

Analog and Digital Signals in Analytical Instruments

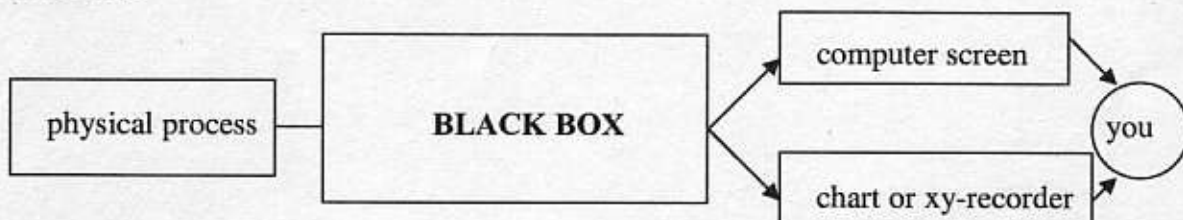
Once upon a time, scientists relied upon little more than their five senses in collecting data. For example, observations of color changes or changes of state (liquid \rightarrow gas was the way to identify and quantify unknowns. No more. Today, the modern scientist employs whatever breakthrough technology is available in physical and engineering science. Not only that, the availability of the computer, in the form of workstations or personal computers, has had a profound effect on what you can do with the data you collect. Consequently, today's scientist (that includes you) must be well versed in how instrumentation advances have revolutionized the measurement science. While most of you will never build your own instruments, and might prefer to treat them as black boxes, it is important at a minimum that you understand the capabilities and limitations of available technology and have the vocabulary that lets you talk with the salesmen. That way, when you hear words like:

digitizer or dynamic range or bandpass filter or transducer or op amp

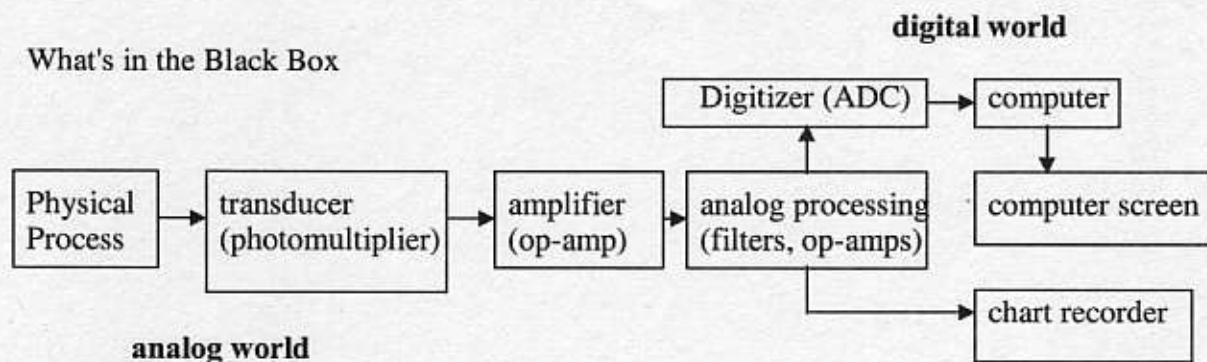
you can nod your head, safe in the knowledge that at the very least, you were once taught the material.

What it all comes down to for scientists exploring the unknown is this: somewhere out there a physical process is occurring that would be really useful in identifying and quantifying some unknown. Maybe it is some electromagnetic radiation bouncing off the sample. Maybe it is a redox reaction being driven by a supply of electrons. The thing is, usually you have a difficult time quantifying what is happening (how much did the color change), and most of the time you can't even see the change (how many X-rays just hit the sample.). What you would like, ideally, is to sit back and watch the result show up in living color on your computer screen, with a nice print-out to boot. Or at the very least, a nice chart recorder or XY-recorder you can photocopy off of from your lab partner. The question to be asked in the next two lectures is, exactly what goes in that box:

The Black Box



Well the answer to what is in the black box can be broken down into just a few categories that we will examine. These are shown in the next figure. First there has to be a translator of some sort that converts the physical phenomenon into something our electronic age can deal with. (We call this a TRANSDUCER.) This transducer most often yields a continuous (analog) signal that travels in an electrical circuit. Digital signals are what are stored in a computer.



Some change in the analog signal is your source of information about the sample. Now there has to be some way to amplify the analog signal which will come out of the transducer at the **nanovolt or microvolt** level. Most transistors in digital circuits like computers operate in the millivolt to low volt level. For example, the on and off voltages in a semiconductor chip can be +5V and 0V, respectively. So those microvolt outputs from a transducer would have little effect if input directly to the computer. Similarly, an oscilloscope or chart recorder pen will respond to voltages in the millivolt to 10V range, again requiring that some form of amplification occur. Operations amplifiers (op-amps) are electronic devices that nicely perform this role of amplifying the signal.

Also of importance in the black box are signal preparation devices that modify the analog signal to provide us with the kind of signal we want to see. For example, RC filters do a nice job of cleaning up unwanted noise so that our data has a smoother or higher S/N appearance (the RC filter does the moving window smooth that we discussed in real time.) Op-amps also perform a wide range of operations on an analog signal, including mathematical functions such as addition, multiplication, differentiation, and integration. All of these operations are performed in real-time (while the experiment is going) on an analog signal. From the point where a signal has been appropriately amplified and cleaned up to our satisfaction, it then can be output directly as an analog signal on a chart recorder or xy-recorder.

Suppose however, we want to put out analog data into a computer? Computers have the advantage that the stored data can be evaluated in a post-processing (opposite of real-time) environment. We literally have all day to play with the data to extract as much information as we can from it and then make it as pretty as possible for others to observe. For example, if we are going to do some kind of Fourier transform deconvolution, or some kind of least squares curve fit or some kind of optimization, or maybe we just want to show the data in a 3-D 65,536 color plot, we need to convert an analog signal into digital signal. A digital signal is the kind required for data to be processed by a computer and stored for later use.

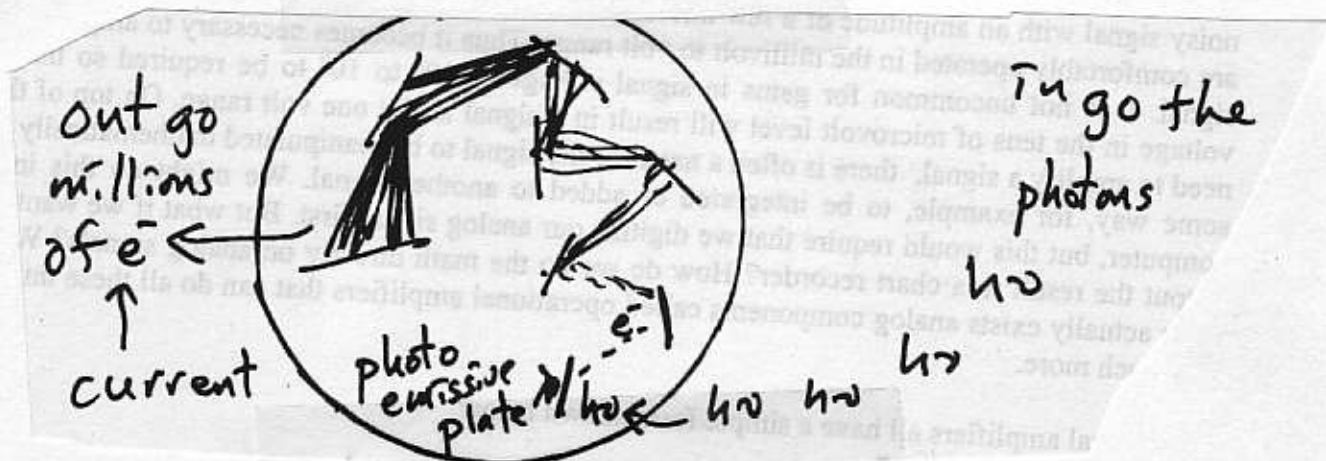
Shown in the figure above are the filled components of the black box. Over the next two lectures we will look at examples of these basic elements of electronic circuits.

ANALOG SIGNALS

Transducers. As you are aware, the mere act of observing a physical phenomenon will perturb it. The extent to which the perturbation of the system occurs can be very important because the tools we use to make and record the observation might potentially introduce erroneous contributions to the measurement we record. Consider for example that we have a chromatograph that does a fine job of separating peppermint oil into 100 components, each of which elute at different times from the end of a chromatographic column. Without some means of detecting the signal, the fact that the separation has occurred will be unknown to us. So we decide to attach a spectrometer as a detector. Each time a compound elutes from the column, light shines on the sample. Some of the light absorbed at wavelengths corresponding to specific types of bonds in each kind of molecule. Again, however, because we cannot see the light (except in the visible region), our sense tell us nothing about what is going on., we are still in the dark. Fortunately, a device is provided to us which converts the physical response (for example, the absorption of light by a molecule) into something we can work with. This device, called a transducer, can come in many forms, but it always generates some sort of measurable change in a way that we can access. For example, we have invented ways to carefully measure changes in voltage, or current, or resistance, or frequency using electronic circuits. So a transducer that measures the absorption of light and provides an output in the form of a change in voltage will be useful.

One common version of a transducer is called a photomultiplier tube (shown below.) A photomultiplier exploits the photoelectric effect (discovering this effect got Einstein a Nobel Prize). In a photomultiplier tube, a photon of light arrives at a phototransmissive surface, and off pops an electron--the fundamental currency in our electronic circuitry. This electron is directed along a series of dynodes, producing more and more electrons along the way until out the other end pops about a million electrons which are a measurable current.

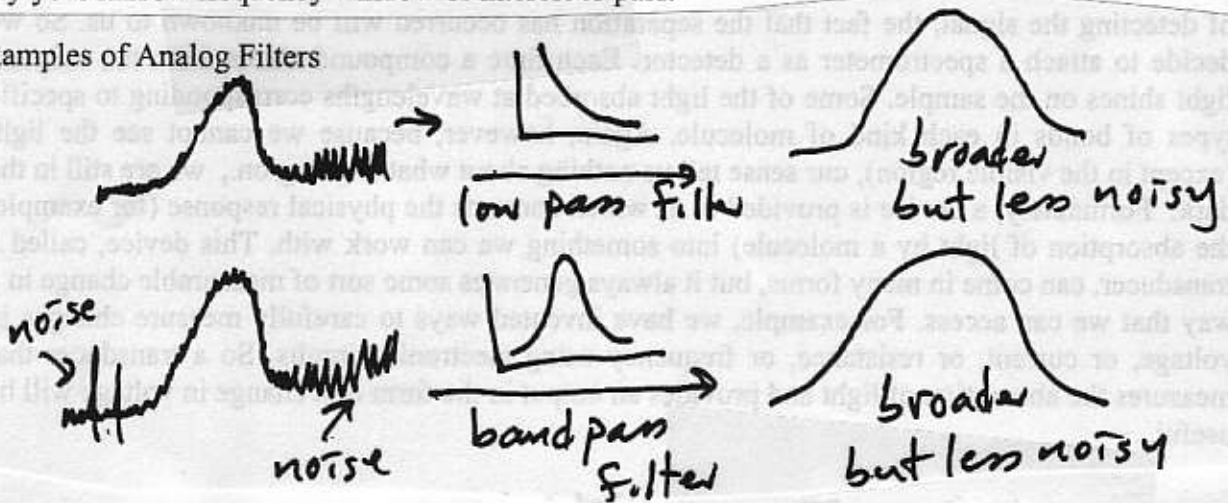
Transducer Example : A Photomultiplier Tube



There are many other types of transducers, including piezoelectric crystals and thermocouples. All share the common ability to convert a physical process (the kind you study in physical chemistry) into something we can more readily manipulate using electronic signals.

Analog Filters. Unfortunately, very often our desired signal sits in the midst of a noisy background that is making it difficult to distinguish a strong signal. Fortunately you will know the frequency region in which you are working; for example, d.c. (zero frequency) for chromatography or 150nm to 300nm for UV spectroscopy. So you can utilize a filter composed of appropriate resistor and capacitor components that allows only frequencies in your frequency window of interest to pass. Thus you might desire a low pass filter that removes high frequency white noise and allows your chromatographic signal (d.c) to pass. Or you might use a high pass filter that removes low frequency flicker noise. Or you might use a bandpass filter that allows only your narrow frequency window of interest to pass.

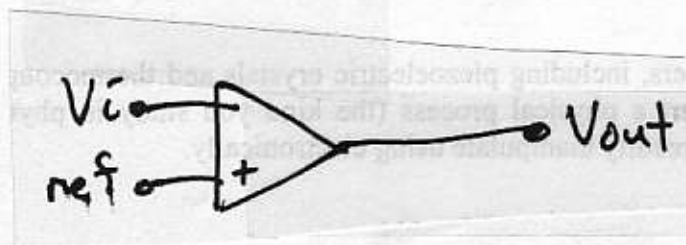
Examples of Analog Filters



Examples of each of these are shown above. Shown on the next page are the circuits for simple RC filter that remove low frequency or high frequency noise. The equations associated with the ratio of output signal for a given input signal are also included. An example of a low pass filter in operation is also shown.

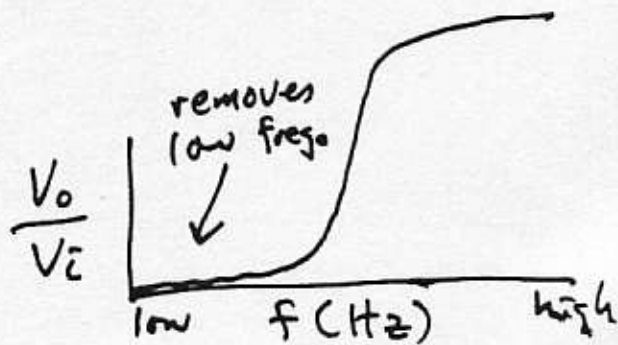
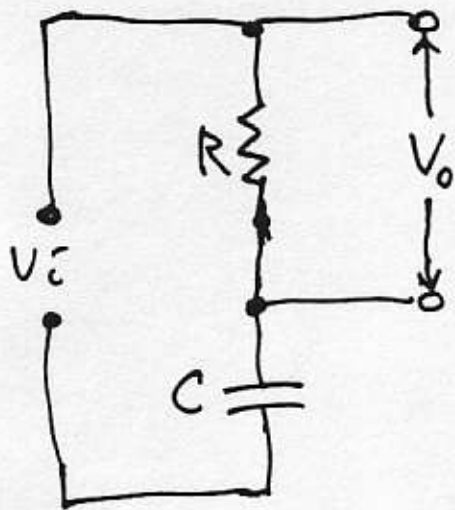
Amplifier Circuits. Okay, so now we have a transducer and a filter that have produced a less noisy signal with an amplitude of a few microvolts. Remember though, that modern instruments are comfortably operated in the millivolt to volt range. Thus it becomes necessary to amplify the signal. It is not uncommon for gains in signal voltage of 10^2 to 10^6 to be required so that a voltage in the tens of microvolt level will result in a signal in the one volt range. On top of the need to amplify a signal, there is often a need for the signal to be manipulated mathematically in some way, for example, to be integrated or added to another signal. We might do this in a computer, but this would require that we digitize our analog signal first. But what if we want to output the result to a chart recorder? How do we do the math directly on analog signals? Well there actually exists analog components called operational amplifiers that can do all these things and much more.

Operational amplifiers all have a simple form shown below



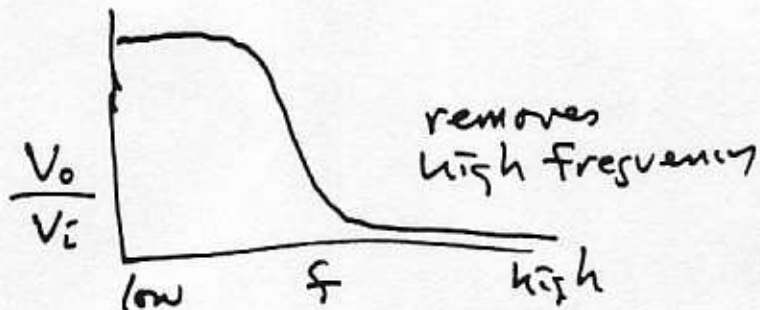
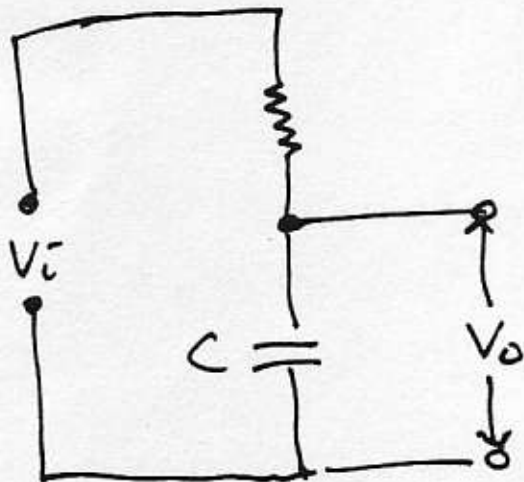
Analog Filters (RC Filters)

high pass

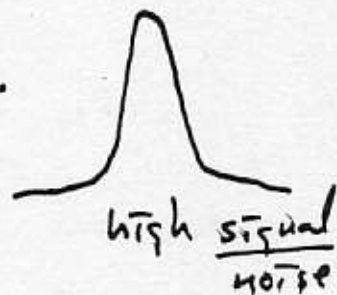
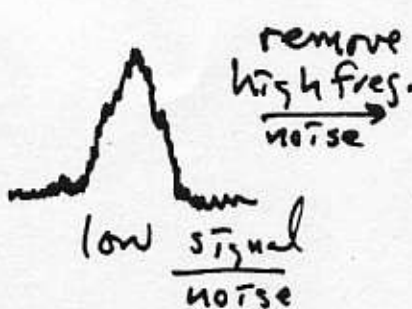


$$\frac{V_o}{V_i} = \frac{R}{\left[R^2 + \left(\frac{1}{2\pi f C} \right)^2 \right]^{1/2}}$$

low pass



$$\frac{V_o}{V_i} = \frac{1}{2\pi f C \left[R^2 + \left(\frac{1}{2\pi f C} \right)^2 \right]^{1/2}}$$



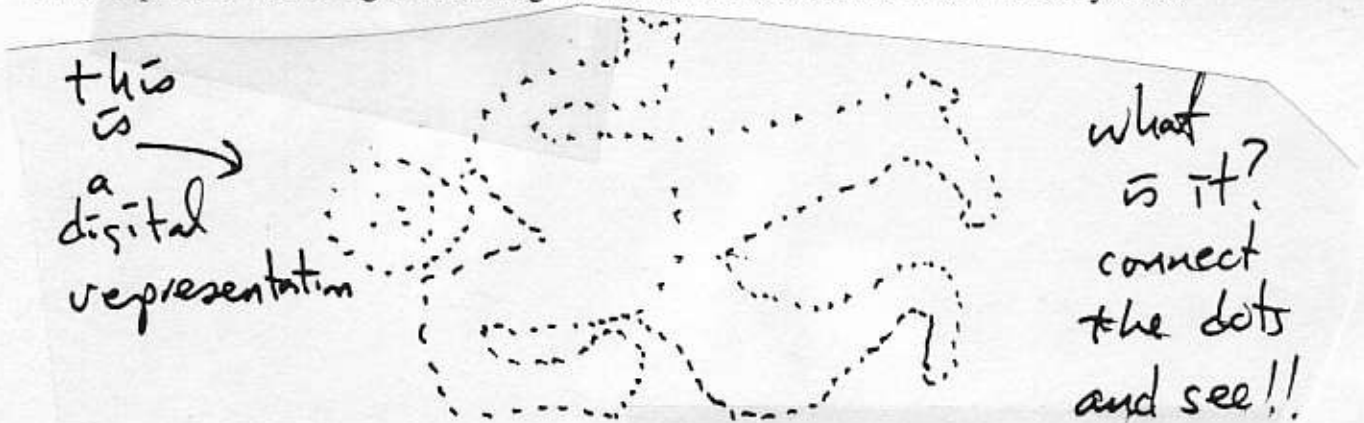
and can be used to convert some input voltage V_{in} , into any desired output voltage, V_{out} we desire. Without going into specifics on how an op-amp works, I can show you several examples of simple OP-AMP circuits that can multiply (amplify), add, integrate, and differentiate.

GIVE ME SOME DATA I CAN PUT MY HANDS ON

Analog Output. There is, of course, the need to convert the processed analog signal into something we take home to show our loved ones. The simplest approach is a chart recorder or XY-recorder, although even with these analog devices, there are severe restrictions on the kind that is acceptable. For example, if the output voltage is too high, the recorder output is off-scale. If the voltage is insufficiently amplified, no signal is measured. Of course, other factors such as the recorder speed and how fast the pen is will also have an affect on whether the data is adequately represented.

Even if the analog output is appropriately scaled, a huge problem remains: there isn't much you can do with the data. At one time this was acceptable, but today when we look at the computational capability of computers, there is a strong desire to increase the flexibility and power of the data processing. Thus, rather than do the processing in real time using op-amps and RC circuits, it is of merit to manipulate the analog signal in a post-processing mode. Unfortunately, computers are not analog; rather, they take advantage of semiconductor technology that employs discrete voltages or switches to define a signal. These discrete voltages are referred to as digital signals. In simple coloring book lingo, in a connect the dots picture, the continuous line you draw to connect the dots is analogous to an analog signal. The discrete, or individual dots are the digital signal.

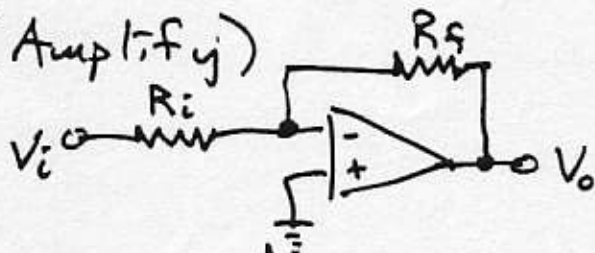
Let's all pretend we are digital to analog converters and connect the dots. What do you see



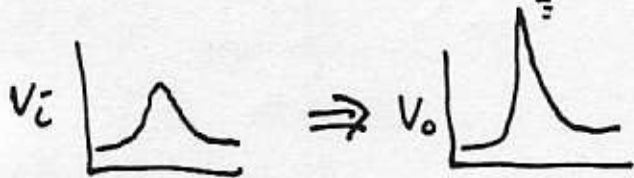
It makes sense that if we want to get from an analog to a digital signal, we will need to construct an analog to digital converter (ADC or digitizer). If we want to do the reverse and convert a digital signal stored in the computer into an analog signal, you need to use a digital to analog (DAC). The obvious advantage of digital signals is the ability to store and mathematically manipulate them whenever we desire. The disadvantage is that the resolution is lost, because now individual data points are stored rather than the continuous signal.

Op Amp Circuits

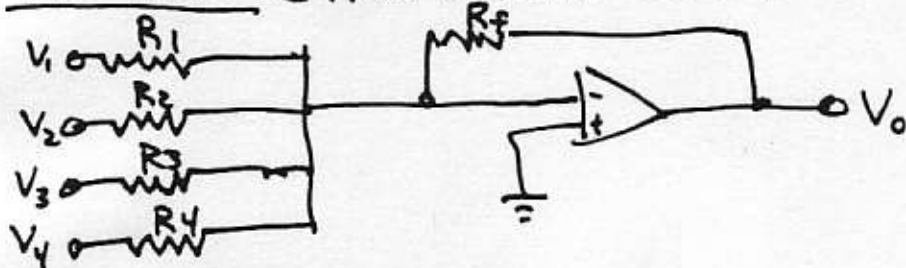
Multiply (Amplify)



$$V_o = -\frac{R_f}{R_i} V_i$$

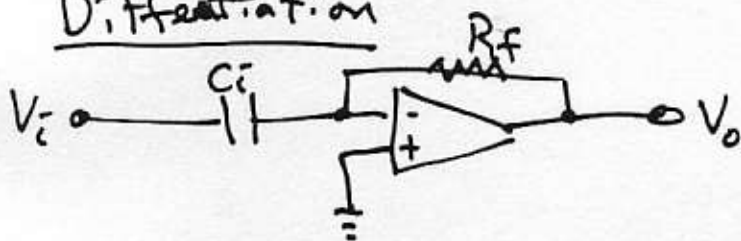


Addition (How a DAC works)

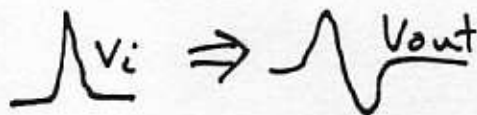


$$V_{out} = -R_f \left(\frac{V_1}{R_1} + \frac{V_2}{R_2} + \dots \right)$$

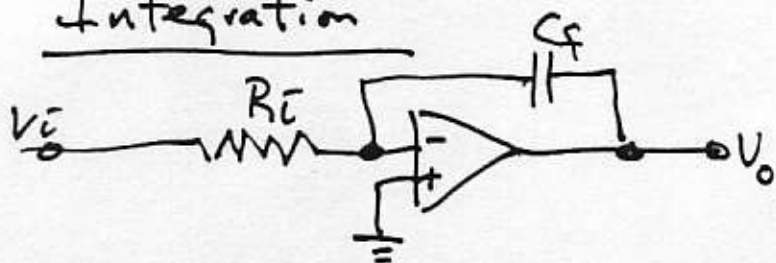
Differentiation



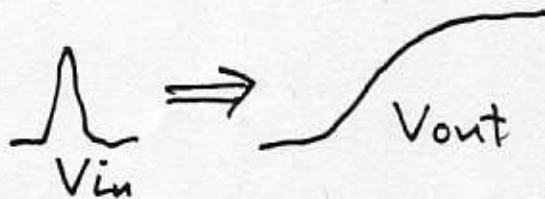
$$V_o = -R_f C_i \frac{dV_{in}}{dt}$$



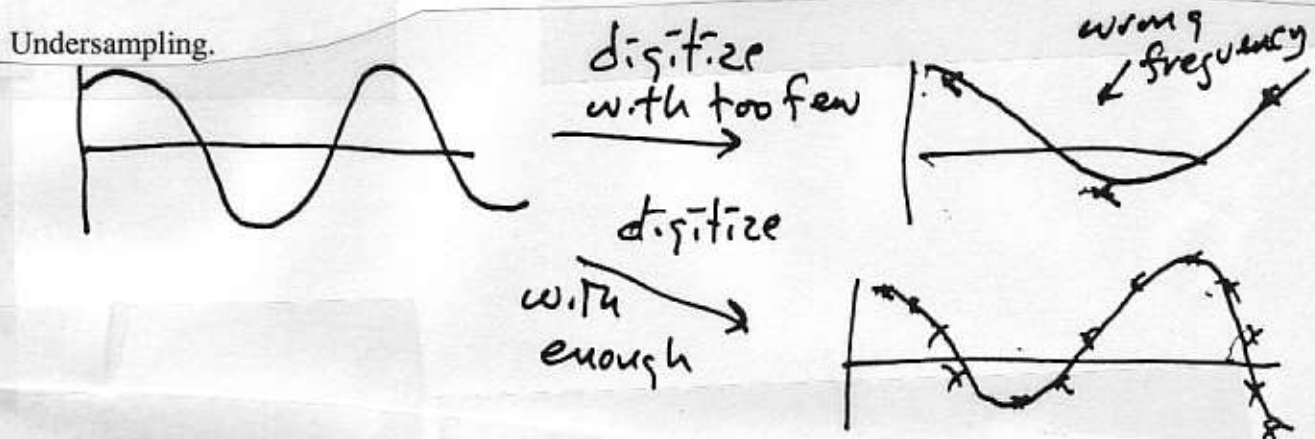
Integration



$$V_o = -\frac{1}{R_i C_f} \int_0^t V_i dt$$



Undersampling. The inability to collect an adequate number of data points is another problem with digitizing signals. If the frequency of the data is undersampled (not collected frequently enough), the actual data is misrepresented. This undersampling phenomenon is called understanding or aliasing and is what happens when Nyquist theorem isn't satisfied. The Nyquist theorem says that when collecting data, always sample it at twice the highest frequency in the spectrum. Shown below is an example of what happens when you don't satisfy the Nyquist sampling rate.



Boundaries and dynamic range. Problems with boundaries come up in digitized signals as well. You can either overflow a digital component like an ADC or microprocessor (the equivalent of your chart recorder going off-scale), or your input signal can be so small, that nothing registers in the device (the equivalent of a flat baseline in your chart recorder.) In a moment we will look at the concept of dynamic range in instrumentation, but first to understand it, we have to have a refresher course in binary numbers.

TIME OUT FOR BINARY NUMBERS

Before going into too much detail about dynamic range in digital electronics, it is important to introduce the nomenclature for describing the magnitude of such number. transistors are based upon the idea of the device being on if an output voltage is 5V, while the device is off if the voltage reads 0V. The concept of having just two states, an on and an off, suggests the advantage of working in binary (base 2) numbers.

As a refresher, here is some binary math. Remember, that in the decimal (base 10 system), columns of number are created which correspond to coefficients of powers of base 10.

Example

$$\begin{array}{ccccccc}
 & & \overbrace{3}^3 & & \overbrace{0}^0 & & \overbrace{7}^7 & & \overbrace{6}^6 \\
 & & \times 10^3 & & \times 10^2 & & \times 10^1 & & \times 10^0 \\
 \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
 3076 \Leftarrow & 3000 & + & 0 & + & 70 & + & 6
 \end{array}$$

Similarly in binary:

$$\begin{array}{ccccccc}
 & & \overbrace{1}^1 & & \overbrace{0}^0 & & \overbrace{1}^1 & & \overbrace{0}^0 & & \overbrace{1}^1 & & \overbrace{1}^1 \\
 & & \times 2^5 & & \times 2^4 & & \times 2^3 & & \times 2^2 & & \times 2^1 & & \times 2^0 \\
 \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
 43 \Leftarrow & 32 & + & 0 & + & 8 & + & 0 & + & 2 & + & 1
 \end{array}$$

We see then a way to convert between base 10 and base 2 (or you can hit that little button on your calculator.)

You will remember from playing video games, that people like to have lots of BITS in their video. The more bits, the more powerful the graphics. So 8-bit ATARI was replaced by 16-bit Nintendo was replaced by 32-bit Sega Genesis. Well a BIT is just a place holder in binary WORD.

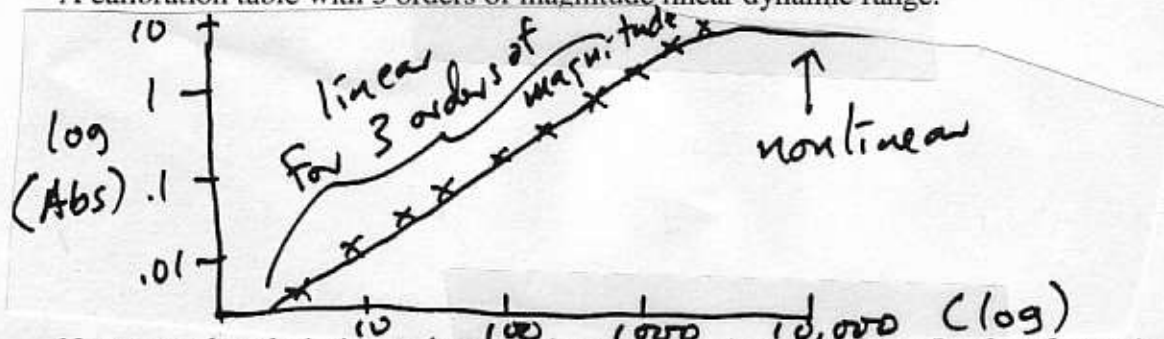
8 bit word _____

16 bit word _____

And we can imagine filling up 8 bits or 16 bits with ones and zeros in various combination. This is the basis for making a language in a transistor or computer.

Dynamic range continued. Dynamic range is an important concept in analytical chemistry. It tells you the range of values over which your experiment will work. For example, in spectroscopy there is this model called Beer's Law that relates light absorbance to concentration of sample. There will be a minimum amount of sample that will produce a signal, and a maximum amount that will produce a signal before the detector saturates. The number of orders of magnitude over which you can vary before the concentration and obtain a response from the detector is the dynamic range. If the response is proportional to the concentration, then the dynamic range is linear. You can always tell the dynamic range of an instrument by constructing a calibration curve and seeing over how many orders of magnitude the line is straight. For example, in the graph below, the linear dynamic range is about 3 orders of magnitude.

A calibration table with 3 orders of magnitude linear dynamic range.



Now a good analytical technique will have a dynamic range of 4 to 5 order of magnitude.

For example, the device will measure from:

10ng to 10 micrograms → 3 orders of magnitude

or

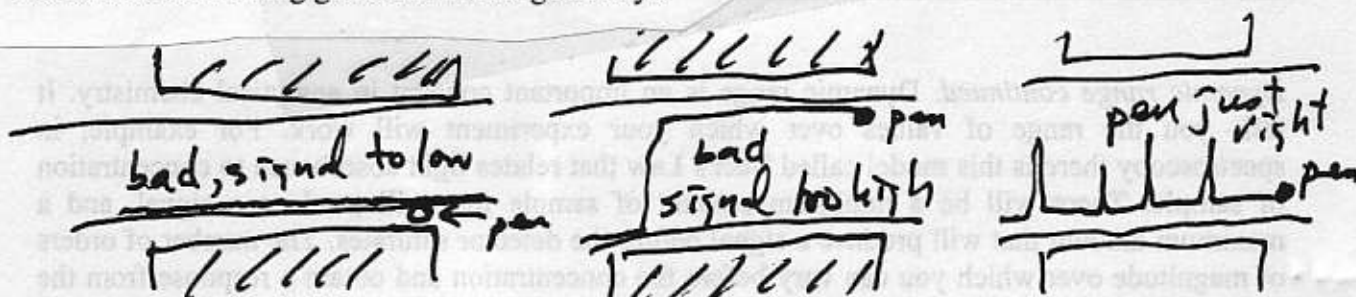
1 microgram to 10 milligrams → 4 orders of magnitude

Note that the dynamic range is not related to detection limits. Instead, a dynamic range defines the BOUNDARIES for performing an experiment successfully. Obviously when you have an unknown, the wider the boundaries, and the easier your job of performing the experiment

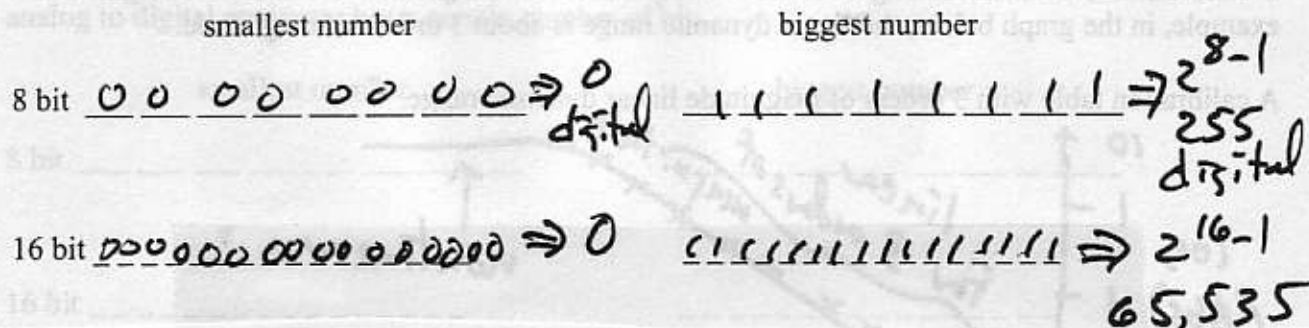
DIGITAL DYNAMIC RANGE in COMPUTERS

But why is dynamic range important in a section on digital signals, and what does any of this have to do with binary numbers? The explanation is that although you might have a technique with a good dynamic range, you still need to be able to view it. For example, consider the following three chart recorder outputs below for the same chromatographic separation. The dynamic range of the detector is the same in each, but the recorder boundaries were incorrectly scaled in two of the outputs, so you obtained no information. This is the problem with dynamic range on an analog instrument.

Chart recorders having good and not-so-good days.



Now consider the same kind of problem on a digital instrument in which your computer or analog to digital converter has a certain number of bits.



Above are written the smallest and largest numbers in binary for an 8-bit computer and a 16-bit computer. The decimal equivalents are listed as well. Can you tell what the approximate dynamic range is for these two devices? It is determined by the number of place holders in the decimal equivalent number: it is the number of orders of magnitude possible in describing the smallest possible number (smallest concentration) and largest possible number (largest concentration). For an 8-bit computer, the decimal equivalent is $2^8 = 256$. This means you have about a two order of magnitude dynamic range to describe your physical system. I don't care if Beer's Law says you could have 10 orders of magnitude for a spectroscopic process. If you use an 8-bit computer, you will get only 2 orders of magnitude dynamic range and everything else will be off-scale.

A table of interesting information for the dynamic range crowd.

bits 2^x	decimal equivalent	dynamic range 10^x	computer jock abbr.
3	8	1	
4	16	1	
6	64	2	
7	128	2	
8	256	2	
10	1,024	3	1K
12	4,096	3	4K
13	8,192	4	8K
16	65,536	5	64K
20	1,048,576	7	1 M

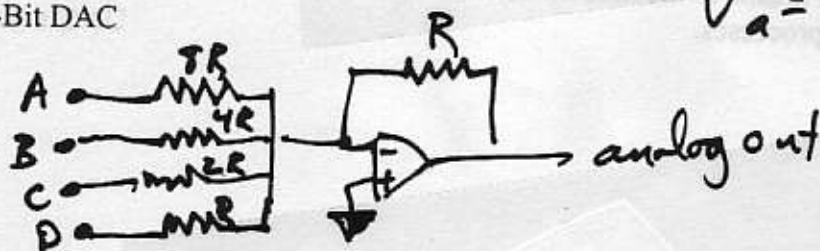
Digital Circuits. Now when I was your age, and real men and women were real men and women, we soldered together our digital circuits with real soldering guns and real solder and real transistors. Nowadays, someone in a third world country does this and Radio Shack sells you the part for about \$15. These digital components are what make up the printed circuit boards you see in everything from computers to automobiles to spaghetti sauce. I'm not going to teach you about counters and scalars and clocks and microprocessors and RAM and CD-ROMS and buses. If you want to remain computer illiterate, that is your business.

But, it is my job to at least tell you how an analytical signal that is analog finds its way into a digital signal that is stored in a computer. This will require that you learn about two kinds of digital circuits: the digital to analog converter (DAC) and the analog to digital converter (ADC).

How DACs and ADCs work.

DACs. You've already seen a DAC. It is the simple addition circuit for op-amps we saw earlier. What makes a summing amplifier into a DAC is the special weighting given each of the resistor. In particular, the resistors are weighted in powers of 2. An example is shown below for a four-bit DAC. The idea is that as often as possible, your binary number is delivered from the DAC and run through an op-amp. The considerations in choosing a DAC are how many bits are possible (this determines the dynamic range of the DAC), and how fast the DAC is (how many times a second it can take a digital number and make it analog.) Thus a 10 bit, 10 MHz DAC puts out a voltage every 100 ns that has a three order of magnitude dynamic range (in other words, it could put out a 1 mV to 1V signal.) While this may sound impressive, it is really routine and inexpensive to purchase (a few dollars).

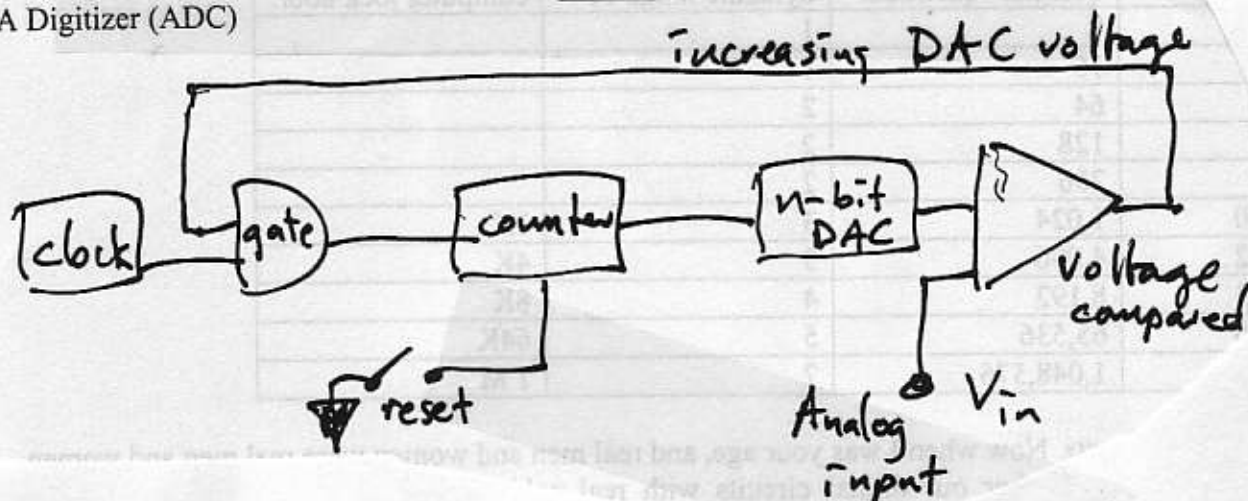
A 4-Bit DAC



$$V_a = -V \left(\frac{D}{1} + \frac{C}{2} + \frac{B}{4} + \frac{A}{8} \right)$$

ADCs. Digitizers are what make the analytical chemistry world go round. They are what provide the important interface between the analog signal coming from a filtered, amplified output of a transducer, and a digital computer. There are many ways to make them. Shown below is a simple example of a digitizer involving a DAC, a counter, and an op-amp comparator.

A Digitizer (ADC)



Here is what happens to make a digital signal from an analog signal. An analog signal, V_{in} , arrives at a comparator op-amp (so called because it makes comparisons). At the same time, a digital counter starts counting in binary (00,01,10,11,...). It is counting from 0 up to the highest number possible for the ADC. Every time the counter increments, it throws the digital number into a DAC (Figure 10) which converts the binary digital number into an analog signal, V_{DAC} . This becomes the comparison signal for V_{in} . If V_{DAC} is less than V_{in} , the counter is incremented by one, a new V_{DAC} analog signal is created, and another comparison to the same V_{in} is made. This process is continued until V_{DAC} equals V_{in} . At that point the counter is stopped and examined. The value in the DAC becomes the stored digital signal in the computer. Then we start all over to get a new digital number,

Note that this single ADC procedure requires that an internal DAC be hundreds to thousands of times faster than the ADC, since it must be used that often just to collect a single ADC digital signal.

As with DACs, ADC price depends upon the number of bits and the speed. You can buy a 10 bit, 10 MHz ADC but it costs a lot more than the equivalent DAC. For one thing, it has inside it a DAC which has to be many times as fast. In fact though, did you know that these days you can buy gigahertz ADCs? In other words, you can buy digitizers that will convert an analog signal into a digital signal 1,000,000,000 times a second! Costs a lot, but that is the capability of modern electronics. What this means to the modern scientist is that incredible opportunities exist for examining extremely fast processes.