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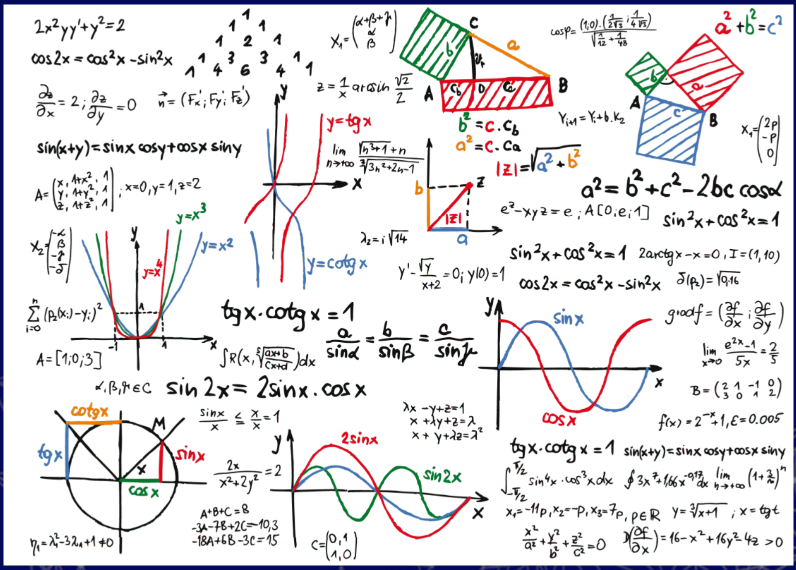
# 109TITRATION

## DERIVATIVES AND PRESERVATIVES



# 109TITRATION

**binary name:** 109titration
**language:** everything working on “the dump”
**compilation:** when necessary, via Makefile, including re, clean and fclean rules

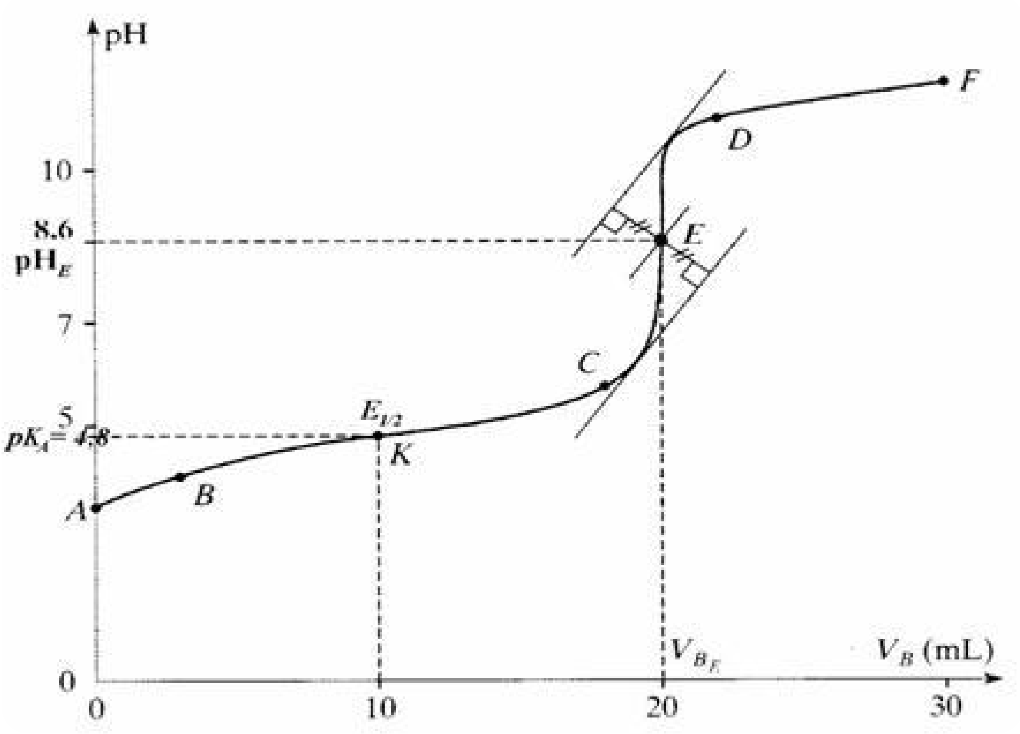
- ✓ The totality of your source files, except all useless files (binary, temp files, objfiles,...), must be included in your delivery.
- ✓ All the bonus files (including a potential specific Makefile) should be in a directory named bonus.
- ✓ Error messages have to be written on the error output, and 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 E210 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 **equivalence point** (*i.e.* 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 equivalence 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 equivalence point is at the intersection between this last line and the curve.

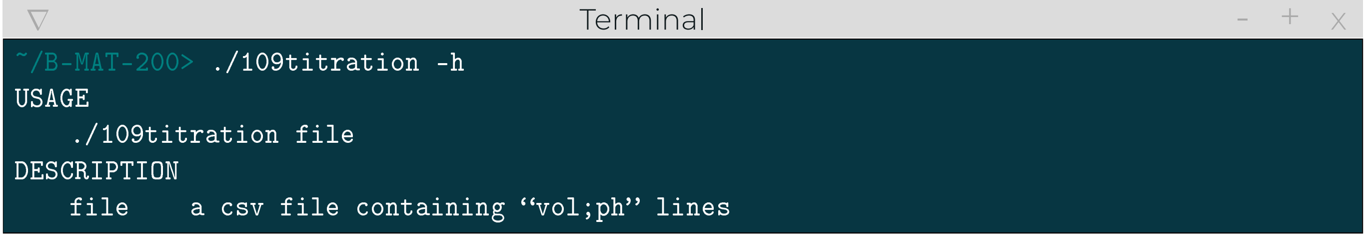


You must code the first approach here. Your program has to read titrant volume (in ml) and pH couples from a csv file, and output:

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

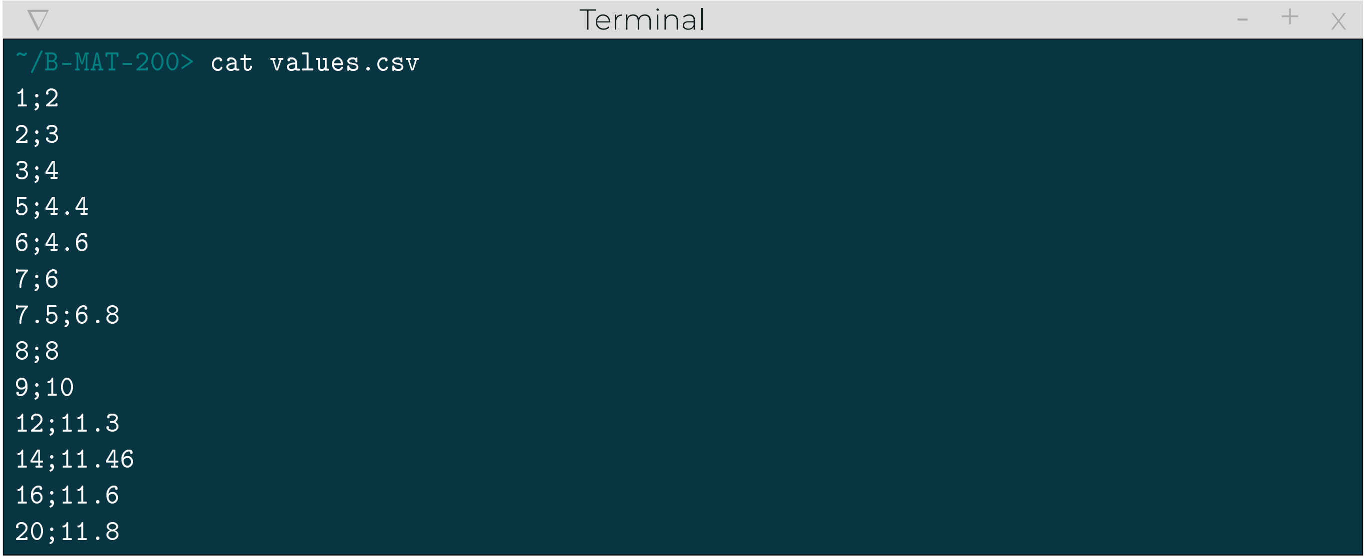
To compute the derivatives, you must use the centered rate defined as the weighted average of the forward and backward rates. Since abscissas are not equidistant here, coefficients must be cleverly put in front of the rates when computing the mean.
**Beware, the coefficients must have a sum of 1!**

## Usage

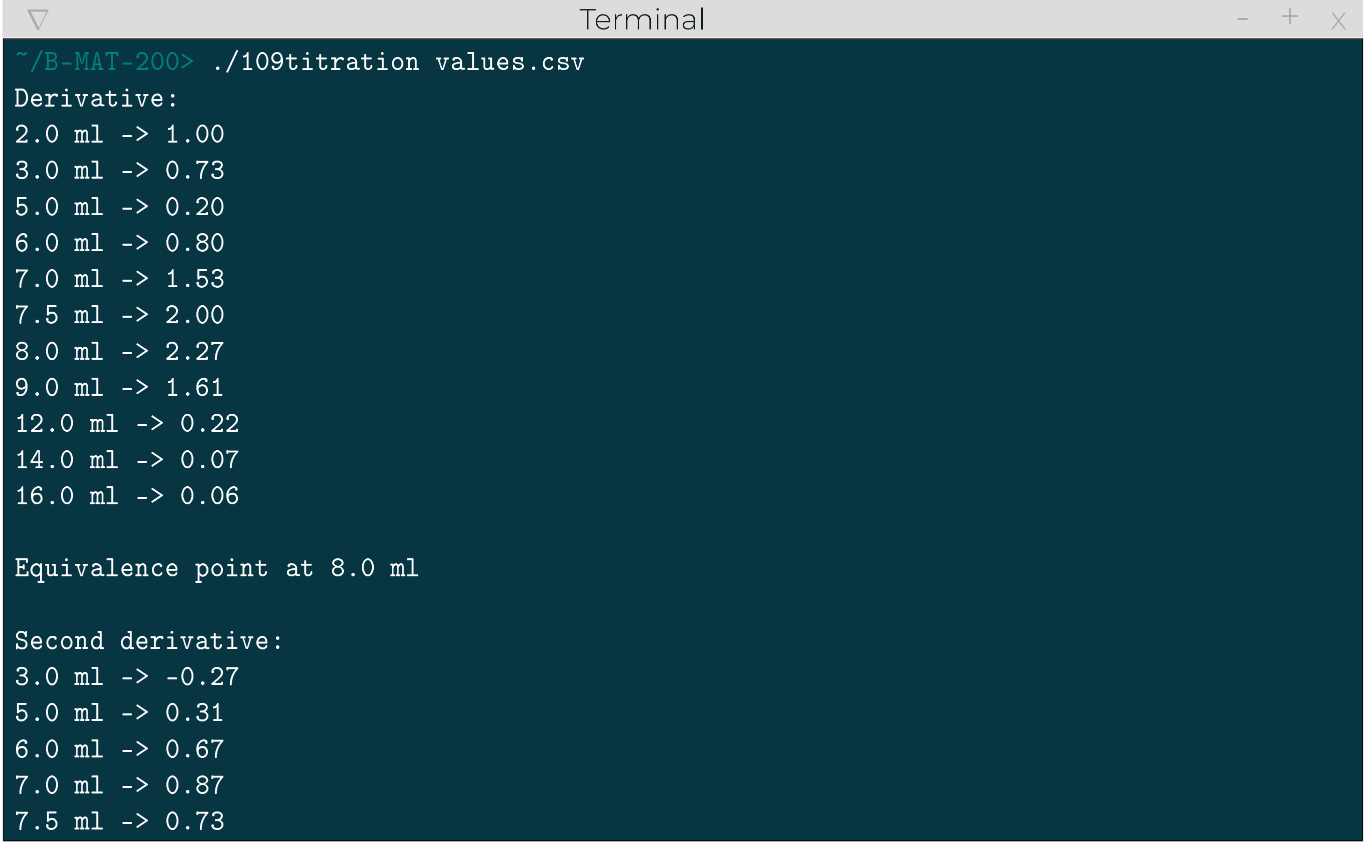


```
~/B-MAT-200> ./109titration -h
USAGE
    ./109titration file
DESCRIPTION
    file     a csv file containing “vol;ph” lines
```

## Examples



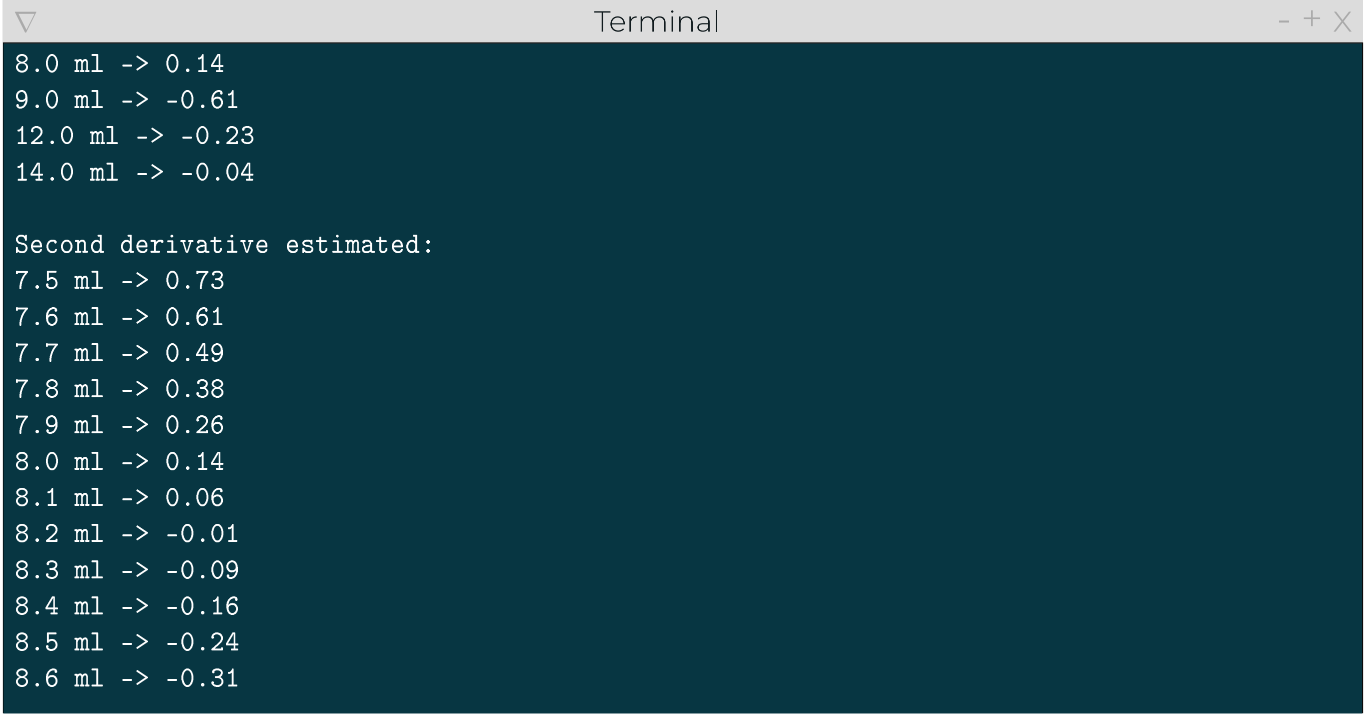
```
~/B-MAT-200> cat values.csv
1;2
2;3
3;4
5;4.4
6;4.6
7;6
7.5;6.8
8;8
9;10
12;11.3
14;11.46
16;11.6
20;11.8
```



```
~/B-MAT-200> ./109titration values.csv
Derivative:
2.0 ml -> 1.00
3.0 ml -> 0.73
5.0 ml -> 0.20
6.0 ml -> 0.80
7.0 ml -> 1.53
7.5 ml -> 2.00
8.0 ml -> 2.27
9.0 ml -> 1.61
12.0 ml -> 0.22
14.0 ml -> 0.07
16.0 ml -> 0.06

Equivalence point at 8.0 ml

Second derivative:
3.0 ml -> -0.27
5.0 ml -> 0.31
6.0 ml -> 0.67
7.0 ml -> 0.87
7.5 ml -> 0.73
```



```
8.0 ml -> 0.14
9.0 ml -> -0.61
12.0 ml -> -0.23
14.0 ml -> -0.04

Second derivative estimated:
7.5 ml -> 0.73
7.6 ml -> 0.61
7.7 ml -> 0.49
7.8 ml -> 0.38
7.9 ml -> 0.26
8.0 ml -> 0.14
8.1 ml -> 0.06
8.2 ml -> -0.01
8.3 ml -> -0.09
8.4 ml -> -0.16
8.5 ml -> -0.24
8.6 ml -> -0.31
```

```
8.7 ml -> -0.39
8.8 ml -> -0.46
8.9 ml -> -0.53
9.0 ml -> -0.61

Equivalence point at 8.2 ml
```

v3

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