Introduction to Nonlinear Optimization (Nonlinear Programming) with Constraints*: Minimization of a nonlinear objective function subject to linear or nonlinear constraints.

Minimize
$$f(\mathbf{x})$$
 where $\mathbf{x} = [x_1, x_2, ..., x_n]^T$ (vector of decision variables)
Subject to $h_i(\mathbf{x}) = b_i$ where $i = 1, 2, ..., m$
 $g_i(\mathbf{x}) \le c_j$ where $j = 1, 2, ..., r$

i.e., we have two types of constraints (equality, inequality)

NOTE: a vector \mathbf{x} is *feasible* if it satisfies all the constraints. The set of all feasible points is called the *feasible region*.

Note[†]: An inequality constraint j is *feasible* when $g_j(x^*) \le 0$ and it is said to be *active* if $g_j(x^*) = 0$ and *inactive* if $g_j(x^*) < 0$

• **Linear Programming** (LP) when the objective function $f(\mathbf{x})$ and the constraints are linear. Example of a linear constraint: $h_i(\mathbf{x}) = \mathbf{a}_i^T \mathbf{x} - b_i$ where $\mathbf{a}_i = [a_1, a_2, ..., a_n]^T$ or $\mathbf{h}(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b}$ where \mathbf{A} is a $(\mathbf{m} \times \mathbf{n})$ matrix. Linear Objective function: $f(\mathbf{x}) = \mathbf{c}^T \mathbf{x}$ where \mathbf{c} is a vector of constant coefficients.

NOTE: Both the objective function and the constraints are *affine* functions.

• Quadratic programming (QP)[‡]: We have a QP problem when f(x) is quadratic function of n variable, $f(x)=1/2x^TQx+c^Tx$ and it is minimized subject to m linear constraints: Ax=b and $x \ge 0$ where c is a vector of constant coefficients and A is an $(m \times n)$ matrix.

^{*} Edgar et al., Optimization of Chemical Proesses, McGRaw Hill, 2nd edition, 2001 [E-H-L]

[†] Martins, Ng, ENGINEERING DESIGN OPTIMIZATION, CUP 2021.

^{*}We may cover LP and QP later if time permits (you may also consult Edgar et al., 2001)

We proceed first with the general constrained NLP problem.

<u>Direct Substitution:</u> Looking at the problem

Minimize
$$f(\mathbf{x})$$
 where $\mathbf{x} = [x_1, x_2, ..., x_n]^T$
Subject to $h_i(\mathbf{x}) = b_i$ where $i = 1, 2, ..., m$
 $g_i(\mathbf{x}) \le c_j$ where $j = 1, 2, ..., r$

We could attempt to eliminate the m equality variables by direct substitution. If there are no inequality constraints and all equality constraints are removed then the objective function $f(\mathbf{x})$ can be differentiated w.r.t. the n-m variables and set the derivatives equal to zero (unconstrained minimization) to obtain \mathbf{x}^* .

Example (E-H):

Minimize
$$f(\mathbf{x}) = 4x_1^2 + 5x_2^2$$

Subject to $2x_1+3x_2=6$

From $2x_1+3x_2=6$ one obtains $x_1=(6-3x_2)/2 \rightarrow f(x_2)=14x_2^2-36x_2+36$. Solution of $df(x_2)/dx_2=0$ or $28x_2-36=0$ or $x_2*=1.286$ and $x_1*=(6-3x_2*)/2=1.071$.

Unfortunately, very few problems in practice offer the possibility of eliminating all equality constraints by direct substitution.

In some cases, suitable transformations enable removal of constraints. For examples, bound constraints $a \le x \le b$ can be removed by the transform

$$x = t_{a,b}(\hat{x}) = \frac{b+a}{2} + \frac{b-a}{2} \left(\frac{2\hat{x}}{1+\hat{x}^2}\right)$$

Example⁴ Minimize
$$x\sin(x)$$
 _Subject to $2 \le x \le 6$

Example. Consider the minimization problem

Minimize.
$$-\exp\left[-\left(x_1x_2 - \frac{3}{2}\right)^2 - \left(x_2 - \frac{3}{2}\right)^2\right]$$

Subject to $x_1 - x_2^2 = 0$
 $x_1 = x_2^2$: $F(x_2) = -\exp\left[-\left(x_1^3 - \frac{3}{2}\right)^2 - \left(x_2 - \frac{3}{2}\right)^2\right]$
 $\frac{\partial F(x_2)}{\partial x_2} = 0$. $x_1^* = 1.358$

⁴ Kochenderfer, M.J., Algorithms for Optimization, MIT press, 2019.

Graphical Solution of a minimization problem. Consider the following problem⁵

The objective function *contours* are plotted by setting the function equal to specific values. The constraint functions are plotted by setting them equal to zero and then choosing the feasible side of the surf ace they represent. The situation in the presence of constraints is shown in the figure below, where the three-dimensional intersection of the various surfaces is projected on the (x_1, x_2) plane.

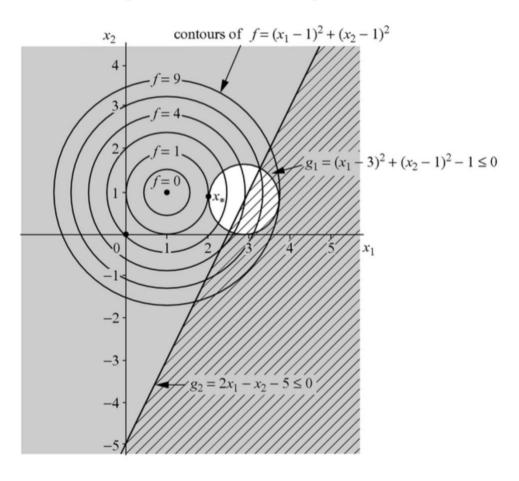


Figure 1.19. Two-dimensional representation of the problem.

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⁵ Papalambros, P.Y., D.J. Wilde, Principles of Optimal Design, 3rd ed, CUP, 2017.

LAGRANGE MULTIPLIERS. Consider a minimization problem with only one equality constraint. The general problem with m equality constraints will be discussed later. Also, inequality constraints are discussed later.

Minimize
$$f(\mathbf{x})$$
 where $\mathbf{x} = [x_1, x_2, ..., x_n]^T$
Subject to $h(\mathbf{x}) = 0$

We introduce a new function $L(\mathbf{x},\lambda)$ called *Langrangian* function. $L(\mathbf{x},\lambda)=f(\mathbf{x})+\lambda h(\mathbf{x})$ with λ called the *Langrange multiplier*. Then the 1st order necessary conditions for a local extremum are [E-H-L]⁶

or
$$\nabla_{x}L(\mathbf{x},\lambda) = \mathbf{0}$$

$$\nabla_{x}(\mathbf{f}(\mathbf{x}) + \lambda \mathbf{h}(\mathbf{x})) = \mathbf{0}$$

This equation as well as the feasibility condition (constraint)

$$h(\mathbf{x})=0$$

constitute the 1st order necessary conditions for a local extremum.

⁶ Edgar et al., *Optimization of Chemical Processes* McGRaw Hill, 2nd edition, 2001

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Example

Minimize $f(x_1,x_2)=x_1+x_2$ Subject to $h(x_1,x_2)=x_1^2+x_2^2-1=0$

$$\frac{\partial L}{\partial x_{1}} = 0 : 1 + 2 \lambda x_{1} = 0 : x_{1} = -\frac{1}{2A} \qquad (1)$$

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Example

Minimize
$$f(\mathbf{x}) = 4x_1^2 + 5x_2^2$$

Subject to $h(x_1,x_2) = 2x_1 + 3x_2 - 6 = 0$

$$L(x_1 \lambda) = 4x_1^2 + 5x_2^2 + \lambda (2x_1 + 3x_2 - 6) = 0$$

$$\frac{\partial L}{\partial x_1} = 0 : 8x_1 + 2\lambda = 0 : x_1 = -\frac{4}{4}$$

$$\frac{\partial L}{\partial x_2} = 0 : 10x_2 + 3\lambda = 0 : 22 = -\frac{3\lambda}{10}$$

$$\frac{\partial L}{\partial x_2} = 0 : 2x_1 + 3x_2 - 6 = 0 \Rightarrow 2x_1 + 3(-\frac{3\lambda}{10}) - 6 = 0 : \lambda = -\frac{60}{14} \approx -4.286$$

$$2(-\frac{2}{4}) + 3(-\frac{3\lambda}{10}) - 6 = 0 : \lambda = -\frac{3\lambda}{10} = 1.286$$

$$x_1^{\alpha} = -\frac{3}{4} = 1.071 ; x_2 = -\frac{3\lambda}{10} = 1.286$$

Extension to multiple (m) equality constraints

Minimize $f(\mathbf{x})$ where $\mathbf{x} = [x_1, x_2, ..., x_n]^T$ are the decision variables *Subject* to $h_j(\mathbf{x}) = b_j$, j = 1, 2, ..., m with b_i being a constant.



We define m Langrangian multipliers λ_j (j=1,2,...,m) corresponding to each constraint: $\lambda = [\lambda_1, \lambda_2, ..., \lambda_m]^T$. The Langrangian for the problem is:

$$L(\mathbf{x},\lambda)=f(\mathbf{x})+\sum_{j=1}^{m}\lambda_{j}[h_{j}(\mathbf{x})-b_{j}]$$

Then the 1st order <u>necessary</u> conditions for a local extremum are [E-H-L]⁷

$$\frac{\partial L}{\partial x_i} = \frac{\partial f}{\partial x_i} + \sum_{j=1}^m \lambda_j \frac{\partial h_j}{\partial x_i} = 0, i = 1, ..., n \text{ and } j = 1, ..., m$$
(A)

$$h_j(\mathbf{x}) = b_j, \quad j=1,2,...,m$$
 (B)

As we see there are n+m equations with n+m unknowns \mathbf{x} and λ . Certain conditions must be satisfied. One such condition is that the gradients of the equality constraints at the optimum \mathbf{x}^* should be *linearly independent*.

The first order necessary conditions are stated formally as follows. Let x* be a local minimum of the problem

Minimize $f(\mathbf{x})$ where $\mathbf{x} = [x_1, x_2, ..., x_n]^T$ are the decision variables *Subject* to $h_j(\mathbf{x}) = b_j$, j = 1, 2, ..., m with b_i being a constant

and assume that the gradients $\nabla h_j(x *)$, j = 1,2,..., m are linearly independent. Then there exists a vector of Langrange multipliers λ^* such that $(\mathbf{x}^*, \lambda^*)$ satisfies the first order necessary conditions (A), and (B)

NOTE: To tell if a point satisfying the 1st order necessary conditions is a minimum, maximum, or neither, 2nd order sufficiency conditions are needed. These are discussed later.

⁷ Edgar et al., Optimization of Chemical Proesses, McGRaw Hill, 2nd edition, 2001

<u>Interpretation of Langrange multipliers for equality constraints</u>⁸⁹ We can carry out a sensitivity analysis to see how an optimal solution changes as the problem data change.

$$f(x) = \frac{1}{2}$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial x}$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial x}$$

$$\frac{\partial f}{\partial x} = -\frac{\partial f}{\partial x}$$

⁸ Vassiliadis et al., *Optimization for Chemical and Biochemical Engineering*, Cambridge Univ Press, 2020

⁹ Edgar et al., Optimization of Chemical Proesses, McGRaw Hill, 2nd edition, 2001

General Problem with r inequality constraints¹⁰. The 1st order necessary conditions for problems with inequality constraints are called *Kuhn-Tucker conditions* (also called *Karush-Kuhn-Tucker conditions*).

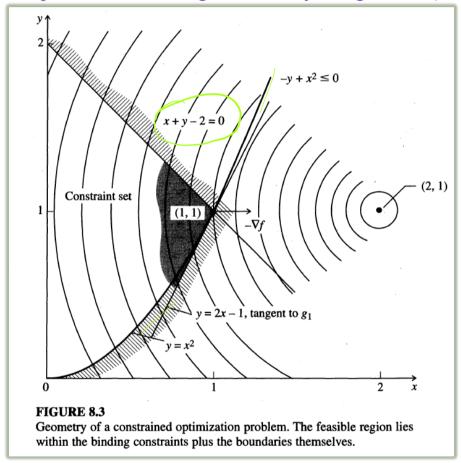
mmimize
$$f(x)$$
 s.t $g_j(x) \leq g_j$ $j=1,2,...,r$

Consider the problem: Minimize $f(x,y)=(x-2)^2+(y-1)^2$ Subject to: $g_1(x,y)=-y+x^2 \le 0$

$$g_2(x,y) = x + y \le 2$$

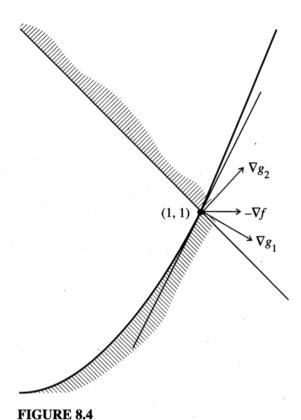
$$g_3(x,y) = y \ge 0$$

The problem is shown geometrically in figure 8.3 (Edgar et al., 2001).



The optimum is at the intersection of the first two constraints at (1,1). Because these two inequality constraints hold as equalities at (1,1), they are called *active* or *binding* constraints at this point. The 3^{rd} constraint holds as a strict inequality at 1,1 and it is an *inactive* or *nonbinding* constraint.

¹⁰ Edgar et al., Optimization of Chemical Processes, McGraw Hill, 2nd edition, 2001



Gradient of objective contained in convex cone.

Note that the negative of the gradient of function f is contained in the cone generated by the gradients of g_1 and g_2^{11} . This leads to the Kuhn-Tucker conditions (KTC): If function f(x) and g(x) are differentiable, a necessary condition for a point x^* to be a constrained minimum of the problem

Minimize
$$f(\mathbf{x})$$

Subject to $g_j(\mathbf{x}) \le c_j = 1,2,...,r$

is that,

at x^* , $-\nabla f(x)$ lies within the cone generated by the gradiends of the binding constraints

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¹¹ Edgar et al., Optimization of Chemical Processes, McGraw Hill, 2nd edition, 2001

Algebraic statement of the Kuhn-Tucker conditions



A <u>necessary condition</u> for a point x^* to be a constrained minimum of the problem: Minimize f(x)

Subject to
$$g_j(\mathbf{x}) \le c_j$$
 $j=1,2,...,r$

is that there must exist Langrange multipliers u_j^* such that $\nabla f(x^*) = \sum_{j \in I} u_j^* [-\nabla g_j(x^*)]$ where $u_j^* \ge 0$. $j \in I$. I is the set of indices of the binding constraints.

These results may be restated to include all the constraints by defining the multiplier u_i^* to be zero if $g_j(x) < c_j$.

Then we can say that $\mathbf{u}_j^* \ge 0$ if $\mathbf{g}_j(\mathbf{x}) = c_j$ and $\mathbf{u}_j^* = 0$ if $\mathbf{g}_j(\mathbf{x}) < c_j$. Thus, the product $\mathbf{u}_j^* [\mathbf{g}_j(\mathbf{x}) - c_j] = 0$ for all j.

The property that inactive inequality constraints have zero Langrange multipliers is called *complementarity slackness*.

In summary, we have as necessary conditions the following

$$\nabla f(\mathbf{x}^{*}) + \sum_{j=1}^{r} \mathbf{u}_{j}^{*} \nabla g_{j}(\mathbf{x}^{*}) = 0$$
 (1)

$$\mathbf{u}_{j}^{*} \geq 0, \ \mathbf{u}_{j}^{*} [g_{j}(\mathbf{x}^{*}) - c_{j}] = 0$$
 (2a)

$$g_{j}(\mathbf{x}^{*}) \leq c_{j} \quad j = 1, 2, ..., r$$
 (2b)

Note: The KTC are closely related to the classical Langrange multipliers results for equality constraints. Form the Langrangian $L(\mathbf{x}, \mathbf{u}) = f(\mathbf{x}) + \sum_{j=1}^{r} \mathbf{u}_{j}^{*} [g_{j}(\mathbf{x}) - c_{j}]$ where \mathbf{u}_{j} are viewed as Langrange multipliers for the inequality constraints $g_{j}(\mathbf{x}) \leq c_{j}$. Then equations 1, 2a, 2b state that $L(\mathbf{x}, \mathbf{u})$ must be stationary in \mathbf{x} at $(\mathbf{x}^{*}, \mathbf{u}^{*})$ with the multipliers \mathbf{u}^{*} satisfying equation 2. The stationarity of L is the same condition as in the equality constraints case. The additional conditions (stated through eqn 2) arise because the constraints here are inequalities.

Example 8.3¹². Minimize $f(\mathbf{x})=x_1x_2$

Subject to $g(\mathbf{x}) = x_1^2 + x_2^2 \le 25$. By the Lagrange multiplier method

CHAPTER 8: Nonlinear Programming with Constraints

279

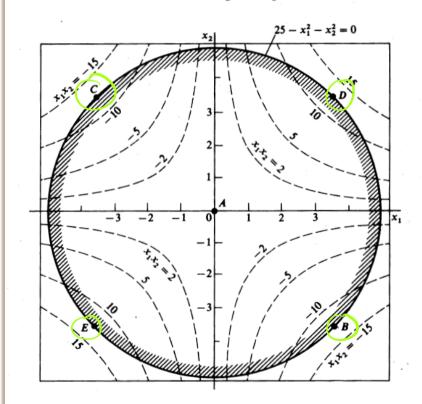


FIGURE E8.3

ure E8.3 the contours of the objective function (hyperbolas) are represented by broken lines, and the feasible region is bounded by the shaded area enclosed by the circle $g(\mathbf{x}) = 25$. Points B and C correspond to the two minima, D and E to the two maxima, and A to the saddle point of $f(\mathbf{x})$.

¹² Edgar et al., Optimization of Chemical Processes, McGraw Hill, 2nd edition, 2001

 $\frac{1}{2} \frac{5/r_{2}}{-\frac{1}{2}} \frac{5/r_{2}}{-\frac{1}{2}} \frac{12.r}{-\frac{1}{2}} \frac{5/r_{2}}{-\frac{1}{2}} \frac{12.r}{-\frac{1}{2}} = \frac{5/r_{2}}{-\frac{1}{2}} \frac{12.r}{-\frac{1}{2}}$ $\frac{1}{2} \frac{5/r_{2}}{-\frac{1}{2}} \frac{12.r}{-\frac{1}{2}} \frac{12.r}{$

<u>Interpretation of Langrange multipliers</u> for inequality constraints¹³ We can carry out a sensitivity analysis

Same a equality Constaint.

1F INACTIVE JHM No impact

11- ACTIVE 71400 LIKE Equality Constaint.

¹³ Vassiliadis et al., *Optimization for Chemical and Biochemical Engineering*, Cambridge Univ Press, 2020; Edgar et al., *Optimization of Chemical Proesses*, McGRaw Hill, 2nd edition, 2001

General Problem with m equality and r inequality constraints

Minimize
$$f(x)$$

S.t $h_i(x) = b_i$ $i = 1, 2, ..., m$
 $g_{i}(x) \neq c_{j}$, $i = 1, 2, ..., m$
 $f(x) = b_{i}(x) = b_{i}$

2nd ORDER NECESSARY (conditions that must be satisfied for a point to be a local minimizer) AND SUFFICIENT CONDITIONS for OPTIMALITY (conditions that will assure that a point is a local minimizer)¹⁴

IF x^4, A^*, u^* sets of necessary bonditions

(Kuhn-Tucker Romt): Thom

The 2nd order Conditions are unified as

follows $y^{T} \nabla_{x}^{2} L (x^*, A^*, u^*) \cdot y = 0$ for all non-zero rectors y such that $J(x^*) \cdot y = 0$ $J(x^*)$ has rows which are the predients of

the constraints'

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¹⁴ Edgar et al., Optimization of Chemical Processes, McGraw Hill, 2nd edition, 2001

EXAMPLE 8.4 Edger et el.

Minimize
$$f(x) = (x_1-1)^2 + x_2^2$$

Siting $g(x) = x_1 - x_2^2 \le 0$

$$L(x,u) = (x_1-1)^2 + x_2^2 + u(x_1-x_2^2)$$
NECESTRAY CONDITIONS $\nabla L(x,u) = 0$, $\nabla u L(x,u) = 0$

$$\frac{\partial L}{\partial x_1} = 0 : 2(x_1-1) + u = 0 \quad (a)$$

$$\frac{\partial L}{\partial x_2} = 0 : 2x_2 - 2ux_2 = 0 \quad (b)$$

$$\frac{\partial L}{\partial x_1} = x_1 - x_2^2 \quad C : S = u(x_1 - x_2^2) = 0 \quad u \neq 0$$

$$\frac{\partial L}{\partial x_2} = x_1 - x_2^2 \quad C : S = u(x_1 - x_2^2) = 0 \quad u \neq 0$$

$$\frac{\partial L}{\partial x_2} = x_1 - x_2^2 \quad C : S = u(x_1 - x_2^2) = 0 \quad u \neq 0$$

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$$\nabla_{x}^{2}L(x,u) = \begin{bmatrix} 2 & 0 \\ 0 & 2(1-u) \end{bmatrix}$$

$$\nabla_{x}^{2}L(x,u) = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix} \quad u=2 \quad x_{1}=x_{2}=0$$

$$y \top \nabla_{x}^{2} L (x^{*}, u^{*}) \cdot y \Rightarrow 0$$
for all mon-zero y such that $J(x^{*}) \cdot y = 0$

$$\frac{\partial g}{\partial x} = \begin{pmatrix} 1 & -2x_{2} \end{pmatrix}, \nabla^{T}g(x^{*}) = \begin{pmatrix} 1 & 0 \end{pmatrix}$$
When $x_{1} = x_{2} = 0$

$$\begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} y_{1} \\ y_{2} \end{pmatrix} = 0$$

$$y = 0 \text{ and } y_{2} \text{ any Volus}$$

$$y = 0 \text{ (a. } y_{2}) = 0$$

$$y \top \nabla_{x}^{2} L (x^{*}, u^{*}) y = \begin{pmatrix} 0 & y_{2} \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} 0 \\ y_{2} \end{pmatrix}$$

$$= -2 y_{2}^{2} < 0$$

$$\begin{pmatrix} x_{2} = 0, 0 \end{pmatrix} \text{ Nut}$$

$$-2 y_{2}^{2} < 0$$

$$\begin{pmatrix} x_{2} = 0, 0 \end{pmatrix} \text{ Nut}$$

$$\begin{pmatrix} x_{1} & y_{1} & y_{2} \\ y_{2} & y_{2} \end{pmatrix} = \begin{pmatrix} x_{1} & y_{2} \\ 0 & y_{2} & y_{2} \end{pmatrix}$$

$$\nabla_{x}^{2} L (x, u) = \begin{pmatrix} 2 & 0 \\ 0 & 2(1-u) \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\nabla_{y}^{2} (x^{*}) = \begin{pmatrix} 1 & -2x_{2} \\ y & y_{2} \end{pmatrix}, \quad \nabla^{T}g(x^{*}) = \begin{pmatrix} 1 & -Y_{2} \\ y_{2} & y_{2} \end{pmatrix}$$

$$\nabla_{y}^{2} (x^{*}) \cdot y = 0 \Rightarrow (1 - Y_{2}) \begin{pmatrix} y_{1} \\ y_{2} \end{pmatrix} = 0$$

$$\frac{y_{1}}{y_{2}} = \frac{Y_{2} \cdot Y_{2}}{Y_{2}}$$

$$\frac{y_{2}}{y_{2}} = \frac{Y_{2} \cdot Y_{2}}{Y_{2}}$$

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$$\frac{y_{2}}{$$