

Numerical Analysis

Lecture 09: Approximation Theory

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Approximation Theory

Introduction

Approximation theory involves two general types of problems.

- ① **Fitting functions to given data** and finding the "best" function in a certain class to represent the data.
- ② When a function is given explicitly, but we wish to **find a "simpler" type of function**, such as a polynomial, to approximate values of the given function.

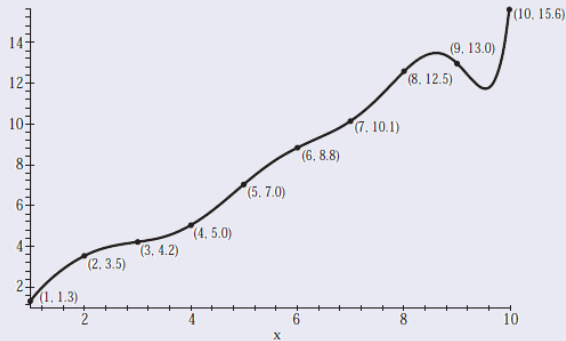
Outline

- 1 Discrete Least Squares Approximation
- 2 Orthogonal Polynomials and Least Squares Approximation
- 3 Rational Function Approximation

Discrete Least Squares Approximation

Example: Curve Fitting with Noise

x_i	y_i	x_i	y_i
1	1.3	6	8.8
2	3.5	7	10.1
3	4.2	8	12.5
4	5.0	9	13.0
5	7.0	10	15.6



Discrete Least Squares Approximation

Example: Curve Fitting with Noise

Assume that the model is $y = a_1x + a_0$, we need to determine a_0 and a_1 based on the observations.

- Minimax problem

$$E_{\infty}(a_0, a_1) = \max_{1 \leq i \leq 10} \{|y_i - (a_1x_i + a_0)|\}$$

- Absolute deviation

$$E_1(a_0, a_1) = \sum_{i=1}^{10} |y_i - (a_1x_i + a_0)|$$

- Linear Least Squares

$$E_2(a_0, a_1) = \sum_{i=1}^{10} [y_i - (a_1x_i + a_0)]^2$$

Linear Least Squares

Linear Least Squares Problem

The general problem of fitting the best least squares line to a collection of data $\{(x_i, y_i)\}_{i=1}^m$ involves minimizing the total error

$$E \equiv E_2(a_0, a_1) = \sum_{i=1}^m [y_i - (a_1 x_i + a_0)]^2$$

with respect to the parameters a_0 and a_1 .

Linear Least Squares

Linear Least Squares Problem

$$\{a_0^*, a_1^*\} = \operatorname{argmin}_{a_0, a_1} \sum_{i=1}^m [y_i - (a_1 x_i + a_0)]^2$$

Solution: (1/3)

$$\frac{\partial E}{\partial a_0} = 0, \quad \text{and} \quad \frac{\partial E}{\partial a_1} = 0$$

That is

$$0 = \frac{\partial}{\partial a_0} \sum_{i=1}^m [y_i - (a_1 x_i + a_0)]^2 = 2 \sum_{i=1}^m (y_i - (a_1 x_i + a_0))(-1)$$

$$0 = \frac{\partial}{\partial a_1} \sum_{i=1}^m [y_i - (a_1 x_i + a_0)]^2 = 2 \sum_{i=1}^m (y_i - (a_1 x_i + a_0))(-x_i)$$

Linear Least Squares

Linear Least Squares Problem

$$\{a_0^*, a_1^*\} = \operatorname{argmin}_{a_0, a_1} \sum_{i=1}^m [y_i - (a_1 x_i + a_0)]^2$$

Solution: (2/3)

These equations simplify to the **normal equations**:

$$a_0 m + a_1 \sum_{i=1}^m x_i = \sum_{i=1}^m y_i$$

and

$$a_0 \sum_{i=1}^m x_i + a_1 \sum_{i=1}^m x_i^2 = \sum_{i=1}^m x_i y_i$$

Linear Least Squares

Solution: (3/3)

The solution to this system of equation is

$$a_0 = \frac{\sum_{i=1}^m x_i^2 \sum_{i=1}^m y_i - \sum_{i=1}^m x_i y_i \sum_{i=1}^m x_i}{m \left(\sum_{i=1}^m x_i^2 \right) - \left(\sum_{i=1}^m x_i \right)^2}$$

and

$$a_1 = \frac{m \sum_{i=1}^m x_i y_i - \sum_{i=1}^m x_i \sum_{i=1}^m y_i}{m \left(\sum_{i=1}^m x_i^2 \right) - \left(\sum_{i=1}^m x_i \right)^2}$$

Linear Least Squares

Linear Least Squares Problem

$$\{a_0^*, a_1^*\} = \operatorname{argmin}_{a_0, a_1} \sum_{i=1}^m [y_i - (a_1 x_i + a_0)]^2$$

$$\mathbf{a}^* = \operatorname{argmin}_{\mathbf{a}} \|\mathbf{y} - \mathbf{X}\mathbf{a}\|_2^2$$

$$0 = -\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{a})$$

Normal equation:

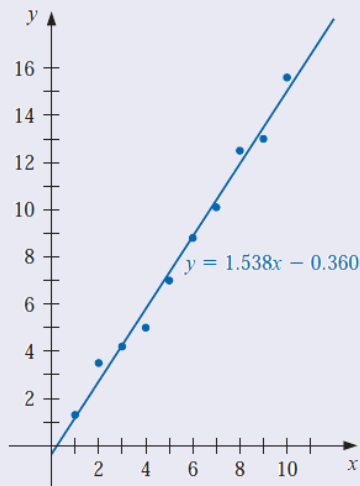
$$\mathbf{X}^T \mathbf{X} \mathbf{a} = \mathbf{X}^T \mathbf{y}$$

$$\Rightarrow \mathbf{a} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Linear Least Squares

Example: Curve Fitting with Noise

x_i	y_i	x_i	y_i
1	1.3	6	8.8
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5	7.0	10	15.6



Polynomial Least Squares

Polynomial Least Squares Problem

The general problem of approximating a set of data, $\{(x_i, y_i)\}_{i=1}^m$, with an algebraic polynomial

$$P_n(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0,$$

of degree $n < m - 1$. The constants a_0, a_1, \cdots, a_n are determined by minimizing the least squares error

$$E = \sum_{i=1}^m (y_i - P_n(x_i))^2$$

Polynomial Least Squares

Polynomial Least Squares Problem

$$\{a_i^*\}_{i=0}^n = \operatorname{argmin}_{\{a_i\}_{i=0}^n} \sum_{i=1}^m (y_i - P_n(x_i))^2$$

Polynomial Least Squares

Polynomial Least Squares Problem

$$\{a_i^*\}_{i=0}^n = \operatorname{argmin}_{\{a_i\}_{i=0}^n} \sum_{i=1}^m (y_i - P_n(x_i))^2$$

$$\begin{aligned} E &= \sum_{i=1}^m (y_i - P_n(x_i))^2 \\ &= \sum_{i=1}^m y_i^2 - 2 \sum_{i=1}^m P_n(x_i) y_i + \sum_{i=1}^m (P_n(x_i))^2 \\ &= \sum_{i=1}^m y_i^2 - 2 \sum_{i=1}^m \left(\sum_{j=0}^n a_j x_i^j \right) y_i + \sum_{i=1}^m \left(\sum_{j=0}^n a_j x_i^j \right)^2 \\ &= \sum_{i=1}^m y_i^2 - 2 \sum_{j=0}^n a_j \left(\sum_{i=1}^m y_i x_i^j \right) + \sum_{j=0}^n \sum_{k=0}^n a_j a_k \left(\sum_{i=1}^m x_i^{j+k} \right) \end{aligned}$$

Polynomial Least Squares

$$\Rightarrow 0 = \frac{\partial E}{\partial a_j} = -2 \sum_{i=1}^m y_i x_i^j + 2 \sum_{k=0}^n a_k \sum_{i=1}^m x_i^{j+k}.$$

This gives $n + 1$ normal equations in the $n + 1$ unknowns a_j .

$$\sum_{k=0}^n a_k \sum_{i=1}^m x_i^{j+k} = \sum_{i=1}^m y_i x_i^j, \text{ for each } j = 0, 1, \dots, n.$$

It is helpful to write the equations as follows:

$$\begin{aligned} a_0 \sum_{i=1}^m x_i^0 + a_1 \sum_{i=1}^m x_i^1 + \dots + a_n \sum_{i=1}^m x_i^n &= \sum_{i=1}^m y_i x_i^0, \\ a_0 \sum_{i=1}^m x_i^1 + a_1 \sum_{i=1}^m x_i^2 + \dots + a_n \sum_{i=1}^m x_i^{n+1} &= \sum_{i=1}^m y_i x_i^1 \end{aligned}$$

Polynomial Least Squares

Example: Nonlinear Curve Fitting with Noise

Fit the data in the following table with the discrete least squares polynomial of degree at most 2.

i	x_i	y_i
1	0	1.0000
2	0.25	1.2840
3	0.50	1.6487
4	0.75	2.1170
5	1.00	2.7183

Polynomial Least Squares

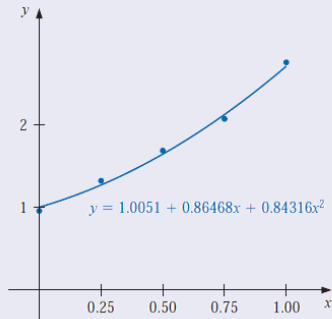
Example2: Nonlinear Curve Fitting with Noise

For this problem, $n = 2$, $m = 5$, and the three normal equations are:

$$5a_0 + 2.5a_1 + 1.875a_2 = 8.7680,$$

$$2.5a_0 + 1.875a_1 + 1.5625a_2 = 5.4514,$$

$$1.875a_0 + 1.5625a_1 + 1.3828a_2 = 4.4015.$$



Outline

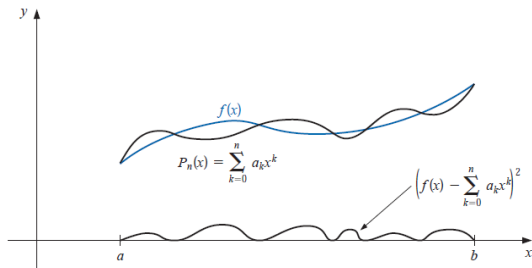
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Approximation of Functions

Approximation of Functions

Suppose $f \in C[a, b]$ and that a polynomial $P_n(x)$ of degree at most n is required that will minimize the error

$$E = \int_a^b [f(x) - P_n(x)]^2 dx = \int_a^b \left(f(x) - \sum_{k=0}^n a_k x^k \right)^2 dx$$



Approximation of Functions

Approximation of Functions

Since

$$E = \int_a^b [f(x)]^2 dx - 2 \sum_{k=0}^n a_k \int_a^b x^k f(x) dx + \int_a^b \left(\sum_{k=0}^n a_k x^k \right)^2 dx,$$

we have

$$\frac{\partial E}{\partial a_j} = -2 \int_a^b x^j f(x) dx + 2 \sum_{k=0}^n a_k \int_a^b x^{j+k} dx.$$

Hence, to find $P_n(x)$, the $(n+1)$ linear **normal equations**

$$\sum_{k=0}^n a_k \int_a^b x^{j+k} dx = \int_a^b x^j f(x) dx, \text{ for each } j = 0, 1, \dots, n.$$

must be solved for the $(n+1)$ unknowns a_j . The normal equations always have a **unique** solution provided that $f \in C[a, b]$.

Approximation of Functions

Example: Approximation of Functions

Find the least squares approximating polynomial of degree 2 for the function $f(x) = \sin \pi x$ on the interval $[0, 1]$.

Approximation of Functions

Example: Approximation of Functions

Find the least squares approximating polynomial of degree 2 for the function $f(x) = \sin\pi x$ on the interval $[0, 1]$.

Solution:(1/2)

The normal equations for $P_2(x) = a_2x^2 + a_1x + a_0$ are

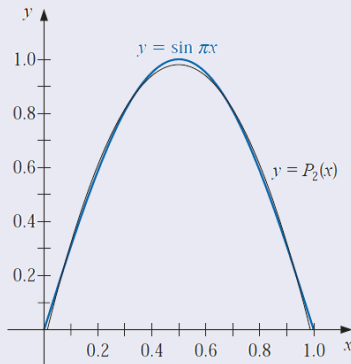
$$\begin{aligned}a_0 \int_0^1 1dx + a_1 \int_0^1 xdx + a_2 \int_0^1 x^2dx &= \int_0^1 \sin\pi xdx, \\a_0 \int_0^1 xdx + a_1 \int_0^1 x^2dx + a_2 \int_0^1 x^3dx &= \int_0^1 x\sin\pi xdx, \\a_0 \int_0^1 x^2dx + a_1 \int_0^1 x^3dx + a_2 \int_0^1 x^4dx &= \int_0^1 x^2\sin\pi xdx.\end{aligned}$$

Approximation of Functions

Solution:(2/2)

Consequently, the least squares polynomial approximation of degree 2 for $f(x) = \sin \pi x$ on $[0, 1]$ is

$$P_2(x) = -4.12251x^2 + 4.12251x - 0.050465.$$



Approximation of Functions

Disadvantages

- ① The coefficients a_0, a_1, \dots, a_n in the linear system are of the form

$$\int_a^b x^{j+k} dx = \frac{b^{j+k+1} - a^{j+k+1}}{j+k+1},$$

a linear system that does not have an easily computed numerical solution.

- ② The calculations that were performed in obtaining the best n th-degree polynomial, $P_n(x)$, do not lessen the amount of work required to obtain $P_{n+1}(x)$.

Linearly Independent Functions

Motivation

Computationally efficient, and once $P_n(x)$ is known, it is easy to determine $P_{n+1}(x)$.

Linearly Independent Functions

Definition: Linearly Independent

The set of functions $\{\phi_0, \dots, \phi_n\}$ is said to be **linearly independent** on $[a, b]$ if, whenever

$$c_0\phi_0(x) + c_1\phi_1(x) + \dots + c_n\phi_n(x) = 0, \quad \text{for all } x \in [a, b],$$

we have $c_0 = c_1 = \dots = c_n = 0$. Otherwise the set of functions is said to be **linearly dependent**.

Linearly Independent Functions

Theorem

Suppose that, for each $j = 0, 1, \dots, n$, $\phi_j(x)$ is a polynomial of degree j . Then $\{\phi_0, \dots, \phi_n\}$ is linearly independent on any interval $[a, b]$.

Proof (1/2)

Let c_0, \dots, c_n be real numbers for which

$$P(x) = c_0\phi_0(x) + c_1\phi_1(x) + \dots + c_n\phi_n(x) = 0, \quad \text{for all } x \in [a, b].$$

- The polynomial $P(x)$ vanishes on $[a, b]$, so it must be the zero polynomial, and the coefficients of all the powers of x are zero.
- In particular, the coefficient of x^n is zero. But $c_n\phi^n(x)$ is the only term in $P(x)$ that contains x_n , so we must have $c_n = 0$.

Linearly Independent Functions

Proof (2/2)

Hence

$$P(x) = \sum_{j=0}^{n-1} c_j \phi_j(x).$$

In this representation of $P(x)$, the only term that contains a power of x^{n-1} is $c_{n-1}\phi_{n-1}(x)$, so this term must also be zero and

$$P(x) = \sum_{j=0}^{n-2} c_j \phi_j(x).$$

In like manner, the remaining constants $c_{n-2}, c_{n-3}, \dots, c_1, c_0$ are all zero, which implies that $\{\phi_0, \phi_1, \dots, \phi_n\}$ is linearly independent on $[a, b]$.

Linearly Independent Functions

Theorem

Suppose that $\{\phi_0(x), \phi_1(x), \dots, \phi_n(x)\}$ is a collection of linearly independent polynomials in Π_n . Then any polynomial in Π_n can be written uniquely as a linear combination of $\phi_0(x), \phi_1(x), \dots, \phi_n(x)$.

Orthogonal Functions

Definition: Weight function

An integrable function w is called a **weight function** on the interval I if $w(x) \geq 0$, for all x in I , but $w(x) \neq 0$ on any subinterval of I .

Example

$$w(x) = \frac{1}{\sqrt{1-x^2}}$$

Orthogonal Functions

Definition: Orthogonal Set of Functions

$\{\phi_0(x), \phi_1(x), \dots, \phi_n(x)\}$ is said to be an **orthogonal set of functions** for the interval $[a, b]$ with respect to the weight function w if

$$\int_a^b w(x) \phi_k(x) \phi_j(x) dx = \begin{cases} 0, & \text{when } j \neq k, \\ \alpha_j > 0, & \text{when } j = k. \end{cases}$$

If, in addition, $\alpha_j = 1$ for each $j = 0, 1, \dots, n$, the set is said to be **orthonormal**.

Orthogonal Functions

Theorem

If $\{\phi_0(x), \phi_1(x), \dots, \phi_n(x)\}$ is an orthogonal set of functions on an interval $[a, b]$ with respect to the weight function w , then the least squares approximation to f on $[a, b]$ with respect to the weight function w is

$$P(x) = \sum_{j=0}^n a_j \phi_j(x),$$

where, for each $j = 0, 1, \dots, n$,

$$a_j = \frac{\int_a^b w(x) \phi_j(x) f(x) dx}{\int_a^b w(x) [\phi_j(x)]^2 dx} = \frac{1}{\alpha_j} \int_a^b w(x) \phi_j(x) f(x) dx$$

Orthogonal Functions

Proof

$$E = E(a_0, \dots, a_n) = \int_a^b w(x) \left[f(x) - \sum_{k=0}^n a_k \phi_k(x) \right]^2 dx.$$

$$0 = \frac{\partial E}{\partial a_j} = 2 \int_a^b w(x) \left[f(x) - \sum_{k=0}^n a_k \phi_k(x) \right] \phi_j(x) dx.$$

$$\int_a^b w(x) f(x) \phi_j(x) dx = \sum_{k=0}^n a_k \int_a^b w(x) \phi_k(x) \phi_j(x) dx = a_j \alpha_j.$$

Orthogonal Functions

Theorem: Gram-Schmidt Process

The set of polynomial functions $\{\phi_0(x), \phi_1(x), \dots, \phi_n(x)\}$ defined in the following way is orthogonal on $[a, b]$ with respect to the weight function w .

$$\phi_0(x) \equiv 1, \quad \phi_1(x) = x - B_1, \quad \text{for each } x \text{ in } [a, b],$$

where

$$B_1 = \frac{\int_a^b xw(x)[\phi_0(x)]^2 dx}{\int_a^b w(x)[\phi_0(x)]^2 dx},$$

and when $k \geq 2$,

$$\phi_k(x) = (x - B_k)\phi_{k-1}(x) - C_k\phi_{k-2}(x), \quad \text{for each } x \text{ in } [a, b],$$

where

$$B_k = \frac{\int_a^b xw(x)[\phi_{k-1}(x)]^2 dx}{\int_a^b w(x)[\phi_{k-1}(x)]^2 dx}, \quad \text{and} \quad C_k = \frac{\int_a^b xw(x)\phi_{k-1}(x)\phi_{k-2}(x) dx}{\int_a^b w(x)[\phi_{k-2}(x)]^2 dx}.$$

Orthogonal Functions

Corollary

For any $n > 0$, the set of polynomial functions $\{\phi_0, \dots, \phi_n\}$ constructed in the Gram-Schmidt process is linearly independent on $[a, b]$ and

$$\int_a^b w(x) \phi_n(x) Q_k(x) dx = 0,$$

for any polynomial $Q_k(x)$ of degree $k < n$.

Orthogonal Functions

Proof:

- For each $k = 0, 1, \dots, n$, $\phi_k(x)$ is a polynomial of degree k , which implies that $\{\phi_0(x), \dots, \phi_n(x)\}$ is a linearly independent set.
- Let $Q_k(x)$ be a polynomial of degree $k < n$. There exist numbers c_0, \dots, c_k such that

$$Q_k(x) = \sum_{j=0}^k c_j \phi_j(x).$$

Because ϕ_n is orthogonal to ϕ_j for each $j = 0, 1, \dots, k$, we have

$$\int_a^b w(x) Q_k(x) \phi_n(x) dx = \sum_{j=0}^k c_j \int_a^b w(x) \phi_j(x) \phi_n(x) dx = \sum_{j=0}^k c_j \cdot 0 = 0.$$

Orthogonal Functions

Legendre Polynomials

The set of **Legendre polynomials**, $\{P_n(x)\}$, is orthogonal on $[-1, 1]$ with respect to the weight function $w(x) \equiv 1$.

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = x^2 - \frac{1}{3}$$

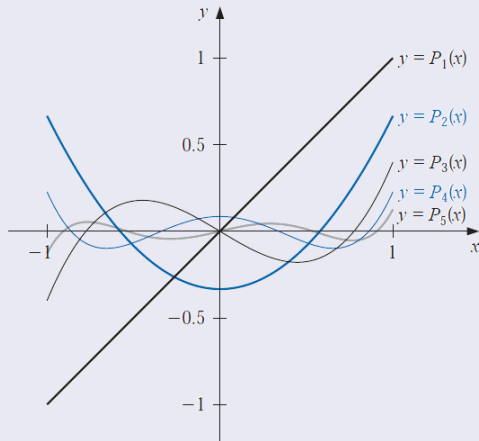
$$P_3(x) = x^3 - \frac{3}{5}x$$

$$P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}$$

$$P_5(x) = x^5 - \frac{10}{9}x^3 + \frac{5}{21}x$$

Orthogonal Functions

Example: Legendre Polynomials



Advantages of Polynomials Approximation

- There are a sufficient number of polynomials to approximate any continuous function on a closed interval to within an arbitrary tolerance;
- Polynomials are easily evaluated at arbitrary values;
- The derivatives and integrals of polynomials exist and are easily determined.

Disadvantages

- Oscillation. This often causes error bounds in polynomial approximation to significantly exceed the average approximation error.

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- 1 Discrete Least Squares Approximation
- 2 Orthogonal Polynomials and Least Squares Approximation
- 3 Rational Function Approximation**

Rational Function Approximation

Definition

A **rational function** r of degree N has the form

$$r(x) = \frac{p(x)}{q(x)},$$

where $p(x)$ and $q(x)$ are polynomials whose degrees sum to N .

Every polynomial is a rational function, so approximation by rational functions gives results that are no worse than approximation by polynomials.

Rational Function Approximation

Pade Approximation

Suppose r is a rational function of degree $N = n + m$ of the form

$$r(x) = \frac{p(x)}{q(x)} = \frac{p_0 + p_1x + \cdots + p_nx^n}{q_0 + q_1x + \cdots + q_mx^m},$$

that is used to approximate a function f on a closed interval I containing zero.

- The **Pade approximation technique** is the extension of Taylor polynomial approximation to rational functions.
- It chooses the $N + 1$ parameters $q_1, q_2, \cdots, q_m, p_0, p_1, \cdots, p_n$ so that $f^{(k)}(0) = r^{(k)}(0)$, for each $k = 0, 1, \cdots, N$.
- When $n = N$ and $m = 0$, the Pade approximation is simply the N th **Maclaurin polynomial**.

Rational Function Approximation

The Pade Approximation Technique

- Consider the difference

$$f(x) - r(x) = f(x) - \frac{p(x)}{q(x)} = \frac{f(x)q(x) - p(x)}{q(x)} = \frac{f(x) \sum_{i=0}^m q_i x^i - \sum_{i=0}^n p_i x^i}{q(x)},$$

and suppose f has the Maclaurin series expansion $f(x) = \sum_{i=0}^{\infty} a_i x^i$. Then

$$f(x) - r(x) = \frac{\sum_{i=0}^{\infty} a_i x^i \sum_{i=0}^m q_i x^i - \sum_{i=0}^n p_i x^i}{q(x)},$$

- The object is to choose the constants q_1, q_2, \dots, q_m and p_0, p_1, \dots, p_n so that

$$f^{(k)}(0) - r^{(k)}(0) = 0, \text{ for each } k = 0, 1, \dots, N.$$

Rational Function Approximation

The Pade Approximation Technique

We choose q_1, q_2, \dots, q_m and p_0, p_1, \dots, p_n so that the numerator

$$(a_0 + a_1x + \dots)(1 + q_1x + \dots + q_mx^m) - (p_0 + p_1x + \dots + p_nx^n),$$

has no terms of degree less than or equal to N .

Then, we can express the coefficient of x^k more compactly as

$$\left(\sum_{i=0}^k a_i q_{k-i} \right) - p_k.$$

The rational function for Pade approximation results from the solution of the $N + 1$ linear equations

$$\left(\sum_{i=0}^k a_i q_{k-i} \right) = p_k, \quad k = 0, 1, \dots, N$$

in the $N + 1$ unknowns $q_1, q_2, \dots, q_m, p_0, p_1, \dots, p_n$.

Rational Function Approximation

Example:

The Maclaurin series expansion for e^{-x} is

$$\sum_{i=0}^{\infty} \frac{(-1)^i}{i!} x^i.$$

Find the Pade approximation to e^{-x} of degree 5 with $n = 3$ and $m = 2$.

Rational Function Approximation

Solution: (1/2)

To find the Pade approximation we need to choose p_0, p_1, p_2, p_3, q_1 , and q_2 so that the coefficients of x^k for $k = 0, 1, \dots, 5$ are 0 in the expression

$$\left(1 - x + \frac{x^2}{2} - \frac{x^3}{6} + \dots\right) (1 + q_1x + q_2x^2) - (p_0 + p_1x + p_2x^2 + p_3x^3)$$

Expanding and collecting terms produces

$$\begin{aligned}x^5 : -\frac{1}{120} + \frac{1}{24}q_1 - \frac{1}{6}q_2 &= 0; & x^2 : \frac{1}{2} - q_1 + q_2 &= p_2; \\x^4 : \frac{1}{24} - \frac{1}{6}q_1 + \frac{1}{2}q_2 &= 0; & x^1 : -1 + q_1 &= p_1; \\x^3 : -\frac{1}{6} + \frac{1}{2}q_1 - q_2 &= p_3; & x^0 : 1 &= p_0.\end{aligned}$$

Rational Function Approximation

Solution: (2/2)

This gives

$$\left\{ p_0 = 1, p_1 = -\frac{3}{5}, p_2 = \frac{3}{20}, p_3 = -\frac{1}{60}, q_1 = \frac{2}{5}, q_2 = \frac{1}{20} \right\}$$

So the Pade approximation is

$$r(x) = \frac{1 - \frac{3}{5}x + \frac{3}{20}x^2 - \frac{1}{60}x^3}{1 + \frac{2}{5}x + \frac{1}{20}x^2}.$$

Assignment

- Reading Assignment: Chap 8.1, 8.2, 8.4