

Cumulative Errata:

A memorandum of minor miscellaneous mistakes.

<http://threeplusone.com/errata>

Gavin E. Crooks

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References

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- [4] G. E. Crooks. Path-ensemble averages in systems driven far from equilibrium. *Phys. Rev. E*, 61(3):2361–2366, 2000. doi:10.1103/PhysRevE.61.2361. (page 2).
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- [13] D. A. Sivak and G. E. Crooks. Thermodynamic metrics and optimal paths. *Phys. Rev. Lett.*, 108(19):190602, 2012. doi:10.1103/PhysRevLett.108.190602. (page 3).

1 Gaussian Statistics Of The Hard-Sphere Fluid (1997) [1]

The lines in Fig. 3 are mislabeled. The dashed line is the fit to the data using an uninformative prior, while the solid line is a fit using the ideal gas prior. The final line of this paper should read "This work was supported by NSF grant number CHE-9508336."

2 Nonequilibrium measurements of free energy differences for microscopically reversible Markovian systems (1998) [2]

The final line of this paper should read "This work was supported by NSF grant number CHE-9508336."

3 Excursions in Statistical Dynamics (1999) [3]

Chapter 1: Missing $M(1)$ After Eq. 1.2, i.e. $M = (M(0), M(1), \dots, M(t-1))$; Section 1.3 (p13), $U(t_3, t_1) = U(t_3, t_2)U(t_2, t_1)$ not $U(t_2, t_1) = U(t_3, t_2)U(t_2, t_1)$;

Eq. 1.19, sign error, should be $-\beta Q$.

Chapter 3: Eq. 3.3 should read $\ln \rho(x(\tau)) - \ln \rho(x(0)) - \beta Q(x(\tau))$ (Sign error, and $x(\tau)$ not $x(t)$). [Kudos: Josh Silverman]

Chapter 4: Free Energies From Nonequilibrium Work Measurements Eq 4.5, wrong sign 3rd line; The statement of Jensen's inequality after Eq 4.15 is should read $\langle \exp(x) \rangle \geq \exp(\langle x \rangle)$ [Kudos: Grant Rotskoff]; Something is wrong with Eq. 4.22, I just haven't got around to figuring out what it is.

Chapter 5: Response theory: The first sentence of the last paragraph of Section 5.3 should read "An approximation for the nonequilibrium entropy can be derived from this expression by substituting the explicit canonical equilibrium probability and ..". The original sounds awful.

The "plausible" approximations in this chapter, from Eq. 5.8 onwards, turn out to be wrong! See "Near-equilibrium measurements of nonequilibrium free energy" by David A. Sivak and myself for the correct answers.

Chapter 7: Pathways to evaporation: Equation 7.3 has several sign errors. It should read

$$P(s(t, i)) = \frac{\exp\left(+\beta H s(t, i) + \beta J \sum_{\{j: <i, j>\}} s(t, i) s(t-1, j)\right)}{2 \cosh\left(-\beta H - \beta J \sum_{\{j: <i, j>\}} s(t-1, j)\right)}$$

There are several misplaced brackets in Eq. 7.4.

$$\frac{\mathcal{P}[s(t, i) = +1, \mathbf{s}]}{\mathcal{P}[s(t, i) = -1, \mathbf{s}]} = \exp\left(+2\beta H + 2\beta J \sum_{\substack{\{j: <i, j>\}, \\ \theta = \pm 1}} s(t + \theta, j)\right) \times \prod_{\{i: <i, j>\}} \left[\frac{\cosh\left(\beta H + \beta J \left(\sum_{\{k: <j, k>, k \neq i\}} s(t, k) - 1\right)\right)}{\cosh\left(\beta H + \beta J \left(\sum_{\{k: <j, k>, k \neq i\}} s(t, k) + 1\right)\right)} \right]$$

Appendix A: Simulation of Langevin Dynamics. It's really not a good idea to use this algorithm to simulate driven Langevin dynamics. See [Using nonequilibrium fluctuation theorems to understand and correct errors in equilibrium and nonequilibrium discrete Langevin dynamics](#), David A. Sivak, John D. Chodera, Gavin E. Crooks (2013) for a discussion of the problem and alternative integrators.

References: Reference 52 contains an extra period.

Minor typos :

Page 6: "flow of energy into into the system"

Page 9: "states energies"

Page 41: "because not only because" in the last sentence of second paragraph

Page 43: "failure can occurs" in last sentence of first para

Page 45: "are essential the same" in the caption

Page 52: parenthetical comment in first para is hard to parse

Page 54: "can derived" should be "can be derived" in second sentence

Page 56: "partial due" should be "partially due" in the caption

[Kudos: Xuenan Li, David Sivak]

4 Path-ensemble averages in systems driven far from equilibrium (2000) [4]

Eq. 14 contains various typos.

5 Statistical Evaluation Of Pairwise Protein Sequence Comparison With The Bayesian Bootstrap, *Bioinformatics* (2005) [5]

Erratum: *Bioinformatics* 21:4138 (2005)

6 Work distribution for the adiabatic compression of a dilute and interacting classical gas, *Phys. Rev. E* (2007) [6]

In Eq. 12 we shouldn't have taken the absolute value of the work in the probability distribution. The equation should read

$$\begin{aligned} \rho(W) &= \int dE_0 P(E_0; \beta) \delta(W - \alpha E_0) \\ &= \frac{\beta}{|\alpha| \Gamma(k)} \left(\frac{\beta W}{\alpha} \right)^{k-1} e^{-\beta W/\alpha} \theta(\alpha W). \end{aligned}$$

We want the equation to be correct both for compression ($\alpha > 0$) and expansion ($\alpha < 0$), but the unit step function $\theta(\cdot)$ and taking the absolute value of α in the normalization takes care of that. [Kudos: David Sivak (2011-09-26)]

Eq. 17 is slightly wrong. We messed up the scaling within the Dirac delta function. It should read:

$$p(E, t) = \int dE_0 P(E_0; \beta) \delta\left(\frac{E}{q_t} - E_0\right) = P(E; \beta/q_t), \quad (1)$$

[Kudos: David Sivak (2011-09-26)]

7 Beyond Boltzmann-Gibbs statistics: Maximum entropy hyperensembles out-of-equilibrium, *Phys. Rev. E* (2007) [7]

The equations contain various sign errors.

Equation 6 should read

$$P(\theta) \propto \exp\left(-\beta\lambda \sum_i \theta_i E_i - \lambda \sum_i \theta_i \log \theta_i\right),$$

Eq. 10 should read

$$\beta F(p) = + \sum_i p_i \ln p_i + \beta \sum_i p_i E_i$$

and the inline equation in the following text should read $F(p) = -S/\beta + \langle E \rangle$.

[Kudos: Eric Van der Straeten; Susanna Still; David Sivak].

8 Measuring thermodynamic length, *Phys. Rev. Lett.* (2007) [8]

The last equation on the second page should be a minus sign after ΔS_{system} , and the Eqs. (10) and (11) should have an extra minus sign “ $-\omega = \dots$ ”. The signs in Eq. 12 are correct; an extra minus sign enters from the definition of g_{ij} , Eq. (4).

[Kudos: David Sivak (2010-01-15)].

Eq. (15) contains extra factors of $1/K$. It should read

$$\begin{aligned} \ell(\Delta\psi_{12}) &= \sum_{k=1}^K \ln \frac{1}{1 + \exp(-\Delta\psi_{12} + (\lambda_2^i - \lambda_1^i) X_{i,1,k})} \\ &+ \sum_{k=1}^K \ln \frac{1}{1 + \exp(-\Delta\psi_{21} + (\lambda_1^i - \lambda_2^i) X_{i,2,k})}. \end{aligned}$$

The following Eq. (16) is correct.

9 Bayesian estimates of free energies from nonequilibrium work data in the presence of instrument noise (2008) [9]

In Fig. 1, ‘Pizeoelectric’ should read ‘Piezoelectric’.

10 Length of Time's Arrow (2008) [10]

Eq. (6) is missing a twiddle. It should read

$$\frac{P(+W|\Lambda)}{P(-W|\tilde{\Lambda})} = e^{\beta W - \beta \Delta F}$$

11 Nonequilibrium candidate Monte Carlo is an efficient tool for equilibrium simulation (2011) [11]

Erratum: *Proc. Natl. Acad. Sci. U.S.A.* 109:9665 (2012) doi:10.1073/pnas.1207617109

12 Thermodynamics of Prediction [12]

Eq. (16) should read $\Delta F_{\text{neq}}[x_{t+1}; s_t \rightarrow s_{t+1}]$.

[Kudos: David Sivak (2015-06-19)]

13 Thermodynamic metrics and optimal paths (2012) [13]

Para beginning “The integral of the excess power...” on page 3: Not our most elegant prose. What we are trying to

say is that we want to imagine $d\lambda/dt$ (velocity of control parameter changes) being inversely proportional to total time allowed for the transition changes (Δt). The excess work should scale as $(\Delta t)^{-1}$, and the excess power at any point λ should scale as $(\Delta t)^{-2}$.

There is an extra sign in the inline application of the fluctuation dissipation theorem after Eq. 6, but Eq. 8 is OK.

Eq. (15): The Fisher information is defined for any parametrizable probability distribution. Thus the π 's (defined in Eq. 1 as equilibrium probabilities) in this equation should be p 's, representing any arbitrary distribution parametrized by λ . It is only in the next sentence, when we specialize to the case of thermal equilibrium, that we get to π 's.

[Kudos: Susanna Still; David Sivak; Grant Rotskoff]