Queens College, CUNY, Department of Computer Science
Numerical Methods
CSCI 361 / 761
Fall 2017
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December 1, 2017

23 Lecture 23

Interpolation and fitting of data

- In this lecture we study some simple examples of **interpolation and fitting of data.**
- We treat only some very simple examples.

23.1 Interpolation: Lagrange polynomial

- Suppose we have a set of points (x_i, y_i), $i = 1, 2, \dots, n$, where the x_i are all distinct (i.e. there is no vertical scatter in the data).
- Without loss of generality we may assume the x_i are sorted from the smallest to the largest, so $x_1 < x_2 < \cdots < x_n$.
- We wish to find a polynomial which passes through all the points.
- We can always find a polynomial of sufficiently high degree which passes through all the points.
- What we seek is the polynomial of *lowest* degree which passes through all the points.
- This polynomial is unique.
- It is called the **Lagrange polynomial**.
- We construct the Lagrange polynomial as follows.
  1. First define the following polynomial

     $$\ell_1(x) = \frac{(x-x_2)(x-x_3)\dots(x-x_n)}{(x_1-x_2)(x_1-x_3)\cdots(x_1-x_n)} \,. \tag{23.1.1}$$

     Note the following:

     (a) The denominator does not vanish, so the polynomial $\ell_1(x)$ is well defined.
     (b) At $x = x_1$, then $\ell_1(x_1) = 1$.
     (c) At all the other points $x = x_2$, $x = x_3$, $\dots$, $x = x_n$, then $\ell_1(x_i) = 0$, $i \neq 1$.
     (d) This is called a **Lagrange basis polynomial**.
     (e) It equals 1 at $x = x_1$ and 0 at all the other points $x = x_i$, $i \neq 1$.
  2. We can easily construct a second Lagrange basis polynomial $\ell_2(x)$, which equals 1 at $x = x_2$ and 0 at all the other points $x = x_i$, $i \neq 2$. The polynomial is obviously

     $$\ell_3(x) = \frac{(x-x_1)(x-x_3)\dots(x-x_n)}{(x_2-x_1)(x_2-x_3)\cdots(x_2-x_n)} \,. \tag{23.1.2}$$

     This time we omit a factor $(x - x_2)$ in the numerator, and the denominator has an obvious pattern.
  3. We can similarly construct a third Lagrange basis polynomial $\ell_3(x)$, which equals 1 at $x = x_3$ and 0 at all the other points $x = x_i$, $i \neq 3$.
  4. The pattern is obvious. We can construct the Lagrange basis polynomial $\ell_j(x)$, which equals 1 at $x = x_j$ and 0 at all the other points $x = x_i$, $i \neq j$.

- The overall Lagrange polynomial $L(x)$ is then given by the following weighted sum of n Lagrange basis polynomials

$$\begin{aligned} L(x) &= y_1\,\ell_1(x) + y_2\,\ell_2(x) + y_3\,\ell_3(x) + \cdots + y_n\,\ell_n(x) \\ &= \sum_{j=1}^{n} y_j\,\ell_j(x)\,. \end{aligned} \tag{23.1.3}$$

  1. Notice that $L(x) = y_1$ at $x = x_1$, because $\ell_1(x_1) = 1$ and all the other basis polynomials vanish $\ell_j(x_1) = 0$ for $j \neq 1$.
  2. Similarly $L(x) = y_2$ at $x = x_2$, because $\ell_2(x_2) = 1$ and all the other basis polynomials vanish $\ell_j(x_2) = 0$ for $j \neq 2$.
  3. And so on: $L(x) = y_3$ at $x = x_3$, etc.

- For only two points $n = 2$, the Lagrange polynomial is the straight line through (x_1, y_1) and (x_2, y_2):

$$L(x) = y_1\,\frac{x - x_2}{x_1 - x_2} + y_2\,\frac{x - x_1}{x_2 - x_1}\,. \tag{23.1.4}$$

- For three points $n = 3$, the Lagrange polynomial is a quadratic

$$L(x) = y_1\,\frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)} + y_2\,\frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)} + y_3\,\frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)}\,. \tag{23.1.5}$$

- **If the three points lie on a straight line, the Lagrange polynomial will simplify to that straight line.**

- There are more efficient numerical techniques to construct the Lagrange polynomial.

- However, we do not have time to discuss the matter in more detail

23.2 Data fitting: linear least squares

- Suppose we have a set of points (x_i, y_i), $i = 1, 2, \dots, n$.
- In this problem, the x_i may not all be distinct, i.e. there may be vertical scatter in the data.
- We wish to find a "best fit" straight line to fit the data.
- In general, a straight line will not pass through all the data points.
- Hence we require a criterion to define what "best fit" means.
- We shall employ the **linear least squares** algorithm.
- Let the straight line to fit the data be given by the formula

$$y = a + bx\,. \tag{23.2.1}$$

- Then at each point, we calculate the difference $d_i = (a + bx_i) - y_i$ and we sum the squares

$$S = \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} (a + bx_i - y_i)^2\,. \tag{23.2.2}$$

- Note that the value of S is always non-negative.
- **The least squares "best fit" straight line is given by the values of a and b which minimize the value of S.**
- Hence we seek the values of a and b such that

$$\frac{\partial S}{\partial a} = 0\,, \qquad \frac{\partial S}{\partial b} = 0\,. \tag{23.2.3}$$

- Note that

$$\frac{\partial S}{\partial a} = 2\sum_{i=1}^{n} (a + bx_i - y_i)\,, \tag{23.2.4a}$$

$$\frac{\partial S}{\partial b} = 2\sum_{i=1}^{n} x_i(a + bx_i - y_i)\,. \tag{23.2.4b}$$

- For brevity, define the following sums

$$s_x = \frac{1}{n}\sum_{i=1}^{n} x_i\,, \tag{23.2.5a}$$

$$s_y = \frac{1}{n}\sum_{i=1}^{n} y_i\,, \tag{23.2.5b}$$

$$s_{xx} = \frac{1}{n}\sum_{i=1}^{n} x_i^2\,, \tag{23.2.5c}$$

$$s_{xy} = \frac{1}{n}\sum_{i=1}^{n} x_i y_i\,. \tag{23.2.5d}$$

- Let the minimum be attained at the values a_* and b_*. Then the equations to solve are

$$\begin{pmatrix} 1 & s_x \\ s_x & s_{xx} \end{pmatrix} \begin{pmatrix} a_* \\ b_* \end{pmatrix} = \begin{pmatrix} s_y \\ s_{xy} \end{pmatrix} . \tag{23.2.6}$$

- The solution is

$$\begin{aligned} \begin{pmatrix} a_* \\ b_* \end{pmatrix} &= \frac{1}{s_{xx} - s_x^2} \begin{pmatrix} s_{xx} & -s_x \\ -s_x & 1 \end{pmatrix} \begin{pmatrix} s_y \\ s_{xy} \end{pmatrix} \\ &= \frac{1}{s_{xx} - s_x^2} \begin{pmatrix} s_{xx}s_y - s_x s_{xy} \\ s_{xy} - s_x s_y \end{pmatrix} . \end{aligned} \tag{23.2.7}$$