Kramers–Kronig transformation

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I. Introduction

Python package to compute Kramers-Kronig relations through a triangular linear sum. If you want to copy and modify my code, feel free to do so.

I will update the method using FFT (Fast Fourier Transform) to speed up my API and add other functions later. If you have recommendations about this, please contact me via the email below.

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Kramers-Kronig 관계를 삼각형 선형결합을 통해 계산하는 Python 패키지입니다. 코드를 수정하고 싶다면 자유롭게 하셔도 됩니다.

FFT (고속 푸리에 변환)를 사용하여 메소드를 업데이트하고 API를 더 빠르게 만들고, 다른 기능도 추가할 예정입니다. 개선하였으면 좋을 것 같은 점이 있다면 아래 이메일로 연락해 주십시오.

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II. Theory

1. Kramers–Kronig relation

If it is said that $f(x) = f_1(x) + if_2(x)$ $(f_1(x), f_2(x) \in \mathbb{R})$, then two relations, f1 and f2, satisfy the following two relationships. These relationships are referred to as the Kramers–Kronig relation.

$$f_1(x) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{f_2(x')}{x'-x}dx' \qquad \text{(Equations 1)}$$

$$f_2(x) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{f_1(x')}{x'-x}dx' \qquad \text{(Equations 2)}$$

If this function is symmetric at x=0 (where f1 is an even function and f2 is an odd function), it satisfies the following relationship. This equation is commonly used in physical situations due to the property of integrating from 0. For example, this can be observed in cases like optical coefficients.

$$f_1(x) = \frac{2}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{x'f_2(x')}{x'-x}dx' \qquad \text{(Equations 3)}$$

$$f_2(x) = \frac{2x}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{f_1(x')}{x'-x}dx' \qquad \text{(Equations 4)}$$

2. Triangular transformation method

Most data obtained through measurements is discrete. To extract the imaginary or real parts from discrete data using the Kramers-Kronig relation, the following method is required.

The function is linear, so it can be represented as the sum of a triangular function, where the height corresponds to the y-values as shown in Figure 1, and the base is formed by the overlapping values of the adjacent function. Therefore, by performing the Kramers-Kronig transformation on this triangular function and linearly adding them, the desired data can be obtained.

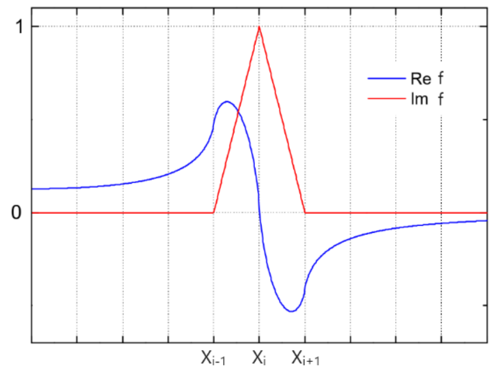

Figure. 1 Triangular method of k-k transformation

Let's set the height of the triangular function to 1. After the Kramers-Kronig transformation, multiplying by the height yields the desired function. The equation for the triangular function is as follows.

$$f^{\wedge}(x') = \begin{cases} (x' - x_{i-1})/(x_i - x_{i-1}) & , \quad x_{i-1} < x' < x_i \\ (x_{i+1} - x')/(x_{i+1} - x_i) & , \quad x_i < x' < x_{i+1} \\ 0 & , \quad otherwise \end{cases}$$

When applying equations 1 through 4 to transform the aforementioned triangular function, the result is as follows.

$$f_1(x) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{f_2{}^{\wedge}(x')}{x' - x} dx' \quad \Rightarrow \quad f_1{}^{\wedge}(x) = \frac{1}{\pi}\left[\frac{x - x_{i-1}}{x_i - x_{i-1}} ln\left|\frac{x_i - x}{x_{i-1} - x}\right| + \frac{x_{i+1} - x}{x_{i+1} - x_i} ln\left|\frac{x_{i+1} - x}{x_i - x}\right| + (x_{i+1} - x_{i-1})\right]$$

$$f_2(x) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{f_1{}^{\wedge}(x')}{x' - x} dx' \quad \Rightarrow \quad f_2{}^{\wedge}(x) = -\frac{1}{\pi}\left[\frac{x - x_{i-1}}{x_i - x_{i-1}} ln\left|\frac{x_i - x}{x_{i-1} - x}\right| + \frac{x_{i+1} - x}{x_{i+1} - x_i} ln\left|\frac{x_{i+1} - x}{x_i - x}\right| + (x_{i+1} - x_{i-1})\right]$$

$$f_1(x) = \frac{2}{\pi}\mathcal{P}\int_{0}^{\infty} \frac{x' f_2{}^{\wedge}(x')}{x'^2 - x^2} dx' \quad \Rightarrow \quad f_1{}^{\wedge}(x) = \frac{1}{\pi}\left[\frac{g(x_{i-1}, x)}{x_i - x_{i-1}} - \frac{x_{i+1} - x_{i-1}}{x_{i+1} - x_i}\frac{g(x_i, x)}{x_i - x_{i-1}} + \frac{g(x_{i+1}, x)}{x_{i+1} - x_i}\right]$$

$$f_2(x) = -\frac{2x}{\pi}\mathcal{P}\int_{0}^{\infty} \frac{f_1{}^{\wedge}(x')}{x'^2 - x^2} dx' \quad \Rightarrow \quad f_2{}^{\wedge}(x) = \frac{1}{\pi}\left[\frac{g(x, x_{i-1})}{x_{i-1} - x_i} - \frac{x_{i+1} - x_{i-1}}{x_{i+1} - x_i}\frac{g(x, x_i)}{x_i - x_{i-1}} + \frac{g(x, x_{i+1})}{x_i - x_{i+1}}\right]$$

$$* \, g(x, y) = (x + y)\ln|x + y| + (x - y)\ln|x - y|$$

3. Extrapolation

To obtain an accurate value, it is necessary to integrate from 0 to ∞, but the actual data available is limited to a finite range. Therefore, for the portions outside the range of the data, estimation through extrapolation is required to fill in the values. In most cases, extrapolation can be performed using the formula where the value tends to decrease as x approaches ∞ as x^{-1} and tends to decrease as x approaches 0 as x^2.

III. API

kk.image_to_real(list_x,list_y)

The function using Equation 1 transforms the imaginary part of the function into the real part.

$$f_1(x) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{f_2(x')}{x'-x}dx' \qquad \text{(Equation 1)}$$

list_x: X-axis data of the data to be transformed. Data format - list

list_y: Y-axis data of the data to be transformed. Data format - list

Result: Y-axis data of the real part. Data format - list

Note: The sizes of the two input lists must be the same. The x-axis of the resulting data matches the input x-axis data.

kk.real_to_image (list_x,list_y)

The function using Equation 2 transforms the real part of the function into the imaginary part.

$$f_2(x) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{f_1(x')}{x'-x}dx' \qquad \text{(Equation 2)}$$

list_x: X-axis data of the data to be transformed. Data format - list

list_y: Y-axis data of the data to be transformed. Data format - list

Result: Y-axis data of the imaginary part. Data format - list

Note: The sizes of the two input lists must be the same. The x-axis of the resulting data matches the input x-axis data.

kkphy.image_to_real (list_x,list_y)

The function using Equation 3 transforms the real part of the function into the imaginary part.

$$f_1(x) = \frac{2}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{x' f_2(x')}{x'-x}dx' \qquad \text{(Equation 3)}$$

list_x: X-axis data of the data to be transformed. Data format - list

list_y: Y-axis data of the data to be transformed. Data format - list

Result: Y-axis data of the real part. Data format - list

Note: The sizes of the two input lists must be the same. The x-axis of the resulting data matches the input x-axis data. Since the imaginary part of the function is an odd function, it converges to zero. Therefore, data converging to zero should be input at the origin.

kkphy.real_to_image (list_x,list_y,x0=1)

The function using Equation 4 transforms the real part of the function into the imaginary part.

$$f_2(x) = \frac{2x}{\pi}\mathcal{P}\int_0^\infty \frac{f_1(x')}{x'-x}dx' \qquad \text{(Equation 4)}$$

list_x: X-axis data of the data to be transformed. Data format - list

list_y: Y-axis data of the data to be transformed. Data format - list

x0: The origin value of the data must be provided separately. If not specified, it is extrapolated and calculated as 1.

Result: Y-axis data of the imaginary part. Data format - list

Note: The sizes of the two input lists must be the same. The x-axis of the resulting data matches the input x-axis data. The real part can converge to a non-zero value since it is an even function. Therefore, it is assumed to converge to a specific value and is calculated accordingly. If no data is provided, it is calculated as 1.

참고자료

[1] Alexey Kuzmenko, 'Guide to RefFIT' (2018)

[2] Tanner, D. B. "Use of x-ray scattering functions in Kramers-Kronig analysis of reflectance." Physical Review B 91.3 (2015): 035123.