Cross-correlations in scaling analyses of phase transitions

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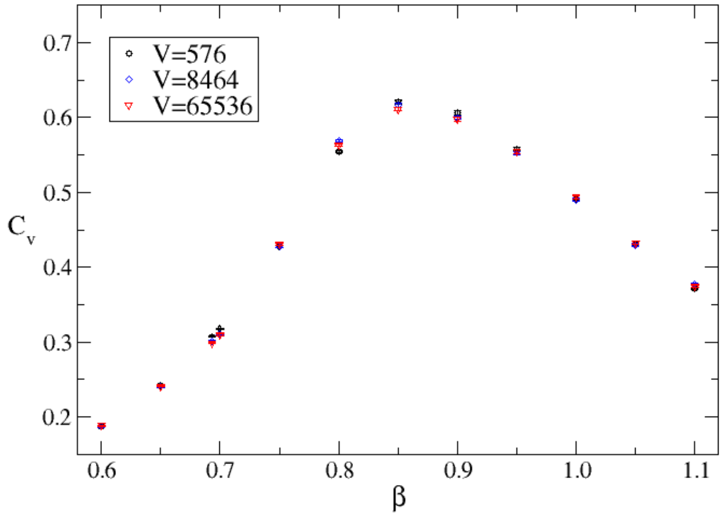
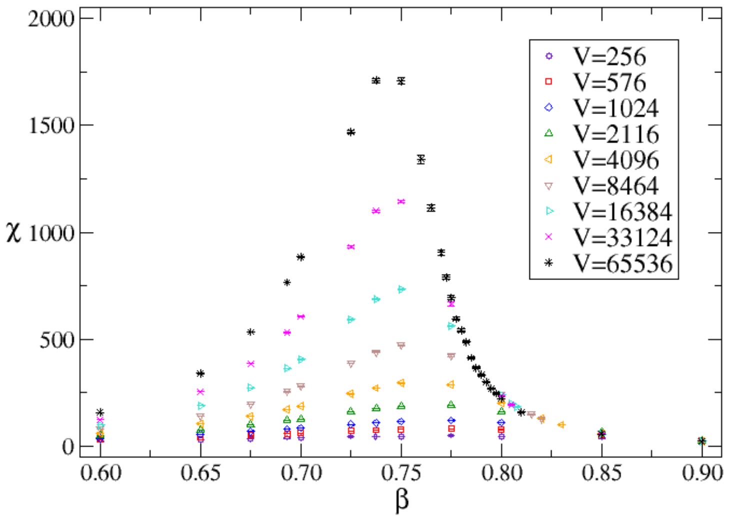
Traditional MCMC simulation study:

Large number of independent simulations for different observables, temperatures, lattice sizes, fields etc.





Traditional MCMC simulation study:

Thermal or finite-size scaling analysis in the vicinity of a phase transition point. Different approaches, one standard technique: consider the maxima of observables,

$$A_{\max}(L) = A_0 L^{\kappa/\nu}(1 + A_1 L^{-\omega} + \ldots)$$

and interpret ν as shift exponent:

$$\beta_{\max}(A, L) - \beta_c = B_0 L^{-1/\nu}(1 + \ldots)$$

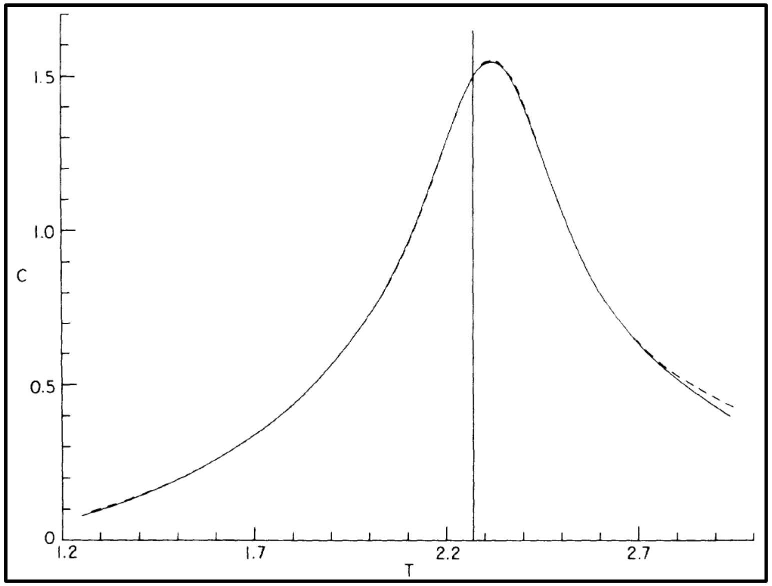
Hence, one needs to perform a number of simulations to track the locations of the maxima, allowing to extract critical exponents, amplitude ratios and the transition coupling.

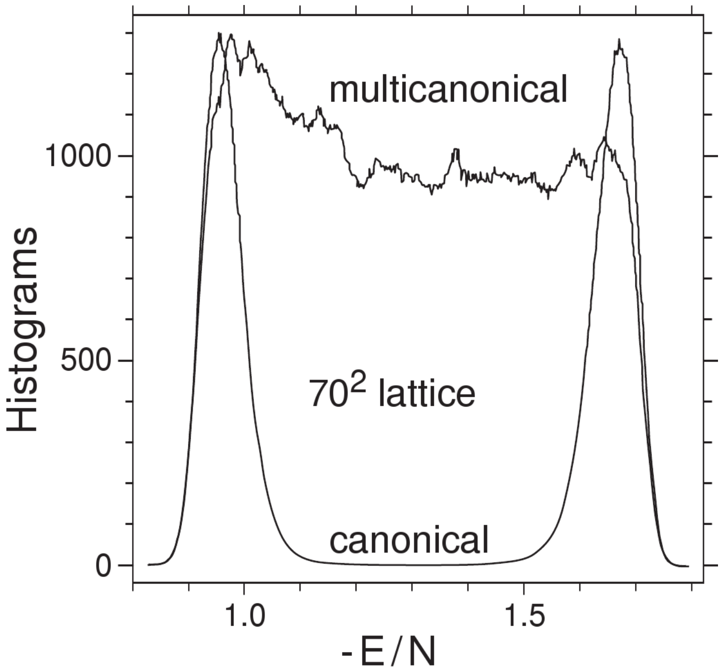
→ Almost unfeasible for larger system sizes!

(Multi-)Histogram reweighting:

Use data from a single simulation at inverse temperature β_0 to extrapolate to $\beta \neq \beta_0$:

$$\hat{A}(\beta) = \frac{\sum_i A_i e^{-(\beta-\beta_0) E_i}}{\sum_i e^{-(\beta-\beta_0) E_i}}$$





Multicanonical/Flat histogram simulation:

One effectively estimates the density of states $\Omega(E)$ to compute

$$\hat{A}(\beta) = \sum_E A(E) \hat{\Omega}(E) e^{-\beta E}$$

Finite-size scaling analysis:

To be specific, consider the FSS analysis of a magnetic system with a continuous phase transition. One standard method (Ferrenberg, Landau, 1991):

- Determine exponent ν via the scaling of the Binder parameter and the logarithmic magnetization derivatives,

$$\left.\frac{dU_{2k}}{d\beta}\right|_{\max} = U_{k,0}L^{1/\nu}(1+U_{k,c}L^{-\omega}+\ldots)$$

$$\left.\frac{d\ln\langle|m|\rangle^{k}}{d\beta}\right|_{\max} = D_{k,0}L^{1/\nu}(1+D_{k,c}L^{-\omega}+\ldots)$$

for $k=1,2,3,\ldots$

Finite-size scaling analysis:

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- Use this value of ν to determine remaining exponents via

$$C_{V,\max}(L) = C_{V,0} L^{\alpha/\nu}(1+\ldots)$$

$$\chi_{\max}(L) = \chi_0 L^{\gamma/\nu}(1+\ldots)$$

$$m_{\inf}(L) = m_0 L^{-\beta/\nu}(1+\ldots)$$

etc.

Finite-size scaling analysis:

To be specific, consider the FSS analysis of a magnetic system with a continuous phase transition. One standard method (Ferrenberg, Landau, 1991):

- As well as the transition coupling via

$$\beta_{\max}(A, L) - \beta_c = B_0 L^{-1/\nu}(1 + \ldots)$$

with

$$A \in \left\{ C_V, \frac{d|m|}{d\beta}, \chi, \frac{d \ln \langle |m|^k \rangle}{d\beta}, \frac{d U_{2k}}{d\beta} \right\}$$

etc.

Finite-size scaling analysis:

This results in a series of estimates for ν ,

$$\{\hat{\nu}_{1,}\hat{\nu}_{2,}\hat{\nu}_{3,}\ldots\}$$

and a similar series of estimates of β as well as possibly further quantities.

How do we find a best final estimate from these?

Final estimates:

Several recipes in use: $\{\hat{x}_1, \ldots, \hat{x}_n\}$

- Use single most precise estimate

Or take an average:

$$\bar{x} = \sum_i \alpha_i \hat{x}_i$$

- Plain average:

$$\alpha_i = 1/n$$

- Error-weighted mean:

$$\alpha_i = Z^{-1} \frac{1}{\sigma^2(\hat{x}_i)}$$

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→ Optimal for uncorrelated data, but $\hat{x}_i$ come from the same simulation!

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- Covariance-weighted mean:

$$\alpha_i = Z^{-1} \sum_j [\Gamma(\hat{x})^{-1}]_{ji}$$

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Or take an average:

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Similarly for variance of averages:

- No correlations:

$$\sigma^2_{\text{uncorr}}(\bar{x}) = \sum_i \alpha_i^2 \sigma^2(\hat{x}_i)$$

- Including correlations:

$$\sigma^2_{\text{corr}}(\bar{x}) = \sum_{i,j} \alpha_i \alpha_j \Gamma_{ij}(\hat{x})$$

Bean-counting: does it really matter?

Check it out with some examples:

Finite-size scaling analysis of the critical points of the FM Ising model in two and three dimensions.

- Single-cluster update simulations at or close to T_c.
- One simulation per lattice size.
- Extract maxima data from histogram reweighting.
- Estimates of ν from maxima of

$$\frac{d\ln\langle|m|\rangle}{d\beta}, \frac{d\ln\langle|m|^2\rangle}{d\beta}, \frac{d\ln\langle|m|^3\rangle}{d\beta}, \frac{dU_2}{d\beta}, \frac{dU_4}{d\beta}$$

- Error estimates from jackknife analysis.
- Estimate covariance matrix via

$$\widehat{\mathrm{COV}}(\hat{\nu}_i, \hat{\nu}_j) = \frac{n-1}{n}\sum_{s=1}^{n}[\hat{\nu}_{i(s)} - \hat{\nu}_{i(.)}][\hat{\nu}_{j(s)} - \hat{\nu}_{j(.)}]$$

2D Ising model:

- Simulations at $\beta_c = 0.440686794...$
- Lattice sizes $L = 16, 24, \ldots, 192.$

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- Lattice sizes $L = 16, 24, \ldots, 192$.
- Correlation coefficients $\rho_{ij} = \Gamma_{ij}/\sigma_i\sigma_j$ and weights:

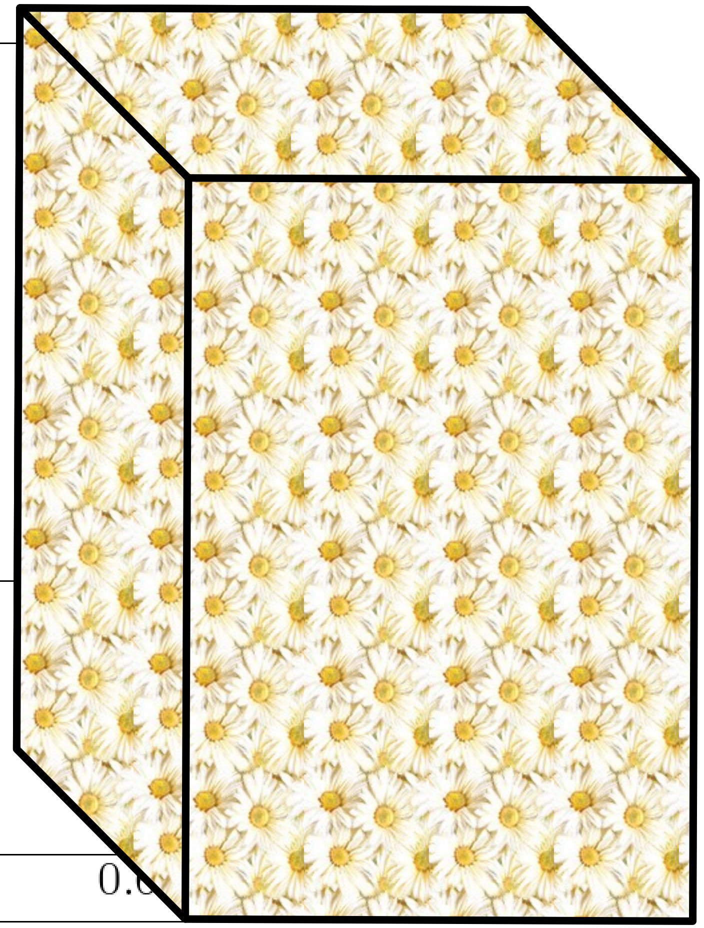
	$\frac{d\ln\langle\vert m\vert\rangle}{d\beta}$	$\frac{d\ln\langle m^2\rangle}{d\beta}$	$\frac{d\ln\langle\vert m\vert^3\rangle}{d\beta}$	$\frac{dU_2}{d\beta}$	$\frac{dU_4}{d\beta}$
$\frac{d\ln\langle\vert m\vert\rangle}{d\beta}$	1.000	0.974	0.939	0.920	0.897
$\frac{d\ln\langle m^2\rangle}{d\beta}$	0.974	1.000	0.991	0.817	0.869
$\frac{d\ln\langle\vert m\vert^3\rangle}{d\beta}$	0.939	0.991	1.000	0.743	0.820
$\frac{dU_2}{d\beta}$	0.920	0.817	0.743	1.000	0.860
$\frac{dU_4}{d\beta}$	0.897	0.869	0.820	0.860	1.000
$\alpha_{i,\mathrm{plain}}$	1.000	1.000	1.000	1.000	1.000
$\alpha_{i,\mathrm{err}}$	0.315	0.271	0.248	0.034	0.132
$\alpha_{i,\mathrm{cov}}$	5.007	−2.426	−0.281	−0.104	−1.196

Case study: 2D Ising model

2D Ising model:

Exponent estimates and averages

		2D		3D
		ν	σ	
$\frac{\mathrm{d}\ln\langle\lvert m\rvert\rangle}{\mathrm{d}\beta}$		1.0085	0.0183	
$\frac{\mathrm{d}\ln\langle m^2\rangle}{\mathrm{d}\beta}$		1.0128	0.0194	
$\frac{\mathrm{d}\ln\langle\lvert m\rvert^3\rangle}{\mathrm{d}\beta}$		1.0175	0.0201	
$\frac{\mathrm{d}U_2}{\mathrm{d}\beta}$		1.0098	0.0281	
$\frac{\mathrm{d}U_4}{\mathrm{d}\beta}$		1.0149	0.0511	
$\bar{x}_{\mathrm{plain}}$	σ_{uncorr}	1.0127	0.0141	
	σ_{corr}		0.0269	
$\bar{x}_{\mathrm{err}}$	σ_{uncorr}	1.0123	0.0102	
	σ_{corr}		0.0208	
$\bar{x}_{\mathrm{cov}}$	σ_{corr}	0.9935	0.0078	
reference value		1		0.[illegible]



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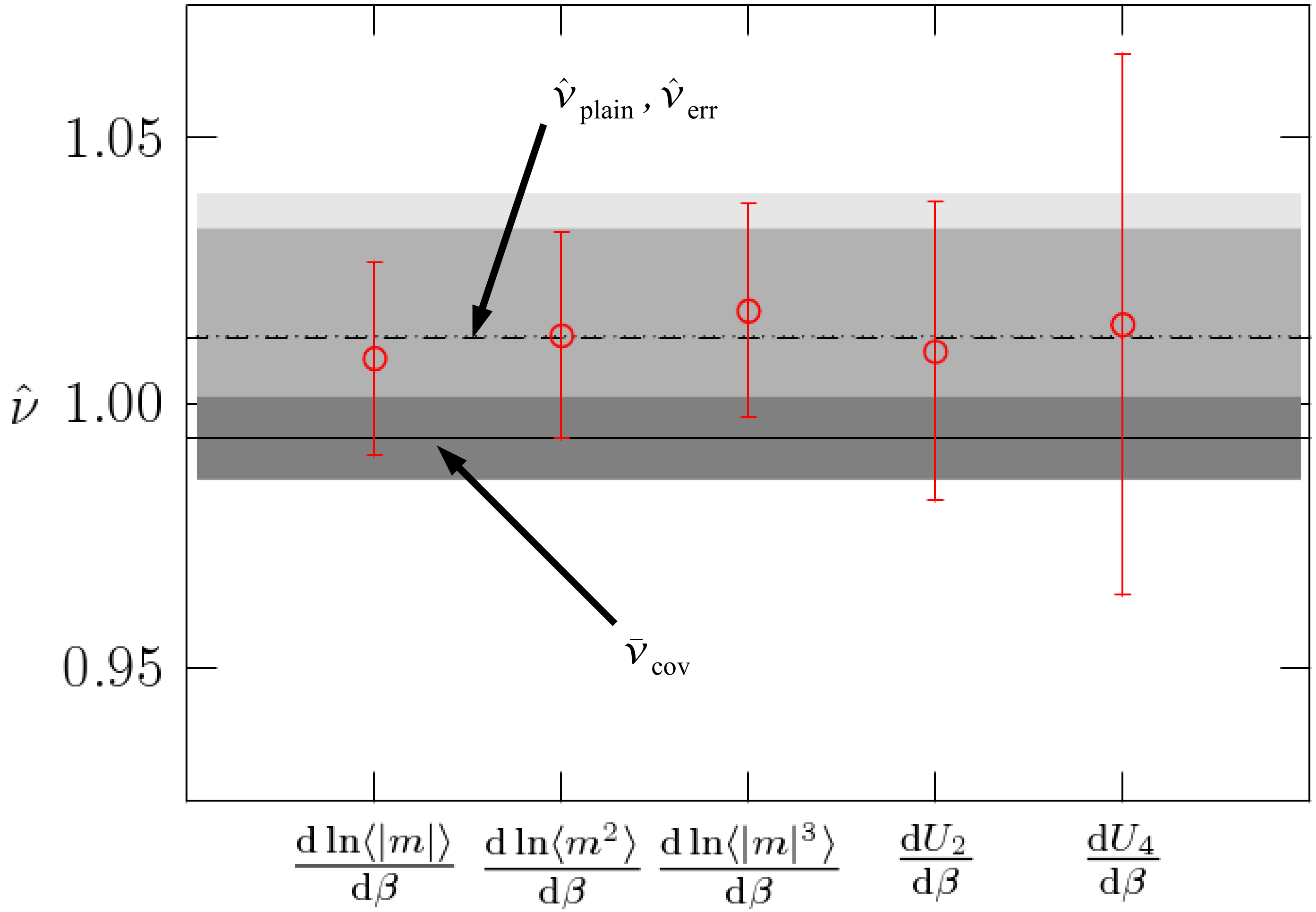
2D Ising model:



3D Ising model:

- Simulations at $\beta_c \approx 0.22165459$.
- Lattice sizes $L = 8, 12, 16, \ldots, 128$.

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3D Ising model:

Exponent estimates and averages

		2D		3D
		ν	σ	
$\frac{\mathrm{d}\ln\langle\lvert m\rvert\rangle}{\mathrm{d}\beta}$		1.0085	0.0183	
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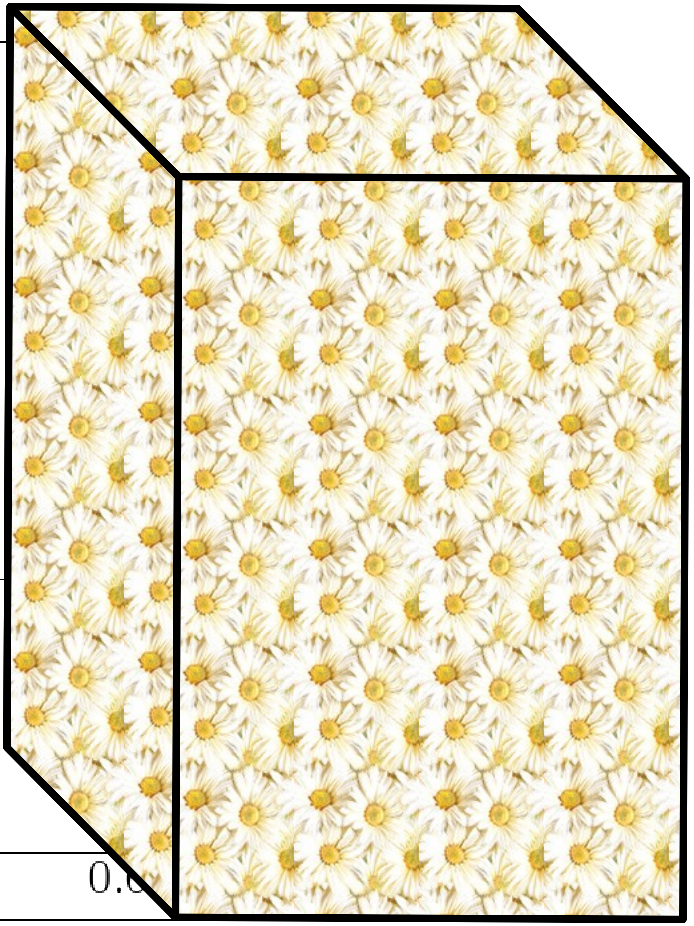

Case study: 3D Ising model

2D Ising model:

Exponent estimates and averages

		2D		3D	
		ν	σ	ν	σ
$\frac{\mathrm{d}\ln\langle\lvert m\rvert\rangle}{\mathrm{d}\beta}$		1.0085	0.0183	0.6358	0.0127
$\frac{\mathrm{d}\ln\langle m^2\rangle}{\mathrm{d}\beta}$		1.0128	0.0194	0.6340	0.0086
$\frac{\mathrm{d}\ln\langle\lvert m\rvert^3\rangle}{\mathrm{d}\beta}$		1.0175	0.0201	0.6326	0.0062
$\frac{\mathrm{d}U_2}{\mathrm{d}\beta}$		1.0098	0.0281	0.6313	0.0020
$\frac{\mathrm{d}U_4}{\mathrm{d}\beta}$		1.0149	0.0511	0.6330	0.0024
$\bar{x}_{\mathrm{plain}}$	σ_{uncorr}	1.0127	0.0141	0.6334	0.0038
	σ_{corr}		0.0269		0.0067
$\bar{x}_{\mathrm{err}}$	σ_{uncorr}	1.0123	0.0102	0.6322	0.0015
	σ_{corr}		0.0208		0.0024
$\bar{x}_{\mathrm{cov}}$	σ_{corr}	0.9935	0.0078	0.6300	0.0017
reference value		1		0.6301	0.0004

Correlations between *different* exponents:

Similar effects occur between estimates of different exponents. Consider, e.g., renormalization group eigenvalues,

$$\begin{aligned} \alpha &= 2 - d/y_t, \\ \beta &= (d - y_h)/y_t, \\ \gamma &= (2y_h - d)/y_t, \\ \delta &= y_h/(d - y_h), \\ \eta &= d + 2 - 2y_h, \\ \nu &= 1/y_t. \end{aligned}$$

and the associated scaling dimensions $x_i = d - y_i$.

Then one has, for instance:

$$d/2 - \gamma/2\nu = x_\sigma = \beta/\nu$$

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Correlations between *different* exponents:

Estimate β/ν and γ/ν from

$$\langle|m|\rangle_{\inf}(L)=m_0 L^{-\beta/\nu}$$

$$\chi_{\max}(L)=\chi_0 L^{\gamma/\nu}$$

and compute $d/2-\gamma/2\nu=x_\sigma=\beta/\nu$:

Correlations between *different* exponents:

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and compute $d/2 - \gamma/2\nu = x_\sigma = \beta/\nu$:

		fits		corr. coeff./weights	
		x_σ	σ	$\langle\vert m\vert\rangle_{\text{inf}}$	$\chi_{\max}$
$\langle\vert m\vert\rangle_{\text{inf}}$		0.1167	0.0054	1.0000	−0.6414
$\chi_{\max}$		0.1271	0.0020	−0.6414	1.0000
$\bar{x}_{\text{plain}}$	σ_{uncorr}	0.1219	0.0027	1.0000	1.0000
	σ_{corr}		0.0021		
$\bar{x}_{\text{err}}$	σ_{uncorr}	0.1261	0.0016	0.0944	0.9056
	σ_{corr}		0.0013		
$\bar{x}_{\text{cov}}$	σ_{corr}	0.1250	0.0010	0.2050	0.7950
reference value		0.125			

Conclusions:

- Substantial cross-correlations between different estimates from single simulation/series of simulations.

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$$\widehat{\mathrm{COV}}(\hat{v}_i, \hat{v}_j) = \frac{n-1}{n} \sum_{s=1}^{n} [\hat{v}_{i(s)} - \hat{v}_{i(.)}][\hat{v}_{j(s)} - \hat{v}_{j(.)}]$$

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- The usual rules of thumb don't (always) work.
- Doing it right can be equivalent to 10-fold simulation time at (almost) not cost.
- Not specific to case study at hand: works (or should work) for
  - different observables: further exponents, transition temperature
  - different situations: soft matter, quantum criticality, first-order transitions
  - Preprint arXiv:0811.3097