CS 314 SUMMER 2012 WEEK 4 NOTES

Lecture 15

July 2nd, 2012

PADÉ APPROXIMATIONS

Approximations for functions that use quotients of polynomials

$$R_{N,M}(x) = \frac{P_N(x)}{Q_M(x)} \quad \text{for a} \leq \text{x} \leq \text{b}$$

$$\text{where } P_N(x) = p_0 + p_1 x + p_2 x^2 + \cdots + p_N x^N$$

$$Q_M(x) = 1 + q_1 + q_2 x^2 + \cdots + q_M x^M$$

The polynomials are constructed so that $f(x)$and $R_{N,M}(x)$ agree at $x = 0$ and the derivatives to $N + M$ agree also at $x = 0$.

Assume that $f(x)$ has the following MacLaurin Expansion [MacLaurin expansion = Taylor expansion when $x = 0$]:

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots$$

Then we form the difference

$$f(x) = \frac{P_N(x)}{Q_M(x)}$$

$$f(x)Q_M(x) - P_N(x) = 0$$

$$(a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k) * (1 + q_1 x + q_2 x^2 + \cdots q_M x^M) - (p_0 + p_1 x + p_2 x^2 + \cdots + p_N x^N = 0$$

Peforming multiplication and factoring, we have

$a_0 - p_0 = 0$ for x^0

$a_1 + a_0 q_1 - p_1 = 0$ for x^1

$a_2 + a_1 q_1 + q_2 a_0 - p_2 = 0$ for x^2

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$q_M a_{N-M} + q_{M-1} a_{N-m-1} \ldots\ldots a_N - p_N = 0$

$q_M a_{N-M+1} + q_{M-1} a_{N+1} \ldots\ldots a_{N+M} = 0$

-We get $N + M + 1$ equations-

Example: Find approximation $\mathbf{R_{2,2}(x)}$ for $\mathbf{f(x) = \frac{\ln(1+x)}{x}}$

Start with MacLaurin expansion:

$$f(x) = 1 - \frac{x}{2} + \frac{x^2}{3} - \frac{x^3}{4} + \frac{x^4}{5} - \cdots$$

$$f(x) = R_{N,M}(x) = \frac{P_N(x)}{Q_M(x)}$$

$$f(x) = R_{2,2}(x) = \frac{P_2(x)}{Q_2(x)} = \frac{p_0 + p_1 x + p_2 x^2)}{1 + q_1 x + q_2 x^2}$$

$$f(x) = \frac{P_N(x)}{Q_N(x)} \text{ at } x = 0$$

$$f(x) Q_N(x) - P_N(x) = 0 \text{ at } x = 0$$

$$\left(1-\frac{x}{2}+\frac{x^2}{3}-\frac{x^3}{4}+\frac{x^4}{5}-\cdots\right)(1+q_1x+q_2x^2)-(p_0+p_1x+p_2x^2)=0$$

$$1-\frac{x}{2}+\frac{x^2}{3}-\frac{x^3}{4}+\frac{x^4}{5}-\cdots q_1x-\frac{q_1x^2}{2}+\frac{q_1x^3}{3}-\frac{q_1x^4}{4}+\frac{q_1x^5}{5}+\cdots$$

$$+q_2x^2-\frac{q_2x^3}{2}+\frac{q_2x^4}{3}-\frac{q_2x^5}{4}+\frac{q_2x^6}{5}+\cdots$$

$$p_0-p_1x-p_2x^2=0 \text{ at } x=0$$

$$(1-p_0)+x\left(-\frac{1}{2}+q_1-p_1\right)+x^2\left(\frac{1}{3}-\frac{q_1}{2}+q_2-p_2\right)+x^3\left(-\frac{1}{4}+\frac{q_1}{3}-\frac{q_2}{2}\right)+x^4(\frac{1}{5}-\frac{q_1}{4}$$
$$+\frac{q_2}{3}=0$$

So we obtain that:

(1) $$1-p_0=0$$

(2) $$-\frac{1}{2}+q_1-p_1=0$$

(3) $$\left(-\frac{1}{3}-\frac{q_1}{2}+q_2-p_2\right)=0$$

(4) $$-\frac{1}{4}+\frac{q_1}{3}-\frac{q_2}{2}=0$$

(5) $$\frac{1}{5}-\frac{q_1}{4}+\frac{q_2}{3}=0$$

Multiplying **(4)** by 3 and **(5)** by 4 and adding,

$$q_1=\frac{3}{10}$$

$$q_2=\frac{6}{5}$$

…Continued from Lecture 15…

From **(3)**

$$p_2 = \frac{1}{3} - \frac{q_1}{2} + q_2 = \frac{1}{3} - \left(\frac{6}{5}\right)\left(\frac{1}{2}\right) + \frac{3}{10} = \frac{10 - 18 + 9}{30} = \frac{1}{30}$$

$$p_2 = \frac{1}{30}$$

From **(2)**

$$p_1 = q_1 - \frac{1}{2} = \frac{7}{10}$$

$$p_1 = \frac{7}{10}$$

From **(1)**

$$p_0 = 1$$

$$R_{2,2}(x) = \frac{p_0 + p_1 x + p_2 x^2}{1 + q_1 x + q_2 x^2}$$

$$= \frac{\left(1 + \frac{7}{10}x\right) + \left(\frac{1}{30}\right)x^2}{1 + \left(\frac{6}{5}\right)x + \frac{3}{10}x^2}$$

$$f(x) = \frac{\ln(1+x)}{x} = \frac{\left(x + \frac{7}{10}x^2\right) + \left(\frac{1}{30}\right)x^3}{1 + \left(\frac{6}{5}\right)x + \frac{3}{10}x^2} = \frac{30x + 21x^2 + x^3}{30 + 36x + 9x^2}$$

$$y = x + 1$$

$x = y - 1$ … Can plug in to the equation

CURVE FITTING

Given a set of points, come up with a curve that best fits the points.

Polynomial Approximation ➔polynomials are passed through every single point

If you have

$$(x_0, y_0), (x_1, y_1), (x_2, y_2), \dots (x_N, y_N)$$

Polynomial Approximation with Lagrange or Newton will give you a polynomial of degree N

We first choose a function like $y = ax + b$ and we have $N + 1$ points $(x_0, y_0) \dots (x_N, y_N)$. Then we find the coefficients (a, b) in this case that minimizes the error.

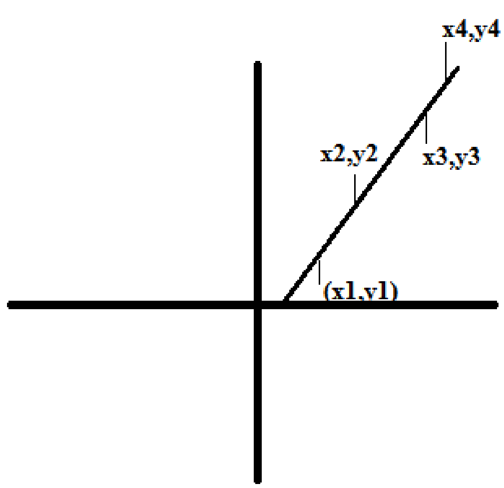
Example: An experiment produces $N + 1$points and we want to find a line that relates these points.

LEAST SQUARES LINE

Assume that we have recorded values $(x_1, y_1), (x_2, y_2), \dots (x_N, y_N)$ and we want to find the line

$$\boldsymbol{y = f(x) = Ax + B}$$

that best fits the recorded data



We have that

$$f(x_k) = y_k + e_k$$

where

$f(x_k)$ is the approximation

y_k is the data sample

e_k is the error

There are several norms that can be used to tell how far $f(x)$ is from the data.

Max Error $$E_\infty(f) = \max(|f(x_k) - y_k|)$$

Average Error $$E_1(f) = \frac{1}{N}\sum_{k=1}^{N}(|f(x_k) - y_k|)$$

➔ **Root Mean Square Error** $$E_2(f) = \frac{1}{N}\sum_{k=1}^{N}(f(x_k) - y_k)^2$$

We use the Root Mean Square Error method because it's easier to derivate to obtain the minimum error.

Given the points $(x_1, y_1), (x_2, y_2), \dots (x_N, y_N)$ the least square line $y = f(x) = Ax + B$ is the line that minimizes the square error $E_2(f)$

The square error for using A,B is

$$E(A, B) = \sum_{k=1}^{N}(Ax_k + B - y_k)^2$$

To minimize error, we obtain the partial derivative of E with respect to A and B

(1) $\frac{\partial E(A,B)}{\partial A} = \sum_{k=1}^{N} 2(Ax_k + B - y_k)(x_k) = 2\sum_{k=1}^{N}(Ax_k^2 + Bx_k - x_k y_k)$

(2) $\frac{\partial E(A,B)}{\partial A} = \sum_{k=1}^{N} 2(Ax_k + B - y_k)(1) = 2\sum_{k=1}^{N}(Ax_k + B - y_k)$

Setting $\frac{\partial E(A,B)}{\partial A} = 0$ in **(1)** we obtain

$$\frac{\partial E(A,B)}{\partial A} = 0 = 2\sum_{k=1}^{N}(Ax_k^2 + Bx_k - x_k y_k)$$

$$0 = \sum_{k=1}^{N} Ax_k^2 + \sum_{k=1}^{N} Bx_k - \sum_{k=1}^{N} x_k y_k$$

(3) $A\sum_{k=1}^{N} x_k^2 + B\sum_{k=1}^{N} x_k - \sum_{k=1}^{N} x_k y_k = 0$

Setting $\frac{\partial E(A,B)}{\partial B} = 0$ in **(2),** we obtain

$$\frac{\partial E(A,B)}{\partial B} = 0 = 2\sum_{k=1}^{N} Ax_k + B - y_k$$

$$0 = \sum_{k=1}^{N} Ax_k + \sum_{k=1}^{N} B - \sum_{k=1}^{N} y_k$$

(4) $A\sum_{k=1}^{N} x_k + NB - \sum_{k=1}^{N} y_k = 0$

(3) and **(4)** give a system of 2 linear equations that can be used to obtain A,B that minimize the error when fitting the curve $y = Ax + B$

Assume the following data,

	x_k	y_k	x_k^2	$x_k y_k$
1	6	7	36	42
2	9	6	81	54
3	14	3	196	42
4	17	1	289	17
5	21	0	441	0
	-------------	-------------	-------------	-------------
	$\sum_{k=1}^{N} x_k = 67$	$\sum_{k=1}^{N} y_k = 17$	$\sum_{k=1}^{N} x_k^2 = 1043$	$\sum_{k=1}^{N} x_k y_k = 155$

Lecture 17

July 5th, 2012

…Continued from Lecture 16…

Least Squares Line

(1) $A \sum_{k=1}^{N} x_k^2 + B \sum_{k=1}^{N} x_k - \sum_{k=1}^{N} x_k y_k = 0$
(2) $A \sum_{k=1}^{N} x_k + NB - \sum_{k=1}^{N} y_k = 0$

We want to approximate $(x_1, y_1), \ldots (x_N, y_N)$ to the line $y = Ax + B$

Using **(1)** and **(2)** to obtain A,B minimizes the square of the error

x_k	y_k	x_k^2	y_k^2
6	7	36	42
9	6	81	54
14	3	196	42
17	1	289	1
21	0	441	0
-------------	-------------	-------------	-------------
$\sum_{k=1}^{N} x_k = 67$	$\sum_{k=1}^{N} y_k = 17$	$\sum_{k=1}^{N} x_k^2 = 1043$	$\sum_{k=1}^{N} x_k y_k = 155$

From **(1)**

(3) $A(1043) + B(67) - 155 = 0$

From **(2)**

(4) $A(67) + B(5) - 17 = 0$

Multiply **(3)** by -5 and **(4)** by 67 to obtain overall

$$A = -0.5013$$

$$B = 10.11$$

Result: $f(x) = y = -0.5013x + 10.11$

Sometimes we would like to fit the data points with the curve

$$(x_0, y_0), \dots .(x_N, y_N) \qquad\qquad f(x) = Ax^M$$

Where M is a known constant and A is unknown

We first compute the error function

$$E(A) = \sum_{k=1}^{N} (Ax_k^M - y_k)^2$$

$$\frac{\partial E(A)}{\partial A} = \sum_{k=1}^{N} 2\,(Ax_k^M - y_k)x_k^M = 0$$

$$2\sum_{k=1}^{N} (Ax_k^{2M} - y_k x_k^M) = 0$$

$$\sum_{k=1}^{N} Ax_k^{2M} - \sum_{k=1}^{N} y_k x_k^M = 0$$

$$A\sum_{k=1}^{N} x_k^{2M} - \sum_{k=1}^{N} y_k x_k^M = 0$$

$$A = (\sum_{k=1}^{N} y_k x_k^M)/(\sum_{k=1}^{N} x_k^{2M})$$

Example: We want to fit the following data in the equation $y = Ax^3$

x_k	y_k	$x_k^3 y_k$	x_k^6
2	5.9	47.2	64
2.3	8.3	100.986	148.04
2.6	10.7	188.06	308.92
2.9	13.7	334.13	594.82
3.2	17.0	557.06	1073.74
		-------------	-------------
		$\sum_{k=1}^{N} x_k^3 y_k = 1227.44$	$\sum_{k=1}^{N} x_k^6 = 2189.52$

$$A = 0.5606$$

$$y = 0.5606x^3$$

What will be covered on the exam:

- Floating Point/Binary Representation
- Propagation of Errors
- Solution of Nonlinear Equations
    - Fixed Point Theorem
    - Types of Convergence/Divergence
        - Monotone Convergence
        - Oscillating Convergence
        - Monotone Divergence
        - Oscillating Divergence
    - Bisection Method
    - False Position Method
        - Horizontal Convergence $|f(x)| < \epsilon$
        - Vertical Convergence $|x_k - x_{k-1}| < \epsilon$
        - Mixed Convergence
        - Well-Conditioned/Ill-Conditioned
    - Newton-Raphson
        - Similarities between Newton –Raphson and Taylor Expansion
        - Numerical Approximation using a derivative

$$f'(x) = \frac{f(x+\epsilon) - f(x)}{\epsilon}$$

        - Order of Convergence
        - When Newton-Raphson may not converge
    - Secant Method
        - It doesn't need a derivative
- Solution of Linear Systems

/Ax=|B

    - Properties of Vectors
    - Vector Algebra
    - Matrices
    - Properties of Matrices
    - Special Matrices
        - Zero matrix
        - Identity matrix

        - Matrix multiplication
        - Inverse of a matrix
    - Upper Triangular System
    - Backward Substitution
    - Gauss Elimination
    - LU Factorization
- Iterative Method for Linear Equation
    - Gauss-Seidel
    - Jacobi
    - Convergence/Strictly Diagonal Dominant Matrices
- Solution of Systems of Non-Linear Equations
    - Newton-Method
- Interpolation and Polynomial Approximation
    - Taylor Approximation
    - Horner's Method
    - Lagrange Approximation
    - Newton Polynomials
        - Divided Differences
    - Padé Approximation with quotient of polynomials

CURVE FITTING WILL NOT BE COVERED

To prepare for the exam:

- Do homework 3 due on Wednesday
- Bring half-page one side with any notes you want to the exam

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Nonlinear Least-Squares Method for $y = ce^{Ax}$

Suppose that we have points $(x_1, y_1) \ldots (x_N\ , y_N)$

We want to fit these points to an exponential curve

$$f(x) = y = ce^{Ax}$$

Using non-linear least squares procedure,

$$E(A, C) = \sum_{k=1}^{N} (f(x_k) - y_k)^2 = \sum_{k=1}^{N} (ce^{Ax_k} - y_k)^2$$

$$\frac{\partial E(A, C)}{\partial A} = \sum_{k=1}^{N} 2(ce^{Ax_k} - y_k)ce^{Ax_k}x_k = 0$$

$$\sum_{k=1}^{N} (ce^{Ax_k}ce^{Ax_k}x_k - y_k ce^{Ax_k}x_k) = 0 = c^2 \sum_{k=1}^{N} e^{2Ax_k}x_k - c \sum_{k=1}^{N} e^{Ax_k}x_k y_k = 0$$

(1) $c \sum_{k=1}^{N} x_k e^{2Ax_k} - \sum_{k=1}^{N} y_k x_k e^{Ax_k} = 0$

$$\frac{\partial E(A, c)}{\partial c} = \sum_{k=1}^{N} 2(ce^{Ax_k} - y_k)e^{Ax_k} = 0$$

(2) $c \sum_{k=1}^{N} e^{2Ax_k} - \sum_{k=1}^{N} y_k e^{Ax_k} = 0$

(1) and **(2)** give a system of 2 nonlinear equations that can be solved using Newton's Method. Method needs to solve non-linear equation. We can avoid this by "linearizing" or converting f(x) to a linear equation before doing least squares.

TRANSFORMATIONS OF DATA LINEARIZATION

Possible to fit curves such as

$y = ce^{Ax}, y = Aln(x) + B$,and $y = \frac{A}{x+B}$ by transforming these equations into a linear curve

$$y = Ax + B.$$

$$y = ce^{Ax}$$

$$\ln(y) = \ln(ce^{Ax})$$

$$\ln(y) = \ln(c) + \ln(e^{Ax})$$

$$\ln(y) = \ln(c) + Ax(\ln(\mathrm{e}))$$

$$\ln(y) = \ln(c) + Ax$$

$$\ln(y) = \ln(c) + Ax$$

where ln(y) is z and ln(c) is B

$$\Rightarrow \; z = Ax + B$$

Example: Assume $(\mathbf{0}, \mathbf{1.3}), (\mathbf{1}, \mathbf{2.5}), (\mathbf{2}, \mathbf{3.5}), (\mathbf{3}, \mathbf{5}), (\mathbf{4}, \mathbf{7.5})$

x_k	y_k	$z_k = \ln(y_k)$	x_k^2	$x_k z_k$
0	1.5	0.4035	0	0
1	2.5	0.9163	1	0.9163
2	3.5	1.2528	4	2.5056
3	5.0	1.6094	9	4.8282
4	7.5	2.0149	16	8.0596
-------------		-------------	-------------	-------------
$\sum_{k=1}^{N} x_k = 10$		$\sum_{k=1}^{N} z_k = 6.1989$	$\sum_{k=1}^{N} x_k^2 = 30$	$\sum_{k=1}^{N} x_k z_k = 16.3097$

Using the Least Square Line,

$$0 = A\sum_{k=1}^{N} x^2 + B\sum_{k=1}^{N} x_k - \sum_{k=1}^{N} x_k z_k$$

$$0 = A\sum_{k=1}^{N} x_k + BN - \sum_{k=1}^{N} z_k$$

Substituting

$$0 = A(30) + B(10) - 16.3097$$

$$0 = (A(10) + B(5) - 6.1989) - 2$$

End up getting,

$$A = 0.3912$$

$$B = 0.4574$$

$$z = Ax + B$$

Where $z = ln(y)$ and $B = ln(c)$

$$B = ln(c)$$

$$C = e\text{^}B = e^{0.4574} = 1.5799$$

So we have

$$y = ce^{Ax}$$

$y = 1.5799e\text{^}(0.3912x)$ minimizes the least squares error for the data above after transformation.

Using non-linear least squares method for $y = ce^{Ax}$, we get

$$y = 1.610899e^{(0.3835705x)}$$

Other substitutions

- $y = \frac{A}{X} + B$ ➔ $y = A\left(\frac{1}{x}\right) + B$
  $y = Az + B$ where z=1/x
- $y = cx^{A}$➔$\ln(y) = Aln(x) + \ln(c)$
  $w = Az + B$ where w=ln(y)
  where z=ln(x)
  where B=ln(c)