

## Lagrange Multipliers

**Constrained Optimization for functions of two variables.** To find the maximum and minimum values of  $z = f(x, y)$ , **objective function**, subject to a **constraint**  $g(x, y) = c$  :

1. Introduce a new variable  $\lambda$ , the **Lagrange multiplier**, consider the function

$$F = f(x, y) - \lambda (g(x, y) - c).$$

2. Find the critical points of  $F$ , that is: all values  $x, y$  and  $\lambda$  such that

$$F_x = f_x - \lambda g_x = 0 \quad F_y = f_y - \lambda g_y = 0 \quad F_\lambda = -g + c = 0 \Rightarrow g = c.$$

3. Evaluate  $f$  at all points from previous step. The largest of these values is the maximum value of  $f$  and the smallest is the minimum value of  $f$ .

In cases when the variables  $x$  or  $y$  are given to be in certain intervals  $a \leq x \leq b$  and  $c \leq y \leq d$ , plug the **endpoints** of the intervals together with the critical points in the function  $f$  to find the largest and the smallest one.

**Constrained Optimization for functions of three variables.** Lagrange Multipliers method generalizes to functions of three variables as well. Let the objective  $f(x, y, z)$  be a function of three variables. To find the maximum and minimum values of  $f$  subject to a constraint  $g(x, y, z) = c$ :

1. Introduce a new variable  $\lambda$  and consider the function

$$F = f(x, y, z) - \lambda (g(x, y, z) - c).$$

2. Find the critical points of  $F$  : all values  $x, y, z$  and  $\lambda$  such that

$$F_x = f_x - \lambda g_x = 0 \quad F_y = f_y - \lambda g_y = 0 \quad F_z = f_z - \lambda g_z = 0 \quad F_\lambda = -g + c = 0$$

3. Evaluate  $f$  at all points from previous step. The largest of these values is the maximum value of  $f$  and the smallest is the minimum value of  $f$ .

**Two constraints.** If there is one objective  $f(x, y, z)$  and two constraints  $g(x, y, z) = c$  and  $h(x, y, z) = d$ , then introduce two new variables  $\lambda$  and  $\mu$  and consider the functions  $F = f - \lambda \cdot (g(x, y, z) - c) - \mu \cdot (h(x, y, z) - d)$ . Find all the critical values of  $F$  from the equations

$$F_x = f_x - \lambda g_x - \mu h_x = 0 \quad F_y = f_y - \lambda g_y - \mu h_y = 0 \quad F_z = f_z - \lambda g_z - \mu h_z = 0$$
$$F_\lambda = -g + c = 0 \Rightarrow g = c \quad F_\mu = -h + d = 0 \Rightarrow h = d$$

and evaluate  $f$  at all the critical points. The largest of these values is the maximum value of  $f$  and the smallest is the minimum value of  $f$ .

### Practice Problems.

- Find the maximum and minimum values of  $f$  subject to the given constraint(s).
  - $f(x, y) = x^2 - y^2$ ;  $x^2 + y^2 = 1$
  - $f(x, y) = x^2y$ ;  $x^2 + 2y^2 = 6$
  - $f(x, y, z) = 2x + 6y + 10z$ ;  $x^2 + y^2 + z^2 = 35$
  - $f(x, y, z) = 3x - y - 3z$ ;  $x + y - z = 0$ ;  $x^2 + 2z^2 = 1$
- Find the points on the surface  $z^2 = xy + 1$  that are closest to the origin.
- Set up a system of equations for finding the dimensions of a rectangular box with the largest volume if the total surface area is  $64 \text{ cm}^2$ . Solve the equations using Matlab and determine the dimensions of such box.
- A cardboard box without a lid is to have volume of  $32,000 \text{ cm}^3$ . Set up a system of equations for finding the dimensions that minimize the amount of cardboard used. Solve the equations using Matlab and determine the dimensions of such box.

### Solutions.

- $F = x^2 - y^2 - \lambda(x^2 + y^2 - 1)$ .  $F_x = 2x - 2x\lambda$ ,  $F_y = -2y - 2y\lambda$ , and  $F_\lambda = -(x^2 + y^2 - 1)$ . Set the three derivatives to 0. From the first equation  $2x - 2x\lambda = 0 \Rightarrow 2x(1 - \lambda) = 0 \Rightarrow 2x = 0$  or  $1 - \lambda = 0 \Rightarrow x = 0$  or  $\lambda = 1$ . So, we have two cases  $x = 0$  and  $\lambda = 1$ . If  $x = 0$ , the last equation becomes  $0^2 + y^2 = 1 \Rightarrow y^2 = 1 \Rightarrow y = \pm 1$ . So, we have two critical points  $(0, \pm 1)$ .

If  $\lambda = 1$ , the second equation becomes  $-2y - 2y = 0 \Rightarrow -4y = 0 \Rightarrow y = 0$ . Then the third equation becomes  $x^2 + 0^2 = 1 \Rightarrow x^2 = 1 \Rightarrow x = \pm 1$ . So, we have another two critical points  $(\pm 1, 0)$ .

Plugging the four critical points in the objective  $f = x^2 - y^2$ , you obtain that the maximum value is  $f(\pm 1, 0) = 1$ , and the minimum value is  $f(0, \pm 1) = -1$ .
  - $F = x^2y - \lambda(x^2 + 2y^2 - 6)$ .  $F_x = 2xy - 2x\lambda$ ,  $F_y = x^2 - 4y\lambda$ , and  $F_\lambda = -(x^2 + 2y^2 - 6)$ . Set the three derivatives to 0. From the first equation  $2xy - 2x\lambda = 0 \Rightarrow 2x(y - \lambda) = 0 \Rightarrow 2x = 0$  or  $y - \lambda = 0 \Rightarrow x = 0$  or  $y = \lambda$ . So, we have two cases  $x = 0$  and  $\lambda = y$ . If  $x = 0$ , the last equation becomes  $0^2 + 2y^2 = 6 \Rightarrow y^2 = 3 \Rightarrow y = \pm\sqrt{3}$ . So, we have two critical points  $(0, \pm\sqrt{3})$ .

If  $\lambda = y$ , the second equation becomes  $x^2 - 4y^2 = 0 \Rightarrow x^2 = 4y^2$ . Then the third equation becomes  $x^2 + 2y^2 = 6 \Rightarrow 4y^2 + 2y^2 = 6 \Rightarrow 6y^2 = 6 \Rightarrow y^2 = 1 \Rightarrow y = \pm 1$ . From  $x^2 = 4y^2$  we have that  $x^2 = 4 \Rightarrow x = \pm 2$ . So, we have another four critical points  $(\pm 2, \pm 1)$ .

Plugging the six critical points in the objective  $f = x^2y$ , you obtain  $f(0, \pm\sqrt{3}) = 0$ ,  $f(\pm 2, 1) = 4$ , and  $f(\pm 2, -1) = -4$ . So, the maximum value is  $f(\pm 2, 1) = 4$ , and the minimum value is  $f(\pm 2, -1) = -4$ .
  - $F = 2x + 6y + 10z - \lambda(x^2 + y^2 + z^2 - 35)$ .  $F_x = 2 - 2x\lambda$ ,  $F_y = 6 - 2y\lambda$ ,  $F_z = 10 - 2z\lambda$ , and  $F_\lambda = -(x^2 + y^2 + z^2 - 35)$ . Set the four derivatives to 0. From the first equation  $x = \frac{2}{2\lambda} = \frac{1}{\lambda}$ . From the second  $y = \frac{6}{2\lambda} = \frac{3}{\lambda}$ . From the third  $z = \frac{10}{2\lambda} = \frac{5}{\lambda}$ . Substitute those values in the last equation and obtain that  $\frac{1}{\lambda^2} + \frac{9}{\lambda^2} + \frac{25}{\lambda^2} = 35 \Rightarrow \frac{35}{\lambda^2} = 35 \Rightarrow \lambda^2 = 1 \Rightarrow \lambda = \pm 1$ . Thus

$x = \frac{1}{\pm 1} = \pm 1$ ,  $y = \frac{3}{\pm 1} = \pm 3$ , and  $z = \frac{5}{\pm 1} = \pm 5$ . So, we have 2 critical points  $(1, 3, 5)$  and  $(-1, -3, -5)$ .

Plugging the two critical points in the objective  $f = 2x + 6y + 10z$ , you obtain the maximum value  $f(1, 3, 5) = 70$ , and the minimum value  $f(-1, -3, -5) = -70$ .

d)  $F = 3x - y - 3z - \lambda(x + y - z) - \mu(x^2 + 2z^2 - 1)$ .  $F_x = 3 - \lambda - 2x\mu$ ,  $F_y = -1 - \lambda$ ,  $F_z = -3 + \lambda - 4z\mu$ ,  $F_\lambda = -(x + y - z)$  and  $F_\mu = -(x^2 + 2z^2 - 1)$ . From the second equation,  $\lambda = -1$ . Eliminating  $\lambda$  from the first two equations gives you:  $F_x = 4 - 2x\mu = 0 \Rightarrow x = \frac{4}{2\mu} = \frac{2}{\mu}$  and  $F_z = -4 - 4z\mu = 0 \Rightarrow z = \frac{-4}{4\mu} = \frac{-1}{\mu}$ . Substituting these  $x$  and  $z$  values in the last equation gives you  $x^2 + 2z^2 = 1 \Rightarrow \frac{4}{\mu^2} + \frac{2}{\mu^2} = 1 \Rightarrow \frac{6}{\mu^2} = 1 \Rightarrow \mu^2 = 6 \Rightarrow \mu = \pm\sqrt{6}$ . Thus,  $x = \frac{\pm 2}{\sqrt{6}}$  and  $z = \frac{-1}{\pm\sqrt{6}} = \frac{\mp 1}{\sqrt{6}}$ .

From the remaining equation  $x + y - z = 0$ , we obtain that  $y = -x + z = \frac{\mp 2}{\sqrt{6}} + \frac{\mp 1}{\sqrt{6}} = \frac{\mp 3}{\sqrt{6}}$ . So, we get two critical points  $(\frac{2}{\sqrt{6}}, \frac{-3}{\sqrt{6}}, \frac{-1}{\sqrt{6}})$  and  $(\frac{-2}{\sqrt{6}}, \frac{3}{\sqrt{6}}, \frac{1}{\sqrt{6}})$ . Plugging these critical points in the objective gives you the maximal value  $f(\frac{2}{\sqrt{6}}, \frac{-3}{\sqrt{6}}, \frac{-1}{\sqrt{6}}) = \frac{12}{\sqrt{6}} = 2\sqrt{6}$  and the minimal value  $f(\frac{-2}{\sqrt{6}}, \frac{3}{\sqrt{6}}, \frac{1}{\sqrt{6}}) = \frac{-12}{\sqrt{6}} = -2\sqrt{6}$ .

2. To find the points on the surface  $z^2 = xy + 1$  that are closest to the origin, the objective is to minimize the distance of the point  $(x, y, z)$  on the surface from  $(0, 0, 0)$ . This distance is  $D = \sqrt{x^2 + y^2 + z^2}$  and the constraint for  $(x, y, z)$  is  $z^2 = xy + 1$ . However, since the root is a strictly increasing function, the minimum of  $D = \sqrt{x^2 + y^2 + z^2}$  will be at the same point as the minimum of  $f = x^2 + y^2 + z^2$  and this function is much easier to work with since the derivatives will be much simpler. So, you can minimize the objective  $f$  subject to the constraint  $z^2 = xy + 1$ .

Consider  $F = x^2 + y^2 + z^2 - \lambda(z^2 - xy - 1)$ .  $F_x = 2x + y\lambda$ ,  $F_y = 2y + x\lambda$ ,  $F_z = 2z - 2z\lambda$ , and  $F_\lambda = -(z^2 - xy - 1)$ . From the first equation  $2x = -y\lambda \Rightarrow x = \frac{-y\lambda}{2}$ . Plugging that in the second equation gives you  $2y - \frac{y\lambda^2}{2} = 0 \Rightarrow 4y - y\lambda^2 = 0 \Rightarrow y(4 - \lambda^2) = 0 \Rightarrow y = 0$  or  $\lambda^2 = 4 \Rightarrow y = 0$  or  $\lambda = \pm 2$ .

In the first case,  $x = 0$  as well and so  $z^2 = xy + 1 \Rightarrow z^2 = 1 \Rightarrow z = \pm 1$ . Thus, we get two critical points  $(0, 0, \pm 1)$ .

In the second case,  $\lambda = \pm 2$  and  $x = \frac{-y\lambda}{2} \Rightarrow x = \mp y$ . The third equation becomes  $F_z = 2z \pm 4z = 0 \Rightarrow (2 \pm 4)z = 0 \Rightarrow z = 0$ . Thus, the constraint becomes  $0^2 = \mp y^2 + 1 \Rightarrow \pm y^2 = 1$ . The equation  $-y^2 = 1$  has no real solutions and the equation  $y^2 = 1$  yields  $y = \pm 1 \Rightarrow x = \mp 1$ . So, we get another two critical points  $(\mp 1, \pm 1, 0)$ .

$f(0, 0, \pm 1) = 0 + 0 + 1 = 1$  and  $f(\mp 1, \pm 1, 0) = 1 + 1 + 0 = 2$ . Thus, the points  $(0, 0, \pm 1)$  on the surface  $z^2 = xy + 1$  are the closest to the origin (not that the points  $(\mp 1, \pm 1, 0)$  are the furthest).

3. Let  $x, y$  and  $z$  denote the three dimensions of the box. Objective: to maximize the volume. Constraint: the surface area is 64. The volume of the box is  $xyz$  so  $f = xyz$  is the objective. The surface area is  $2xy + 2xz + 2yz$ . So, the constraint is  $2xy + 2xz + 2yz = 64 \Rightarrow xy + xz + yz = 32$ .  $F = xyz - \lambda(xy + xz + yz - 32)$ .

$$F_x = yz - \lambda y - \lambda z = 0, \quad F_y = xz - \lambda x - \lambda z = 0,$$

$$F_z = xy - \lambda x - \lambda y = 0, \quad \text{and} \quad F_\lambda = -(xy + yz + xz - 32).$$

To solve this system using Matlab, you can represent  $\lambda$  by  $l$  for brevity and use

$$[l,x,y,z]=\text{solve}('y*z-l*y-l*z = 0', 'x*z-l*x-l*z = 0', 'x*y-l*x-l*y = 0', 'x*y+y*z+x*z-32=0')$$

Note that the list of the variables in the brackets is in alphabetical order to match the order in the Matlab answer. The answer is  $x = y = z = \frac{4\sqrt{6}}{3}$  cm. These dimensions produce the maximum value since the minimal volume is 0 (which happens when one of the three dimensions is trivial).

4. Objective: to minimize the surface area. Constraint: the volume is 32,000. The surface area of a box without the top is  $xy + 2xz + 2yz$  so  $f = xy + 2xz + 2yz$  is the objective. The constraint is  $xyz = 32,000$ .  $F = xy + 2xz + 2yz - \lambda(xyz - 32,000)$ .

$$F_x = y + 2z - yz\lambda = 0, \quad F_y = x + 2z - xz\lambda = 0,$$

$$F_z = 2x + 2y - xy\lambda = 0, \quad \text{and} \quad F_\lambda = -(xyz - 32,000).$$

You can solve it in Matlab using similar command as in the previous problem. The answer is  $x = y = 40$  cm, and  $z = 20$  cm. These dimensions produce the minimal surface area since the surface area of, for example  $x = y = z = \sqrt[3]{32000} = 31.75$  produce larger value of  $f$ .

## Hardy-Weinberg Theorem for phenotypes

The goal of this section is twofold.

1. to generalize the familiar scenario from your freshmen biology and math classes with two possible phenotypes to the case with three possible phenotypes and
2. to find extreme values of certain frequency functions using Lagrange multipliers.

**Two phenotypes reminder.** An allele is a particular variation of a gene that determines the genetic makeup of an organism. In your freshmen biology and math classes, you considered cases with two possible allele types (phenotypes) carrying certain trait.

Recall first the familiar case with two phenotypes (for example left or right handed, free or attached earlobe, tongue rollers or not etc): there is a dominant allele  $A$  (carries dominant trait: right-handedness, free earlobe, tongue rolling etc) and a recessive allele  $a$  (carries recessive trait). In each cell, chromosomes come in pairs, so the possible combinations (genotypes) are:  $AA$ ,  $Aa = aA$ , and  $aa$ .

If  $p$  denotes the frequency of  $A$  and  $q$  the frequency of  $a$ , the Hardy-Weinberg theorem is stating that

$$p + q = 1 \Rightarrow (p + q)^2 = p^2 + 2pq + q^2 = 1$$

**Hardy-Weinberg Theorem for three phenotypes. Blood type example.** In some cases, there are three possible phenotypes. For example, three blood type phenotypes  $A$ ,  $B$  and  $O$  determine six possible genotypes  $AA$ ,  $AO = OA$ ,  $BB$ ,  $BO = OB$ ,  $AB = BA$ , and  $OO$ . The alleles  $A$  and  $B$  are

dominant over  $O$ , so person with  $AO = OA$  combination will display trait carried by  $A$ . This person is said to have **blood type A**. A person with  $AA$  combination is said to have blood type  $A$  as well.

Similarly, a person has blood type  $B$  if any of the combinations  $BB$  or  $BO = OB$  occur. A person has blood type  $AB$  if the combination  $AB = BA$  occurs. The alleles  $A$  and  $B$  are “equally strong” so this combination yields a new blood type different from both  $A$  and  $B$ . Finally, a person has blood type  $O$  if the combination  $OO$  occurs. Thus, six possible genotypes determine four possible phenotypes.

If  $p, q$  and  $r$  denote the frequencies of  $A, B$  and  $O$  respectively, the The Hardy Weinberg Theorem states that

$$p + q + r = 1 \Rightarrow (p + q + r)^2 = p^2 + q^2 + r^2 + 2pq + 2pr + 2qr = 1.$$

The table below illustrates the world frequencies of the four blood types.

| Blood Type      | $O$ | $A$ | $B$ | $AB$ |
|-----------------|-----|-----|-----|------|
| World Frequency | 45% | 40% | 11% | 4%   |

**Using Lagrange Multipliers.** The terms, homozygous and heterozygous, refer to a person having pair of identical alleles or two different alleles, in both two and three allele type cases. Thus, in the three allele type case, the proportion of heterozygous individuals in a population is  $HE = 2pq + 2pr + 2qr$  and the proportion of homozygous individuals in a population is  $HO = p^2 + q^2 + r^2$ .

Use the fact that  $p + q + r = 1$ , to find the following:

1. the maximum and minimum proportions of heterozygous individuals in a given population, and
2. the maximum and minimum proportions of homozygous individuals in a given population.

### Solutions.

1. Consider  $F = 2pq + 2pr + 2qr - \lambda(p + q + r - 1)$ . Finding critical points:  $F_p = 2q + 2r - \lambda = 0$ ,  $F_q = 2p + 2r - \lambda = 0$ ,  $F_r = 2p + 2q - \lambda = 0$ ,  $F_\lambda = -(p + q + r - 1) = 0$ . Subtracting the first equation from the second gives you  $2p - 2q = 0 \Rightarrow p = q$ . Subtracting the first equation from the third gives you  $2p - 2r = 0 \Rightarrow p = r$ . So,  $p = q = r$ . Substituting that in the fourth one  $p + q + r = 1$  gives you that  $3p = 1 \Rightarrow p = \frac{1}{3}$ . So,  $p = q = r = \frac{1}{3}$ . This gives you one critical point  $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ .

Note that  $p, q$  and  $r$  take value between 0 and 1 so these endpoints determine other possible candidates for minimal and maximal values. Since  $p+q+r = 1$ , if one of  $p, q, r$  is 1, the rest have to be 0. Thus, points  $(1, 0, 0)$ ,  $(0, 1, 0)$  and  $(0, 0, 1)$  should also be considered.  $HE((\frac{1}{3}, \frac{1}{3}, \frac{1}{3})) = \frac{2}{9} + \frac{2}{9} + \frac{2}{9} = \frac{2}{3} = 66.67\%$ . The value of  $HE$  at any of the other three remaining points is 0, so 0 is the minimal and  $2/3$  is the maximal value.

2. Consider  $F = p^2 + q^2 + r^2 - \lambda(p + q + r - 1)$ . Finding critical points:  $F_p = 2p - \lambda = 0$ ,  $F_q = 2q - \lambda = 0$ ,  $F_r = 2r - \lambda = 0$ ,  $F_\lambda = -(p + q + r - 1) = 0$ . From the first three equations  $p = q = r = \frac{\lambda}{2}$ . Substituting that in the fourth one  $p + q + r = 1$  gives you that  $3p = 1 \Rightarrow p = \frac{1}{3}$ . So,  $p = q = r = \frac{1}{3}$ . This gives  $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$  and the endpoints 0 and 1 for  $p, q$  and  $r$  another three points  $(1, 0, 0)$ ,  $(0, 1, 0)$  and  $(0, 0, 1)$  just as in part (a).  $HO(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}) = \frac{1}{9} + \frac{1}{9} + \frac{1}{9} = \frac{1}{3} = 33.33\%$ . The value of  $HO$  at any of the other three remaining points is 1, so 1 is the maximal and  $1/3$  is the minimal value.