Information Theory Primer

With an Appendix (see section 1) on Logarithms
Postscript version: ftp://ftp.ncifcrf.gov/pub/delila/primer.ps
web versions: http://www.lecb.ncifcrf.gov/∼toms/paper/primer/

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This primer is written for molecular biologists who are unfamiliar with information theory. Its purpose is to introduce you to these ideas so that you can understand how to apply them to binding sites [1, 2, 3, 4, 5, 6, 7, 8, 9]. Most of the material in this primer can also be found in introductory texts on information theory. Although Shannon's original paper on the theory of information [10] is sometimes difficult to read, at other points it is straight forward. Skip the hard parts, and you will find it enjoyable. Pierce later published a popular book [11] which is a great introduction to information theory. Other introductions are listed in reference [1]. A workbook that you may find useful is reference [12]. Shannon's complete collected works have been published [13]. Information about ordering this book is given in

> http://www.lecb.ncifcrf.gov/∼toms/bionet.info-theory.faq.html
> #REFERENCES-Information_Theory

Other papers and documentation on programs can be found at

> http://www.lecb.ncifcrf.gov/∼toms/

Note: If you have trouble getting through one or more steps in this primer, please send email to me describing the exact place(s) that you had the problem. If it is appropriate, I will modify the text to smooth the path. My thanks go to the many people whose stubbed toes led to this version.

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Information and Uncertainty

Information and uncertainty are technical terms that describe any process that selects one or more objects from a set of objects. We won't be dealing with the meaning or implications of the information since nobody knows how to do that mathematically. Suppose we have a device that can produce 3 symbols, A, B, or C. As we wait for the next symbol, we are *uncertain* as to which symbol it will produce. Once a symbol appears and we see it, our uncertainty *decreases*, and we remark that we have received some *information*. That is, information is a decrease in uncertainty. How should uncertainty be measured? The simplest way would be to say that we have an "uncertainty of 3 symbols". This would work well until we begin to watch a second device at the same time, which, let us imagine, produces symbols 1 and 2. The second device gives us an "uncertainty of 2 symbols". If we combine the devices into one device, there are six possibilities, A1, A2, B1, B2, C1, C2. This device has an "uncertainty of 6 symbols". This is not the way we usually think about information, for if we receive two books, we would prefer to say that we received twice as much information than from one book. That is, we would like our measure to be additive.

It's easy to do this if we first take the logarithm of the number of possible symbols because then we can add the logarithms instead of multiplying the number of symbols. In our example, the first device makes us uncertain by $\log(3)$, the second by $\log(2)$ and the combined device by $\log(3)+\log(2)=\log(6)$. The base of the logarithm determines the units. When we use the base 2 the units are in bits (base 10 gives digits and the base of the natural logarithms, e, gives nats [14] or nits, though I don't have a reference for the latter). Thus if a device produces one symbol, we are uncertain by $\log_2 1 = 0$ bits, and we have no uncertainty about what the device will do next. If it produces two symbols our uncertainty would be $\log_2 2 = 1$ bit. In reading an mRNA, if the ribosome encounters any one of 4 equally likely bases, then the uncertainty is 2 bits.

So far, our formula for uncertainty is $\log_2(M)$, with M being the number of symbols. The next step is to extend the formula so it can handle cases where the symbols are not equally likely. For example, if there are 3 possible symbols, but one of them never appears, then our uncertainty is 1 bit. If the third symbol appears rarely relative to the other two symbols, then our uncertainty should be larger than 1 bit, but not as high as $\log_2(3)$ bits. Let's begin by rearranging the formula like this:

$$\begin{aligned} \log_2(M) &= -\log_2(M^{-1}) \\ &= -\log_2(\frac{1}{M}) \\ &= -\log_2(P) \end{aligned} \tag{1}$$

so that $P = 1/M$ is the probability that any symbol appears. (If you don't remember this trick of 'pulling the sign out', recall that $\log M^b = b \log M$ and let $b = -1$.)

Now let's generalize this for various probabilities of the symbols, P_i, so that the probabilities sum to 1:

$$\sum_{i=1}^{M} P_i = 1. \tag{2}$$

(Recall that the $\sum$ symbol means to add the P_i together, for i starting at 1 and ending at M.) The surprise that we get when we see the ith kind of symbol was called the "surprisal" by Tribus [15] and is defined by analogy with $-\log_2 P$ to be:

$$u_i = -\log_2(P_i). \tag{3}$$

For example, if P_i approaches 0, then we will be *very surprised* to see the ith symbol (since it should almost never appear), and the formula says u_i approaches ∞. On the other hand, if P_i=1, then we won't be surprised at all to see the ith symbol (because it should always appear) and u_i = 0.

Uncertainty is the *average surprisal* for the infinite string of symbols produced by our device. For the moment, let's find the average for a string that has an alphabet of N symbols. Suppose that the ith type of symbol appears N_i times so that

$$N = \sum_{i=1}^{M} N_i. \tag{4}$$

There will be N_i cases where we have surprisal u_i. The average surprisal for the N symbols is:

$$\frac{\sum_{i=1}^{M} N_i u_i}{\sum_{i=1}^{M} N_i}. \tag{5}$$

By substituting N for the denominator and bringing it inside the upper sum, we obtain:

$$\sum_{i=1}^{M} \frac{N_i}{N} u_i \tag{6}$$

If we do this measure for an infinite string of symbols, then the frequency N_i/N becomes P_i, the probability of the ith symbol. Making this substitution, we see that our average surprisal (H) would be:

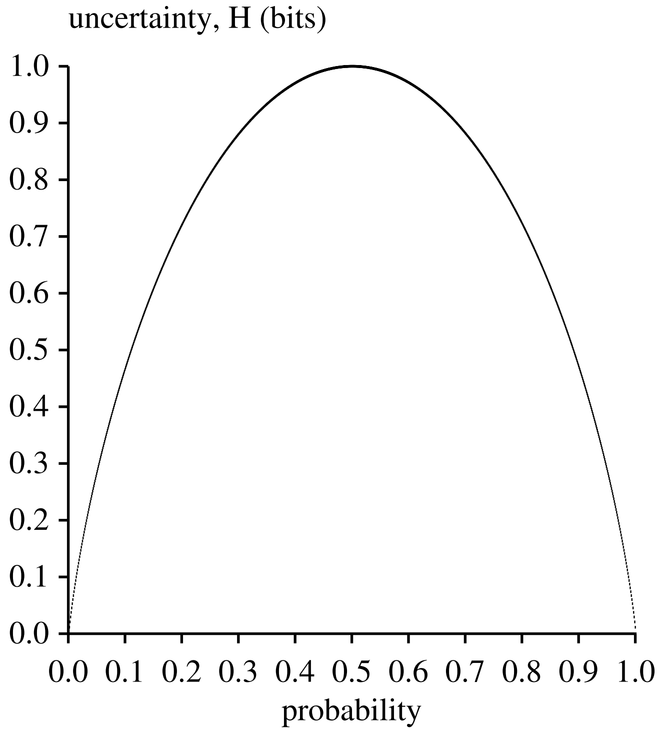
$$H = \sum_{i=1}^{M} P_i u_i. \tag{7}$$

Finally, by substituting for u_i, we get Shannon's famous general formula for uncertainty:

$$\boxed{H = -\sum_{i=1}^{M} P_i \log_2 P_i \quad \text{(bits per symbol).}} \tag{8}$$

Shannon got to this formula by a much more rigorous route than we did, by setting down several desirable properties for uncertainty, and then deriving the function. Hopefully the route we just followed gives you a feeling for how the formula works.

To see how the H function looks, we can plot it for the case of two symbols. This is shown below[1]:



Notice that the curve is symmetrical, and rises to a maximum when the two symbols are equally likely (probability = 0.5). It falls towards zero whenever one of the symbols becomes dominant at the expense of the other symbol.

As an instructive exercise, suppose that all the symbols are equally likely. What does the formula for H (equation (8)) reduce to? You may want to try this yourself before reading on.

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[1]The program to create this graph is at http://www.lecb.ncifcrf.gov/∼toms/delila/hgraph.html

Equally likely means that $P_i = 1/M$, so if we substitute this into the uncertainty equation we get:

$$H_{equiprobable} = -\sum_{i=1}^{M} \frac{1}{M} \log_2 \frac{1}{M} \tag{9}$$

Since M is not a function of i, we can pull it out of the sum:

$$\begin{aligned}
H_{equiprobable} &= -(\frac{1}{M} \log_2 \frac{1}{M}) \sum_{i=1}^{M} 1 && (10)\\
&= -\left(\frac{1}{M} \log_2 \frac{1}{M}\right) M \\
&= -\log_2 \frac{1}{M} && (11)\\
&= \log_2 M
\end{aligned}$$

which is the simple equation we started with. It can be shown that for a given number of symbols (ie., M is fixed) the uncertainty H has its largest value only when the symbols are equally probable. For example, an unbiased coin is harder to guess than a biased coin. As another exercise, what is the uncertainty when there are 10 symbols and only one of them appears? (clue: $\lim_{p \to 0} p \log p = 0$ by setting $p = 1/M$ and using l'Hôpital's rule, so $0 \log_2 0 = 0$.)

What does it mean to say that a signal has 1.75 bits per symbol? It means that we can convert the original signal into a string of 1's and 0's (binary digits), so that *on the average* there are 1.75 binary digits for every symbol in the original signal. Some symbols will need more binary digits (the rare ones) and others will need fewer (the common ones). Here's an example. Suppose we have $M = 4$ symbols:

$$A \quad C \quad G \quad T \tag{12}$$

with probabilities (P_i):

$$P_A = \frac{1}{2}, \quad P_C = \frac{1}{4}, \quad P_G = \frac{1}{8}, \quad P_T = \frac{1}{8}, \tag{13}$$

which have surprisals ($-\log_2 P_i$):

$$u_A = 1 \text{ bit}, \quad u_C = 2 \text{ bits}, \quad u_G = 3 \text{ bits}, \quad u_T = 3 \text{ bits}, \tag{14}$$

so the uncertainty is

$$H = \frac{1}{2} \cdot 1 + \frac{1}{4} \cdot 2 + \frac{1}{8} \cdot 3 + \frac{1}{8} \cdot 3 = 1.75 \text{ (bits per symbol)}. \tag{15}$$

Let's recode this so that the number of binary digits equals the surprisal:

$$\begin{aligned}
A &= 1 \\
C &= 01 \\
G &= 000 \\
T &= 001 && (16)
\end{aligned}$$

so the string

$$ACATGAAC \tag{17}$$

which has frequencies the same as the probabilities defined above, is coded as

$$10110010001101. \tag{18}$$

14 binary digits were used to code for 8 symbols, so the average is 14/8 = 1.75 binary digits per symbol. This is called a Fano code. Fano codes have the property that you can decode them without needing spaces between symbols. Usually one needs to know the "reading frame", but in this example one can figure it out. In this particular coding (equations (16)), the first binary digit distinguishes between the set containing A, (which we symbolize as A) and the set C,G,T, which are equally likely. The second digit, used if the first digit is 0, distinguishes C from G,T. The final digit distinguishes G from T. Because each choice is equally likely (in our original definition of the probabilities of the symbols), every binary digit in this code carries 1 bit of information. *Beware!* This won't always be true. A binary digit can supply 1 bit *only* if the two sets represented by the digit are equally likely (as rigged for this example). If they are not equally likely, one binary digit supplies less than one bit. (Recall that H is at a maximum for equally likely probabilities.) So if the probabilities were

$$P_A = \frac{1}{2}, \quad P_C = \frac{1}{6}, \quad P_G = \frac{1}{6}, \quad P_T = \frac{1}{6}, \tag{19}$$

there is no way to assign a (finite) code so that each binary digit has the value of one bit (by using larger blocks of symbols, one can approach it).[2] In the rigged example, there is no way to use fewer than 1.75 binary digits per symbol, but we could be wasteful and use extra digits to represent the signal. The Fano code does reasonably well by splitting the symbols into successive groups that are equally likely to occur; you can read more about it in texts on information theory. The uncertainty measure tells us what could be done ideally, and so tells us what is impossible. For example, the signal with 1.75 bits per symbol could not be coded using only 1 binary digit per symbol.

Tying the Ideas Together

In the beginning of this primer we took information to be a decrease in uncertainty. Now that we have a general formula for uncertainty, (8), we can express information using this formula. Suppose that a computer contains some information in its memory. If we were to look at individual flip-flops, we would have an uncertainty H_{before} bits per flip-flop. Suppose we now clear part of the computer's memory (by setting the values there to zero), so that there is a new uncertainty, smaller than the previous one: H_{after}. Then the computer memory has lost an average of

$$R = H_{before} - H_{after} \tag{20}$$

bits of information per flip-flop. If the computer was completely cleared, then $H_{after} = 0$ and $R = H_{before}$.

[2]This is because the fractions in equations (19) evaluate to irrational numbers when the logarithm is base 2, and since a Fano code divides by rational numbers, no binary Fano code can be made that exactly matches.

Now consider a teletype receiving characters over a phone line. If there were no noise in the phone line and no other source of errors, the teletype would print the text perfectly. With noise, there is some uncertainty about whether a character printed is really the right one. So before a character is printed, the teletype must be prepared for any of the letters, and this prepared state has uncertainty H_{before}, while after each character has been received there is still some uncertainty, H_{after}. This uncertainty is based on the probability that the symbol that came through is not equal to the symbol that was sent, and it measures the amount of noise.

Shannon gave an example of this in section 12 of [10] (pages 33-34 of [13]). A system with two equally likely symbols transmitting every second would send at a rate of 1 bit per second without errors. Suppose that the probability that a 0 is received when a 0 is sent is 0.99 and the probability of a 1 received is 0.01. "These figures are reversed if a 1 is received." Then the uncertainty after receiving a symbol is $H_{after} = -0.99 \log_2 0.99 - 0.01 \log_2 0.01 = 0.081$, so that the actual rate of transmission is $R = 1 - 0.081 = 0.919$ bits per second.[3] The amount of information that gets through is given by the decrease in uncertainty, equation (20).

Unfortunately many people have made errors because they did not keep this point clear. The errors occur because people implicitly assume that there is no noise in the communication. When there is no noise, $R = H_{before}$, as with the completely cleared computer memory. That is *if there is no noise, the amount of information communicated is equal to the uncertainty before communication.* When there is noise and someone assumes that there isn't any, this leads to all kinds of confusing philosophies. One must always account for noise.

One Final Subtle Point. In the previous section you may have found it odd that I used the word "flip-flop". This is because I was intentionally avoiding the use of the word "bit". The reason is that there are two meanings to this word, as we mentioned before while discussing Fano coding, and it is best to keep them distinct. Here are the two meanings for the word "bit":

1. A binary digit, 0 or 1. This can only be an integer. These 'bits' are the individual pieces of data in computers.

2. A *measure* of uncertainty, H, or information R. This can be any real number because it is an average. It's the measure that Shannon used to discuss communication systems.

[3] Shannon used the notation $H_y(x)$, meaning the conditional uncertainty at the receiver y given the message sent from x, for what we call H_{after}. He also used the term "equivocation".

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1 APPENDIX: A Tutorial On Logarithms

Understanding the Log Function. In the mathematical operation of addition we take two numbers and join them to create a third:

$$1+1=2. \tag{21}$$

We can repeat this operation:

$$1+1+1=3. \tag{22}$$

Multiplication is the mathematical operation that extends this:

$$3\times 1=3. \tag{23}$$

In the same way, we can repeat multiplication:

$$2\times 2=4. \tag{24}$$

and

$$2\times 2\times 2=8. \tag{25}$$

The extension of multiplication is exponentiation:

$$2\times 2=2^2=4. \tag{26}$$

and

$$2\times 2\times 2=2^3=8. \tag{27}$$

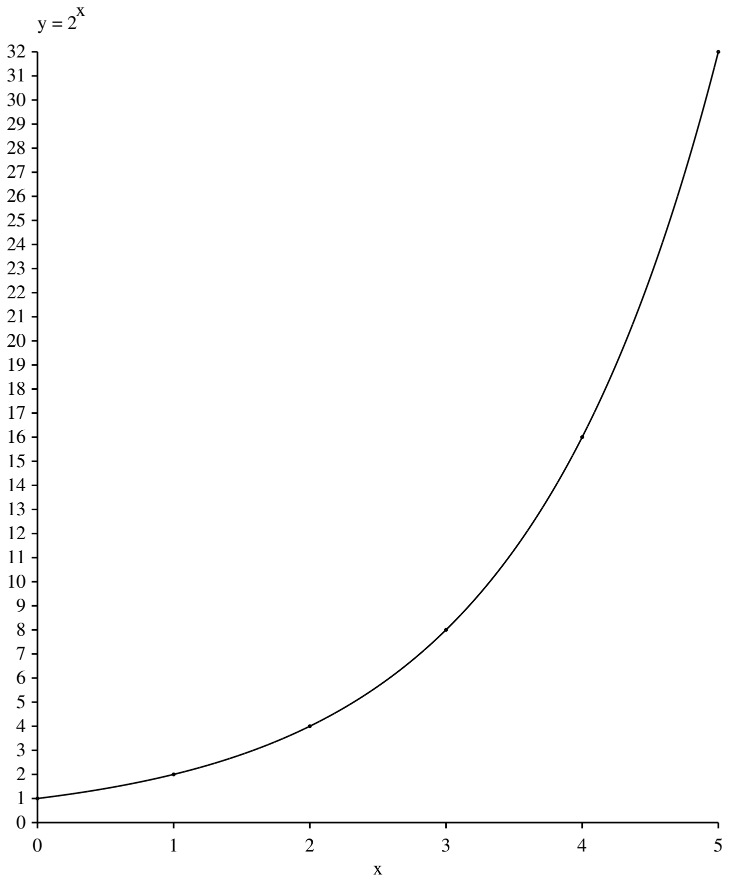
This is read "two raised to the third is eight". Because exponentiation simply counts the number of multiplications, the exponents add:

$$2^2\times 2^3=2^{2+3}=2^5. \tag{28}$$

The number '2' is called the base of the exponentiation. If we raise an exponent to another exponent, the values multiply:

$$\left(2^2\right)^3=2^2\times 2^2\times 2^2=2^{2+2+2}=2^{2\times 3}=2^6. \tag{29}$$

The exponential function $y = 2^x$ is shown in this graph[4]:



Now consider that we have a number and we want to know how many 2's must be multiplied together to get that number. For example, given that we are using '2' as the base, how many 2's must be multiplied together to get 32? That is, we want to solve this equation:

$$2^B = 32. \tag{30}$$

Of course, $2^5 = 32$, so $B = 5$. To be able to get a hold of this, mathematicians made up a new function called the logarithm:

$$\log_2 32 = 5. \tag{31}$$

We pronounce this as "the logarithm to the base 2 of 32 is 5". It is the "inverse function" for exponentiation:

$$2^{\log_2 a} = a \tag{32}$$

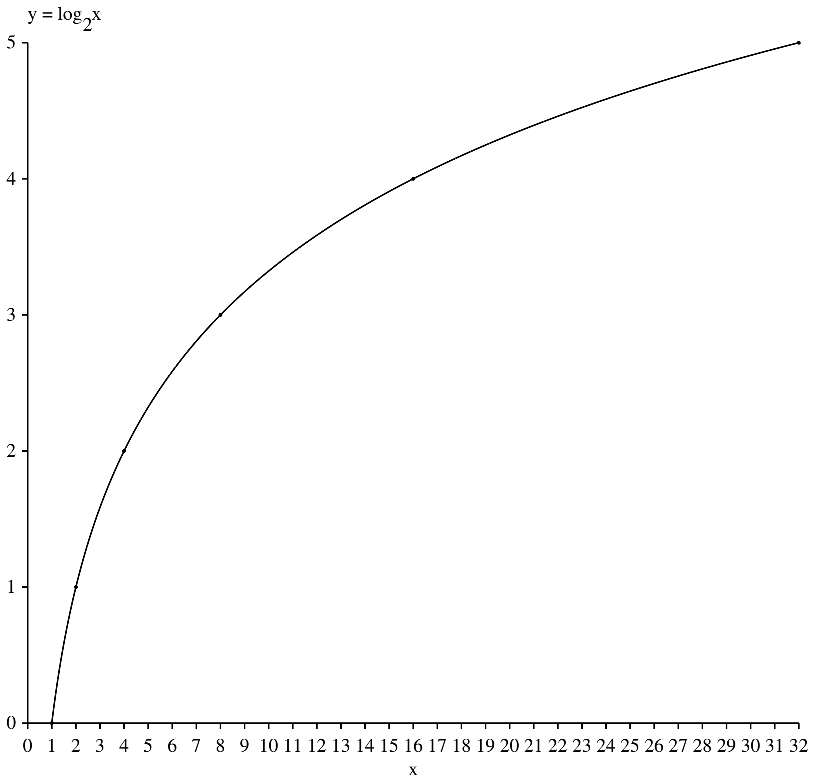
and

$$\log_2(2^a) = a. \tag{33}$$

The logarithmic function $y = \log_2 x$ is shown in this graph[5]:

[4]The program to create this graph is at http://www.lecb.ncifcrf.gov/∼toms/delila/expgraph.html

[5]The program to create this graph http://www.lecb.ncifcrf.gov/∼toms/delila/expgraph.html



This graph was created by switching the x and y of the exponential graph, which is the same as flipping the curve over on a 45° line. Notice in particular that $\log_2(1) = 0$ and $\log_2(0) = -\infty$.

The Addition Law. Consider this equation:

$$\boxed{2^{a+b} = 2^a \times 2^b} \tag{34}$$

which is just a generalization of equation (28). Take the logarithm of both sides:

$$\log_2 2^{a+b} = \log_2 \left(2^a \times 2^b\right) \tag{35}$$

Exponentiation and the logarithm are inverse operations, so we can collapse the left side:

$$a + b = \log_2 \left(2^a \times 2^b\right) \tag{36}$$

Now let's be tricky and substitute: $\log_2 x = a$ and $\log_2 y = b$:

$$\log_2 x + \log_2 y = \log_2 \left(2^{\log_2 x} \times 2^{\log_2 y}\right) \tag{37}$$

Again, exponentiation and the logarithm are inverse operations, so we can collapse the two cases on the right side:

$$\boxed{\log_2 x + \log_2 y = \log_2 (x \times y)} \tag{38}$$

This is the additive property that Shannon was interested in.

The "Pull Forward" Rule. From equation (32):

$$a = 2^{\log_2 a}. \tag{39}$$

Raise both sides to the u:

$$a^u = \left(2^{\log_2 a}\right)^u. \tag{40}$$

Now, we can combine the exponents by multiplying, as in (29):

$$a^u = 2^{u \log_2 a}. \tag{41}$$

Finally, take the log base 2 of both sides and collapse the right side:

$$\boxed{\log_2 a^u = u \log_2 a} \tag{42}$$

This can be remembered as a rule that allows one to "pull" the exponent forward from inside the logarithm.

How to Convert Between Different Bases. Calculators and computers generally don't calculate the logarithm to the base 2, but we can use a trick to make this easy. Start by letting:

$$x = \log_z a / \log_z b \tag{43}$$

Rearrange it as:

$$\log_z a = x \log_z b. \tag{44}$$

Now use a "reverse pull forward" (!):

$$\log_z a = \log_z b^x \tag{45}$$

and drop the logs:

$$a = b^x. \tag{46}$$

Now take the log base b:

$$\log_b a = \log_b b^x. \tag{47}$$

This simplifies to:

$$\log_b a = x. \tag{48}$$

But we know what x is from equation (43):

$$\log_b a = \log_z a / \log_z b \tag{49}$$

The conversion rule to get logarithms base 2 from any base z is:

$$\boxed{\log_2(a) = \log_z(a) / \log_z(2)} \tag{50}$$

Notice that since the z does not appear on the left hand side it doesn't matter what kind of logarithm you have available, because you can always get to another base using this equation! Try this example on your calculator:

$$\log_2(32) = \frac{\log_{\text{whatever!}}(32)}{\log_{\text{whatever!}}(2)}. \tag{51}$$

You should get '5'.

Tricks With Powers of 2. In calculus we learn about the natural logarithm with base $e = 2.718281828459045\ldots$[6] Calculations with this base can easily be done by a computer or calculator, but they are difficult for most people to do in their head.

In contrast, the powers of 2 are easy to memorize and remember:

choices M	bits B
1	0
2	1
4	2
8	3
16	4
32	5
64	6
128	7
256	8
512	9
1024	10

where $2^B = M$ and $\log_2 M = B$.

We can use this table and a trick to make quick estimates of the logs of higher numbers. Notice that

$$2^{10} = 1024 \approx 1000 = 10^3. \tag{52}$$

So to take the log base 2 of 4×10^6, we think:

$$\begin{aligned}
\log_2(4 \times 10^6) &= \log_2(4) + \log_2(10^6) && (53)\\
&= 2 + \log_2(10^3 \times 10^3) && (54)\\
&= 2 + \log_2(10^3) + \log_2(10^3) && (55)\\
&\approx 2 + \log_2(2^{10}) + \log_2(2^{10}) && (56)\\
&\approx 2 + 10 + 10 && (57)\\
&\approx 22 && (58)
\end{aligned}$$

The actual value is 21.93.

[6] Want to impress your friends by memorizing this number? Note that after the 2.7 (you are you your own for that!) we have two 1828's followed by a 45°-90°-45°triangle.