SAND2024-02140R

Sandia National Laboratories

Operated for the United States Department of Energy
by National Technology and Engineering Solutions
of Sandia, LLC.

Albuquerque, New Mexico 87185
Livermore, California 94550

date: February 26, 2024

to: Distribution

from: Michael R. Buche (1558)

subject: Laplace's method applied to functional integrals

Abstract

In statistical thermodynamics, partition functions are required to evaluate the current state. It is typically impossible to analytically calculate the resulting configuration integrals, but it is sometimes possible to obtain approximations in the limit of steep potential energies [1]. This approach directly leverages Laplace's method for approximating integrals [2] and has been quite successful in recent applications [3–6]. Motivated by models with an infinite number of degrees of freedom [7, 8], this approach should be extended to the statistical thermodynamics of fields. To that end, Laplace's method is developed for functional integrals.

Mathematics

Consider a partition function Z given by the functional path integral

$$Z = \int f(x)\, e^{-\lambda\phi(x)}\, \mathcal{D}x, \tag{1}$$

where $f(x)$ and $\phi(x)$ are functionals of the path $x(s)$. For simplicity, $\phi(x)$ is assumed to be

$$\phi(x) = \frac{1}{2}\int \big[x(s) - x_0\big]^2 ds, \tag{2}$$

which is minimized at $x(s) = x_0$, i.e., $\phi(x_0) = 0$. For $\lambda \gg 1$, the partition function Z should be well approximated by some functional integral analog of Laplace's method [1, 2]. It is assumed that $x(s) = x_0$ lies within the interior of the path integration, and that the functional derivatives of $f(x)$ with respect to x, denoted as $f^{(n)} = \delta^n f/\delta x^n$, exist. For $\lambda \gg 1$, the path integral Z can be approximated by instead integrating over the paths in the narrow region $|x(s) - x_0| < \epsilon$. Subsequently, $f(x)$ can be approximated in that region using the functional Taylor series [9] of $f(x)$ about $x(s) = x_0$,

$$f(x) \sim f(x_0) + \int \frac{\delta f(x_0)}{\delta x(s)} \, \Delta x(s) \, ds + \frac{1}{2} \iint \frac{\delta^2 f(x_0)}{\delta x(s) \delta x(s')} \, \Delta x(s) \Delta x(s') \, ds \, ds' + \cdots . \tag{3}$$

where $\Delta x(s) = x(s) - x_0$. Since the functional derivatives are evaluated at the constant function x_0 they can be removed from the integrals, and then Z can be approximated by

$$Z \sim \int_{x_0-\epsilon}^{x_0+\epsilon} \left\{ f(x_0) + \frac{\delta f(x_0)}{\delta x} \int \Delta x(s) \, ds + \cdots \right\} e^{-\frac{\lambda}{2} \int \Delta x(s) \, ds} \, \mathcal{D}x. \tag{4}$$

Following Laplace's method [2], the range of integration is then extended back to all paths since the contribution from outside the narrow region $|x(s) - x_0| < \epsilon$ is small. The functional Taylor series remains and can be written more succinctly in terms of a sum, yielding

$$Z \sim \int \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\delta^n f(x_0)}{\delta x^n} \left[\int \Delta x(s) \, ds \right]^n e^{-\frac{\lambda}{2} \int \Delta x(s) \, ds} \, \mathcal{D}x. \tag{5}$$

Applying the change of variables $u(s) = \sqrt{\lambda} \, \Delta x(s)$, $\mathcal{D}u = \sqrt{\lambda} \, \mathcal{D}x$ simplifies this result to

$$Z \sim \frac{1}{\sqrt{\lambda}} \int \sum_{n=0}^{\infty} \frac{1}{n! \sqrt{\lambda^n}} \frac{\delta^n f(x_0)}{\delta x^n} \left[\int u(s) \, ds \right]^n e^{-\frac{1}{2} \int u^2(s) \, ds} \, \mathcal{D}u. \tag{6}$$

The zeroth term in the series is simply the path integral of the exponential functional.

$$A = \int e^{-\frac{1}{2} \int u^2(s) \, ds} \, \mathcal{D}u. \tag{7}$$

Utilizing path integration by parts [10], the second term is found to equal the first,

$$\int \left[\int u(s) \, ds \right]^2 e^{-\frac{1}{2} \int u^2(s) \, ds} \, \mathcal{D}u = A, \tag{8}$$

and repeatedly applying the same process allows all even terms to be obtained as

$$\int \left[\int u(s) \, ds \right]^{2m} e^{-\frac{1}{2} \int u^2(s) \, ds} \, \mathcal{D}u = A(2m-1)!!. \tag{9}$$

It can be similarly shown that all odd terms are zero. Z is then approximated for $\lambda \gg 1$ by

$$Z \sim \frac{A}{\sqrt{\lambda}} \, f(x_0) \left[1 + \sum_{m=1}^{\infty} \frac{(2m-1)!!}{\lambda^m (2m)!} \frac{f^{(2m)}(x_0)}{f(x_0)} \right]. \tag{10}$$

If $\phi(x)$ is not a harmonic functional of x, there will be additional terms involving $\phi^{(n)}(x_0)$. Also, this approximation heavily depends on the assumption that x_0 is a constant function.

Acknowledgements

Sandia National Laboratories is a multimission laboratory managed and operated by the National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

References

[1] M. R. Buche, Cornell University, Ph.D. thesis (2021).

[2] C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers I: Asymptotic Methods and Perturbation Theory* (Springer, New York, 2013).

[3] M. R. Buche, M. N. Silberstein, and S. J. Grutzik, Phys. Rev. E **106**, 024502 (2022).

[4] J. Mulderrig, B. Talamini, and N. Bouklas, J. Mech. Phys. Solids **174**, 105244 (2023).

[5] M. R. Buche and J. M. Rimsza, Phys. Rev. E **108**, 064503 (2023).

[6] M. R. Buche and S. J. Grutzik, Phys. Rev. E **109**, 015001 (2024).

[7] J. F. Marko, Phys. Rev. E **57**, 2134 (1998).

[8] M. Grasinger and P. Sharma, J. Mech. Phys. Solids **184**, 105527 (2024).

[9] M. Ernzerhof, Phys. Rev. A **50**, 4593 (1994).

[10] A. Zee, *Quantum Field Theory in a Nutshell* (Princeton University Press, NJ, 2010).

External Distribution:

Matthew Grasinger (AFRL)
Jason Mulderrig (AFRL)
Steven Strogatz (Cornell)

Internal Distribution:

Ken Cundiff (1558)
Scott Grutzik (1558)
Kevin Long (1558)
Stacy Nelson (1558)