Appendix A
Variational Derivatives and Integrals

Definitions and useful properties of functionals, variational derivatives and functional integrals are collected here, and illustrated for the well known example of a classical scalar field.

A.1 Functional Derivatives

A functional, $F[f]$, is a mapping from a set of functions on configuration space to the real or complex numbers. We will denote the value of f at x by f_x. The functional derivative of $F[f]$ is defined via the variation of F with respect to f, i.e.,

$$\delta F := F[f + \delta f] - F[f] = \int \mathrm{d}x \, \frac{\delta F}{\delta f_x} \, \delta f_x \tag{A.1}$$

for arbitrary infinitesimal variations $f \to f + \delta f$. Thus the functional derivative is a field density, $\delta F/\delta f$, having the value $\delta F/\delta f_x$ at position x. Note that this definition is analogous to the definition of the partial derivative of a function $g(x)$ via

$$g(x + \varepsilon) - g(x) = \varepsilon \cdot \nabla g(x)$$

for arbitrary infinitesimal variations $x \to x + \varepsilon$. It follows directly from Eq. (A.1) that the functional derivative satisfies product and chain rules analogous to ordinary differentiation.

The choice $F[f] = f_{x'}$ in Eq. (A.1) yields

$$\delta f_{x'}/\delta f_x = \delta(x - x'). \tag{A.2}$$

Moreover, if the field depends on some parameter, t say, then choosing $\delta f_x = f_x(t + \delta t) - f_x(t)$ in Eq. (A.1) yields

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$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \int \mathrm{d}x \, \frac{\delta F}{\delta f_x} \frac{\partial f_x}{\partial t} \tag{A.3}$$

for the rate of change of F with respect to t. As another useful example, for a functional of the form $F = \int dx \, g(x, f, \nabla f)$ one has

$$\begin{aligned}
\delta F &= \int dx \, [g(x, f + \delta f, \nabla f + \nabla(\delta f)) - g(x, f, \nabla f)] \\
&= \int dx \left[\frac{\partial g}{\partial f} \delta f + \frac{\partial g}{\partial \nabla f} \nabla(\delta f) \right] \\
&= \int dx \left[\frac{\partial g}{\partial f} - \nabla \cdot \frac{\partial g}{\partial \nabla f} \right] \delta f,
\end{aligned}$$

where integration by parts has been used in the last line, assuming that the variations and/or the derivatives of g vanish at infinity. Hence from Eq. (A.1) one has

$$\delta F/\delta f = \partial g/\partial f - \nabla \cdot \partial g/\partial(\nabla f) \tag{A.4}$$

for this case. This formula is easily extended when g also depends on higher derivatives of f.

A.2 Functional Integrals

Functional integrals correspond to integration of functionals over the space of functions (or equivalence classes thereof). We will consider here a measure Df on this vector space which is *translation invariant*, i.e., $\int Df \equiv \int Df'$ for any translation $f' = f + h$ (which follows immediately, for example, from approaches to functional integration based on discretising the space of functions). In particular, this property implies the useful result

$$\int \mathrm{D}f \, \frac{\delta F}{\delta f} = 0 \quad \text{for} \quad \int \mathrm{D}f \, F[f] < \infty. \tag{A.5}$$

Equation (A.5) follows by noting that the finiteness condition and translation invariance imply

$$0 = \int \mathrm{D}f \, (F[f + \delta f] - F[f]) = \int \mathrm{d}x \, \delta f_x \left(\int \mathrm{D}f \, \frac{\delta F}{\delta f_x} \right) \tag{A.6}$$

for arbitrary infinitesimal translations, where we use f_x to denote the value of f at x.

Thus, for example, if $F[f]$ has a finite expectation value with respect to some probability density functional $P[f]$, then Eq. (A.5) yields the "integration by parts" formula

$$\int \mathrm{D}f \; P \frac{\delta F}{\delta f} = -\int \mathrm{D}f \; \frac{\delta P}{\delta f} F. \tag{A.7}$$

Moreover, from Eq. (A.5) the total probability, $\int \mathrm{D}f \; P$, is conserved for any probability flow satisfying a continuity equation of the form

$$\frac{\partial P}{\partial t} + \int \mathrm{d}x \; \frac{\delta}{\delta f_x} [P V_x] = 0, \tag{A.8}$$

providing that the average flow rate, $\langle V_x \rangle$, is finite.

Finally, consider a functional integral of the form

$$I[F] = \int \mathrm{D}f \; \xi(F, \delta F/\delta f), \tag{A.9}$$

where ξ denotes any function of some functional F and its functional derivative. Variation of $I[F]$ with respect to F then gives, to first order,

$$\begin{aligned} \Delta I &= I[F + \Delta F] - I[F] \\ &= \int \mathrm{D}f \; \left\{ \frac{\partial \xi}{\partial F} \Delta F + \int \mathrm{d}x \; \frac{\partial \xi}{\partial(\delta F/\delta f_x)} \frac{\delta(\Delta F)}{\delta f_x} \right\} \\ &= \int \mathrm{D}f \; \left\{ \frac{\partial \xi}{\partial F} - \int \mathrm{d}x \; \frac{\delta}{\delta f_x} \left[\frac{\partial \xi}{\partial(\delta F/\delta f_x)} \right] \right\} \Delta F \\ &\quad + \int \mathrm{d}x \int \mathrm{D}f \; \frac{\delta}{\delta f_x} \left\{ \left[\frac{\partial \xi}{\partial(\delta F/\delta f_x)} \right] \Delta F \right\}. \end{aligned} \tag{A.10}$$

Assuming that the functional integral of the expression in curly brackets in the last term is finite, this term vanishes from Eq. (A.5), yielding the result

$$\Delta I = \int \mathrm{D}f \; \frac{\Delta I}{\Delta F} \Delta F \tag{A.11}$$

analogous to Eq. (A.1), where the variational derivative $\Delta I/\Delta F$ is defined by

$$\frac{\Delta I}{\Delta F} := \frac{\partial \xi}{\partial F} - \int \mathrm{d}x \; \frac{\delta}{\delta f_x} \left[\frac{\partial \xi}{\partial(\delta F/\delta f_x)} \right]. \tag{A.12}$$

A.3 Example: Ensemble Hamiltonian for a Classical Scalar Field

To illustrate the application of the above concepts, we consider a classical scalar field, its corresponding ensemble Hamiltonian, and the equations of motion that follow from this ensemble Hamiltonian.

Field theories present well known mathematical and conceptual difficulties. As a consequence, the equations are formal in nature and it is necessary to examine each individual field theory to establish the validity of the ensemble formalism when applied to particular cases. This is done whenever particular field theories are discussed in the monograph. In the case of a field theory, the configuration is described by some field $\phi(x)$ (which may comprise multi-component fields that that carry a set of indices, which we omit here to simplify the notation). The probability density $P[\phi]$ is a functional, defined over the space of fields. We can consider a Hamiltonian description of the time evolution of the field, and introduce an auxiliary quantity $S[\phi]$ that is canonically conjugate to $P[\phi]$, as discussed in Chap. 5.

As an example, consider a classical scalar field ϕ. In the classical Hamilton–Jacobi formulation reviewed in Chap. 5, the equation for ϕ is given by

$$\frac{\partial S}{\partial t} + \int \mathrm{d}x \left[\frac{1}{2} \left(\frac{\delta S}{\delta \phi} \right)^2 + |\nabla \phi|^2 + V(\phi) \right] = 0. \tag{A.13}$$

The ensemble Hamiltonian $\mathscr{H}$ is the functional integral corresponding to the mean energy of the field,

$$\mathscr{H}[P, S] := \int \mathrm{D}f \, \mathrm{d}x \, P \left[\frac{1}{2} \left(\frac{\delta S}{\delta \phi} \right)^2 + |\nabla \phi|^2 + V(\phi) \right]. \tag{A.14}$$

The Hamiltonian equations of motion for the dynamical variables P and S,

$$\frac{\partial P}{\partial t} = \frac{\Delta \mathscr{H}}{\Delta S}, \qquad \frac{\partial S}{\partial t} = -\frac{\Delta \mathscr{H}}{\Delta P}, \tag{A.15}$$

reduce via Eq. (A.12) to the Hamilton–Jacobi equation, Eq. (A.13), as required, and to the continuity equation

$$\frac{\partial P}{\partial t} + \int \mathrm{d}x \, \frac{\delta}{\delta \phi} \left(P \, \frac{\delta S}{\delta \phi} \right) = 0. \tag{A.16}$$

Comparison with Eq. (A.8) shows that the local rate of change of the field is $V = \delta S / \delta \phi$.

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