# HAB 619 Introduction to Scientific Computing in Sports Science



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# **SERDAR ARITAN**

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Optimization - finding value of a parameter that maximizes or minimizes a function with that parameter

- Talking about <u>mathematical optimization</u>, not optimization of computer code!
- "function" is mathematical function, not python language def
- Can have multiple parameters
- Can have multiple functions
- Parameters can appear linearly or nonlinearly

#### Linear programming

- Most often used kind of optimization
- Tremendous number of practical applications
- "Programming" means determining feasible programs (plans, schedules, allocations) that are optimal with respect to a certain criterion and that obey certain constraints
- A feasible program is a solution to a linear programming problem and that satisfies certain constraints
- In linear programming
- Constraints are linear inequalities
- Criterion is a linear expression
- Expression called the objective function
- In practice, objective function is often the cost of or profit from some activity

#### **Diet Problem**

You are given a group of foods, their nutritional values and costs. You know how much nutrition a person needs. What combination of foods can you serve that meets the nutritional needs of a person but costs the least?



Mathematical formulation

The variables  $x_1, x_2, ... x_n$  satisfy the inequalities

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n \le b_1$$

$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n \le b_2$$

$$\vdots$$

$$a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n \le b_m$$

and  $x_1 \ge 0$ ,  $x_2 \ge 0$ , ...  $x_n \ge 0$ . Find the set of values of  $x_1$ ,  $x_2$ , ...  $x_n$  that minimizes (maximizes)

$$x_1 f_1 + x_2 f_2 + \cdots + x_n f_n$$

Note that  $a_{pq}$  and  $f_i$  are known

Mathematical matrix formulation

Find the value of x that minimizes (maximizes)  $f^Tx$  given that  $x \ge 0$  and  $Ax \le b$ , where

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{21} & \cdots & a_{21} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \text{and } f = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}$$



#### General procedure

- Restate problem in terms of equations and inequalities
- Rewrite in matrix and vector notation
- Call function linprog from scipy.optimize to solve



Example – diet problem

Nowadays kids diet comes from the four basic food groups - chocolate dessert, ice cream, soda, and cheesecake. They checks in a store and finds one of each kind of food, namely, a brownie, chocolate ice cream, Pepsi, and one slice of pineapple cheesecake. Each day they needs at least 500 calories, 6 gr of chocolate, 10 gr of sugar, and 8 gr of fat. Using the table on the next slide that gives the cost and nutrition of each item, figure out how much he should buy and eat of each of the four items he found in the store so that he gets enough nutrition but spends as little as possible.





## Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice





## Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
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Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

#### What are unknowns?

 $x_1$  = number of brownies to eat each day

 $x_2$  = number of scoops of chocolate ice cream to eat each day

 $x_3$  = number of bottles of Coke to drink each day

x<sub>4</sub> = number of pineapple cheesecake slices to eat each day
 In linear programming "unknowns" are called decision variables





#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

Objective is to minimize cost of food. Total daily cost is

Cost = (Cost of brownies) + (Cost of ice cream) (Cost of Coke) + (Cost of cheesecake)

- Cost of brownies =  $(Cost/brownie) \times (brownies/day)$  $= 2.5 x_1$
- Cost of ice cream =  $x_2$
- Cost of Coke =  $1.5x_3$
- Cost of cheesecake =  $4x_4$





#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

#### Therefore, need to minimize

min 
$$2.5x_1 + x_2 + 1.5x_3 + 4x_4$$



#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

#### Constraint 1 - calorie intake at least 500

- Calories from brownies = (calories/brownie)(brownies/day)
   = 400x<sub>1</sub>
- Calories from ice cream = 200x<sub>2</sub>
- Calories from Coke = 150x<sub>3</sub>
- Calories from cheesecake =  $500x_4$

So constraint 1 is  $400x_1 + 200x_2 + 150x_3 + 500x_4 \ge 500$ 



#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

#### Constraint 2 - chocolate intake at least 6 gr

- Chocolate from brownies = (Chocolate/brownie)(brownies/day)
   = 3x<sub>1</sub>
- Chocolate from ice cream = 2x<sub>2</sub>
- Chocolate from Coke = 0x<sub>3</sub> = 0
- Chocolate from cheesecake =  $0x_4 = 0$

So constraint 2 is 
$$3x_1 + 2x_2 \ge 6$$





#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

#### Constraint 3 - sugar intake at least 10 gr

- Sugar from brownies = (sugar/brownie)(brownies/day)  $= 2x_{1}$
- Sugar from ice cream =  $2x_2$
- Sugar from Coke =  $4x_3$
- Sugar from cheesecake =  $4x_4$

So constraint 3 is 
$$2x_1 + 2x_2 + 4x_3 + 4x_4 \ge 10$$





#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

#### Constraint 4 - fat intake at least 8 gr

- (fat/brownie)(brownies/day) from brownies Fat  $= 2x_{1}$
- Fat from ice cream =  $4x_2$
- Fat from Coke =  $1x_3$
- Fat from cheesecake =  $5x_4$

So constraint 4 is 
$$2x_1 + 4x_2 + x_3 + 5x_4 \ge 8$$



#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

Finally, we assume that the amounts eaten are non-negative, i.e., we ignore throwing up. This means that we have

$$x_1 \ge 0, x_2 \ge 0, x_3 \ge 0, \text{ and } x_4 \ge 0$$





#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

Putting it all together, we have to minimize

$$2.5x_1 + x_2 + 1.5x_3 + 4x_4$$

#### subject to the constraints

And

$$x_1 \ge 0$$
$$x_2 > 0$$

$$x_2 \ge 0$$

$$x_3 \ge 0$$

$$x_4 \ge 0$$

$$400x_1 + 200x_2 + 150x_3 + 500x_4 \ge 500$$
$$3x_1 + 2x_2 \ge 6$$
$$2x_1 + 2x_2 + 4x_3 + 4x_4 \ge 10$$
$$2x_1 + 4x_2 + x_3 + 5x_4 \ge 8$$





#### Example – diet problem

Food	Calories	Chocolate	Sugar	Fat	Cost (serving)
Brownie	400	3	2	2	\$2.50 / brownie
Chocolate ice cream	200	2	2	4	\$1.00 / scoop
Coke	150	0	4	1	\$1.50 / bottle
Pineapple cheesecake	500	0	4	5	\$4.00 / slice

In matrix notation, want to

minimize  $f^T x$  subject to  $Ax \ge b$  and  $x \ge 0$ 

where

$$A = \begin{bmatrix} 400 & 200 & 150 & 500 \\ 3 & 2 & 0 & 0 \\ 2 & 2 & 4 & 4 \\ 2 & 4 & 1 & 5 \end{bmatrix}, \quad b = \begin{bmatrix} 500 \\ 6 \\ 10 \\ 8 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}, \quad \text{and } f = \begin{bmatrix} 2.5 \\ 1 \\ 1.5 \\ 4 \end{bmatrix}$$



scipy.optimize.linprog solves linear programming

minimize 
$$f^T x$$
 such that 
$$\begin{cases} A \cdot x \le b \\ Aeq \cdot x = beq \\ lb \le x \le ub \end{cases}$$

where x, b, beq, lb, and ub are vectors and A and Aeq are matrices.

- Can use one or more of the constraints
- "Ib" means "lower bound", "ub" means "upper bound" Often have lb = 0 and  $ub = \infty$ , i.e., no upper bound





scipy.optimize programming solver is linprog()

scipy.optimize.linprog(f, A\_ub=None, b\_ub=None, A\_eq=None, b\_eq=None, bounds=None,
method='interior-point', callback=None, options=None, x0=None)

Linear programming: minimize a linear objective function subject to linear equality and inequality constraints.

f 1-D array

The coefficients of the linear objective function to be minimized.

A ub 2-D array, optional

The inequality constraint matrix. Each row of A\_ub specifies the coefficients of a linear inequality constraint on x.

b\_ub 1-D array, optional

The inequality constraint vector. Each element represents an upper bound on the corresponding value of



# minimize $f^T x$ subject to $Ax \ge b$ and $0 \le x$

$$A = \begin{bmatrix} 400 & 200 & 150 & 500 \\ 3 & 2 & 0 & 0 \\ 2 & 2 & 4 & 4 \\ 2 & 4 & 1 & 5 \end{bmatrix}, \quad b = \begin{bmatrix} 500 \\ 6 \\ 10 \\ 8 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}, \quad \text{and } f = \begin{bmatrix} 2.5 \\ 1 \\ 1.5 \\ 4 \end{bmatrix}$$

#### NumPy:

minimize 
$$f^T x$$
 such that 
$$\begin{cases} A \cdot x \not \ge b \\ Aeq \cdot x = beq \\ lb \le x \le ub \end{cases}$$

Note two differences:



linprog() solves linear programming problem

**ISSUE 1** - We have  $Ax \ge b$  but need  $Ax \le b$ 

One way to handle is to note that

if  $Ax \ge b$  then  $-Ax \le -b$ , so can have **numpy**. **negative** use constraint

$$(-A)x \leq (-b)$$

**ISSUE 2** - We have  $0 \le x$  but linprog() wants  $lb \le x \le ub$ . Handle by omitting ub in call of **linprog()**. If omitted, linprog() assumes no upper bound.

```
import numpy as np
from scipy.optimize import linprog
# objective function
f = np.array([2.5, 1.0, 1.5, 4.0])
# constraint matrix
A = np.array([[400, 200, 150, 500],
              [3.0, 2.0, 0.0, 0.0],
              [2.0, 2.0, 4.0, 4.0],
              [2.0, 4.0, 1.0, 5.0]])
# inequality constraint vector
b = np.array([500.0, 6.0, 10.0, 8.0])
x1 bounds = (0, None)
x2 bounds = (0, None)
x3 bounds = (0, None)
x4 bounds = (0, None)
result = linprog(f, A ub=np.negative(A), b ub=np.negative(b), \
         bounds=[x1 bounds, x2 bounds, x3 bounds, x4 bounds])
```

```
NumPy
```

```
>>> print(result)
con: array([], dtype=float64)
    fun: 4.5000000466017935
message: 'Optimization terminated successfully.'
    nit: 7
    slack: array([2.50000005e+02, 4.03549727e-09, 4.82628302e-08,
4.9999998e+00])
    status: 0
    success: True
>>> x = np.array(result.x)
>>> print(x)
[1.42673815e-08 2.99999998e+00 1.00000001e+00 3.35245816e-09]
```



Optimal solution is  $x = [0 \ 3 \ 1 \ 0]$ . In words, kids Numpy should eat 3 scoops of ice cream and drink 1 Coke each day.

A constraint is binding if both sides of the constraint inequality are equal when the optimal solution is substituted.

For 
$$\mathbf{x} = [0 \ 3 \ 1 \ 0]$$
 the set

Becomes 
$$750 \ge 500$$
,  $6 \ge 6$   $3x_1 + 2x_2 \ge 6$   $2x_1 + 2x_2 + 4x_3 + 4x_4 \ge 10$   $13 \ge 8$   $2x_1 + 4x_2 + x_3 + 5x_4 \ge 8$ 

so the chocolate and sugar constraints are binding. The other two are nonbinding



How many calories, and how much chocolate, sugar and fat NumPy will he get each day?

```
>> print(np.negative(A) @ x)
[-750.0000052
                 -6.
                              -10.00000005 -12.99999998
750.0 calories
 6.0 chocolate
 10.0 sugar
 13.0 fat
```

How much money will this cost?

```
>>> print(f @ x)
4.5000000466017935 # dollars
```



#### **Special Kinds of Solutions**

Usually a linear programming problem has a unique (single) optimal solution. However, there can also be:

- No feasible solutions
- An unbounded solution. There are solutions that make the objective function arbitrarily large (max problem) or arbitrarily small (min problem)
- An infinite number of optimal solutions. The technique of goal programming is often used to choose among alternative optimal solutions.



A scipy.optimize.OptimizeResult consisting of the fields:

NumPv x 1-D array

The values of the decision variables that minimizes the objective function while satisfying the constraints.

fun float

The optimal value of the objective function c @ x.

slack 1-D array

The (nominally positive) values of the slack variables, b ub - A ub @ x.

con 1-D array

The (nominally zero) residuals of the equality constraints, b\_eq - A\_eq @ x.

successbool

True when the algorithm succeeds in finding an optimal solution.

statusint

An integer representing the exit status of the algorithm.

0 : Optimization terminated successfully.

1 : Iteration limit reached.

2 : Problem appears to be infeasible.

3 : Problem appears to be unbounded.

4 : Numerical difficulties encountered.

nitint

The total number of iterations performed in all phases.

messagestr

A string descriptor of the exit status of the algorithm.