Contents

1 Introduction ................................................................. 1
  1.1 The Goal: Classical Statistical Mechanics as a Black Box Tool ............................................. 1
  1.2 Nested Sampling in Bayesian Statistics and in Statistical Mechanics ........................................... 3
  1.3 Outline of the Thesis .................................................. 4
  1.4 A History of Nested Sampling ........................................ 5
  References ........................................................................ 6

2 A Primer in Probability ..................................................... 7

Part I Statistical and Thermal Physics

3 Introduction ..................................................................... 13
  3.1 Phase Space .............................................................. 13
  3.2 Classical and Statistical Mechanics ............................... 13
  3.3 Hamilton’s Equations of Motion .................................... 14
  3.4 Statistical Equilibrium ................................................ 14
  3.5 Correlation Lengths and Statistically Independent Subsystems .................................................. 15
  3.6 Fluctuations ............................................................. 15

4 Phase Space Probability Distributions for Various External Conditions ........................................ 19
  4.1 Isolated Systems: Fixed $N$, $E$ and $V$ ......................... 19
     4.1.1 Distributions for $U$, $K$ ........................................ 20
     4.1.2 Principle of Equal Equilibrium Probability .............. 22
  4.2 Systems That Exchange Energy with the Universe: Fixed $N$, $T$, and $V$ ................................. 22
  4.3 Systems That Exchange Both Energy and Volume with the Universe: Fixed $N$, $T$, and $P$ ......... 25
12 Hamiltonian Monte Carlo for Nested Sampling

12.1 Galilean Monte Carlo

12.2 Molecular Dynamics Nested Sampling in the Total Hamiltonian

12.3 Nested Sampling in the Total Hamiltonian at Fixed \( N \) and \( P \)

12.3.1 MTK Dynamics

12.3.2 Choice of \( W_{\text{MTK}} \)

12.3.3 Hamiltonian Monte Carlo Scheme

12.3.4 Initialisation

12.3.5 HMC Acceptance Rate

12.3.6 Thermal Distributions

12.3.7 Comparison of MDNS with MCMC

12.4 Summary

12.5 Further Work

References

Part IV Conclusion

13 Summary and Further Work

13.1 Summary

13.2 Further Work

Appendix A: Model Selection for Gaussian Mixtures

Appendix B: Soft K-Means Algorithm, Version 2
Classical Statistical Mechanics with Nested Sampling
Baldock, R.J.N.
2017, XII, 144 p. 30 illus., 25 illus. in color., Hardcover
ISBN: 978-3-319-66768-3