In[820]:=

```
(*Jared Frazier*)
(*Microstates-M7*)
(*Description:

Relate the multiplicity of macrostates to principles of thermodynamics.

*)
(*Date: 02/15/2021*)
Clear["Global`*"]

(***********************************************************************)
                (*Part 1 -- The Multiplicity of Macrostates*)
(***********************************************************************)



(*Subroutines in for multiplicity function*)
totalStatesM[N_] := 2 ^ N
multiplicity[N_, n_] := N! / (n! * (N-n)!)
probability[Ω_, M_] := Ω / M
entropy[Ω_] := 1 * Log[Ω]

(*
:Purpose: Compute multiplicity table with variable macrostates.

:param macrostatesN_: Number of macrostates in the system.
:param state1_: Define a state a particle can have (e.g. "H", 1, "L", etc.).
:param state2_: Define another state a particle can have.
:param q3_: Should be True for question 3 and changes output for microstates column.

:return: <Table object> representing multiplicity
*)
computeMultiplicityTable[macrostatesN_, state1_, state2_, q3_] := (
    multiplicityTable = Table[0, macrostatesN+1, 5];
    pos = 1;
    For[n = macrostatesN, n >= 0, n--,  (*'n' the number of heads for a given macrostate varies*)
        (*Initial macrostate*)
        macroList = List[];

        (*Write "H" to list based on 'n'*)
        For[i = 1, i ≤ n, i++,
            AppendTo[macroList, state1];
        ];

        (*Complete list with "T"s*)
        For[i = 1, i ≤ macrostatesN-n, i++,
            AppendTo[macroList, state2];
        ];

        (*List of microstates corresponding to that macrostate*)
```

```
        microList = Permutations[macroList];

        (*Concatenated microList*)
        concatenatedMicroList = List[];
        microListDims = Dimensions[microList];
        For[row = 1, row ≤ microListDims[[1]], row++,
            AppendTo[concatenatedMicroList, StringRiffle[microList[[row]], ""]];
        ];

        (*Set microstate str for table*)
        omega = multiplicity[macrostatesN, n];
        If [q3,
            (*TRUE*)
            on = 0;
            off = 0;
            (*Iterate through macrostate string and count number of 'on' and 'off' states*)
            For [i = 1, i ≤ macrostatesN, i++,
                If [ToString[microList[[1, i]]] == state1, on++, off++]
            ];
            (*Set the on/off string*)
            resultString = ToString[on] <> "/" <> ToString[off];,

            (*FALSE*)
            (*Create column microstate string*)
            resultString = "";
            For[i = 1, i ≤ omega, i++,
                resultString = StringJoin[resultString, ToString[Part[concatenatedMicroList, i]]]
                If[i ≠ omega, resultString = StringJoin[resultString, "\n"]];
            ];
        ]

        (*Create the table*)
        capitalM = totalStatesM[macrostatesN];
        multiplicityTable[[pos, 1]] = n;                                (*Macrostate*)
        multiplicityTable[[pos,2]] = resultString;             (*Microstates*)
        multiplicityTable[[pos, 3]] = omega;
        multiplicityTable[[pos, 4]] = probability[omega, capitalM];    (*Probabiltity*)
        multiplicityTable[[pos, 5]] = SetPrecision[entropy[omega], 4]; (*Entropy*)
        pos++;
    ];

    (*Return the table*)
    headerTable = Prepend[multiplicityTable, {"Macrostate", "Microstates", "Multiplicity", "Proba
    Return[finalTable = Transpose[headerTable]];
)


Print["(************************************************************************)
                (*Part 1 -- The Multiplicity of Macrostates*)
```

```
(***************************************************************************)"]
tenCoinTable = computeMultiplicityTable[10, "H", "T", False];
Grid[tenCoinTable, Frame->All]
Print["Is the 10 coin distribution more peaked than the 4 coin distribution?\n
Yes, the 10 coin distribution is significantly more peaked as 10 coins lends
to a greater number of microstates per macrostate."]


(***************************************************************************)
      (*Part 2 -- Evolution of Macrostates for a non-isolated system*)
(***************************************************************************)
(*Coin flip function*)
coinFlip := RandomChoice[{"H","T"}]

(*Lists for results*)
yNumHeads = List[];       (*Counts number of heads after a given toss*)
yNumTails = List[];       (*Counts number of tails after a given toss*)
xNumTosses = Range[100];  (*1 to 100th toss list*)


Print["(***************************************************************************)
      (*Part 2 -- Evolution of Macrostates for a non-isolated system*)
(***************************************************************************)"]

Print["What macrostate will be reached in the process of flipping N ordered
coins randomly starting from the NH state?"]

(*Do 100 tosses*)
For [toss = 1, toss <= 100, toss++,
    cntHeads = 0;
    cntTails = 0;
    (*Do 100 coin flips*)
    For [flip = 1, flip ≤ 100, flip++,
        If [coinFlip == "H", cntHeads++, cntTails++];
    ];
    (*Append to parallel lists*)
    AppendTo[yNumHeads, cntHeads];
    AppendTo[yNumTails, cntTails];
]

(*Graph results*)
headData = Transpose[{xNumTosses, yNumHeads}];
tailData = Transpose[{xNumTosses, yNumTails}];
ListPlot [
    {headData, tailData},
    PlotRange→Full,
    ImageSize→{750, 750},
    PlotLegends→{"Heads",
                 "Tails"},
```

```
    PlotLabel→"Number of Coin Faces Appearing from 100 Flips vs. Number of Simulations (Coin Toss
    AxesLabel→{"Number of Coin Tosses", "Number of Face"}
]

(*Calculate entropy*)
yEntropyList = List[];
For [i = 1, i ≤ Length[yNumHeads], i++,
    AppendTo[yEntropyList, entropy[multiplicity[100, Part[yNumHeads, i]]]];
]


(*Graph entropy*)
entropyData = Transpose[{xNumTosses, yEntropyList}];
ListPlot[
    entropyData,
    ImageSize→Large,
    PlotLabel→"Entropy vs. Number of Simulations (Coin Tosses)",
    AxesLabel→{"Number of Coin Tosses", "S = k ln(Ω)"}
]

Print["What pattern can you find during the process (how does the macrostate evolve)?
Is there a tendency toward equilibrium?\nThe macrostate generally oscillates around the
expected value for the macrostate which is 50.\n\nWhat happens in terms of entropy?\nThe entropy
also seems to remain in a constrained region on the graph, which is to be expected if multiplicity
is somewhat consistent.
"]



(*****************************************************************************)
     (*Part 3 -- Dependence on Statistical Multiplicity on the volume*)
(*****************************************************************************)
Print["(*****************************************************************************)
     (*Part 3 -- Dependence of Statistical Multiplicity on the volume*)
(*****************************************************************************)"]
Print["Compute L/R Multiplicity for N=4"]
volumeTable = computeMultiplicityTable[4, "L", "R", True];
Grid[volumeTable, Frame->All]
Print["Which macrostate is the largest multiplicity?
n=2 macrostate has the largest multiplicity of 6."]
Print["\nDo your findings support that particles occupy the entire volume after removing a restra
Yes, my findings support the statistical nature of the observation that
particles spread out in the available volume."]


(*****************************************************************************)
                         (*Part 4 -- Gas diffusion*)
(*****************************************************************************)
(*Initial Lists*)
initMacrostate = {"A", "A", "A", "A", "B", "B", "B", "B"};
```

```
allPermutations = Permutations[initMacrostate];

(*This will be a list of strings holding all {?A, ?B/?A, ?B} format*)
macrostateList = List[];

(*Each row in allPermutations is a list with 8 columns containing permutations of AAAABBBB*)
For [row = 1, row ≤ Length[allPermutations], row++,
    (*Counting macrostates
    OnLeft is defined as columns 1-4
    OnRight is defined as columns 5-8
    *)
    cntAOnLeft = 0;
    cntAOnRight = 0;
    cntBOnLeft = 0;
    cntBOnRight = 0;

    (*Macrostate string of "?A, ?B/?A, ?B" format*)
    macrostateString = "";

    (*Count particles on left side*)
    For [letter = 1, letter ≤ 4, letter++,
        If [ToString[allPermutations[[row, letter]]] == "A",
        cntAOnLeft++,
        cntBOnLeft++
        ];
    ];

    (*Count particles on right side*)
    For [letter = 5, letter ≤ 8, letter++,
        If [ToString[allPermutations[[row, letter]]] == "A",
            cntAOnRight++,
            cntBOnRight++
        ];
    ];

    (*Build the macrostateList*)
    toAdd = ToString[cntAOnLeft] <> "A, " <> ToString[cntBOnLeft] <> "B/" <> ToString[cntAOnRigh
    AppendTo[macrostateList, toAdd];
]

(*Count multiplicity*)
noDuplicateMacrostatesList = DeleteDuplicates[macrostateList];
multiplicityCounterList = List[];                              (*Parallel to noDuplicateMacrosta
(*Iterate through noDuplicateMacrostatesList and the total macrostateList to count multiplicity*)
For [i = 1, i ≤ Length[noDuplicateMacrostatesList], i++,
    multiplicityCounter = 0;
    For [mstate = 1, mstate ≤ Length[macrostateList], mstate++,
        (*If the current macrostateList element matches the current noDuplicateMacrostatesList el
        If [Part[macrostateList, mstate] == Part[noDuplicateMacrostatesList, i],
            multiplicityCounter++;
```

```
        ];
    ];
    AppendTo[multiplicityCounterList, multiplicityCounter];
]

Print["(*************************************************************************)
                        (*Part 4 -- Gas diffusion*)
(*************************************************************************)"]

(*Format and display table*)
question4Table = Prepend[Transpose[{noDuplicateMacrostatesList, multiplicityCounterList}], {"Macr
Grid[question4Table, Frame→All]

Print["The equilibrium composition is 2A, 2B/2A, 2B based on the table above."]



(*************************************************************************)
                          (*Part 5 -- Heat Flow*)
(*************************************************************************)
Print["(*************************************************************************)
                          (*Part 5 -- Heat Flow*)
(*************************************************************************)"]
Print["What are the total energies and multiplicities of the isolated systems B {0111} and A {001
Print["The blue and gray columns represent system B and A, respectively. The total energy
of system B (n=3) is 3 and the multiplicity is 4. The total energy of system
A (n=2) is 2 and the multiplicity is 6.\n"]
isolatedSystems = computeMultiplicityTable[4, "1", "0", False];
Grid[isolatedSystems, Frame→All, Background -> {{None, None, LightBlue, LightGray, None, None}}]
Print["Calculate the multiplicity of the overall system with total energy of 5 units?
What is the expected direction of heat flow?"]
Print["The brown column represents the combined system with total energy of 5.
The multiplicity of this system is 56 from the table. The direction of heat flow is
such that the total energy of the system is 4. This means heat from either A or B  must be
lost to the surroundings such that the overall system only has 4 units of energy."]
combinedSystems = computeMultiplicityTable[8, "1", "0", False];
Grid[combinedSystems, Frame→All, Background→{{None, None, None,None, LightBrown}}]
```

```
(*************************************************************************)
                (*Part 1 -- The Multiplicity of Macrostates*)
(*************************************************************************)
```

Macrostate	10	9	8	7	6	5	4	3	2	1	0

Microstates	HHHHHHHHHH	HHHHHHHHHT	HHHHHHHHTT	HHHHHHHTTT	HHHHHHTTTT	HHHHHTTTTT	HHHHTTTTTT	HHHTTTTTTT	HHTTTTTTTT	HTTTTTTTTT	TTTTTTTTTT
		HHHHHHHHTH	HHHHHHHTHT	HHHHHHTHTT	HHHHHTHTTT	HHHHTHTTTT	HHHTHTTTTT	HHTHTTTTTT	HTHTTTTTTT	THTTTTTTTT	
		HHHHHHHTHH	HHHHHHHTTH	HHHHHHTTHT	HHHHHTTHTT	HHHHTTHTTT	HHHTTHTTTT	HHTTHTTTTT	HTTHTTTTTT	TTHTTTTTTT	
		HHHHHHTHHH	HHHHHHTHHT	HHHHHHTTTH	HHHHHTTTHT	HHHHTTTHTT	HHHTTTHTTT	HHTTTHTTTT	HTTTHTTTTT	TTTHTTTTTT	
		HHHHHTHHHH	HHHHHHTHTH	HHHHHTHHTT	HHHHHTTTTH	HHHHTTTTHT	HHHTTTTHTT	HHTTTTHTTT	HTTTTHTTTT	TTTTHTTTTT	
		HHHHTHHHHH	HHHHHHTTHH	HHHHHTHTHT	HHHHTHHTTT	HHHHTTTTTH	HHHTTTTTHT	HHTTTTTHTT	HTTTTTHTTT	TTTTTHTTTT	
		HHHTHHHHHH	HHHHHTHHHT	HHHHHTHTTH	HHHHTHTHTT	HHHTHHTTTT	HHHTTTTTTH	HHTTTTTTHT	HTTTTTTHTT	TTTTTTHTTT	
		HHTHHHHHHH	HHHHHTHHTH	HHHHHTTHHT	HHHHTHTTHT	HHHTHTHTTT	HHTHHTTTTT	HHTTTTTTTH	HTTTTTTTHT	TTTTTTTHTT	
		HTHHHHHHHH	HHHHHTHTHH	HHHHHTTHTH	HHHHTHTTTH	HHHTHTTHTT	HHTHTHTTTT	HTHHTTTTTT	HTTTTTTTTH	TTTTTTTTHT	
		THHHHHHHHH	HHHHHTTHHH	HHHHHTTTHH	HHHHTTHHTT	HHHTHTTTHT	HHTHTTHTTT	HTHTHTTTTT	THHTTTTTTT	TTTTTTTTTH	
			HHHHTHHHHT	HHHHTHHHTT	HHHHTTHTHT	HHHTHTTTTH	HHTHTTTHTT	HTHTTHTTTT	THTHTTTTTT		
			HHHHTH	HHHHTH	HHHHTT	HHHTTH	HHTHTT	HTHTTT	THTTHT		

Multiplicity	1	10	45	120	210	252	210	120	45	10	1
Probability	$\frac{1}{1024}$	$\frac{5}{512}$	$\frac{45}{1024}$	$\frac{15}{128}$	$\frac{105}{512}$	$\frac{63}{256}$	$\frac{105}{512}$	$\frac{15}{128}$	$\frac{45}{1024}$	$\frac{5}{512}$	$\frac{1}{1024}$
Entropy	0	2.303	3.807	4.787	5.347	5.529	5.347	4.787	3.807	2.303	0

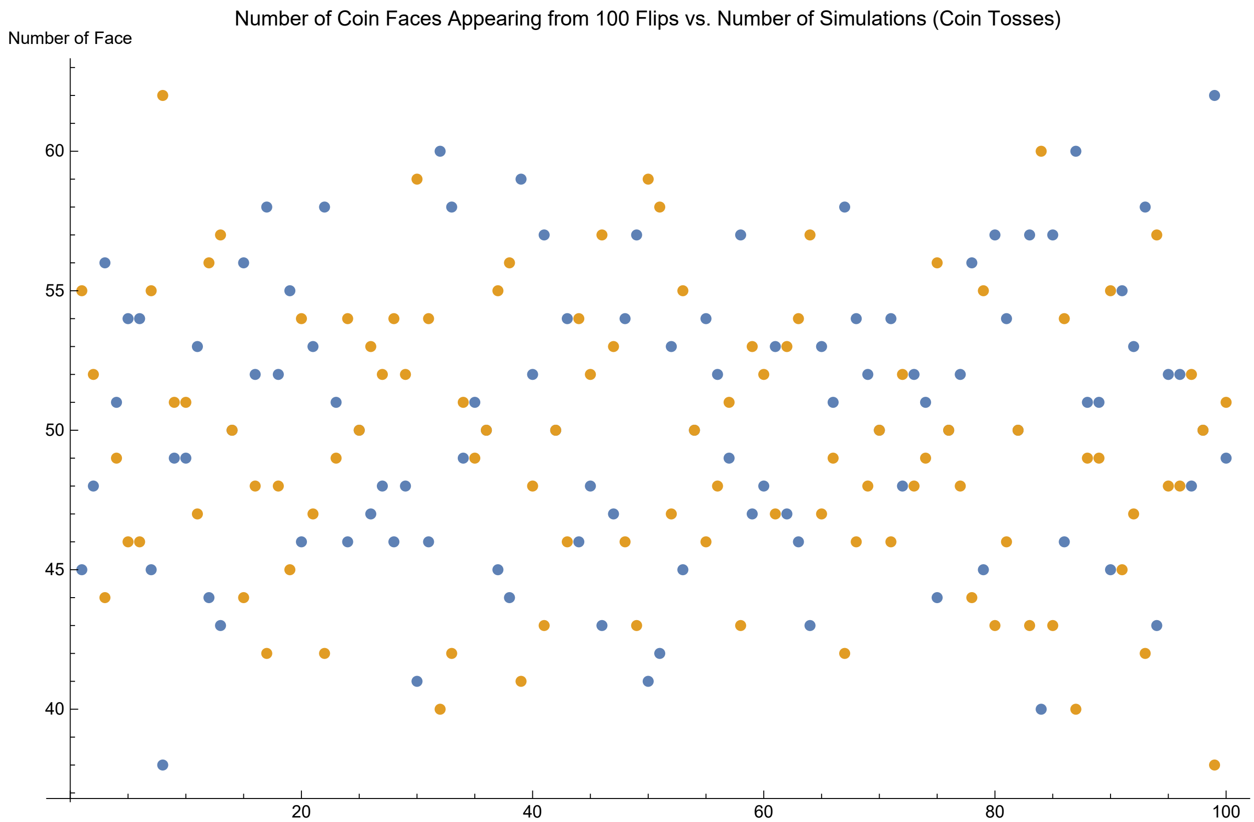
Is the 10 coin distribution more peaked than the 4 coin distribution?

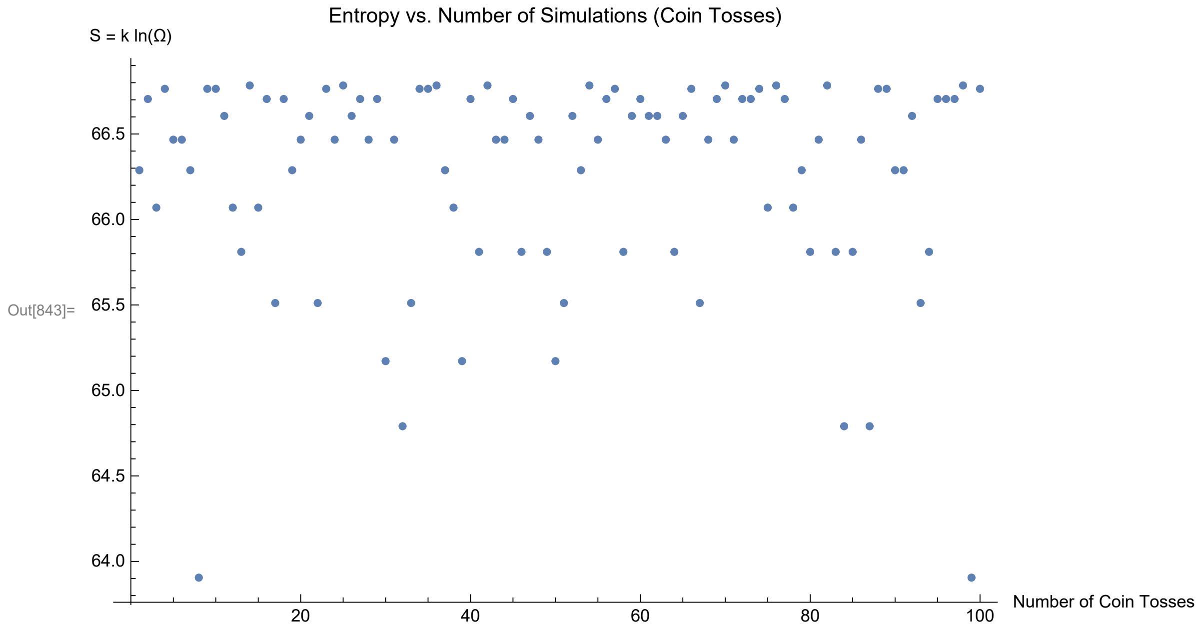
Yes, the 10 coin distribution is significantly more peaked as 10 coins lends to a greater number of microstates per macrostate.

```
(*************************************************************************)
      (*Part 2 -- Evolution of Macrostates for a non-isolated system*)
(*************************************************************************)
```

What macrostate will be reached in the process of flipping N ordered coins randomly starting from the NH state?

Out[839]=


Number of Coin Faces Appearing from 100 Flips vs. Number of Simulations (Coin Tosses)
Number of Face
60
55
50
45
40
20
40
60
80
100



What pattern can you find during the process (how does the macrostate evolve)?
Is there a tendency toward equilibrium?
The macrostate generally oscillates around the
expected value for the macrostate which is 50.

What happens in terms of entropy?
The entropy
also seems to remain in a constrained
region on the graph, which is to be expected if multiplicity
is somewhat consistent.

```
(**********************************************************************)
     (*Part 3 -- Dependence of Statistical Multiplicity on the volume*)
(**********************************************************************)
```

Compute L/R Multiplicity for N=4

Out[848]=

Macrostate	4	3	2	1	0
Microstates	4/0	3/1	2/2	1/3	0/4
Multiplicity	1	4	6	4	1
Probability	$\frac{1}{16}$	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{1}{4}$	$\frac{1}{16}$
Entropy	0	1.386	1.792	1.386	0

Which macrostate is the largest multiplicity?
n=2 macrostate has the largest multiplicity of 6.

Do your findings support that particles occupy the entire volume after removing a restraint?
Yes, my findings support the statistical nature of the observation that
particles spread out in the available volume.

```
(**********************************************************************)
                         (*Part 4 -- Gas diffusion*)
(**********************************************************************)
```

Out[860]=

Macrostate	Multiplicity
4A, 0B/0A, 4B	1
3A, 1B/1A, 3B	16
2A, 2B/2A, 2B	36
1A, 3B/3A, 1B	16
0A, 4B/4A, 0B	1

The equilibrium composition is 2A, 2B/2A, 2B based on the table above.

```
(**************************************************************************)
                          (*Part 5 -- Heat Flow*)
(**************************************************************************)
```

What are the total energies and multiplicities of the isolated systems B {0111} and A {0011}?

The blue and gray columns represent system B and A, respectively. The total energy of system B (n=3) is 3 and the multiplicity is 4. The total energy of system A (n=2) is 2 and the multiplicity is 6.

Out[866]=

Macrostate	4	3	2	1	0
Microstates	1111	1110 1101 1011 0111	1100 1010 1001 0110 0101 0011	1000 0100 0010 0001	0000
Multiplicity	1	4	6	4	1
Probability	$\frac{1}{16}$	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{1}{4}$	$\frac{1}{16}$
Entropy	0	1.386	1.792	1.386	0

Calculate the multiplicity of the overall system with total energy of 5 units?
What is the expected direction of heat flow?

The brown column represents the combined system with total energy of 5.
The multiplicity of this system is 56 from the table. The direction of heat flow is such that the total energy of the system is 4. This means heat from either A or B must be lost to the surroundings such that the overall system only has 4 units of energy.

Macrostate	8	7	6	5	4	3	2	1	0

Microstates	11111111	11111110 11111101 11111011 11110111 11101111 11011111 10111111 01111111	11111100 11111010 11111001 11110110 11110101 11110011 11101110 11101101 11101011 11100111 11011110 11011101 11011011 11010111 11001111 10111110 10111101 10111011 10110111 1010111	11111000 11110100 11110010 11110001 11101100 11101010 11101001 11100110 11100101 11100011 11011100 11011010 11011001 11010110 11010101 11010011 11001110 11001101 11001011 1100011	11110000 11101000 11100100 11100010 11100001 11011000 11010100 11010010 11010001 11001100 11001010 11001001 11000110 11000101 11000011 10111000 10110100 10110010 10110001 1010110	11100000 11010000 11001000 11000100 11000010 11000001 10110000 10101000 10100100 10100010 10100001 10011000 10010100 10010010 10010001 10001100 10001010 10001001 10000110 1000010	11000000 10100000 10010000 10001000 10000100 10000010 10000001 01100000 01010000 01001000 01000100 01000010 01000001 00110000 00101000 00100100 00100010 00100001 00011000 0001010	10000000 01000000 00100000 00010000 00001000 00000100 00000010 00000001	00000000

Multiplicity	1	8	28	56	70	56	28	8	1
Probability	$\frac{1}{256}$	$\frac{1}{32}$	$\frac{7}{64}$	$\frac{7}{32}$	$\frac{35}{128}$	$\frac{7}{32}$	$\frac{7}{64}$	$\frac{1}{32}$	$\frac{1}{256}$
Entropy	0	2.079	3.332	4.025	4.248	4.025	3.332	2.079	0