Queens College, CUNY, Department of Computer Science

Numerical Methods

CSCI 361 / 761

Spring 2018

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due Friday, April 27, 2018, 11.59 pm

26 Homework lecture 26

- **As experience has demonstrated, if you do not understand the above expressions/questions, THEN ASK.**
- **If you do not understand the words/sentences in the lectures, THEN ASK.**
- **Send me an email, explain what you do not understand.**
- **Do not just keep quiet and produce nonsense in exams.**

26.1 General information

- We shall compute the Fourier transform of a function and the inverse transform numerically.
- This 'question' is to provide background information to set up the calculation.
- The definition of the Fourier transform of a function $f(x)$ is

$$F(k) = \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx\,. \tag{26.1.1}$$

- The inverse Fourier transform is given by

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk\,. \tag{26.1.2}$$

- However, eqs. (26.1.1) and (26.1.2) are not directly useful for numerical computation.
- **Explain why the integrals in eq. (26.1.1) and eq. (26.1.2) are improper integrals.**
- Therefore we must modify eqs. (26.1.1) and (26.1.2) to obtain proper integrals.
- Let $a > 0$ be a real positive constant.
- **We shall set $a = 1$ in this homework assignment.**
- Set $x_{\rm min} = -4a$ and $x_{\rm max} = 4a$.
- Set $k_{\rm min} = -6\pi/a$ and $k_{\rm max} = 6\pi/a$.
- Use $n = 1024$ subintervals for the numrical integration.
- Define the integration stepsizes $\Delta x = (x_{\rm max} - x_{\rm min})/n$ and $\Delta k = (k_{\rm max} - k_{\rm min})/n$.
- We shall consider only a real function $f(x)$. Suppose also that it is an even function $f(-x) = f(x)$. Now note that $\sin(kx)$ is an odd function of x. Hence the product $f(x)\sin(kx)$ is an odd function of x. Therefore its integral will cancel to zero over a symmetric interval $|x| \le 4a$.
- Hence we simplify eq. (26.1.1) to the following proper integral:

$$F(k) = \int_{x_{\rm min}}^{x_{\rm max}} f(x)\, \cos(kx)\, dx\,. \tag{26.1.3}$$

- The resulting function $F(k)$ will clearly be real. It is also even $F(-k) = F(k)$ because $\cos(kx)$ is an even function of k. Hence for the inverse transform, the product $F(k)\sin(kx)$ is an odd function of k. Therefore its integral will cancel to zero over a symmetric interval $|k| \le 6\pi/a$.
- Hence we simplify eq. (26.1.2) to the following proper integral:

$$f(x) = \frac{1}{2\pi} \int_{k_{\rm min}}^{k_{\rm max}} F(k)\, \cos(kx)\, dk\,. \tag{26.1.4}$$

- **Explain why the integrals in eqs. (26.1.3) and (26.1.4) are proper.**

  1. *Actually, if you have paid attention to the class material, you will realize they are* ***not*** *proper integrals, because we do not yet know what $f(x)$ and $F(k)$ are yet.*
  2. But I do not assign trick questions.
  3. We shall only consider well behaved functions so the integrals in eqs. (26.1.3) and (26.1.4) are proper.

- **Allocate arrays `double FT[...]` and `double IFT[...]` of lengths $\geq n+1$.**

- Use can also use `std::vector<double> FT(n+1,0.0)` and `std::vector<double> IFT(n+1,0.0)`.

- You will be supplied with an input function $f(x)$ in later questions in this assignment.

- Calculate the Fourier transform numerically as follows.

  1. Let $k_j = k_{\min} + j\Delta k$, for $j = 0, \ldots, n$. Note that these are $n+1$ values.
  2. **Use the trapezoid rule with n subintervals to compute the integral**

$$\mathrm{FT[j]} = \int_{x_{\min}}^{x_{\max}} f(x)\,\cos(k_j x)\,dx\,. \tag{26.1.5}$$

  3. **Note that you must calculate $n+1$ integrals, to obtain `FT[j]` for $j = 0, \ldots, n$.**
  4. **Each integral is a trapezoid rule calculation with n subintervals.**
  5. **Hence overall there are $O(n^2)$ computations.**

- **Hence we have an array `FT[j]` at $n+1$ points $k_j = k_{\min} + j\Delta k$, for $j = 0, \ldots, n$.**

- For the inverse transform, we perform a similar calculation, in reverse:

  1. Let $x_i = x_{\min} + i\Delta x$, for $i = 0, \ldots, n$. Note that these are $n+1$ values.
  2. **Use the trapezoid rule with n subintervals to compute the integral**

$$\mathrm{IFT[i]} = \int_{k_{\min}}^{k_{\max}} F(k)\,\cos(kx_i)\,dk\,. \tag{26.1.6}$$

  3. **For the trapezoid rule, the values of k are *exactly the points k_j listed above.***
  4. **Therefore the values of $F(k)$ *are exactly the numbers in the array* `FT[j]`.**
  5. That is why you must save the array `FT`.
  6. **Once again there are $n+1$ integrals, to obtain `IFT[i]` for $i = 0, \ldots, n$.**
  7. Hence again there are $O(n^2)$ computations.

- Hence we obtain an array `IFT[i]` at $n+1$ points $x_i = x_{\min} + i\Delta x$, for $i = 0, \ldots, n$.

- **Hence at the end we have two arrays `FT[j]` and `IFT[i]` both with $n+1$ elements.**

26.2 Triangle function

- Let $a > 0$ be a real positive constant.
- The **triangle function** is defined via

$$f_{\rm tri}(x) = \begin{cases} \dfrac{1}{2a}\Bigl(1 - \dfrac{|x|}{2a}\Bigr) & (|x| \le 2a) \\ 0 & (|x| > 2a)\,. \end{cases} \tag{26.2.1}$$

- The Fourier transform of the triangle function was derived in the lectures:

$$F_{\rm tri}(k) = \frac{\sin^2(ka)}{(ka)^2}\,. \tag{26.2.2}$$

- We shall compute the Fourier transform and inverse numerically.
- **Set $a = 1$ in this question.**
- Set $n = 1024$ for the numerical integration.
  1. **Compute the array `FT[j]` using eq. (26.1.5).**
  2. **Compute the array `IFT[j]` using eq. (26.1.6).**
- Plot some graphs to see how well the numerical values in the arrays match the known formulas.
  1. **Plot a graph of $f_{\rm tri}(x)$ and `IFT[i]` for $-4a \le x \le 4a$.**
  2. Recall that $x_i = x_{\rm min} + i\Delta x$ for $i = 0, \dots, n$ (totally $n+1$ points from $x_{\rm min}$ and $x_{\rm max}$).
  3. **Plot a graph of $F_{\rm tri}(k)$ and `FT[j]` for $-6 \le k/(\pi a) \le 6$.**
  4. Recall that $k_j = k_{\rm min} + j\Delta k$ for $j = 0, \dots, n$ (totally $n+1$ points from $k_{\rm min}$ and $k_{\rm max}$).
  5. To obtain nicer numbers on the horizontal axis, plot the value of $k/(\pi a)$, so the values go from -6 to 6.
- *If you have done your work correctly, you should obtain very good agreement in both graphs.*
  The value of `IFT[i]` *should agree very well with* $f_{\rm tri}(x)$.
  The value of `FT[j]` *should agree very well with* $F_{\rm tri}(k)$.

26.3 Window function

- Let $a > 0$ be a real positive constant.
- The **window function** is defined via

$$f_{\text{win}}(x) = \begin{cases} \dfrac{1}{2a} & (|x| \le a) \\ 0 & (|x| > a)\,. \end{cases} \tag{26.3.1}$$

- Note that the window function is discontinuous and cuts off to zero at $|x| = a$ not $2a$.
- The Fourier transform of the window function was derived in the lectures:

$$F_{\text{win}}(k) = \frac{\sin(ka)}{ka}\,. \tag{26.3.2}$$

- We shall compute the Fourier transform and inverse numerically.
- **Set $a = 1$ in this question.**
- Set $n = 1024$ for the numerical integration.
  1. **Compute the array `FT[j]` using eq. (26.1.5).**
  2. **Compute the array `IFT[j]` using eq. (26.1.6).**
- Plot some graphs to see how well the numerical values in the arrays match the known formulas.
- **We plot the graph of the Fourier transform first.**
  1. **Plot a graph of $F_{\text{tri}}(k)$ and `FT[j]` for $-6 \le k/(\pi a) \le 6$.**
  2. Recall that $k_j = k_{\text{min}} + j\Delta k$ for $j = 0, \dots, n$ (totally $n + 1$ points from k_{min} and k_{max}).
  3. To obtain nicer numbers on the horizontal axis, plot the value of $k/(\pi a)$, so the values go from -6 to 6.
  4. *If you have done your work correctly, you should obtain good agreement of* `FT[j]` *and* $F_{\text{win}}(k)$.
- Next, we plot the graph of the window function and inverse Fourier transform.
- **We shall observe some problems.**
  1. **Plot a graph of $f_{\text{win}}(x)$ and `IFT[i]` for $-4a \le x \le 4a$.**
  2. Recall that $x_i = x_{\text{min}} + i\Delta x$ for $i = 0, \dots, n$ (totally $n + 1$ points from x_{min} and x_{max}).
- **The graphs of $f_{\text{win}}(x)$ and `IFT[i]` will not match.**
- There are difficulties when a function is discontinuous.
- This is a manifestation of the **Gibbs–Wilbraham phenomenon.**
- We shall study the Gibbs–Wilbraham phenomenon in the context of Fourier series.
- **Stop here.** Do not attempt to process the graphs or the functions further.

26.4 Odd function

- Let us use an odd real function $f(-x) = -f(x)$.
- Let $a > 0$ be a real positive constant.
- Let us analyze the function

$$f_s(x) = \begin{cases} \dfrac{1}{a}\,\sin(\dfrac{\pi x}{a}) & (|x| \le a) \\ \\ 0 & (|x| > a)\,. \end{cases} \tag{26.4.1}$$

- The funcion is a sine, but we cut it off to zero for $|x| > a$. The sine equals zero at $x = \pm a$, hence $f_s(x)$ is continuous.
- The formula for the Fourier transform $F_s(k)$ is a difference of two sinc functions:

$$F_s(k) = -i\left[\frac{\sin(\pi - ka)}{\pi - ka} - \frac{\sin(\pi + ka)}{\pi + ka}\right]. \tag{26.4.2}$$

- Limits must be taken at the two values $k = \pm\pi/a$ to avoid $0/0$ expressions.
- *What shall we do with this function?* The Fourier transform is pure imaginary.
- Let us not panic. Since the function is odd, let us employ a sine transform and redefine

$$F_s(k) = \int_{-\infty}^{\infty} f_s(x)\,\sin(kx)\,dx\,. \tag{26.4.3}$$

- With this definition, $F_s(k)$ is real and odd in k: $F_s(-k) = -F_s(k)$.
- Using a sine transform, the answer is a real function:

$$F_s(k) = \begin{cases} \dfrac{\sin(\pi - ka)}{\pi - ka} - \dfrac{\sin(\pi + ka)}{\pi + ka} & (k \ne \pm\pi/a) \\ \\ 1 - \dfrac{\sin(\pi + ka)}{\pi + ka} & (k = \pi/a) \\ \\ \dfrac{\sin(\pi - ka)}{\pi - ka} - 1 & (k = -\pi/a)\,. \end{cases} \tag{26.4.4}$$

- We must restructure our computations to use $\sin(kx)$ instead of $\cos(kx)$.

- Calculate the sine transform and inverse numerically as follows.

  1. Let $k_j = k_{\min} + j\Delta k$, for $j = 0, \ldots, n$. Note that these are $n+1$ values.
  2. **Use the trapezoid rule with n subintervals to compute the integral**

  $$\mathrm{FT[j]} = \int_{x_{\min}}^{x_{\max}} f(x)\, \boldsymbol{\sin(k_j x)}\, dx\,. \tag{26.4.5}$$

  3. For the inverse transform, we perform a similar calculation, in reverse:
  4. Let $x_i = x_{\min} + i\Delta x$, for $i = 0, \ldots, n$. Note that these are $n+1$ values.
  5. **Use the trapezoid rule with n subintervals to compute the integral**

  $$\mathrm{IFT[i]} = \int_{k_{\min}}^{k_{\max}} F(k)\, \boldsymbol{\sin(k x_i)}\, dk\,. \tag{26.4.6}$$

- **Set $a = 1$ in this question.**
- Set $n = 1024$ for the numerical integration.

  1. **Compute the array `FT[j]` using eq. (26.4.5).**
  2. **Compute the array `IFT[j]` using eq. (26.4.6).**

- Plot some graphs to see how well the numerical values in the arrays match the known formulas.

  1. **Plot a graph of $f_s(x)$ and `IFT[i]` for $-4a \le x \le 4a$.**
  2. Recall that $x_i = x_{\min} + i\Delta x$ for $i = 0, \ldots, n$ (totally $n+1$ points from $x_{\min}$ and $x_{\max}$).
  3. **Plot a graph of $F_s(k)$ and `FT[j]` for $-6 \le k/(\pi a) \le 6$.**
  4. Recall that $k_j = k_{\min} + j\Delta k$ for $j = 0, \ldots, n$ (totally $n+1$ points from $k_{\min}$ and $k_{\max}$).
  5. To obtain nicer numbers on the horizontal axis, plot the value of $k/(\pi a)$, so the values go from -6 to 6.

- *If you have done your work correctly, you should obtain good agreement in both graphs.*
  In the case of $f_s(x)$, the graph of `IFT[i]` *will display some wiggles or small amplitude oscillations.*
  The graph of the sine transform `FT[j]` *should agree very well with $F_s(k)$.*

The derivation of the Fourier transform of $f_s(x)$ is as follows:

$$\begin{aligned}
F_s(k) &= \frac{1}{a} \int_{-a}^{a} \sin(\frac{\pi x}{a})\, e^{-ikx}\, dx \\
&= -\frac{i}{a} \int_{-a}^{a} \sin(\frac{\pi x}{a})\, \sin(kx)\, dx \\
&= -\frac{i}{2a} \int_{-a}^{a} \Big[\cos((\frac{\pi}{a} - k)x) - \cos((\frac{\pi}{a} + k)x) \Big]\, dx \\
&= -\frac{i}{2a} \left[\frac{\sin((\frac{\pi}{a} - k)x)}{\frac{\pi}{a} - k} - \frac{\sin((\frac{\pi}{a} + k)x)}{\frac{\pi}{a} + k} \right]_{-a}^{a} \\
&= -\frac{i}{a} \left[\frac{\sin((\frac{\pi}{a} - k)a)}{\frac{\pi}{a} - k} - \frac{\sin((\frac{\pi}{a} + k)a)}{\frac{\pi}{a} + k} \right] \\
&= -i \left[\frac{\sin(\pi - ka)}{\pi - ka} - \frac{\sin(\pi + ka)}{\pi + ka} \right].
\end{aligned} \tag{26.4.7}$$

26.5 Comment on computational complexity

- The complexity of our calculations of the Fourier transform and inverse were of $O(n^2)$.
- Later we shall learn the **Fast Fourier Transform (FFT)** which hss $O(n \log_2 n)$ complexity.