Monte Carlo versus Langevin methods for nonpositive definite weights

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We point out that a standard Monte Carlo algorithm can be made to converge in some cases for nonpositive definite weights. Comparison of Monte Carlo and Langevin algorithms for two simple models with complex actions shows the Monte Carlo method to be always superior; it is more reliable and gives smaller statistical error when both converge, and converges in cases where the Langevin method does not.

Recently there have been claims in the literature that Langevin simulation methods offer the possibility to do stochastic calculations in cases where the standard Metropolis Monte Carlo algorithm is not applicable in the presence of nonpositive weights.[1-7] The purpose of this Brief Report is to point out that in fact a standard Monte Carlo algorithm does often converge in cases with a complex action, and that there is no evidence that the Langevin method converges in cases where the Monte Carlo method does not. In fact, we show here for two simple models that the Monte Carlo method always converges where the Lagevin method does, and gives better answers, and it even converges in cases where the Langevin method does not.

Consider the Monte Carlo evaluation of an integral

$$\bar{f}(\mathbf{x})=\frac{\int d\{x_i\}e^{-\beta S(\mathbf{x})}f(\mathbf{x})}{\int d\{x_i\}e^{-\beta S(\mathbf{x})}} . \tag{1}$$

For complex β, it is clear that $e^{-\beta S(\mathbf{x})}$ cannot be interpreted as a probability. However, one can still use its absolute value as a probability and lump the phase onto the quantity to be averaged over.[8] That is, for $\beta=\beta'+i\beta''$

$$\bar{f}(\mathbf{x})=\frac{\int d\{x_i\}e^{-\beta' S(\mathbf{x})-i\beta''(\mathbf{x})}f(\mathbf{x})}{\int d\{x_i\}e^{-\beta' S(\mathbf{x})-i\beta''(\mathbf{x})}}=\frac{\langle f(\mathbf{x})e^{-i\beta'' S(\mathbf{x})}\rangle}{\langle e^{-i\beta'' S(\mathbf{x})}\rangle} , \tag{2}$$

where the average $\langle\ \rangle$ is taken with weight

$$\frac{e^{-\beta' S(\mathbf{x})}}{\int d\{x_i\}e^{-\beta' S(\mathbf{x})}} , \tag{3}$$

which, being positive definitely, can be interpreted as a probability in a Metropolis algorithm.

If the original integral in Eq. (1) converges so will a Monte Carlo evaluation of Eq. (2), provided that the integral

$$\int d\{x_i\}e^{-\beta' S(\mathbf{x})}<\infty . \tag{4}$$

In practice, of course, the variance of the computed value of $\bar{f}(\mathbf{x})$ by Eq. (2) could be very large if $\langle e^{-i\beta''(\mathbf{x})}\rangle$ is very small. For a quadratic action

$$S(\mathbf{x})=\tfrac{1}{2}\sum_{i,j}x_iA_{ij}x_j , \tag{5}$$

it is clear that the integral of Eq. (1) is finite for any $f(\mathbf{x})$, provided that

$$\mathrm{Re}\lambda_i>0,\ i=1,2,\ldots,N , \tag{6}$$

where λ_i are the eigenvalues of the matrix A. In that case, Eq. (4) is also automatically satisfied.

To compute Eq. (1) using a Langevin equation method, one solves[9]

$$\frac{dx_i}{dt}=-\frac{\partial S}{\partial x_i}+\eta_i(t) , \tag{7}$$

with η_i a white noise, satisfying

$$\langle\eta_i(t)\rangle=0,\ \langle\eta_i(t)\eta_j(t')\rangle=2\delta_{ij}\delta(t-t') \tag{8}$$

by discretizing Eq. (7) and computing $\bar{f}(\mathbf{x})$ from a time average. For a quadratic action (5), one shows easily that Eq. (6) is necessary and sufficient for the Langevin method to converge. For general S and complex β there seems to be no general theorem on the convergence of the Langevin equation method.[1]

We have studied the two models discussed recently by Hamber and Ren.[3] The first one is

$$S(x)=\cos x . \tag{9}$$

We have calculated $\langle\cos x\rangle$ by Monte Carlo and Langevin methods. The exact statistical average is given by

$$\langle\cos x\rangle=I_1(\beta)/I_0(\beta) , \tag{10}$$

where $I_\nu(z)$ is the modified Bessel function of the first kind. The corresponding Langevin equation is

$$dx/dt=-\beta\sin x+\eta(t) . \tag{11}$$

Let $z=e^{ix}$, then Eq. (11) can be discretized as[3]

$$z_{i+1}=z_i\exp\left[-\frac{dt\beta}{2}\left(z_i-\frac{1}{z_i}\right)+i\sqrt{24dt}\,\eta_i\right] , \tag{12}$$

where η_i is a random number uniformly distributed in $(-\frac{1}{2},\frac{1}{2})$ and dt is the step size. It is well known that the systematic error introduced by discretizing Eq. (11) into Eq. (12) is proportional to dt. To have systematic error within the statistical error and for another reason given below, we choose $dt=0.0005$ in all of our Langevin calculations. There is not much difference in computer time needed for one sweep between Monte Carlo and Langevin simulation (1.4:1). We typically did 10^6 Monte Carlo sweeps and 2×10^6 iterations in Langevin simulation for comparison. In Table I we present our results obtained from exact calculation and both Monte Carlo and Langevin methods. As can be seen, the Monte Carlo results converge very nicely for all values of $\mathrm{Im}\beta$ and give smaller statistical errors than the Langevin results. In both cases, we did several runs with different initial conditions like starting point $x(0)$ and random number seed, and we found that the Monte Carlo results are very stable, but the Langevin simulations are very dependent on the initial condition (the difference between two runs sometimes is far off the statistical error); the data shown in Table I are the best ones of several runs. The convergence gets worse when the phase angle of β gets large and the solution blows up for $\beta=i|\beta|$ (Hamber and Ren also found similar behavior[3]), while the Monte Carlo method still gives the right answer in that case. The results for $\mathrm{Re}\beta<0$ can be obtained trivially from the symmetry relation

$$\langle\cos x\rangle(-\beta^*)=-[\langle\cos x\rangle(\beta)]^* \ . \tag{13}$$

For this model there should be no convergence problem because the action is bounded. This is indeed the case in the

TABLE I. Comparison between Monte Carlo (MC) results (10^6 sweeps) and Langevin results (2×10^6 iterations) for the action $S(x)=\cos x$.

$\lvert\beta\rvert$	Phase (deg)	$\langle\cos x\rangle$ (exact)	$\langle\cos x\rangle$ (MC)	$\langle\cos x\rangle$ (Langevin)
1.0	0.0	(0.4464, 0.0000)	(0.4467, 0.0000)	(0.4532, 0.0000)
			(0.0010, 0.0000)	(0.0087, 0.0000)
	10.0	(0.4444, 0.0621)	(0.4445, 0.0621)	(0.4689, 0.0059)
			(0.0011, 0.0001)	(0.0081, 0.0025)
	20.0	(0.4379, 0.1260)	(0.4375, 0.1261)	(0.4924, 0.1058)
			(0.0012, 0.0002)	(0.0202, 0.0167)
	30.0	(0.4255, 0.1933)	(0.4250, 0.1934)	(0.5065, 0,1070)
			(0.0010, 0.0004)	(0.0149, 0.0182)
	60.0	(0.3165, 0.4225)	(0.3173, 0.4221)	(0.3453, 0.0484)
			(0.0015, 0.0007)	(0.0233, 0.0194)
	80.0	(0.1281, 0.5538)	(0.1294, 0.5534)	No convergence
			(0.0014, 0.0007)	
	90.0	(0.0000, 0.5751)	(0.0009, 0.5747)	No convergence
			(0.0015, 0.0007)	
3.0	0.0	(0.8100, 0.0000)	(0.8098, 0.0000)	(0.8109, 0.0000)
			(0.0006, 0.0000)	(0.0049, 0.0000)
	10.0	(0.8141, 0.0386)	(0.8139, 0.0388)	(0.8173, 0.0352)
			(0.0006, 0.0003)	(0.0051, 0.0020)
	20.0	(0.8269, 0.0762)	(0.8269, 0.0765)	(0.8251, 0.0667)
			(0.0005, 0.0005)	(0.0046, 0.0030)
	30.0	(0.8501, 0.1110)	(0.8502, 0.1109)	(0.8479, 0.0976)
			(0.0005, 0.0006)	(0.0041, 0.0038)
	60.0	(1.0200, 0.1125)	(1.0184, 0.1123)	(0.8328, 0.1024)
			(0.0014, 0.0014)	(0.0107, 0.0078)
	80.0	(1.0644, −0.6112)	(1.0625, −0.6098)	No convergence
			(0.0037, 0.0041)	
	90.0	(0.0000, −1.3038)	(0.0055, −1.3059)	No convergence
			(0.0079, 0.0047)	
5.0	0.0	(0.8934, 0.0000)	(0.8929, 0.0000)	(0.8934, 0.0000)
			(0.0004, 0.0000)	(0.0020, 0.0000)
	10.0	(0.8955, 0.0200)	(0.8951, 0.0202)	(0.8952, 0.0197)
			(0.0004, 0.0002)	(0.0021, 0.0007)
	30.0	(0.9116, 0.0555)	(0.9117, 0.0555)	(0.9101, 0.0556)
			(0.0004, 0.0004)	(0.0016, 0.0017)
	45.0	(0.9292, 0.0751)	(0.9292, 0.0754)	(0.9288, 0.0773)
			(0.0005, 0.0004)	(0.0017, 0.0024)
	60.0	(0.9440, 0.0996)	(0.9433, 0.0998)	(0.9486, 0.0908)
			(0.0007, 0.0008)	(0.0035, 0.0031)
	80.0	(1.0614, 0.4612)	(1.0610, 0.4654)	No convergence
			(0.0032, 0.0039)	
	90.0	(0.0000, 1.8445)	(0.0035, 1.8364)	No convergence
			(0.0145, 0.0099)	

TABLE II. Comparison between Monte Carlo results (2×10^6 sweeps) and Langevin results (10^7 iterations) for $\langle x^2\rangle$ for the action $S(x)=\frac{1}{4}x^4$ and $|\beta|=1$.

Phase (deg)	$\langle x^2\rangle$ (exact)	$\langle x^2\rangle$ (MC)	$\langle x^2\rangle$ (Langevin)
0.0	(0.6760, 0.0000)	(0.6762, 0.0000)	(0.6719, 0.0000)
		(0.0008, 0.0000)	(0.0048, 0.0000)
30.0	(0.6529, −0.1750)	(0.6525, −0.1749)	(0.6556, −0.1748)
		(0.0010, 0.0006)	(0.0052, 0.0020)
60.0	(0.5854, −0.3380)	(0.5838, −0.3389)	(0.5820, −0.3347)
		(0.0013, 0.0011)	(0.0050, 0.0042)
80.0	(0.5178, −0.4345)	(0.5161, −0.4358)	(0.5194, −0.4456)
		(0.0029, 0.0029)	(0.0058, 0.0062)

Monte Carlo simulation. In the Langevin method, however, no convergence is obtained when β approaches the imaginary axis. Hamber and Ren attributed this to the infinite number of poles in $\langle \cos x\rangle$ along the imaginary axis, and they found that dt must be smaller than 0.001. We used a smaller dt (0.0005), and we found that for different random number seeds the solution patterns $x(t)$ for up to 10^6 steps ($t=50$) in the complex plane look very different. It seems that for β close to the imaginary axis the stochastic forces affect the stability of the numerical integration procedure seriously and the problem is not only introduced by the discretization (remember that the measuring time is proportional to $1/dt$). On the other hand, when $\beta=i|\beta|$, the average quantity in the Monte Carlo method is

$$\langle F(x)\rangle=\frac{\int_a^b dx\,\exp\{\mathrm{Re}[S(x)]\}F(x)}{\int_a^b dx\,\exp\{\mathrm{Re}[S(x)]\}}=\int_a^b dx\,F(x)\Big/\int_a^b dx\ , \tag{14}$$

where a,b are finite numbers. By the Metropolis algorithm, each move $x\rightarrow x'=(b-a)\mathrm{ran}[0,1]+a$ is always accepted and $[\sum_{i=1}^N F(x_i)]/N$ is nothing but the integral $\int_a^b dx F(x)$ as long as ran[0,1] is a truly uniformly distributed random number. So for this model, the Monte Carlo method clearly has better convergence than the Langevin method and is more reliable.

The second example studied was the noncompact action

$$S(x)=\tfrac{1}{4}x^4\ . \tag{15}$$

The exact statistical average is easy to evaluate:[3]

$$\langle x^{2n}\rangle=\left[\frac{4}{\beta}\right]^{n/2}\left[\Gamma\left[\frac{n}{2}+\frac{1}{4}\right]\Big/\Gamma\left[\frac{1}{4}\right]\right]\ , \tag{16}$$

where $\Gamma(z)$ is the usual Γ function. For this model, the statistical integral is meaningless for $\mathrm{Re}\beta<0$ and both the Monte Carlo and Langevin methods converge only for $\mathrm{Re}\beta>0$. We calculated $\langle x^2\rangle$ and $\langle x^4\rangle$ using both Monte Carlo and Langevin methods. The associated Langevin equation is

$$dx/dt=-\beta x^3+\eta(t)\ , \tag{17}$$

and a simple finite-difference form of this equation is

$$x_{i+1}=x_i-dt\,\beta x_i^3+\sqrt{24dt}\,\eta_i\ . \tag{18}$$

In this case, the computer time for one iteration in the Langevin equation is four times less than for the Monte Carlo, so we did 10^7 iterations for the Langevin equation and 2×10^6 iterations for the Monte Carlo equation. We chose $dt=0.001$ here and did several runs for the same β due to the same reasons as before. The results for $|\beta|=1$ and various values of the phase are shown in Table II and Table III. For $\langle x^2\rangle$ Monte Carlo again gives substantially smaller statistical errors for the same amount of computer time. For $\langle x^4\rangle$ and large phase angle the errors are comparable in both methods. However, the Langevin solution sometimes blows up as one gets closer to the imaginary axis and we only show the best results obtained; the Monte Carlo solution is much more stable. We also tried the Langevin method for $\mathrm{Re}\beta<0$. There we again found that the solution pattern $x(t)$ in the complex plane is strongly

TABLE III. Same as Table II, for $\langle x^4\rangle$.

Phase (deg)	$\langle x^4\rangle$ (exact)	$\langle x^4\rangle$ (MC)	$\langle x^4\rangle$ (Langevin)
0.0	(1.0000, 0.0000)	(1.0008, 0.0000)	(1.0050, 0.0000)
		(0.0023, 0.0000)	(0.0115, 0.0000)
30.0	(0.8660, −0.5000)	(0.8664, −0.4993)	(0.8771, −0.5040)
		(0.0024, 0.0024)	(0.0113, 0.0079)
60.0	(0.5000, −0.8660)	(0.5004, −0.8699)	(0.5060, −0.8804)
		(0.0049, 0.0060)	(0.0076, 0.0139)
80.0	(0.1736, −0.9848)	(0.1662, −0.9797)	(0.1796, −0.9828)
		(0.0173, 0.0167)	(0.0107, 0.0166)

dependent on the initial conditions, even if one uses a small dt, and it is not possible to obtain convergence to the analytic continuation of Eq. (16), contrary to the conclusion of Hamber and Ren.[3]

In summary, we have shown that the Monte Carlo method can also be used to deal with complex actions and gives better answers than the Langevin method for two simple examples. Thus, at present there is no evidence that the Langevin method is superior to the Monte Carlo method for systems with complex actions, contrary to what seems to be widely believed.

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