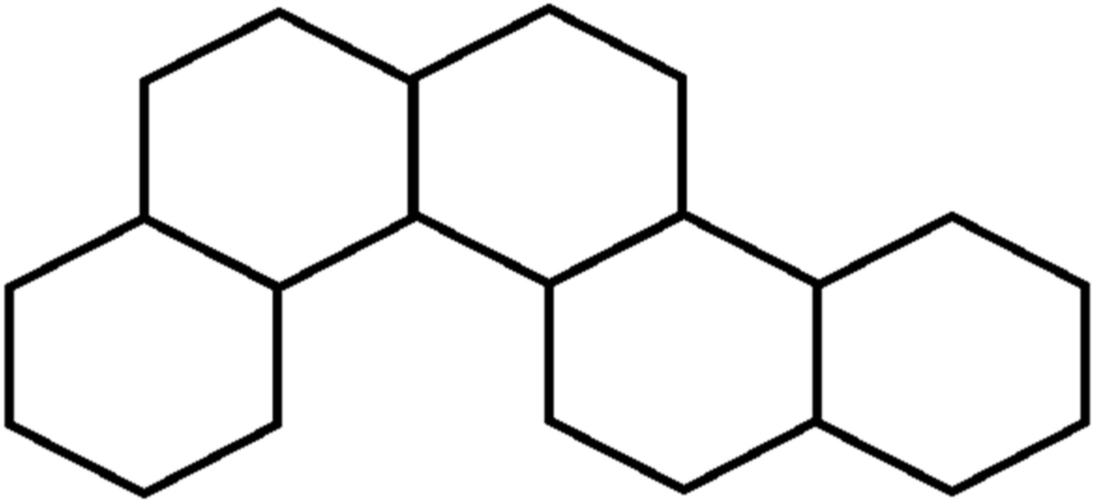
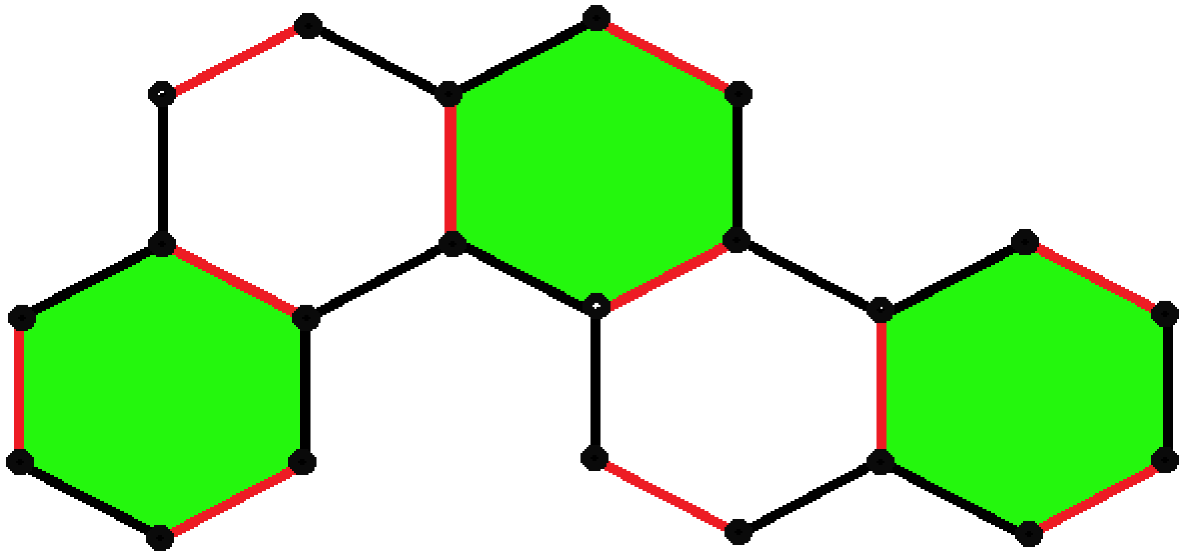
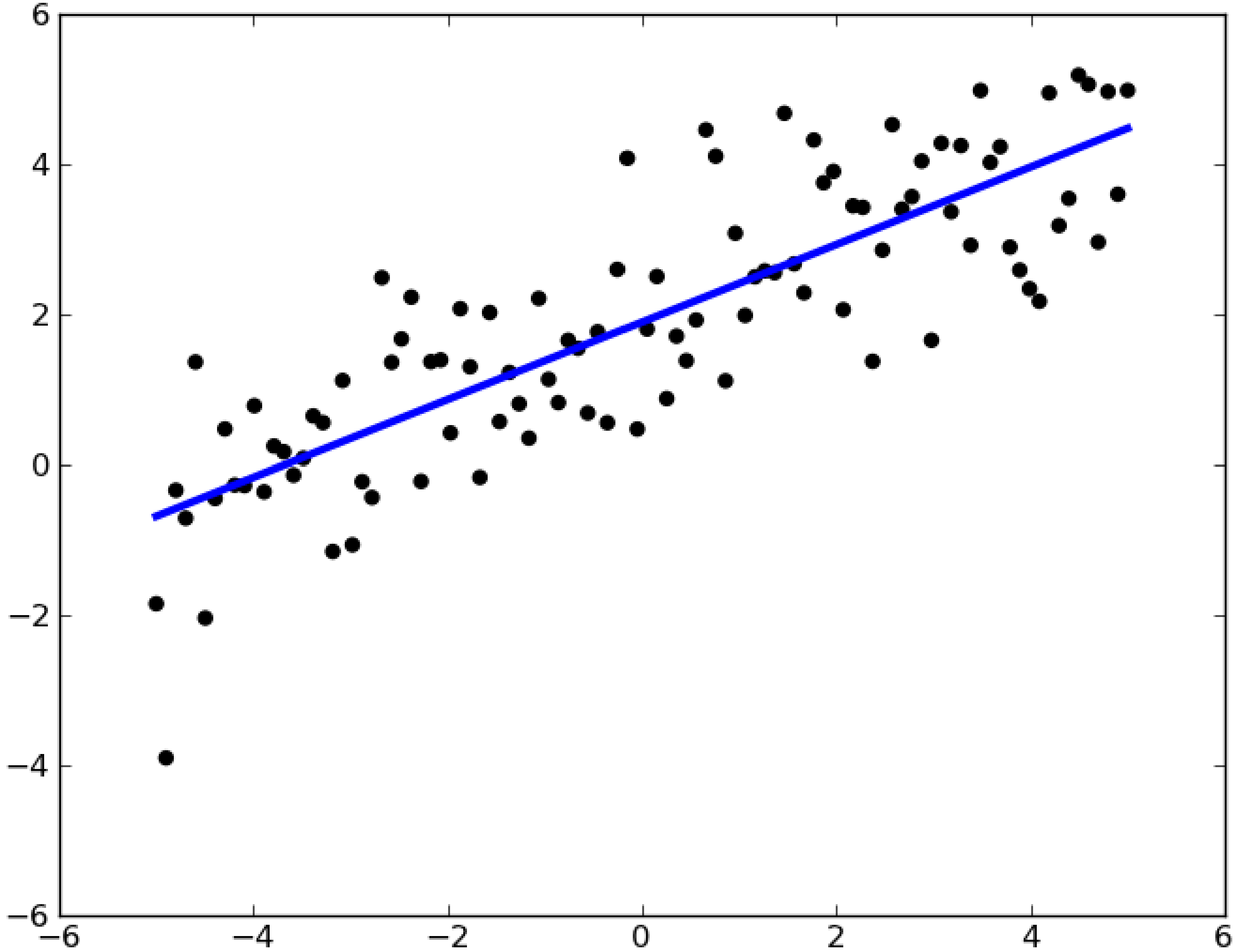
Matching: collection of disjoint edges.
Benzenoid hexagon: has 3 matching edges.
Fries number: Maximum over all perfect matchings of the number of benzenoid hexagons.
Clar number: Maximum over all perfect matchings of the number of independent benzenoid hexagons.
Find the Fries number and Clar number of this benzenoid:







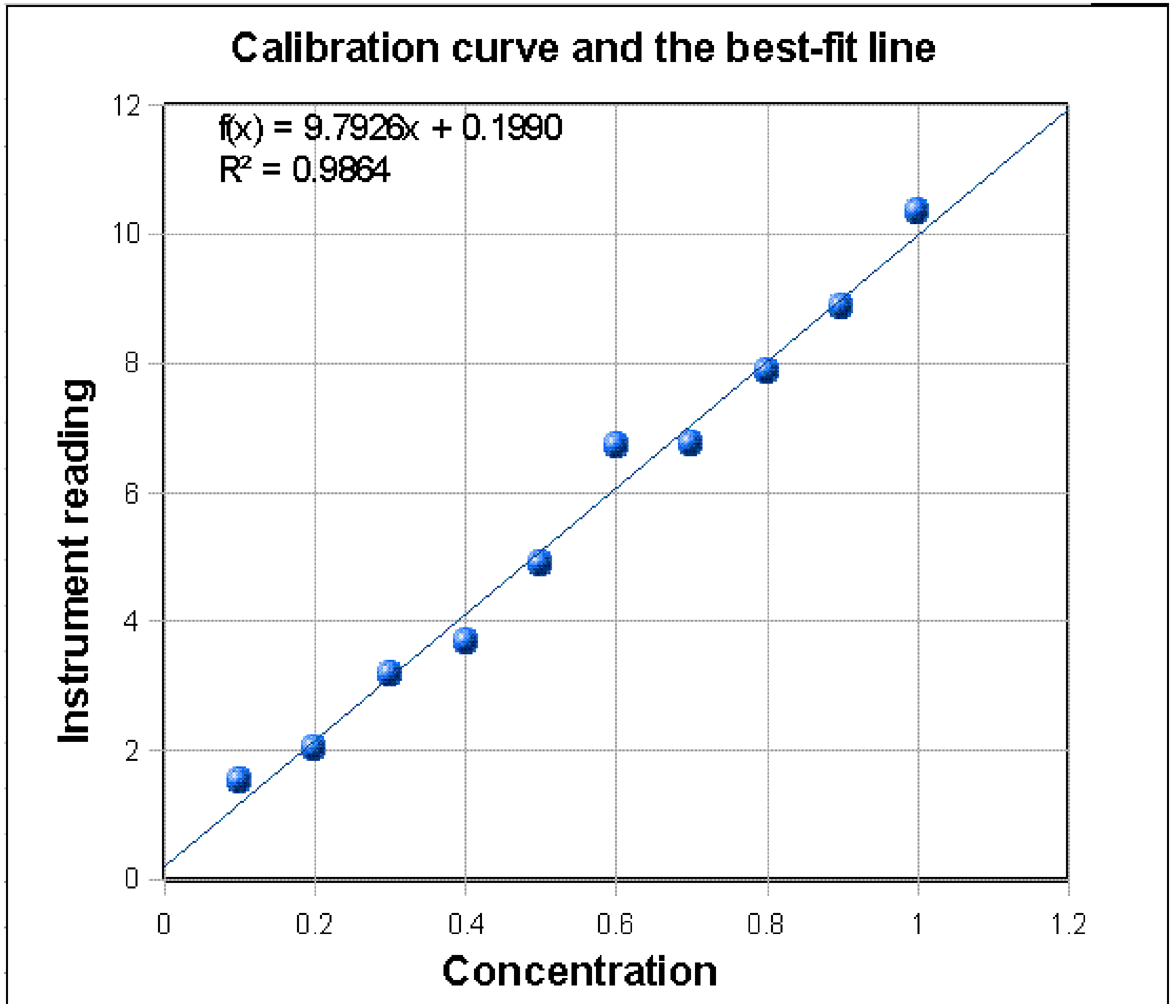
http://scikit-learn.org/0.8/auto_examples/linear_model/plot_ols.html

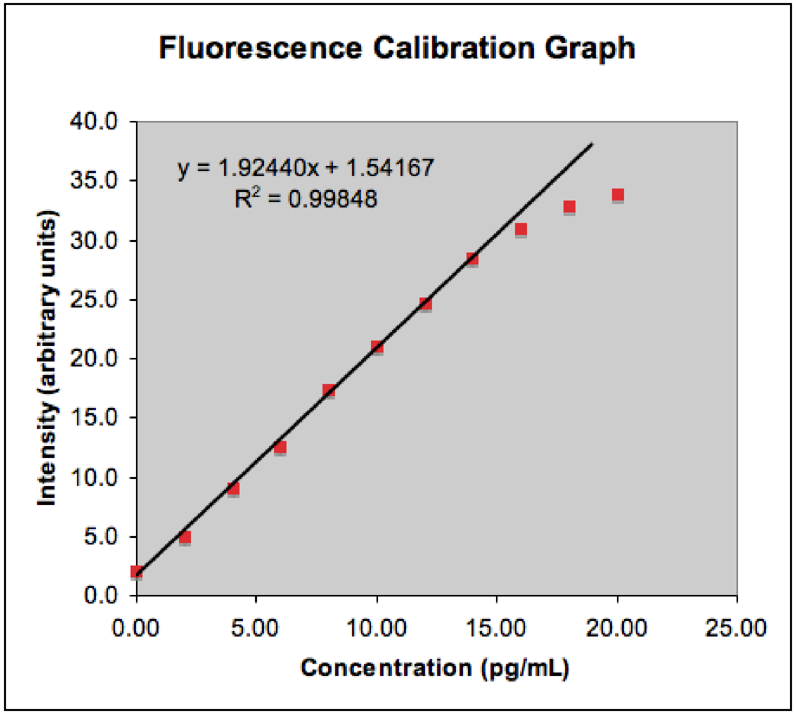
Algorithms for best L1 and L∞ linear approximations on a discrete set

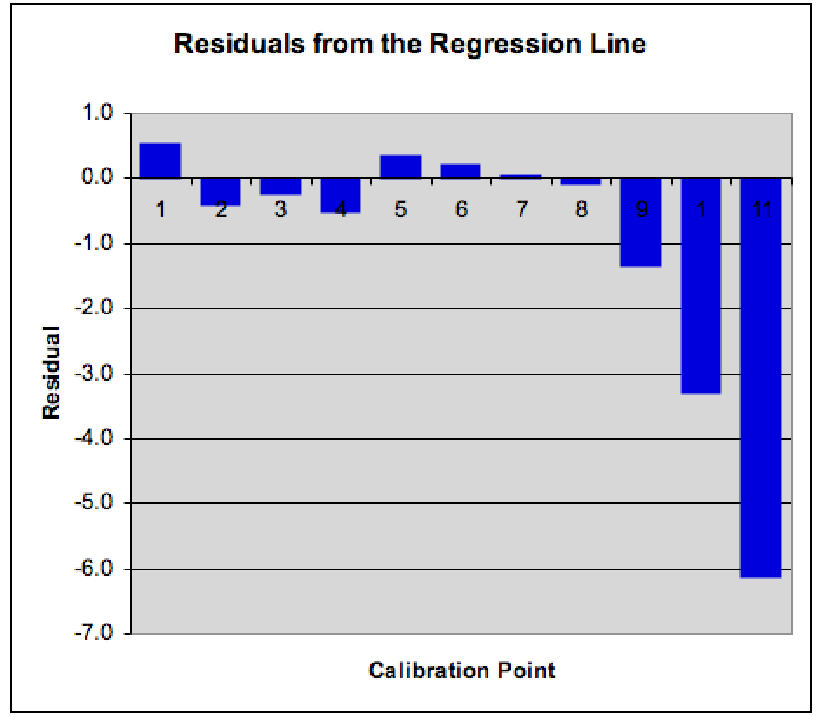
Authors	Ian Barrodale, Andrew Young
Publication date	1966/5/29
Journal	Numerische Mathematik
Volume	8
Issue	3
Pages	295-306
Publisher	Springer Berlin/Heidelberg
Description	Abstract This paper supplies algorithms for the best approximation to a real-valued function, defined as a table of values, by a linear approximating function in both the L 1 and L∞ norms. The algorithms are modified simplex algorithms which due to the particular structures of the tableaux have been condensed and require minimal storage space. Both algorithms are given as Algol procedures and sample times are noted for several examples.

Ian Barrodale

Chemistry calibration: The data points don't all fall in a perfect straight line because of random noise and measurement error in the instrument readings and possibly also volumetric errors in the concentrations of the standards (which are usually prepared in the laboratory by diluting a stock solution).
http://terpconnect.umd.edu/~toh/spectrum/CurveFitting.html







Least squares fitting.

Some applications in the geosciences of a best fit line:

- flood frequency curves
- earthquake forecasting
- Meteorite impact prediction
- earthquake frequency vs. magnitude
- climate change

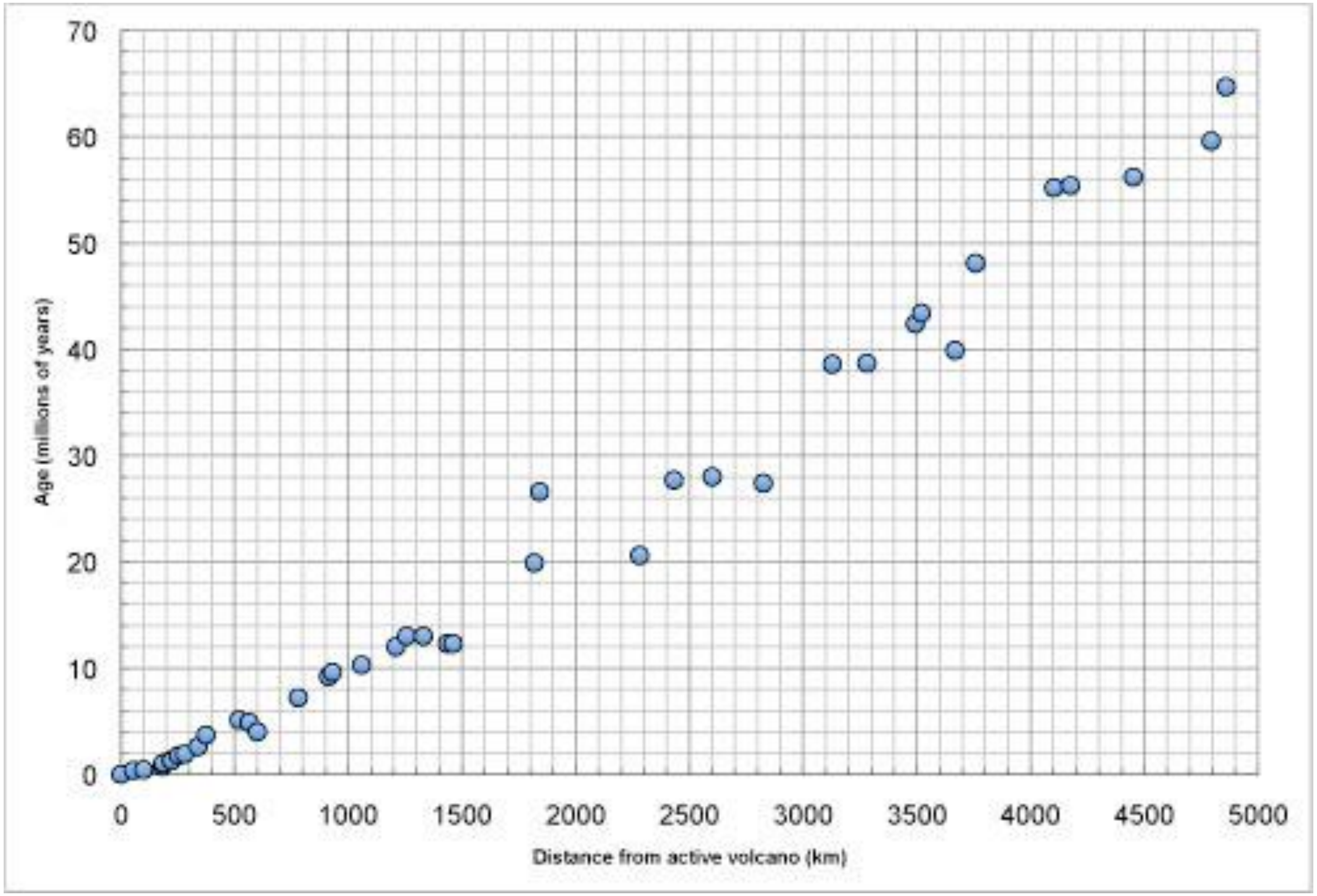
Examples on next slides taken from:

http://serc.carleton.edu/mathyouneed/graphing/bestfit.html

http://serc.carleton.edu/mathyouneed/graphing/bestfit_sample.html

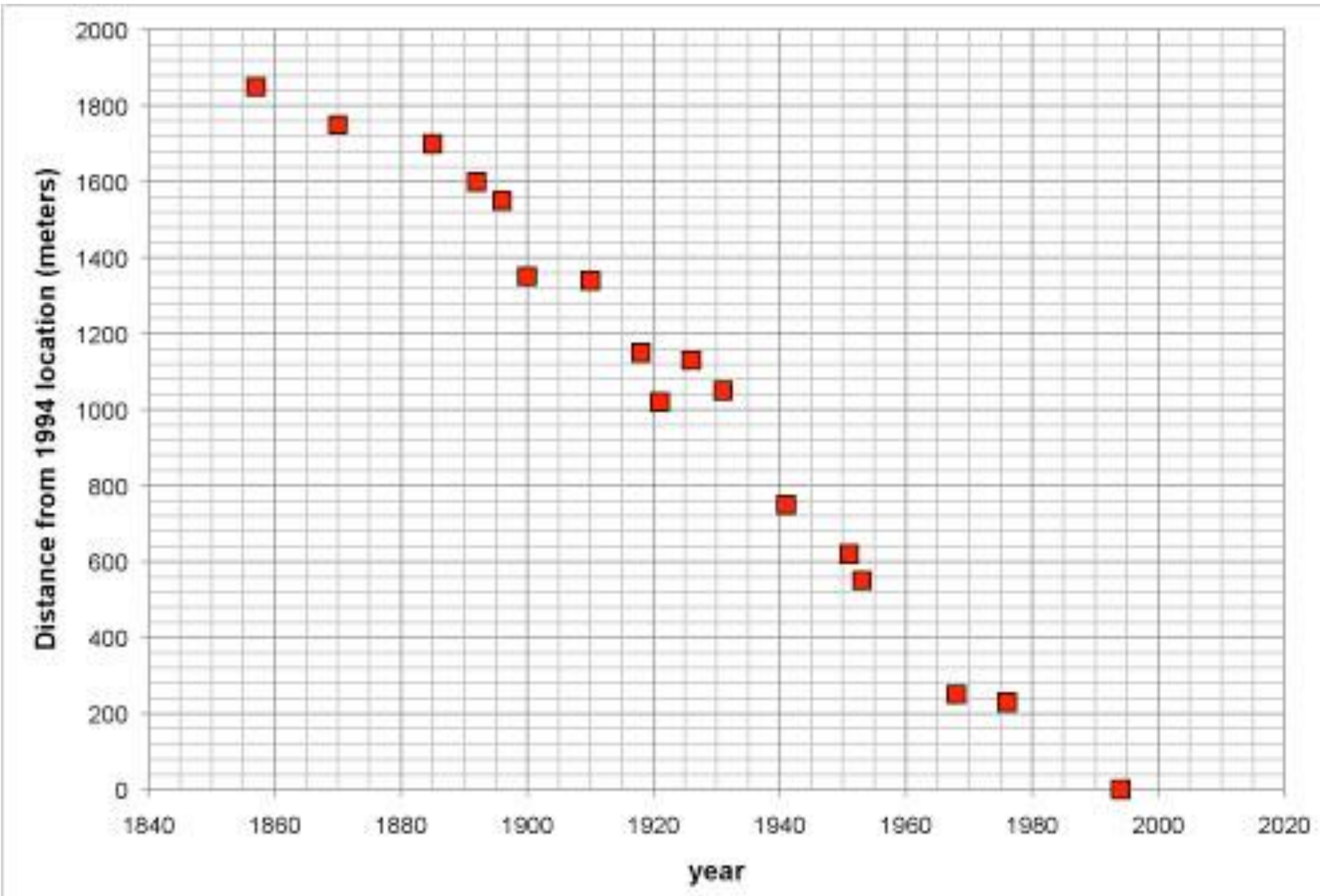
Plate motion problem

Hawaii is a hot spot, a volcano that is generated by a fixed plume of magma. The Pacific plate moves over the hot spot and we can use the location of a volcano through time to determine the rate at which the Pacific plate moves. The graph below shows a plot of the age of volcanoes vs. location relative to Kilauea (the present active volcano).



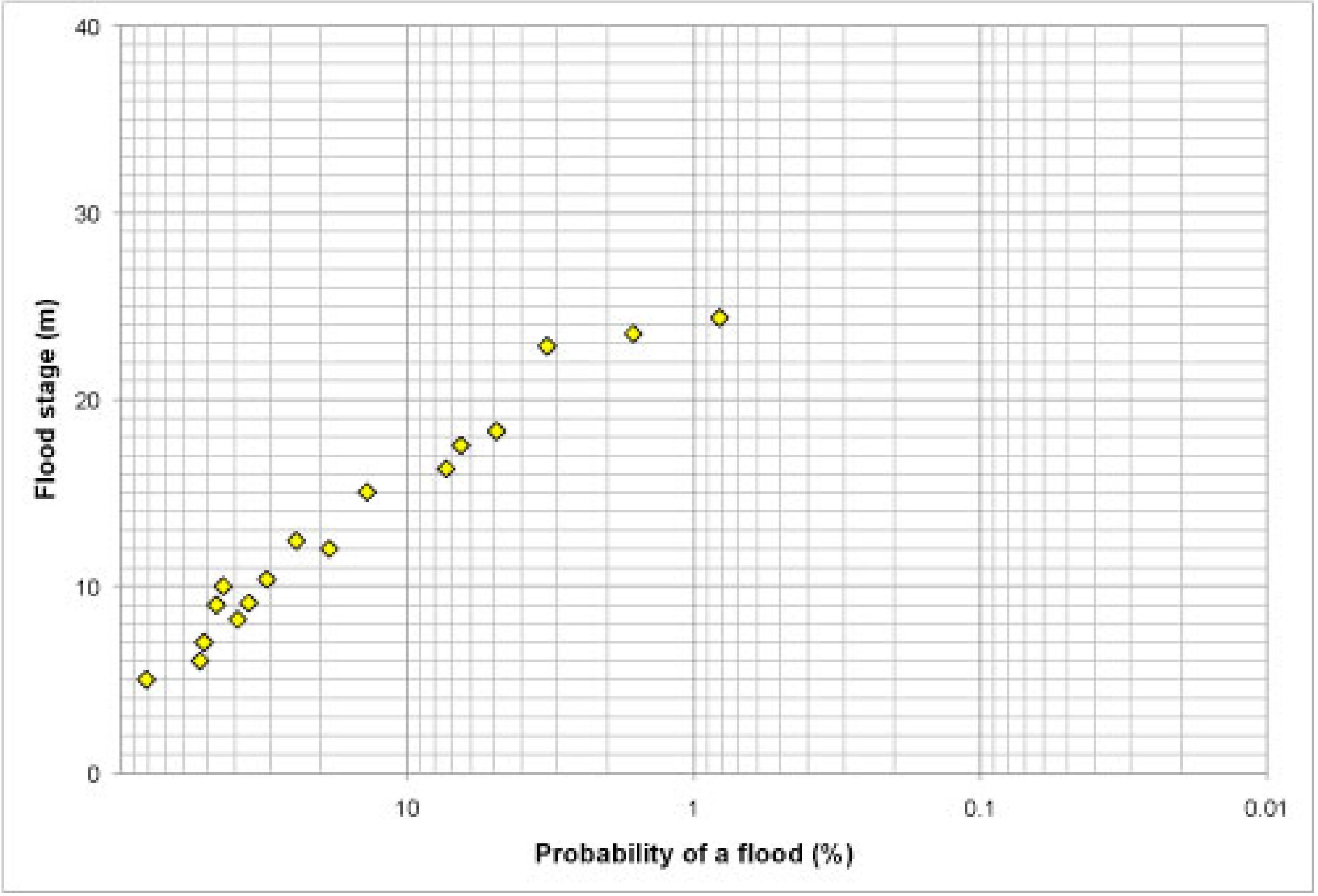
Glacial Retreat problem

Global climate change has affected mountain glaciers all over the world. At Nisqually Glacier on Mount Rainier in Washington State, scientists have measured the retreat of the glacier from 1858 through 1994. The data from 1858-1994 is plotted on the graph below, using the location in 1994 as the 0 km point.



Flooding problem

Many communities built on flood plains want to know whether a flood will impact their lives. Geoscientists can give inhabitants an estimate of the probability of a flood hitting an area based on past patterns. Below is a plot (on a type of graph paper called semi-log, where the x-axis is a logarithmic scale) of the probability of a river rising to a given stage (meters above normal).



Curve Fitting: from Ian Barrodale's talk

L_1-norm: Minimize sum of the absolute values of the differences between the function values and the linear approximation of the function.

L_∞-norm: Minimize the absolute value of the maximum difference between the function value and the linear approximation.

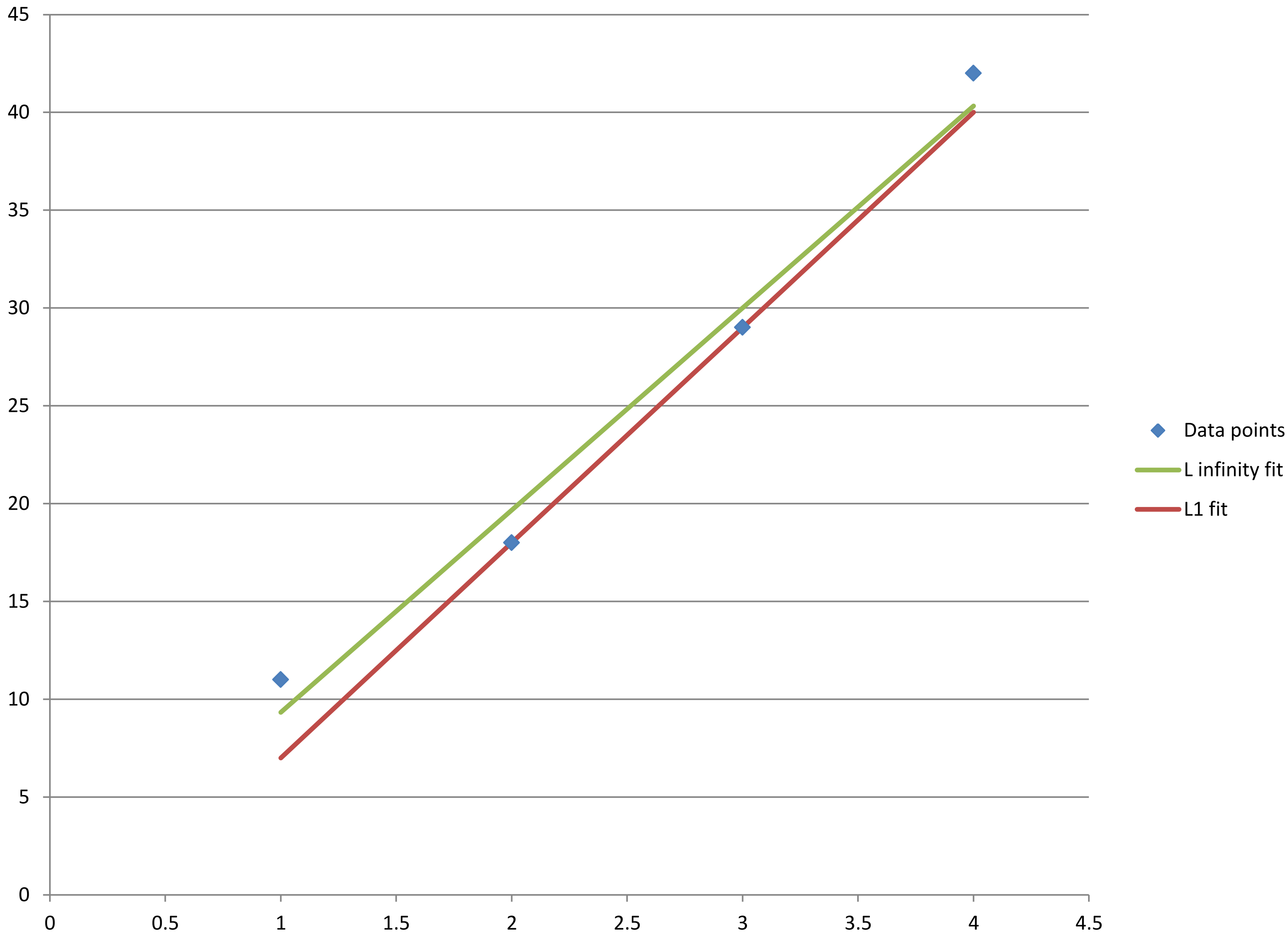
x	y	L_1-fit	L_1 error	L_∞-fit	L_∞ error
1	11	7	4	$9\ ^1/_3$	$1\ ^2/_3$
2	18	18	0	$19\ ^2/_3$	$-1\ ^2/_3$
3	29	29	0	30	-1
4	42	40	2	$40^1/_3$	$1\ ^2/_3$

L_1: $y = -4 + 11x$

Error $= 4 + 0 + 0 + 2 = 6$

L_∞: $y = -1 + 10\ ^1/_3\ x$

Error $= \mathrm{Max}\{\ |5/3|, |-5/3|,\ |-1|,\ |5/3|\} = 5/3$


45
40
35
30
25
20
15
10
5
0
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
Data points
L infinity fit
L1 fit

How do we formulate the fitting problem as a linear program for each of these norms?

In both cases we want to find a_0 and a_1 so that the linear approximation is:

$$y = a_0 + a_1\,x = a_0\,1 + a_1\,x$$

x	y
1	11
2	18
3	29
4	42

L_1-norm: minimize the sum of the absolute values of the differences.

Minimize $|d_1| + |d_2| + |d_3| + |d_4|$
subject to
$d_1 = 11 - (a_0 1 + a_1 1)$
$d_2 = 18 - (a_0 1 + a_1 2)$
$d_3 = 29 - (a_0 1 + a_1 3)$
$d_4 = 42 - (a_0 1 + a_1 4)$

x	y
1	11
2	18
3	29
4	42

This is not in standard form.

To manage the absolute values:

Minimize $|d_1| + |d_2| + |d_3| + |d_4| =$

$$u_1 + v_1 + u_2 + v_2 + u_3 + v_3 + u_4 + v_4$$

subject to

$d_1 = u_1 - v_1 = 11 - (a_0 1 + a_1 1)$

$d_2 = u_2 - v_2 = 18 - (a_0 1 + a_1 2)$

$d_3 = u_3 - v_3 = 29 - (a_0 1 + a_1 3)$

$d_4 = u_4 - v_4 = 42 - (a_0 1 + a_1 4)$

$u_1, u_2, u_3, u_4 \geq 0$

$v_1, v_2, v_3, v_4 \geq 0$

The value of u_i is > 0 if d_i is strictly positive.

The value of v_i is > 0 if d_i is strictly negative.

Change to Maximize:

Minimize

$u_1 + v_1 + u_2 + v_2 + u_3 + v_3 + u_4 + v_4$

becomes

Maximize

$-u_1 - v_1 - u_2 - v_2 - u_3 - v_3 - u_4 - v_4$

Missing non-negativity constraints on the a_0 and a_1:

$u_1 - v_1 = 11 - (a_0\, 1 + a_1\, 1)$
$u_2 - v_2 = 18 - (a_0\, 1 + a_1\, 2)$
$u_3 - v_3 = 29 - (a_0\, 1 + a_1\, 3)$
$u_4 - v_4 = 42 - (a_0\, 1 + a_1\, 4)$

Set $a_0 = b_0 - c_0$
Set $a_1 = b_1 - c_1$

$b_0, b_1, c_0, c_1 \geq 0$

Maximize $0\ b_0 + 0\ c_0 + 0\ b_1 + 0\ c_1$

$-u_1 - v_1 - u_2 - v_2 - u_3 - v_3 - u_4 - v_4$

subject to

$$u_1 - v_1 = 11 - (\ (b_0 - c_0)\ 1 + \ (b_1 - c_1)\ \ 1)$$
$$u_2 - v_2 = 18 - (\ (b_0 - c_0)\ 1 + \ (b_1 - c_1)\ \ 2)$$
$$u_3 - v_3 = 29 - (\ (b_0 - c_0)\ 1 + \ (b_1 - c_1)\ \ 3)$$
$$u_4 - v_4 = 42 - (\ (b_0 - c_0)\ 1 + \ (b_1 - c_1)\ \ 4)$$

Finally, change each equality constraint:

$$u_1 - v_1 \leq 11 - (\ (b_0 - c_0)\ 1 + \ (b_1 - c_1)\ \ 1)$$
$$u_1 - v_1 \geq 11 - (\ (b_0 - c_0)\ 1 + \ (b_1 - c_1)\ \ 1)$$
$$\Longrightarrow$$
$$-u_1 + v_1 \leq -11 + (\ (b_0 - c_0)\ 1 + \ (b_1 - c_1)\ \ 1)$$

```
X13= 11 - 1 B0 + 1 C0 - 1 B1 + 1 C1 - 1 U1 + 0 U2
        + 0 U3 + 0 U4 + 1 V1 + 0 V2 + 0 V3 + 0 V4
X14= 18 - 1 B0 + 1 C0 - 2 B1 + 2 C1 + 0 U1 - 1 U2
        + 0 U3 + 0 U4 + 0 V1 + 1 V2 + 0 V3 + 0 V4
X15= 29 - 1 B0 + 1 C0 - 3 B1 + 3 C1 + 0 U1 + 0 U2
        - 1 U3 + 0 U4 + 0 V1 + 0 V2 + 1 V3 + 0 V4
X16= 42 - 1 B0 + 1 C0 - 4 B1 + 4 C1 + 0 U1 + 0 U2
        + 0 U3 - 1 U4 + 0 V1 + 0 V2 + 0 V3 + 1 V4

X17=-11 + 1 B0 - 1 C0 + 1 B1 - 1 C1 + 1 U1 + 0 U2
        + 0 U3 + 0 U4 - 1 V1 + 0 V2 + 0 V3 + 0 V4
X18=-18 + 1 B0 - 1 C0 + 2 B1 - 2 C1 + 0 U1 + 1 U2
        + 0 U3 + 0 U4 + 0 V1 - 1 V2 + 0 V3 + 0 V4
X19=-29 + 1 B0 - 1 C0 + 3 B1 - 3 C1 + 0 U1 + 0 U2
        + 1 U3 + 0 U4 + 0 V1 + 0 V2 - 1 V3 + 0 V4
X20=-42 + 1 B0 - 1 C0 + 4 B1 - 4 C1 + 0 U1 + 0 U2
        + 0 U3 + 1 U4 + 0 V1 + 0 V2 + 0 V3 - 1 V4
-----------------------------------------------
z = 0   + 0 B0 + 0 C0 + 0 B1 + 0 C1 - 1 U1 - 1 U2
        - 1 U3 - 1 U4 - 1 V1 - 1 V2 - 1 V3 - 1 V4
```

```
The optimal solution: -6
Minimization problem has solution: 6

B0 =   0     C0 =   4

B1 =  11     C1 =   0

U1 =   4     U2 =   0
V1 =   0     V2 =   0

U3 =   0     U4 =   2
V3 =   0     V4 =   0
```

The L_1-norm:
The result from running my program.

The optimal solution: -6.0

[So the error is 6]

$X1 = b_0 = 0 \quad X2 = c_0 = 4$

$X3 = b_1 = 11 \quad X4 = c_1 = 0$

$a_0 = b_0 - c_0 = -4$

$a_1 = b_1 - c_1 = 11$

So the curve is

$y = -4 + 11\,x$

The L_∞-norm:

Minimize $w = \text{Max}\{|d_1|, |d_2|, |d_3|, |d_4|\}$

subject to

$d_1 = u_1 - v_1 = 11 - (a_0 1 + a_1 1)$

$d_2 = u_2 - v_2 = 18 - (a_0 1 + a_1 2)$

$d_3 = u_3 - v_3 = 29 - (a_0 1 + a_1 3)$

$d_4 = u_4 - v_4 = 42 - (a_0 1 + a_1 4)$

$w \geq |d_1|$: $w \geq u_1$ and $w \geq v_1$

$w \geq |d_2|$: $w \geq u_2$ and $w \geq v_2$

$w \geq |d_3|$: $w \geq u_3$ and $w \geq v_3$

$w \geq |d_4|$: $w \geq u_4$ and $w \geq v_4$

$u_1, u_2, u_3, u_4 \geq 0, \quad v_1, v_2, v_3, v_4 \geq 0$

Same equations as L_1 case except W variable included:

```
X14= 11 - 1 B0 + 1 C0 - 1 B1 + 1 C1 - 1 U1 + 0 U2
        + 0 U3 + 0 U4 + 1 V1 + 0 V2 + 0 V3 + 0 V4 + 0 W
X15= 18 - 1 B0 + 1 C0 - 2 B1 + 2 C1 + 0 U1 - 1 U2
        + 0 U3 + 0 U4 + 0 V1 + 1 V2 + 0 V3 + 0 V4 + 0 W
X16= 29 - 1 B0 + 1 C0 - 3 B1 + 3 C1 + 0 U1 + 0 U2
        - 1 U3 + 0 U4 + 0 V1 + 0 V2 + 1 V3 + 0 V4 + 0 W
X17= 42 - 1 B0 + 1 C0 - 4 B1 + 4 C1 + 0 U1 + 0 U2
        + 0 U3 - 1 U4 + 0 V1 + 0 V2 + 0 V3 + 1 V4 + 0 W

X18=-11 + 1 B0 - 1 C0 + 1 B1 - 1 C1 + 1 U1 + 0 U2
        + 0 U3 + 0 U4 - 1 V1 + 0 V2 + 0 V3 + 0 V4 + 0 W
X19=-18 + 1 B0 - 1 C0 + 2 B1 - 2 C1 + 0 U1 + 1 U2
        + 0 U3 + 0 U4 + 0 V1 - 1 V2 + 0 V3 + 0 V4 + 0 W
X20=-29 + 1 B0 - 1 C0 + 3 B1 - 3 C1 + 0 U1 + 0 U2
        + 1 U3 + 0 U4 + 0 V1 + 0 V2 - 1 V3 + 0 V4 + 0 W
X21=-42 + 1 B0 - 1 C0 + 4 B1 - 4 C1 + 0 U1 + 0 U2
        + 0 U3 + 1 U4 + 0 V1 + 0 V2 + 0 V3 - 1 V4 + 0 W
```

```
X22= 0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 - 1 U1 + 0 U2
       + 0 U3 + 0 U4 + 0 V1 + 0 V2 + 0 V3 + 0 V4 + 1 W
X23= 0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 + 0 U1 - 1 U2
       + 0 U3 + 0 U4 + 0 V1 + 0 V2 + 0 V3 + 0 V4 + 1 W
X24= 0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 + 0 U1 + 0 U2
       - 1 U3 + 0 U4 + 0 V1 + 0 V2 + 0 V3 + 0 V4 + 1 W
X25= 0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 + 0 U1 + 0 U2
       + 0 U3 - 1 U4 + 0 V1 + 0 V2 + 0 V3 + 0 V4 + 1 W

X26= 0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 + 0 U1 + 0 U2
       + 0 U3 + 0 U4 - 1 V1 + 0 V2 + 0 V3 + 0 V4 + 1 W
X27= 0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 + 0 U1 + 0 U2
       + 0 U3 + 0 U4 + 0 V1 - 1 V2 + 0 V3 + 0 V4 + 1 W
X28= 0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 + 0 U1 + 0 U2
       + 0 U3 + 0 U4 + 0 V1 + 0 V2 - 1 V3 + 0 V4 + 1 W
X29= 0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 + 0 U1 + 0 U2
       + 0 U3 + 0 U4 + 0 V1 + 0 V2 + 0 V3 - 1 V4 + 1 W

----------------------------------------------
z=   0 + 0 B0 + 0 C0 + 0 B1 + 0 C1 - 0 U1 + 0 U2
       + 0 U3 + 0 U4 + 0 V1 + 0 V2 + 0 V3 + 0 V4 -  1 W
```

The optimal solution: -1 2/3

Solution to the minimization problem: 1 2/3

B0 =	0.0000	C0 =	1.0000
B1 =	10.3333	C1 =	0.0000

U1 =	1.6667	U2 =	0.0000
V1 =	0.0000	V2 =	1.6667

U3 =	0.0000	U4 =	1.6667
V3 =	1.0000	V4 =	0.0000

W = 1.6667

The L_∞-norm:

The result from running my program.

The optimal solution: -1.666667

[So the error is $1\,{}^{2}/_{3}$]

$X1 = b_0 = 0$ $\quad$ $X2 = c_0 = 1$

$X3 = b_1 = 10\,{}^{1}/_{3}$ $\quad$ $X4 = c_1 = 0$

$a_0 = b_0 - c_0 = -1$

$a_1 = b_1 - c_1 = 10\,{}^{1}/_{3}$

So the curve is: $y = -1 + 10\,{}^{1}/_{3}\,x$

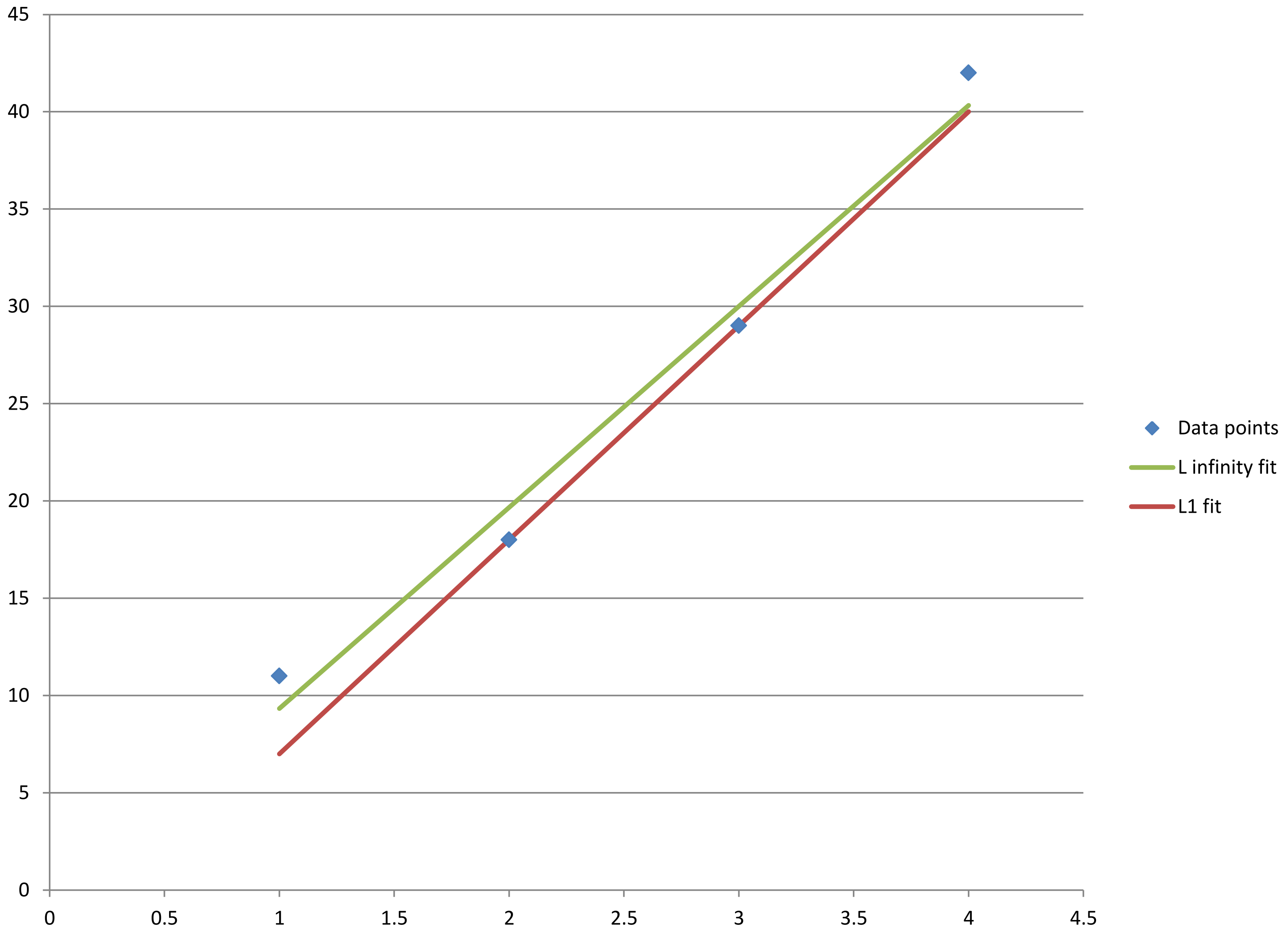
x	y	L_1-fit	L_1 error	L_∞-fit	L_∞ error
1	11	7	4	$9\,{}^{1}/_{3}$	$1\,{}^{2}/_{3}$
2	18	18	0	$19\,{}^{2}/_{3}$	$-1\,{}^{2}/_{3}$
3	29	29	0	30	-1
4	42	40	2	$40\,{}^{1}/_{3}$	$1\,{}^{2}/_{3}$

L_1: $y= -4 + 11x$

Error $= 4 + 0 + 0 + 2 = 6$

L_∞: $y= -1 + 10\,{}^{1}/_{3}x$

Error $=$ Max$\{ |5/3|,|-5/3|, |-1|, |5/3|\} = 5/3$



45
40
35
30
25
20
15
10
5
0
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
Data points
L infinity fit
L1 fit