#### ASTR 535 : Observational Techniques

Uncertainties and Error Propagation Probability distribution functions and their statistics

#### Learning objectives

- Understand the concept of probability distribution functions and basic quantities used to describe them: mean, variance, standard deviation.
- Understand the difference between population quantities and sample quantities.
- Understand the impact of outliers and advantages and disadvantages of using robust estimators

#### Motivation

- In most empirical science, where one is making measurements, it is critical to understand the uncertainty on the measurement
- Being able to predict the expected uncertainty is critical to experimental design
- In the case of measuring light, there are multiple sources of uncertainty
  - Statistical uncertainty in counting photons, both from object and sky
  - Instrumental uncertainties
- Note that uncertainty analysis is often called error analysis, and uncertainties are often called errors
- Distinction between random and systematic uncertainties: precision and accuracy

# Light

- For a given incident photon flux, the detected flux in a series of exposures will yield a range of measured photon fluxes
- we describe this by a probability distribution function (PDF), which gives the relative frequency of getting different measurements for a given true value (which we are trying to discern)

# Probability distribution functions

• PDF gives probability of getting different measurements given some true value. By definition

 $\int p(x)dx = 1$ 

• PDF can be characterized with some simple statistics

• Mean

$$\mu = \int x \, p(x) dx$$

• Variance ( $\sigma^2$ ) or standard deviation ( $\sigma$ )

$$\sigma^2 = \int (x - \mu)^2 p(x) dx$$

#### Population vs sample statistics

- Sample statistics or, estimators of the population statistics
- Sample mean

 $\langle x \rangle \equiv \frac{\sum x}{N}$  (where x implies  $x_i$ , the individually measured values)

• Sample variance

$$s^{2} \equiv \frac{\sum (x - \langle x \rangle)^{2}}{N - 1} = \frac{\sum x^{2} - \frac{(\sum x)^{2}}{N}}{N - 1}$$

- Sample mean and variance are *consistent* estimators, i.e. they converge to the population values as the number of points approaches infinity
- With finite samples, they are only *estimators* of the population values

# Outliers and their effects

- Sample estimators may be heavily affected by outliers
- More robust estimators
  - For mean:
    - Median : middle value in a sorted list (perhaps average of two if N is even)
    - Mode : most common value (more appropriate for discrete measurements)
    - Max reject : reject highest value and take mean of rest
    - Min-max reject : reject highest and lowest value and take mean of rest
    - $\sigma$  clipping : reject points greater/less than n- $\sigma$  (need to have robust value of  $\sigma$ !)
  - For standard deviation
    - Mean absolute deviation :

$$\sum |x - \langle x \rangle|$$

- Note that more robust may mean less efficient (i.e. less precise)
  - E.g., uncertainty of median is 1.25x uncertainty of mean (for normal distribution, large N)

#### ASTR 535 : Observational Techniques

Uncertainties and Error Propagation Some standard probability distribution functions

#### Learning objectives

- Understand the Poisson distribution and when it applies.
- Know how the variance/standard deviation of the Poisson distribution is related to the mean of the distribution.
- Know what a Gaussian (normal) distribution is, including the full functional form of it.
- Understand under what circumstances the Poisson distribution is similar to a normal distribution.

# Probability distribution function for counting photons

- For photons, the PDF of observed counts given some true incident count is given by the Poisson distribution
- Poisson distribution is derived from the binomial distribution

$$P(x,n,p) = \frac{n!px (1-p)^{(n-x)}}{x!(n-x)!}$$

which gives the probability of observing a particular value, x, given a total number of events, n, and a probability of observing x in a given event, p, under the assumption that events are independent

• Can derive mean and variance:

 $\mu = np$  $\sigma^2 = np(1-p)$ 

# Poisson distribution

- For counting photons,
  - we don't know n or p
  - we know that p << 1</li>
  - we either know the mean or can estimate it by making a measurement
- In this limit, the binomial distribution approaches the Poisson distribution

$$P(x,\mu) = \frac{\mu^x e^{-\mu}}{x!}$$

• For the variance, the binomial np(1-p) for p<<1 gives:

# Poisson distribution

- Applies for discrete quantities
- Can't count less than zero!
- Distribution is not symmetric, esp. for low means
- At high means, approaches a Gaussian (normal) distribution
- Poisson distribution is applicable to any counting experiment, and is sometimes called counting statistics



# Gaussian (normal) distribution

- Gaussian distribution is important for several reasons
  - Poisson approaches Gaussian for large mean
  - Gaussian describes some other noise sources in observing, in particular, the instrumental noise known as readout noise
  - Many quantities in nature appear to be distributed according to a normal distribution, perhaps due to the *central limit theorem*
- But certainly, not all PDFs are Gaussian!

#### Gaussian (normal) distribution

$$P(x,\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$



#### ASTR 535 : Observational Techniques

Uncertainties and Error Propagation Using uncertainties and confidence limits

#### Learning objectives

- Understand different circumstances under which you need to understand uncertainties and their importance
- Know how uncertainties are represented and how confidence intervals are used
- Understand how to assess whether a data series is consistent with a hypothesis and the stated uncertainties

### Importance of uncertainties: applications

- Exposure time calculation : how much time is needed to bring uncertainties to required level
- Is observed scatter consistent with expectation?
  - If not, need to revise expectation or investigate uncertainties
- Distinguish scientific hypotheses

#### Uncertainties

- Distribution of uncertainties is given by the probability distribution function of experimental outcomes
- Often simply characterized by the standard deviation  $\rightarrow$  the error bar
- Interpretation of the error bar does depend on the nature of the PDF, but often is interpreted under the assumption of normally distributed uncertainties

# Confidence levels

- Say you observe some value well off of the mean value
- Calculate the probability of getting a value as far or farther from the mean as a particular measured value
- Integrate under the Gaussian: the error function (erf)
- $1\sigma$ ,  $2\sigma$ ,  $3\sigma$  results, etc.



Shape of the normal distribution



No. of standard deviations from the mean

# $\chi^2$

- Say you have a series of measurements, and an assumption or hypothesis about the nature of the source, e.g., it is constant in time: is scatter of a set of points consistent with expectation?
- Can calculate chi-squared statistic  $\chi^{2} = \frac{\sum (obs_{i} - modeli)^{2}}{\sigma_{i}^{2}}$
- For a given number of data points, one can calculate probability of getting a particular value of  $\chi^2$  or larger
- Quick estimate: reduced  $\chi^2$  :  $\chi^2_{\nu} = \chi^2$  / dof

Where dof is the "degrees of freedom" = number of points minus number of parameters



#### ASTR 535 : Observational Techniques

**Uncertainties and Error Propagation** 

Noise equation

#### Learning objectives

- Understand the concept of S/N and fractional error.
- Know how S/N depends on the signal for the Poisson-limited case.
- Understand how Poisson uncertainties in the background contributes to the S/N of an object, and how the background contribution depends on both the brightness of the background but also on the image quality because the amount of background included in the measurement
- Understand readout noise and how it represented by a normal distribution with zero mean. Know under what circumstances readout noise is an important contributor to the total noise.

# Signal-to-noise

• The precision of a measurement can be quantified by the fractional uncertainty, i.e., for signal S

fractional uncertainty  $\equiv \frac{\sigma_s}{s}$ 

• Astronomers often use the inverse of this, and call the uncertainty the noise, to get the signal-to-noise (S/N, SNR) of a measurement:

$$\frac{S}{N} \equiv \frac{S}{\sigma_S}$$

 So, clearly, higher S/N is better, and corresponds to lower fractional uncertainty

#### Noise source: signal

- In the simplest case, the only noise source is Poisson uncertainties from the source itself, where  $\sigma_s = \sqrt{S}$ , so  $\frac{S}{N} = \frac{S}{\sqrt{S}} = \sqrt{S}$
- We can break this down to see how it depends on source photon flux, collecting area, and exposure time given S = S'Tt

$$\frac{S}{N} = \sqrt{S'Tt}$$

but you don't need to separately know S', T, and t to get S/N!

- S/N scales with  $\sqrt{t}$
- S/N scales with  $\sqrt{S'}$ , i.e. source brightness

# Noise source: background

- In many cases, we also have to account for "background" emission
- "background" is extended, so is a surface brightness
- Amount of "background" in a measurement depends on area of the sky in which source photons are collected, because one gets background over that area

$$B = Tt \int \frac{B_{\lambda}}{hc/\lambda} q_{\lambda} d\lambda$$

where B is a surface brightness, and the total background counts is AB

where A is the area (solid angle) over which we collect source photons We can express B in flux/solid angle and A in solid angle or, alternatively, express B in flux/pixel and A in pixels

# Noise source: background

• Since we collect both source and background photons, the Poisson statistics comes from the total photons we collect:

$$\sigma = \sqrt{S + AB}$$

- To measure the signal from the object alone, we make a separate estimate of the background, B, usually by looking around the object, and subtract it from the measurement of the object
- Even if we measure B exactly, and subtract it off, the uncertainty arising from the photons we count (S+B) remains

$$\frac{S}{N} = \frac{S}{\sqrt{S + AB}}$$

• This highlights the relevance of both dark skies (lower *B*) and sharper images, which allow for lower *A* 

#### Noise source: background

$$\frac{S}{N} = \frac{S}{\sqrt{S + AB}}$$

- Breaking out the dependence on collecting area and exposure time  $\frac{S}{N} = \frac{S'Tt}{\sqrt{S'Tt + AB'Tt}}$
- Again, S/N scales with  $\sqrt{t}$
- But now, S/N scales with S' directly

#### Noise source: signal and background limited

$$\frac{S}{N} = \frac{S}{\sqrt{S + AB}}$$

Signal-limited

$$\frac{S}{N} = \frac{S}{\sqrt{S}} = \frac{S'Tt}{\sqrt{S'Tt}} = \sqrt{S'Tt}$$

Background-limited

$$\frac{S}{N} = \frac{S}{\sqrt{AB}} = \frac{S'Tt}{\sqrt{AB'Tt}} = \frac{S'}{\sqrt{AB}}\sqrt{Tt}$$

Once you are background-limited, S/N drops linearly with source photon flux

#### Noise source: readout noise

• An additional source of noise arises with some types of detectors, e.g., CCDs, and is called *readout noise*, which is distributed as a normal distribution for each pixel with zero mean and standard deviation,  $\sigma_{rn}$  (generally called the readout noise)

$$\frac{S}{N} = \frac{S}{\sqrt{S + AB + Npi_x \sigma_{rn}^2}}$$

- Unlike the signal and background terms, however, the readout noise term does not depend on exposure time or collecting area
- In the readout noise limited case, S/N scales with S like in the background case
- Minimize  $\sigma_{rn}$  with better detectors and electronics, and also by trying to ensure pixel scale is a good match to images, so N<sub>pix</sub> is minimized

# What regime are different types of observations?

- Imaging
  - Bright objects (much brighter than sky) : signal-limited
  - Fainter objects : background-limited
  - In optical, typical sky surface brightness ranges from 18-22 mag/square arcsec
  - In near-IR, typical sky surface brightness ranges from 12-15 mag/square arcsec
  - Image quality also matter
- Spectroscopy
  - Both object and background light is dispersed (in most applications)
  - Readout noise can become important, especially for short exposures

#### ASTR 535 : Observational Techniques

**Uncertainties and Error Propagation** 

**Error propagation** 

#### Learning objectives

• Know the uncertainty (error) propagation formula and be able to apply it in a general case

#### Motivation

- say we want to make some calculations (e.g., calibration, unit conversion, averaging, conversion to magnitudes, calculation of colors, etc.) using these observations: we need to be able to estimate the uncertainties in the calculated quantities that depend on our measured quantities.
- Specific example: when we added in readout noise in the noise equation, why did we add the uncertainty in quadrature?

## Propagation of uncertainties

• Say you have some quantities (u,v,...) with known uncertainties ( $\sigma_u$ ,  $\sigma_v$ ,...) and you combine these into some new quantity, x

x = f(u,v,...)

What is  $\sigma_x$ ?

• If uncertainties are small:

$$x_i - \langle x \rangle \approx (ui - \langle u \rangle) \frac{\partial x}{\partial u} + (v_i - \langle v \rangle) \frac{\partial x}{\partial v}$$

e.g.

$$\begin{array}{l} x = u + v \\ x = uv \end{array}$$

#### Propagation of uncertainties

By definition, the uncertainty  $\sigma_x$  is given by  $\sigma_x^2 = \lim(N \to \infty) \frac{1}{N} \sum (x_i - \langle x \rangle)^2$ 

(sample variance approaches population variance as N approaches  $\infty$ ) Substituting our expression for  $(x_i - \langle x \rangle)$ :  $\sigma_x^2 = \lim(N \to \infty) \frac{1}{N} \left[ \sum (u_i - \langle u \rangle)^2 (\frac{\partial x}{\partial u})^2 + \sum (v_i - \langle v \rangle)^2 (\frac{\partial x}{\partial v})^2 + 2 \sum (u_i - \langle u \rangle) (v_i - \langle v \rangle) (\frac{\partial x}{\partial u}) (\frac{\partial x}{\partial v}) \right]$  $= \sigma_u^2 (\frac{\partial x}{\partial u})^2 + \sigma_v^2 (\frac{\partial x}{\partial v})^2 + \sigma_{uv}^2 (\frac{\partial x}{\partial u}) (\frac{\partial x}{\partial v})$ 

#### Covariance

Last term is the covariance:

$$\sigma_{uv}^2 = \lim(N \to \infty) \frac{1}{N} [\sum (u_i - \langle u \rangle) (v_i - \langle v \rangle)]$$

Which accounts for the possibility that the uncertainties in two quantities could be *correlated;* deviation in one quantity is correlated with deviation in another

If uncertainties are uncorrelated, then summing over all points, positive deviations in one variable, will be multiplied by equal numbers of positive and negative deviations in the other, so the covariance will be zero

#### Uncorrelated uncertainties

$$\sigma_x^2 = \sigma_u^2 \left(\frac{\partial x}{\partial u}\right)^2 + \sigma_v^2 \left(\frac{\partial x}{\partial v}\right)^2$$

- Some examples:
  - Addition

$$x = u + v$$
  
$$\sigma_x^2 = \sigma_u^2 + \sigma_v^2$$

• Multiplication

$$x = uv$$
  

$$\sigma_x^2 = v^2 \sigma_u^2 + u^2 \sigma_v^2$$

• Logarithm

$$x = \ln u$$
$$\sigma_x^2 = \frac{\sigma_u^2}{u^2}$$

(note that  $\log x = \log e \ln x$ )

in logarithms, uncertainties in the log correspond to fractional uncertainties in the raw quantity

#### Example: readout noise

$$\frac{S}{N} = \frac{S}{\sqrt{S + AB + Npix\sigma_{rr}^2}}$$

 Without readout noise, the uncertainty from Poisson statistics (source and background, with perfect background subtraction) is:

$$\sigma_S = \sqrt{S + AB}$$

- Readout noise adds an additional distribution: a Gaussian with zero mean and standard deviation  $\sigma_{\rm rn}$  for each pixel
- Summing over pixels (addition), noise adds in quadrature, to give a total variance of  $N_{pix}\sigma_{~rn}^2$
- This is added to the signal, with zero mean, so total readout noise is added in quadrature

# Distribution of resultant uncertainties

- We have characterized the uncertainty PDF with the standard deviation, but a given standard deviation could arise with different PDFs
- In general, the shape of the PDF of the derived quantity is not necessarily the shape of the PDF of any of the input quantities
- If two normally distributed variables are combined by addition i.e. the uncertainties add in quadrature – then the resulting PDF is also normally distributed

#### ASTR 535 : Observational Techniques

Uncertainties and Error Propagation Summing and averaging measurements

#### Learning objectives

- Understand under what circumstances you can split exposures without a noise penalty, and under what circumstances you cannot. Understand some of the reasons why you might want to split an exposure into shorter pieces
- Understand how to properly average measurements and estimate the uncertainty on the sample mean
- Understand how the distinction between sample variance and true variance can lead to biases when calculating a weighted mean, and how to overcome this.

# Summing exposures

- Say you take multiple exposures of an object and want to sum the counts,  $C_{i,}$  given an uncertainty  $\sigma$  on each
- Uncertainty on the sum is  $\sigma\sqrt{N}$ , from error propagation

# Summing / splitting exposures

- What about the uncertainty of a single long exposure vs the uncertainty of a series of shorter exposures?
- For a single exposure

$$\sigma = \sqrt{S'Tt + AB'Tt + Npi_x\sigma_{rn}^2}$$

where we've explicitly included exposure time

• Summing N exposures

$$\sigma_N^2 = N\sigma^2$$

$$\sigma_N = \sqrt{NS'Tt + NAB'Tt + NN_{pix}\sigma_{rn}^2}$$

• One long exposure with exposure time Nt

$$\sigma_{Long} = \sqrt{S'TNt + AB'TNt + Npix\sigma_{rn}^2}$$

Difference is only in the readout noise term, which makes sense (1 readout vs N readouts, same number of photons)

 $\rightarrow$  If individual exposures are not readout-noise limited, then there is no noise penalty

# Splitting exposures

- For long exposures, there are benefits to splitting exposures, but make sure that individual exposure have sufficient signal to dominate readout noise
  - Tracking
  - Monitoring of conditions
  - Cosmic ray rejection
  - Increasing dynamic range by avoiding saturation
- There are also some potential disadvantages
  - Increased readout time
  - Increased data volume

#### Averaging measurements

 In some circumstances, we might be in the position of wanting to average measurements, e.g., from a set of measurements taken with different exposure times, on different nights, or from different telescopes

# Averaging measurements : equal uncertainties

• For a series of measurements with equal uncertainty on each, the maximum likelihood estimate of the population mean is the sample mean:

$$\langle x \rangle = \frac{\sum xi}{N}$$

The variance of  $\sum x_i$  is  $N\sigma^2$ 

The variance of  is then 
$$\frac{N\sigma^2}{N^2} = \frac{\sigma^2}{N}$$
  
The uncertainty of the mean is  $\frac{\sigma}{\sqrt{N}} = \sqrt{\frac{\sum(x_i - \langle x \rangle)^2}{N(N-1)}}$ 

i.e. the uncertainty goes down by the square root of the number of samples

# Averaging with unequal uncertainties

• If the uncertainties are not the same on all points, the *weighted mean* provides the best estimate of the population mean:

$$\langle x \rangle = \frac{\sum \frac{x_i}{\sigma_i^2}}{\sum \frac{1}{\sigma_i^2}}$$

Propagation of uncertainties gives the uncertainty on the weighted mean:

$$\sigma < x > = \frac{1}{\sum \frac{1}{\sigma_i^2}}$$

# Weighted mean: a subtlety

- For the weighted mean, the weights,  $1/\sigma_i^2$  use the population variances
- But we generally only have the sample variances, which are estimates of the population variances!
- This can lead to biases if the estimates are not determined self consistently
- Example:
  - three measurements give photon counts of 40, 50, and 60 photons
  - Considered independently, one might adopt variances of 40, 50, and 60 photons, respectively
  - Using a weighted mean would then give a biased result, since the 40 measurement will be weighted more
  - For three identical measurements of the same thing, you might recognize the fallacy, but there are certainly cases in which you would want to use a weighted mean
  - Remedy: weight the measurements self-consistently!

#### ASTR 535 : Observational Techniques

**Uncertainties and Error Propagation** 

Random vs systematic uncertainties

#### Learning objectives

- Understand the distinction between random and systematic errors
- Understand how comparing observed scatter with expected scatter may be critical to discovering systematic errors

#### Random and systematic errors

- Random uncertainties describe scatter around the true value
- Systematic uncertainties describe the possibility that observed values are offset from the true value
- Sometimes described as precision (random scatter) and accuracy (offset from true value)
- Systematic uncertainties are often the most problematic as they often arise from unknown things
  - If a source of systematics is known, one can attempt to mitigate it and/or to estimate its amplitude

# Example: flat fielding

- Typically, imaging systems don't have a uniform response across the field of view
  - Non-uniformities can arise from vignetting in the system, non-uniform filter response, non-uniform detector response, etc.
- If this was ignored, it would lead to systematics as a function of position: objects in areas with lower sensitivity would be measured fainter
- Of course, it is not ignored: one uses a "flat field", an observation of a (supposedly) uniformly illuminated field to calibrate out the non-uniform response
- But what is a "uniformly illuminate field" and how uniform is it?
  - Any deviations from "uniformity" lead to systematic errors
- How can you test for this?
  - One possibility: take images of the same object at multiple locations



# Example: HST/WFPC2 CTE

- For the HST/WFPC2, calibration was done by observing stars that had calibrated magnitudes from ground-base observations
- In the resulting analysis, the scatter for brighter stars was larger than expected given the noise model (signal + background + readout noise)
- Looking at scatter:
  - Not correlated with color (transformation term)
  - Correlated with row position on detector!
- Discovery of an (iunfortunate) unforeseen effect: charge transfer losses!
- Discovered by comparing observed scatter to expected scatter!

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#### The Photometric Performance and Calibration of WFPC2<sup>1</sup>

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FIG. 5—Residuals from the flight-to-ground WFPC2 transformations for F555W (left) and F814W (right) as a function of color (top) and magnitude (bottom). Different point types represent the four different chips (PC1, triangles; WF2, squares; WF3, pentagons; WF4, hexagons).

# Finding unknown systematics

- Check to see if observed scatter is consistent with known sources of uncertainty.
  - If not, there's something you need to understand!
  - Look for correlations of deviations with other quantities
  - Don't overestimate random uncertainties!

#### ASTR 535 : Observational Techniques

**Uncertainties and Error Propagation** 

Digital photometry

#### Learning objectives

- Understand the basic principles of doing aperture photometry on images
- Understand the S/N tradeoffs with aperture size depending on source and background brightness
- Understand the basic principles of doing crowded field photometry

# Digital aperture photometry

- Find your object(s)
- For all pixels within some radius of the object (the aperture), sum the data values, which gives Tot = S+BA
  - Radius should include a significant fraction of the light of the star (more later)
- For all pixels in some annulus around the object, determine a robust mean, B
  - Annulus should cover enough area such that the uncertainty of the robust mean is small (N(annulus)>>N(aperture), otherwise you introduce another source of uncertainty
- Determine BA given area of aperture
- Determine readout noise given area of aperture and  $\sigma_{\rm rn}$  for the detector
- Determine S = Tot BA
- Determine uncertainty: N =  $\sqrt{S + BA + Npix \sigma_{rn}^2}$
- Note that, as described here, if you determine B as background per pixel, then A is the number of pixels in the aperture, which is the same as N<sub>pix</sub>
- Relatively straightforward to implement a simple prescription, but see also the astropy-affliciated package, photutils





# Photometry

- Choice of aperture radius
  - Larger gets more light
  - Larger includes more background
  - Tradeoff depends on source and background brightness
- Differential photometry
  - If comparing to other object(s) in field, need aperture radius to provide consistent fraction of light across frame



# Crowded field photometry

If there are many objects, such that they are "overlapping", then digital aperture photometry clearly won't work!

Here, things become more complicated

- Find stars
- Determine shape of a star (PSF) from some isolated star(s)
- Simultaneously fit groups of stars, solving for brightnesses and also centers (since your initial estimates may have been biased by neighbors
- Include pixel uncertainties when doing the fit
- Adopt derived parameter uncertainties
- Implementations: DAOPHOT, DoPHOT, DolPhot, implementations in astropy-affiliate photutils

