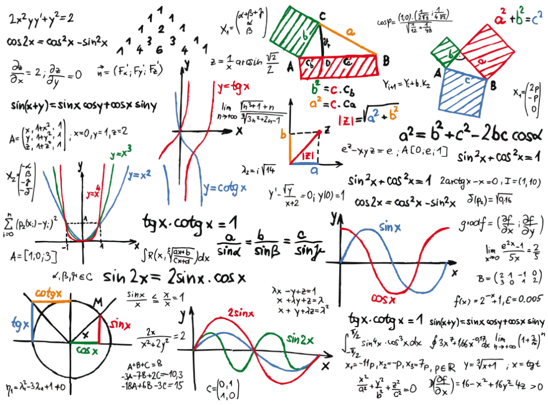
B2 - Mathematics

B-MAT-200

109titration

Derivatives and Preservatives



2.0

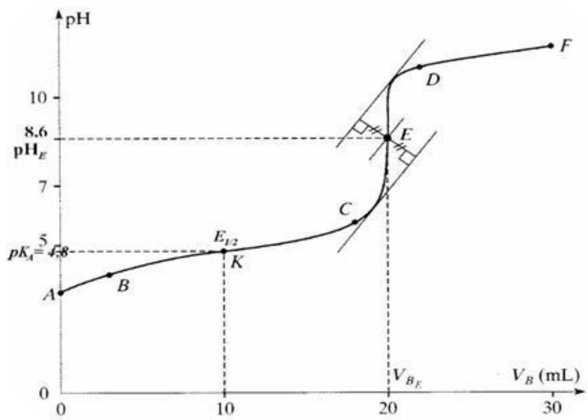
109titration

binary name:	109titration
repository name:	109titration_*$ACADEMIC_YEAR*
repository rights:	ramassage-tek
language:	C, C++, python3, perl, ruby, php or bash
compilation:	when necessary, via Makefile, including re, clean and fclean rules

- Your repository must contain the totality of your source files, but no useless files (binary, temp files, obj files,...).
- All the bonus files (including a potential specific Makefile) should be in a directory named *bonus*.
- Error messages have to be written on the error output, and the program should then exit with the 84 error code (0 if there is no error).

The benzoic acid is used in industry as a food preservative under the E220 code. It is a white silky-looking solid. To determine the concentration of this additive in a soda, one can realize a pH titration: a strong base (the titrant) is progressively added to a sample of the soda (the analyte), and pH is then read.

The generated curve is typical, and has an area where pH brutally increases: it is the pH-jump.



To find the concentration of preservative in the soda, the volume of added titrant at the **equivalent point** (ie at the middle of the pH-jump) must be read. There are two main approaches to do so:

- **the derivative method**, which consists in calculating the derivative of the curve; the equivalent point matches with the maximum of this derivative,
- **the parallel tangents method**, which consists in drawing two parallel tangents from one part and another of the pH-jump, then to draw a third straight line equidistant from the two first. The equivalent point is at the intersection between this last line and the curve.

You must code the first approach here. Your program has to read titrant volume (in ml) and pH couples from a csv file, and output:

1. the derivative values for each given volume,
2. the closest point from the equivalent point amongst those given points,
3. the second derivative values for each given volume,
4. an approximation of the second derivative values every 0.1 ml around the above closest point from the equivalent point,
5. the proper equivalent point, estimated from the second derivative.

> To approximate the derivative, the centered rate is defined in the course as the mean of the forward and backward rates. Since abscissas are not equidistant here, coefficients must be cleverly put in front of the rates when computing the mean.
> **Beware, the coefficients must have a sum of 1!**

Usage

Terminal

```
~/B-MAT-200> ./109titration -h
USAGE
    ./109titration file

DESCRIPTION
    file     a csv file containing "vol;ph" lines
```

Examples

Terminal

```
~/B-MAT-200> cat values.csv
1;2
2;3
3;4
5;4.4
6;4.6
7;6
7.5;6.8
8;8
9;10
12;11.3
14;11.46
16;11.6
20;11.8
```

```
Terminal
~/B-MAT-200> ./109titration values.csv
Derivative:
2.0 ml -> 1.00
3.0 ml -> 0.47
5.0 ml -> 0.20
6.0 ml -> 0.80
7.0 ml -> 1.47
7.5 ml -> 2.00
8.0 ml -> 2.13
9.0 ml -> 0.83
12.0 ml -> 0.29
14.0 ml -> 0.07
16.0 ml -> 0.06

Equivalent point at 8.0 ml

Second derivative:
3.0 ml -> -0.27
5.0 ml -> 0.11
6.0 ml -> 0.63
7.0 ml -> 0.80
7.5 ml -> 0.67
8.0 ml -> -0.78
9.0 ml -> -0.46
12.0 ml -> -0.15
14.0 ml -> -0.06

Second derivative estimated:
7.5 ml -> 0.67
7.6 ml -> 0.38
7.7 ml -> 0.09
7.8 ml -> -0.20
7.9 ml -> -0.49
8.0 ml -> -0.78
8.1 ml -> -0.75
8.2 ml -> -0.72
8.3 ml -> -0.69
8.4 ml -> -0.65
8.5 ml -> -0.62
8.6 ml -> -0.59
8.7 ml -> -0.56
8.8 ml -> -0.52
8.9 ml -> -0.49
9.0 ml -> -0.46

Equivalent point at 7.7 ml
```