



University
of Manitoba

Matrix methods – Least squares problems

MATH 2740 – Mathematics of Data Science – Lecture 06

Julien Arino

FIGS-slides-admin/Gemini_Gjulien.arino@umanitoba.ca7iz9.jpeg

Department of Mathematics @ University of Manitoba

Fall 202X

The University of Manitoba campuses are located on original lands of Anishinaabeg, Ininew, Anisininew, Dakota and Dene peoples, and on the National Homeland of the Red River Métis. We respect the Treaties that were made on these territories, we acknowledge the harms and mistakes of the past, and we dedicate ourselves to move forward in partnership with Indigenous communities in a spirit of Reconciliation and collaboration.

Outline

Least squares problems

FIGS-slides-admin/Gemini_Generated_Image_iyzqdwiyzqdwiyzq.jpeg

Least squares problems

FIGS-slides-admin/Gemini_Generated_Image_c06eixc06eixc06e.jpeg

Least squares problems

Getting the Canadian census data

Least squares problem – Initial considerations

Least squares problem

Fitting something more complicated

Grabing the Canadian census data

We want to consider the evolution of the population of Canada through time

For this, we grab the Canadian census data

Search for (Google) “Canada historical census data csv”, since csv (comma separated values) is a very easy format to use with R

Here, we find a csv for 1851 to 1976

We follow the link to Table A2-14, where we find another link, this time to a csv file.
This is what we use in R

Grabing the Canadian census data

The function `read.csv` reads in a file (potentially directly from the web)

Assign the result to the variable `data`. We then use the function `head` to show the first few lines in the result.

```
data_old = read.csv("https://www150.statcan.gc.ca/n1/en/pub/11-516-x/section
head(data_old)
```

```
##      X Series.A2.14.
```

```
## 1 NA
```

```
## 2 NA      Year
```

```
## 3 NA
```

```
## 4 NA
```

```
## 5 NA
```

```
## 6 NA
```

```
##      Population.of.Canada..by.province..census.dates..1851.to.1976 X.1
```

```
## 1 NA
```

```
## 2      Canada NA Newf
```

```
## 3 NA
```

Obviously, this does not make a lot of sense. This is normal: take a look at the first few lines in the file. They take the form

```
head(data_old)
```

```
##      X Series.A2.14.
```

```
## 1 NA
```

```
## 2 NA          Year
```

```
## 3 NA
```

```
## 4 NA
```

```
## 5 NA
```

```
## 6 NA
```

```
## Population.of.Canada..by.province..census.dates..1851.to.1976 X.1
```

```
## 1                                                                NA
```

```
## 2                                                                Canada NA Newf
```

```
## 3                                                                NA
```

```
## 4                                                                NA
```

```
## 5                                                                2 NA
```

```
## 6                                                                NA
```

The first line here does this; it is easy to deal with this: the function `read.csv` takes the optional argument `skip=`, which indicates how many lines to skip at the beginning. The second line is also empty, so let us skip it too.

```
data_old = read.csv("https://www150.statcan.gc.ca/n1/en/pub/11-516-x/section
                    skip = 2)
```

```
head(data_old)
```

##	X	Year	Canada	X.1	Newfound.	Prince	X.2	Nova	New	Quebe	
## 1	NA			NA	land	Edward	NA	Scotia	Brunswick		
## 2	NA			NA		Island	NA				
## 3	NA		2	NA	3	4	NA	5	6		
## 4	NA			NA			NA				
## 5	NA	1976	22,992,604	NA	557,725	118,229	NA	828,571	677,250	6,234,44	
## 6	NA			NA			NA				
##		Ontario	Manitoba	X.3	Saskat.	X.4	Alberta	X.5	British	X.6	Yuk
## 1				NA	chewan	NA		NA	Columbia	NA	Territo
## 2				NA		NA		NA		NA	
## 3		8	9	NA	10	NA	11	NA	12	NA	

Here, there is the further issue that to make things legible, the table authors used 3 rows (from 2 to 4) to encode for long names (e.g., Prince Edward Island is written over 3 rows). Note, however, that 'read.csv' has rightly picked up on the first row being the column names.

(You could also use the function 'read_csv' from the package 'readr' to read in the file. This function is a bit more flexible than 'read.csv' and can handle such cases more easily. However, it is not part of the base R package, so you would need to install it first.)

Because we are only interested in the total population of the country and the year, let us simply get rid of the first 4 rows and of all columns except the second (Year) and third (Canada)

```
data_old = data_old[5:dim(data_old)[1], 2:3]
```

```
head(data_old, n=4)
```

```
##      Year      Canada
```

```
## 5 1976 22,992,604
```

```
## 6
```

```
## 7 1971 21,568,311
```

Still not perfect:

- there are some empty rows;
- the last few rows need to be removed too, they contain remarks about the data;
- the population counts contain commas;
- it would be better if years were increasing.

Let us fix these issues.

For 1 and 2, this is easy: remark that the Canada column is empty for both issues. Now remark as well that below Canada (and Year, for that matter), it is written `<chr>`. This means that entries in the column are characters. Looking for empty content therefore means looking for empty character chains.

So to fix 1 and 2, we keep the rows where Canada does not equal the empty chain. To get rid of commas, we just need to substitute an empty chain for ",".

To sort, we find the order for the years and apply it to the entire table.

Finally, as remarked above, for now, both the year and the population are considered as character chains. This means that in order to plot anything, we will have to indicate that these are numbers, not characters.

```

data_old = data_old[which(data_old$Canada != ""),]
data_old$Canada = gsub(",", "", data_old$Canada)
order_data = order(data_old$Year)
data_old = data_old[order_data,]
data_old$Year = as.numeric(data_old$Year)
data_old$Canada = as.numeric(data_old$Canada)
data_old

```

```

##      Year      Canada
## 23 1851    2436297
## 22 1861    3229633
## 21 1871    3689257
## 20 1881    4324810
## 19 1891    4833239
## 17 1901    5371315
## 16 1911    7206643
## 15 1921    8787949
## 14 1931   10376786

```

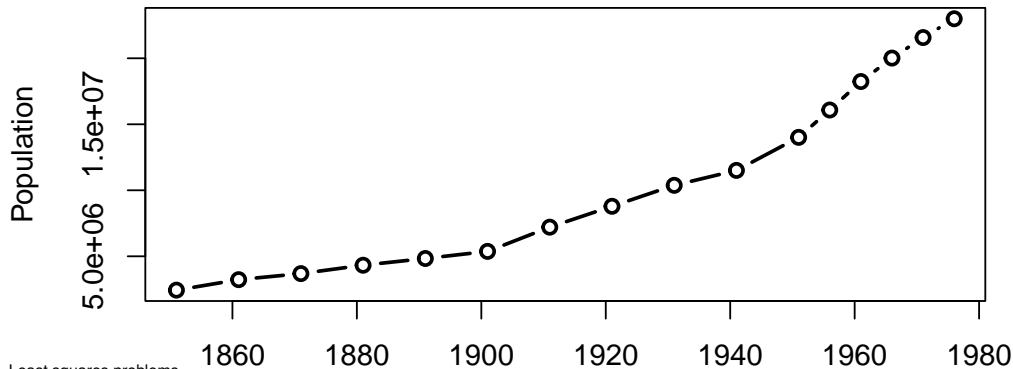
Row numbers are a little weird, so let us fix this.

```
row.names(data_old) = 1:dim(data_old)[1]
```

```
data_old
```

```
##      Year      Canada
## 1  1851    2436297
## 2  1861    3229633
## 3  1871    3689257
## 4  1881    4324810
## 5  1891    4833239
## 6  1901    5371315
## 7  1911    7206643
## 8  1921    8787949
## 9  1931   10376786
## 10 1941   11506655
## 11 1951   14009429
## 12 1956   16080791
## 13 1961   18238247
```

```
plot(data_old$Year, data_old$Canada,  
     type = "b", lwd = 2,  
     xlab = "Year", ylab = "Population")
```



But wait, this is only to 1976..! Looking around, we find another table here. There's a download csv link in there, let us see where this leads us. The table is 720KB, so surely there must be more to this than just the population. To get a sense of that, we dump the whole data.frame, not just its head.

```
data_new = read.csv("https://www12.statcan.gc.ca/census-recensement/2011/dp-  
head(data_new, 10)
```

##	GEOGRAPHY.NAME	CHARACTERISTIC	YEAR.S.	TOTAL	FLAG_TOTAL
## 1	Canada Population	(in thousands)	1956	16081	
## 2	Canada Population	(in thousands)	1961	18238	
## 3	Canada Population	(in thousands)	1966	20015	
## 4	Canada Population	(in thousands)	1971	21568	
## 5	Canada Population	(in thousands)	1976	22993	
## 6	Canada Population	(in thousands)	1981	24343	
## 7	Canada Population	(in thousands)	1986	25309	
## 8	Canada Population	(in thousands)	1991	27297	
## 9	Canada Population	(in thousands)	1996	28847	
## 10	Canada Population	(in thousands)	2001	30007	

Haha, this looks quite nice but has way more information than we need: we just want the population of Canada and here we get 9960 rows. Also, the population of Canada is expressed in thousands, so once we selected what we want, we will need to multiply by 1,000.

There are many ways to select rows. Let us proceed as follows: we want the rows where the geography is "Canada" and the characteristic is "Population (in thousands)". Let us find those indices of rows that satisfy the first criterion, those that satisfy the second; if we then intersect these two sets of indices, we will have selected the rows we want.

```
idx_CAN = which(data_new$GEOGRAPHY.NAME == "Canada")
idx_char = which(data_new$CHARACTERISTIC == "Population (in thousands)")
idx_keep = intersect(idx_CAN, idx_char)
head(idx_keep, n = 8)

## [1] 1 2 3 4 5 6 7 8
```

Yes, this looks okay, so let us keep only these

```
data_new = data_new[idx_keep,]  
head(data_new, n = 8)
```

##	GEOGRAPHY.NAME	CHARACTERISTIC	YEAR.S.	TOTAL	FLAG_TOTAL
## 1	Canada	Population (in thousands)	1956	16081	
## 2	Canada	Population (in thousands)	1961	18238	
## 3	Canada	Population (in thousands)	1966	20015	
## 4	Canada	Population (in thousands)	1971	21568	
## 5	Canada	Population (in thousands)	1976	22993	
## 6	Canada	Population (in thousands)	1981	24343	
## 7	Canada	Population (in thousands)	1986	25309	
## 8	Canada	Population (in thousands)	1991	27297	

We want to concatenate this `data.frame` with the one from earlier

To do this, we need the two data frames to have the same number of columns and, actually, the same column names and entry types (notice that `YEAR.S.` in `data_new` is a column of characters)

What remains to do

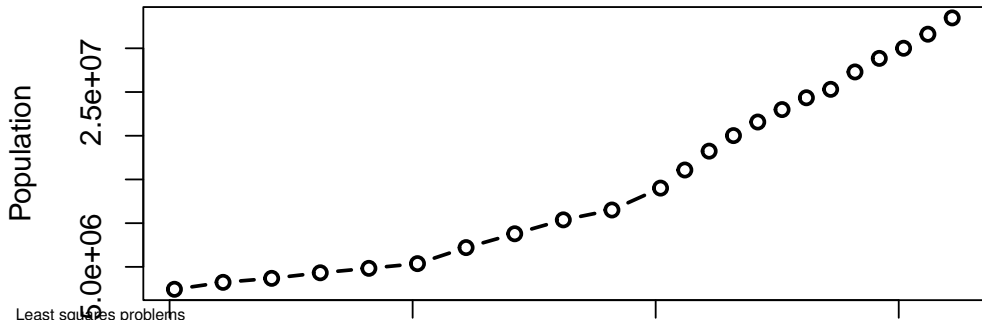
- ▶ Rename the columns in the pruned old data (`data_pruned`) to `year` and `population`. Personally, I prefer lowercase column names.. `and` `population` is more informative than `Canada`
- ▶ Keep only the relevant columns in `data_new`, rename them accordingly and multiply population by 1,000 there
- ▶ Transform `year` in `data_new` to numbers
- ▶ We already have data up to and including 1976 in `data_old`, so get rid of that in `data_new`
- ▶ Append the rows of `data_new` to those of `data_pruned`

```
colnames(data_old) = c("year", "population")
data_new = data_new[,c("YEAR.S.", "TOTAL")]
colnames(data_new) = c("year", "population")
data_new$year = as.numeric(data_new$year)
data_new = data_new[which(data_new$year>1976),]
data_new$population = data_new$population*1000

data = rbind(data_old, data_new)
```

Let us plot the result

```
plot(data$year, data$population,  
     type = "b", lwd = 2,  
     xlab = "Year", ylab = "Population")
```



Save the processed data

In case we need the data elsewhere, we save the data to a `csv` file

```
write.csv(data, file = "../CODE/Canada_census.csv")
```

Using `readr` saves the data without row numbers (by default), so we can do this instead

```
readr::write_csv(data, file = "../CODE/Canada_census.csv")
```

Least squares problems

Getting the Canadian census data

Least squares problem – Initial considerations

Least squares problem

Fitting something more complicated

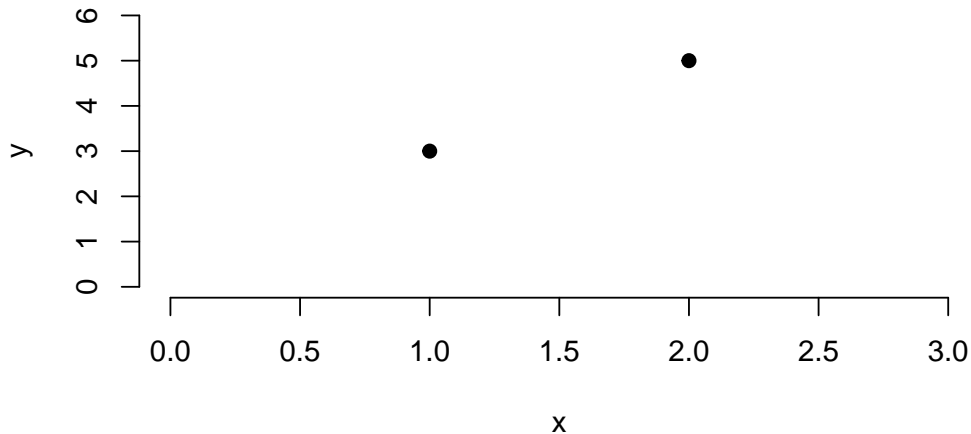
We just collected the census data for Canada

Suppose we want to predict the population of Canada in 20 years given the historical population growth seen in the previous plot. What can we do?

If there were just two points, we could easily "drive" a line through these two points. However, we have much more than two points, so we will use *fitting*, *i.e.*, try to make a curve come as close to possible to the points

We start with a line, giving rise to **linear least squares**

Least squares approximation – A trivial case



We want to find the equation of a line $y = a + bx$ that goes through these two points, i.e., we seek a and b such that

$$3 = a + b$$

$$5 = a + 2b$$

i.e., they satisfy $y = a + bx$ for $(x, y) = (1, 3)$ and $(x, y) = (2, 5)$

This is a linear system with 2 equations and 2 unknowns a and b

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 3 \\ 5 \end{pmatrix}$$

We know from the “famous” linear algebra in a nutshell theorem that this system has a unique solution if the matrix

$$M = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}$$

is invertible

$\det(M) = 1$, so we are good, we'll find a and b easily..

Now let's add another point

```
points = list()
points$x = c(1,2,3)
points$y = c(3,5,4) # So the points are (1,3), (2,5) and (3,4)
plot(points$x, points$y,
      pch = 19, cex = 2, bty = "n",
      xlim = c(0, 3.5), ylim = c(0,6), xlab = "x", ylab = "y")
```

These points are clearly not colinear, so there is not one line going through the 3

We end up with an *overdetermined* system

$$3 = a + b$$

$$5 = a + 2b$$

$$4 = a + 3b$$

i.e.,

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 3 \\ 5 \\ 4 \end{pmatrix}$$

We have verified visually that the points are not colinear, so this system has no solution.

(If you had to do it for good, you consider two vectors stemming from these 3 points and compute the angle between them or check that one is a multiple of the other).

So let us instead try to find the line that comes "closest" to the 3 points.

```
A = matrix(c(1,1,1,2), nr = 2, nc = 2, byrow = TRUE)
rhs = matrix(c(3,5), nr = 2, nc = 1)
coefs = solve(A,rhs) # To invert A, in R, you use solve(A), to solve  $Ax=b$ , y
plot(points$x, points$y,
     pch = 19, cex = 2, bty = "n",
     xlim = c(0, 3.5), ylim = c(0,6), xlab = "x", ylab = "y")
abline(coef = coefs, lwd = 2)
```

Obviously, not sensational..

```
plot(points$x, points$y,  
      pch = 19, cex = 2, bty = "n",  
      xlim = c(0, 3.5), ylim = c(0,6), xlab = "x", ylab = "y")  
abline(coef = coefs, lwd = 2)  
abline(a = 3, b = 0.5, lwd = 2, col = "red")
```

How do we find "how far away"?

- We could use projections onto the line (which we know minimises the distance) -
- However, this will be a problem if we later decide that rather than a straight line, we want to use something more "funky" like a quadratic or an exponential

So instead, we compare, for a given value x , the distance between the true value y and the value of y obtained using the curve (line, here) that we use to fit the data. Let (x_i, y_i) be the data points, i.e., here, $(x_1, y_1) = (1, 3)$, $(x_2, y_2) = (2, 5)$ and $(x_3, y_3) = (3, 4)$

Now suppose we use a line with equation $y = a + bx$ and that we pick a value for a and b . Then at x_1 ,

$$\tilde{y}_1 = a + bx_1 = a + b$$

at x_2

$$\tilde{y}_2 = a + bx_2 = a + 2b$$

and at x_3 ,

$$\tilde{y}_3 = a + bx_3 = a + 3b$$

Consider x_1 , for instance. The error we made by using the line with coefficients (a, b) is $\overrightarrow{(x_1, y_1)(x_1, \tilde{y}_1)}$.

For future use, let us create a function for $y = a_0 + a_1 x$.

```
my_line = function(x, a_0, a_1){  
  return(a_0 + a_1*x)  
}
```

Functions are super useful when programming

```
my_line(1,2,3)  
## [1] 5  
  
my_line(a_0 = 2, a_1 = 3, x = 1)  
## [1] 5  
  
my_line(x = c(1,2,3), a_0 = 2, a_1 = 3)  
## [1] 5 8 11
```

```

a = 3
b = 0.5 # The line has equation  $y=a+bx$ 
plot(points$x, points$y,
      pch = 19, cex = 2, bty = "n",
      xlim = c(0, 3.5), ylim = c(0,6), xlab = "x", ylab = "y")
abline(a = a, b = b, lwd = 2)
abline(v = c(1,2,3)) # If we used abline(h=c(0,1)), we would get horizontal
p = my_line(c(1,2,3), a, b)
points(c(1,2,3), p, pch = 19, cex = 2, col = "red")

```

Let us return to the error

$$\overrightarrow{(x_1, y_1)(x_1, \tilde{y}_1)}$$

We have

$$\overrightarrow{(x_1, y_1)(x_1, \tilde{y}_1)} = (x_1 - x_1, y_1 - \tilde{y}_1) = (0, y_1 - \tilde{y}_1)$$

Let us call

$$\varepsilon_1 = y_1 - \tilde{y}_1$$

We can compute ε_2 and ε_3 too. And we can then form the ****error vector****

$$\mathbf{e} = (\varepsilon_1, \varepsilon_2, \varepsilon_3)^T$$

The norm of \mathbf{e} , $\|\mathbf{e}\|$, then tells us how much error we are making for the choice of (a, b) we are using

The norm of \mathbf{e} , $\|\mathbf{e}\|$, tells us how much error we are making for the choice of (a, b) we are using

So our objective is to find (a, b) such that $\|\mathbf{e}\|$ is minimal

We could use various norms, but the Euclidean norm has some very interesting properties, so we use

$$\|\mathbf{e}\| = \sqrt{\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2}$$

The linear least squares problem

Given a collection of data points $(x_1, y_1), \dots, (x_n, y_n)$, find the coefficients a, b of the line $y = a + bx$ such that

$$\|\mathbf{e}\| = \sqrt{\varepsilon_1^2 + \dots + \varepsilon_n^2} = \sqrt{(y_1 - \tilde{y}_1)^2 + \dots + (y_n - \tilde{y}_n)^2}$$

is minimal, where $\tilde{y}_i = a + bx_i$, for $i = 1, \dots, n$

Let us first hack a brute force solution! (For the example we have been using this far)

We have our three points in the list 'points', the function `my_line` that computes the value \tilde{y} given x and a, b , so let us make a new function that, given a, b , computes e . We'll also pass the points 'points'

```
error = function(a_0, a_1, points) {  
  y_tilde = my_line(points$x, a_0 = a_0, a_1 = a_1)  
  e = points$y - y_tilde  
  return(sqrt(sum(e^2)))  
}  
error(a_0 = 2, a_1 = 3, points)  
  
## [1] 7.874008  
  
error(a_0 = 3, a_1 = 0.5, points)  
  
## [1] 1.224745  
  
error(a_0 = 3.1, a_1 = 0.48, points)
```

Genetic algorithms

Let's use something cool: a *genetic algorithm*

- Genetic algorithms are a stochastic *optimisation* method. There are other types, e.g., gradient descent (deterministic) - The idea is to use a mechanism mimicking evolution's drive towards higher fitness - The function value is its fitness
- We try different genes (here, different values of a, b) and evaluate their fitness..
- keep the good ones - We mutate or crossover genes, throw in new ones, etc. - We keep doing this until we reach a stopping criterion - We then return the best gene we found

```

if (!require("GA", quietly = TRUE)) {
  install.packages("GA")
  library(GA)
}
GA = ga(type = "real-valued",
        fitness = function(x) -error(a_0 = x[1], a_1 = x[2], points),
        suggestions = c(a_0 = 2, a_1 = 3),
        lower = c(-10, -10), upper = c(10, 10),
        popSize = 200, maxiter = 150)
# plot(GA)
GA

## An object of class "ga"
##
## Call:
## ga(type = "real-valued", fitness = function(x) -error(a_0 = x[1], a_1
##
## Available slots:

```


Least squares problems

Getting the Canadian census data

Least squares problem – Initial considerations

Least squares problem

Fitting something more complicated

The least squares problem (simplest version)

Definition 1

Given a collection of points $(x_1, y_1), \dots, (x_n, y_n)$, find the coefficients a, b of the line $y = a + bx$ such that

$$\|\mathbf{e}\| = \sqrt{\varepsilon_1^2 + \dots + \varepsilon_n^2} = \sqrt{(y_1 - \tilde{y}_1)^2 + \dots + (y_n - \tilde{y}_n)^2}$$

is minimal, where $\tilde{y}_i = a + bx_i$ for $i = 1, \dots, n$

We just saw how to solve this by brute force using a genetic algorithm to minimise $\|\mathbf{e}\|$, let us now see how to solve this problem “properly”

For a data point $i = 1, \dots, n$

$$\varepsilon_i = y_i - \tilde{y}_i = y_i - (a + bx_i)$$

So if we write this for all data points,

$$\varepsilon_1 = y_1 - (a + bx_1)$$

$$\vdots$$

$$\varepsilon_n = y_n - (a + bx_n)$$

In matrix form

$$\mathbf{e} = \mathbf{b} - A\mathbf{x}$$

with

$$\mathbf{e} = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}, A = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \mathbf{x} = \begin{pmatrix} a \\ b \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

The least squares problem (reformulated)

Definition 2 (Least squares solutions)

Consider a collection of points $(x_1, y_1), \dots, (x_n, y_n)$, a matrix $A \in \mathcal{M}_{mn}$, $\mathbf{b} \in \mathbb{R}^m$. A **least squares solution** of $A\mathbf{x} = \mathbf{b}$ is a vector $\tilde{\mathbf{x}} \in \mathbb{R}^n$ s.t.

$$\forall \mathbf{x} \in \mathbb{R}^n, \quad \|\mathbf{b} - A\tilde{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$$

Needed to solve the problem

Definition 3 (Best approximation)

Let V be a vector space, $W \subset V$ and $\mathbf{v} \in V$. The **best approximation** to \mathbf{v} in W is $\tilde{\mathbf{v}} \in W$ s.t.

$$\forall \mathbf{w} \in W, \mathbf{w} \neq \tilde{\mathbf{v}}, \quad \|\mathbf{v} - \tilde{\mathbf{v}}\| < \|\mathbf{v} - \mathbf{w}\|$$

Theorem 4 (Best approximation theorem)

Let V be a vector space with an inner product, $W \subset V$ and $\mathbf{v} \in V$. Then $\text{proj}_W(\mathbf{v})$ is the best approximation to \mathbf{v} in W

Let us find the least squares solution

$\forall \mathbf{x} \in \mathbb{R}^n$, $A\mathbf{x}$ is a vector in the **column space** of A (the space spanned by the vectors making up the columns of A)

Since $\mathbf{x} \in \mathbb{R}^n$, $A\mathbf{x} \in \text{col}(A)$

\Rightarrow least squares solution of $A\mathbf{x} = \mathbf{b}$ is a vector $\tilde{\mathbf{y}} \in \text{col}(A)$ s.t.

$$\forall \mathbf{y} \in \text{col}(A), \quad \|\mathbf{b} - \tilde{\mathbf{y}}\| \leq \|\mathbf{b} - \mathbf{y}\|$$

This looks very much like Best approximation and Best approximation theorem

Putting things together

We just stated: The least squares solution of $A\mathbf{x} = \mathbf{b}$ is a vector $\tilde{\mathbf{y}} \in \text{col}(A)$ s.t.

$$\forall \mathbf{y} \in \text{col}(A), \quad \|\mathbf{b} - \tilde{\mathbf{y}}\| \leq \|\mathbf{b} - \mathbf{y}\|$$

We know (reformulating a tad):

Theorem 5 (Best approximation theorem)

Let V be a vector space with an inner product, $W \subset V$ and $\mathbf{v} \in V$. Then $\text{proj}_W(\mathbf{v}) \in W$ is the best approximation to \mathbf{v} in W , i.e.,

$$\forall \mathbf{w} \in W, \mathbf{w} \neq \text{proj}_W(\mathbf{v}), \quad \|\mathbf{v} - \text{proj}_W(\mathbf{v})\| < \|\mathbf{v} - \mathbf{w}\|$$

$$\implies W = \text{col}(A), \mathbf{v} = \mathbf{b} \text{ and } \tilde{\mathbf{y}} = \text{proj}_{\text{col}(A)}(\mathbf{b})$$

So if $\tilde{\mathbf{x}}$ is a least squares solution of $A\mathbf{x} = \mathbf{b}$, then

$$\tilde{\mathbf{y}} = A\tilde{\mathbf{x}} = \text{proj}_{\text{col}(A)}(\mathbf{b})$$

We have

$$\mathbf{b} - A\tilde{\mathbf{x}} = \mathbf{b} - \text{proj}_{\text{col}(A)}(\mathbf{b}) = \text{perp}_{\text{col}(A)}(\mathbf{b})$$

and it is easy to show that

$$\text{perp}_{\text{col}(A)}(\mathbf{b}) \perp \text{col}(A)$$

So for all columns \mathbf{a}_i of A

$$\mathbf{a}_i \cdot (\mathbf{b} - A\tilde{\mathbf{x}}) = 0$$

which we can also write as $\mathbf{a}_i^T (\mathbf{b} - A\tilde{\mathbf{x}}) = 0$

For all columns \mathbf{a}_i of A ,

$$\mathbf{a}_i^T (\mathbf{b} - A\tilde{\mathbf{x}}) = 0$$

This is equivalent to saying that

$$A^T (\mathbf{b} - A\tilde{\mathbf{x}}) = \mathbf{0}$$

We have

$$\begin{aligned} A^T (\mathbf{b} - A\tilde{\mathbf{x}}) = \mathbf{0} &\iff A^T \mathbf{b} - A^T A\tilde{\mathbf{x}} = \mathbf{0} \\ &\iff A^T \mathbf{b} = A^T A\tilde{\mathbf{x}} \\ &\iff A^T A\tilde{\mathbf{x}} = A^T \mathbf{b} \end{aligned}$$

The latter system constitutes the **normal equations** for $\tilde{\mathbf{x}}$

Least squares theorem

Theorem 6 (Least squares theorem)

$A \in \mathcal{M}_{mn}$, $\mathbf{b} \in \mathbb{R}^m$. Then

1. $A\mathbf{x} = \mathbf{b}$ always has at least one least squares solution $\tilde{\mathbf{x}}$
2. $\tilde{\mathbf{x}}$ least squares solution to $A\mathbf{x} = \mathbf{b} \iff \tilde{\mathbf{x}}$ is a solution to the normal equations $A^T A \tilde{\mathbf{x}} = A^T \mathbf{b}$
3. A has linearly independent columns $\iff A^T A$ invertible.
In this case, the least squares solution is unique and

$$\tilde{\mathbf{x}} = \left(A^T A\right)^{-1} A^T \mathbf{b}$$

We have seen 1 and 2, we will not show 3 (it is not hard)

Least squares problems

Getting the Canadian census data

Least squares problem – Initial considerations

Least squares problem

Fitting something more complicated

Suppose we want to fit something a bit more complicated..

For instance, instead of the affine function

$$y = a + bx$$

suppose we want to do the quadratic

$$y = a_0 + a_1x + a_2x^2$$

or even

$$y = k_0 e^{k_1 x}$$

How do we proceed?

Fitting the quadratic

We have the data points $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ and want to fit

$$y = a_0 + a_1x + a_2x^2$$

At (x_1, y_1) ,

$$\tilde{y}_1 = a_0 + a_1x_1 + a_2x_1^2$$

\vdots

At (x_n, y_n) ,

$$\tilde{y}_n = a_0 + a_1x_n + a_2x_n^2$$

In terms of the error

$$\begin{aligned}\varepsilon_1 &= y_1 - \tilde{y}_1 = y_1 - (a_0 + a_1 x_1 + a_2 x_1^2) \\ &\vdots \\ \varepsilon_n &= y_n - \tilde{y}_n = y_n - (a_0 + a_1 x_n + a_2 x_n^2)\end{aligned}$$

i.e.,

$$\mathbf{e} = \mathbf{b} - A\mathbf{x}$$

where

$$\mathbf{e} = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}, A = \begin{pmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix}, \mathbf{x} = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Theorem 6 applies, with here $A \in \mathcal{M}_{n3}$ and $\mathbf{b} \in \mathbb{R}^n$

Fitting the exponential

Things are a bit more complicated here

If we proceed as before, we get the system

$$\begin{aligned}y_1 &= k_0 e^{k_1 x_1} \\ &\vdots \\ y_n &= k_0 e^{k_1 x_n}\end{aligned}$$

$e^{k_1 x_i}$ is a nonlinear term, it cannot be put in a matrix

However. take the \ln of both sides of the equation

$$\ln(y_i) = \ln(k_0 e^{k_1 x_i}) = \ln(k_0) + \ln(e^{k_1 x_i}) = \ln(k_0) + k_1 x_i$$

If $y_i, k_0 > 0$, then their \ln are defined and we're in business..

$$\ln(y_i) = \ln(k_0) + k_1 x_i$$

So the system is

$$\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{b}$$

with

$$\mathbf{A} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \mathbf{x} = (k_1), \mathbf{b} = (\ln(k_0)) \text{ and } \mathbf{y} = \begin{pmatrix} \ln(y_1) \\ \vdots \\ \ln(y_n) \end{pmatrix}$$