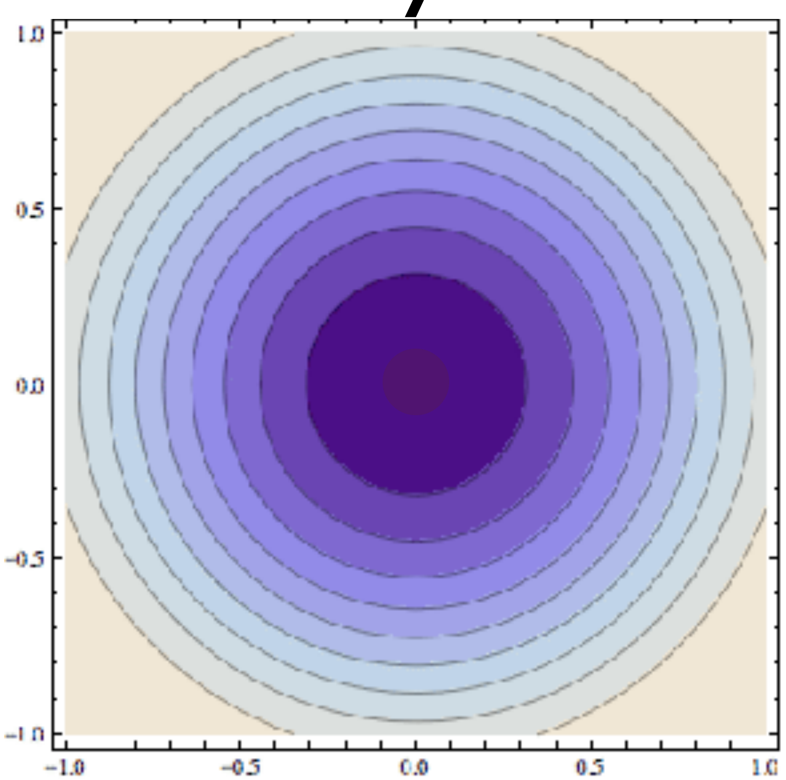
Parameter Estimation & Maximum Likelihood

Marisa Eisenberg
Epid 814

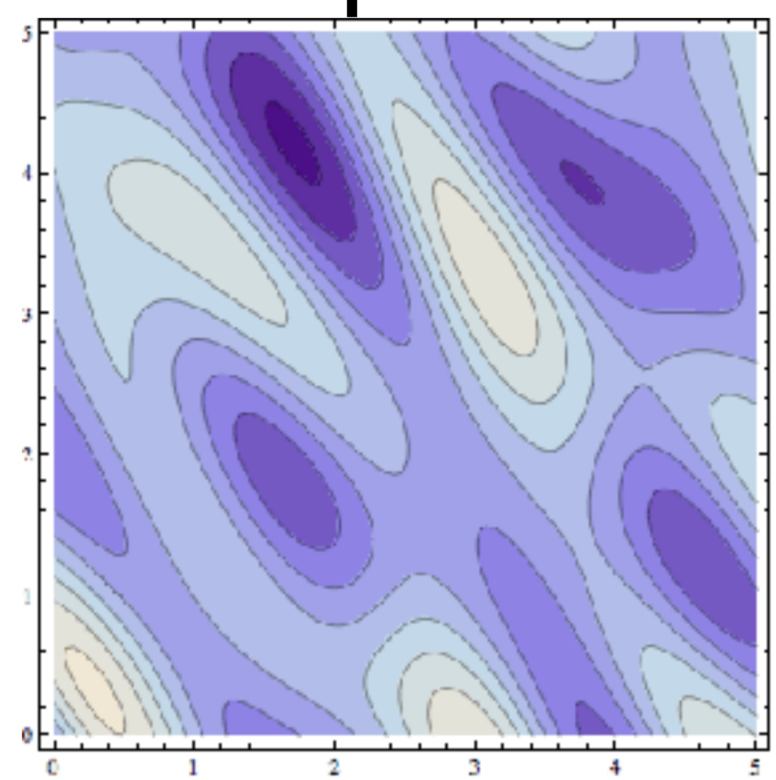
Parameter Estimation

- In general—search parameter space to find optimal fit to data
- Or to characterize distribution of parameters that matches data

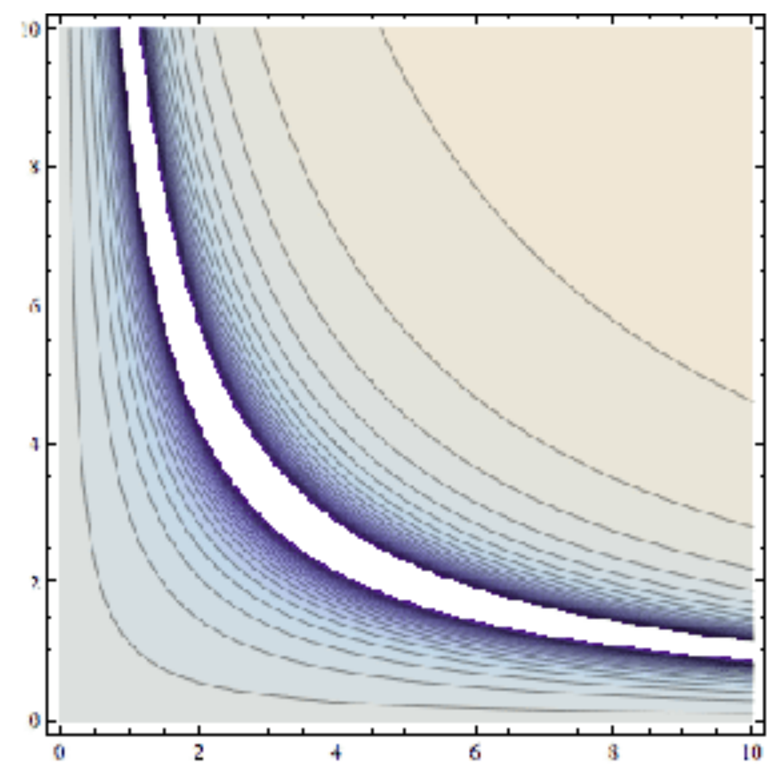
Yay!



Multiple Mins

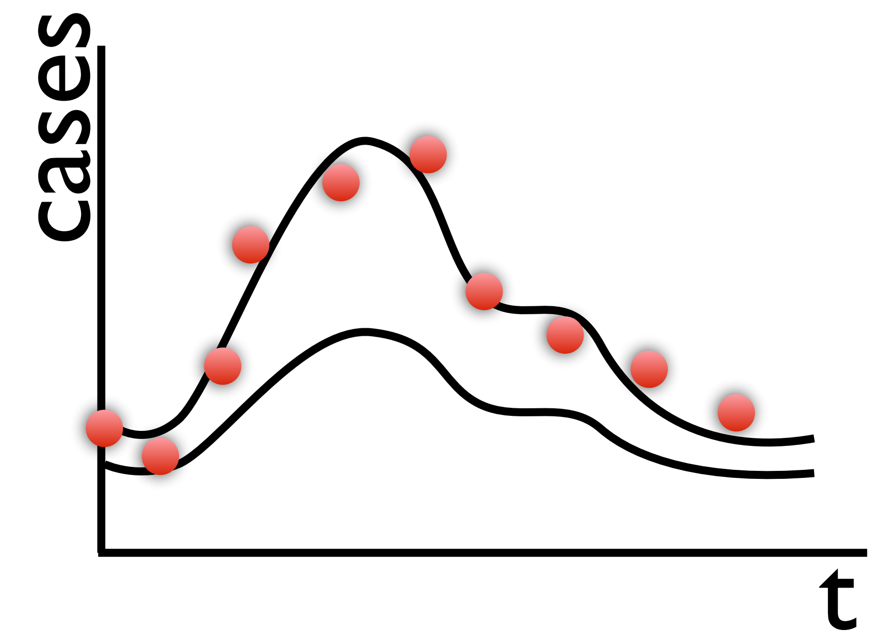


Struct. UnID



Parameter Estimation

- Basic idea: parameters that give model behavior that more closely matches data are 'best' or 'most likely'



- Frame this from a statistical perspective (inference, regression)
  - Can determine 'most likely' parameters or distribution, confidence intervals, etc.

How to frame this statistically?

- **Maximum Likelihood Approach**
- Idea: rewrite the ODE model as a statistical model, where we suppose we know the general form of the density function but not the parameters values
- Then if we knew the parameters we could calculate probability of a particular observation/data:

$$P(z \mid p)$$

data parameters

Maximum Likelihood

- **Likelihood Function**

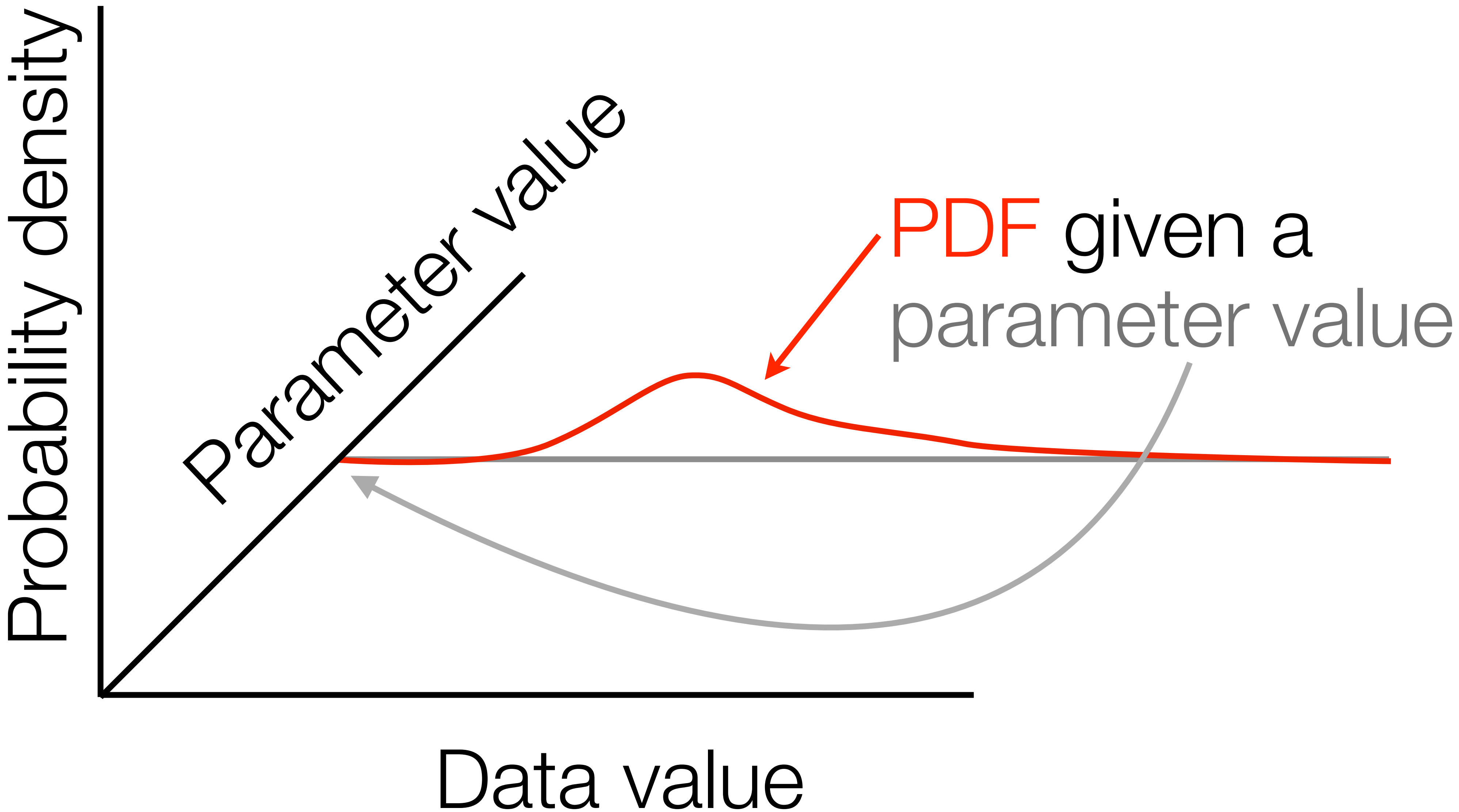
$$P(z \mid p) = f(z, p) = L(p \mid z)$$

- Re-think the distribution as a function of the data instead of the parameters

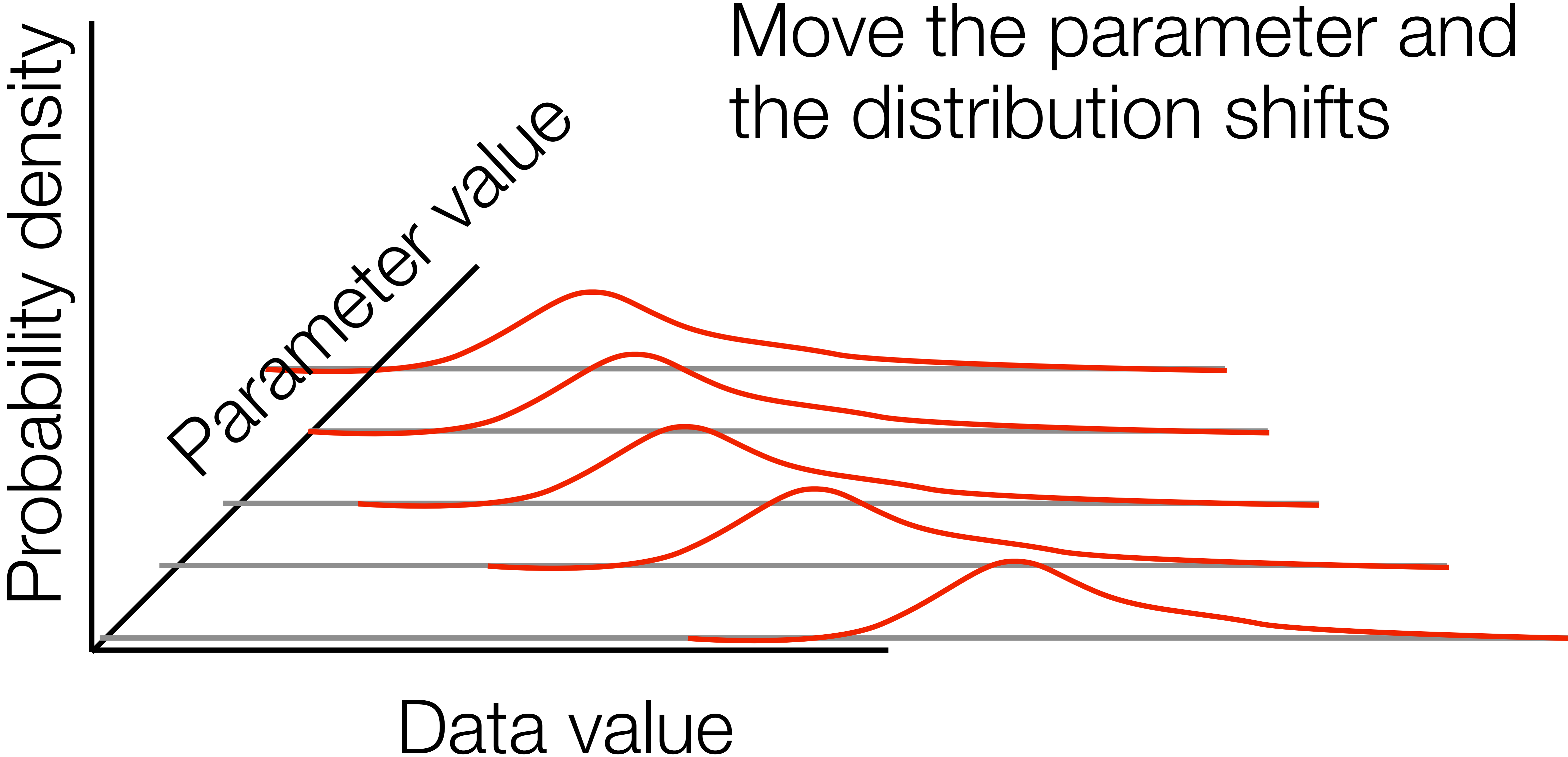
- E.g. $f(z \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(z-\mu)^2}{2\sigma^2} \right) = L(\mu, \sigma^2 \mid z)$

- Find the value of p that maximizes L(p|z) - this is the maximum likelihood estimate (**MLE**) (most likely given the data)

Likelihood Function

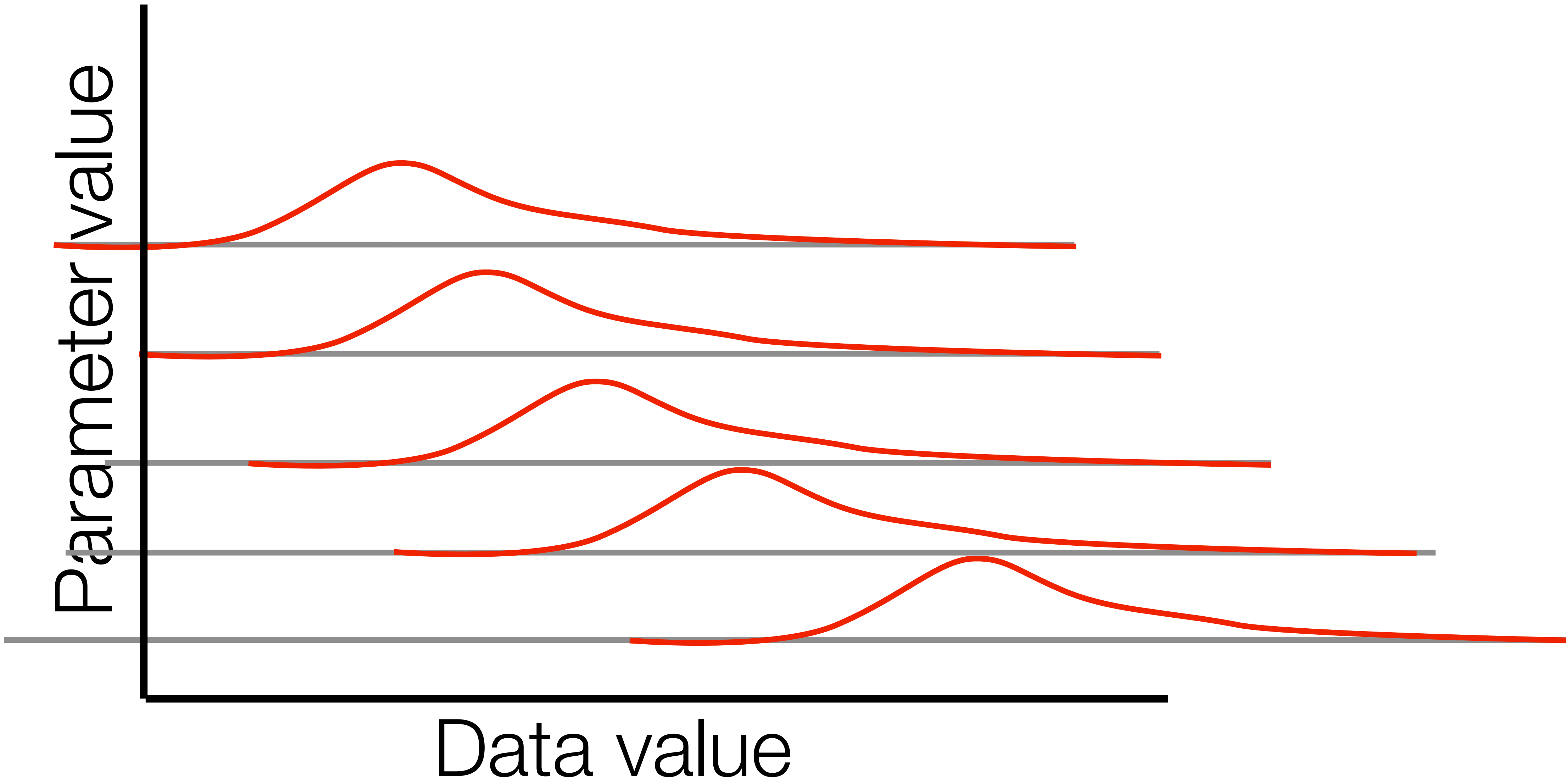


Likelihood Function

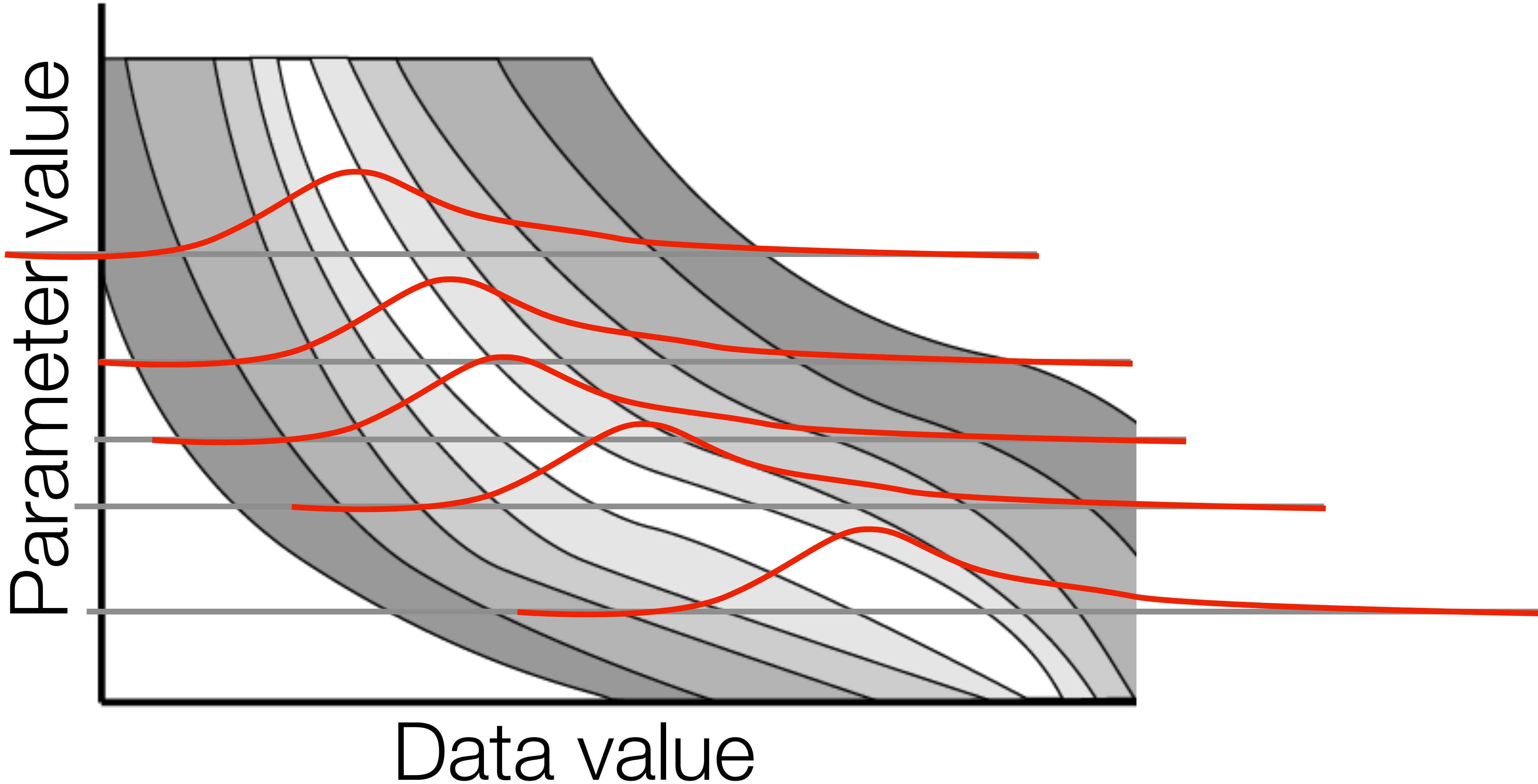


Move the parameter and the distribution shifts

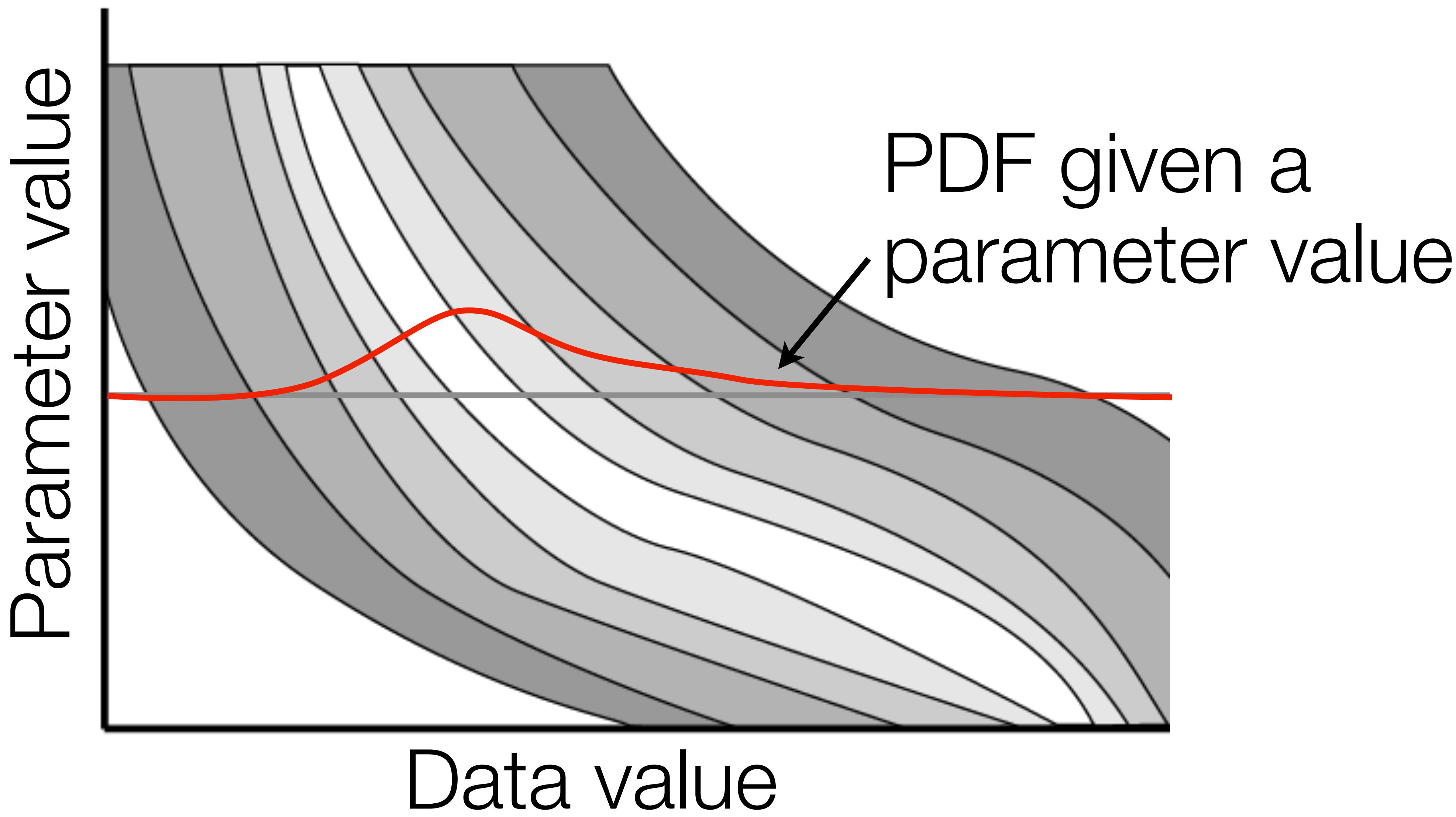
Likelihood Function



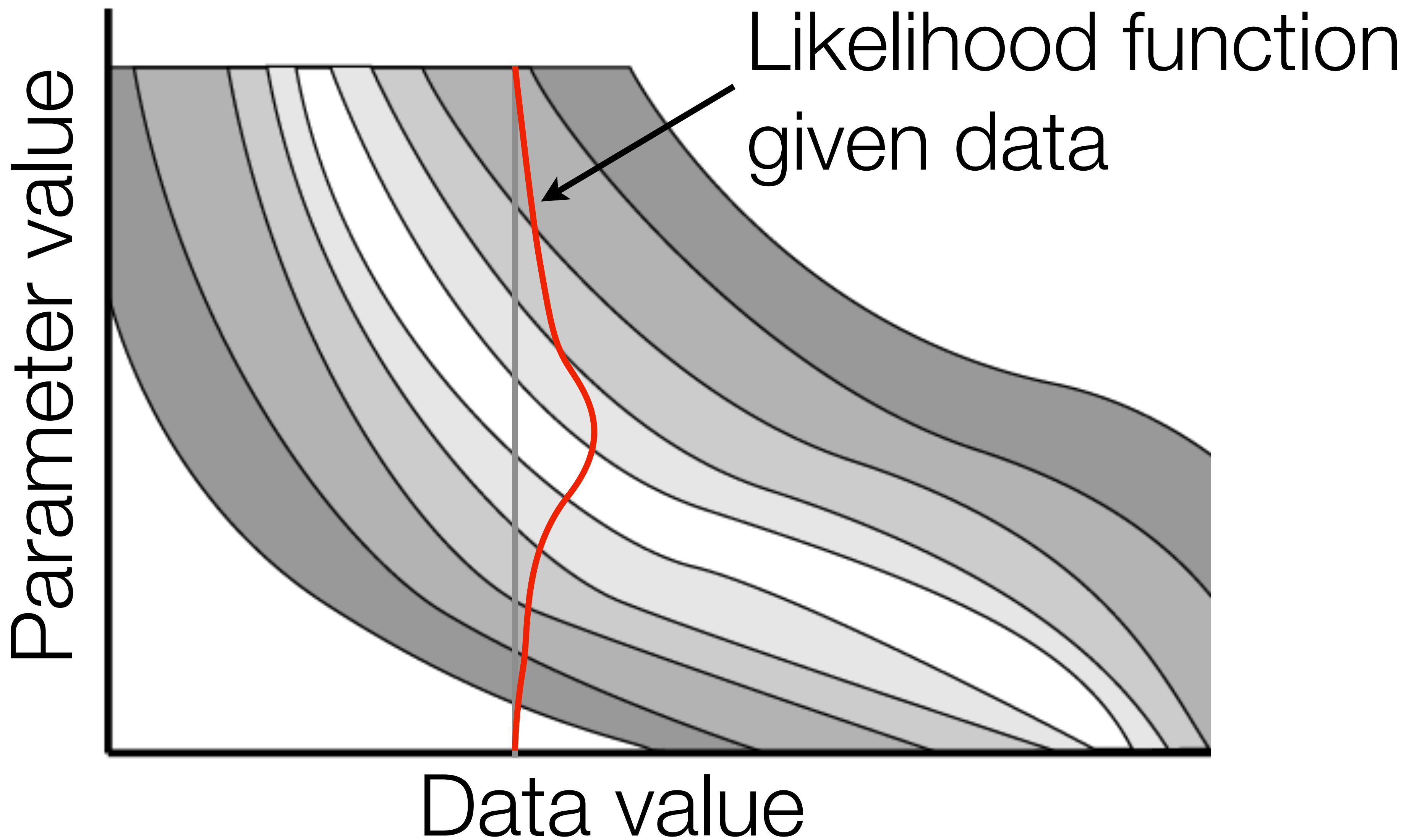
Likelihood Function



Likelihood Function



Likelihood Function



Maximum Likelihood

- **Consistency** - with sufficiently large number of observations n, it is possible to find the value of p with arbitrary precision (i.e. converges in probability to p)

- **Normality** - as the sample size increases, the distribution of the MLE tends to a Gaussian distribution with mean and covariance matrix equal to the inverse of the Fisher information matrix

- **Efficiency** - achieves CR bound as sample size$\longrightarrow\infty$ (no consistent estimator has lower asymptotic mean squared error than MLE)

Example - ODE Model with Gaussian Error

- Model:

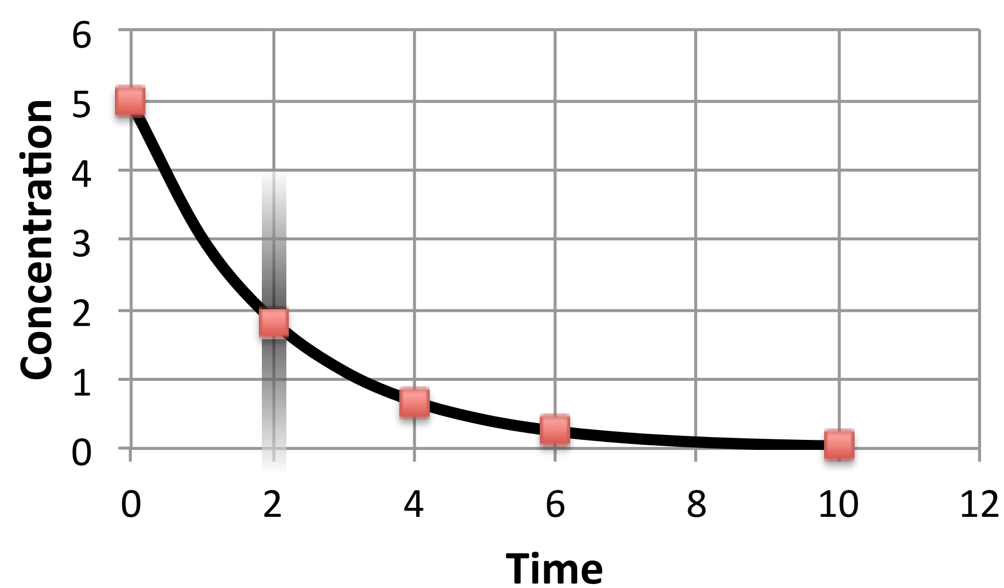
$$\dot{x} = f\left(x, t, p\right)$$

$$y = g(x, t, p)$$

- Suppose data is taken at times $t_1, t_2, \ldots, t_n$
- Data at t_i = $z_i = y\left(t_i\right) + e_i$
- Suppose error is gaussian and unbiased, with known variance σ^2 (can also be considered an unknown parameter)

Example - ODE Model with Gaussian Error

- The measured data z_i at time i can be viewed as a sample from a Gaussian distribution with mean y(x, t_i,p) and variance σ^2



- Suppose all measurements are independent (is this realistic?)

Example - ODE Model with Gaussian Error

- Then the likelihood function can be calculated as:

Gaussian PDF: $$f\left(z_i \mid \mu, \sigma^2\right) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(z_i - \mu\right)^2}{2\sigma^2}\right)$$

Example - ODE Model with Gaussian Error

- Then the likelihood function can be calculated as:

Gaussian PDF: $$f\left(z_i \mid \mu,\sigma^2\right) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{\left(z_i-\mu\right)^2}{2\sigma^2}\right)$$

Formatted for model: $$f\left(z_i \mid y\left(x,t_i,p\right),\sigma^2\right) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{\left(z_i-y\left(t_i,p\right)\right)^2}{2\sigma^2}\right)$$

Example - ODE Model with Gaussian Error

- Then the likelihood function can be calculated as:

Gaussian PDF: $$f\left(z_i \mid \mu,\sigma^2\right) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{\left(z_i-\mu\right)^2}{2\sigma^2}\right)$$

Formatted for model: $$f\left(z_i \mid y\left(x,t_i,p\right),\sigma^2\right) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{\left(z_i-y\left(t_i,p\right)\right)^2}{2\sigma^2}\right)$$

Likelihood function assuming independent observations:

$$L\left(y\left(t_i,p\right),\sigma^2 \mid z_1,\ldots,z_n\right) = f\left(z_1,\ldots,z_n \mid y\left(t_i,p\right),\sigma^2\right)$$

$$= \prod_{i=1}^{n} f\left(z_i \mid y\left(t_i,p\right),\sigma^2\right)$$

Example - ODE Model with Gaussian Error

$$L\left(y\left(t_i, p\right), \sigma^2 \mid z_1, \ldots, z_n\right) = f\left(z_1, \ldots, z_n \mid y\left(t_i, p\right), \sigma^2\right)$$

$$= \prod_{i=1}^{n} f\left(z_i \mid y\left(t_i, p\right), \sigma^2\right)$$

$$= \left(\frac{1}{2\pi\sigma^2}\right)^{n/2} \exp\left(-\frac{\sum_{i=1}^{n}\left(z_i - y\left(t_i, p\right)\right)^2}{2\sigma^2}\right)$$

Example - ODE Model with Gaussian Error

- It is often more convenient to minimize the Negative Log Likelihood (-LL) instead of maximizing the Likelihood
  - Log is well behaved, minimization algorithms common

$$-LL = -\ln\left(\left(\frac{1}{2\pi\sigma^2}\right)^{n/2}\exp\left(-\frac{\sum_{i=1}^{n}\left(z_i - y\left(t_i, p\right)\right)^2}{2\sigma^2}\right)\right)$$

Example - ODE Model with Gaussian Error

$$-LL = -\ln\left(\left(\frac{1}{2\pi\sigma^2}\right)^{n/2} \exp\left(-\frac{\sum_{i=1}^{n}\left(z_i - y\left(t_i, p\right)\right)^2}{2\sigma^2}\right)\right)$$

$$-LL = -\left(-\frac{n}{2}\ln\left(2\pi\right) - n\ln\left(\sigma\right) - \frac{\sum_{i=1}^{n}\left(z_i - y\left(t_i, p\right)\right)^2}{2\sigma^2}\right)$$

Example - ODE Model with Gaussian Error

$$-LL = \frac{n}{2}\ln(2\pi) + n\ln(\sigma) + \frac{\sum_{i=1}^{n}\left(z_i - y(t_i, p)\right)^2}{2\sigma^2}$$

If σ is known, then first two terms are constants & will not be changed as p is varied—so we can minimize only the 3rd term and get the same answer

$$\min_p(-LL) = \min_p\left(\frac{\sum_{i=1}^{n}\left(z_i - y(t_i, p)\right)^2}{2\sigma^2}\right)$$

Example - ODE Model with Gaussian Error

- Similarly for denominator:

$$\min_p\left(-LL\right) = \min_p\left(\frac{\sum_{i=1}^{n}\left(z_i - y\left(t_i, p\right)\right)^2}{2\sigma^2}\right) = \min_p\left(\sum_{i=1}^{n}\left(z_i - y\left(t_i, p\right)\right)^2\right)$$

- This is just least squares!

- So, least squares is equivalent to the ML estimator when we assume a constant known variance

Maximum Likelihood Summary for ODEs

- Can calculate other ML estimators for different distributions
- Not always least squares-ish! (mostly not)
- Although surprisingly, least squares does fairly decently a lot of the time

Example - Poisson ML

- For count data (e.g. incidence data), the Poisson distribution is often more realistic than Gaussian

- Likelihood function?

Example - Poisson ML

- Model:

$$\dot{x} = f\left(x, t, p\right)$$

$$y = g(x, t, p)$$

- Data z_i is assumed to be Poisson with mean $y\left(t_i\right)$
- Assume all data points are independent
- Poisson PMF:

$$f\left(z_i \mid y\left(t_i\right)\right) = \frac{y\left(t_i\right)^{z_i} e^{-y\left(t_i\right)}}{z_i\,!}$$

Example - Poisson ML

- Likelihood function:

$$L\left(y(t,p) \mid z_1,\ldots,z_n\right) = f\left(z_1,\ldots,z_n \mid y(t,p)\right)$$

$$= \prod_{i=1}^{n} f\left(z_i \mid y(t,p)\right)$$

$$= \prod_{i=1}^{n} \frac{y(t_i)^{z_i}\, e^{-y(t_i)}}{z_i\,!}$$

Poisson ML

- Negative log likelihood:

$$-LL = -\ln\left(\prod_{i=1}^{n} \frac{y(t_i)^{z_i}\, e^{-y(t_i)}}{z_i\,!}\right)$$

$$= -\sum_{i=1}^{n} \ln\left(\frac{y(t_i)^{z_i}\, e^{-y(t_i)}}{z_i\,!}\right)$$

$$= -\sum_{i=1}^{n} z_i \ln\left(y(t_i)\right) + \sum_{i=1}^{n} y(t_i) + \sum_{i=1}^{n} \ln(z_i)$$

- Last term is constant

Example - Poisson ML

- Poisson ML Estimator:

$$\min_p(-LL) = \min_p\left(-\sum_{i=1}^{n} z_i \ln\left(y(t_i)\right) + \sum_{i=1}^{n} y(t_i)\right)$$

- Other common distributions - negative binomial (overdispersion), zero-inflated poisson or negative binomial, etc.

Maximum Likelihood Summary for ODEs

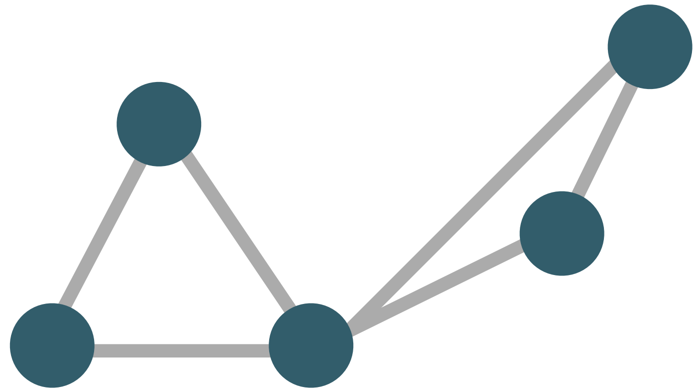
- Basic approach - suppose only measurement error
- Data is given by distribution where model output is the mean
- Suppose each time point of data is independent
- Use PDF/PMF to calculate the likelihood
- Take the negative log likelihood, minimize this over the parameter space

Maximum Likelihood for other kinds of models

- Can be quite different!
- May require more computation to evaluate (e.g. stochastic models)
- May also be structured quite differently! (e.g. network or individual-based models)

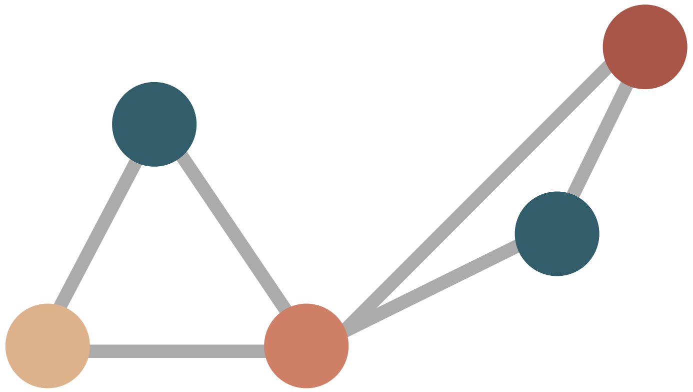
Tiny Network Example

- Data: infection pattern on the network
- Model: suppose constant probability *p* of infecting along an edge
- What's the likelihood?



Tiny Network Example

- Data: infection pattern on the network
- Model: suppose constant probability *p* of infecting along an edge, assuming we start with first case
- What's the likelihood?
- Let's see how we would calculate it for a specific data set



- L(p,data) = P(susc nodes did not get sick)
  x P(infected nodes did get sick)

Very (very!) brief intro to Bayesian Approaches to Parameter Estimation

- Allows one to account for prior information about the parameters
    - E.g. previous studies in a similar population
- Update parameter information based on new data
- Recall Bayes' Theorem:

$$P(p \mid z) = P(params \mid data) = \frac{P(z \mid p) \cdot P(p)}{P(z)}$$

Very (very!) brief intro to Bayesian Approaches to Parameter Estimation

- Allows one to account for prior information about the parameters
    - E.g. previous studies in a similar population
- Update parameter information based on new data
- Recall Bayes' Theorem:

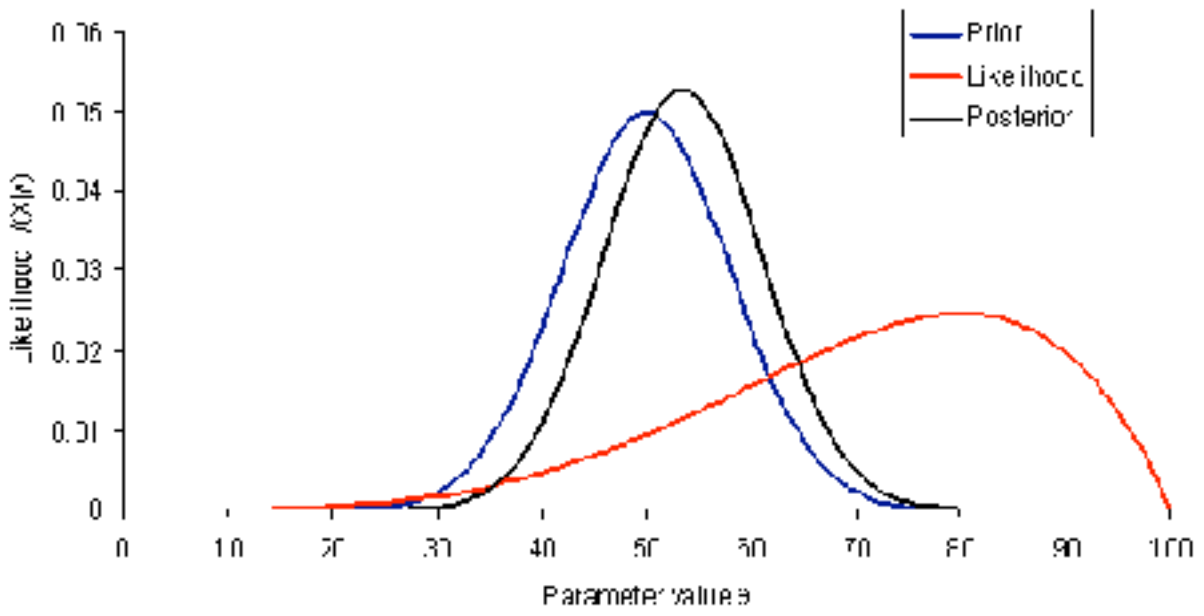
Likelihood → $P(z \mid p)$; Prior distribution → $P(p)$

$$P(p \mid z) = P(params \mid data) = \frac{P(z \mid p) \cdot P(p)}{P(z)}$$

Normalizing constant → $P(z)$
(can be difficult to calculate!)

Bayesian Parameter Estimation

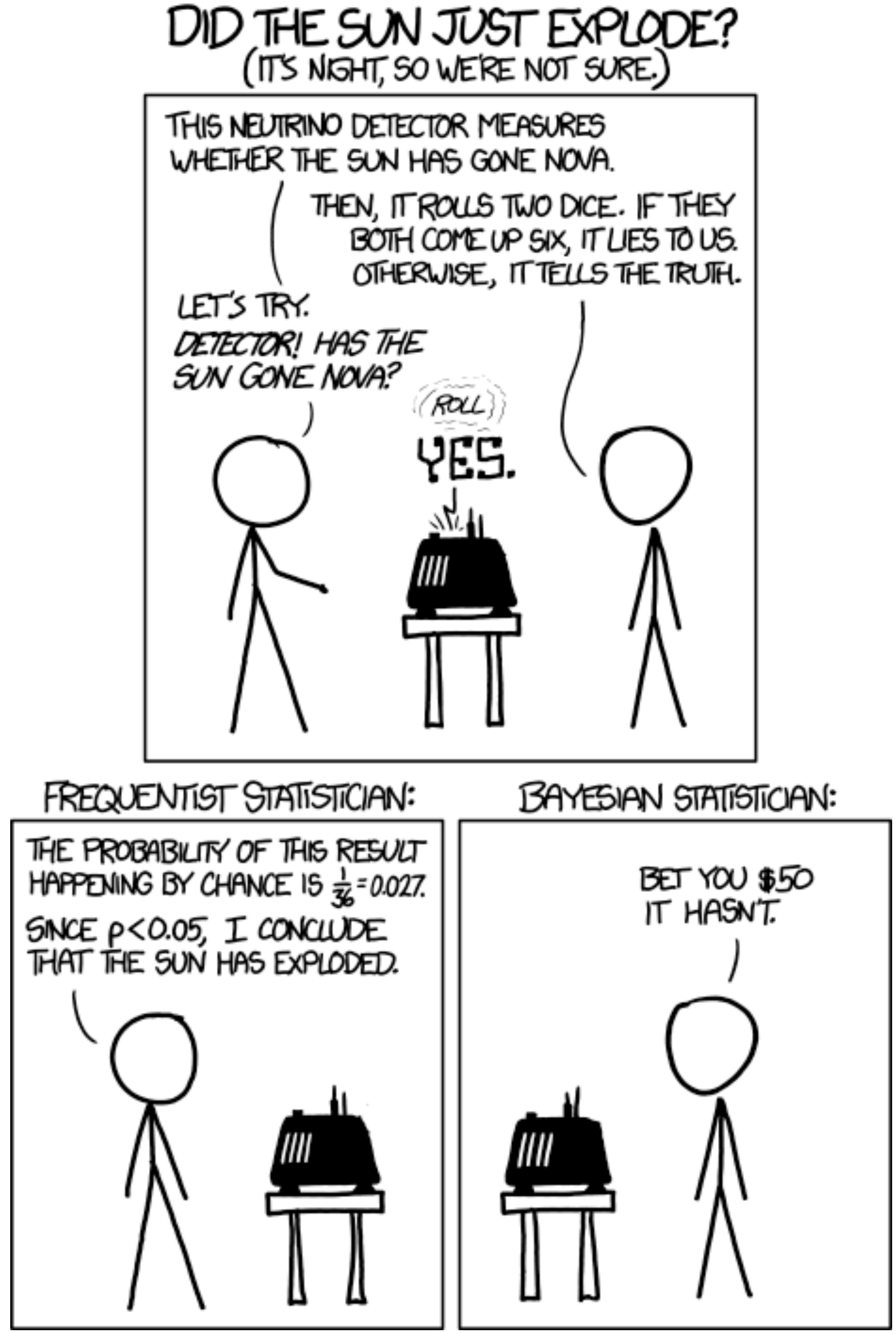
- From prior distribution & likelihood distribution, determine the posterior distribution of the parameter



- Can repeat this process as new data is available

Bayesian Parameter Estimation

- Treats the parameters inherently as distributions (belief)
- Philosophical battle between Bayesian & frequentist perspectives
- Word of caution on choosing your priors
- Denominator issues - MAP Approach



from XKCD:
http://xkcd.com/1132/