PY4C01 - Numerical Methods II

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January 16, 2012

Notes

Useful information

Books:

- "A first course in computational physics", Paul deVries
- "Computational Physics", Nicholas J. Giordano and Hisao Nakanishi
- "Partial Differential Equations - AN Introduction", Walter A. Strauss
- "Numerical recipes in C++, 3rd ed.", William H. Press et al. .The "bible" of numerical methods. Very good reference book.

Lecture Notes and Problem Sets:

`http://www.tcd.ie/Physics/People/Matthias.Moebius/teaching/`

Notes

Fourier Analysis and its applications

Fourier analysis originated from the study of heat conduction: Jean Baptiste Joseph Fourier (1768-1830)
Fourier analysis enables a function (signal) to be decomposed into its frequency components.
Wide range of applications:

- Spectrum analysis
- Digital filtering (e.g. electronics, image processing), Deconvolution
- Audio compression (MP3 etc.)
- Solving differential equations

Notes

Definition of Fourier series

Consider a periodic function $f(t)$ with period $T = 2\pi$ such that

$$f(t + 2\pi) = f(t), \tag{1}$$

Any periodic function can be expressed as an infinite Fourier series of *sin* and *cos* functions with frequencies that are integer multiples of $\omega = 2\pi/T = 1$, the frequency of the function:

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos(nt) + b_n \sin(nt) \right), \tag{2}$$

where $a_0, a_1, \ldots b_1, \ldots, b_n$ are the Fourier coefficients.

Notes

Convergence

Theorem

Dirichlet's theorem If $f(t)$ is periodic of period 2π, if for $-\pi < t < \pi$ the function $f(t)$ has a finite number of maximum and minimum values and a finite number of discontinuities, and if $\int_{-\pi}^{\pi} f(t)dt$ is finite, then the Fourier series converges to $f(t)$ at all points where $f(t)$ is continuous, and at discontinuities it converges to the arithmetic mean of the right-hand and left-hand limits of the function.

For all practical purposes, these conditions hold and the series converges.

Notes

Fourier series as an expansion of orthogonal functions

The Fourier series can be viewed as an expansion of orthogonal functions that form a complete set over any 2π interval:

$$\int_{-\pi}^{\pi} \sin(mt)\sin(nt)dt = \begin{cases} \pi\delta_{m,n} & \text{if } m \neq 0 \\ 0 & \text{if } m = 0 \end{cases} \quad (3)$$

$$\int_{-\pi}^{\pi} \cos(mt)\cos(nt)dt = \begin{cases} \pi\delta_{m,n} & \text{if } m \neq 0 \\ 2\pi & \text{if } m = n = 0 \end{cases} \quad (4)$$

$$\int_{-\pi}^{\pi} \sin(mt)\cos(nt)dt = 0 \text{ all integral } m \text{ and } n \quad (5)$$

From these orthogonality relations we can derive the Fourier coefficients a_n and b_n

Notes

Fourier coefficients

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(t)\cos(nt)dt \quad (6)$$

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(t)\sin(nt)dt \quad (7)$$

You can prove this by substituting the Fourier series for $f(t)$ (eqn. (2)) in to the above relations and use the orthogonality equations (eqns. (3,4,5).

Notes

Example - the square wave

Consider the unit step function (i.e square wave):

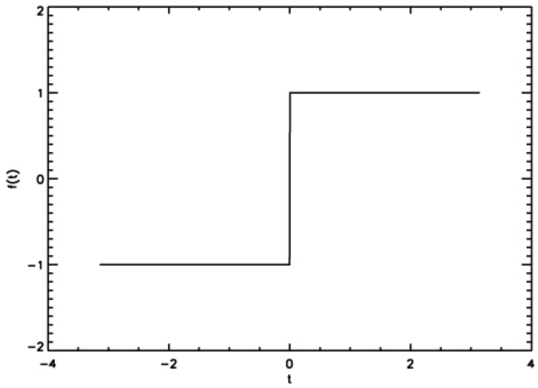
$$f(t) = \begin{cases} -1 & \text{for } -\pi < t < 0 \\ +1 & \text{for } 0 < t < \pi \end{cases} \quad (8)$$

Since the function is odd, all a_n's are zero. The b_n's are given by

$$\begin{aligned} b_n &= \frac{1}{\pi}\int_{-\pi}^{0}(-1)\sin(nt)dt + \frac{1}{\pi}\int_{0}^{\pi}(+1)\sin(nt)dt \\ &= \frac{2}{\pi}\int_{0}^{\pi}\sin(nt)dt = \frac{2}{n\pi}[-\cos(nt)]_0^{\pi} \\ &= \frac{2}{n\pi}[1-\cos(n\pi)] \\ &= \begin{cases} 0, & n = 2,4,6,\ldots \\ 4/n\pi, & n = 1,3,5,\ldots \end{cases} \end{aligned}$$

Notes

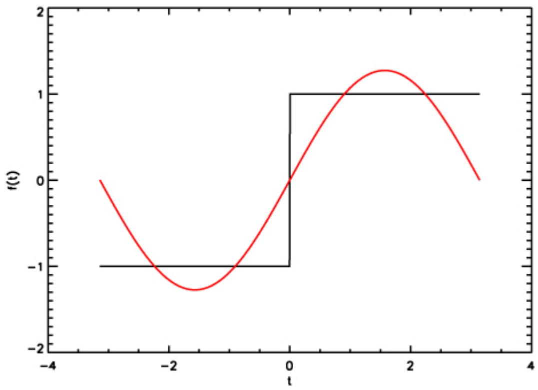
Fourier series of square wave



Notes

Fourier Analysis | The Fourier series
The Fourier transform

Fourier series of square wave: N=1



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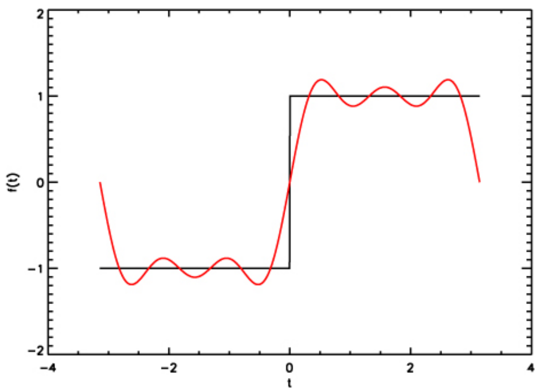
Notes

Fourier Analysis | The Fourier series
The Fourier transform

Fourier series of square wave: N=5



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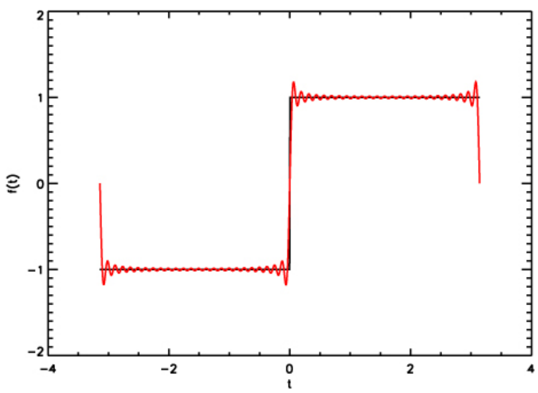
Notes

Fourier Analysis | The Fourier series
The Fourier transform

Fourier series of square wave: N=50



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Notes

Remarks

- The amplitude of the high frequency sine waves falls of $1/n$. Therefore convergence is slow.
- In general: For discontinuous functions, like the square wave, the coefficients decrease as $1/n$. For continuous functions with discontinuous slopes (e.g. full wave rectifier), coefficients typically decrease as $1/n^2$.
- Overshoot at discontinuities is called "Gibbs phenomenon".
- In electronics, square wave pulses are common. If apparatus does not pass the high frequencies, square wave will be rounded off.

Notes

Fourier series of complex functions

Definition of Fourier series can easily be extended to complex functions. Using the identity $e^{ix} = \cos(x) + i\sin(x)$ we can rewrite Fourier series (eqn.(2)) as

$$f(t) = \sum_{n=-\infty}^{\infty} c_n e^{int}, \tag{9}$$

where

$$c_n = \begin{cases} (a_n - ib_n)/2, & n > 0, \\ a_0/2 & n = 0, \\ (a_{|n|} + ib_{|n|})/2 & n < 0 \end{cases} \tag{10}$$

which can be obtained by integration

$$c_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(t)e^{-int}dt \tag{11}$$

Notes

Fourier series of functions with arbitrary period

So far, considered functions periodic on a 2π interval. Can easily extend to functions with any period T:

Consider a periodic function $f(t)$ with period T, and corresponding angular frequency $\omega = 2\pi/T$.
Let $t \to \omega t = 2\pi t/T$. Then the complex Fourier series (eqn. (9)) becomes

$$f(t) = \sum_{n=-\infty}^{\infty} c_n e^{in\omega t}, \tag{12}$$

where,

$$c_n = \frac{1}{T}\int_{-T/2}^{T/2} f(t)e^{-in\omega t}dt \tag{13}$$

Notes

Fourier series of functions with arbitrary period

Similarly for the Fourier series of real functions (eqn. (2)) becomes:

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty}\left(a_n\cos(n\omega t) + b_n\sin(n\omega t)\right), \tag{14}$$

where,

$$a_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t)\cos(n\omega t)dt \tag{15}$$

$$b_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t)\sin(n\omega t)dt \tag{16}$$

Function is expressed as a series of *sin* and *cos* functions with frequencies that are integer multiples of ω, the frequency of the function.

Notes

Fourier series - summary

- Fourier series decomposes periodic signal into its frequency components.
- Even discontinuous functions or functions with discontinuous slopes (where Taylor expansion fails) can be expressed in a converging Fourier series.
- Solving differential equations. e.g. harmonic oscillator with some periodic driving force.

Notes

From Fourier series to Fourier transform

Concept of Fourier series can be expanded to **non-periodic** functions. Consider the Fourier series for functions with period T in complex representation:

$$f(t) = \sum_{n=-\infty}^{\infty} c_n e^{in\Delta\omega t}, \tag{17}$$

with

$$c_n = \frac{\Delta\omega}{2\pi}\int_{-T/2}^{T/2} f(t)e^{-in\Delta\omega t}dt, \tag{18}$$

where we have written $\omega = \Delta\omega$, since the discrete frequencies $n\omega$ are separated by $\Delta\omega = 2\pi/T$.

Notes

From Fourier series to Fourier transform

Now define

$$c_n = \frac{\Delta\omega}{\sqrt{2\pi}} g(n\Delta\omega), \tag{19}$$

so that

$$g(n\Delta\omega) = \frac{1}{\sqrt{2\pi}}\int_{-T/2}^{T/2} f(t)e^{-in\Delta\omega t}dt, \tag{20}$$

$$f(t) = \sum_{n=-\infty}^{\infty} \Delta\omega g(n\Delta\omega)e^{in\Delta\omega t}. \tag{21}$$

Take the limit as $T \to \infty$. Then, $n\Delta\omega$ becomes the **continuous** variable ω and the summation becomes an integral as $\Delta\omega = 2\pi/T \to d\omega$.

Notes

The Fourier transform

"time domain" $$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(\omega)e^{i\omega t}d\omega, \tag{22}$$

"frequency domain" $$g(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt \tag{23}$$

We define $g(\omega)$ to be the Fourier transform of $f(t)$:

Fourier transform $$\mathfrak{F}[f(t)] = g(\omega) \tag{24}$$

inverse transform $$\mathfrak{F}^{-1}[g(\omega)] = f(t) \tag{25}$$

Notes

Remarks:

- As with the Fourier series, the Fourier transform is used to obtain information on the frequency spectrum. However, $\mathfrak{F}[f(t)] = g(\omega)$ is complex in general, even if $f(t)$ is real. Fourier transform is often represented in terms of its magnitude and phase: $g(\omega) = |g(\omega)|e^{i\theta(\omega)}$, where $\theta = \tan^{-1}(Im(g(\omega)/Re(g(\omega)))$.
- Prefactor $(1/\sqrt{2\pi})$ of the transforms depends on convention. Here we chose them to be distributed symmetrically.
- Often, the Fourier transform is used to go from the time domain to the frequency domain. However, mathematically, the original transform could be considered the inverse and vice versa. Therefore, the sign in the exponential also depends on the convention.

Notes

The Dirac delta function

If Fourier transform are consistent, then inserting $f(t)$ into $g(\omega)$ should lead to an identity:

$$g(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\underbrace{\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(\omega')e^{i\omega' t}d\omega'\right)}_{f(t)} e^{-i\omega t}dt \quad (26)$$

$$= \int_{-\infty}^{\infty}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(\omega'-\omega)t}dt\right] g(\omega')d\omega' \quad (27)$$

The term in the square brackets $[\dots]$ has to be the Dirac delta function:

$$\delta(\omega'-\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(\omega'-\omega)t}dt \quad (28)$$

Notes

The Dirac delta function

Consider the same integral with finite limits:

$$\delta(\omega'-\omega)_\tau = \frac{1}{2\pi}\int_{-\tau}^{\tau} e^{i(\omega'-\omega)t}dt = \frac{\sin((\omega'-\omega)\tau)}{\pi(\omega'-\omega)}$$

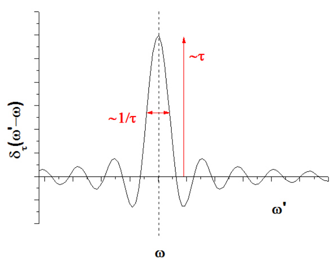
For $(\omega'-\omega) \approx 0$, the this can be approximated as

$$\frac{\sin((\omega'-\omega)\tau)}{\pi(\omega'-\omega)} \approx \frac{1}{\pi(\omega'-\omega)}\left[\tau(\omega'-\omega) - \frac{\tau^3(\omega'-\omega)^3}{3!} + \dots\right]$$

$$\approx \frac{\tau}{\pi} - \frac{\tau^3}{3!\pi}(\omega'-\omega)^2 + \dots$$

Notes

The Dirac delta function



The peak height is $\propto \tau$ and the width is $\propto 1/\tau$, therefore the area under the curve remains (approximately) constant.

Notes

The Dirac delta function

Eqns.(27) and (28) have to hold for any function $g(\omega)$. Set $g(\omega) = 1$:

$$1 = \int_{-\infty}^{\infty} \delta(\omega' - \omega) d\omega' \qquad (29)$$

However, according to eqn. (28), $\delta(0) = \infty$.

Delta function is a distribution, not a function, and has only a meaning inside an integrand!

Notes

Properties of the Fourier transform

Linearity: $\mathfrak{F}[f_1(t) + f_2(t)] = \mathfrak{F}[f_1(t)] + \mathfrak{F}[f_2(t)]$.

Shifting:

$$\begin{aligned}
\mathfrak{F}[f(t-t_0)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t-t_0) e^{-i\omega t} dt \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\tau) e^{-i\omega(\tau+t_0)} d\tau \\
&= e^{-i\omega t_0} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\tau) e^{-i\omega\tau} d\tau \\
&= e^{-i\omega t_0} g(\omega),
\end{aligned}$$

where $\tau = t - t_0$. Similarly, $\mathfrak{F}^{-1}[g(\omega - \omega_0)] = e^{i\omega_0 t} f(t)$

Notes

Properties of the Fourier transform

Scaling: Let $\mathfrak{F}[f(t)] = g(\omega)$ and $\alpha > 0$. Then,

$$\begin{aligned}
\mathfrak{F}[f(\alpha t)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(\alpha t) e^{-i\omega t} dt \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\alpha} \int_{-\infty}^{\infty} f(t') e^{-i\omega t'/\alpha} dt' \\
&= \frac{1}{\alpha} g(\omega/\alpha),
\end{aligned}$$

where substitution $t' = \alpha t$ was made. For $\alpha < 0$, we obtain

$$\mathfrak{F}[f(\alpha t)] = -\frac{1}{\alpha} g(\omega/\alpha)$$

Notes

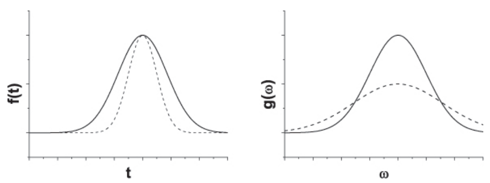
Properties of the Fourier transform

Therefore,

$$\mathfrak{F}[f(\alpha t)] = \frac{1}{|\alpha|} g(\omega/\alpha)$$

Similarly, $\mathfrak{F}^{-1}[g(\beta t)] = \frac{1}{|\beta|} f(t/\beta)$.

This is a crucial relation !. As function $f(t)$ becomes more localized, its Fourier transform becomes broader in frequency domain.



Notes

Parseval's theorem

Consider the integral $I = \int_{\infty}^{\infty} f_1(t)^* f_2(t) dt$. Substitute Fourier transforms of $f_1(t)$ and $f_2(t)$:

$$\begin{aligned}
I &= \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g_1(\omega) e^{i\omega t} d\omega\right]^* \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g_2(\omega') e^{i\omega' t} d\omega'\right] dt \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g_1^*(\omega) g_2(\omega') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega'-\omega)t} dt\right] d\omega d\omega' \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g_1^*(\omega) g_2(\omega') \delta(\omega' - \omega) d\omega d\omega' \\
&= \int_{-\infty}^{\infty} g_1^*(\omega) g_2(\omega) d\omega
\end{aligned}$$

For $f_1(t) = f_2(t)$, we obtain Parseval's theorem:

$$\int_{-\infty}^{\infty} \underbrace{|f(t)|^2}_{\text{Power}} dt = \int_{-\infty}^{\infty} \underbrace{|g(\omega)|^2}_{\text{Power spectrum}} d\omega \tag{30}$$

Notes

Higher dimensions

So far considered 1D Fourier transform. Generalization to higher dimensions as follows:

2D:

$$\mathfrak{F}[f(x,y)] = g(k_x, k_y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y) e^{-i(k_x x + k_y y)} dx dy$$

3D:

$$\begin{aligned}
\mathfrak{F}[f(x,y,z)] &= g(k_x, k_y, k_z) \\
&= \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y,z) e^{-i(k_x x + k_y y + k_z z)} dx dy dz \\
&= g(\vec{k}) = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int_{-\infty}^{\infty} f(\vec{r}) e^{-i\vec{k}\vec{r}} d\vec{r}
\end{aligned}$$

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