8.08/8.S308 - Problem Set 1 - IAP Year

Due before January 9, 23:59

Problems that are referred to as "graduate" count as bonus problems for undergraduate students. This first problem set is essentially a reminder/test of the Mathematical prerequisites for the course.

Problem 1—Probabilities

Consider a random variable X of probability density p. Then $p(x)dx$ is the probability that the random variable X takes a values in $[x, x+dx]$, as $dx \to 0$.The n^{th} moment of X is denoted by $m_n = \langle X^n \rangle = \int dx x^n p(x)$. The generating function of the moments of p is $Z(h) = \langle e^{hX} \rangle$. It satisfies

$$\langle X^n \rangle = \frac{d^n Z}{dh^n}\bigg|_{h=0} \qquad \text{so that} \qquad Z(h) = \sum_{n\geq 0} \langle X^n \rangle \frac{h^n}{n!} \ . \tag{1}$$

The function $W(h) = \ln Z(h)$ is the generating function of the cumulants (also called "connected moments") of p. By definition, the n^{th} cumulant κ_n of p is $\kappa_n = \frac{d^n}{dh^n} W(h)\Big|_{h=0}$. We will use the notation $\kappa_n = \langle X^n \rangle_c$, where c stands for "cumulant" or "connected". One thus has $W(h) = \sum_{n\geq 1} h^n \langle X^n \rangle_c/(n!)$.

1.1) Determine the m_n's and κ_n's for $p(x) = \exp(-|x|)/2$.

1.2) For an arbitrary $p(x)$, show that $\kappa_1 = m_1$ and $\kappa_2 = m_2 - m_1^2$. Find similar relations for κ_3 in terms of m_3, m_2 and m_1, and for κ_4 in terms of m_4, m_3, m_2 and m_1. For this question, you may want to us that $\ln(1+u) \simeq u - \frac{u^2}{2} + \frac{u^3}{3} - \frac{u^4}{4} + \mathcal{O}(u^4)$ as $u \to 0$.

1.3) Show that, for an even $p(x)$, the relationship between κ_4 and the moments simplifies into $\kappa_4 = m_4 - 3m_2^2$. Conclude that, if $p(x)$ is a Gaussian with vanishing mean, $\langle X^4 \rangle = 3\langle X^2 \rangle^2$. The fourth cumulant is important in that it shows that cumulants are *not* the moments of the centered random variable $X - \langle X \rangle$.

Problem 2—Fourier transforms and series

Let f_n be a function defined on an N-site lattice, $n = 1, \ldots, N$, with N assumed to be even. We denote the lattice spacing by a so that $L = Na$ is the total length of the lattice. We define

$$\tilde{f}_q = \sum_{n=1}^{N} e^{iqna} f_n \ . \tag{2}$$

2.1) Show that if $q = \frac{2\pi k}{Na}$, with $k = -\frac{N}{2} + 1, \ldots, \frac{N}{2}$, then $f_n = \frac{1}{N} \sum_q \tilde{f}_q e^{-iqna}$. *Bonus:* Show that $\sum_q e^{iq(k-n)a} = N\delta_{k,n}$. If short of time, feel free to use this identity without proving it.

Note that such Fourier transforms are defined up to an arbitrary normalization factor A through

$$\tilde{f}_q = \frac{1}{A} \sum_{n=1}^{N} e^{iqna} f_n; \quad \text{and} \quad f_n = \frac{A}{N} \sum_q e^{-iqna} \tilde{f}_q \ . \tag{3}$$

This is reflected in the diversity of conventions that are commonly found in the literature.

2.2) We denote $x = na$ and take the $N \to \infty, a \to 0$ limits, with $L = Na$ kept fixed. To this end, we adopt the convenient convention $A = \frac{1}{a}$. This is the limit of a continuous but finite interval. Express $\tilde{f}_q$ as an integral involving $f(x)$, using the convergence of the Riemann sum $\sum_n a g_n \sim_{N\to\infty} \int dx g(x)$. How does one obtain $f(x)$ if $\tilde{f}_q$ is given? What are the acceptable values of q?

2.3) We now consider $N \to \infty$ with $L/N = a$ fixed. This is the limit of an infinite lattice. Show that, in this limit, $f_n = a \int_{-\pi/a}^{\pi/a} \frac{dq}{2\pi} \tilde{f}_q e^{-iqna}$. (We are back to the convention $A = 1$.)

2.4) Let $f(\tau)$ be a periodic function with period β, prove that $f(\tau) = \sum_{n\in\mathbb{Z}} \tilde{f}_{\omega_n} e^{-i\omega_n \tau}$ where ω_n and $\tilde{f}_{\omega_n}$ will be given in terms of f.

Problem 3—Gaussian integrals

3.1) We consider $a > 0$. Compute $I(a, 0)^2$, where

$$I(a,b) = \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2 - bx} \tag{4}$$

hint: you may want to write I^2 as a two-dimensional integral that can be computed in polar coordinates.

3.2) Compute $I(a, b)$.

3.3) By taking derivates of I, compute

$$\int_{-\infty}^{\infty} dx\, x^2 e^{-\frac{1}{2}ax^2 - bx} \tag{5}$$

The rest of this problem counts as a *Graduate* problem. Let $\mathbf{x} = (x_1, \ldots, x_n)$ and $\mathbf{h} = (h_1, \ldots, h_N)$ be n-component vectors. We define

$$Z(\mathbf{h}) = \int d\mathbf{x} e^{-\frac{1}{2}x_i \Gamma_{ij} x_j + h_i x_i}, \tag{6}$$

where Γ is, for now, a positive definite $n \times n$ matrix. We use the notation $\frac{1}{2}x_i\Gamma_{ij}x_j - h_i x_i$ for $\frac{1}{2}\mathbf{x} \cdot (\Gamma x) - \mathbf{h} \cdot \mathbf{x}$, *i.e.* we implicitly sum over repeated indices. We also defined $P(\mathbf{x}) = \frac{1}{Z(\mathbf{0})} e^{-\frac{1}{2}\mathbf{x}\cdot(\Gamma\mathbf{x})}$ and the angular brackets mean $\langle \ldots \rangle \equiv \int d\mathbf{x} \ldots P(\mathbf{x})$.

3.4) Check that $\langle e^{\mathbf{h}\cdot\mathbf{x}} \rangle = Z(\mathbf{h})/Z(\mathbf{0})$.

3.5) Why can we always restrict our analysis to the case where Γ is symmetric? This property will be assumed in the rest of this problem.

3.6) Prove that

$$\frac{1}{2}\mathbf{x} \cdot (\Gamma \mathbf{x}) - \mathbf{h} \cdot \mathbf{x} = \frac{1}{2}(\mathbf{x} - \Gamma^{-1}\mathbf{h}) \cdot [\Gamma(\mathbf{x} - \Gamma^{-1}\mathbf{h})] - \frac{1}{2}(\Gamma^{-1}\mathbf{h}) \cdot [\Gamma(\Gamma^{-1}\mathbf{h})]\,. \tag{7}$$

Show then that

$$\langle e^{\mathbf{h}\cdot\mathbf{x}} \rangle = e^{\frac{1}{2}\mathbf{h}\cdot(\Gamma^{-1}\mathbf{h})}\,. \tag{8}$$

This is the generalization of the computation of $I(a, b)$ to N variables, $b^2/2a$ has now became a matrix relation.

3.7) With our choice for P above, $P(\mathbf{x}) = P(-\mathbf{x})$, so that $\langle \mathbf{x} \rangle = 0$. Consider instead the new probability density obtained by including the field term $\mathbf{h} \cdot \mathbf{x}$: $\tilde{P}(\mathbf{x}) \propto e^{-\frac{1}{2}x_i \Gamma_{ij} x_j + h_i x_i}$. Show, using symmetry consideration, that $\langle \mathbf{x} \rangle = \Gamma^{-1}\mathbf{h}$.

3.8) Since Γ is symmetric, it can be diagonalized into a matrix D such that $\Gamma = QDQ^T$, with $Q^T = Q^{-1}$. By changing variables from $\mathbf{x}$ to $\mathbf{y} = Q^{-1}\mathbf{x}$, compute $Z(\mathbf{0})$ to show that

$$\int dx e^{-\frac{1}{2}\mathbf{x}\cdot\Gamma\mathbf{x}} = \frac{(2\pi)^{N/2}}{\sqrt{\det \Gamma}} \tag{9}$$

This is the generalization of the derivation of $I(a, 0)$ to N variables.

Problem 4—Dirac distribution

The Dirac distribution $\delta(x)$ can be defined from

$$\int_{-\infty}^{\infty} f(x)\delta(x) = f(0) \tag{10}$$

4.1) Show that $\delta(ax) = \frac{1}{|a|}\delta(x)$.

4.2) Compute the Fourier transform of $\delta(x)$, $\hat{\delta}(k) = \int_{-\infty}^{\infty} dx\, e^{ikx}\delta(x)$ and show that

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{-ikx} \tag{11}$$

4.3) Consider a probability density $p(x)$ and define the average of an observable $f(x, x_0)$ with respect to x as $\langle f(x, x_0)\rangle_x = \int dx f(x, x_0)p(x)$. Show that $p(x) = \langle \delta(x - x_0)\rangle_{x_0}$.

4.4) Consider two independent Gaussian random variables x and y of averages $\bar{x}$ and $\bar{y}$ and of variance σ_x^2 and σ_y^2. Using the result of question 4.3, compute $p(z = \alpha x + \beta y)$. *Hint*: you may want to use Eq.(11) to turn $\delta(z - z_0)$ into a more useful expression.

Problem 5—Functional derivatives (*Graduate*)

Let $q(t)$ be a function of t and let $S[q]$ be a functional of q (i.e. a map from the space of functions $q(t)$ into the field of real or complex numbers). The functional derivative of S with respect to $q(t_0)$ is defined as follows. Let $q_{\epsilon,t_0}(t) = q(t) + \epsilon\delta(t - t_0)$, then

$$\frac{\delta S}{\delta q(t_0)} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left(S[q_{\epsilon,t_0}] - S[q]\right) . \tag{12}$$

An equivalent definition is to say that when $q \to q + \delta q$ (meaning that the trajectory $q(t)$ is perturbed by $\delta q(t)$), the functional changes from S to $S + \delta S$, with

$$\delta S = \int \frac{\delta S}{\delta q(t')}\delta q(t')dt' \tag{13}$$

to first order in δq. This relation defines the functional derivative $\delta S/\delta q(t')$, which is a functional of q and a function of t'.

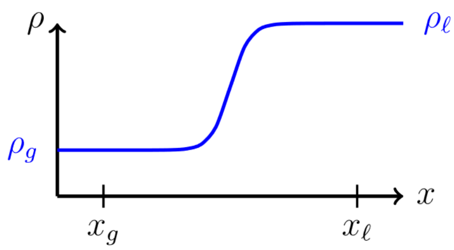

Figure 1: *A profile separating high-density and low-density regions*

5.1) Compute $\frac{\delta q(t_1)}{\delta q(t_2)}$.

5.2) If S can be written in the form $S[q] = \int_0^\infty dt L(q(t), \dot{q}(t))$, where L is a function of $q(t)$ and $\dot{q}(t)$, prove that

$$\frac{\delta S}{\delta q(t_0)} = \frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} \ , \tag{14}$$

were everything is evaluated at $t = t_0$.

5.3) Consider a free energy $\mathcal{F}[\rho] = \int dx \Big(f(\rho(x)) + \frac{\kappa}{2}[\partial_x \rho(x)]^2 \Big)$. Show that the free energy is extremalized (minimized, really), by a profile that satisfies

$$\kappa \partial_{xx} \rho(x) = f'(\rho(x)) \tag{15}$$

Show that, for the phase-separated profile shown in Fig. 1, the free-energy density f is equal in the coexisting phases, i.e. $f(\rho_g) = f(\rho_\ell)$