Chapter 3: Approximation Theory

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Summer 2015 / Numerical Analysis
Overview

Discrete Least Squares Approximation

Orthogonal Polynomials

Rational Function Approximation

Fast Fourier Transforms
$l_p$-norms and Error functions

The $l_p$ norm of an $n$-vector $\vec{v}$ is

$$||\vec{v}||_p = \left( \sum_{k=1}^{n} |v_k|^p \right)^{1/p}.$$ 

Let $S = \{(x_k, y_k)\}_{k=1}^{n}$ be a set of discrete data points derived from an unknown function $f$ and let $g$ be a function with parameters $\{a_j\}_{j=1}^{m}$. We say that $g$ approximates $f$ (or the data set) with $l_p$ error of

$$E_p(a_1, a_2, \ldots, a_m) = \sum_{k=1}^{n} |y_k - g(x_k)|^p.$$
Example 1

Suppose the approximating function is 
\[ g(x) = a_1 e^{a_2 x} + a_3. \]
Then the \( l_1 \) error would be

\[
E_1(a_1, a_2, a_3) = \sum_{k=1}^{n} |y_k - (a_1 e^{a_2 x_k} + a_3)|.
\]

Finding the best fit parameters in an absolute sense would require minimizing the \( l_\infty \) error:

\[
E_\infty(a_1, a_2, a_3) = \max_{1 \leq k \leq n} \{|y_k - (a_1 e^{a_2 x_k} + a_3)|\}.
\]

Both of these error functions lead to difficult minimization problems.
Square Error

The Euclidean or **Square error** function,

\[ E \equiv E_2(a_1, \ldots, a_m) = \sum_{k=1}^{n} (y_k - g(x_k))^2, \]

is the commonly used error function because of it’s convenient minimization properties and the following:

**Theorem 2**

*(From Analysis)* For all \( p, q \in \mathbb{Z}^+ \cup \{\infty\} \) and all \( n \in \mathbb{Z}^+ \), there exist \( m, M \in \mathbb{R}^+ \) such that for all \( \vec{v} \in \mathbb{R}^n \),

\[ m\|\vec{v}\|_p \leq \|\vec{v}\|_q \leq M\|\vec{v}\|_p. \]
Suppose that \( \{ \phi_j \}_{j=1}^m \) are a set of “basis” functions and \( g(x) = a_1 \phi_1(x) + a_2 \phi_2(x) + \ldots + a_m \phi_m(x) \). Then \( g \) approximates a data set \( S \) with square error given above. To minimize this error we solve the system

\[
\frac{\partial E}{\partial a_j} = 0, \ 1 \leq j \leq m
\]

of linear equations.

**Example 3**

Straight-line, linear least-squares approximation uses \( g(x) = a_1 x + a_2 \) as the approximating function.
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Function Norms

Suppose $f \in C[a, b]$, then the $L_p$ norm of $f$ is given by

$$
||f||_p = \left( \int_a^b |f(x)|^p \, dx \right)^{1/p}.
$$

Suppose $g$ is an approximating function for $f$. Then the $L_p$ error between $f$ and $g$ is

$$
E_p = \int_a^b |f(x) - g(x)|^p \, dx
$$

where $g$ (and then $E_p$) may depend on parameters $a_1, a_2, ..., a_m$. 
Square Error for Functions

As with the discrete case, the common error that is used for functions is the \textbf{square error}, when \( p = 2 \).

**Example 4**
Suppose \( g \) is an \( m^{th} \) degree polynomial. Then the square error is

\[
E \equiv E_2(a_0, \ldots, a_m) = \int_a^b \left( f(x) - \sum_{k=0}^{m} a_k x^k \right)^2 \, dx.
\]

To minimize this error over the parameter space we solve the linear system of \textbf{normal equations}:

\[
\frac{\partial E}{\partial a_k} = 0, \quad k = 0, 1, \ldots, m.
\]
The above system of normal equations leads to:

\[
\begin{bmatrix}
1 & \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{m+1} \\
\frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \cdots & \frac{1}{m+2} \\
\frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \cdots & \frac{1}{m+3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{1}{m+1} & \frac{1}{m+2} & \frac{1}{m+3} & \cdots & \frac{1}{2m+1}
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
a_2 \\
\vdots \\
a_m
\end{bmatrix}
= 
\begin{bmatrix}
\int_a^b f(x) \, dx \\
\int_a^b xf(x) \, dx \\
\int_a^b x^2 f(x) \, dx \\
\vdots \\
\int_a^b x^m f(x) \, dx
\end{bmatrix}
\]

The coefficient matrix is called a Hilbert matrix, which is a classic example for demonstrating round-off error difficulties.
Linear Independence of Functions

Definition 5
A set of functions \( \{ f_1, f_2, \ldots, f_n \} \) is said to be **linearly independent** on \([a, b]\) if

\[
a_1 f_1(x) + a_2 f_2(x) + \cdots + a_n f_n(x) = 0, \quad \forall x \in [a, b]
\]

\[\Leftrightarrow a_1 = a_2 = \cdots = a_n = 0.\]

Otherwise the set of functions is **linearly dependent**.

Example 6
Is \( \{1, x, x^2\} \) linearly independent? How about \( \{1, \cos(2x), \cos^2(x)\} \)?
Definition 7
Let \( f, g \in C[a, b] \). The \( L_2 \) inner product of \( f \) and \( g \) is given by

\[
\langle f, g \rangle = \int_{a}^{b} f(x)g(x) \, dx.
\]

Note that the \( L_2 \) norm of \( f \) is then \( \|f\|_2 = \sqrt{\langle f, f \rangle} \).

Definition 8
Two functions \( f \) and \( g \), both in \( C[a, b] \), are said to be orthogonal if \( \langle f, g \rangle = 0 \).
Weighted Inner Products

**Definition 9**
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 \( I \).

The purpose of a weight function is to assign more importance to approximations on certain portions of the interval.

**Definition 10**
For \( f \) and \( g \) in \( C[a, b] \) and \( w \) a weight function on \( [a, b] \),

\[
\langle f, g \rangle_w = \int_a^b w(x)f(x)g(x) \, dx
\]

is a weighted inner product.
Weighted Errors

The error function associated with a weighted inner product is

\[ E(a_0, \ldots, a_m) = \int_a^b w(x) (f(x) - g(x))^2 \, dx \]

where the approximating function \( g \) depends on the parameters \( a_k \).

**Example 11**

Suppose \( \{\phi_0, \phi_1, \ldots, \phi_m\} \) is a set of linearly independent functions on \([a, b]\) and \( w \) is a weight function for \([a, b]\). Given \( f \in C[a, b] \), we want to find the best fit approximation

\[ g(x) = \sum_{k=0}^{m} a_k \phi_k(x). \]
Example Continued

That is, we wish to minimize the above error. This leads to a system of normal equations of the form

$$\langle f, \phi_j \rangle_w = \sum_{k=0}^{m} a_k \langle \phi_k, \phi_j \rangle_w.$$ 

If we can choose the functions in \( \{ \phi_0, \phi_1, \ldots \phi_m \} \) to be pairwise orthogonal (with respect to the weight \( w \)), then the minimizing parameters would be given by

$$a_k = \frac{\langle f, \phi_k \rangle_w}{\langle \phi_k, \phi_k \rangle_w}.$$
Example 12

Show that \( \{1, \sin(kx), \cos(kx)\}_{k=1}^{m} \) form an orthogonal set of functions with respect to \( w(x) \equiv 1 \) on \([-\pi, \pi]\).

Example 13

Find an orthogonal set of polynomials that span the space of third degree polynomials with respect to \( w(x) \equiv 1 \) on \([-1, 1]\). This uses a **Gram-Schmidt process**. These polynomials are the first four **Legendre Polynomials**.
Homework

Homework assignment 5, due: TBA
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Why?

Polynomials are good in that:

- Any continuous function can be approximated on a closed interval to within an arbitrary tolerance.
- Polynomials are easy to evaluate at arbitrary values.
- The derivatives and integrals of polynomials exist and are easy to determine.

Polynomials do tend to oscillate dramatically. So in discrete approximations, the approximating polynomial may have small $l_2$ error even though the $L_2$ error between the polynomial and the underlying function is large. Polynomials do not do well with discontinuities, especially singularities.
Rational Functions

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

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

where

$$p(x) = p_0 + p_1 x + ... + p_n x^n$$

and

$$q(x) = q_0 + q_1 x + ... + q_m x^m$$

with $n + m = N$.

Rational functions often do a better job of approximating functions (with the same effort) as polynomials, and can include discontinuities. Note that, without loss of generality, we may set $q_0 = 1$. 

This is an extension of Taylor polynomials to rational functions. It chooses parameters so that $f^{(k)}(0) = r^{(k)}(0)$ for $k = 0, 1, ..., N$. When $n = N$ and $m = 0$, the Padé approximation is simply the $N^{th}$ degree Maclaurin polynomial.

Suppose $f(x)$ has a Maclaurin expansion: $f(x) = \sum a_ix^i$. Then

$$f(x) - r(x) = \frac{f(x)q(x) - p(x)}{q(x)} = \sum_{i=0}^{\infty} a_ix^i \frac{m}{\sum_{i=0}^{n} q_i x^i} - \sum_{i=0}^{n} p_i x^i \frac{n}{q(x)}.$$
Minding the p’s and q’s

The objective is to find the constants $p_i$ and $q_i$ so that

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

This means $f - r$ has a root of multiplicity $N + 1$ at $x = 0$. That is, the numerator of $f(x) - r(x)$ has no non-zero terms of degree less than $N + 1$. So,

$$\sum_{i=0}^{k} a_i q_{k-i} - p_k = 0$$

where we set $p_i = 0$ for $i = n + 1, n + 2, \ldots, N$ and $q_i = 0$ for $i = m + 1, m + 2, \ldots N$. 
Example 14

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

**Solution:** expand the following and collect terms, setting coefficients of $x^j$ to zero for $j = 0, 1, ..., 5$.

\[
\left(1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} + \ldots\right) \left(1 + q_1 x + q_2 x^2\right)
\]
\[
- \left(p_0 + p_1 x + p_2 x^2 + p_3 x^3\right).
\]

To get $p_0 = 1$, $p_1 = -\frac{3}{5}$, $p_2 = \frac{3}{20}$, $p_3 = -\frac{1}{60}$, $q_1 = \frac{2}{5}$, and $q_2 = \frac{1}{20}$.
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Euler’s Formula

\[ e^{ix} = 1 + (ix) + \frac{(ix)^2}{2!} + \frac{(ix)^3}{3!} + \frac{(ix)^4}{4!} + \frac{(ix)^5}{5!} + \ldots \]

\[ = \left( 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \ldots \right) + i \left( x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots \right) \]

\[ = \cos(x) + i \sin(x), \]

where \( i = \sqrt{-1} \). So we can write

\[ a_k \cos(kx) + b_k \sin(kx) = c_k e^{kx}, \]

where \( a_k \) and \( b_k \) are real, and \( c_k \) is complex.
Trigonometric Polynomials

Given $2m$, evenly spaced, data points $\{x_j, y_j\}$ from a function $f$, we can transform the data in a linear way so that it is assumed that $x_j = -\pi + (j/m)\pi$ for $j = 0, 1, 2, ..., 2m - 1$. Then we can find $a_k$ and $b_k$ so that

$$S_m(x) = \frac{a_0 + a_m \cos(mx)}{2} + \sum_{k=1}^{m-1} (a_k \cos(kx) + b_k \sin(kx))$$

interpolates the transformed data. That is, when

$$a_k = \frac{1}{m} \sum_{j=0}^{2m-1} y_j \cos(kx_j) \quad \text{and} \quad b_k = \frac{1}{m} \sum_{j=0}^{2m-1} y_j \sin(kx),$$

the $l_2$ error between $S_m(x)$ and the data is zero.
Using Symmetry

Euler’s formula gives us \( S_m(x) = \frac{1}{m} \sum_{k=0}^{2m-1} c_k e^{ikx} \) where \( c_k = \sum_{k=0}^{2m-1} y_j e^{ik\pi j/m} \). From this we have \( a_k + ib_k = \frac{(-1)^k}{m} c_k \).

Suppose \( m = 2^p \) for some positive integer \( p \), then for \( k = 0, 1, 2, \ldots, m - 1 \), we have

\[
c_k + c_{m+k} = \sum_{j=0}^{2m-1} y_j e^{ik\pi j/m} (1 + e^{ij\pi}).
\]

But \( 1 + e^{ij\pi} = 2 \) if \( j \) is even and zero if \( j \) is odd, so there are only \( m \) nonzero terms in the sum and we can write

\[
c_k + c_{m+k} = 2 \sum_{l=0}^{m-1} y_{2l} e^{ik\pi (2l)/m} = 2 \sum_{l=0}^{m-1} y_{2l} e^{ik\pi l/(m/2)}.
\]
Similarly,

\[ c_k - c_{m+k} = 2e^{ik\pi/m} \sum_{l=0}^{m-1} y_{2l+1} e^{ik\pi l/(m/2)}. \]

Note that these two relationships allow us to calculate all of the \( c_k \)'s but the sums now require \( 2m^2 + m \) complex multiplications instead of \( (2m)^2 \) multiplications calculating the coefficients directly.

These sums have the same form as the sum for calculating the \( c_k \)'s directly except we replace \( m \) with \( m/2 \). Thus, we can repeat the process (another \( p - 1 \) times) to further reduce the number of complex multiplications to \( 3m + m\log_2(m) = O(m\log_2(m)) \). If \( m = 1024 \), that is about 13,300 complex multiplications instead of about 4,200,000 using the direct method.
Example 15

Play with Matlab to investigate FFT using functions like $\sin(nx)$ and $\cos(nx)$ for various values of $n \in \mathbb{Z}^+$. Then try $f_1(x) = 1 - x^2$ and $f_2(x) = x^3$ on $[-1, 1]$.
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Dr. White

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