Least-squares approximation (LSA)

Ágnes Baran, Csaba Noszály

Least-squares approximation (LSA)

In nutshell:

- Collect the data.
- Select the most appropriate model.
- Compute the best instance of the chosen model
- Use the model (predicting)

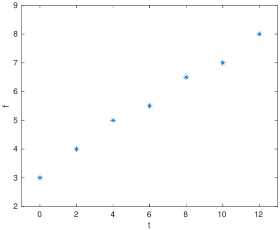
Example

A cylindrical, 0.5m height tank is being filled with water at a constant rate. Peter starts to observe the height of water (at $t = 0$) in the tank. The measurements are summarized in the table below.

t_i (min)	0	2	4	6	8	10	12
f_i (cm)	3	4	5	5.5	6.5	7	8

The following questions arise:

- What is the height of the water in the tank at $t = 20$?
- When will be the tank full?
- When was the tank empty?



Because of the circumstances (constant rate, the shape of the tank) we choose the linear model:

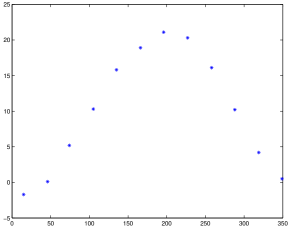
$$F(t) = x_1 + x_2 t$$

Monthly average temperatures in Budapest 1901-1950.

t_i	15	46	74	105	135	166	196	227	258	288	319	349
f_i	-1.7	0.1	5.2	10.3	15.8	18.9	21.1	20.3	16.1	10.2	4.2	0.5

This time, the periodicity presenting in the data suggests of using the model:

$$F(t) = x_1 + x_2 \cos\left(2\pi \frac{t-14}{365}\right)$$



Least squares approximations

We have the observations:

$$f_1, f_2, \dots, f_m \in \mathbb{R}$$

at time moments:

$$t_1, t_2, \dots, t_m \in \mathbb{R}$$

We assume that the observed phenomenon can be described by a `model`:

$$F(t) = \sum_{j=1}^{n} x_j \varphi_j(t)$$

- the φ_j's are `given` functions, the building blocks of our model.
- the x_j's are real numbers, the `unknown` coefficients of the model.

There are infinitely many functions of this type. We are going to choose the one, for which

$$J(x) = \sum_{i=1}^{m} (F(t_i) - f_i)^2$$

is `minimal`.

The model F determined in this way is called a `least-squares` approximation of the data.

Common models

`linear model`

$n = 2$ and $\varphi_1(t) \equiv 1$, $\varphi_2(t) = t$:

$$F(t) = x_1 + x_2 t$$

Common models

`polynomial model`

$\varphi_1(t) \equiv 1$, $\varphi_2(t) = t$, ..., $\varphi_n(t) = t^{n-1}$:

$$F(t) = x_1 + x_2 t + x_3 t^2 + \cdots + x_n t^{n-1}$$

Common models

`trigonometric model`

$n = 3$ and $\varphi_1(t) \equiv 1$, $\varphi_2(t) = \sin(\pi t)$, $\varphi_3(t) = \cos(\pi t)$:

$$F(t) = x_1 + x_2 \sin(\pi t) + x_3 \cos(\pi t)$$

We can express our model by means of matrices and vectors:

$$A = \begin{pmatrix} \varphi_1(t_1) & \varphi_2(t_1) & \dots & \varphi_n(t_1) \\ \varphi_1(t_2) & \varphi_2(t_2) & \dots & \varphi_n(t_2) \\ \vdots & & & \\ \varphi_1(t_m) & \varphi_2(t_m) & \dots & \varphi_n(t_m) \end{pmatrix} \in \mathbb{R}^{m\times n},$$

$$f = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{pmatrix} \in \mathbb{R}^m, \qquad x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \in \mathbb{R}^n,$$

$$Ax = \begin{pmatrix} F(t_1) \\ F(t_2) \\ \vdots \\ F(t_m) \end{pmatrix}$$

The function to be minimized:

$$J(x) = \sum_{i=1}^{m} (F(t_i) - f_i)^2 = \|Ax - f\|_2^2$$

In calculus, it is proved that at the minimum location the partial derivatives are zero:

$$\frac{\partial J(x)}{\partial x_k} = 0, \quad k = 1, \ldots, n.$$

Which can be rearranged in the form:

$$A^T A x = A^T f$$

It is the `Gaussian normal-equation`.

Gaussian normal-equation

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- it always has a solution
- the solution gives the coefficients of the best model in the "least squares" sense
- If A has linearly independent columns, then the solution is unique.
- If the column vectors of A forms linearly dependent system, then there are infinitely many solutions. This situation is called singularity. ($A^T A$ is singular)

In case of singularity we need:

- to get (collect) more data
- to simplify the model (drop out some of the φ_j's)

Example

Linear model: $F(t) = x_1 + x_2 t$, $\varphi_1(t) \equiv 1$ and $\varphi_2(t) = t$

$$A = \begin{pmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \\ 1 & t_m \end{pmatrix}$$

$$A^T A = \begin{pmatrix} m & \sum_{i=1}^{m} t_i \\ \sum_{i=1}^{m} t_i & \sum_{i=1}^{m} t_i^2 \end{pmatrix}, \qquad A^T f = \begin{pmatrix} \sum_{i=1}^{m} f_i \\ \sum_{i=1}^{m} t_i f_i \end{pmatrix}$$

Singularity (the column vectors of A is dependent system):

$$t_1 = t_2 = \cdots = t_m$$

Example

Polynomial model: $F(t) = x_1 + x_2 t + x_3 t^2 + \dots + x_n t^{n-1}$, that is

$$\varphi_1(t) \equiv 1, \varphi_2(t) = t, ..., \varphi_n(t) = t^{n-1}$$

$$A = \begin{pmatrix} 1 & t_1 & t_1^2 & \dots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \dots & t_2^{n-1} \\ \vdots & & & & \\ 1 & t_m & t_m^2 & \dots & t_m^{n-1} \end{pmatrix}$$

Polynomial model

Example

$$A^T A = \begin{pmatrix} m & \sum_{i=1}^m t_i & \sum_{i=1}^m t_i^2 & \dots & \sum_{i=1}^m t_i^{n-1} \\ \sum_{i=1}^m t_i & \sum_{i=1}^m t_i^2 & \sum_{i=1}^m t_i^3 & \dots & \sum_{i=1}^m t_i^n \\ \sum_{i=1}^m t_i^2 & \sum_{i=1}^m t_i^3 & \dots & \dots & \\ \vdots & & & & \\ \sum_{i=1}^m t_i^{n-1} & & & \dots & \sum_{i=1}^m t_i^{2n-2} \end{pmatrix}$$

Polynomial model

$$A^T f = \begin{pmatrix} \sum_{i=1}^{m} f_i \\ \sum_{i=1}^{m} f_i t_i \\ \sum_{i=1}^{m} f_i t_i^2 \\ \vdots \\ \sum_{i=1}^{m} f_i t_i^{n-1} \end{pmatrix}$$

The solution is unique, if there are at least n different number among $t_1, t_2, \ldots, t_m$.

Example

Determine the linear LSA for the data given below!

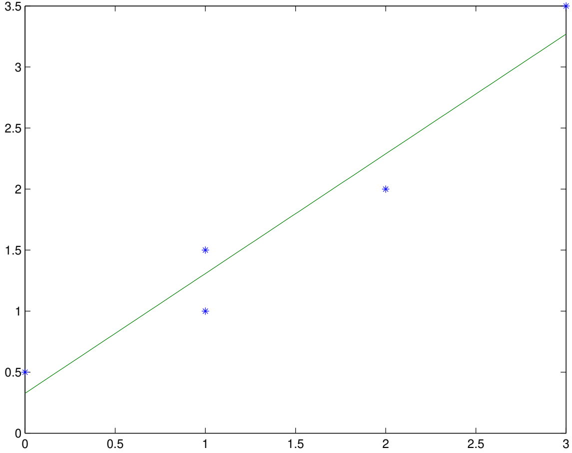
t_i	0	1	1	2	3
f_i	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{7}{2}$

The (general) model: $F(t) = x_1 + x_2 \cdot t$

$$\begin{pmatrix} 5 & 7 \\ 7 & 15 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \frac{17}{2} \\ 17 \end{pmatrix}$$

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{1}{26} \begin{pmatrix} 15 & -7 \\ -7 & 5 \end{pmatrix} \begin{pmatrix} \frac{17}{2} \\ 17 \end{pmatrix} = \begin{pmatrix} \frac{17}{52} \\ \frac{51}{52} \end{pmatrix}$$

The actual model: $F(t) = \frac{17}{52} + \frac{51}{52} t$


3.5
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
2.5
3

Example

Determine the linear LSA for the data given below!

t_i	2	2	2	2	2
f_i	1	1	2	2	2

The model: $F(t) = x_1 + x_2 \cdot t$

$$\begin{pmatrix} 5 & 10 \\ 10 & 20 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 8 \\ 16 \end{pmatrix}$$

$$5x_1 + 10x_2 = 8$$

$$x_2 = s \in \mathbb{R}, \qquad x_1 = \frac{8}{5} - 2s$$

Setting $s = 0$, we get an instance of solutions: $F(t) \equiv \frac{8}{5}$

LSA in Octave/Matlab

Example

Determine the linear LSA for the data given below!

t_i	1	1.1	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2
f_i	8	8.9	9	9.8	10	11	11.5	11.5	12.5	13	13.7	14

LSA in Octave/Matlab

Solution:

Use the function `polyfit`! The call:

```
>> p=polyfit(t,f,m)
```

will return the coefficients of the LSA polynomial `p` of degree `m` for the data points (t_i, f_i), as given in vectors `t` and `f`. The coefficients in `p` are in `decreasing` order.

```
>> t=[1 1.1 1.1:0.1:2];
>> f=[8 8.9 9 9.8 10 11 11.5 11.5 12.5 13 13.7 14];
>> p=polyfit(t,f,1)
p=
  5.8235    2.5338
```

LSA in Octave/Matlab

The equation of the line:

$$f(t) = 5.8235t + 2.5338$$

LSA in Octave/Matlab

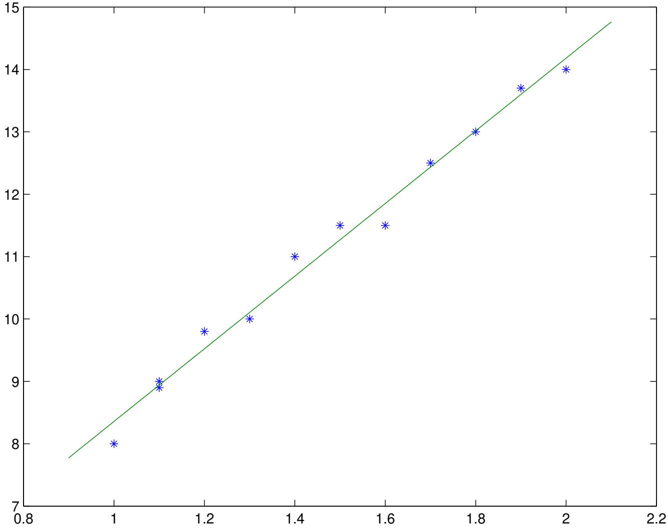
The equation of the line:

$$f(t) = 5.8235t + 2.5338$$

A plot of the data and the corresponding LSA line can be made as follows:

```
>> xx=linspace(0.9,2.1);
>> yy=polyval(p,xx);
>> figure; plot(t,f,'*',xx,yy)
```

Where the function `polyval` evaluates the polynomial `p` at locations given in `xx`.



15
14
13
12
11
10
9
8
7
0.8
1
1.2
1.4
1.6
1.8
2
2.2

Exercise 1

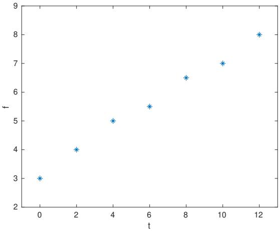
A cylindrical, 0.5m height tank is being filled with water at a constant rate. Peter starts to observe the height of water (at $t = 0$) in the tank. The measurements are summarized in the table below.

t_i (min)	0	2	4	6	8	10	12
f_i (cm)	3	4	5	5.5	6.5	7	8

Answer the questions below:

- What is the height of the water in the tank at $t = 20$?
- When will be the tank full?
- When was the tank empty?

Examining the data plot, the linear connection between `t` and `f` seems acceptable.



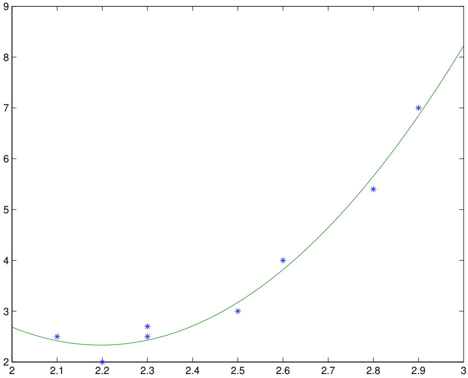
Solution:

Simple application of the built-in `polyval`. Note that the values that we get evaluating the LSA function only give approximations of the real values!

Exercise 2

Determine the quadratic (2nd order polynomial) LSA for the points (t_i, f_i)!
What is the (mean) value of the process at $t = 4$?

t_i	2.1	2.2	2.3	2.3	2.5	2.6	2.8	2.9
f_i	2.5	2	2.5	2.7	3	4	5.4	7

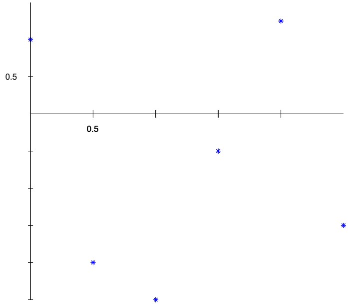

9
8
7
6
5
4
3
2
2
2.1
2.2
2.3
2.4
2.5
2.6
2.7
2.8
2.9
3

Example

Determine LSA for the given points using the model:

$$F(t) = x_1 + x_2 \cos(\pi t) + x_3 \sin(\pi t)$$

t_i	0	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$
f_i	1	-2	$-\frac{5}{2}$	$-\frac{1}{2}$	$\frac{5}{4}$	$-\frac{3}{2}$


0.5
0.5

Setting up the Gaussian normal equation:

$\varphi_1(t) \equiv 1$, $\varphi_2(t) = \cos(\pi t)$, $\varphi_3(t) = \sin(\pi t)$

$$A = \begin{pmatrix} 1 & \cos(\pi t_1) & \sin(\pi t_1) \\ 1 & \cos(\pi t_2) & \sin(\pi t_2) \\ \vdots & & \\ 1 & \cos(\pi t_6) & \sin(\pi t_6) \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

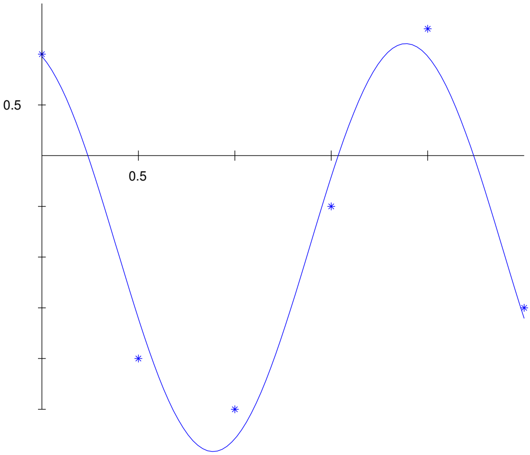
$$A^T A = \begin{pmatrix} 6 & 1 & 1 \\ 1 & 3 & 0 \\ 1 & 0 & 3 \end{pmatrix}, \qquad A^T f = \begin{pmatrix} -\frac{17}{4} \\ \frac{19}{4} \\ -3 \end{pmatrix}$$

We get the (unique) solution:

$$x = \begin{pmatrix} -\frac{29}{32} \\ \frac{181}{96} \\ -\frac{67}{96} \end{pmatrix}$$

So, the actual model is

$$F(t) = -\frac{29}{32} + \frac{181}{96}\cos(\pi t) - \frac{67}{96}\sin(\pi t)$$


0.5
0.5

Example

Determine LSA for the given points using the model:

$$F(t) = x_1 + x_2 \cos(\pi t) + x_3 \sin(\pi t)$$

t_i	0	$\frac{1}{2}$	2	$\frac{5}{2}$
f_i	1	-2	$\frac{5}{4}$	$-\frac{3}{2}$

$$A = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \qquad f = \begin{pmatrix} 1 \\ -2 \\ \frac{5}{4} \\ -\frac{3}{2} \end{pmatrix}$$

The columns of A form dependent system: the model is singular. (actually $A^T A$ is)

Handling singularity:

- get more data (sometimes impossible)
- simplify the model (always can be done)

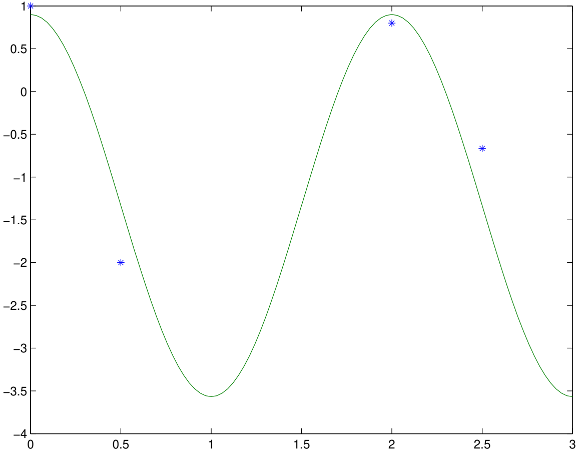
This time we will simplify our model: we drop out the sin term:

$$F(t) = x_1 + x_2 \cos(\pi t)$$

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 0 \end{pmatrix}, \qquad f = \begin{pmatrix} 1 \\ -2 \\ \frac{5}{4} \\ -\frac{3}{2} \end{pmatrix}$$

Solving the SLE $A^T A x = A^T f$, we get unique LSA solution for the simplified model:

$$x = \begin{pmatrix} -1.3333 \\ 2.2333 \end{pmatrix}$$


1
0.5
0
−0.5
−1
−1.5
−2
−2.5
−3
−3.5
−4
0
0.5
1
1.5
2
2.5
3

LSA in Octave/Matlab

Example

Determine the LSA for the given data, using the model:

$$F(t) = x_1 + x_2 \cos(\pi t) + x_3 \sin(\pi t)$$

t_i	0.1	0.5	1.2	1.5	2	2.1	2.4	3	3.2
f_i	3.9	2.6	-0.8	0.3	3.2	3.8	3.2	-0.7	-0.9

LSA in Octave/Matlab

Solution:
The parameters are obtained by solving:

$$A^T A x = A^T f$$

where:

$$A = \begin{pmatrix} 1 & \cos(\pi t_1) & \sin(\pi t_1) \\ 1 & \cos(\pi t_2) & \sin(\pi t_2) \\ \vdots & & \\ 1 & \cos(\pi t_9) & \sin(\pi t_9) \end{pmatrix}, \quad f = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_9 \end{pmatrix}, \quad x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

Building up the matrix A based on the data:

```
>> t=[0.1 0.5 1.2 1.5 2 2.1 2.4 3 3.2]';
>> f=[3.9 2.6 -0.8 0.3 3.2 3.8 3.2 -0.7 -0.9]';
>> A=[ones(9,1), cos(pi*t), sin(pi*t)];
```

Remember that `t` and `f` should be column vectors.

Solve the normal equation:

```
>> x=(A'*A)\(A'*f)
x =
   1.4372
   2.0310
   1.1711
```

Substituting the parameters into the model, we get:

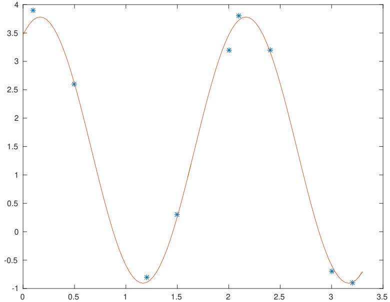
$$F(t) = 1.4372 + 2.0310\cos(\pi t) + 1.1711\sin(\pi t)$$

Plot the data and the model!

```
>> xx=linspace(0,3.3);
>> yy=x(1)+x(2)*cos(pi*xx)+x(3)*sin(pi*xx);
>> figure; plot(t,f,'*',xx,yy)
```

In one block:

```
t=[0.1 0.5 1.2 1.5 2 2.1 2.4 3 3.2]';
f=[3.9 2.6 -0.8 0.3 3.2 3.8 3.2 -0.7 -0.9]';
A=[ones(9,1), cos(pi*t), sin(pi*t)];
x=(A'*A)\(A'*f);
xx=linspace(0,3.3);
yy=x(1)+x(2)*cos(pi*xx)+x(3)*sin(pi*xx);
figure; plot(t,f,'*',xx,yy)
```



4
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
-1
0
0.5
1
1.5
2
2.5
3
3.5

Exercise 3

Determine the linear LSA for the given data!

t_i	1	1.2	1.4	1.4	1.5	1.7	1.9	2
f_i	6.2	7	8	7.9	8.4	9.2	10	10.6

Exercise 4

Determine the 3-rd order polynomial LSA for the given data!

t_i	0.5	0.8	1.1	1.3	1.5	1.7	1.9	2.1	2.3
f_i	2.5	2.3	1.8	1.3	0.9	0.4	0.1	-0.05	-0.01

Exercise 5

Determine the LSA for the given data, using the model:

$$F(t) = x_1 + \frac{x_2}{t}$$

t_i	1	1.2	1.4	1.4	1.5	1.7	1.9	2	2.1	2.2
f_i	4.2	3.8	3.4	3.3	3.3	3	2.8	2.8	2.75	2.7

Exercise 6

Determine the LSA for the given data, using the model:

$$F(t) = x_1 \sin(t) + x_2 \sin(2t) + x_3 \sin(3t)$$

t_i	0.1	0.5	1.2	1.5	2	2.1	2.4	3	3.2	3.4	3.8	4	4.2	4.6	5
f_i	1	4.1	3	1	-1.5	-1.6	-1.7	-0.4	0.1	0.7	1.6	1.8	1.6	0.2	-2.5

Exercise 7

Determine the LSA for the given data, using the model:

$$F(t) = x_1 + x_2 ln(t)$$

t_i	0.1	0.5	1.2	1.5	2	2.1	2.4	3	3.2
f_i	-0.6	1.5	2.5	2.9	3.2	3.3	3.5	3.8	3.9

Exercise 8

Determine the LSA for the given data, using the model:

$$F(t) = x_1 + x_2 \cos\left(2\pi \frac{t-14}{365}\right)$$

t_i	15	46	74	105	135	166	196	227	258	288	319	349
f_i	-1.7	0.1	5.2	10.3	15.8	18.9	21.1	20.3	16.1	10.2	4.2	0.5

Exercise 9

Determine the linear LSA for the given data!

t_1	0	1	2	3
f_i	0.5	1.5	2	3

Exercise 10

Determine the linear LSA for the given data!

t_i	0	1	1	2	3
f_i	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$

Exercise 11

Determine the LSA for the given data, using the model:

$$F(t) = x_1 + \frac{x_2}{t}$$

t_i	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1
f_i	8	6	4	$\frac{5}{2}$

Exercise 12

Determine the LSA for the given data, using the model:

$$F(t) = x_1 + x_2 \cdot \sin^2\left(\frac{t\pi}{2}\right)$$

t_i	0	$\frac{1}{2}$	1	2
f_i	$\frac{1}{2}$	1	1	0

Data for the exercises

The datas in text file