Notes on Statistical Mechanics and Thermodynamics relevant to Machine Learning

compiled by D. Gueorguiev, 1/7/2025

# Starting Note

This document does not aim to discuss in depth the topics covered in the classic Statistical Mechanics books. Rather the interest here is in the statistical models and underlying physical mechanisms relevant to certain problems in the Machine Learning field in order to establish a clear link to and to provide useful insights to Machine Learning algorithms of interest.

# Introductory Material

## Classical Ideal Gas

The abstraction ‘Ideal Gas’ and the mathematical model behind it have many applications outside the Physical Sciences. Thus we start our journey into the world of Statistical Mechanics and Thermodynamics with the definition of Ideal Gas.

An ideal gas is different from real gases by the absence of interactions between particles which constitute the gas.

While idea gas is unrealistic model for real gasses it can be thought as a limit scenario for real gasses with sufficiently low densities. The simple model of ideal gas does not capture phase transitions present in real gasses.

## Phase Space of a Classical Gas

Let us consider particles contained in some specified volume. Each particle has a well-defined position and momentum. The position of every particle is represented as a point in some abstract space (*position space*) with an axis for every coordinate of every particle. The generalized coordinates of this abstract space are given as

(1)

The momentum of every particle can be represented as a point in momentum space – an abstract -dimensional space (*momentum space*), with axes for every component of the momentum of every particle.

(2)

The complete microscopic state of the system can be described by a point in *phase space* – an abstract -dimensional space with axes for every coordinate and every momentum component for all particles. Phase space is the union of configuration space and momentum space, .

(3)

The *kinetic energy* of the -th particle is given by the usual expression . The *total kinetic energy* of the system is the sum of the kinetic energies of all particles in the system.

(4)

Since, by definition, there are no interactions between the particles in an ideal gas, the potential energy of the system is zero.

(5)

**Distinguishability**:

Particles in the system are considered *distinguishable* so that the exchange of two particles results in a different microscopic sate. Thus every point in phase space represents a different microscopic state.

**Thermodynamic Entropy:**

Let us denote with the thermodynamic entropy of a system – this quantity is associated with particular microstate defined by thermodynamic parameters such as temperature, volume, and energy. is related to the number of microstates which can result in a given microstate with the following expression:

( Gibbs’ entropy law )

**Independence of Positions and Momenta:**

# References

[1] [An Introduction to Statistical Mechanics and Thermodynamics, Robert H. Swendsen, 2012](https://github.com/dimitarpg13/information_theory_and_statistical_mechanics/blob/main/literature/books/An-Introduction-to-Statistical-Mechanics-and-Thermodynamics-Swendsen-2012.pdf)

[2] [Statistical Physics by L.D. Landau and E.M. Lifshitz, 2nd Edition, 1970 (orig. 1958)](https://github.com/dimitarpg13/information_theory_and_statistical_mechanics/blob/main/literature/books/LandauLifshitz-StatisticalPhysics_1958.pdf)