

Lecture 2: Functional Differentiation

1 Introduction: Functionals

A *functional* maps functions to numerical values. Many common functionals take the form of integrals. For example, the normalization of a quantum mechanical wavefunction is

$$I[\psi] = \int_{-\infty}^{\infty} |\psi(x)|^2 dx. \quad (1)$$

Some other example are the length of a curve $y(x)$,

$$L[y] = \int_a^b \sqrt{1 + [y'(x)]^2} dx, \quad (2)$$

or the kinetic energy of a wavefunction,

$$K[\psi] = \int_{-\infty}^{\infty} \psi^*(x) \frac{\hbar^2}{2m} \frac{d}{dx} \psi(x) dx \quad (3)$$

or the coulomb energy of a charge density,

$$V_{\text{coul}}[\rho] = \int \int \frac{\rho(r)\rho(r')}{\epsilon|r-r'|} d^3r d^3r'. \quad (4)$$

The notation for a functional is to enclose the functional argument in square brackets.

Note that functionals do not have to be integrals of functions, they can be more general. In fact, a famous theorem by Hohenberg and Kohn (1964) says that the ground-state energy of interacting electrons in an external potential is simply a functional of their ground-state density $E[\rho]$. Of course, this functional is very complicated and unknown, but approximate schemes for evaluating $E[\rho]$ have been very successful. Density functional theory now plays a central role in condensed matter theory, and earned Walter Kohn the 1998 Nobel Prize in Chemistry.

2 Derivatives on integrals that *are not* functional derivatives

If the value of an integral is a function $I(x)$, the derivative of this function is not a functional derivative. Before getting to functional derivatives, we'll review the ordinary derivatives of integrals.

If the limits of integration are constant, the order of integration and differentiation can be reversed,

$$\frac{dI(x)}{dx} = \frac{d}{dx} \int_a^b f(x, t) dt \quad (5)$$

$$= \int_a^b \frac{\partial f(x, t)}{\partial x} dt \quad (6)$$

When the limits of integration themselves depend on x , that dependence must also be included,

$$\frac{dI(x)}{dx} = \frac{d}{dx} \int_{u(x)}^{v(x)} f(x, t) dt \quad (7)$$

$$= f(x, v(x)) \frac{dv(x)}{dx} - f(x, u(x)) \frac{du(x)}{dx} + \int_{u(x)}^{v(x)} \frac{\partial f(x, t)}{\partial x} dt \quad (8)$$

3 Functional derivatives

Functional derivatives can be intuitively understood in analogy to partial derivatives. Consider N discrete charges, with a different applied potential on each charge. Ignoring the interaction between charges (which makes no contribution to the present discussion), the energy due to the applied potential is

$$E(\phi_1, \dots, \phi_n) = \sum_i q_i \phi_i, \quad (9)$$

where ϕ_i is the applied external potential at site i . We could then ask how this applied energy changes as we vary the charge at one site. This is simply the partial derivative,

$$\frac{\partial E}{\partial \phi_i} = q_i. \quad (10)$$

That is, varying the external potential at a site measures the charge on the site. Although this is a rather trivial example, varying an external potential to probe the state of a system is a common technique in theoretical physics.

A functional derivative is the continuous analog of this process. The energy of a line of charge sitting in an external potential (where we again ignore interactions within the charge itself) is a functional

$$E[\phi] = \int_{-\infty}^{\infty} \rho(r) \phi(r) dr. \quad (11)$$

The rate of change in the energy as the external field ϕ is changed at point r is a *functional derivative*,

$$\frac{\delta E}{\delta \phi(r')} \equiv \lim_{\epsilon \rightarrow 0} \frac{E[\phi(r) + \epsilon \delta(r - r')] - E[\phi(r)]}{\epsilon} \quad (12)$$

$$= \lim_{\epsilon \rightarrow 0} \frac{\int \rho(r) \phi(r) + \epsilon \rho(r) \delta(r - r') dr - \int \rho(r) \phi(r) dr}{\epsilon} \quad (13)$$

$$= \int \rho(r) \delta(r - r') dr \quad (14)$$

$$= \rho(r'). \quad (15)$$

Thus, varying the external potential at a point measures the charge density at the point.

4 Common functional derivatives

All the following results are written out in one dimension, but actually apply to functions in any number of dimensions. The first example is the functional derivative of the integral of a function,

$$\frac{\delta}{\delta\eta(x)} \int dx' \eta(x') = 1. \quad (16)$$

To prove this result, simply use the definition for a functional derivative, Eq. (12),

$$\frac{\delta}{\delta\eta(x)} \int dx' \eta(x') = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[\int [\eta(x') + \epsilon\delta(x' - x)] dx - \int \eta(x') dx \right] \quad (17)$$

$$= \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \int \epsilon\delta(x' - x) dx \quad (18)$$

$$= 1. \quad (19)$$

The next example is the functional derivative of a function,

$$\frac{\delta}{\delta\eta(x)} \eta(x') = \lim_{\epsilon \rightarrow 0} \frac{[\eta(x') + \epsilon\delta(x' - x)] - \eta(x')}{\epsilon} \quad (20)$$

$$= \lim_{\epsilon \rightarrow 0} \frac{\epsilon\delta(x - x')}{\epsilon} \quad (21)$$

$$= \delta(x - x'). \quad (22)$$

Here is a less trivial example,

$$\frac{\delta}{\delta\eta(x)} \int dx' \frac{1}{2} [\partial_{x'} \eta(x')]^2 = -\partial_x^2 \eta(x). \quad (23)$$

To derive this, you must drop the term of order epsilon and do an integration by parts. The δ -function in these equations makes these mathematical steps less rigorous, so it is helpful (and probably mathematically necessary) to think of the δ -function as an ordinary function and take the limit of its spike becoming infinity after the other limits of integrating over the width of the delta function and ϵ becoming zero).

$$\frac{\delta}{\delta\eta(x)} \int dx' \frac{1}{2} [\partial_{x'} \eta(x')]^2 = \lim_{\epsilon \rightarrow 0} \frac{\int dx' \frac{1}{2} [\partial_{x'} (\eta(x') + \epsilon\delta(x' - x))]^2 - \int dx' \frac{1}{2} [\partial_{x'} \eta(x')]^2}{\epsilon} \quad (24)$$

$$= \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \int dx' \partial_{x'} (\eta(x') \partial_x \epsilon\delta(x' - x)) \quad (25)$$

$$= [\partial_x \eta(x')]_{-\infty}^{\infty} \delta(x' - x) - \int dx' \delta(x' - x) \partial_{x'}^2 \eta(x') \quad (26)$$

$$= -\partial_x^2 \eta(x). \quad (27)$$

As a final example, we take the functional derivative of the integral of a function of a function,

$$\frac{\delta}{\delta\eta(x)} \int dx f(\eta(x)) = \lim_{\epsilon \rightarrow 0} \frac{\int f(\eta(x) + \epsilon\delta(x)) dx - \int f(\eta(x)) dx}{\epsilon} \quad (28)$$

$$= \lim_{\epsilon \rightarrow 0} \frac{\int f(\eta(x)) + \epsilon\delta(x) f'(\eta(x)) + O(\epsilon^2) dx - \int f(\eta(x)) dx}{\epsilon} \quad (29)$$

$$= f'(\eta(x)) \quad (30)$$

$$(31)$$

5 Physical applications of functional derivatives

Functional derivatives describe the response of a functional to an infinitesimal change in the function at each point. They are used in several areas of theoretical physics.

5.1 Statistical Mechanics

For continuous systems, the partition function Z is actually a functional of the state of the system, $Z[\phi(r)]$. Here $\phi(r)$ is the Landau order parameter, for example the magnetization. Functional derivatives give the response of the system to small changes and also correlation functions. Goldenfeld's *Lectures on Phase Transitions and the Renormalization Group* (Addison-Wesley, Reading, 1992) makes use of functional derivatives.

5.2 Quantum Mechanics

Quantum mechanics is usually formulated in terms of linear operators, with the Schrödinger equation expressed in matrix form or as a differential equation. An alternative approach is to formulate quantum mechanics in terms of path integrals or functional integrals. The formulation as a functional integral is quite useful for many-body physics and field theories. In these formulations, a *generating function* $Z[\psi]$ describes the system (N.B. this ψ is not the wavefunction). Expectation values for propagators describing response functions and correlation functions are expressed in terms of functional derivatives (Negele and Orland, 1992).

5.3 Classical Mechanics

In classical mechanics, the action $S = \int T - V dt$ is a functional of the systems trajectory, $x(t)$. The functional derivatives of the action are

$$\frac{\delta S}{\delta x(t)} = \frac{\delta}{\delta x(t)} \int \frac{1}{2} m (\partial_{t'} x(t'))^2 - V(x(t')) dt' \quad (32)$$

$$= -m \frac{d^2 x}{dt^2} - \frac{dV}{dx}. \quad (33)$$

Requiring $\frac{\delta S}{\delta x}$ to be zero gives Newton's equation for one dimensional motion in a potential, $\partial_t^2 x = -\partial_x V(x)$. The requirement that the action functional be insensitive to small changes in the trajectory is part of the principle of least action. The mathematics for finding a function that minimizes a function is known as variational calculus, and is the subject of the next lecture.

References

Hohenberg and Kohn, Phys. Rev. B **136**, B864 (1964).

Negele and Orland, *Quantum Many-Particle Systems* (Addison-Wesley, Reading, 1992).