Physics 2660

Lecture 10

<u>Today</u>

Comments on chi-squared fits

• Bitwise operators and binary files

• Generating arbitrary distributions of pseudo-random numbers for functions that can be inverted and binned data

1



- As scientists, we're also "in search of the unknown". We're looking for the physical laws of the universe. We can't see what's far out in front of us, though, so we have to slowly feel our way along, one experiment at a time.
- The tools that tell us if there's something solid in front of us, or just air, are statistical measures like chisquared. Today we'll start out by looking at other tools, and some of the limitations of chi-squared.



- First, a note about the importance of fitting models to data.
- Fitting is widely used in every field of science and engineering, including the physical sciences, biology and the social sciences. It's one of the most important computational techniques for you to learn. As soon as you start collecting data of any kind, you'll want to fit some theoretical model to it, and you'll want to know how well that model fits.
- That's why we're spending a substantial amount of time talking about it.

The Art of Curve Fitting:

There are many things that may make it difficult or impossible to get a model to fit your data well. Some of them are:

- Using an incorrect model to represent data.
- Making a poor choice of starting parameters.

Perhaps they are too far from correct values? Also, some programs have trouble with starting parameters at 0.0.

• Sometimes parameters land on unphysical values during the χ^2 minimization process: 1/0, log(-1), 10^300, sqrt(negative #), ...

• Sometimes the fitting program has difficulty settling into stable values for the parameters (convergence):

- Maybe you're fitting too many parameters at once, while far from the minimum χ^2 .

- Maybe you've chosen a poor set of model parameters: high correlations, large differences in scale among parameters (leading to rounding errors), ...





The term "pull distribution" is used in Physics, but I'm not sure how widely used this term is in other fields. Some people just call it the "histogram of the fit residuals".









Sometimes we assume that our data has been generated according to a particular probability distribution (a Gaussian distribution, for example). We can check whether this is likely to be true by looking at the distribution's Cumulative Distribution Function.



This particular example shows the CDF of a Gaussian distribution centered at zero. Notice that the value of the CDF is 0.5 when x=0. This just tells us that there's a 50% chance of observing an x value less than zero.



The pages on Wikipedia for the various probability distrubutions are great. Each one shows graphs of the distribution's PDF and CDF, along with their functional forms.



- The ECDF is computed from "unbinned" data (i.e., you don't histogram the data and look at the bins, you look at the raw, unhistogrammed numbers).
- To construct an ECDF just sort the data numbers, x_i, in order of increasing value. Then, if the number of values is N, plot x_i on the x-axis and i/N on the y-axis.



The Kolmogorov-Smirnov (KS) test provides us with a mathematical way of testing to see if a set of data is likely to have been generated by a given probability distribution.



Here's a table of such probabilities for various values of $D_{\mbox{\tiny N}}$ and N.



The next section deals with manipulating individual bits within data. This is a topic we haven't talked about yet, and we'll spend some time on it in the next couple of lectures, a lab, and a homework assignment.

Bits and Bytes: Until now, we've only dealt with data in 8-bit chunks called "bytes". All of the variable types we've used have sizes that are integer multiples of 8 bits. 8 bits: 1 1 1 1 1 Byte For g++ on Galileo: sizeof(int) 4 bytes used to store an integer returns 4 sizeof(double) 8 bytes used to store a double returns 8 sizeof(char) returns 1 1 byte used to store a char But sometimes we want to flip individual bits. Let's look at how that can be done. 17



We often think of a set of bits like this as a checklist, where we can "set" a bit, by making it a 1, or "unset" it by making it a 0.

Bitwise Operators:

C provides several operators for manipulating individual bits:

&	a&b	Bitwise and
	a b	Bitwise <i>or</i>
<<	a< <b< td=""><td>Left shift</td></b<>	Left shift
>>	a>>b	Right shift
1	~a	Bitwise inverse

Don't confuse the & and | operators with the & & and | | operators we've used before.

Let's see what these new operators do.

19

Bitwise And:

The "&" operator performs a "bitwise and" on its two arguments. The bits of the returned value are computed by "and"ing together the corresponding bits of the two arguments. If both bits are "1", then the resulting bit is "1", otherwise, it's "0".







This seems like an odd thing to want to do, but we'll see what it's good for soon.





Don't confuse this with the logical "!" operator.



Also note that 1<<0 is just equal to 1.

Notice that this gives us an easy way to make powers of two. Instead of, for example, writing:

pow(2,4)

for 2⁴, we could just write:

1<<4

And, as you might imagine, the latter is much faster.



- See what's happening here? Most of the bits in "1<<n" are zero (there's only one non-zero bit). When a bit from "a" gets anded with one of these zeros, the result will always be zero, since "anything & 0" is zero.
- This means that all but one of the bits in the result will always be zero. The only bit in question is the bit that gets anded with "1". If this bit of "a" is zero, then the result has zero. Otherwise, the result has a one.



You can think of "1<<4" as a "mask" that only lets one bit through. (Bit number 4, in this case.) The "1" in the bit pattern of "1<<4" is like a hole in the mask, allowing us to see through to the value of the corresponding bit in "a", underneath.



- In this example, all but one of the bits in "1<<3" is zero. Since "anything | 0" is just "anything", most of the bits in the result will have the same values they have in "a".
- The one exception is the bit of "a" that's above the "1" in "1<<3". Since "anything | 1" is always 1, this bit of the result will always be 1.



- Most of the bits in ~(1<<4) are ones. There's only one zero bit. Since "anything & 1" is just "anything", most of the bits in the result will have the same values they have in "a".
- The one exception is the bit of "a" above the "0". Since "anything & 0" is always zero, this bit will always be zero.

Example Program:



Note how we use 1<<n to write out the powers of two.

Hexadecimal Representation:

Binary numbers are long, and it's easy to mis-type a 1 or 0. Because of this, we often represent binary numbers in "hexadecimal" (base 16) form. Hex notation works better than our normal "decimal" (base 10) system for this because each hex digit is equivalent to exactly 4 bits (half a byte).

In hex notation, there are 16 digits instead of the 10 we usually use, or the 2 (0 and 1) that are used in binary. Here's how you count in hex:

0, 1, 2, 3, 4, 5, 6, 7, 8, 9, A, B, C, D, E, F Decimal equivalents → 10,11,12,13,14,15						
Decimal	Binary	<u>Hex</u>	Here are some examples showing decimal, binary and hex equivalents for a few numbers.			
1	00000001	01				
10	00001010	0A				
42	00101010	2A				
100	01100100	64	31			
128	10000000	80				
255	11111111	FF				





- The history of the "0x" notation goes like this: a long time ago, people often used "octal" (base 8) notation with computers. In C, you can write octal numbers by just prefixing a zero in front of the number, like "012". The leading zero indicates that this number is to be interpreted in something other than base 10.
- To accomodate hexadecimal numbers, C added an "x" after the zero. (For "heXadecimal".) The C compiler interprets "0x12" something like this:
- "Here comes a non-decimal number. Oh, and by the way, it's hexadecimal. And the digits are 1,2."

Data S	Storage:							
When variab	nen storing bit-wise data, we usually use one of the "unsigned" iable types.							
Why? simple	Why? With these types, the representation of a number in memory is simple: the bits are just a binary representation of the number.							
Other	Other data types encode sign (+/-), exponent information and other things in some of the bits, making it hard to predict how your data values will change when you change a particular bit.							
things values	in some of the bits, making it has will change when you change a Typical values:	d to predict h particular bit	now your data					
things values	in some of the bits, making it has will change when you change a Typical values: sizeof(unsigned char)	rd to predict h particular bit 1 byte	now your data <mark>8</mark> bits					
things values	in some of the bits, making it has will change when you change a Typical values: sizeof(unsigned char) sizeof(unsigned short)	rd to predict r particular bit 1 byte 2 bytes	now your data 8 bits 16 bits					
things values	<pre>in some of the bits, making it has will change when you change a Typical values: sizeof(unsigned char) sizeof(unsigned short) sizeof(unsigned int)</pre>	rd to predict h particular bit 1 byte 2 bytes 4 bytes	8 bits 16 bits 32 bits					

Since the "unsigned" variable types have such a simple, direct representation in memory, we can quickly do multiplication or division by powers of 2 on them by using the bitwise shift operators:

unsigned int i = 42; unsigned int j;

j = i<<1; // Multiply i by 2. j = i<<2; // Multiply i by 4.

j = i>>1; // Divide i by 2. j = i>>2; // Divide i by 4.



So, what kinds of things might we use these operators for? Here's an example of one kind of application where bitwise operations might be useful.



If we could flip the bits on and off, like light switches, we could control the robot's behavior.

Setting Command Bits:

We can define individual motion commands, using the left shift operator:

unsigned char FWD_STEP	= 1<< 0;	// 1	i.e. 00000001
unsigned char BAK_STEP	= 1<< 1;	// 2	i.e. 00000010
unsigned char RGT_TURN	= 1<< 2;	// 4	i.e. 00000100
unsigned char LFT_TURN	= 1<< 3;	// 8	i.e. 00001000
unsigned char RGT_ARM_UP	= 1<< 4;	// 16	i.e. 00010000
unsigned char LFT_ARM_UP	= 1<< 5;	// 32	i.e. 00100000
unsigned char LFT_LOOK	= 1<< 6;	// 64	i.e. 01000000
unsigned char RGT_LOOK	= 1<< 7;	//128	i.e. 10000000

Then compound commands can easily be constructed using bitwise operators. For example:

unsigned char FWD_LEFT	= FWD_STEP LFT_TURN;	// 00001001
unsigned char BAK_RIGHT	= BAK_STEP RGT_TURN;	// 00000110

Note that, in reality, we would need to define the precedence of these actions, since they don't commute. (E.g., a forward step followed by a left turn isn't the same as a left turn followed by a forward step.) 37

We'll do more with bitwise operations in this week's lab.

Part 3: Arbitrary Random Number Distributions



- Here's an arbitrary random picture of a bullfrog from the pond down the street.
- We've talked a lot about a couple of probability distributions: the Gaussian (Normal) distribution and the uniform distribution. We've seen how it's possible to generate random numbers according to each of these.
- But what if we want to generate random numbers in some other distribution? Is there some general way to generate random numbers in a given, arbitrary distribution?



- If you remember the Barnsley Fern problem we did a few weeks ago, you may recall that it required us to pick one of four functions (f1, f2, f3, or f4) at random, with a different probability for picking each function.
- We could represent that as a Probability Density Function, like the graph above. The height of the blue line just represents the probability of picking each function.



We could integrate this PDF and come up with a CDF, like the one shown in red.



Do you recall how we picked which function to use? We chose a uniformly-distributed random number, U, between 0 and 1, and then said:

- if U between 0.00 and 0.01 pick f1
- if U between 0.01 and 0.86 pick f2
- if U between 0.86 and 0.93 pick f3
- if U between 0.93 and 1.000 pick f4

When we did this, we were just integrating the PDF in our heads, and creating the CDF.



- The uniformly-distributed random number we picked just corresponds to the vertical axis on the graph. Following the blue dashed line, it told us which function to pick.
- It turns out that you can use the same procedure to generate random numbers in any distribution you want. All you need to know is the distribution's CDF.



For example, here's the PDF (dark blue) and CDF (red) for a Gaussian (Normal) distribution. By picking a uniformly-distributed random number between 0 and 1 on the y-axis, we could get a number N from the x-axis. The values of N picked in this way would be distributed in a Gaussian way. If we histogrammed these numbers, we'd see the familiar Gaussian bell curve.



- The devil is in the details, though. We'd like to be able to generate U, then stick U into some formula that gives us N. The CDF, though, gives us a formula for getting U from N (the exact opposite of what we want).
- Can we invert the CDF to get a function that does what we want?
- The actual form of the CDF for a Gaussian is shown in the formula at the bottom. Can we solve this equation for N as a function of U?



- Yes, we can! The formula for the "inverse CDF" of a unit Normal distribution is shown at the top. Using this, we could just generate uniformly-distributed U values on the x axis, and plug those values into the function to get the corresponding normally-distributed N values.
- There's a practical problem with this, though. In the regions that are circled at either end of the graph, the function is zooming up (or down) very fast. This means that a small change in U in this region will cause a large change in N. Note that these regions are only two or three standard deviations away from N=0.
- Once we're beyond a few sigma away from N=0, we'll find that small computational errors will multiply rapidly, and our results for N will become meaningless.
- This is why we don't typically use this method to generate normally-distributed numbers. Instead, we use tricks like the Box-Muller method that our "randn" function uses.

The Exponential Distribution:

Although the inverse-CDF method doesn't work well for all distributions (even when it can be calculated!), there are some distributions for which it works just fine.

One example is the exponential probability distribution, which is sometimes used to describe the probable lifetime of devices like lightbulbs, as a function of time after turning them on.



Some distributions work better, though. Here's an example of one that does.



And here's an example, showing how you can use the inverse CDF of the exponential distribution to actually generate numbers distributed this way.



- Of course we are often interested in distributions for which the CDF isn't known, or can't be inverted.
- There are a couple of methods we could use to generate numbers distributed in any way at all. First, we could approximate the inverse of the CDF and its inverse by using a fixed number of samples. We've done similar things for the purpose of integration (estimating the area underneath a curve). Let's see how that works.



First, slice up the x axis, and find the height of each slice.



- As we're making slices from left to right, store the sum of all the slices so far into an array element. When we're done, the array will contain our Cumulative Distribution Function (or an approximation of it).
- (Of course, we'll need to normalize it to a maximum value of 1. We can do this by dividing all of the aray elements by the last, largest element.)
- We can use this CDF to generate random numbers distributed like the original PDF. Just generate a uniformly-distributed random number, U, then loop through our array elements until we find one with a value greater than U. The N value corresponding to this array element is the one we want.
- By using a smaller step size, we can increase the accuracy.



- It turns out that there's another, easier but slower way to generate random numbers in any distribution you want. It's essentially another Monte Carlo method, similar to the Monte Carlo integration techniques we looked at earlier.
- Say, for example, we want to generate random numbers according to some funky probability distribution like the red line in the graph above. All we need to do is generate some random points. For each point, we check to see if it's underneath the red curve. If it is, then we return this point's x value as our random number. If it's not, we try again.

Monte Carlo Explanation:

This technique is slow, but it will always work, even for the oddest approbability distributions.

How does it work?



As we generate random points, it's more likely for a point to fall under the curve at x values where the curve is high (there's more room underneath), so more of our random numbers will come from these places.

At x values where the curve is low, points will be less likely to fall underneath the curve, so we'll get fewer random numbers from there.



Last week, in the homework problem involving a projectile with air resistance, we solved a differential equation numerically, using a technique called Euler's method. Let's look at another way of solving these equations.





Consider the problem above, involving velocity and time. We aren't explicitly given the relationship between velocity and time, but we're told that dv/dt is some function that we can evaluate, and we're told an initial condition. We want to find v at a later time value.



As you can see, the estimate in this case isn't very close to the true value at all. Maybe if we divided the x distance up into a hundred steps (instead of one) we'd get a better value. But that would involve a lot of computations, and take a lot of time.



- There's a whole family of Runge-Kutta methods, but generally when people say "the Runge-Kutta method" they mean the 4th order one. It gives good results, and higher-order versions are significantly more difficult to calculate.
- As we'll see in the pages that follow, the Runge-Kutta method gives results that are much more accurate than we'd get using a similar number of computations with the Euler method.



Note that we find the slope by just evaluating our function, f(x,y) at this point.





- We're now using slopes obtained from four different points: one point at each end of the trajectory (the original position and point 5), and two points in the middle (points 2 and 4).
- Using these slopes, we've found four estimates of the final position: points 1, 3, 5 and 6.



The final weighted average is a pretty good approximation to the true value. Note that it only required a few calculations to get it. Compare this to the possibly hundreds of steps that would be reqired to get a simlar accuracy from the Euler method, and you'll see the appeal of the RK4 method.

Next Time:

- More on bitwise operations
- Dynamic memory allocation





Thanks!