# 140415 NTF Entropy Equations with Stirling’s Approximation

NOTE TO FILE:

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## References:

1. 140209 How to write a function in Excel
2. 140409 NTF Discussion with Dr Yakovenko.
3. 140412 NTF Entropy in a Histogram.
4. 140414 Stirling’s Approximation.xlsm (a spreadsheet).
5. 140414 Stirling’s Approximation.

## Background

This note covers some material also covered in other notes. The purpose of this note is simply to work through the details of the mathematical development of my formulae for entropy from first principles. There are a couple of logical gaps, but it is mostly here.

I proceed in three steps, with three variations on the formulae:

* **SMALL N – (N < 170)** – Development of some exact formulae that do not involve the use of Stirling’s approximation. These formula require the evaluation of terms involving ln(N!). Many computational engines are unable to evaluate these formulae when A is large. For example, MS Excel cannot evaluate it for A > 170.
* **LARGE N – (N > 1,000,000)** – A journey into the use of Stirling’s approximation, which enables easy evaluation for large N, but is not very accurate for small-to-medium-sized N. This is the classic approximation used in thermodynamics where the numbers of molecules are immense. The division between medium-sized and large-sized is entirely arbitrary, and not based on any analysis. However, my interest is in using the formula in agent-based models (ABMs) where N is always small to medium in size. I can use the exact formulae for small A, but for medium-sized N, I might be able to do better than these classical formulae.
* **MEDIUM N – (170 <= N <= 1,000,000)** – An exploration of a variation on Stirling’s approximation that can be used for medium-sized values of N. For practical purposes, I consider 1M to be larger than most ABMs, and smaller than most thermodynamic systesms. But, in fact, the revised version of Stirling’s formula should be good for large A as well, I believe.

## Before applying Stirling’s approximation:

Historically, Boltzmann defined entropy with the following formula:

By this he converted Clausius’ empirical definition into a “statistical mechanics” definition. This definition seems somewhat arbitrary to me. I cannot challenge it. I cannot see the reason for it. It is opaque to me. So I accept it as probably reasonable, and use it. So, my approach to entropy in ABMs is based on Boltzmann’s interpretation of Clausius’ work.

S is at a maximum when all of the bins have an equal number of agent in them. To produce an index, I need a constant formula for the maximum entropy possible.

Then I can make an exact formula for the entropic index.

These three formula – for S, Smax and Sindex – are exact formulae, and are good for 0 <= A <= 170.

## Stirling’s approximation – In two forms:

Classic form:

My revised form:

where

 and

## Stirling’s approximation – Classic form:

According to Wikipedia article referenced above, Stirling’s approximation to A! is an infinite series, and only the first few terms are used in the classic derivation of the formula for entropy. Working with the classic form first, start where I left off above. Here I reconstruct that classic derivation, and use it to build a formula for an entropic index:

Making the substitution:

Let

 and

So, making a substitution and changing the sign on the sum by inverting the argument of ln():

Add and subtract a term:

Combine the two middle terms:

Combine the first and last terms:

But, noting that

So

or

Using that, and substituting pi = α / A = 1 / K, when S is at its maximum:

Then I can make an approximate formula for the entropic index.

These three formulae – for S, Smax and Sindex – are those typically used in thermodynamics, where the numbers of active agents (atoms) are numbered using Avogadro’s number (of the order 1023).

## Stirling’s approximation – Revised formula

The Wikipedia article referenced above describes a variety of ways to derive variations on Stirling’s formulae, and a variety of expansions as series. All are asymptotic solutions which start at some distance from the value ln(A!), i.e. start with some large relative error, which then improves, quickly at first, then gradually, in an asymptotic fashion. Here is a chart from that description, for one of the series.



So, the question in my mind is, does my “empirically determined” variation on Stirling’s approximation perform better than a two-term truncated expansion? It seems that it does, in the area of interest, i.e. from 170 <= A <= 1M.

Here’s my empirically determined improvement on Stirling’s approximation:

where

 and

Here I repeat my above construction, but using this variation, and use it to build a formula for an entropic index:

Making the substitution:

As before the (-A) of the first term cancels the sum of the ai in the second term and they disappear. We are left with this two-term expression, the first term of which is identical to the previous formula, and the second term of which is the corrective expression.

By the same procedure used above, the first term is simplified to the classical approximation for entropy:

To simplify the right side, let

 and

And note that:

So

Where C is a corrective term.

Four of the five terms are constants and can be gathered:

Putting the two pieces together again:

Using that, and substituting pi = α / A = 1 / K, and using the simplified form for the first term found above, when S is at its maximum:

Wow. Pretty complicated! But it is a constant, so once computed, it is not a waster of computer resources. It is just a normalizing constant.

Then I can make an approximate formula for the entropic index.

As A approaches infinity the corrective term, both top and bottom, rises at a rate of ln(A) while the base term rises at a rate of A. This implies that the relative error approaches zero as A approaches infinity. This is no guarantee that it performs as well as the classical formula for large A, but it seems to perform better on the domain [170, 1M].

These three formulae – for S, Smax and Sindex – are intended to give me improved relative error in that mid-range in which MS Excel cannot support analysis of ABM entropy, and Stirling’s approximation has higher relative error due to its “asymptotic” characteristics, i.e. between 170 and 1M.

Do these simplify if I substitute approximate values for ξ (=0.5) and ψ (=1.0)?

Apparently not! So, I have built-to-purpose formulae that are complicated and lack credibility.

## Decision:

Which formulae do I use when analyzing entropy using MS Excel and when building entropy into ABMs?

The problem seems to arise when I try to use one technique to approximate all occurrences of factorials. Factorials of many sizes can arise in a single determination of entropy for a single configuration. So, maybe there is no one-size-fits-all formula for computing entropy in a histogram. In fact, for computational purposes, I can decide which formula I wish to use at the time of use, for each individual factorial. This means I would have some kind of dynamic hybrid of all of the above formulae each time I compute S, Smax or Sindex.

This means that for small A I get exact answers, and that is where my personal work is. For larger A, associated with larger ABMs, some approximations will be applied, but only when the subsidiary factorials are large. The results will then be consistent with usage in thermodynamics and elsewhere where very large factorials dominate, but accurate for the small factorials that appear in ABMs.

In MS Excel and in C++ I will construct a LawnOfFactorial() function which switches between the exact calculation and the classic two-term Sterling’s approximation at the threshold of A = 170.

I will use this dynamic hybrid approach in each computation of S and Sindex.

This will give me reasonable accuracy (within the limits of relative error of Stirling’s approximation, when applied), but is, I think, somewhat uncommon as an approach, and therefore may lose credibility.