New method for the extrapolation of finite-size data to infinite volume

Sergio Caracciolo\textsuperscript{a}, Robert G. Edwards\textsuperscript{b}, Sabino J. Ferreira\textsuperscript{c}, Andrea Pelissetto\textsuperscript{d} and Alan D. Sokal\textsuperscript{e,}\textsuperscript{*}

\textsuperscript{a}Dipartimento di Fisica and INFN, Università degli Studi di Lecce, Lecce 73100, ITALIA
\textsuperscript{b}SCRI, Florida State University, Tallahassee, FL 32306, USA
\textsuperscript{c}Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, MG 30161, BRASIL
\textsuperscript{d}Dipartimento di Fisica and INFN – Sezione di Pisa, Università degli Studi di Pisa, Pisa 56100, ITALIA
\textsuperscript{e}Department of Physics, New York University, 4 Washington Place, New York, NY 10003, USA

We present a simple and powerful method for extrapolating finite-volume Monte Carlo data to infinite volume, based on finite-size-scaling theory. We discuss carefully its systematic and statistical errors, and we illustrate it using three examples: the two-dimensional three-state Potts antiferromagnet on the square lattice, and the two-dimensional \(O(3)\) and \(O(\infty)\) \(\sigma\)-models. In favorable cases it is possible to obtain reliable extrapolations (errors of a few percent) even when the correlation length is 1000 times larger than the lattice.

Quantum field theorists are interested primarily in infinite systems; but Monte Carlo simulations must perforce be carried out on lattices of finite linear size \(L\), limited by computer memory and speed. This raises the problem of extrapolating finite-volume data to \(L = \infty\). We present here a simple and powerful method for performing this extrapolation, based on finite-size-scaling theory [1]; and we discuss carefully its systematic and statistical errors. We illustrate the method using three examples: the two-dimensional three-state Potts antiferromagnet on the square lattice [2], and the two-dimensional \(O(3)\) and \(O(\infty)\) \(\sigma\)-models [3,4]. We have found — much to our surprise — that in favorable cases it is possible to obtain reliable extrapolations (errors of a few percent) at \(\xi / L\) as large as 10–1000. More details can be found in [5].

Consider, for starters, a model controlled by a renormalization-group (RG) fixed point having \textit{one} relevant operator. Let us work on a periodic lattice of linear size \(L\). Let \(\xi(\beta, L)\) be a suitably defined finite-volume correlation length (we use the second-moment correlation length defined by equations (4.11)–(4.13) of [6]), and let \(\mathcal{O}\) be any long-distance observable (e.g. the correlation length or the susceptibility). Then finite-size-scaling theory [1] predicts that

\[
\frac{\mathcal{O}(\beta, L)}{\mathcal{O}(\beta, \infty)} = f_\mathcal{O} \left( \frac{\xi(\beta, \infty)}{L} \right) + O(\xi^{-\omega}, L^{-\omega})
\]

where \(f_\mathcal{O}\) is a universal function and \(\omega\) is a correction-to-scaling exponent. Hence, if \(s\) is any fixed scale factor (usually we take \(s = 2\)),

\[
\frac{\mathcal{O}(\beta, sL)}{\mathcal{O}(\beta, L)} = F_\mathcal{O} \left( \frac{\xi(\beta, L)}{L} \right) + O(\xi^{-\omega}, L^{-\omega})
\]

where \(F_\mathcal{O}\) can be expressed in terms of \(f_\mathcal{O}, f_k\).

Our method proceeds as follows [7]: Make Monte Carlo runs at numerous pairs \((\beta, L)\) and \((\beta, sL)\). Plot \(\mathcal{O}(\beta, sL)/\mathcal{O}(\beta, L)\) versus \(\xi(\beta, L)/L\), using those points satisfying both \(\xi(\beta, L) \geq \xi_{\text{min}}\) and \(L \geq \text{some value} L_{\text{min}}\). If all these points fall with good accuracy on a single curve — thus verifying the Ansatz (2) for \(\xi \geq \xi_{\text{min}}, L \geq L_{\text{min}}\) — choose a smooth fitting function \(F_\mathcal{O}\). Then, using the functions \(F_\xi\) and \(F_\mathcal{O}\), extrapolate the pair \((\xi, \mathcal{O})\) successively from \(L \rightarrow sL \rightarrow s^2L \rightarrow \ldots \rightarrow \infty\).

We have chosen to use functions \(F_\mathcal{O}\) of the form

\[
F_\mathcal{O}(x) = 1 + a_1 e^{-1/x} + \ldots + a_n e^{-n/x}
\]

This form is partially motivated by theory, which tells us that \(F(x) \rightarrow 1\) exponentially fast as \(x \rightarrow \infty\)
0 [10]. Typically a fit of order $3 \leq n \leq 12$ is sufficient; we increase $n$ until the $\chi^2$ of the fit becomes essentially constant. The resulting $\chi^2$ value provides a check on the systematic errors arising from corrections to scaling and/or from the inadequacies of the form (3).

The statistical error on the extrapolated value of $O_\infty(\beta) \equiv O(\beta, \infty)$ comes from three sources: (i) error on $O(\beta, L)$, which gets multiplicatively propagated to $O_\infty$; (ii) error on $\xi(\beta, L)$, which affects the argument $x \equiv \xi(\beta, L)/L$ of the scaling functions $F_\xi$ and $F_\omega$; and (iii) statistical error in our estimate of the coefficients $a_1, \ldots, a_n$ in $F_\xi$ and $F_\omega$. The errors of type (i) and (ii) depend on the statistics available at the single point $(\beta, L)$, while the error of type (iii) depends on the statistics in the whole set of runs. Errors (i)+(ii) [resp. (i)+(ii)+(iii)] can be quantified by performing a Monte Carlo experiment in which the input data at $(\beta, L)$ [resp. the whole set of input data] are varied randomly within their error bars and then extrapolated.

The discrepancies between the extrapolated values from different lattice sizes at the same $\beta$ — to the extent that these exceed the estimated statistical errors — indicate the presence of systematic errors and thus the necessity of increasing $L_{\text{min}}$ and/or $\xi_{\text{min}}$ and/or $n$.

A figure of (de)merit of the method is the relative variance on the extrapolated value $O_\infty(\beta)$, multiplied by the computer time needed to obtain it. We expect this relative variance-time product [for errors (i)+(ii) only] to scale as

$$\text{RVTP}(\beta, L) \approx \xi_\infty(\beta)^{d+z_{\text{int}G}} \xi_{\text{C}} \left( \frac{\xi_\infty(\beta)}{L} \right)$$

where $d$ is the spatial dimension and $z_{\text{int}G}$ is the dynamic critical exponent of the Monte Carlo algorithm being used; here $\xi_{\text{C}}$ is a combination of several static and dynamic finite-size-scaling functions, and depends both on the observable $O$ and on the algorithm but not on the scale factor $s$. As $\xi_\infty/L$ tends to zero, we expect $\xi_{\text{C}}$ to diverge as $(\xi_\infty/L)^{-d}$ (it is wasteful to use a lattice $L \gg \xi_\infty$). As $\xi_\infty/L$ tends to infinity, we expect $\xi_{\text{C}} \sim (\xi_\infty/L)^p$ [5], but the power $p$ can be either positive or negative. If $p > 0$, there is an optimum value of $\xi_\infty/L$; this determines the best lattice size at which to perform runs for a given $\beta$. If $p < 0$, it is most efficient to use the smallest lattice size for which the corrections to scaling are negligible compared to the statistical errors.

Our first example [2] is the two-dimensional three-state Potts antiferromagnet on the square lattice, which is believed to have a critical point at $\beta = \infty$ [11]. We used the Wang-Swendsen-Koteckê cluster algorithm [12], which appears to have no critical slowing-down ($\tau_{\text{int,M} \approx \text{avg} < 5$ uniformly in $\beta$ and $L$) [2]. We ran on lattices $L = 32, 64, 128, 256, 512, 1024, 1536$ at 153 different pairs $(\beta, L)$ in the range $5 \leq \xi_\infty \leq 20000$. Each run was between $2 \times 10^5$ and $2.2 \times 10^7$ iterations, and the total CPU time was modest by our standards (about 2 years on an IBM RS-6000/370). We took $\xi_{\text{min}} = 10$ and $L_{\text{min}} = 128$ and used a quintic fit in (3); the result for $F_\xi$ is shown in [2,9] ($\chi^2 = 75.41, 66$ DF, level = 20%). The extrapolated values from different lattice sizes at the same $\beta$ agree within the estimated statistical errors ($\chi^2 = 43.08, 75$ DF, level > 99%). The result for $G_\xi$ is shown in [5]; the errors are roughly constant for $\xi_\infty/L \geq 0.4$ but rise sharply for smaller $\xi_\infty/L$. In practice we were able to obtain $\xi_\infty$ to an accuracy of about 1% (resp. 2%, 3%, 5%) at $\xi_\infty \approx 1000$ (resp. 2000, 5000, 10000).

Next let us consider [3,4] the two-dimensional $O(3)$ $\sigma$-model (see Caracciolo’s talk for more details). We used the Wolff embedding algorithm with standard Swendsen-Wang updates; again critical slowing-down appears to be completely eliminated. We ran on lattices $L = 32, 48, 64, 96, 128, 192, 256, 384, 512$ at 180 different pairs $(\beta, L)$ in the range $20 \leq \xi_\infty \leq 10^2$. Each run was between $10^5$ and $5 \times 10^6$ iterations, and the total CPU time was 7 years on an IBM RS-6000/370. We took $\xi_{\text{min}} = 20$ and used a tenth-order fit. There appear to be weak corrections to scaling (of order $\leq 1.5\%$) in the region $0.3 \leq \xi_L/L \leq 0.7$ for lattices with $L \leq 64-96$. We therefore chose $L_{\text{min}} = 128$ for $\xi_L/L \leq 0.7$, and $L_{\text{min}} = 64$ for $\xi_L/L > 0.7$. The result for $F_\xi$ is shown in [4,5] ($\chi^2 = 72.91, 73$ DF, level = 48%). The result for $G_\xi$ is shown in [5]; at large $\xi_\infty/L$ it decreases sharply, with a power $p \approx -2$ in agree-
ment with theory [5]. In practice we obtained $\xi_\infty$ to an accuracy of about 0.2% (resp. 0.7%, 1.1%, 1.6%) at $\xi_\infty \approx 10^3$ (resp. $10^4$, $10^5$, $10^6$).

We also carried out a "simulated Monte Carlo" experiment for the $O(N)$ $\sigma$-model at $N = \infty$, by generating data from the exact finite-volume solution plus random noise of 0.1% for $L = 64, 96, 128, 0.2\%$ for $L = 192, 256$ and 0.5% for $L = 384, 512$ [which is the order of magnitude we attain in practice for $O(3)$]. We considered 35 values of $\beta$ in the range $20 \leq \xi_\infty \leq 10^6$. We used $\xi_{\text{min}} = 20$ and $L_{\text{min}} = 64$ (in fact much smaller values could have been used, as corrections to scaling are here very small) and a ninth-order fit; for two different data sets we get $\chi^2 = 114$ (resp. 118) with 166 DF. In practice we obtain $\xi_\infty$ with an accuracy of 0.6% (resp. 1.2%, 2%, 3%) at $\xi_\infty \approx 10^3$ (resp. $10^4$, $10^5$, $10^6$).

Here we can also compare the extrapolated values $\xi_\infty^{\text{extr}}(\beta)$ with the exact values $\xi_\infty^{\text{exact}}(\beta)$. Defining $R = \sum_\beta |\xi_\infty^{\text{extr}}(\beta) - \xi_\infty^{\text{exact}}(\beta)|^2 / \sigma^2(\beta)$, we find for the two data sets $R = 17.19$ (resp. 25.81) with 35 DF. Only 6 (resp. 9) points differ from the exact value more than one standard deviation, and none by more than two.

Details on all of these models will be reported separately [2,4].

The method is easily generalized to a model controlled by an RG fixed point having $k$ relevant operators. It suffices to choose $k - 1$ dimensionless ratios of long-distance observables, call them $R = (R_1, \ldots, R_{k-1})$; then the function $F_\beta$ will depend parametrically on $R(\beta, L)$. In practice one can divide $R$-space into "slices" within which $F_\beta$ is empirically constant within error bars, and perform the fit (3) within each slice. We have used this approach to study the mixed isovector/isotensor $\sigma$-model, taking $R$ to be the ratio of isovector to isotensor correlation length [3,4].

The method can also be applied to extrapolate the exponential correlation length (inverse mass gap). For this purpose one must work in a system of size $L^{d-1} \times T$ with $T \gg \xi_{\text{exp}}(\beta, L)$ (cf. [8]).

We wish to thank Martin Hasenbusch and especially Jae-Kwon Kim for sharing their data with us, and for challenging us to push to ever larger values of $\xi / L$. This research was supported by CNR, INFN, CNPq, FAPEMIG, DOE contracts DE-FG05-85ER25000 and DE-FG05-92ER40742, NSF grant DMS-9200719, and NATO CRG 910251.

REFERENCES

2. S.J. Ferreira and A.D. Sokal, hep-lat/9405015; and in preparation.
7. Our method has many features in common with those of Lüscher, Weisz and Wolff [8] and Kim [9]. In particular, all these methods share the property of working only with observable quantities ($\xi$, $O$ and $L$) and not with bare quantities ($\beta$). Therefore, they rely only on "scaling" and not on "asymptotic scaling"; and they differ from other FSS-based methods such as phenomenological renormalization.