

		Course schedule	Required learning
04/07	Class 1	Discretizing differential equations	Discretize differential equations using forward, backward, and central difference, with high order, and evaluate the discretization error
04/11	Class 2	Finite difference methods	Understand stability of low and high order time integration, and use it to solve convection, diffusion, and wave equations
04/14	Class 3	Finite element methods	Understand the concepts of Galerkin methods, test functions, isoparametric elements, and use it to solve elasticity equations.
04/18	Class 4	Spectral methods	Explain the advantages of orthogonal basis functions such as Fourier, Chebyshev, Legendre, and Bessel.
04/21	Class 5	Boundary element methods	Understand the relation between inverse matrices, δ functions and Green's functions, and solve boundary integral equations.
04/25	Class 6	Molecular dynamics	Understand the significance of symplectic time integrators and thermostats, and solve the dynamics of interacting molecules.
04/28	Class 7	Smooth particle hydrodynamics (SPH)	Evaluate the conservation and dissipation properties of differential operators formed from radial basis functions.
05/02	Class 8	Particle mesh methods	How to conserve higher order moments for interpolations schemes when both particle and mesh-based discretizations are used.

Fourier transform

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i x \xi} dx,$$

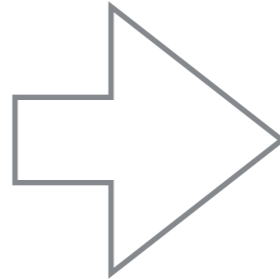
$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi) e^{2\pi i \xi x} d\xi,$$



Discrete Fourier transform

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i x \xi} dx,$$

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi) e^{2\pi i \xi x} d\xi,$$

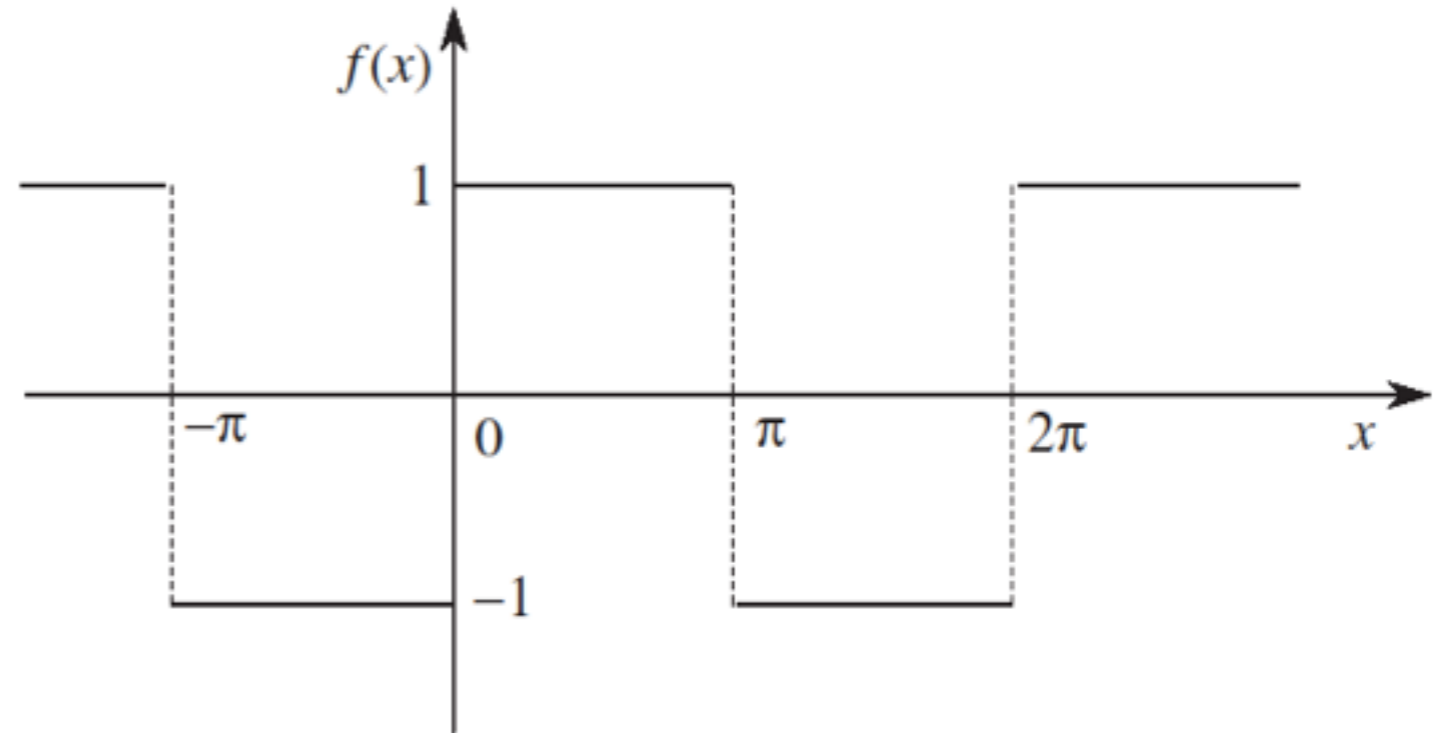


$$f(x_n) = \sum_{k=-N/2}^{N/2} \hat{f}_k e^{ikx_n}$$

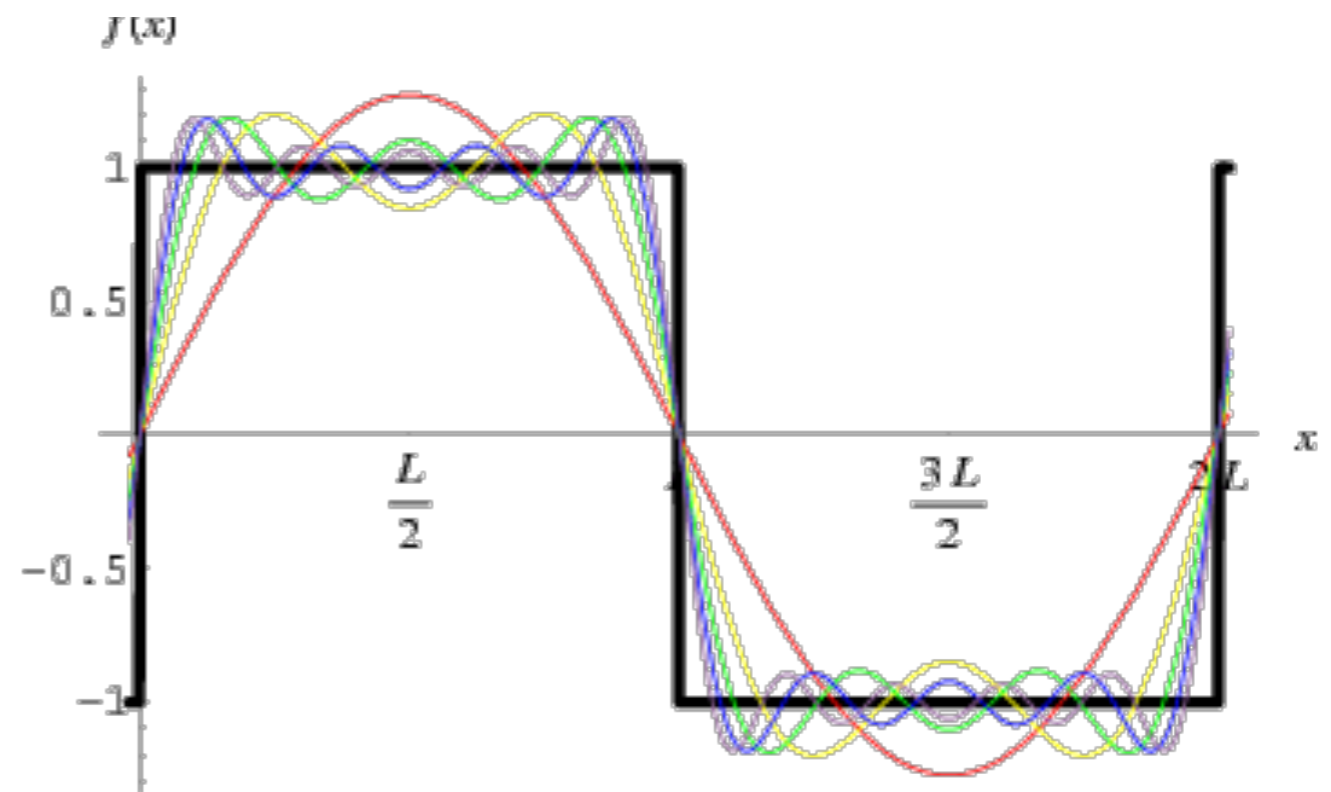
$$\hat{f}_k = \sum_{n=0}^N f(x_n) e^{-ikx_n}$$

Periodic square function

$$f(x) = \begin{cases} 1 & \text{if } 0 \leq x < \pi \\ -1 & \text{if } \pi \leq x < 2\pi \end{cases}$$



k	$\text{Re}(\hat{f}_k)$	$\text{Im}(\hat{f}_k)$	$ \hat{f}_k $
0	0	0	0
1	0.125	-0.628	0.641
2	0	0	0
3	0.125	-0.187	0.225
4	0	0	0
5	0.125	-0.084	0.150
6	0	0	0
7	0.125	-0.025	0.127
8	0	0	0

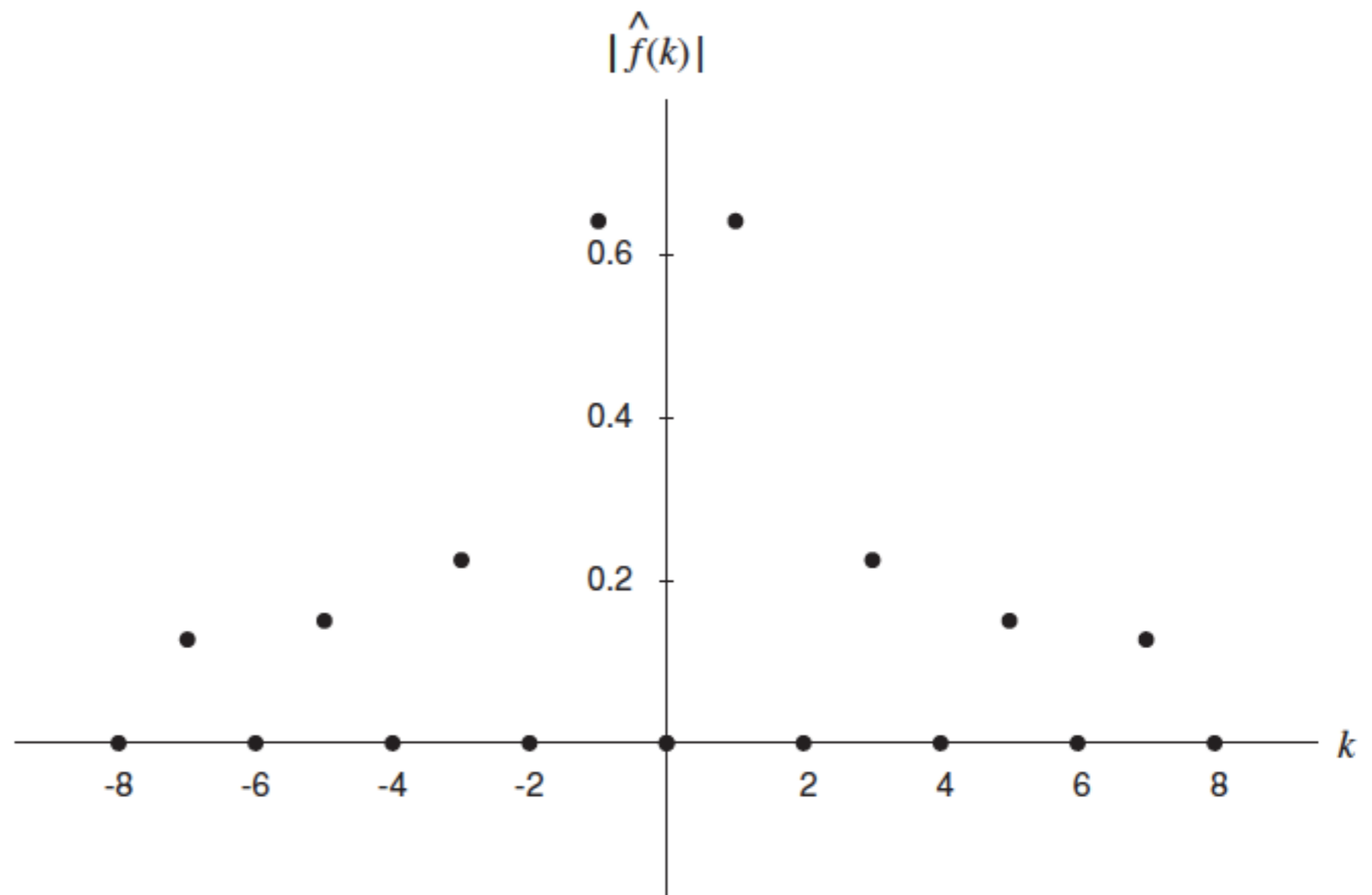


Fourier transform of a real function

$$\hat{f}_{-k} = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{ikx_j}$$

$$\hat{f}_{-k}^* = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-ikx_j}$$

$$\hat{f}_{-k} = \hat{f}_k^*$$



Product of functions in Fourier space

$$H(x) = f(x)g(x)$$

$$\hat{H}_m = (\hat{f}g)_m = \frac{1}{N} \sum_{j=0}^{N-1} f_j g_j e^{-imx_j}$$

$$\hat{H}_m = \frac{1}{N} \sum_{j=0}^{N-1} \sum_k \sum_{k'} \hat{f}_k \hat{g}_{k'} e^{ikx_j} e^{ik'x_j} e^{-imx_j}$$

$$\hat{H}_m = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \hat{g}_{m-k}$$

Product of two functions

$$f(x) = \sin 2x$$

$$g(x) = \sin 3x$$

$$\hat{f}_k = \begin{cases} \mp i/2 & \text{if } k = \pm 2 \\ 0 & \text{otherwise,} \end{cases}$$

$$\hat{g}_k = \begin{cases} \mp i/2 & \text{if } k = \pm 3 \\ 0 & \text{otherwise.} \end{cases}$$

$$H(x) = f(x)g(x).$$

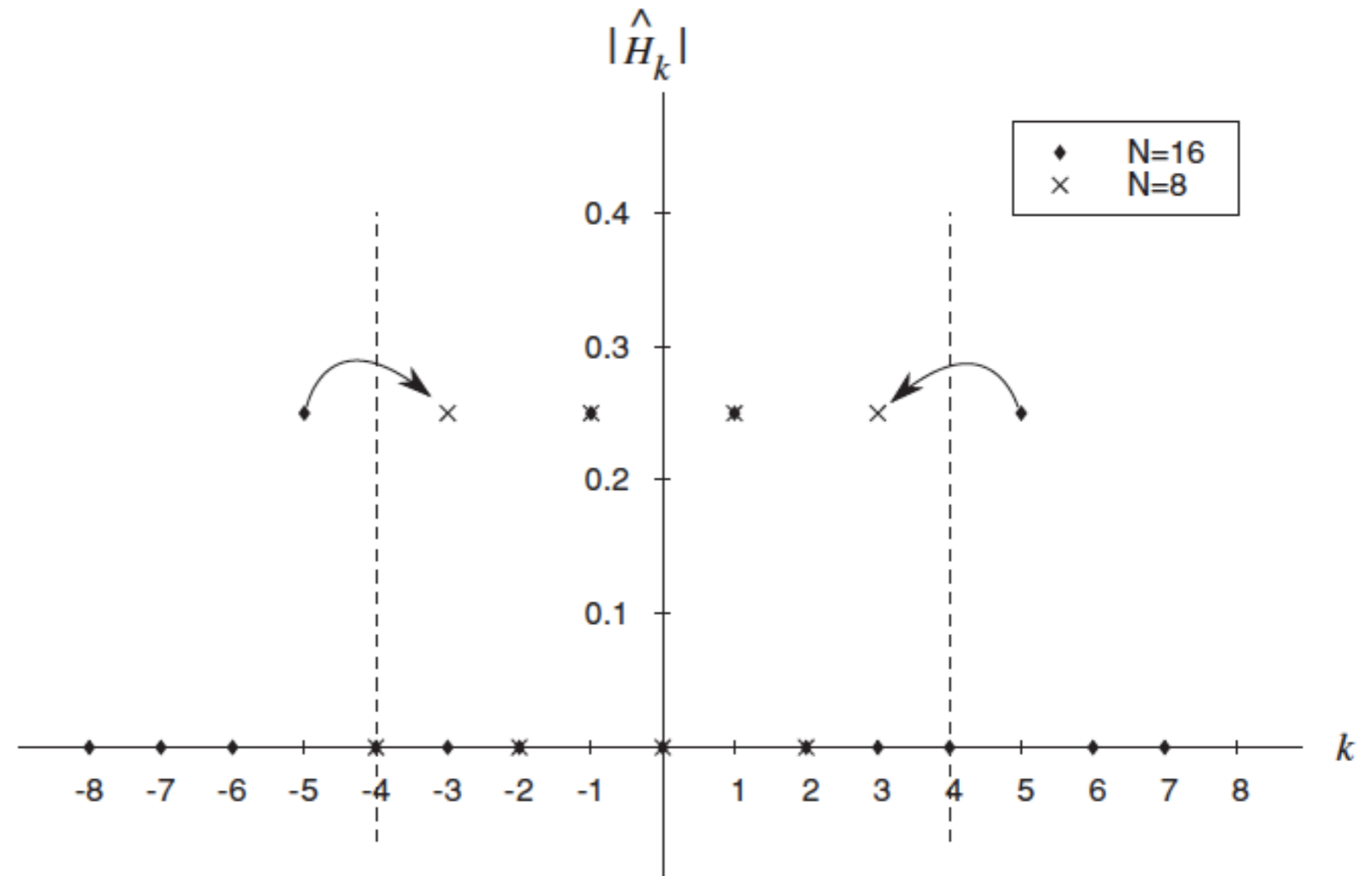
$$\hat{H}_m = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \hat{g}_{m-k}$$

$$H(x) = 0.5(\cos x - \cos 5x)$$

$$\hat{H}_k = \begin{cases} 1/4 & \text{if } k = \pm 1 \\ -1/4 & \text{if } k = \pm 5 \\ 0 & \text{otherwise} \end{cases}$$

Aliasing

$$\hat{H}_m = \sum_{k=-N/2}^{N/2-1} \hat{f}_k \hat{g}_{m-k}$$



Derivative in Fourier space

$$f(x_n) = \sum_{k=-N/2}^{N/2} \hat{f}_k e^{ikx_n}$$

$$f'(x_n) = \sum_{k=-N/2}^{N/2} ik \hat{f}_k e^{ikx_n}$$

Derivative in Fourier space

$$f(x) = \cos 3x$$

$$f'(x) = -3 \sin 3x$$

$$\widehat{Df}_k = \begin{cases} -(3/2)i & \text{if } k = -3 \\ (3/2)i & \text{if } k = 3 \\ 0 & \text{otherwise.} \end{cases}$$

$$f(x) = 2\pi x - x^2$$

$$f'(x) = 2\pi - 2x$$

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