

There will be 8 lectures by Prof. Baiesi - the first two about some mathematical tools, and then about scattered arguments, to show how to apply the theoretical physics framework to various topics.

(Lesson 3 of
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0.1 Moments and Generating Functions

Consider a continuous function $f: \mathbb{R} \rightarrow \mathbb{R}$, $x \mapsto f(x)$. The n -th **moment** of f about a point $c \in \mathbb{R}$ is defined as the integral:

$$\mu_n = \int_{-\infty}^{\infty} (x - c)^n f(x) dx$$

Moments provide a way to quantify, in a certain sense, the *shape* of f . For example, if $f(x)$ is a linear density ($[\text{kg m}^{-1}]$), then the 0-th moment is the total mass, the first one (with $c = 0$) is the center of mass, and the second is the *moment of inertia*.

Moments are especially useful if $f(x)$ is a probability density function (pdf), i.e. a non-negative normalized function. In this case the first moment about 0 is the **mean**:

$$\mu_1 \equiv \int_{-\infty}^{\infty} x f(x) dx = \mathbb{E}[X] \equiv \mu; \quad X \sim f$$

where X is a random variable sampled from f . Note that, if not specified, a moment is intended to be centered around $c = 0$ (it is a *raw moment* or *crude moment*).

The *central second moment*, that is μ_2 with $c = \mu$ is the **variance**:

$$\int_{-\infty}^{\infty} (x - \mu)^2 f(x) dx \equiv \mathbb{E}[(X - \mu)^2] = \text{Var}[X]$$

A **moment-generating function** of a real-valued random variable is a certain function $f: \mathbb{R}^n \rightarrow \mathbb{R}$, $\mathbf{x} \mapsto f(\mathbf{x})$ that can be used to *compute* the moment of the distribution where X comes from.

More precisely, for a random variable X , the moment-generating function M_X is defined as:

$$M_X(t) \equiv \mathbb{E}[e^{tX}], \quad t \in \mathbb{R}$$

In fact, recall that:

$$e^{tX} = 1 + tX + \frac{t^2 X^2}{2!} + \dots$$

Hence, as the *expected value* is a linear operator:

$$\begin{aligned} M_X(t) &= \mathbb{E}[e^{tX}] = 1 + t \mathbb{E}[X] + \frac{t^2 \mathbb{E}[X^2]}{2!} + \dots = \\ &= 1 + t\mu_1 + \frac{t^2 \mu_2}{2!} + \dots \end{aligned}$$

Note that the distribution's moments are the coefficients of the power series that defines $M_X(t)$.

In fact, the more general definition of a **generating function** is that of a power-series with “hand-picked” coefficients a_n , such that by simply knowing the function one can compute a_n in an iterative way.

To recover a certain μ_n we start by differentiating M_X n times with respect to t , such that the first $n - 1$ terms vanish:

$$\frac{d^n}{dt^n} M_X(t) = \underbrace{\frac{n(n-1)\dots 1}{n!}}_{=1} \mu_n + \frac{(n+1)n\dots 2}{(n+1)!} t \mu_{n+1} + \dots$$

Then, by setting $t = 0$, all μ_r with $r > n$ vanish, leaving only the desired μ_n :

$$\left. \frac{d^n}{dt^n} M_X(t) \right|_{t=0} = \mu_n$$

Finally, we note that a moment-generating function can be constructed even for a multi-dimensional vector $\mathbf{X} = (X_1, \dots, X_n)^T$ of random variables, by simply taking a scalar product in the exponential:

$$M_{\mathbf{X}}(\mathbf{t}) \equiv \mathbb{E} \left(e^{\mathbf{t}^T \mathbf{X}} \right) \quad \mathbf{t} \in \mathbb{R}^n$$

0.2 Multivariate Gaussian

Consider now a normal pdf in $d = 1$:

$$f(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left(-\frac{(x - \mu)^2}{2\sigma^2} \right)$$

We denote a random variable sampled from $f(x; \mu, \sigma)$ as $X \sim \mathcal{N}(\mu, \sigma)$.

Suppose that we have multiple random variables $\{X_i\}_{i=1,\dots,n}$, each normally distributed ($X_i \sim \mathcal{N}(\mu_i, \sigma_i)$), with covariance matrix $\Sigma \in \mathbb{R}^{n \times n}$ defined as:

$$\Sigma_{ij} = \mathbb{E}[(X_i - \mu_i)(X_j - \mu_j)]$$

Their joint pdf is given by a **multivariate normal distribution** :

$$f(x_1, \dots, x_n; \boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{(2\pi)^n \det(\Sigma)}} \exp \left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right)$$

0.3 Moments and Gaussians

We want now to compute the moment generating function for a multivariate gaussian, that is the value of the integral:

$$M_{\mathbf{X}}(\mathbf{t}) = \int_{\mathbb{R}^n} e^{\mathbf{t} \cdot \mathbf{x}} f(\mathbf{x}; \boldsymbol{\mu}, \Sigma) d^n x \quad (1)$$

Let's start from the easiest case, and work our way out to the most general one.

Recall that the **gaussian integral**, i.e. the 0-th moment of a normal univariate distribution is:

$$\int_{-\infty}^{\infty} \exp\left(-\frac{a}{2}x^2\right) dx = \sqrt{\frac{2}{a}}\pi$$

Proof. The integral as is can't be computed in terms of elementary functions. However, its square can be calculated:

$$\left(\int_{-\infty}^{\infty} dx \exp\left(-\frac{a}{2}x^2\right)\right)^2 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \exp\left(-\frac{a}{2}(x^2 + y^2)\right)$$

Transforming to polar coordinates:

$$= \int_0^{2\pi} d\theta \int_0^{\infty} dr \exp\left(-\frac{a}{2}r^2\right) r = -\frac{2\pi}{a} \exp\left(-\frac{a}{2}r^2\right) \Big|_0^{\infty} = \frac{2\pi}{a}$$

and we arrive at the desired result by simply taking the square root.

Consider now the integral of the multivariate case, with $\boldsymbol{\mu} = \mathbf{0}$ (meaning we applied a translation from the general case):

$$Z(\Sigma) = \int_{\mathbb{R}^n} d^n \mathbf{x} \exp\left(-\frac{1}{2} \mathbf{x}^T \Sigma^{-1} \mathbf{x}\right)$$

Notice that the inverse of the covariance matrix $\Sigma^{-1} \equiv A$ is a symmetric positive-definite matrix, thus can be used to define a quadratic form:

$$\mathbb{A}(\mathbf{x}) = \sum_{i,j=1}^n x_i A_{ij} x_j$$

The integral can be computed by applying a change of variables, *rotating* \mathbf{x} such that A becomes diagonal:

$$\mathbf{y} = O\mathbf{x}; \quad O \in \mathbb{R}^{n \times n}; \quad O^T = O^{-1}, \det(O) = 1$$

where O is an orthogonal matrix, with a set of orthogonal eigenvectors of A as columns, such that:

$$OAO^{-1} = \text{diag}(a_1, \dots, a_n)$$

with a_i being the eigenvalues of A .

Note that, as $\det(O) = 1$, the volume element in the integral does not change. So, by substituting:

$$\mathbf{x} = O^{-1}\mathbf{y}; \quad \mathbf{x}^T = \mathbf{y}^T (O^{-1})^T = \mathbf{y}^T O$$

in the integral, we get:

$$\begin{aligned} Z(A) &= \int_{\mathbb{R}^n} d^n \mathbf{y} \exp \left(-\frac{1}{2} \mathbf{y}^T O A O^T \mathbf{y} \right) = \int_{\mathbb{R}^n} d^n \mathbf{y} \exp \left(-\frac{1}{2} \sum_{i=1}^n a_i y_i^2 \right) = \\ &= \prod_{i=1}^n \int_{\mathbb{R}} dy_i \exp \left(-\frac{1}{2} a_i y_i^2 \right) = (2\pi)^{n/2} \prod_{i=1}^n a_i^{-1/2} \stackrel{(a)}{=} (2\pi)^{n/2} (\det(A))^{-1/2} \end{aligned} \quad (2)$$

where in (a) we noted that the determinant of a matrix is the product of its eigenvalues.

We are now ready to consider the more general case of (1), by simply adding a linear term in the exponential of $Z(A)$:

$$Z(A, \mathbf{b}) \equiv \int_{-\infty}^{\infty} d^n \mathbf{x} \exp \left(-\frac{1}{2} \mathbb{A}(\mathbf{x}) + \mathbf{b} \cdot \mathbf{x} \right) \quad \mathbf{b} \cdot \mathbf{x} = \sum_{i=1}^n b_i x_i \quad (3)$$

To compute this integral, a trick is to translate the maximum of the exponential to the origin. So we start by differentiating:

$$\frac{\partial}{\partial x_i} \left(\frac{1}{2} \mathbb{A}(\mathbf{x}) - \mathbf{b} \cdot \mathbf{x} \right) \stackrel{!}{=} 0 \quad \forall i \quad (4)$$

Note that:

$$\begin{aligned} \frac{\partial}{\partial x_i} \mathbb{A}(\mathbf{x}) &= \frac{\partial}{\partial x_i} \sum_{ab} x_a A_{ab} x_b = \sum_{ab} \delta_{ai} A_{ab} x_b + \sum_{ab} x_a A_{ab} \delta_{bi} = \\ &= \sum_b A_{ib} x_b + \sum_a x_a A_{ai} \end{aligned}$$

By renaming the first summation variable to a , we get:

$$= \sum_a (A_{ia} + A_{ai}) x_a \stackrel{(b)}{=} 2 \sum_a A_{ia} x_a = 2A\mathbf{x}$$

where in (b) we used the fact that A is symmetrical ($A_{ij} = A_{ji}$). Substituting in (4):

$$\frac{1}{2} 2 \sum_j A_{ij} x_j = b_i \quad \forall i \stackrel{(c)}{\Leftrightarrow} A^T \mathbf{x} = \mathbf{b} \stackrel{(d)}{\Leftrightarrow} \mathbf{x}^* = A^{-1} \mathbf{b}$$

In (c) we noted that b_i is the scalar product between the i -th column of A and \mathbf{x} , leading to the transpose in the matrix notation. Of course, as $A = A^T$, in (d) we simply dropped the transpose.

We can now apply the coordinate change:

$$\mathbf{x} = \mathbf{x}^* + \mathbf{y}$$

Substituting in the exponential argument:

$$\begin{aligned} -\frac{\mathbb{A}(\mathbf{x})}{2} + \mathbf{b} \cdot \mathbf{x} &= -\frac{1}{2} \mathbf{x}^T A \mathbf{x} + \mathbf{x}^T \mathbf{b} = -\frac{1}{2} (\mathbf{x}^* + \mathbf{y})^T A (\mathbf{x}^* + \mathbf{y}) + (\mathbf{x}^* + \mathbf{y})^T \mathbf{b} = \\ &= -\frac{1}{2} [\mathbf{x}^{*T} A \mathbf{x}^* + \mathbf{y}^T A \mathbf{y} + \cancel{\mathbf{x}^{*T} A \mathbf{y}} + \cancel{\mathbf{y}^T A \mathbf{x}^*}] + \mathbf{x}^{*T} A \mathbf{x}^* + \cancel{\mathbf{y}^T A \mathbf{x}^*} \end{aligned} \quad (5)$$

Note, in fact, that $\mathbf{y}^T A \mathbf{x}^* = (\mathbf{x}^{*T} A^T \mathbf{y})^T = (\mathbf{x}^{*T} A \mathbf{y})^T$ because A is symmetric, and then $(\mathbf{x}^{*T} A \mathbf{y})^T = \mathbf{x}^{*T} A \mathbf{y}$ because they are scalars.

Then:

$$\mathbf{x}^{*T} A \mathbf{x}^* = (A^{-1} \mathbf{b})^T A A^{-1} \mathbf{b} = \mathbf{b}^T (A^{-1})^T \mathbf{b} = \mathbf{b}^T A^{-1} \mathbf{b} = \mathbf{b} \cdot \mathbf{x}^*$$

And substituting in (5):

$$-\frac{\mathbb{A}(\mathbf{x})}{2} + \mathbf{b} \cdot \mathbf{x} = -\frac{1}{2} \mathbf{y}^T A \mathbf{y} + \underbrace{\frac{1}{2} \mathbf{b} \cdot \mathbf{x}^*}_{\omega_2(\mathbf{b})}$$

To simplify notation, let's define:

$$\omega_2(\mathbf{b}) = \frac{1}{2} \sum_{i,j=1}^n b_i (A^{-1})_{ij} b_j = \frac{1}{2} \mathbf{b} \cdot \mathbf{x}^* \quad (6)$$

As the change of variables involves only a translation by a constant value, the volume element in the integral does not change, leading to:

$$Z(A, \mathbf{b}) = \int_{-\infty}^{\infty} d^n \mathbf{y} \exp \left(-\frac{\mathbb{A}(\mathbf{y})}{2} + \omega_2(\mathbf{b}) \right)$$

Note that $\omega_2(\mathbf{b})$ is constant, thus can be extracted from the integral:

$$= e^{\omega_2(\mathbf{b})} \int_{-\infty}^{\infty} d^n \mathbf{y} \exp \left(-\frac{\mathbb{A}(\mathbf{y})}{2} \right) \stackrel{(2)}{=} e^{\omega_2(\mathbf{b})} (2\pi)^{n/2} (\det A)^{-1/2} \quad (7)$$

Another way to solve the integral for $Z(A, \mathbf{b})$ is by using the matrix equivalent of “completing the square”. We start by considering the argument of the exponential in (3):

$$-\frac{1}{2} (\mathbf{x}^T A \mathbf{x} - 2 \mathbf{b}^T \mathbf{x})$$

$\mathbf{x}^T A \mathbf{x}$ has the role of the square, and $-2 \mathbf{b}^T \mathbf{x}$ that of the double product.

We can then sum and subtract a constant vector \mathbf{c} in order to rewrite:

$$\mathbf{x}^T A \mathbf{x} - 2 \mathbf{b}^T \mathbf{x} + \mathbf{c} - \mathbf{c} = \mathbf{y}^T A \mathbf{y} - \mathbf{c}$$

for some $\mathbf{y} \in \mathbb{R}^n$.

Comparing to a generic square:

$$(\mathbf{a} + \mathbf{b})^T A (\mathbf{a} + \mathbf{b}) = \mathbf{a}^T A \mathbf{a} + \mathbf{b}^T A \mathbf{b} + 2 \mathbf{a}^T A \mathbf{b}$$

we note that $\mathbf{a} = \mathbf{x}$ and $\mathbf{b} = -A^{-1}\mathbf{b}$, leading to:

$$\mathbf{x}^T A \mathbf{x} - 2\mathbf{b}^T \mathbf{x} = (\mathbf{x} - A^{-1}\mathbf{b})^T A (\mathbf{x} - A^{-1}\mathbf{b}) - \mathbf{b}^T A^{-1}\mathbf{b}$$

Defining $A^{-1}\mathbf{b} \equiv \mathbf{x}^*$ and $\mathbf{y} = \mathbf{x} - \mathbf{x}^*$ then leads to the same calculations as before.

Exercise 1 (Multivariate Gaussian Integral):

Compute $Z(A)$ and $Z(A, \vec{b})$ with:

$$A = \begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix}; \quad b = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Note that $\det A = 8$, and:

$$A^{-1} = \frac{1}{8} \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}$$

So, by simply using (2) and (7):

$$\begin{aligned} Z(A, 0) &= \frac{(2\pi)^{2/2}}{\sqrt{8}} = \frac{\pi}{\sqrt{2}} \\ \frac{1}{2} \begin{pmatrix} 1 & 0 \end{pmatrix} \frac{1}{8} \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \frac{3}{16} \\ Z(A, \mathbf{b}) &= \frac{\pi}{\sqrt{2}} \exp\left(\frac{3}{16}\right) \end{aligned}$$

0.3.1 Gaussian expectation values

The result in (7) is exactly what we need to compute the moment generating function for the multivariate normal (1).

So, we can finally compute moments:

$$\langle x_{k_1} x_{k_2} \dots x_{k_l} \rangle \equiv \frac{1}{Z(A)} \int d^n \mathbf{x} x_{k_1} x_{k_2} \dots x_{k_l} \exp\left(-\frac{1}{2} \mathbb{A}(\mathbf{x})\right)$$

by simply deriving the generating function $Z(A, \mathbf{b})$ with respect to certain variables in \mathbf{b} . For example:

$$\langle x_k \rangle = \frac{1}{Z(A)} \frac{\partial}{\partial b_k} Z(A, \vec{b}) = \frac{1}{Z(A)} \int d^n \mathbf{x} x_k \exp\left(-\frac{\mathbb{A}(\mathbf{x})}{2} + \mathbf{b}^T \mathbf{x}\right)$$

For the general case:

$$\begin{aligned}\langle x_{k_1} x_{k_2} \dots x_{k_l} \rangle &= (2\pi)^{-n/2} (\det A)^{-1/2} \left[\frac{\partial}{\partial b_{k_1}} \frac{\partial}{\partial b_{k_2}} \dots \frac{\partial}{\partial b_{k_l}} Z(A, \mathbf{b}) \right]_{\mathbf{b}=\mathbf{0}} = \\ &= \frac{\partial}{\partial b_{k_1}} \frac{\partial}{\partial b_{k_2}} \dots \frac{\partial}{\partial b_{k_l}} e^{\omega_2(\mathbf{b})} \Big|_{\mathbf{b}=\mathbf{0}}\end{aligned}$$

In physics, we say that b_k is “coupled” to x_k , and that $Z(A, \mathbf{b})$ is used as “generating function” for \mathbf{x} .

0.3.2 Wick’s Theorem

From the previous formula we know that:

$$\frac{\partial}{\partial b_i} \text{ pulls down a } b_i$$

Explicitly, recall that:

$$\omega_2(\mathbf{b}) = \frac{1}{2} \mathbf{b}^T A^{-1} \mathbf{b}$$

and so:

$$\frac{\partial}{\partial b_i} e^{\omega_2(\mathbf{b})} = \frac{1}{2} e^{\omega_2 \mathbf{b}} \frac{\partial}{\partial b_i} \sum_{tk} b_t A_{tk}^{-1} b_k = e^{\omega_2 \mathbf{b}} \sum_k A_{ik}^{-1} b_k$$

If we now set $\mathbf{b} = \mathbf{0}$, the result will be 0, meaning that:

$$\langle x_i \rangle = \frac{\partial}{\partial b_i} \frac{Z(A, \mathbf{b})}{Z(A)} = 0$$

This result is expected, as in $Z(A, \mathbf{b})$ all random variables are centered in 0.

However, note that if we derive one more time, with respect to some b_l :

$$\frac{\partial}{\partial b_i} \frac{\partial}{\partial b_l} e^{\omega_2(\mathbf{b})} = e^{\omega_2 \mathbf{b}} \sum_s A_{ls}^{-1} b_s \sum_k A_{ik}^{-1} b_k + e^{\omega_2 \mathbf{b}} A_{il}^{-1}$$

And now, if we set $\mathbf{b} = \mathbf{0}$, the result may be $\neq 0$.

Note that if we derive one more time we return to the previous situation - and the result will be also 0.

In general, every moment of odd-order is 0, due to the symmetry of the gaussian, we have:

$$\langle x_i x_j x_k \rangle = 0$$

So the expectation value of the product of different random variables, sampled from the same gaussian distribution centered on 0, is only non-zero for an even

number of variables. This result is known as the **Wick's theorem** (also known in literature as the **Isserlis theorem**).

By extending this argument, one can find a way to compute the even-order moments, leading to the following formula (which we will not prove):

$$\langle x_{k_1} x_{k_2} \dots x_{k_l} \rangle = \sum_{P \in \sigma(K)} A_{k_{P_1} k_{P_2}}^{-1} A_{k_{P_3} k_{P_4}}^{-1} \dots A_{k_{P_{l-1}} k_{P_l}}^{-1} = \sum_{P \in \sigma(K)} \langle x_{k_{P_1}} x_{k_{P_2}} \rangle \dots \langle x_{k_{P_{l-1}}} x_{k_{P_l}} \rangle$$

where (k_p, k_q) are a pair of indices from $K = \{k_1, \dots, k_l\}$, and P is a permutation of K , so that (k_{P_1}, k_{P_2}) is the first pair of indices after the permutation P . The sum is over all the distinct ways of partitioning $l = 2s$ variables in pairs to obtain distinct products of s groups.

So, the total number of terms to be added will be $(2s)!/(2^s s!)$ - that is the total number of permutation of $2s$ elements, where the order within couples does not matter (2^s) and neither the order of the couples themselves ($s!$).

Note that:

$$\frac{(2s)!}{2^s s!} = (2s-1)!! = (2s-1)(2s-3)(2s-5) \dots$$

Where $!!$ denotes the *double factorial*, not to be confused with the factorial of a factorial (which requires brackets: $(a!)!$).

Exercise 2 (Wick's theorem):

Consider a univariate normal distribution:

$$f(x) = \frac{1}{Z(A)} \exp\left(-\frac{a}{2}x^2\right)$$

Show that:

$$\begin{aligned} \langle x^2 \rangle &= \frac{1}{a} \\ \langle x^4 \rangle &= \frac{3}{a^2} = 3(\langle x^2 \rangle)^2 \end{aligned}$$

Here the A matrix is just the scalar $a = \sigma^{-2}$. As the pdf is univariate, there is only one index possible $K = \{1\}$. As $(2-1)!! = 1!! = 1$, there is only one term in the summation, thus:

$$\langle x^2 \rangle = A_{11}^{-1} = \frac{1}{a}$$

For the 4-th order, however, we have more combinations: $(4-1)!! = 3!! = 3 \cdot 1 = 3$. Again, there is only one possible index, so all terms will be the same:

$$\langle x^4 \rangle = A_{11}^{-1} A_{11}^{-1} + A_{11}^{-1} A_{11}^{-1} + A_{11}^{-1} A_{11}^{-1} = \frac{3}{a^2} = 3(\langle x^2 \rangle)^2$$

0.4 Steepest Descent Integrals

It is possible to use gaussian integrals to solve a more general set of integrals, thanks to the *Steepest Descent approximation*.

We start with an integral of the form:

$$I(\lambda) \equiv \int_S d^n x \exp\left(-\frac{F(\mathbf{x})}{\lambda}\right) \quad (8)$$

where λ is a small parameter (the approximation is more and more accurate as $\lambda \rightarrow 0$), $F(\mathbf{x})$ has a global minimum in $\mathbf{x}_0 \in (a, b)$ and $S \subseteq \mathbb{R}^n$ is a sufficiently large region.

Note that, if λ is lowered, the integral is dominated by the neighborhood of the minimum \mathbf{x}_0 . In fact:

$$h(\mathbf{x}) \equiv \exp\left(-\frac{F(\mathbf{x})}{\lambda}\right); \quad \frac{h(\mathbf{x}_0)}{h(\mathbf{x})} = \exp\left(-\frac{1}{\lambda}(F(\mathbf{x}_0) - F(\mathbf{x}))\right)$$

As $F(\mathbf{x}_0) - F(\mathbf{x}) < 0$, the ratio becomes exponentially higher if $\lambda \rightarrow 0$. Basically, for $\lambda \rightarrow 0$, the integrand function becomes “more and more similar to a gaussian”.

To compute the integral, then, we translate the coordinates about \mathbf{x}_0 :

$$\mathbf{x} = \mathbf{x}_0 + \sqrt{\lambda} \mathbf{y} \quad d^n \mathbf{x} = \lambda^{n/2} d^n \mathbf{y}$$

Then we perform a second order Taylor expansion about $\lambda = 0$ and $\mathbf{x} = \mathbf{x}_0$:

$$\frac{1}{\lambda} F(\mathbf{x}) = \frac{1}{\lambda} F(\mathbf{x}_0) + \frac{1}{\lambda} \sum_i \cancel{\partial_{x_i} F(\mathbf{x}_0) y_i \sqrt{\lambda}} + \frac{1}{\lambda} \frac{1}{2!} \sum_{ij} \partial_{x_i x_j}^2 F(\mathbf{x}_0) y_i y_j \lambda + O(\lambda^{1/2})$$

where we cancelled the first derivative, as \mathbf{x}_0 is a stationary point for F .

Substituting back in the integral we get:

$$I(\lambda) = \lambda^{n/2} \exp\left(-\frac{F(\mathbf{x}_0)}{\lambda}\right) \int_{S'} d^n \mathbf{y} \exp\left[-\frac{1}{2} \sum_{ij} \partial_{x_i x_j}^2 F(\mathbf{x}_0) y_i y_j - R(\mathbf{y})\right]$$

This is a gaussian integral $Z(A)$, with A being the Hessian of F evaluated at the minimum \mathbf{x}_0 (or, equivalently, at the maximum of $-F(\mathbf{x})$).

Now, for λ sufficiently small, we can ignore $R(\mathbf{y})$ and compute the integral with (2), leading to the approximation:

$$I(\lambda) \underset{\lambda \rightarrow 0}{\approx} (2\pi\lambda)^{n/2} [\det \partial_{x_i x_i}^2 F(\mathbf{x}_0)]^{-1/2} \exp\left(-\frac{F(\mathbf{x}_0)}{\lambda}\right) \quad (9)$$

Doing this, we implicitly integrated over the entire \mathbb{R}^n . This is fine because, for $\lambda \rightarrow 0$, the gaussian is “peaked” in a small region around \mathbf{x}_0 , and vanishes exponentially moving further away.

The Steepest Descent approximation generalizes Laplace's method for calculating integrals, which has a much simpler expression for the limited case of univariate integrals:

$$I(s) = \int g(z) e^{sf(z)} dz \underset{s \rightarrow \infty}{\approx} \frac{(2\pi)^{1/2} g(z_c) e^{sf(z_c)}}{|sf''(z_c)|^{1/2}} \quad (10)$$

with $f, g \in \mathbb{R}$, and z_c is the maximum of f , i.e. $f(z_c) \geq f(z) \forall z \in (a, b)$. This formula is useful in physics: s can model the system's size, and $s \rightarrow \infty$ is then the limit for a large system.

Example 1 (Stirling approximation):

We can use the Steepest Descent approximation to derive the formula for the Stirling approximation of factorials.

Recall that a factorial is merely the Γ function evaluated on \mathbb{N} :

$$s! = \int_0^\infty x^s e^{-x} dx$$

We then perform a change of variables:

$$x = zs$$

so that:

$$s! = s^{s+1} \int_0^\infty e^{s(\ln z - z)} dz$$

This is an integral in the form:

$$\int \exp\left(-\frac{F(x)}{\lambda}\right)$$

if we let $\lambda = 1/s$ and $F(z) = z - \ln z$. So we need to find the minimum of $F(z)$:

$$\begin{aligned} F'(z) &= \frac{d}{dz}(z - \ln z) = 1 - \frac{1}{z} \stackrel{!}{=} 0 \Rightarrow z_c = 1 \\ F''(z) &= \frac{1}{z^2} \Rightarrow F''(z_c) = 1 > 0 \end{aligned}$$

We can now apply (9), leading to:

$$s! \underset{s \rightarrow \infty}{\approx} \left(\frac{2\pi}{s}\right)^{1/2} (1)^{1/2} e^{-s} = \sqrt{2\pi} s^{s+\frac{1}{2}} e^{-s}$$

Note that the same result can be obtained by using the much simpler (10), with $g(z) \equiv 1$ and $f(z) = \ln z - z$.

Exercise 3 (Steepest Descent Approximation):

Compute the Steepest Descent Approximation for the following integral (for $s \rightarrow \infty$):

$$I(s) = \int_{-\infty}^{\infty} e^{sx - \cosh x} dx$$

By collecting a s in the exponential argument:

$$I(s) = \int_{-\infty}^{\infty} \exp \left(s \left(x - \frac{\cosh x}{s} \right) \right) dx$$

we can bring back to the form of (8) with $F(x) = \cosh x/s - x$ and $\lambda = s^{-1}$. We find the minimum of $F(x)$ by differentiating:

$$\begin{aligned} F'(x) &= \frac{\sinh x}{s} - 1 \stackrel{!}{=} 0 \Rightarrow x_0 = \sinh^{-1} s \\ F''(x) &= \frac{\cosh x}{s} \Rightarrow F''(x_0) = \frac{\cosh \sinh^{-1} s}{s} = \frac{\sqrt{1+s^2}}{s} > 0 \end{aligned}$$

Finally, by applying (9) we obtain the result:

$$\begin{aligned} I(s) &\underset{s \rightarrow \infty}{\approx} \sqrt{\frac{2\pi}{s}} \sqrt{\frac{s}{\sqrt{1+s^2}}} \exp \left(\frac{\sqrt{1+s^2}}{s} - \sinh^{-1} s \right) = \\ &= \frac{\sqrt{2\pi}}{(1+s^2)^{1/4}} \exp \left(\frac{\sqrt{1+s^2}}{s} - \sinh^{-1} s \right) \end{aligned}$$

Note that, for this peculiar case, the simple 1D formula does not work (why?) - and so one should proceed with the general method (full steps: find maximum, second derivative...).

Exercise 4 (Laplace's formula):

Compute:

$$I(N) = \int_0^{\infty} \cos(x) \exp \left(-N \left[\left(x - \frac{\pi}{3} \right)^2 + \left(x - \frac{\pi}{3} \right)^4 \right] \right) dx$$

in the limit $N \rightarrow \infty$.

For this exercise we can use Laplace's formula (10) with:

$$g(x) = \cos(x) \quad f(x) = - \left[\left(x - \frac{\pi}{3} \right)^2 + \left(x - \frac{\pi}{3} \right)^4 \right]$$

By looking at $f(x)$ one can see directly that it has a global maximum in $x_0 = \pi/3$. In fact:

$$f'(x) = - \left[2 \left(x - \frac{\pi}{3} \right) + 4 \left(x - \frac{\pi}{3} \right)^3 \right] \stackrel{!}{=} 0 \Leftrightarrow x_0 = \frac{\pi}{3}$$

$$f''(x) = - \left[2 + 12 \left(x - \frac{\pi}{3} \right)^2 \right] \Rightarrow f''(x_0) = -2 < 0$$

And so we arrive at:

$$I(N) \underset{N \rightarrow \infty}{\approx} \frac{(2\pi)^{1/2} \cos(\pi/3) e^{N \cdot 0}}{|N(-2)|^{1/2}} = \frac{1}{2} \sqrt{\frac{\pi}{N}}$$