Function approximation: Fourier, Chebyshev, Lagrange

- Orthogonal functions
- Fourier Series
- Discrete Fourier Series
- Fourier Transform: properties
- Chebyshev polynomials
- Convolution
- DFT and FFT

**Scope:** Understanding where the Fourier Transform comes from. Moving from the continuous to the discrete world. The concepts are the basis for pseudospectral methods and the spectral element approach.
The Problem

we are trying to approximate a function \( f(x) \) by another function \( g_N(x) \) which consists of a sum over \( N \) orthogonal functions \( \Phi(x) \) weighted by some coefficients \( a_n \).

\[
f(x) \approx g_N(x) = \sum_{i=0}^{N} a_i \Phi_i(x)
\]
... and we are looking for optimal functions in a least squares (l2) sense ...

\[ \| f(x) - g_N(x) \|_2 = \left[ \int_a^b \left( f(x) - g_N(x) \right)^2 \, dx \right]^{1/2} = \text{Min!} \]

... a good choice for the basis functions \( \Phi(x) \) are orthogonal functions. 

What are orthogonal functions? Two functions \( f \) and \( g \) are said to be orthogonal in the interval \([a,b]\) if

\[ \int_a^b f(x)g(x) \, dx = 0 \]

How is this related to the more conceivable concept of orthogonal vectors? Let us look at the original definition of integrals:
Orthogonal Functions

\[ \int_{a}^{b} f(x)g(x)\,dx = \lim_{N \to \infty} \sum_{i=1}^{N} f_i(x)g_i(x)\Delta x \]

... where \( x_0 = a \) and \( x_N = b \), and \( x_i - x_{i-1} = \Delta x \) ...

If we interpret \( f(x_i) \) and \( g(x_i) \) as the \( i \)th components of an \( N \) component vector, then this sum corresponds directly to a scalar product of vectors. The vanishing of the scalar product is the condition for orthogonality of vectors (or functions).

\[ f_i \cdot g_i = \sum_{i} f_i g_i = 0 \]
Let us assume we have a piecewise continuous function of the form

\[ f(x + 2\pi) = f(x) \]

... we want to approximate this function with a linear combination of \(2\pi\) periodic functions:

\[ 1, \cos(x), \sin(x), \cos(2x), \sin(2x), \ldots, \cos(nx), \sin(nx) \]

\[ \Rightarrow f(x) \approx g_N(x) = \frac{1}{2} a_0 + \sum_{k=1}^{N} \left\{ a_k \cos(kx) + b_k \sin(kx) \right\} \]
... are these functions orthogonal?

\[
\int_{-\pi}^{\pi} \cos(jx) \cos(kx) \, dx = \begin{cases} 
0 & j \neq k \\
2\pi & j = k = 0 \\
\pi & j = k > 0 
\end{cases}
\]

\[
\int_{-\pi}^{\pi} \sin(jx) \sin(kx) \, dx = \begin{cases} 
0 & j \neq k, j, k > 0 \\
\pi & j = k > 0 
\end{cases}
\]

\[
\int_{-\pi}^{\pi} \cos(jx) \sin(kx) \, dx = 0 \quad j \geq 0, k > 0
\]

... YES, and these relations are valid for any interval of length \(2\pi\).

Now we know that this is an orthogonal basis, but how can we obtain the coefficients for the basis functions?

from minimising \(f(x) - g(x)\)
optimal functions $g(x)$ are given if
\[
\left\| g_n(x) - f(x) \right\|_2 = \text{Min} ! \quad \text{or} \quad \frac{\partial}{\partial a_k} \left\{ \left\| g_n(x) - f(x) \right\|_2 \right\} = 0
\]

... with the definition of $g(x)$ we get ...

\[
\frac{\partial}{\partial a_k} \left\| g_n(x) - f(x) \right\|_2^2 = \frac{\partial}{\partial a_k} \left[ \int_{-\pi}^{\pi} \left( \frac{1}{2} a_0 + \sum_{k=1}^{N} \{ a_k \cos(kx) + b_k \sin(kx) \} - f(x) \right)^2 \, dx \right]
\]

leading to

\[
g_N(x) = \frac{1}{2} a_0 + \sum_{k=1}^{N} \{ a_k \cos(kx) + b_k \sin(kx) \} \quad \text{with}
\]

\[
a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(kx) \, dx, \quad k = 0,1,\ldots, N
\]

\[
b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(kx) \, dx, \quad k = 1,2,\ldots, N
\]
Orthogonal functions

Fourier approximation of \(|x|\)

\[ f(x) = |x|, \quad -\pi \leq x \leq \pi \]

leads to the Fourier Series

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

.. and for \(n<4\) \(g(x)\) looks like

![Graph comparing the original function and its Fourier approximation]
... another Example ...

\[ f(x) = x^2, \quad 0 < x < 2\pi \]

leads to the Fourier Serie

\[
g_N(x) = \frac{4\pi^2}{3} + \sum_{k=1}^{N} \left\{ \frac{4}{k^2} \cos( kx ) - \frac{4\pi}{k} \sin( kx ) \right\}
\]

.. and for \( N < 11 \), \( g(x) \) looks like
Fourier - discrete functions

... what happens if we know our function $f(x)$ only at the points

$$x_i = \frac{2\pi}{N} i$$

it turns out that in this \textit{particular} case the coefficients are given by

$$a_k^* = \frac{2}{N} \sum_{j=1}^{N} f(x_j) \cos(kx_j), \quad k = 0,1,2,...$$

$$b_k^* = \frac{2}{N} \sum_{j=1}^{N} f(x_j) \sin(kx_j), \quad k = 1,2,3,...$$

.. the so-defined Fourier polynomial is the unique interpolating function to the function $f(x_j)$ with $N=2m$

$$g_m^*(x) = \frac{1}{2} a_0^* + \sum_{k=1}^{m-1} \left\{ a_k^* \cos(kx) + b_k^* \sin(kx) \right\} + \frac{1}{2} a_m^* \cos(kx)$$
Orthogonal functions

... with the important property that ...

\[ g^*_m(x_i) = f(x_i) \]

... in our previous examples ...

\[ f(x) = |x| \Rightarrow f(x) - \text{blue} ; \ g(x) - \text{red}; \ x_i - '+' \]
Fourier series - convergence

\[ f(x) = x^2 \Rightarrow f(x) \text{ - blue}; \ g(x) \text{ - red}; \ x_i \text{ - ‘+’} \]
Fourier series - convergence

\[ f(x) = x^2 \Rightarrow f(x) \text{ - blue; } g(x) \text{ - red; } x_i \text{ - +} \]
Gibb’s phenomenon

\[ f(x) = x^2 \Rightarrow f(x) \text{ - blue; } g(x) \text{ - red; } x_i \text{ - ‘+’} \]

The overshoot for equi-spaced Fourier interpolations is \( \approx 14\% \) of the step height.
We have seen that Fourier series are excellent for interpolating (and differentiating) periodic functions defined on a regularly spaced grid. In many circumstances physical phenomena which are not periodic (in space) and occur in a limited area. This quest leads to the use of **Chebyshev polynomials**.

We depart by observing that \( \cos(n\varphi) \) can be expressed by a polynomial in \( \cos(\varphi) \):

\[
\begin{align*}
\cos(2\varphi) &= 2\cos^2\varphi - 1 \\
\cos(3\varphi) &= 4\cos^3\varphi - 3\cos\varphi \\
\cos(4\varphi) &= 8\cos^4\varphi - 8\cos^2\varphi + 1
\end{align*}
\]

... which leads us to the definition:
cos(n \varphi) = T_n(\cos(\varphi)) = T_n(x), \quad x = \cos(\varphi), \quad x \in [-1,1], \quad n \in \mathbb{N}

... for the Chebyshev polynomials $T_n(x)$. Note that because of $x=\cos(\varphi)$ they are defined in the interval $[-1,1]$ (which - however - can be extended to $\mathbb{R}$). The first polynomials are

\[
T_0(x) = 1 \\
T_1(x) = x \\
T_2(x) = 2x^2 - 1 \\
T_3(x) = 4x^3 - 3x \\
T_4(x) = 8x^4 - 8x^2 + 1
\]

where

\[
|T_n(x)| \leq 1 \quad \text{for} \quad x \in [-1,1] \quad \text{and} \quad n \in \mathbb{N}_0
\]
The first ten polynomials look like $[0, -1]$

The $n$-th polynomial has extrema with values 1 or -1 at

$$x_k^{(ext)} = \cos\left( \frac{k\pi}{n} \right), \quad k = 0, 1, 2, 3, ..., n$$
These extrema are not equidistant (like the Fourier extrema)

\[ x_k^{(ext)} = \cos\left( \frac{k\pi}{n} \right), \quad k = 0, 1, 2, 3, \ldots, n \]
... are the Chebyshev polynomials orthogonal?

Chebyshev polynomials are an orthogonal set of functions in the interval \([-1,1]\) with respect to the weight function \(1/\sqrt{1-x^2}\) such that

\[
\int_{-1}^{1} T_k(x) T_j(x) \frac{dx}{\sqrt{1-x^2}} = \begin{cases} 
0 & \text{for } k \neq j \\
\pi/2 & \text{for } k = j > 0 \\
\pi & \text{for } k = j = 0
\end{cases}, \quad k, j \in \mathbb{N}_0
\]

... this can be easily verified noting that

\[x = \cos \varphi, \quad dx = -\sin \varphi d\varphi\]

\[T_k(x) = \cos(k\varphi), \quad T_j(x) = \cos(j\varphi)\]
... we are now faced with the same problem as with the Fourier series. We want to approximate a function $f(x)$, this time not a periodical function but a function which is defined between $[-1,1]$. We are looking for $g_n(x)$

$$f(x) \approx g_n(x) = \frac{1}{2} c_0 T_0(x) + \sum_{k=1}^{n} c_k T_k(x)$$

... and we are faced with the problem, how we can determine the coefficients $c_k$. Again we obtain this by finding the extremum (minimum)

$$\frac{\partial}{\partial c_k} \left[ \int_{-1}^{1} \left\{ g_n(x) - f(x) \right\}^2 \frac{dx}{\sqrt{1-x^2}} \right] = 0$$
... to obtain ...

\[ c_k = \frac{2}{\pi} \int_{-1}^{1} f(x) T_k(x) \frac{dx}{\sqrt{1 - x^2}}, \quad k = 0, 1, 2, \ldots, n \]

... surprisingly these coefficients can be calculated with FFT techniques, noting that

\[ c_k = \frac{2}{\pi} \int_{0}^{\pi} f(\cos \varphi) \cos k\varphi d\varphi, \quad k = 0, 1, 2, \ldots, n \]

... and the fact that \( f(\cos \varphi) \) is a \( 2\pi \)-periodic function ...

\[ c_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(\cos \varphi) \cos k\varphi d\varphi, \quad k = 0, 1, 2, \ldots, n \]

... which means that the coefficients \( c_k \) are the Fourier coefficients \( a_k \) of the periodic function \( F(\varphi) = f(\cos \varphi) \)!
what happens if we know our function $f(x)$ only at the points

$$x_i = \cos \frac{\pi}{N} i$$

in this particular case the coefficients are given by

$$c_k^* = \frac{2}{N} \sum_{j=1}^{N} f(\cos \varphi_j) \cos(k \varphi_j), \quad k = 0,1,2,\ldots N/2$$

... leading to the polynomial ...

$$g_m^*(x) = \frac{1}{2} c_0^* T_0 + \sum_{k=1}^{m} c_k^* T_k(x)$$

... with the property

$$g_m^*(x) = f(x) \quad \text{at} \quad x_j = \cos(\frac{\pi j}{N}) \quad j = 0,1,2,\ldots, N$$
Chebyshev - collocation points - $|x|$

$f(x) = |x| \Rightarrow f(x) - \text{blue}; g_n(x) - \text{red}; x_i - '+'$

8 points

16 points

Orthogonal functions
Orthogonal functions

Chebyshev - collocation points - $|x|$

\[ f(x) = |x| \Rightarrow f(x) \text{ - blue}; g_n(x) \text{ - red}; x_i \text{ - ‘+’} \]

32 points

128 points
Orthogonal functions

Chebyshev - collocation points - $x^2$

$f(x) = x^2 \Rightarrow f(x) - \text{blue}; g_n(x) - \text{red}; x_i - '+'$

8 points

N = 8

64 points

N = 64

The interpolating function $g_n(x)$ was shifted by a small amount to be visible at all!
Chebyshev vs. Fourier - numerical

This graph speaks for itself! Gibb’s phenomenon with Chebyshev?
Orthogonal functions

Chebyshev vs. Fourier - Gibb’s

\[ f(x) = \text{sign}(x - \pi) \Rightarrow f(x) - \text{blue}; \ g_N(x) - \text{red}; \ x_i - '+' \]

Gibb’s phenomenon with Chebyshev? YES!
Chebyshev vs. Fourier - Gibb’s

Chebyshev

Fourier

\[ f(x) = \text{sign}(x - \pi) \Rightarrow f(x) - \text{blue} ; g_N(x) - \text{red} ; x_i - \text{‘+’} \]
Fourier vs. Chebyshev

**Fourier**

\[ x_i = \frac{2\pi}{N} i \]

periodic functions

\[ \cos(nx), \sin(nx) \]

\[ g_m^*(x) = \frac{1}{2} a_0^* \]
\[ + \sum_{k=1}^{m-1} \left\{ a_k^* \cos(kx) + b_k^* \sin(kx) \right\} \]
\[ + \frac{1}{2} a_m^* \cos(kx) \]

**Chebyshev**

\[ x_i = \cos \frac{\pi}{N} i \]

limited area [-1,1]

\[ T_n(x) = \cos(n\varphi), \]
\[ x = \cos \varphi \]

\[ g_m^*(x) = \frac{1}{2} c_0^* T_0 + \sum_{k=1}^{m} c_k^* T_k(x) \]
Orthogonal functions

Fourier vs. Chebyshev (cont’d)

### Fourier

\[
a^*_k = \frac{2}{N} \sum_{j=1}^{N} f(x_j) \cos(kx_j)
\]

\[
b^*_k = \frac{2}{N} \sum_{j=1}^{N} f(x_j) \sin(kx_j)
\]

- Gibb’s phenomenon for discontinuous functions
- Efficient calculation via FFT
- Infinite domain through periodicity

### Chebyshev

\[
c^*_k = \frac{2}{N} \sum_{j=1}^{N} f(\cos\varphi_j) \cos(k\varphi_j)
\]

- Limited area calculations
- Grid densification at boundaries
  - Coefficients via FFT
  - Excellent convergence at boundaries
  - Gibb’s phenomenon
The Fourier Transform Pair

\[ F(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) e^{i\omega t} \, dt \]

\[ f(t) = \int_{-\infty}^{\infty} F(\omega) e^{-i\omega t} \, d\omega \]

Forward transform

Inverse transform

Note the conventions concerning the sign of the exponents and the factor.
Some properties of the Fourier Transform

Defining as the FT:

\[ f(t) \Rightarrow F(\omega) \]

- **Linearity**

\[ af_1(t) + bf_2(t) \Rightarrow aF_1(\omega) + bF_2(\omega) \]

- **Symmetry**

\[ f(-t) \Rightarrow 2\pi F(-\omega) \]

- **Time shifting**

\[ f(t + \Delta t) \Rightarrow e^{i\omega\Delta t} F(\omega) \]

- **Time differentiation**

\[ \frac{\partial^n f(t)}{\partial t^n} \Rightarrow (-i\omega)^n F(\omega) \]
Differentiation theorem

- Time differentiation
  \[ \frac{\partial^n f(t)}{\partial t^n} \Rightarrow (-i\omega)^n F(\omega) \]

\[ \exp(-\pi t^2) \]

\[ \exp(-\pi w^2) \]

\[ \frac{d}{dt}(\exp(-\pi t^2)) \]

\[ i2\pi w \exp(-\pi w^2) \]
The **convolution** operation is at the heart of **linear systems**.

**Definition:**

\[
f(t) \ast g(t) = \int_{-\infty}^{\infty} f(t')g(t-t')dt' = \int_{-\infty}^{\infty} f(t-t')g(t')dt'
\]

**Properties:**

\[
f(t) \ast g(t) = g(t) \ast f(t)
\]

\[
f(t) \ast \delta(t) = f(t)
\]

\[
f(t) \ast H(t) = \int_{-\infty}^{t} f(t)dt
\]

H(t) is the Heaviside function:
A convolution in the time domain corresponds to a multiplication in the frequency domain.

… and vice versa …

A convolution in the frequency domain corresponds to a multiplication in the time domain

\[ f(t) \ast g(t) \Rightarrow F(\omega)G(\omega) \]

\[ f(t)g(t) \Rightarrow F(\omega) \ast G(\omega) \]

The first relation is of tremendous practical implication!
The Fourier Transform can be derived from the problem of approximating an arbitrary function.

A regular set of points allows exact interpolation (or derivation) of arbitrary functions.

There are other basis functions (e.g., Chebyshev polynomials, Legendre polynomials) with similar properties.

These properties are the basis for the success of the spectral element method.