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Moment Generating Function

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The Moment Generating Function

? context.

The Question

Suppose that we make multiple observations of some quantity Q. Let q_i be the result of the i^{th} observation, $i = 1, \ldots, N$. From these observations, we can estimate the *moments*

$$\mu_\ell = \frac{1}{N} \sum_{i=1}^{N} q_i^\ell, \qquad \ell = 0, 1, \ldots \tag{1}$$

Of course, $\mu_0 = 1$, and μ_1 is just the average over the observations. μ_2 can be used to estimate the *variance* of the observations,

$$\left\langle (q - \langle q \rangle)^2 \right\rangle = \mu_2 - \mu_1^2$$

[The square root of this quantity is often referred to as the *standard deviation* of the observations.]

That all the q_i are not identical implies that there is something statistical in the data set. We say that Q is a *stochastic variable* and we* characterize the statistics in terms of a *distribution function*, $f(q)$,

$$\mu_\ell = \int_{-\infty}^{\infty} q^\ell \, f(q) \, dq, \quad \ell = 0, 1, \ldots \tag{2}$$

The question is, how can we deduce $f(q)$ from observations of the moments? How can we *invert* the relation (2)?

The Fourier Integral Transform

Let us start with the Fourier series representation of a function $f(x)$. If $f(x)$ is defined in $-\frac{1}{2}L \le x \le \frac{1}{2}L$, then we can calculate

$$c_n = \frac{1}{L} \int_{-\frac{L}{2}}^{\frac{L}{2}} dx \, e^{-2\pi i n x/L} f(x), \quad n = 0, \pm 1, \pm 2, \ldots \tag{3a}$$

* In this case, *we* means physical scientists. Mathematicians use a different terminology.

$f(x)$ can, in turn, be reconstructed from the Fourier series coefficients c_n,

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \, e^{2\pi i n x/L}. \tag{3b}$$

The sum (3b) gives a function that is periodic in x: $f(x+L) = f(x)$, all x.

Let us reexpress (3) in terms of *wave vectors*

$$k_n = \frac{2\pi n}{L}, \quad n = 0, \pm 1, \pm 2, \ldots$$

Then

$$\left\{ \begin{aligned} L\, c(k_n) &= \int_{-L/2}^{L/2} dx \, e^{-i k_n x} f(x), \\ f(x) &= \sum_{n=-\infty}^{\infty} \tfrac{1}{L} L\, c_n \, e^{i k_n x}. \end{aligned} \right. \tag{4}$$

As $L \to \infty$, the discrete variable k_n approaches a continuous variable, $\Delta k = k_{n+1} - k_n = \frac{2\pi}{L} \to 0$, and

$$\sum_{n=-\infty}^{\infty} \frac{1}{L} \mathcal{F}(k_n) = \sum_{n=-\infty}^{\infty} \frac{\Delta k}{2\pi} \mathcal{F}(k_n) \to \int_{-\infty}^{\infty} \frac{dk}{2\pi} \mathcal{F}(k).$$

If $L\, c(k_n) \to 2\pi\, g(k)$ as $L \to \infty$, (4) becomes

$$\left\{ \begin{aligned} g(k) &= \tfrac{1}{2\pi} \int_{-\infty}^{\infty} dx \, e^{-i k x} f(x), \\ f(x) &= \int_{-\infty}^{\infty} dk \, g(k) \, e^{i k x}. \end{aligned} \right. \tag{5}$$

The $f(x)$, $g(k)$ in (5) are *Fourier Transform* pairs. [Different definitions move the 2π factor around and/or replace $i \to -i$.]

The Dirac Delta Function

Using both equations in (5),

$$\begin{aligned} f(x) &= \int_{-\infty}^{\infty} dk\, g(k)\, e^{i\,k\,x} \\ &= \int_{-\infty}^{\infty} dk \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} dy\, e^{-i\,k\,y}\, f(y) \right) e^{i\,k\,x} \\ &= \int_{-\infty}^{\infty} dy\, f(y)\, \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{i\,k\,(x-y)} \end{aligned}$$

which can only be true for all $f(x)$ if

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{i\,k\,(x-y)} = \delta(x-y). \tag{6}$$

The Moment Generating Function

If

$$\Psi = \sum_n c_n \chi_n$$
$$\hat{Q}\, \chi_n = \lambda_n\, \chi_n, \quad \text{all } n,$$

then

$$\mu_\ell = \left\langle \Psi | \hat{Q}^\ell \Psi \right\rangle = \sum_n |c_n|^2\, \lambda_n^\ell \tag{7}$$

Combining (2) and (7) gives

$$\int_{-\infty}^{\infty} dq\, q^\ell\, f(q) = \sum_n |c_n|^2\, \lambda_n^\ell, \quad \ell = 0, 1, \ldots \tag{8}$$

Summing the terms in (8) weighted by $\frac{i^\ell s^\ell}{\ell!}$ gives a function of s,

$$\int_{-\infty}^{\infty} dq\, e^{i\,q\,s}\, f(q) = \sum_n |c_n|^2\; e^{i\,\lambda_n\,s} \quad \ell = 0, 1, \ldots \tag{9}$$

called the *moment generating function* since all moments can be obtained by expanding this expression in s.

What is the Distribution on q?

Equation (9) identifies the Fourier transform of $f(q)$. Thus $f(q)$ can be identified by inverse Fourier transforming,

Probability of seeing eigen values depends on the amplitude

$$
\begin{aligned}
f(q) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} ds\, e^{-iqs} \sum_n |c_n|^2\, e^{i\lambda_n s} \\
&= \sum_n |c_n|^2 \frac{1}{2\pi} \int_{-\infty}^{\infty} ds\, e^{-i(q-\lambda_n)s} \\
&= \sum_n |c_n|^2\, \delta(q - \lambda_n)
\end{aligned}
\tag{10}
$$

This shows that the only possible values of q that could be observed are the eigenvalues of $\hat{Q}$. The only possible values that can be observed are determined by the operator associated with the observable. These values have no relation to the actual state Ψ of the system.

The *probability* that $q = \lambda_n$ will be observed, however, depends upon $|c_n|^2$, i.e., on the actual state of the system.