

The background is a dark blue gradient with faint, light blue geometric patterns. On the left side, there are several concentric circles and a curved scale with numerical markings from 150 to 260 in increments of 10. Some of the circles have arrows indicating a clockwise direction. The overall aesthetic is technical and scientific.

# BASIC STATISTICS III

# CHI SQUARED AND LIKELIHOOD

Individual values of Chi squared – comparison of observed residuals from a model to expected residuals (uncertainties)

$$\chi^2 = \sum_i \frac{(O_i - E_i)^2}{\sigma_i^2}$$

These individual values come from an underlying Chi squared probability distribution.

The likelihood of a model given a data set is proportional to  $e^{-\chi^2/2}$  because we assume the residuals follow normal distributions.

# FITTING

- traditional maximum likelihood:  
“best fit” models/parameters
- the right fit for the question
- the Bayesian approach:  
probability *distributions* for models/parameters

# TRADITIONAL MAXIMUM LIKELIHOOD

- likelihood proportional to  $e^{-\chi^2/2}$
- $\min \chi^2 \rightarrow \max \text{likelihood}$
- “maximum likelihood estimators” (MLEs) of parameters  $\alpha_i$  of a model are usually found by  $\frac{\partial L}{\partial \alpha_i} = 0$  or equivalently 
$$\frac{\partial \ln(L)}{\partial \alpha_i} = 0$$
- if residuals are Gaussian, called “ordinary least-squares” (OLS) fitting – minimizes rms deviations

# TRADITIONAL MAXIMUM LIKELIHOOD

- Example: model  $y = \alpha X + \beta$  with equal Gaussian errors  $\sigma$

- $\chi^2 = \sum_i \frac{(Y_i - (\alpha X_i + \beta))^2}{\sigma^2} \rightarrow \text{max likelihood}$

- $\frac{\partial \ln(L)}{\partial \alpha} = 0 \rightarrow \frac{\partial \ln(e^{-\frac{\chi^2}{2}})}{\partial \alpha} = 0 \rightarrow \sum_i \frac{(Y_i - (\alpha X_i + \beta)) X_i}{\sigma^2} = 0$

- $\frac{\partial \ln(L)}{\partial \beta} = 0 \rightarrow \frac{\partial \ln(e^{-\frac{\chi^2}{2}})}{\partial \beta} = 0 \rightarrow \sum_i \frac{(Y_i - (\alpha X_i + \beta))}{\sigma^2} = 0$

- two eqns, two unknowns – solve to get result in tutorial:

$$\alpha = \frac{\bar{X}\bar{Y} - \overline{XY}}{(\bar{X})^2 - \overline{X^2}} \text{ and } \beta = \bar{Y} - \bar{X}\alpha$$

(so for this simple case, no numerical  $\chi^2$  minimization is needed; harder for more parameters or different  $\sigma_i$ )

# TRADITIONAL MAXIMUM LIKELIHOOD

- uncertainties on MLEs estimated by  $1/E(-H)$  = inverse of expectation of negative “Hessian matrix”
- Hessian matrix example:  $y = \alpha X + \beta$

$$\text{Hessian}(\alpha, \beta) = \begin{bmatrix} \frac{\partial^2}{\partial \alpha^2} \log L(\alpha, \beta) & \frac{\partial^2}{\partial \alpha \partial \beta} \log L(\alpha, \beta) \\ \frac{\partial^2}{\partial \alpha \partial \beta} \log L(\alpha, \beta) & \frac{\partial^2}{\partial \beta^2} \log L(\alpha, \beta) \end{bmatrix}$$

note covariance terms!

- complicated to compute Hessians, typically done numerically
- considering  $\beta^2$  term, can see errors on parameters generally decrease as  $\frac{1}{\sqrt{N}} \rightarrow$  more data is better



# TRADITIONAL MAXIMUM LIKELIHOOD

Even simple line fitting gets complicated really quickly...

- Isobe+ (1990):  $OLS(y|x)$ ,  $OLS(x|y)$ , bisector fit
- Beers+ (1990): biweight for robust (outlier-resistant) fitting
- A. Trotters' 2011 UNC PhD thesis: "I present a new, broadly applicable statistical technique... for fitting model distributions to data in two dimensions, where the data have intrinsic uncertainties in both dimensions, and extrinsic scatter in both dimensions that is greater than can be accounted for by the intrinsic uncertainties alone."

# THE RIGHT FIT FOR THE QUESTION

- Hogg, Bovy, and Lang (2010) model fitting review (<http://arxiv.org/pdf/1008.4686v1.pdf>) claims you must choose  $\text{OLS}(y|x)$  or  $\text{OLS}(x|y)$  based on comparing  $\sigma_x$  and  $\sigma_y$
- fair enough if you're after the underlying relationship between  $x$  &  $y$ , but what if that's not your question? (see earlier Feigelson & Babu (1992) fitting review)

EXAMPLE: For the Tully-Fisher Relation,

- 1) which fit is best if you want a relation useful to predict  $L$ , and in this case how should you trim the data?
- 2) which fit is best if you want to study the residual dependence on third parameters at fixed  $L$ , and again how should you trim the data?
- 3) which fit is best if you want to study the TFR itself, assuming  $V$  has the most scatter, and there is selection bias on  $L$ ?



# THE BAYESIAN APPROACH: ~~MAXIMUM~~ LIKELIHOOD DISTRIBUTIONS

- construct space of models with expected ranges of parameters
- $\text{prob}(\text{model} | \text{data}) \propto \text{prob}(\text{data} | \text{model}) \times \text{prob}(\text{model})$
- for uniform priors on model params, posterior probability of each model is proportional to its likelihood,  $e^{-\chi^2/2}$
- integrate probability over “nuisance parameters” (“marginalize” over them) to get probability distribution for the parameter of interest (doesn’t even need to be an input parameter...)

# THE BAYESIAN APPROACH: ~~MAXIMUM~~ LIKELIHOOD DISTRIBUTIONS

## More uses of this approach:

- Compare whole classes of models A and B (e.g. straight line or curved?) by integrating over parameters:

$$\text{“Bayes Factor”} = \frac{\int_{\alpha} p_A(X_i|\alpha, A)p(\alpha|A)}{\int_{\alpha} p_B(X_i|\alpha, B)p(\alpha|B)}$$

- Get probability distributions for model quantities other than the model parameters, e.g., galaxy stellar masses from SPS fits to galaxy SEDs (galaxy stellar mass is not an input to the model, in fact indeterminate before fit)