Mathematical Modeling
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Optimization.
Numerical Optimization. Linear Programming

Problems asking for a set of optimal conditions (maxima or minima) in relation to a certain situation appear very often. In this case, a mathematical model is created to find these optimal conditions.

We distinguish two types of optimization problems:

i) **Unconstrained Optimization.** Problems where a set of optimal conditions needs to be find without any additional constraints on the variables.

ii) **Constrained Optimization.** Problems where a set of optimal conditions needs to be find subject to a set of additional constraints on the variables.

An **unconstrained optimization** problem in a single variable can be solved using methods of Calculus 1.

1. Find the first derivative. Solve for zeros (critical points).

2.   - Either: find the second derivative. If it is positive at a critical point a, then there is a minimum at a. If it is negative at a critical point a, then there is a maximum at a.

   - Or: use the sign of the first derivative to determine which critical points are maxima and which are minima.

For a function in two variables, recall the following. To find the maximum and minimum values of $z = f(x, y)$:

1. Find the first partial derivatives f_x and f_y. Then find all points (a, b) where both partial derivatives are zero. Such points are called critical points.

2. Find the second partial derivatives f_{xx}, f_{xy}, f_{yx} and f_{yy}, and find the determinant $D = \begin{vmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{vmatrix} = f_{xx}f_{yy} - f_{xy}f_{yx}$.

3. Then,

    a) If $D > 0$ and $f_{xx}(a, b) > 0$, then $f(a, b)$ is a local **minimum**.
    b) If $D > 0$ and $f_{xx}(a, b) < 0$, then $f(a, b)$ is a local **maximum**.
    c) If $D < 0$, then $f(a, b)$ is **not** a local minimum or maximum. It is a saddle point.

To solve a **constrained optimization** problem in two variables, following the steps listed below might be helpful:

1. Sketch a diagram if possible.

2. Select the variables to represent the independent variables and the quantity to be maximized or minimized.

3. Write down the equation for the quantity to be minimized or maximized, **objective equation**. Write down the equation(s) that relates the independent variables, **constraint equation(s)**.

4. Solve the constraint for one variable and substitute in the objective. Find the zeros of the first derivative.

5. Plug those critical points into the objective. The smallest value is the minimum and the largest is the maximum.

6. Interpret the solution.

If the objective contains two independent variables, the solution can be found using simple methods of Calculus 1.

Example 1. An open top box is made with a square base and should have a volume of 6000 cubic inches. If the material for the sides costs $.20 per square inch and the material for the base costs $.30 per square inch, determine the dimensions of the box that minimize the cost of the materials.

Solution. List the variables: let x denotes the side of the base, y denotes the height and C denotes the cost. Objective: to minimize the cost function $C = .20 \cdot 4 \cdot xh + .30x^2$. Constraint: volume $= 6000$. So, $x^2h = 6000$. From the constraint we have that $h = 6000/x^2$. Substituting this in the objective, we arrive to a function in a single variable $C = \frac{4800}{x} + .3x^2$. Finding a minimum, we obtain $x = 20$. Then $h = 15$. The minimal cost is $ 360.

If the objective constrains contains more than two independent variables, Lagrange multipliers method can be helpful. Recall the following.

Let $y = f(x_1, x_2, \ldots, x_n)$ be a multivariable function. To find the maximum and minimum values of f subject to a constraint $g(x_1, x_2, \ldots, x_n) = 0$, we introduce a new variable λ, a **Lagrange multiplier**, and find the critical values of function $F = f - \lambda \cdot g$:

1. Find all the critical points $(x_1, x_2, \ldots, x_n, \lambda)$ of F.

2. 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.

If there are **two constraints** $g(x_1, x_2, \ldots, x_n) = 0$ and $h(x_1, x_2, \ldots, x_n) = 0$, then we introduce two new variables λ and μ and find the critical values of function $F = f - \lambda \cdot g - \mu \cdot h$. The second step is the same. This method generalizes to more than two constraints.

Example 2. A cardboard box without a lid is to have volume of 32,000 cm^3. Set up the equations for finding the dimensions that minimize the amount of cardboard used. Use Matlab if you have trouble solving the equations by hand.

Solution. List the variables: dimension of the box x, y, z. Objective: to minimize surface area $S = xy + 2xz + 2yz$. Constraint volume is 32000 so $xyz = 32000$. $F = xy + 2xz + 2yz - \lambda(xyz - 32000)$. Setting the partial derivatives of F equal to zero produces equations: $y + 2z - yz\lambda = 0$,

$x + 2z - xz\lambda = 0$, $\quad 2x + 2y - xy\lambda = 0$, and $xyz = 32,000$. Solving these equations would yield: square base of side $x = y = 40$ cm, and height $z = 20$ cm.

Numerical Optimization Methods

If the derivative of a function to be maximized is too complex so that finding its zeros might take too much time to find, finding the exact values of the critical points (and thus maximum and minimum as well) can be replaced by the numerical methods. Let us assume that we need to find the extreme value of $f(x)$ on interval $[a, b]$ and such that

1. $f(x)$ has exactly one maximum or minimum in the interior of $[a, b]$. Such function is called a **unimodal function**.

2. If 1. is not satisfied, you need to divide the interval $[a, b]$ in subintervals such $f(x)$ is unimodal on each interval.

The idea of a numerical optimization method we shall consider here. The algorithm below finds the **maximum value**. Finding the minimal value is analogous.

1. Divide $[a, b]$ into two overlapping intervals $[a, x_2]$ and $[x_1, b]$ choosing the test points x_1 and x_2 according to some chosen criterion.

2. Compute $f(x_1)$ and $f(x_2)$. There are 2 cases.

Case 1 $f(x_1) \geq f(x_2)$, the solution cannot lie in $[x_2, b]$. Let the left endpoint remain a, choose x_2 to be the new right endpoint and repeat the first two steps.

Case 2 $f(x_1) < f(x_2)$, the solution cannot lie in $[a, x_1]$. Let the right endpoint remain b, choose x_1 to be the new right endpoint and repeat the first two steps.

3. Keep repeating steps 1 and 2 *while* the length of the interval is larger than a given small number. This number is usually referred to as the **tolerance**.

4. Finally, the value $\frac{a+b}{2}$ approximates the x-value of the maximum. The corresponding y-value is $f(\frac{a+b}{2})$.

The points x_1 and x_2 in the first step can be chosen on several different ways. If these points are chosen so that

$$x_1 = \frac{a+b}{2} - \varepsilon \quad \text{and} \quad x_2 = \frac{a+b}{2} + \varepsilon$$

where ε is some (relatively small) number, the resulting method is called the **Dichotomous Search Method**.

Recall that the golden ratio $r = 0.618$ (see the handout on Difference Equations) is the positive solution of the equation $x^2 + x - 1 = 0$. If the golden ratio is used so that

$$x_1 = a + (1 - r)(b - a) \quad \text{and} \quad x_2 = a + r(b - a)$$

that is x_1 is the endpoint of the $1 - r$-th portion of $[a, b]$) and x_2 is the endpoint of the r-th portion of $[a, b]$, the resulting method is called the **Golden Section Search Method.**

The following M-file computes x and y values of the maximum point of an unimodal function f on an interval $[a, b]$ using the Dichotomous Search Method with a given tolerance t and using s to compute the endpoints x_1 and x_2 of two overlapping intervals in each step.

```
function [xmax, ymax]=dichotomous(a, b, f, s, t)
while b-a>t
   x1=(a+b)/2-s;
   x2=(a+b)/2+s;
   if f(x1)>=f(x2)
      a=a; b=x2;
   else b=b; a=x1;
   end
end
xmax=(a+b)/2;
ymax=f(xmax);
```

A similar M-file can be obtained for the Golden Section Search Method. The above M-file can also be modified to calculate **minimum value** of an unimodal function.

Note that the numerical optimization can be used for every least-squares fit (recall that every least-squares fit involves optimization of the sum of squares of differences $(y_i - f(x_i))$).

Linear Programming

If the objective is to optimize a linear function in two or more variables that is subject to the given constraints which are also linear equations, such problem can be solved using method called linear programming. Thus, let

Constraints = set of linear inequalities.   Objective = quantity that needs to be optimized.

Then perform the following steps:

1. **Interpret the problem.** Draw a table if possible.

2. **Assign the variables.** Label the unknowns and a variable for quantity that has to be optimized.

3. Set up the model: **write down the objective and constraints**.

4. **Graph the constraints** on the same chart.

5. **Find the feasible region.** The constraints divide the coordinate system into a few regions. Just one of them is a region that will satisfy **all** of the constraints. Such region is called the feasible region. Considering the inequalities (or simply plugging a point from the inside of each region in all of the constraints) determine which of the regions is feasible.

6. **Find the corner points** of your feasible region. Plug all the corner points into the *objective* equation. Compare the values: the smallest value is the minimum, the largest is the maximum value.

7. **Interpret the solution** in terms of the problem.

Example 3. A patient just had surgery and is required to have at least 84 units of drug D_1 and 120 units of drug D_2 each day. Assume that an over dosage of either drug is harmless. Each gram of substance M contains 10 units of D_1 and and 8 units of drug D_2 and each gram of substance N contains 2 units of D_1 and 4 units of D_2. Now suppose that both M and N contain an undesirable drug D_3, 3 units per gram in M and 1 unit per gram in N. Find how many grams of substances M and N should be taken in order to meet the requirements and minimize the intake of D_3 at the same time.

Solution. Define the variables: $x =$ number of grams of M, $y =$ number of grams of N, amount of D_1 taken$= 10x + 2y$, amount of D_2 taken$= 8x + 4y$, amount of D_3 taken $= 3x + y$. Objective: to minimize $D_3 = 3x + y$. Constraints

$$D_1 \geq 81, D_2 \geq 120, x \geq 0, y \geq 0.$$

This gives you

$$10x + 2y \geq 81, 8x + 4y \geq 120, x \geq 0, y \geq 0$$

The lines $10x + 2y = 81, 8x + 4y = 120, x = 0$, and $y = 0$ divide the plane in four regions. Testing the region determines the unbounded region to be the feasible one. It has 3 corner points (0,42), (15,0) and (4,22). Plugging all three of them in D_3 gives you that the point (4, 22) yields the smallest value of D_3 and so 4 grams of M and 22 grams of N should be taken.

Practice Problems.

1. Write M-files for Dichotomous and Golden Section Search Methods. Test the files to find the maximum of $f(x) = -4x^2 + 3.2x + 3$ on interval [-2,2] with a tolerance 0.2 (for Dichotomous method you can use $\varepsilon = 0.01$).

2. A team of engineers considered a physical system in order to determine the optimal conditions for an industrial flow process. Let x represent the flow rate of dye into the coloring process of cotton fabric. Based on this rate, the reaction differs with the other substances in the process as evidenced by the step function defined as

$$f(x) = \begin{cases} 2 + 2x - x^2 & 0 \leq x \leq 1.5 \\ -x + 17/4 & 1.5 < x \leq 4 \end{cases}$$

This function has exactly one maximum on interval [0,4]. Find the flow that maximizes the reaction of the other substances $f(x)$. Through experimentation, the engineers have found that the process is sensitive to within about 0.02 of the actual value of x.

3. A special dietary supplement regiment is designed for a patient. The liquid portion of the diet is to provide at most 696 calories, at least 105 units of vitamin A, and at least 150 units of vitamin C daily. The clinic sells two special dietary drinks X-tra and E-er-G. A cup of X-tra provides 58 calories, 10.5 units of vitamin A and 23 units of vitamin C. A cup of dietary drink N-er-G provides 80 calories, 15 units of vitamin A and 10 units of vitamin C. X-tra costs 18 cents per cup and N-er-G costs 20 per cup. Find how many cups should be taken daily in order to satisfy the requirements and minimize the cost at the same time.

4. A patient is required to have at least 60 milligrams of nifeldipin, at least 1100 micrograms of hydrochloride, at most 1000 micrograms of diezepamum, and at least 31 milligram of ibuprofen daily. These substances are to be consumed by taking a certain amount of Vianol and Gantric, both of which contain unwanted sodium-sulphate. Each gram of Vianol contains 140 micrograms of diezepamum, 13 milligrams of ibuprofen, 705 micrograms of hydrochlorid, 20 milligrams of nifeldipin, and 23 milligrams of sodium-sulphate. Each gram of Gantric contains 100 micrograms of diezepamum, 3.5 milligrams of ibuprofen, 310 micrograms of hydrochlorid, 15 milligrams of nifeldipin, and 12 milligrams of sodium-sulphate. How many grams of Vianol and Gantric should be taken to fulfill the requirements for diezepamum, ibuprofen, hydrochloride and nifeldipin and to minimize the intake of sodium-sulphate?

Solutions.

1. Using the Dichotomous Search Method: $x = .363$ $y = 3.6345$ increasing the tolerance, you can get closer to the exact answer $x = 0.4$. Using the Golden Section Search Method: $x = .403$ $y = 3.64$.

2. Use either Dichotomous or Golden Section search method. You can use a simple if.. else branch to compute the value of $f(x)$ for a given value of x. With the tolerance of 0.02, the golden section method gives you $x = 1.01$ and $y = 2.9999$. The exact value of maximum is $(1, 3)$.

3. $x =$ number of cups of X-tra, $y =$ number of cups of N-er-G. Objective: to minimize $C = 18x + 20y$. Constraints: $58x + 80y \le 69$, $10.5x + 15y \ge 105$, $23x + 10y \ge 150$, $x \ge 0$ and $y \ge 0$. The feasible region has 4 corner points and $(5, 3.5)$ minimizes the cost.

4. $x =$ number of grams of Vianol, $y =$ number of grams of Gantric. Objective $f = 23x + 12y$. Constraints: $20x + 15y \ge 60$, $.705x + .310y \ge 1.1$, $.14x + .1y \le 1$, $13x + 3.5y \ge 31$, $x \ge 0$ and $y \ge 0$. Get $x = 2.04$ and $y = 1.28$. at that point $f = 62.28$.