A NOTE ON APPROXIMATION TECHNIQUES USED TOR PROCESS OPTIMIZATION

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DRC-06-61-84

December, 1984

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ABSTRACT

The need for increasingly complex models for process simulation has led several researchers to develop more efficient steady-state simulation strategies. In a common approach, rigorous physical property calculations are replaced by simplified ones which approximate locally the behavior of the rigorous ones. Periodically the rigorous models are executed to check if the simplified ones are still accurate enough, and, if not, parameters for the simplified ones are adjusted so both the rigorous and simplified models again predict the same values locally. Convergence is assumed when no adjustments are needed for these parameters and the simplified model is converged.

This approach works well for phase equilibrium and even general process simulation problems. Some researchers have extended this approach to optimization problems as well. In this Note we discuss problems which arise when adapting this approach for process optimization problems. We also present three examples where the use of simplified models can lead to detection of false optima or convergence failures.

INTRODUCTION

In order to model physical and chemical properties efficiently, engineers have usually resorted to simplified correlations and shortcut procedures. As physical property and unit operations models have become more complex, these procedures have found wide use in computer-aided process design and simulation.

To aid in solving flash problems with complex models, approximate methods have been proposed [1,2] which embed simplified models into the calculation loop. Parameters for these models are found by matching properties calculated by the simplified models with those computed by the rigorous models. The flash problem is then solved using the simplified models. After solution, parameters are updated by matching properties again and the iteration repeats. Using this procedure investigators have reported significant reductions in computational effort (see [1-4]).

Boston and Britt [3] proposed the "inside-out" flash algorithm which totally recasts the problem in terms of simplified models. Here the major iterations deal with updating the parameters for simplified models and matching their properties with a rigorous model. Since rigorous models are evaluated in an outer iteration loop, considerably less effort is required than with conventional procedures. The investigators report that the algorithm works well for several types of flash problems and physical systems. Extensions of this approach have also been made to absorption and distillation problems [4].

Recently, this approach has also been extended to general plant-wide simulation and optimization problems. Again, parameters for simplified process models (such as Kremser equations and extent of conversion reactors) are found by matching the models with rigorous model properties in the outer loop. The simplified simulation or optimization problem is then solved and control returns to the outer iteration loop where model parameters are updated. Applied to general simulation and optimization problems, this approach requires far less computational effort than with other approaches [5,6] because rigorous model properties are calculated much less often. For the sake of brevity we will refer to this approach as the "inside-out" procedure.

What is overlooked, however, is that for optimization problems, the approach based on simplified models can converge to a solution that may not necessarily correspond to the optimum found when only rigorous methods are used. In the next section we discuss why this situation may arise and present three examples that illustrate difficulties for simplified models in converging to the optimum predicted by using only rigorous models. The first two examples show that convergence to the true optimal solution is not obtained, while the third example fails to converge to any solution when one in fact exists.

Comparison of Rigorous and Inside-Out Optimization Procedures

The inside–out procedure consists of applying simplified models over a small region to approximate rigorous hard-to-calculate models. Let a be properties calculated by the rigorous models p(x,y,a,r) such as K values or liquid and vapor enthalpies, where:

x are decision variables such as reactor pressure

y are process (dependent) variables such as stream flowrates or compositions

T are values from process database such as pure component properties or cost coefficients.

The optimization problem, when modelled rigorously, can be described as:

$$\begin{aligned} &\text{Min} \quad rf(x, y_f<^*) \\ &\text{s.t.} \quad g(x,y,or) \,*0 \qquad\qquad (1) \\ &\qquad\quad \mathbf{h(x,y,\alpha)} - 0 \\ &\qquad\quad or - p(x_f y, offY) - o \end{aligned}$$

where we distinguish between process equations that contain rigorous models (o - p(x,y,o,Y)) and the rest (h(x,y,a) = 0). At the optimum the Karush-Kuhn-Tucker (KKT) conditions for this problem are:

$$\begin{bmatrix} \nabla \\ \nabla_{\alpha}\phi \end{bmatrix} + \begin{bmatrix} \nabla_x g & -V'' \\ \nabla & -\nabla \\ \nabla & I-\nabla_{\alpha} p \end{bmatrix} \begin{bmatrix} -u \\ v \\ t \end{bmatrix} = 0 \qquad (2)$$

$$g(x,y,\alpha) \leq 0$$

$$h(x,y,\alpha) = 0$$

$$\alpha t - p(x,y,cr,Y) = o$$

$$a \geq 0$$

$$\alpha^{T} g(Xty»cr) = 0$$

where u,v, and t are corresponding multipliers for the three types of constraints.

Consider the inside-out formulation of this optimization problem. Here the rigorous Models are replaced by simplified models, a-K(x,y,a,B) = 0, with parameters S determined by setting

$$\text{or} - p<x,y,cr,Y) = K(x,y,\alpha,\beta) \qquad (3)$$

in the outer iteration. The "inside-out" optimization algorithm [5] is thus:

Step 0) Guess B^{α},x,y, select a tolerance e and set i=0.

Step 1) Solve the optimization problem with simplified models.

$$\bar{x},\bar{y} - \arg\{\text{Min } rf(x,y,ar) \quad \text{s.t. } g(x,y,Qf) < 0 \quad h(x,y,of) = 0 \quad a - K(x,y,ar,3^{i}) =\bullet 0\} \qquad (4)$$

Step 2) Solve for $\bar{a}$ «.$p(\bar{x}_9\bar{y}_9<\bar{i}9Y)$«

Step 3) Calculate $\bar{B}$ from $\bar{a}$ and $K(\bar{x},\bar{y},\bar{a},?)$. Define $f = \bar{B}\text{-}8^{i}$. If $f^{T}f$ < c, stop. Otherwise, let $fl^{i+1} = B^{i} - H f$, where H is the Jacobian (af/38) or its approximation, depending on the outer loop convergence method.

Step 4) Set i = i+1, and go to Step 1).

The following conditions will hold at the final solution from Step 1).

$$\begin{bmatrix} v \\ V \\ 7_{Of}{}^{4} \end{bmatrix}^{\bullet} + \begin{bmatrix} \nabla_{x}g & {}^{7}X^{h} & -V \\ V & {}^{7}{}_{y}{}^{h} & -V \\ V & {}^{7}h_{or} & 1\text{-}7_{or}K \end{bmatrix} \begin{bmatrix} u \\ v \\ t \end{bmatrix} = 0 \qquad (5)$$

$$g(x,y,\alpha) < 0$$
$$h(x,y,\alpha) = 0$$
$$ce - K(x_t y_{>Q} r,3) - 0$$
$$u^{T}g(x,y,or) - 0$$

In order for the optimum of the rigorous problem $(\hat{x},\hat{y},\hat{a})$ to match the solution from Step 1, it is* clear by comparing (2) and (5) that a sufficient condition is that $V_x K = V_{x^{r>}} p$, $V_y K = V_{y^{r}} p$ and $V_a K = 7_{o^{r}} p$ at the optimum. Otherwise, the inside-out algorithm may not recognize the rigorous optimum and not terminate at this point. To illustrate this problem, consider the following examples.

Example 1 (Recognition of different optima)

The simple algebraic optimization problem:

$$\begin{aligned} \text{Min} \quad & (a - 1/2)^2 + (x - I)^2 \\ \text{s.t.} \quad & \alpha \geq 0 \ , \ x \geq 0 \\ & a - [(x\text{-}1)^3 + (x\text{-}1)^2 + l] - 0 \end{aligned} \qquad (6)$$

is pictured in Figure 1. Here Che "rigorous model" is defined by the equality constraint:

$$cr - (x-1)^3 + (x-1)^2 + 1 \tag{7}$$

and we propose the simple, approximate model:

$$a - K(x,3) \approx x + 3 \tag{8}$$

The inside-out optimization problem thus becomes:

Match: $$\bar{a} - (\bar{x}-1)^3 + (\bar{x}-1)^2 + 1 - \bar{x} + 0 \tag{9}$$

Solve: $$\text{Mia} \quad (cr-1/2)^2 + (x-1)^2 \tag{10}$$

$$a \geq 0 \quad x \geq 0$$

$$cr - (x + 3) - 0$$

The optimum of the rigorous problem is clearly at point A in Figure 1. Because the sets y and h are empty in this problem, the optimality conditions are:

$$\begin{bmatrix} \nabla_x \phi \\ \nabla_\alpha \phi \end{bmatrix} + \begin{bmatrix} \nabla_x g_1 & \nabla_x g_2 & -\nabla_x p \\ \nabla_\alpha g_1 & \nabla_\alpha g_2 & 1-\nabla_\alpha p \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ t \end{bmatrix} = 0 \tag{11}$$

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 5 \\ t \end{bmatrix} = 0$$

g_1 and g_2 are not active so $u_1 = u_2 = 0$ and $t = -1$. Applying these conditions at point A for the simplified problem shows the following:

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} -1 & 0 & -1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ t \end{bmatrix} = 0 \tag{12}$$

Again, the inequality constraints are inactive and $u_1 = u_2 = 0$, but now no value of t can satisfy the above conditions. In fact, if we initialize at point A, the inside-out algorithm actually moves away to point B. We illustrate this behavior with the following iterations:

i = 0 : Start at optimum, point A. x = 1, a = 1

The solution to:

$$\begin{aligned} &\textbf{Min} && (cr-1/2) + (x-1)^2 \\ &\text{s.t.} && cr \wedge 0 \ , \ x \pounds 0 \\ & && cr - (x + fl) - 0 \end{aligned}$$

is $x - r - 3*/2$ **if** $a \wedge 0$ **and** $x \wedge 0$.

Step 0) $x + P^\circ - (x-1)^3 + (x-1)^2 + 1$ **at point A**

1) $3^\circ - 0 \ , \ \bar{x} - 3/4$

2) $\bar{\bar{\alpha}} - (\bar{x}-1)^3 + (\bar{x}-1)^2 + 1 - 1.046*$

3) $\bar{f} - \bar{a} - \bar{x} - 0.2969$

$f - f - 3^1 - 0.2969$

Use discrete Newton method to calculate B^i for next iteration: 6' = 0.1, $\bar{x}^*$ - 0.7, ?• = 0.363, f• = ?' -B' = 0.263

$$\overline{d\beta} \cdot \quad \beta' - \beta$$

$$\beta^1 = \beta^\circ - \pounds^1 \| f \| 0\,1856$$

i = 1 :

1) $3^1 - 0.856$, $\bar{x} - 0.322$

2) $\bar{a} - 1.148$

3) $F - 0.826 \quad f - F - 3^1 - -0.03$

Use secant method for next 6

$$B^Z - 3^1 - f^1 \frac{<eV>}{(f_{i-1} - f_{i-2})} - 0.777$$

i = 2 :

1) $3^* - 0.777$, $\bar{x} - 0.3615$

2) $\bar{or} - 1.1474$

3) $F « 0.786 \quad f - F - 3 - 9\text{-}10^{-3}$

$$\beta^3 = \beta^2 - f^2 \frac{(\beta^2 - \beta^1)}{(f^2 - f^1)} = 0.795$$

i » 3 ;

1) $3 - 0.795 \quad \bar{x} - 0.3525$

2) $\bar{a} - 1.1475$

3) $F - 0.795$, $f - F - 3 « 0$

As seen in Figure 1, the solution at point B of the inside-out optimization problem is feasible but clearly suboptimal. In the next example, we see that even if the KKT conditions of the inside-out problem are satisfied at the optimum of the rigorous problem, failure can still occur if the gradients of the rigorous and approximate models are not the same at all points.

Example 2 (Convergence to wrong solution)

Consider the following optimization problem and the corresponding inside-out problem with a very simple approximate model:

Rigorous		Inside-Out		
		$\bar{\alpha} = \bar{x} = \beta$		
Min	$\alpha^2 + x^2$	Min	$\alpha^2 + x^2$	(13)
s.t.	$\alpha = x$	s.t.	$\alpha - \frac{x}{2} - 1 \leq 0$	
	$\alpha - \frac{x}{2} - 1 \leq 0$		$\alpha = \beta$	
	$(p = x)$		$(K = \beta)$	

Starting at some point C where $x = \alpha \geq 1$ and following the same analysis as in Example 1, the inside-out algorithm converges to point B in Figure 2. From the figure it is readily seen that point A is the optimum of the rigorous problem and is also a KKT point for the inside-out problem. If one starts at $x = \alpha < 1$, the inside-out algorithm also converges to point A. Otherwise, the inside-out algorithm chooses the wrong constraint set because the gradients of the simplified and rigorous models are different.

Example 3 (No convergence)

This example shows that on some problems the inside-out algorithm may fail to converge even if the rigorous problem is well-posed. Given below is a small optimization problem and its corresponding inside-out problem, again with a very simple approximate model.

Rigorous		Inside-Out		
		$\bar{\alpha} = \bar{x} = \beta$		
Min	αx	Min	αx	(14)
s.t.	$\alpha = x$	s.t.	$1 \leq x \leq 1$	
	$-1 \leq x \leq 1$		$\alpha = \beta$	
	$(p = x)$		$(K = \beta)$	

From Figure 3, the solution to both the rigorous and the inside-out problem can be seen at point E. However, if one applies the procedure described and demonstrated above, at any point other than E, the inside-out algorithm cycles between points A, B, C and D. On the other hand, the rigorous problem itself is well-posed; it is merely Min x^2 s.t. $-1 \leq x \leq 1$.

CONCLUSIONS

The discussion and examples in the previous section demonstrate the need for great care when solving optimization problems with simplified model embedding. Because determination of the optimum and performance of optimization algorithms are directly influenced by accuracy of the objective function and constraint gradients, more attention should be paid to derivative information when choosing simplified models and calculating parameters* However, most shortcut models, such as Antoine equations or distillation models with constant relative volatility, overlook this information and can lead to suboptimal points.

The reason for the difference in solutions has a very simple conceptual basis. Application of the inside-out procedure leads to the optimum of the simplified model at a point where the simplified and rigorous models match. However, as has been demonstrated with the above examples, this point is not always the same as the rigorous model optimum.

This leads us to the open question as to whether appropriate simplified models can be found for process optimization. At present, we can offer two observations:

a) A necessary condition for an appropriate simplified model for optimization is that it recognize the rigorous model optimum as a KKT point. A stronger condition would be that the gradients of the simplified and rigorous model be the same at the optimum. This, however, implies nothing about convergence to KKT points inherent in the simple model that may be absent with the rigorous model. Example 2 illustrates a problem with this feature.

b) A sufficient condition for an appropriate simplified model is that it match the gradients of the rigorous model at all points. Clearly, this condition is not very helpful because it implies that only the rigorous model is appropriate.

The use of simplified models for process simulation has been used to advantage for complex process models. However, much interesting and challenging work remains in order to embed these models properly into an optimization framework.

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FIGURE CAPTIONS

Figure 1 Recognition of Different Optima

Figure 2 Convergence to Wrong Solution

Figure 3 No Convergence

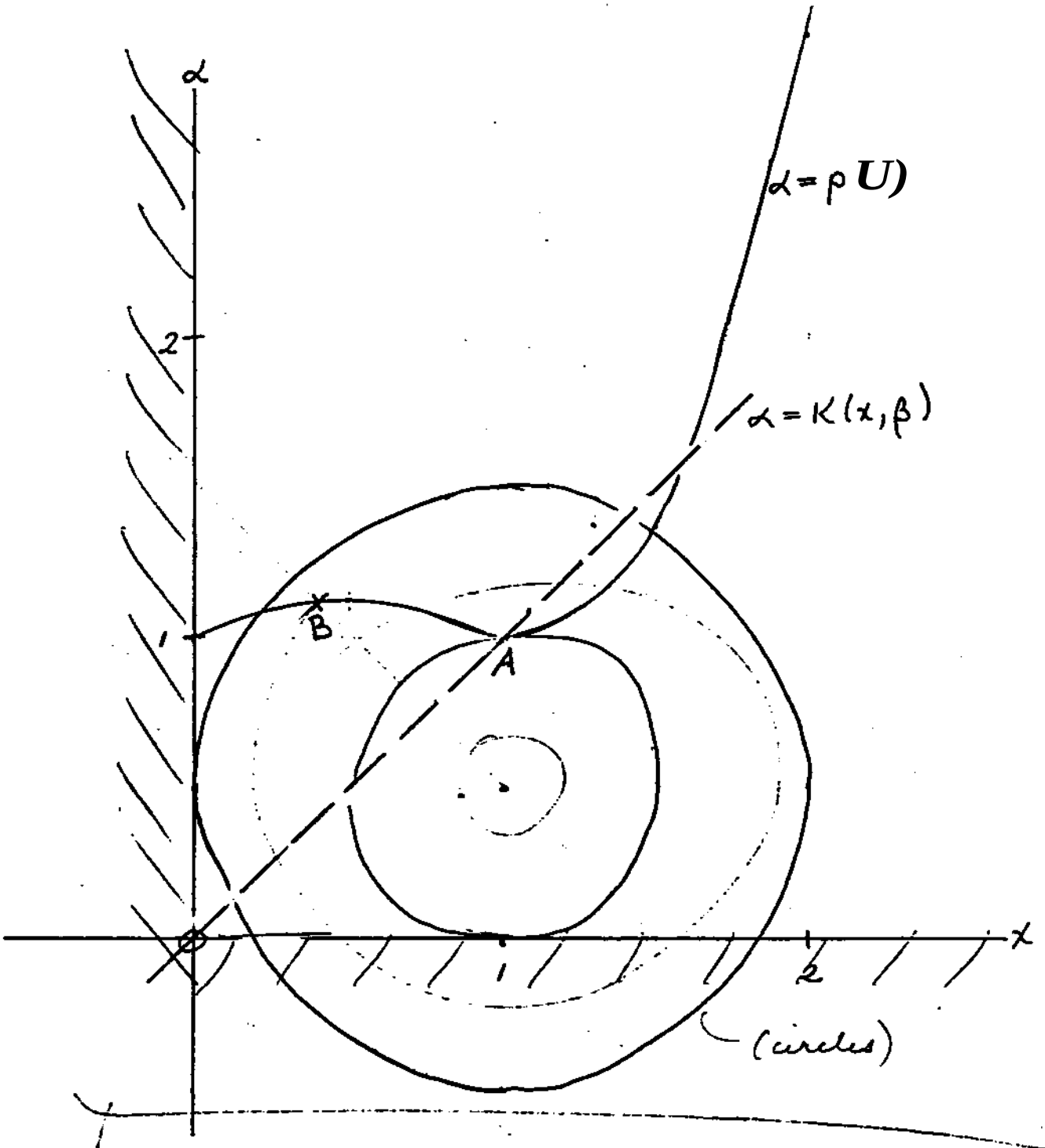

Figure 1

Recognition of Different Optima

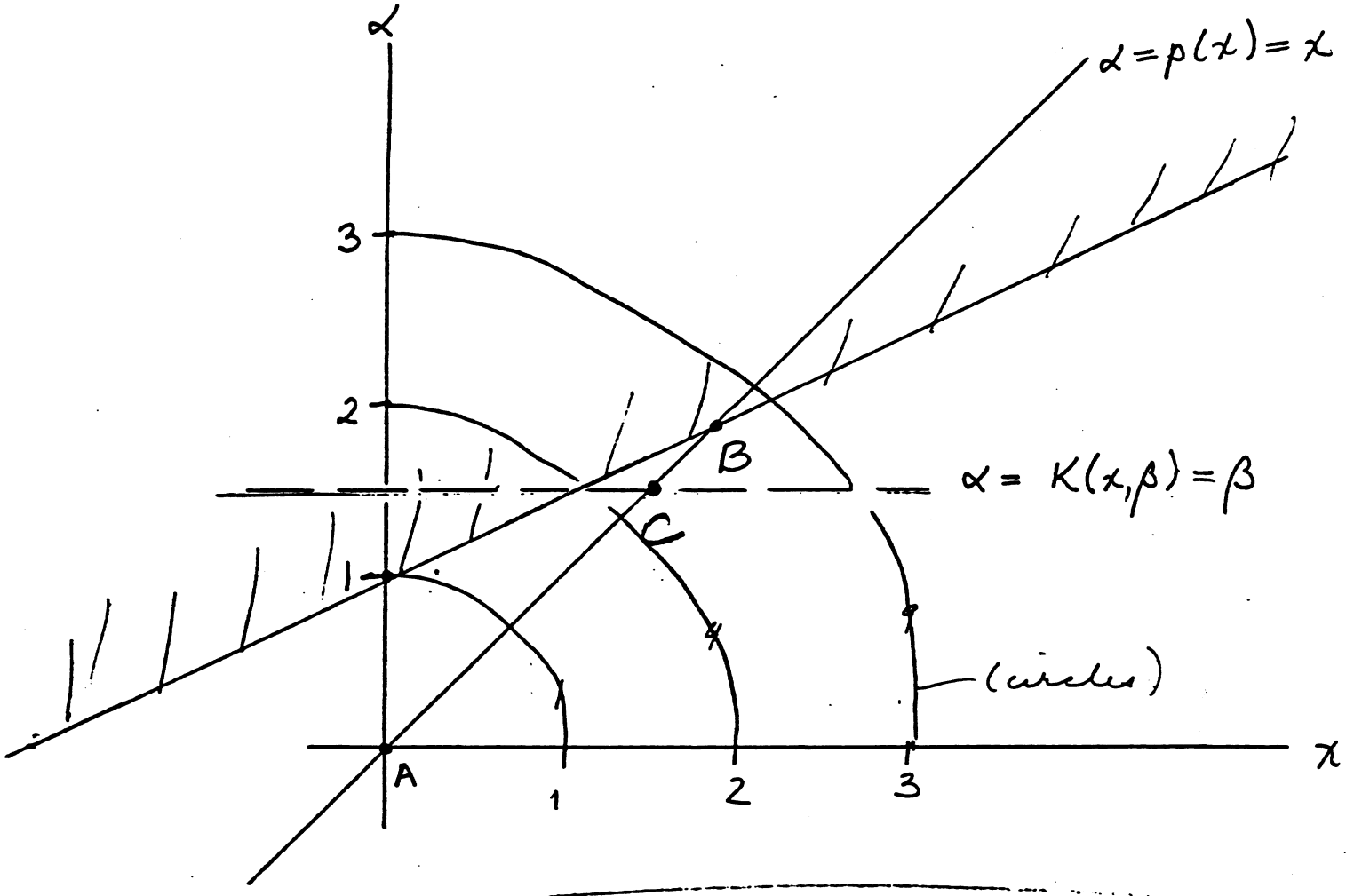

Figure 2
Convergence to Wrong Solution

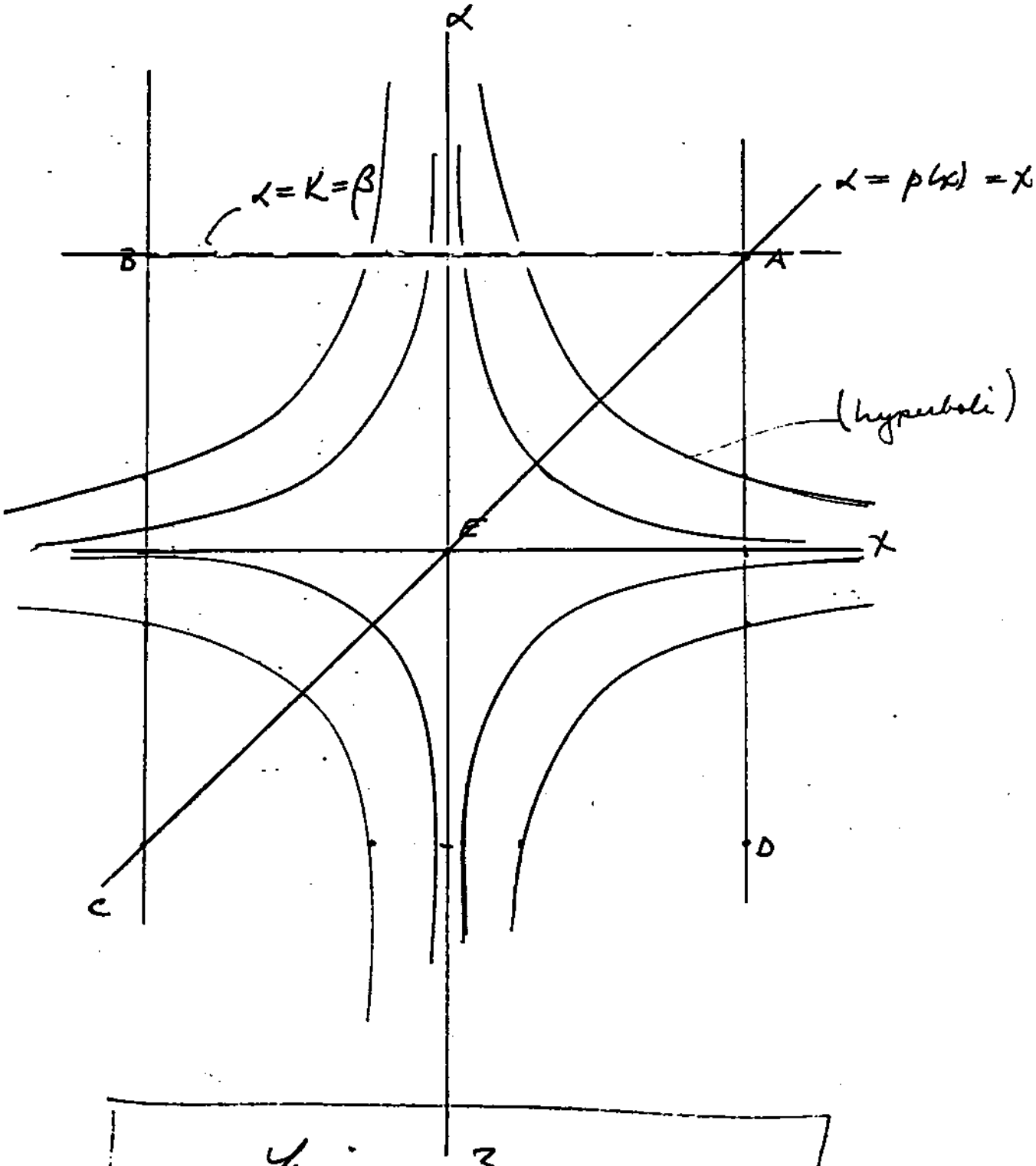

Figure 3
No Commencement