neq \max_k \left|\frac{dF}{dz_k}\right| \\ -\frac{dF}{dz_j} \text{ if } \left|\frac{dF}{dz_j}\right| = \max_k \left|\frac{dF}{dz_k}\right| \end{cases}$$

Rosen [16] proposed a similar orthogonal gradient projection algorithm which deals with linear constraints and uses - F as the search direction. Others [17,18,19] used quasi-Newton methods [20] with the reduced gradient.

In dealing with nonlinear constraints all reduced gradient algorithms linearize the constraints at the current iteration and calculate the reduced gradient. Some algorithms [21,14] then project into the hyperplane of the linearized constraints. Others, however, calculate the search direction and then adjust the basic variables so that equality constraints are always satisfied. This involves a few

Newton iterations of the form:

$$y^{i+1} = y^i - \left[\frac{\partial h^i}{\partial y^i} \right]^{-1} h(z^i, y^i) \qquad \text{with } z^i \text{ fixed}$$

At present there are three widely used optimization programs based on the active set strategy. GRG2[22] converges the equality constraints for every function evaluation. It uses quasi-Newton search directions on the reduced problem when the number of degrees of freedom is small or conjugate gradients when the reduced problem is large. A similar approach is used by VMP[18] but here a different projection strategy is used for the reduced problem.

MINOS[14] can project into the tangent hyperplane of the constraints without always satisfying equality constraints. This algorithm has been implemented as a very sophisticated and efficient package. Results on optimization test problems have shown that MINOS performs very well[23].

Penalty Function Methods

This is the earliest of the constrained optimization approaches [24,25]. Popularized by Fiacco and McCormick [26] as Sequential Unconstrained Minimization Techniques (SUMT), early penalty function concepts are now obsolete although extensions of their ideas have led to more current and efficient algorithms.

The SUMT philosophy involves the solution of a series of unconstrained problems on penalty functions made up of the objective function and constraints. Several types of penalty functions have been proposed. Two typical functions are the interior penalty:

$$P_I(x) = f(x) - \frac{1}{\alpha_i} \sum_{j=1}^{m} \frac{1}{g_i(x)}$$

(which uses feasible points and handles inequality constraints only) and the exterior penalty

$$P_E = f(x) + \alpha_i \left[\sum_{j=1}^{m} [\max(0, g_j(x))]^2 + \sum_{j=1}^{k} h_j^2 \right]$$

(which uses infeasible points). For a given α_i, the penalty function is minimized at $\bar{x}_i$, say. As α_i tends to infinity the sequence of $\bar{x}_i$ tends to the optimum $\bar{x}$. Figure 4 shows this approach on a one-dimensional problem. Penalty functions have the advantage of not having to track nonlinear constraints as active set strategies do. However, as $\alpha_i \to \infty$ the penalty function becomes more and more ill-conditioned, leading to a sequence of $\bar{x}_i$ that terminates before the optimum is found. Also, penalty functions are only as good as the unconstrained minimization algorithm used. If the surface is not

convex, the algorithm will fail and the penalty function algorithm terminates prematurely.

An exact penalty function:

$$P00 - f(x) + \alpha \; ||_{g+}, h||_p$$

- where $g_j^- = \max(0, g)$ and $||a||_p$ - p-norm of vector a -

$$= \left(\sum |a^p\right)^{1/p}$$

does not requires to tend to infinity to find the optimum. If [2]

$$a - \geq ||u, v|| < P\text{-iyp}$$

where u,v are the KKT multipliers at the optimum, then the minimum of the nonlinear programming problem is found at the minimum of the exact penalty. The disadvantage to this penalty function, however, is that * . it is not differentiate at the boundary of the constraints.

Another way of avoiding the requirement that or** is to add the terms $u^T g + v^T h$ to the exterior penalty function given above. For a finite or it can easily be shown that the minimum of this function under certain conditions will satisfy Kuhn-Tucker conditions for the HLP. The function:

$$L(x,u,v,\alpha) = f(x) + \alpha \left\| g_+ \right\|^2 + u^T g + v^T h + \alpha \left\| h \right\|^2$$

or equivalently

$$L(x,u,v,\alpha) = f(X) + \sum_{j=1}^{m} [(\alpha g_j + u_j)_+^2 - u_j^2] + \alpha \left\| h \right\|^2 + v^T h$$

is known as the augmented Lagrangian and was originally applied only to equality constraints[27]. The extension to inequality constraints leads to the above expression [28].

The optimization proceeds by minimizing L(x,u,v#) with respect to x, keeping u and v fixed. If constraints are satisfied, stop. Otherwise update u and v to maximize the augmented Lagrangian. The penalty parameter, or, is periodically increased if constraint violations are not reduced. The algorithm follows naturally from considering Kuhn-Tucker saddlepoint conditions[1]

$$f6H + u^T g(\bar{x}) + v^T h(\bar{x}) = f\,CX) + u^T g(\bar{x}) + v^T h(\bar{x}) = f(x) + \bar{x}i\backslash(k) + v^T h(x)$$

and merely consists of

$$\underset{U,V}{\text{Max}}\,[\underset{X}{\text{Min}}(L(x,u,v,cr)]$$

Several unconstrained algorithms have been applied to the inner minimization and outer maximization of L(x,u,v,cr). An excellent review of these augmented Lagrangian or multiplier methods is given in [29].

Successive Approximation Methods

These methods can be summarized by the following steps [30].

1. Form an approximate model of the NLP at the current point that can be solved by a standard algorithm (Linear or Quadratic Programming).

2. Let the solution d^i from the standard algorithm determine the search direction for the next point. If the direction is zero, stop.

3. Find a stepsize X along this search direction that gives a point which is "better" than the current point. Go to 1) with $x^{i+1} = x^1 + Xd^1$.

As mentioned above, the approximate model is solved either as a linear or quadratic program. For linear programming the approximate model is a simple linearization about the current point x^i, i.e.,

$$\begin{aligned} \text{Min} \quad & f(x^1)^{\wedge} \\ \text{s.t.} \quad & g(xj)jd = -g(xj) \\ & h(x^1)^{\wedge} = -htx^1) \end{aligned}$$

where d is the search direction found by the LP. Often limits must be placed on d because the LP model cannot take advantage of curvature of the original surface. In fact, adjustment of the extrapolation limit on d is very critical in the neighborhood of the optimum as oscillations usually occur.

Since their development in the late fifties and early sixties [30,31], SLP models have been widely used for refinery optimization and other large process problems that are mostly linear[32,33].

If a model approximation is made to a quadratic program the result is:

$$\begin{aligned} \text{Min} \quad & f(x^1)^{\wedge} + -|d^T Bd \\ \text{s.t.} \quad & g(3\text{Ç}^i) + gix^*)^T d = 0 \\ & h(ar) + hjx^1)^{\wedge} = 0 \end{aligned}$$

Again the nonlinear problem is linearized about x* but a quadratic term is added to the objective function. The matrix B is the Hessian of the Lagrangian at x^L[34]:

$$V_{xx}L(x^i,u^i,v^i) * V_{xx}f(x^i) + V_{xx}g(x^i)u^i + V_{xx}h(x^i)v^i$$

or its quasi-Newton[19] approximation. Here the multipliers u^1, v* are shadow prices from the quadratic program. Placing an extrapolation limit on d is not as critical here as with SLP, because the quadratic objective function includes curvature information from the NLP. In fact, if B is a quasi-Newton approximation to v L(x,u,v) and remains positive definite, no extrapolation limit on d is™ required.

For SLP methods the stepsize in step 3 is usually set to one and movement is dictated by the size of extrapolation limit. With SQP methods the stepsize is found by minimizing an exact penalty function along the search direction. Although this procedure worfcs very well, some difficulties have been reported[35,36].

SQP methods were initially discovered in 1963 [37,38] but have only recently been seriously improved and developed [34,39,40]. In general, applications of this method have been very successful. However some questions and difficulties must still be resolved.

Comparison of Methods

Of the strategies described above, only active set and successive quadratic programming methods should be seriously considered. Although penalty function methods provide a good conceptual grasp of the constrained problem, they are much less efficient and lead to computational problems as the penalty parameter goes to infinity.

Two very powerful computer packages that use active set strategies are MINOS[41] and 6RG2[22]. In numerical studies these codes have been shown to be very robust and efficient. Although the SQP method is easy to program with the aid of a standard quadratic programming package, only one version (VF02AD from the Harwell library) is commercially available at present [42]. In numerical comparisons [40,13], the SQP method has even outperformed some active set strategies. Current research on this method should make it more efficient, robust and reliable.

Conclusions - Tips for solving Optimization Problems

Having surveyed briefly some aspects of optimization techniques and applications, we conclude with a few guidelines for formulating optimization problems and choosing methods to solve them.

When formulating the optimization model, consider the simpler aspects first. Only when one understands the behavior and limitations of a simple model should he proceed, stepwise, to a more complicated one[43]. Starting with too complicated a model leaves no opportunities to backtrack and correct the formulation if the optimization fails.

Once formulated, the model and optimization approach should be checked for sensitivity to changes in the scientist's data. He should carefully consider what information the optimization study will provide and how changing prices, variable feedstocks and fluctuating equipment performance will affect these results.

Before applying an optimization technique to the model the scientist should check for inconsistent constraints or equations. For instance, the optimization will surely fail if two compositions sum up to one and both are constrained above 60%! Moreover, many inconsistencies appear subtly and are difficult to spot. Also the scientist should, if necessary, scale the variables so that they have similar orders of magnitude. The same should be done with objective and constraint functions and their gradients. Although poorly scaled models do not affect the theoretical solution of the problem, they introduce computational problems due to the computer's fixed precision.

Finally, in choosing an optimization method to solve the model, one should consider the following questions:

1. Are the modelled functions continuous and differentiate?
   If not, only very inefficient and time-consuming direct search

methods offer any guarantee of success. Although the optimization techniques surveyed above may still solve the problem, they could also jam into a corner and stay there.

2. Can gradients be calculated analytically?

Although the objective and constraint functions may be smooth, it may be difficult to calculate analytical gradients. Instead the derivative is obtained by perturbing the variable and measuring the effect on the function. To get an accurate measure of the gradient, the perturbation size must be chosen carefully. A good rule of thumb is to let the perturbation size be $\sqrt{\epsilon_f}T$ where ϵ_f is the relative function error [44].

3. What fcind of equality constraints are present and how should they be treated?

Each time the objective function is evaluated the algorithm could solve all of the equality constraints first. On the other hand, it could just linearize the constraints and project the objective function onto the linearized space. The latter approach allows the simulataneous optimization of the objective function and convergence of equalities.

If the number of equalities is small and the system is easily solved, following a feasible path is always a safe policy. Failure of the algorithm always yields an improved and usable point.

If the system of equations is large and difficult to solve, a feasible path policy may be grossly inefficient. Fortunately, SLP, SQP and MINOS are well-suited to the linearized approach. In the absence of degrees of freedom they all degenerate to a damped Newton method for solving nonlinear equations. Moreover, if the constraints are linear, this problem can be handled very easily by the above three methods.

Summary

In this paper we surveyed some current methods for constrained optimization. Presently, the best methods are active set strategies, such as MINOS and GRG2, and SQP methods.

We began with a simple analogy to constrained optimization and formulated three chemical problems as nonlinear programs. After reviewing current optimization techniques we concluded with some guidelines for their application.

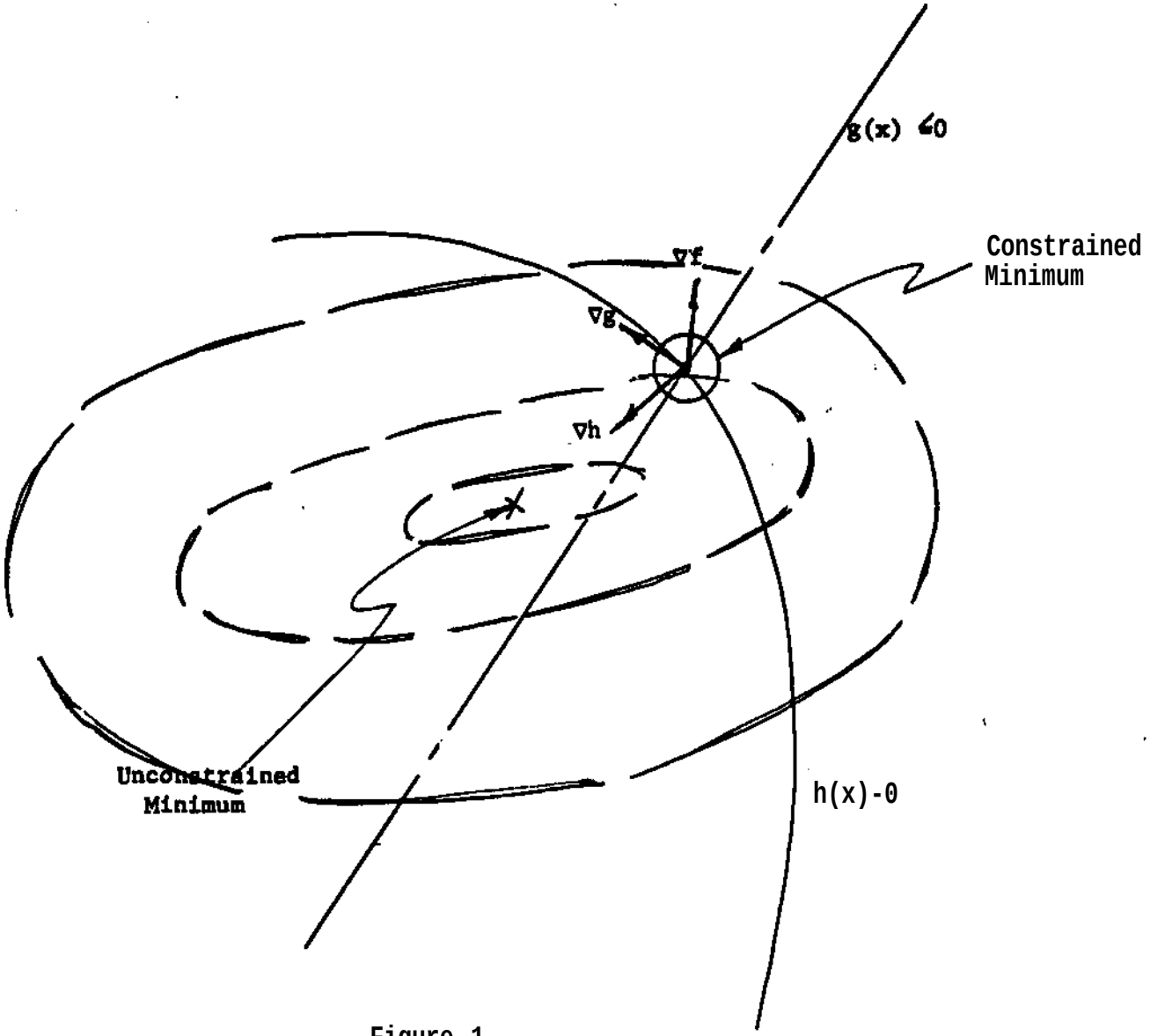
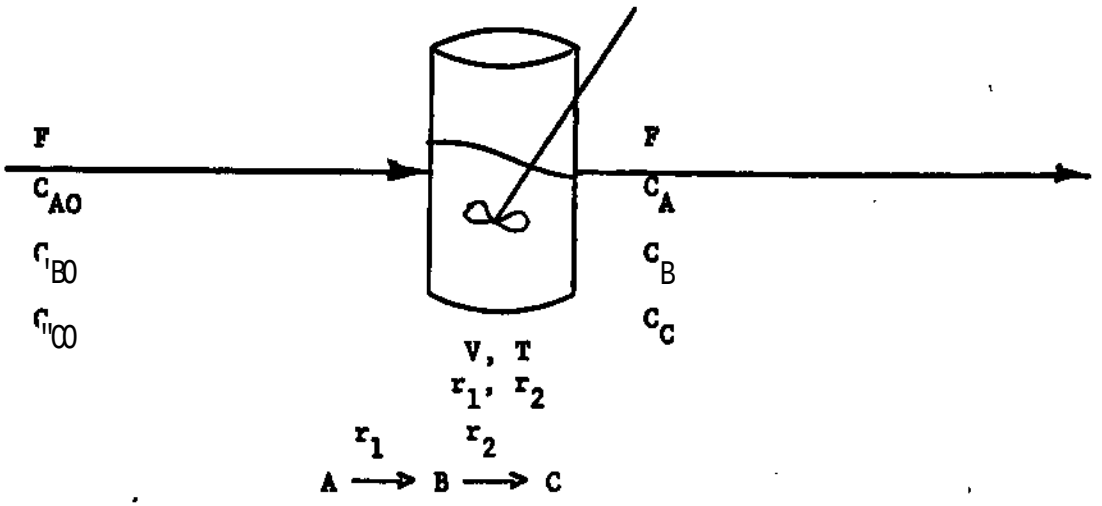


Figure 1.

Two-Dimensional Contour of Smooth Valley



$$r_1 = k_{10}\exp(-E_1/RT)c_A^m c_B^n$$

$$V \quad {}^{k}20^{ex}P<-{}^{E}2/{}^{RT}>{}^{C}A^{Pc}BV$$

Figure 2. Stirred Tank Reactor Nonlinear **Regression**

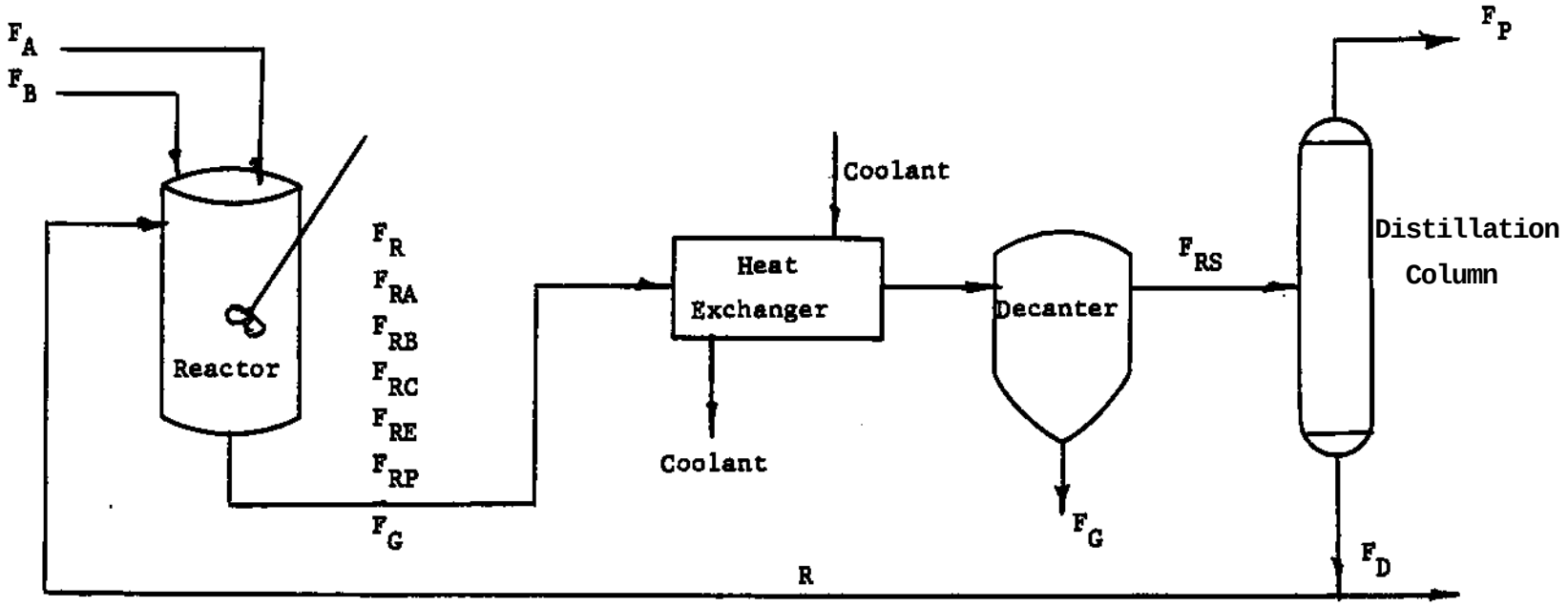


Figure *3.*
Williams-Otto Problem
Flow Diagram

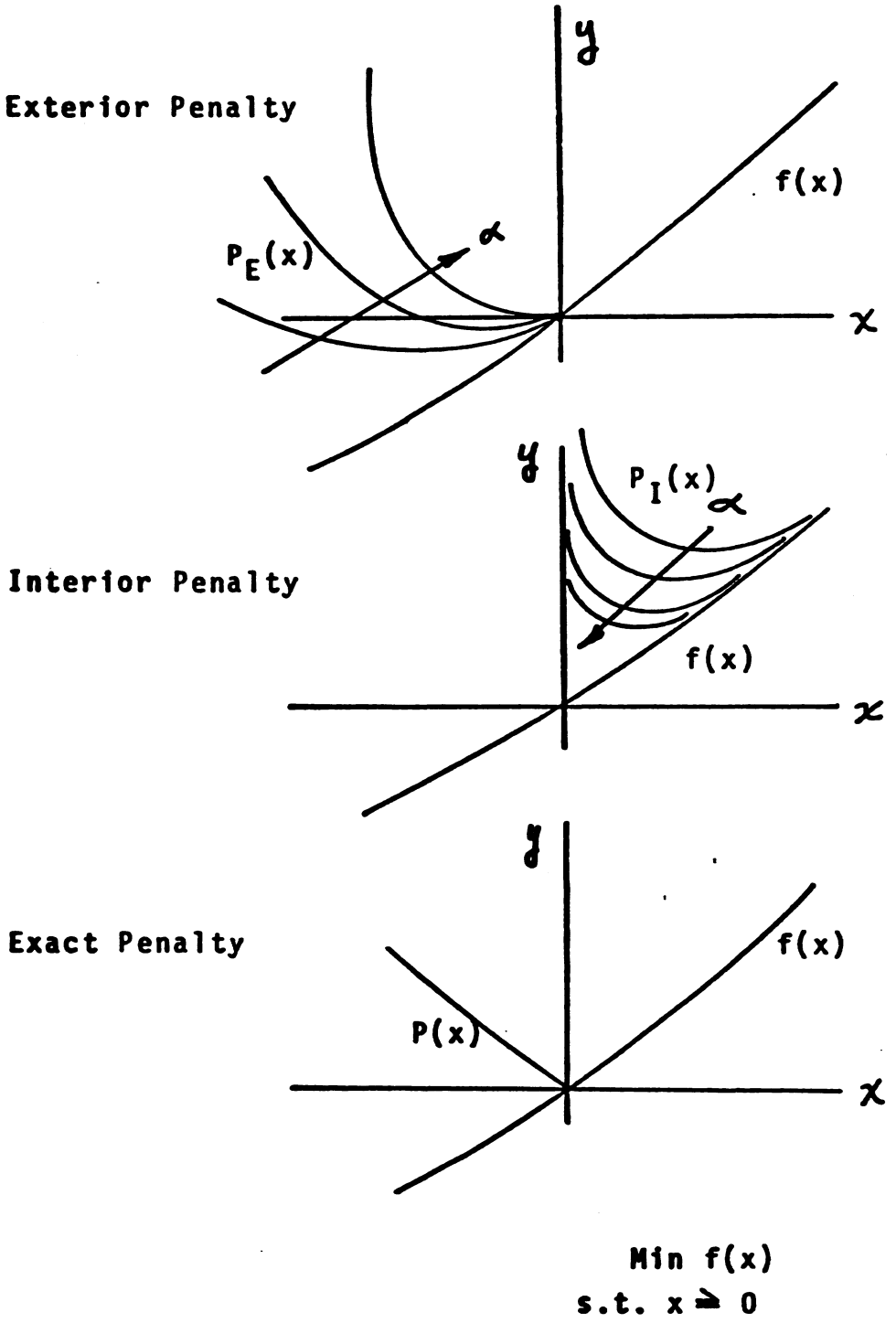


Figure 4.

Penalty Functions for

Constrained Minimization

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