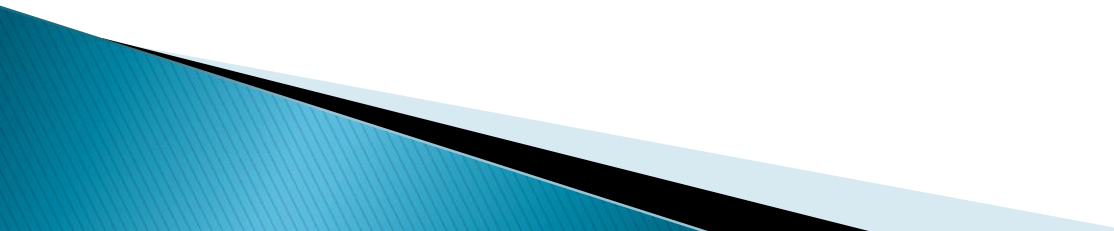


# Testing Goodness of Fit

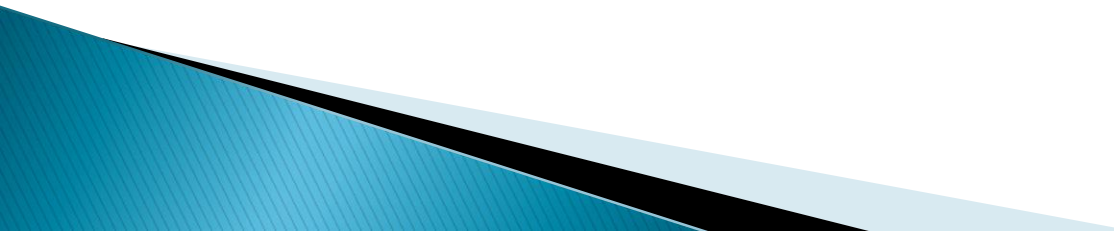
Dr. Wolfgang Rolke  
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- 

# The Archetypical Statistics Problem:

- There is a theory
  - There is data from an experiment
  - Does the data agree with the theory?
- 

# Example: Is the die fair?

Theory: die is fair ( $p_i = 1/6$ )

Experiment: roll die 1000 times

If die is fair one would expect  $1000 * 1/6 = 167$   
1's, 2's and so on

Data:

| 1   | 2   | 3   | 4   | 5   | 6   |
|-----|-----|-----|-----|-----|-----|
| 187 | 168 | 161 | 147 | 176 | 161 |

➤ Good fit?

# Most Famous Answer: Pearson $\chi^2$

Sir Karl Pearson 1900,  
*“On the criterion that a  
given system of  
deviations from the  
probable in the case of  
correlated system of  
variables is such that it  
can be reasonably  
supposed to have arisen  
from random sampling”,*  
Phil. Mag (5) 50, 157–175



Use as measure of deviations

$$\chi^2 = \sum \frac{(O-E)^2}{E}$$

O: observed counts

E: expected counts

Agreement is bad if  $\chi^2$  is large

But why  $\sum \frac{(O-E)^2}{E}$ , why not (say)  $\sum \frac{(O-E)^2}{O}$  or  $\sum |O - E|$  or  $\max\{|O - E|\}$  ?

|   | 1   | 2   | 3   | 4   | 5   | 6   |
|---|-----|-----|-----|-----|-----|-----|
| O | 187 | 168 | 161 | 147 | 176 | 161 |
| E | 167 | 167 | 167 | 167 | 167 | 167 |

$$X^2 = \frac{(187 - 167)^2}{167} + \dots + \frac{(161 - 167)^2}{167} = 5.72$$

Is 5.72 “large”?

If die is fair and rolled 1000 times, how large would  $X^2$  typically be?

# Pearson's Reasoning

$N_i$  = frequency of outcome  $i$ ,  $i = 1, \dots, k$

$(N_1, \dots, N_k) \sim \text{Multinomial}(n, p_1, \dots, p_k)$

$E[N_i] = np_i$ ,  $\text{Var}[N_i] = np_i(1 - p_i)$

$\frac{N_i - np_i}{\sqrt{np_i(1-p_i)}} \sim_{app} N(0, 1)$  by CLT

$\left( \frac{N_i - np_i}{\sqrt{np_i(1-p_i)}} \right)^2 = \frac{(N_i - np_i)^2}{np_i(1-p_i)} \sim_{app} \chi^2(1)$

so maybe  $\sum_{i=1}^k \frac{(N_i - np_i)^2}{np_i(1-p_i)} \sim_{app} \chi^2 ?$

but  $N_1 + \dots + N_k = n$  fixed (not independent)

$$k = 2 : (N_1, N_2) = (N, n - N)$$

$$\chi^2 = \sum_{i=1}^k \frac{(N_i - E_i)^2}{E_i} =$$

$$\frac{(N - np)^2}{np} + \frac{(n - N - n(1 - p))^2}{n(1 - p)} =$$

$$\frac{(N - np)^2}{np} + \frac{(n - N - n + np)^2}{n(1 - p)} =$$

$$\left( \frac{1}{np} + \frac{1}{n(1 - p)} \right) (N - np)^2 =$$

$$\left( \frac{1 - p + p}{np(1 - p)} \right) (N - np)^2 =$$

$$\frac{(N - np)^2}{np(1 - p)} = \left( \frac{N - np}{\sqrt{np(1 - p)}} \right)^2 \sim \chi^2(1)$$

Pearson:  $X^2$  has a chi square distribution with  $k-1$  degrees of freedom ( $k$ =number of categories)

Here: mean of  $\chi^2(5) = 5$

So our  $X^2 = 5.72$  is not unusually large, die is fair.

In the derivation of the distribution of  $X^2$  we used the CLT approximation, so this needs a sufficiently large sample size. But how large does it have to be?

Famous answer:  $E \geq 5$

William G. Cochran The [chi-squared] test of goodness of fit. *Annals of Mathematical Statistics* 1952; 25:315–345.

Seems to have picked 5 for no particular reason. Later research showed this is quite conservative.



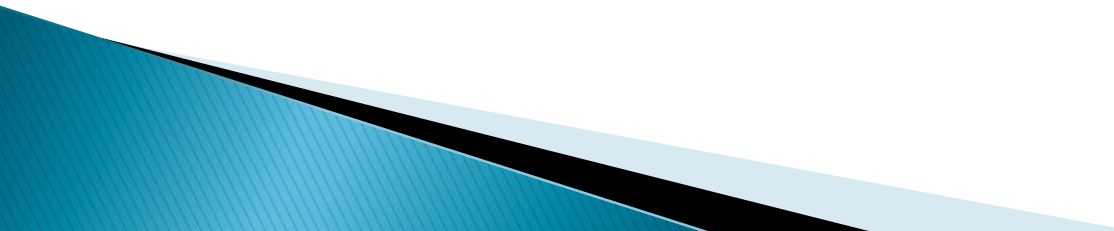
# Hypothesis Testing Basics

- ▶ Type I error: reject true null hypothesis
- ▶ Type II error: fail to reject false null hypothesis

1: A HT **has to have** a true type I error probability no higher than the nominal one

2: The probability of committing the type II error **should** be as low as possible (subject to 1)

Historically 1 was achieved either by finding an exact test or having a large enough sample.



# Another Derivation of $\chi^2$

Neyman, Jerzy; Pearson, Egon S. (1933). "On the Problem of the Most Efficient Tests of Statistical Hypotheses". *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*. 231 (694–706):  
In a test of a simple vs simple hypotheses likelihood ratio test is most powerful



$$L(p_1, \dots, p_k) \sim p_1^{N_1} \dots p_k^{N_k}$$

$$\Lambda = \frac{L(p_1, \dots, p_k)}{\max\{L(p_1, \dots, p_k) : n_1 + \dots + n_k = n\}} =$$

$$\frac{L(p_1, \dots, p_k)}{L(N_1/n, \dots, N_k/n)} = \frac{p_1^{N_1} \dots p_k^{N_k}}{\left(\frac{N_1}{n}\right)^{N_1} \dots \left(\frac{N_k}{n}\right)^{N_k}} =$$

$$\left(\frac{np_1}{N_1}\right)^{N_1} \dots \left(\frac{np_k}{N_k}\right)^{N_k}$$

Samuel S. Wilks: “*The Large-Sample Distribution of the Likelihood Ratio for Testing Composite Hypotheses*”, The Annals of Mathematical Statistics, Vol. 9, No. 1 (Mar., 1938), pp. 60–62

$$-2\log\Lambda \sim \chi^2(k - 1)$$

$$-2 \log \Lambda = -2 \log \left[ \left( \frac{np_1}{N_1} \right)^{N_1} \cdots \left( \frac{np_k}{N_k} \right)^{N_k} \right] =$$

$$2 \sum n_i \log \frac{N_i}{np_i} =$$

$$2 \sum n_i \log \left( \frac{N_i}{np_i} - 1 + 1 \right) =$$

$$2 \sum n_i \log \left( \frac{N_i - np_i}{np_i} + 1 \right)$$

$\log(x + 1) \approx x + x^2/2$  Taylor expansion

$$-2 \log \Lambda \approx 2 \sum n_i \left( \frac{N_i - np_i}{np_i} + \left( \frac{N_i - np_i}{np_i} \right)^2 / 2 \right) =$$

$$2 \sum n_i \frac{N_i - np_i}{np_i} + \sum \left( \frac{N_i - np_i}{np_i} \right)^2 \approx X^2$$

because  $N_i \approx np_i$ , so  $N_i - np_i \approx 0$

$$\text{so } 2 \sum n_i \frac{N_i - np_i}{np_i} \approx 0$$

# The Degree of Freedom Controversy

Not

$H_0: F = \text{Normal}(0,1)$       (**simple** hypothesis)

but

$H_0: F = \text{Normal}$       (**composite** hypothesis)

Idea: find estimates of parameters, use those.

Any change in test? Pearson said no.

In 1915 Greenwood and Yule publish an analysis of a 2x2 table and note that there is a problem.

In 1922, 1924 and 1926 Sir Karl Fisher published several papers showing that Pearson was wrong.

If  $m$  parameters are estimated

$$X^2 \sim \chi^2(k - 1 - m)$$

The 1922 paper is the first ever to use the term “degrees of freedom”.

In some ways this is an astonishing result: it does not seem to matter how well one can estimate the parameter (aka what sample size is used)

Does it matter what method of estimation is used? Yes, and it has to be minimum chisquare!

Except these days everyone is using maximum likelihood, and then this result can be wrong

Pearson didn't acknowledge Fisher was right until 1935!



# Mendel–Fisher Controversy

Mendel, J.G. (1866). "Versuche über Pflanzenhybriden", *Verhandlungen des naturforschenden Vereines in Brünn*, Bd. IV für das Jahr, 1865, *Abhandlungen*: 3–47

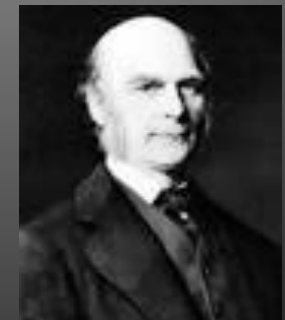


Discovery of Mendelian inheritance

Immediate impact on Science: ZERO!

Darwin could have used this when he wrote *On The Origin of Species*.

His cousin Francis Galton (inventor of regression!) could have told him.



Around 1900, Hugo de Vries and Carl Correns first independently repeat some of Mendel's experiments and then rediscover Mendel's writings and laws.

Finally Mendel becomes the “Father of Genetics”

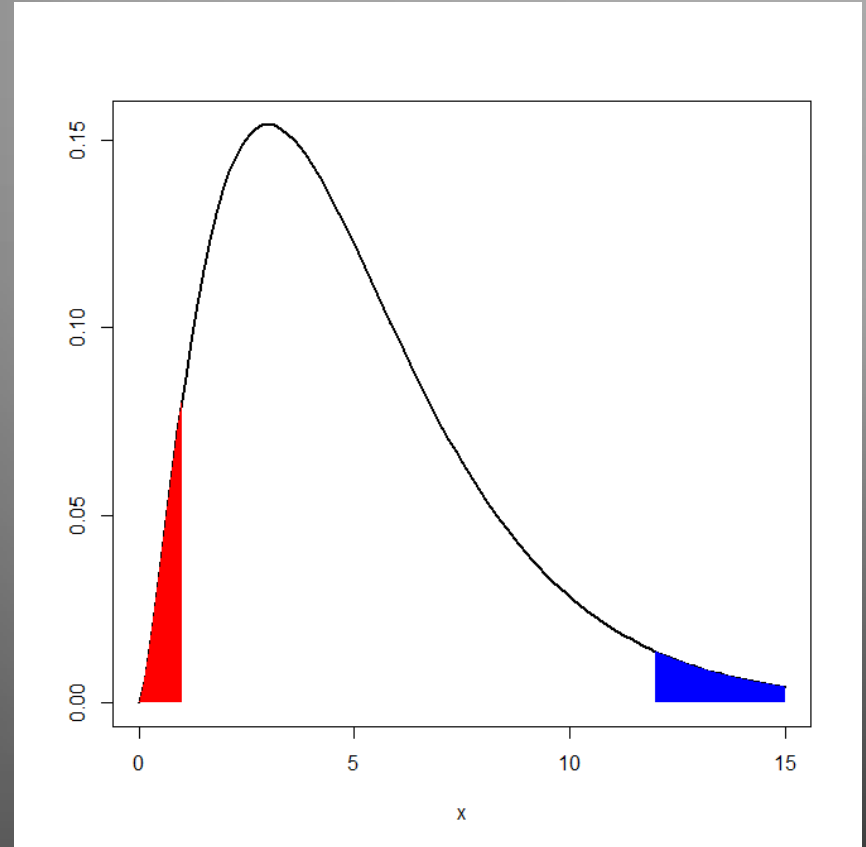
*Fisher, R.A. (1936). "Has Mendel's work been rediscovered?". *Annals of Science*. 1 (2): 115–137.*

Fisher re-analyzed Mendel's data and applied the  $\chi^2$  test to all of them together. He finds an (almost) perfect agreement. But inheritance is intrinsically random, the agreement should not be that good.

Fisher's words: “too good to be true”

$\chi^2$  large (blue area)  
→ difference between O  
and E to large  
→ theory doesn't agree  
with data

$\chi^2$  small (red area)  
→ difference between O  
and E to small  
→ Cheating!



More than 50 papers published since 1936 have tried to figure out what happened.

For a long time: it was the Gardener!

Another explanation, which seems to have gained momentum in recent years: It was early in the history of experimentation, modern ideas of how to avoid (even unconscious) biases were not yet developed.

Allan Franklin, A. W. F. Edwards, Daniel J. Fairbanks, Daniel L. Hartl and Teddy Seidenfeld. *“Ending the Mendel–Fisher Controversy”*, University of Pittsburgh Press, 2008.



# Variations on $\chi^2$

|                                              |                                                                                                |
|----------------------------------------------|------------------------------------------------------------------------------------------------|
| Cressie-Read                                 | $\frac{1}{n\lambda(\lambda-1)} \sum O \left\{ \left( \frac{O}{E} \right)^\lambda - 1 \right\}$ |
| Pearson ( $\lambda = 1$ )                    | $\sum \frac{(O-E)^2}{E}$                                                                       |
| log likelihood ratio ( $\lambda = 0$ )       | $2 \sum O \log\left(\frac{O}{E}\right)$                                                        |
| Freeman-Tukey ( $\lambda = -1/2$ )           | $4 \sum [\sqrt{O} - \sqrt{E}]^2$                                                               |
| Neyman modified $\chi^2$ ( $\lambda = -2$ )  | $\sum \frac{(O-E)^2}{O}$                                                                       |
| modified likelihood ratio ( $\lambda = -1$ ) | $2 \sum E \log\left(\frac{E}{O}\right)$                                                        |

Question used to be: which converges fastest to  $\chi^2$ ?

But these day null distribution can be found most easily using Monte Carlo simulation!

# Monte Carlo Simulation

```
function(B=1e4) {  
  O<-c(187,168,161,147,176,161)  
  E<-rep(1,6)/6*1000  
  TS.Data<-rep(0,5)  
  TS.Data[1]<-sum( (O-E)^2/E)  
  TS.Data[2]<-2*sum(O*log(O/E))  
  TS.Data[3]<-4*sum( (sqrt(O)-sqrt(E))^2)  
  TS.Data[4]<-sum( (O-E)^2/O)  
  TS.Data[5]<-2*sum(E*log(E/O))  
  TS.Sim<-matrix(0,B,5)  
  for(i in 1:B) {  
    O<-table(sample(1:6,size=1000,replace=T))  
    TS.Sim[i,1]<-sum( (O-E)^2/E)  
    TS.Sim[i,2]<-2*sum(O*log(O/E))  
    TS.Sim[i,3]<-4*sum( (sqrt(O)-sqrt(E))^2)  
    TS.Sim[i,4]<-sum( (O-E)^2/O)  
    TS.Sim[i,5]<-2*sum(E*log(E/O))  
  }  
  list(TS.Data,apply(TS.Sim,2,quantile,0.95))  
}
```

| Method                    | Data | 95 <sup>th</sup> |
|---------------------------|------|------------------|
| Pearson                   | 5.72 | 10.95            |
| log likelihood ratio      | 5.76 | 10.97            |
| Freeman-Tukey             | 5.75 | 10.95            |
| Neyman modified           | 5.73 | 11.08            |
| modified likelihood ratio | 5.73 | 11.00            |

# Question today: Which Method has highest Power?

```
function(B=1e4) {  
  crit95<-c(10.95, 10.97, 10.95, 11.08,  
  11.00)  
  E<-rep(1,6)/6*1000  
  TS.Sim<-matrix(0,B,5)  
  for(i in 1:B) {  
    O<-  
    table(sample(1:6,size=1000,replace=T,  
      prob=c(1.25,1,1,1,1,1)))  
    TS.Sim[i,1]<-sum( (O-E)^2 / E)  
    TS.Sim[i,2]<-2*sum(O*log(O/E))  
    TS.Sim[i,3]<-4*sum( (sqrt(O)-sqrt(E))^2  
    TS.Sim[i,4]<-sum( (O-E)^2 / O)  
    TS.Sim[i,5]<-2*sum(E*log(E/O))  
  }  
  power<-rep(0,5)  
  for(i in 1:5) power[i]<-  
    sum(TS.Sim[,i]>crit95[i])/B  
  power  
}
```

| Method                    | Power  |
|---------------------------|--------|
| Pearson                   | 55.47% |
| log likelihood ratio      | 53.95% |
| Freeman-Tukey             | 53.33% |
| Neyman modified           | 50.50% |
| modified likelihood ratio | 52.26% |

# Fisherian Significance Testing vs Neyman–Pearson

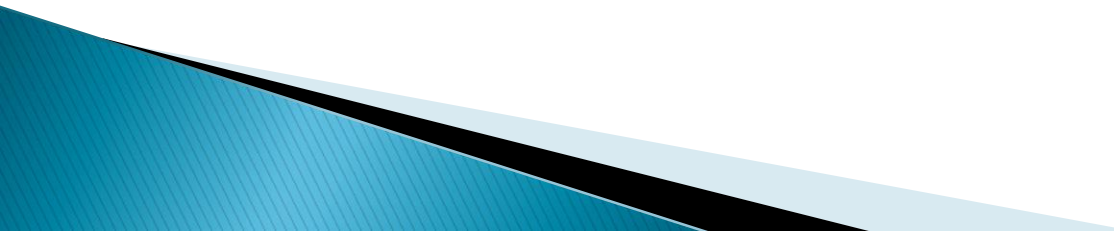
Fisher's question: does data agree with theory?

Neyman–Pearson's question: should one reject the null hypothesis in favor of some specific alternative?

Main advantage of Neyman–Pearson style test: can decide which method is better (aka has a higher power)

Today's procedure is a hybrid of both

GOF testing much closer to Fisherian significance testing, except when we have a specific alternative in mind

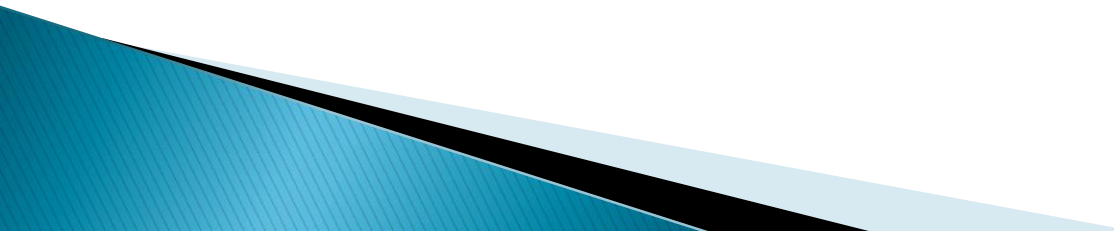


George Box: All models are wrong, but some are useful

Probability models are theoretical constructs, one can not expect them to be perfect fits in real life (“there is no perfect circle in nature”)

→ how close an agreement between null and data is needed depends on context

→ related to choice of type I error probability  $\alpha$ , 5%? 1%?  $5\sigma$  (I hope not!)

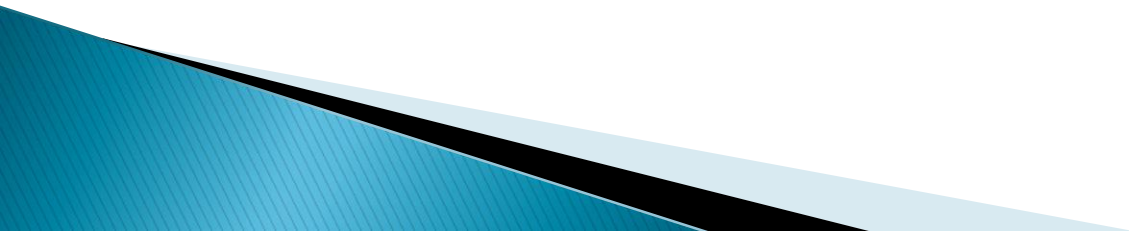


# Overfitting

Usual question: is our theory a good enough model for the data?

We also should worry about: is our model better than it should be?

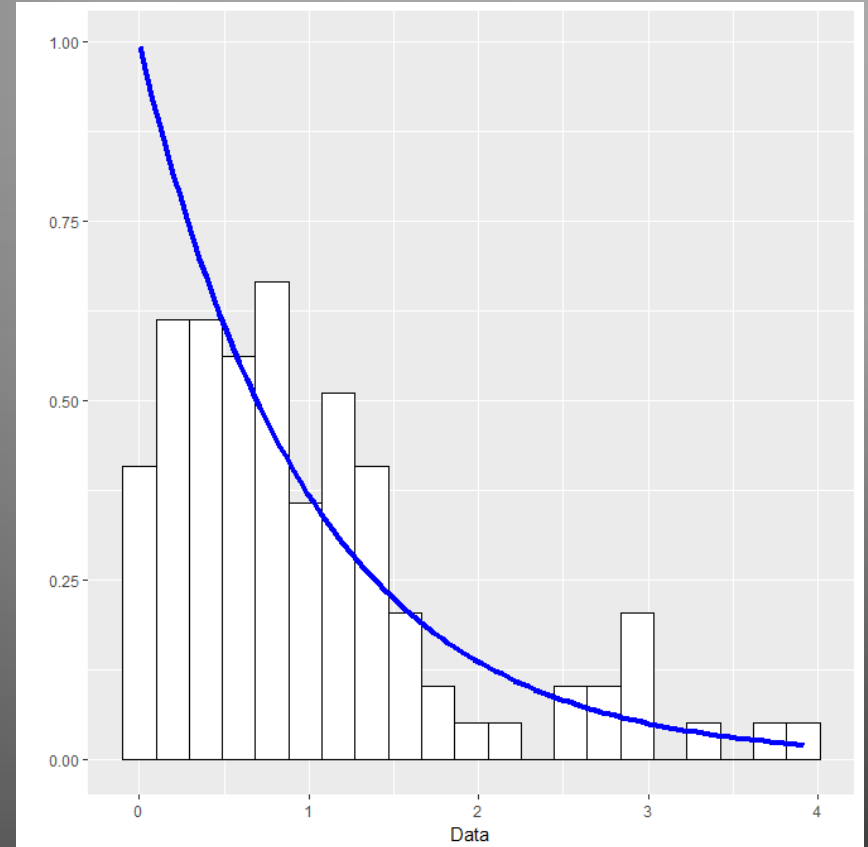
➤ Overfitting!



# Exponential Model – Good Fit?

$\chi^2$  (6 bins): p value =  
0.111

KS test: p value =  
0.117



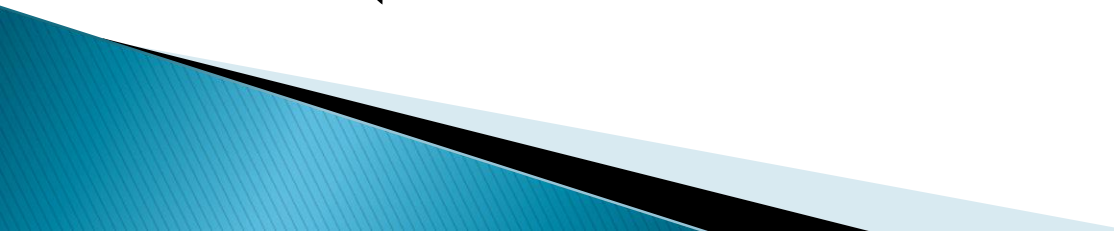
Typical procedure (especially for background fits):

Start with low degree polynomial

Add higher degrees until fit looks good

If GOF done by “visual inspection” quite likely leads to overfitting.

Additional problem: Version of “look-elsewhere effect” (aka simultaneous inference)



# Continuous Data

Need to bin the data

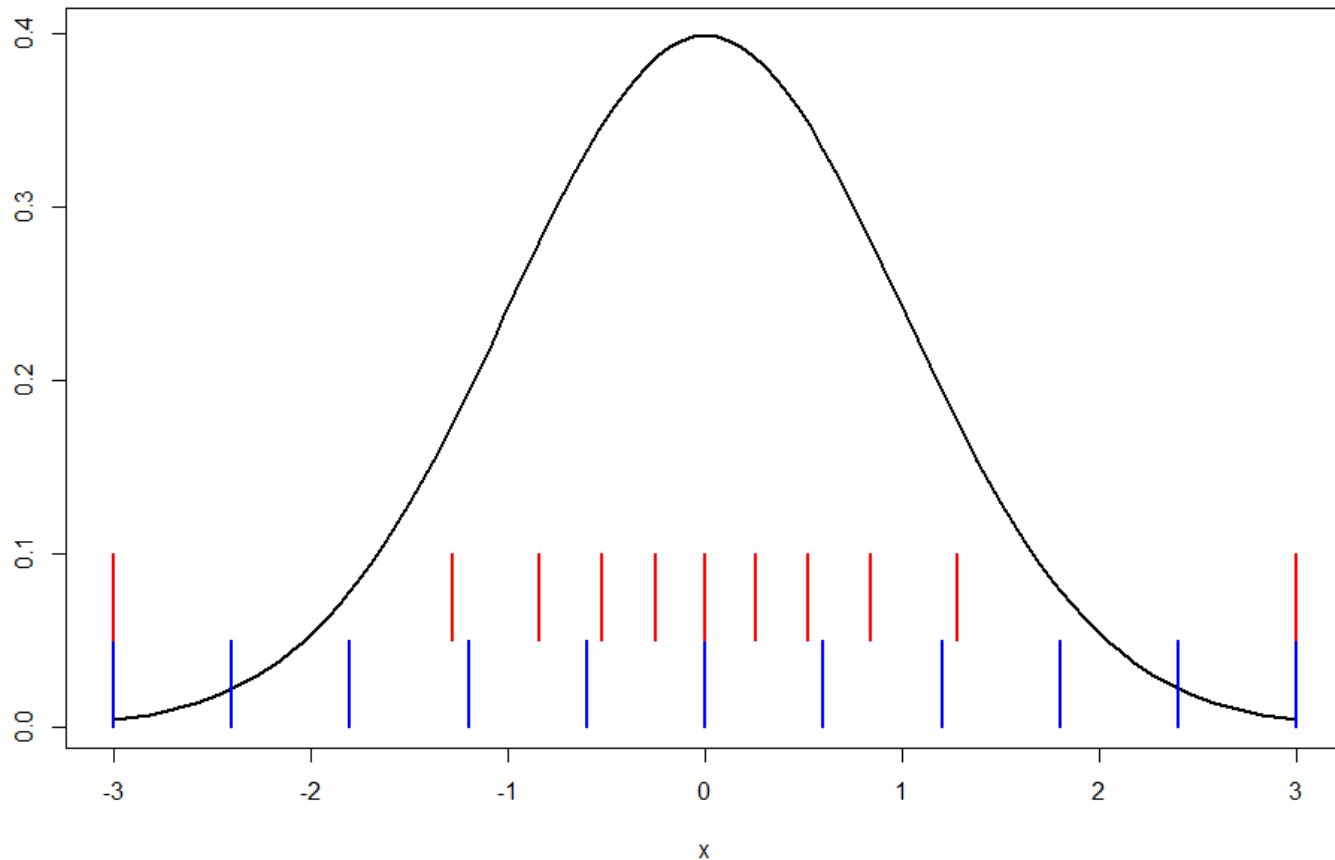
In principle any binning is ok

Two Questions:

- 1) What kind of bins?
- 2) How many bins?

# What kind of bins?

Equi-distant – Equi-probable

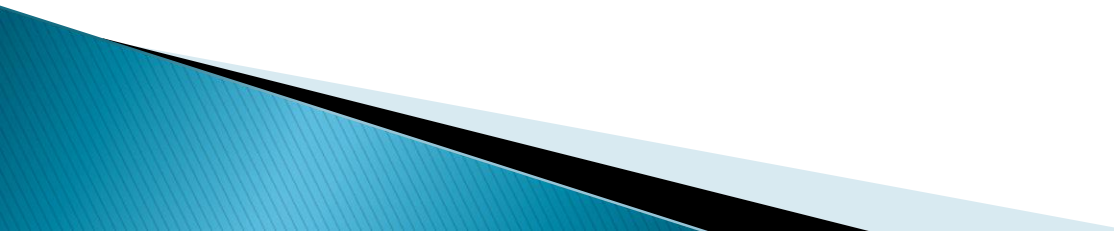


Most studies suggest equi-probable is better

One advantage:  $E=1/k \gg 5$  for all bins, no need to adjust binning

Major advantage: In general leads to tests with higher power

Bins can be found easily as quantiles of  $F$  or as quantiles of data



# How many bins?

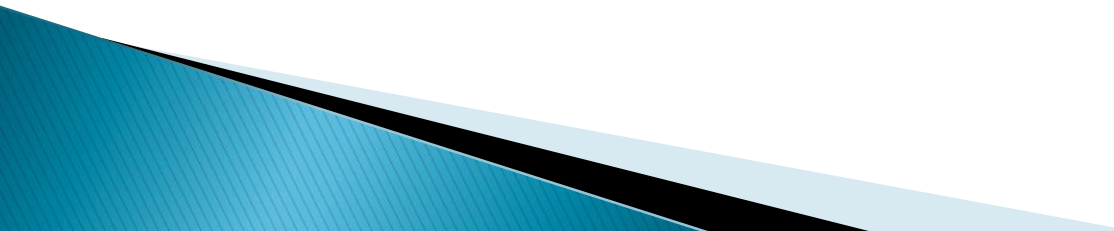
Textbook answer:  $k = 2n^{2/5}$

D'Agostini and Stephens (1986) “*Goodness-of-Fit Techniques*”

But: really depends on alternative

Example:  $H_0: X \sim U[0,1]$  vs  $H_a: X \sim \text{Linear}$

Optimal  $k$ :  $k=2$ !



# EDF Methods

**EDF: Empirical Distribution Function**

$$\hat{F}(x) = \frac{1}{n} \sum_{i=1}^n I_{(-\infty, x]}(X_i) = \frac{\# \text{ of events } \leq x}{n}$$

$\hat{F}(x) \rightarrow F(x)$  uniformly (Glivenko–Cantelli lemma)

so

$$D\{\hat{F}(x), F(x)\}$$

where  $D$  is some distance measure on function space can be used for goodness-of-fit test.

## Theorem: (Probability Integral Transform)

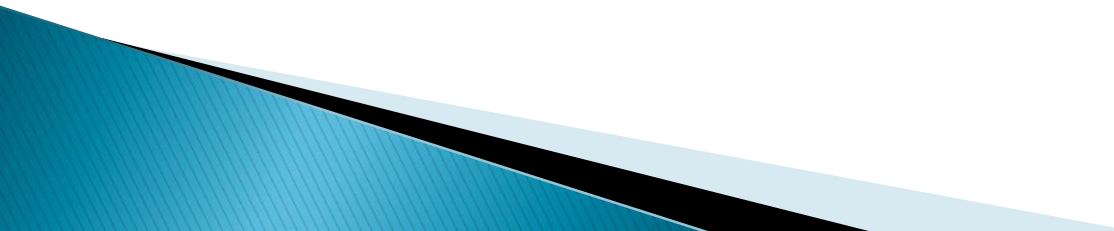
Let  $X$  be a continuous random variable with distribution function  $F$ , then the random variable

$Y = F(X)$  has a uniform  $(0,1)$  distribution.

Consequence:  $D$  is distribution free, aka does not depend on  $F$ .

One table to rule them all!

Except this does not work if parameters are estimated from data!

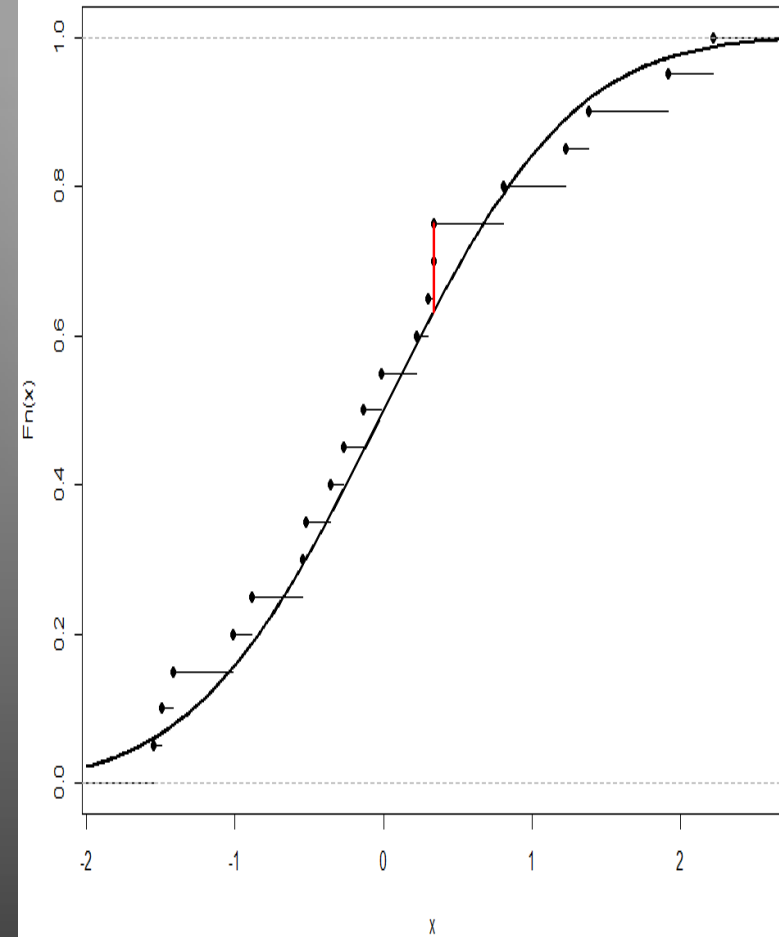


# Kolmogorov–Smirnov

$$KS = \max\{|\hat{F}(x) - F(x)|; x\} = \max\left\{\left|\frac{i}{n} - F(X_{(i)})\right|, \left|F(X_{(i)}) - \frac{i-1}{n}\right|\right\}$$

Kolmogorov A (1933). "Sulla determinazione empirica di una legge di distribuzione". G. Ist. Ital. Attuari. 4: 83–91.

Smirnov N (1948). "Table for estimating the goodness of fit of empirical distributions". Annals of Mathematical Statistics. 19: 279–281



# Alternatives

## Anderson-Darling

Anderson, T. W.; Darling, D. A. (1952). "Asymptotic theory of certain "goodness-of-fit" criteria based on stochastic processes". *Annals of Mathematical Statistics*. 23: 193-212.

$$AD = n \int_{-\infty}^{\infty} \frac{(\hat{F}(x) - F(x))^2}{F(x)[1 - F(x)]} dF(x)$$

## Cramer-vonMises

Cramér, H. (1928). "On the Composition of Elementary Errors". *Scandinavian Actuarial Journal*. 1928 (1): 13-74.

doi:10.1080/03461238.1928.10416862.

von Mises, R. E. (1928). *Wahrscheinlichkeit, Statistik und Wahrheit*. Julius Springer.

$$CM = \int_{-\infty}^{\infty} (\hat{F}(x) - F(x))^2 d\hat{F}(x)$$

And more...

Modern theory based on convergence of  $\hat{F}$  to Gaussian process

None of these allows estimation of parameters except in some special cases:

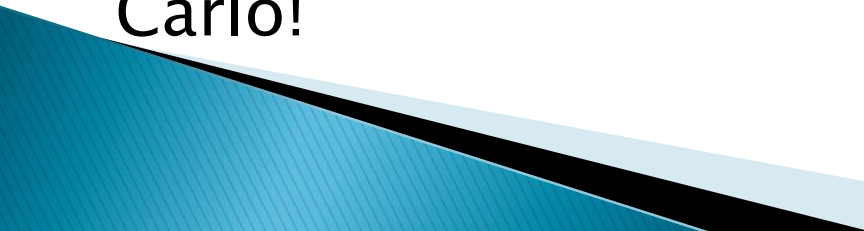
$H_0: X \sim \text{Normal}$

Hubert Lilliefors (1967), "*On the Kolmogorov-Smirnov test for normality with mean and variance unknown*", Journal of the American Statistical Association, Vol. 62. pp. 399–402.

$H_0: X \sim \text{Exponential}$

Hubert Lilliefors (1969), "*On the Kolmogorov-Smirnov test for the exponential distribution with mean unknown*", Journal of the American Statistical Association, Vol. 64 . pp. 387–389.

But then again, just find null distribution via Monte Carlo!



# R package KScorrect

Uses maximum likelihood to estimate parameters and Monte Carlo simulation to estimate null distribution

## Example:

```
> x<-rexp(1000,1)
> LcKS(x,"pexp")$p.value
[1] 0.3998
```

- "pnorm" for normal,
- "pmixnorm" for (univariate) normal mixture,
- "plnorm" for lognormal (log-normal, log normal),
- "punif" for uniform,
- "plunif" for loguniform (log-uniform, log uniform),
- "pexp" for exponential,
- "pgamma" for gamma,
- "pweibull" for Weibull.

Later I will show you another way to do GOF testing!

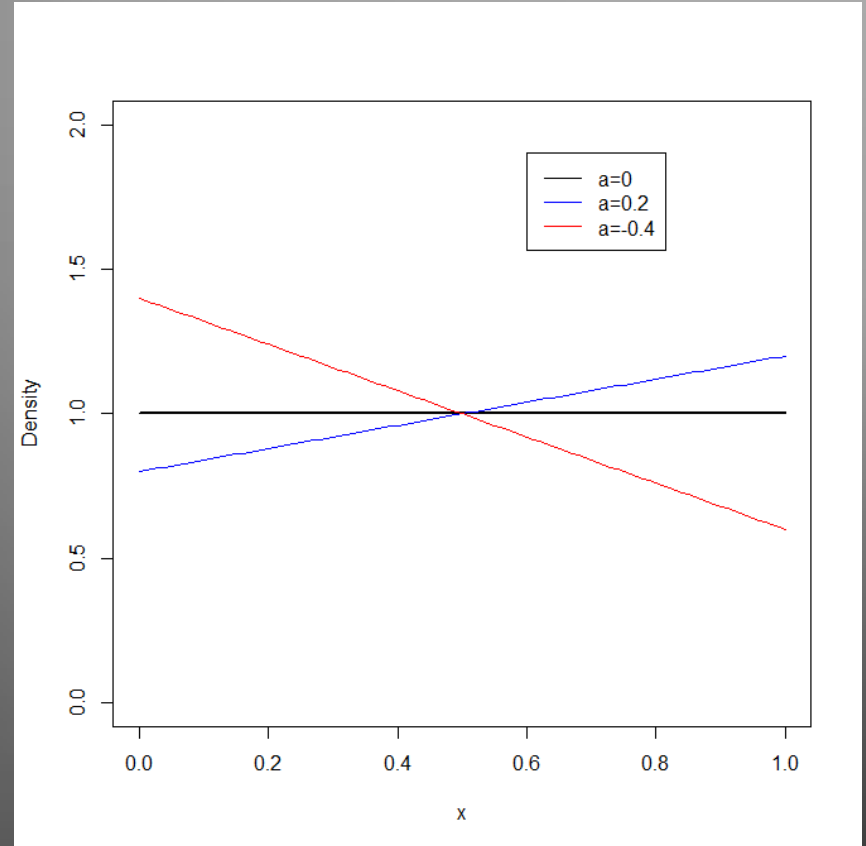
# $\chi^2$ vs K-S

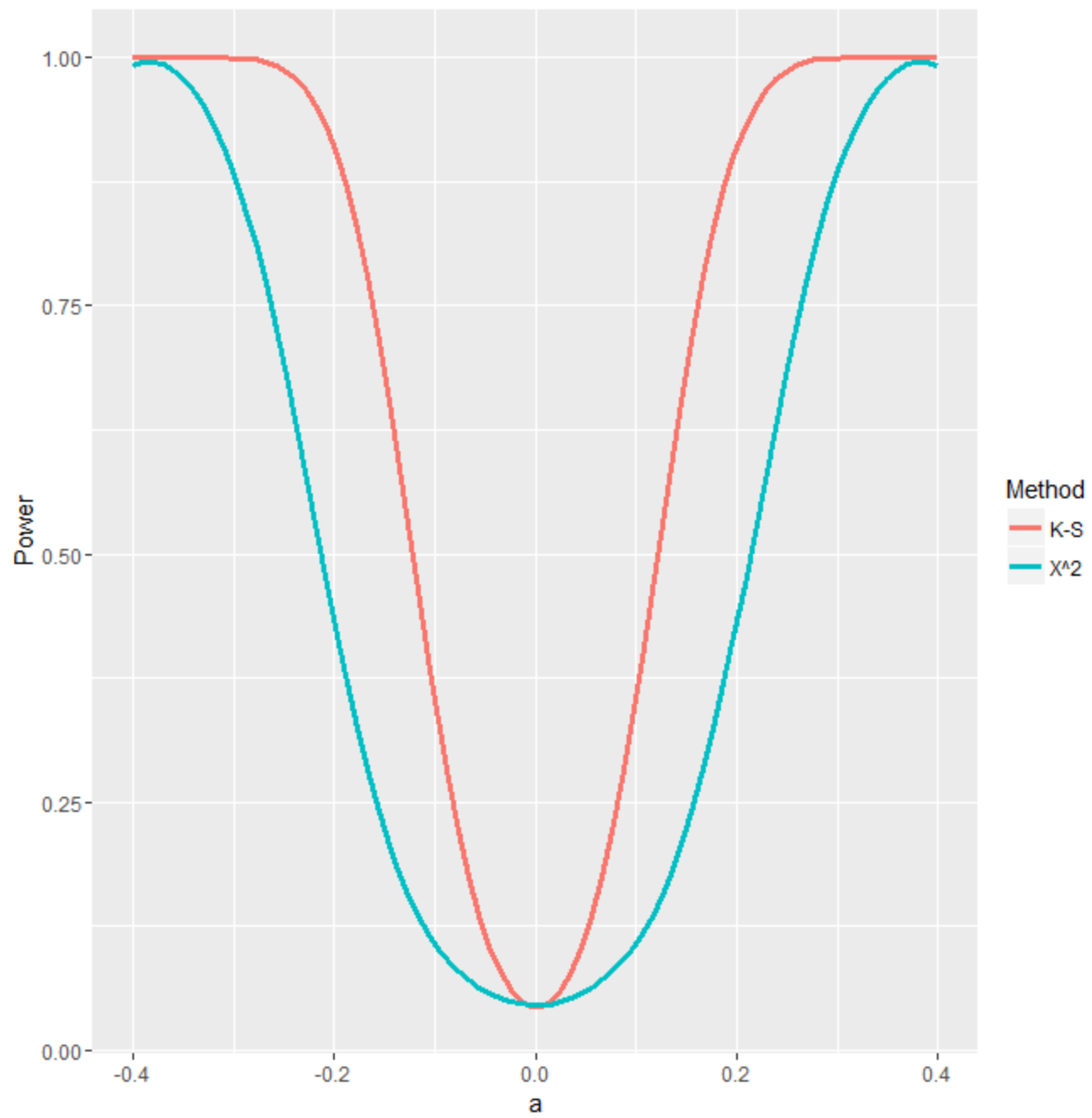
$$H_0: F = \text{Uniform}[0,1]$$

$$H_a: F = \text{Linear} [0,1]$$

Sample size:  $n=1000$

$\chi^2$ : 32 bins  
(here Equi-distant =  
Equi-probable )

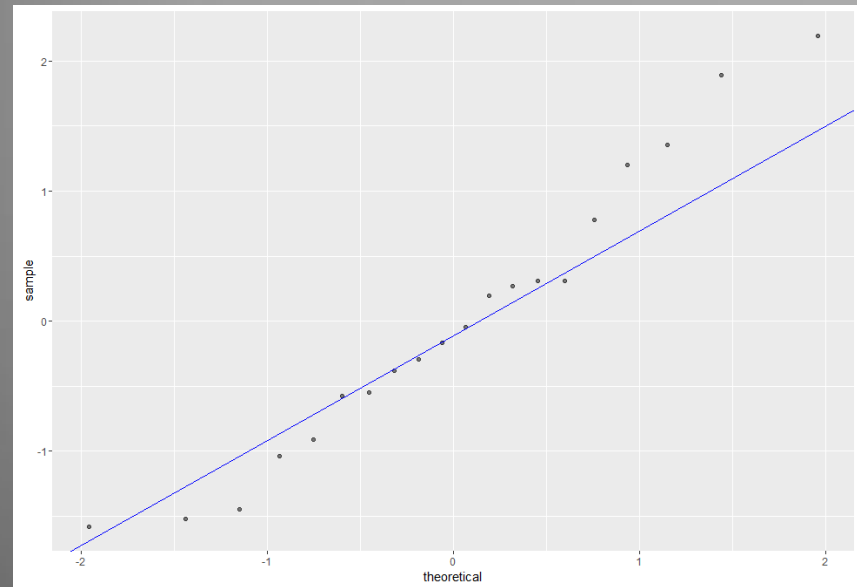




# Probability Plots

Plot quantiles  
of F vs sample  
quantiles

If F is correct  
model, points  
form a straight  
line



# Turn this into a formal test

Again Probability Integral Transform:

$$X \sim F \rightarrow F(X) \sim U[0,1]$$

$$(U_1, \dots, U_n) \text{ iid } U[0,1]$$

Order Statistic

$$U_{(1)} < \dots < U_{(n)}$$

$$U_{(k)} \sim \text{Beta}(k, n - k + 1)$$

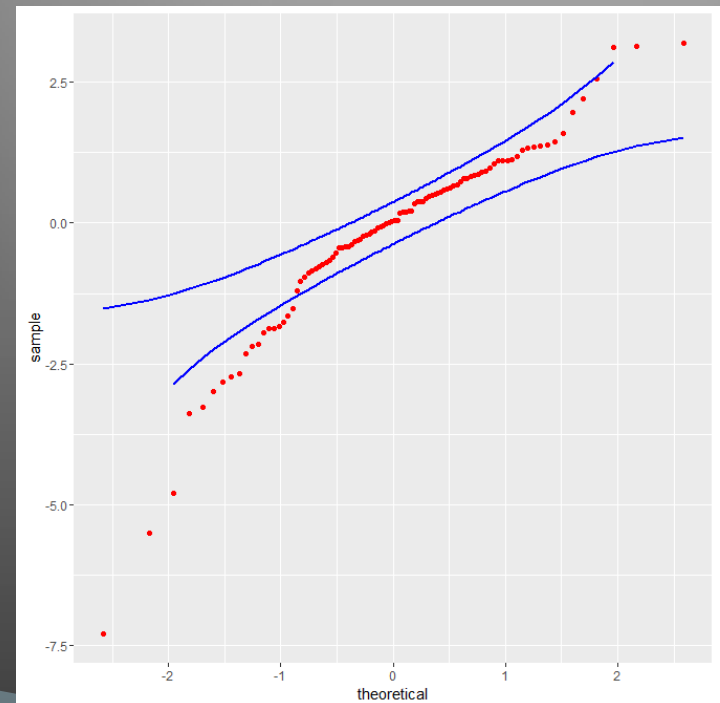
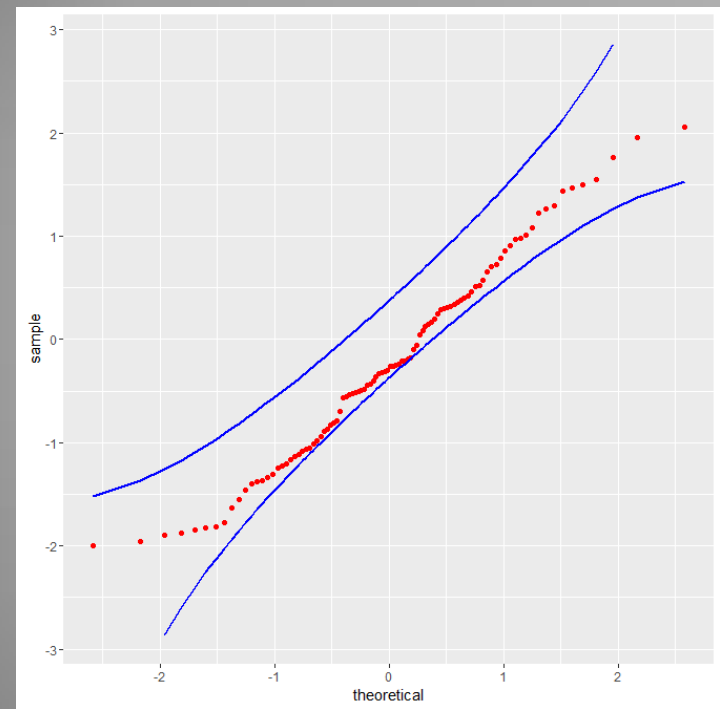
Find pointwise confidence intervals from quantiles of Beta distribution

Turn into simultaneous confidence band by adjusting nominal confidence level

Sivan Aldor–Noima, Lawrence D. Brown, Andreas Buja , Robert A. Stine and Wolfgang Rolke, “*The Power to See: A New Graphical Test of Normality*”, The American Statistician (2013), Vol 67/4

Andreas Buja, Wolfgang Rolke  
“*Calibration for Simultaneity:  
(Re) Sampling Methods for  
Simultaneous Inference with  
Applications to Function  
Estimation and Functional  
Data*”, Technical Report,  
Wharton School of Business,  
Univ. of Pennsylvania

R routines:  
<http://academic.uprm.edu/wrolke/research/publications.htm>



# Smooth Tests

Old idea – goes back to Neyman (1937) – but with some recent improvements.

Basic idea: embed density  $f$  in family of densities  $\{g_k\}$  indexed by some parameter vector  $\Theta = (\theta_1, \dots, \theta_k)$  which includes true density for some  $k$  and such that

$$H_0: \text{true density is } f \leftrightarrow H_0: \Theta = \mathbf{0}$$

$$g_k(x; \theta, \beta) = C(\theta, \beta) \exp \left\{ \sum_{j=1}^k \theta_j h_j(x; \beta) \right\} f(x; \beta)$$

$\{h_j\}$  should be orthonormal family of functions, i.e.

$$\int_{-\infty}^{\infty} h_i(x) h_j(x) dx = \delta_{ij}$$

optimal choice of  $\{h_j\}$  depends on  $f$ !

Typical choices for  $\{h_j\}$ :

Legendre Polynomials, Fourier series,

$h_j(x) = \sqrt{2} \cos(j\pi x)$ , Haar functions, ....

Basics of the test:

$$U_j = \frac{1}{\sqrt{n}} \sum_{i=1}^n h_j(X_i)$$

$$T_k = \sum_{j=1}^k U_j^2$$

$$T_k \rightarrow_d \chi_k^2$$

Interesting feature: partial tests  $(\theta_1, \dots, \theta_m) = 0$  for  $m < k$  can give insight into HOW null is wrong.

testing composite hypotheses is possible

Quite unusual: best method for estimating parameters: MoM (method of moments)

Example:

$$X_1, \dots, X_n \text{ iid } N(\mu, \sigma)$$

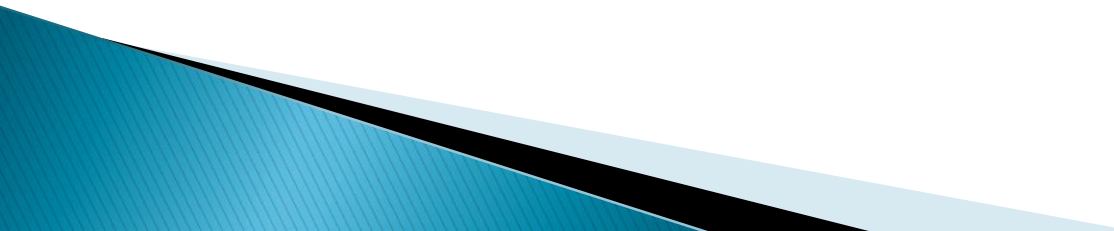
$$\mu = E[X_1] \simeq \frac{1}{n} \sum_{i=1}^n X_i$$

$$\sigma^2 = \text{Var}(X_1) = E[X_1^2] - E[X_1]^2$$

$$E[X_1^2] \simeq \frac{1}{n} \sum_{i=1}^n X_i^2$$

$$\sigma^2 \simeq \frac{1}{n} \sum_{i=1}^n X_i^2 - \left( \frac{1}{n} \sum_{i=1}^n X_i \right)^2$$

# And many more...

- ▶ Tests based on moments
  - ▶ Tests specific for a distribution (Normal: more than 20 tests)
  - ▶ A good place to start: “Comparing Distributions”, Olivier Thais, Springer
- 

# Multidimensional Data

$\chi^2$  tests: Curse of Dimensionality (R. Bellman)

Example:  $H_0: (X_1, \dots, X_d) \sim U[0,1]^d$

We want  $E \geq 5$  and we want 10 bins in each dimension. What  $n$  do we need?

$$d=1: E = n/10 \cong 5 \rightarrow n \cong 50$$

$$d=2: E = n/10^2 \cong 5 \rightarrow n \cong 500$$

$$d=3: E = n/10^3 \cong 5 \rightarrow n \cong 5000$$

...

$$d=10: E = n/10^{10} \cong 5 \rightarrow n \cong 50 \text{ billion}$$

# EDF Tests

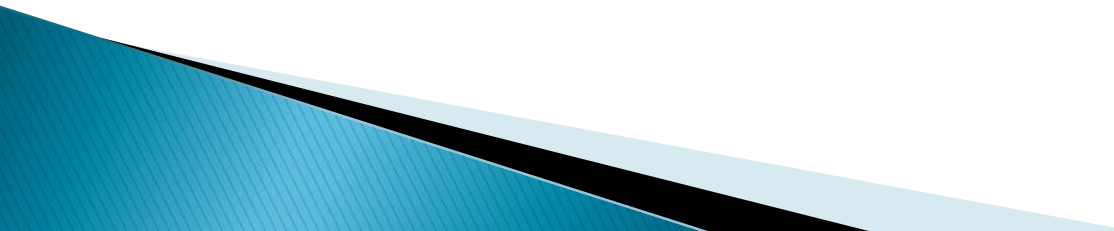
EDF needs an ordering.

What comes first in  $R^2$ :  $(0,1)$  or  $(1,0)$ ?

One can impose an ordering but in  $R^d$  there are  $2^d - 1$  ways to do it!

Also, Probability Integral Transform no longer works, so KS test is no longer distribution free.

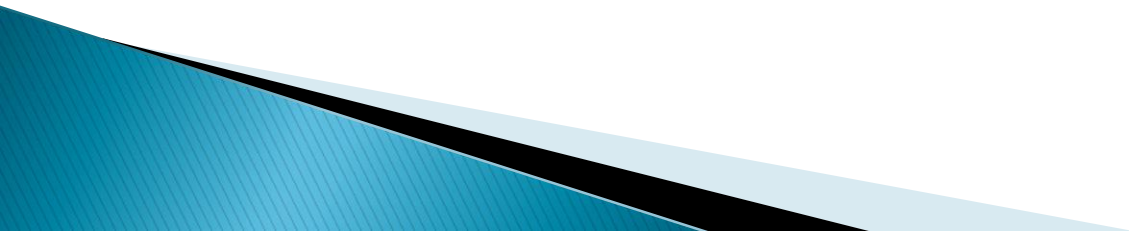
But one can always use MC to find null distribution.



GOF tests beyond 2 or 3 dimensions unlikely to be very useful.

At the very least will require gigantic data sets

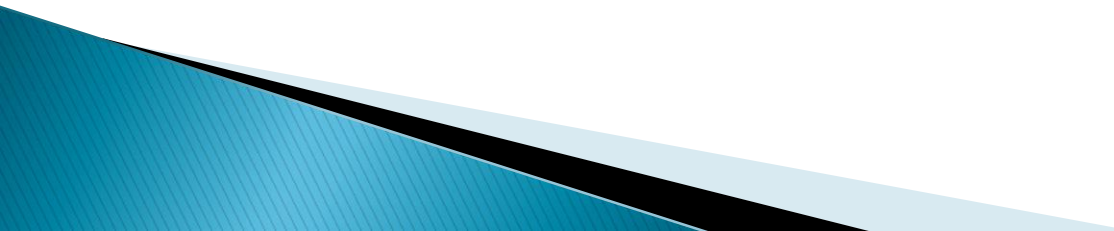
Still a wide open problem!



# Special Cases

Often data has special features that need to be taken into account

**Example: High Energy Physics**

- 1) Data is truncated
  - 2) Sample size is random
  - 3) Data is binned
- 

# Truncated Data

- ▶ Data in High Energy Physics is always truncated to a finite interval.
- ▶ Care needs to be taken with normalization  
(aka  $\int_{-\infty}^{\infty} f(x)dx = 1$ )

# Sample Size

In HEP experiments sample size is not fixed a-priori but is a consequence of the run time

$$n \sim \text{Poisson}(\lambda)$$

If  $n$  is fixed:  $(N_1, \dots, N_k) \sim \text{Multinomial}(n, p_1, \dots, p_k)$

But if  $n$  is Poisson

$$N_i \sim \text{Poisson}(\lambda p_i) \text{ and } N_1, \dots, N_k \text{ independent!}$$

(Theory of Marked Poisson processes)

Consequence:  $X^2 \sim \chi^2(k)$  (not  $k-1$ )

Not an issue if null distribution is found via MC

# Binned Data

Data in HEP is often already binned for various reasons, for example detector resolution

Still need to consider rebinning for chi square tests.

How about Kolmogorov–Smirnov?

$$KS = \max \left\{ \left| \frac{i}{n} - F(X_{(i)}) \right|, \left| F(X_{(i)}) - \frac{i-1}{n} \right| \right\}$$

But we only know  $b_i < X_{(i)} < b_{i+1}$

Obvious answer:  $x_i = \frac{b_i + b_{i+1}}{2}$  midpoint

Better answer: spread out  $N_i$  points in  $(b_i, b_{i+1})$  according to  $F$ .

Can be quite slow (requires finding quantiles of  $F$ , solve many non-linear equations), in practise spreading them uniformly almost as good.

# 2-Sample Problem

Say we have

$$X_1, \dots, X_n \sim F \text{ and } Y_1, \dots, Y_m \sim G$$

and we want to test

$$H_0: F = G \text{ vs } H_0: F \neq G$$

At first this seems a very different problem, but fairly generally a method for one can be turned into a method for the other.

**Example:** Kolmogorov–Smirnov

GOF:  $KS = \max\{|\hat{F}(x) - F(x)|; x\}$

2-Sample:  $KS = \max\{|\hat{F}(x) - \hat{G}(x)|; x\}$

# Permutation Tests

Under  $H_0: F = G$

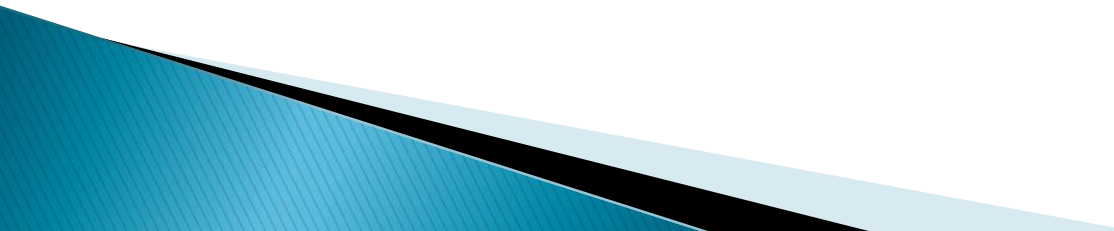
so

$$X_1, \dots, X_n, Y_1, \dots, Y_m \sim F$$

samples are independent, so any reordering is equally likely.

Basic permutation test:

Find random permutation of data, split in vectors of size  $n$  and  $m$ , calculate test statistic, repeat many times. Compare to actual data.



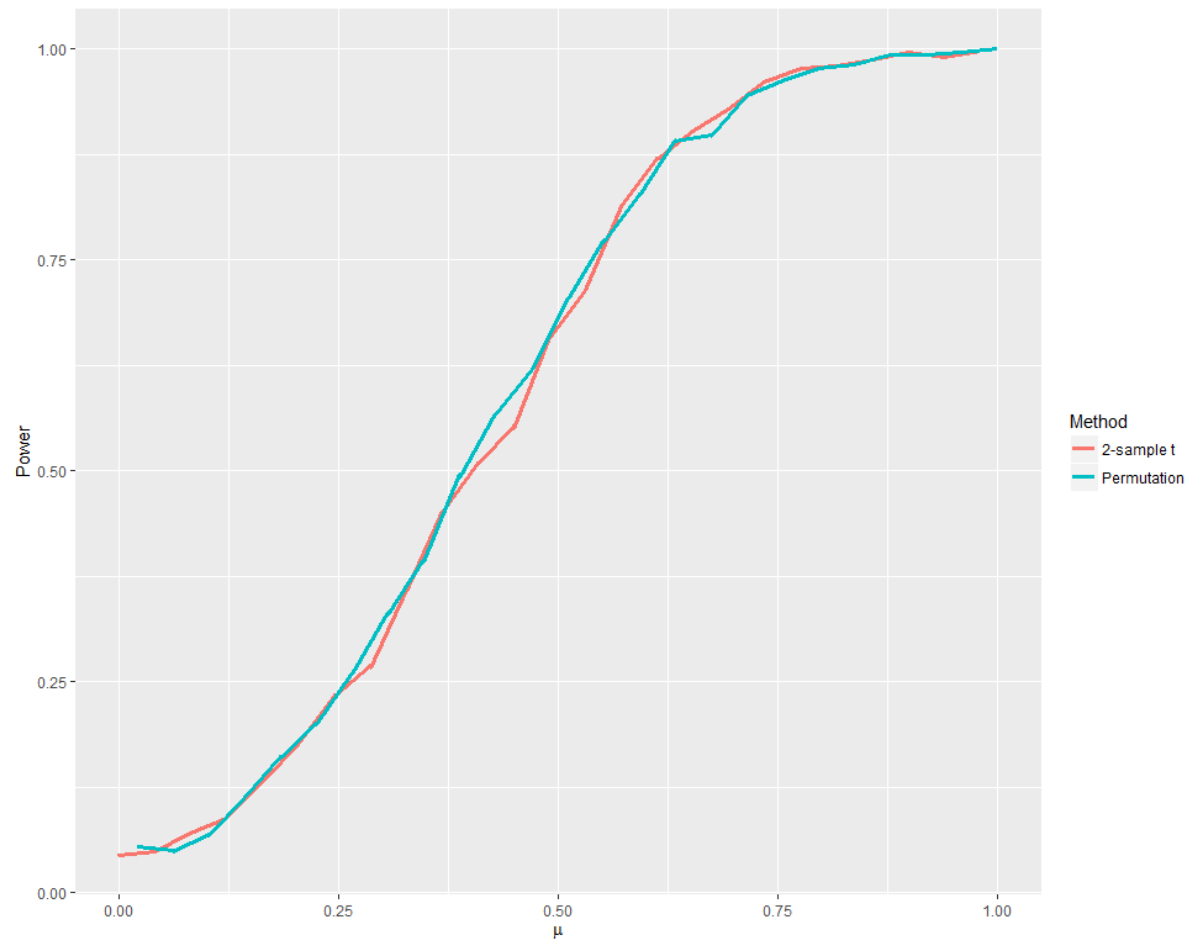
# Power

$$F = N(0,1) \quad G = N(\mu, 1)$$

in example:  $n=50$

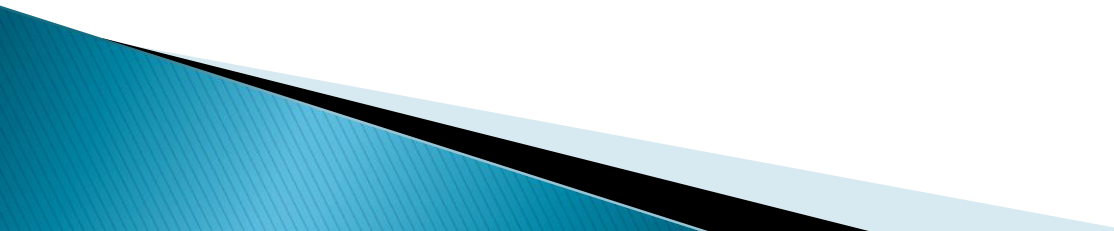
Compare to classic 2-sample t test:

$$TS = \frac{\bar{X} - \bar{Y}}{s_p \sqrt{\frac{1}{n} + \frac{1}{m}}} \sim t_{n+m-2, \alpha/2}$$

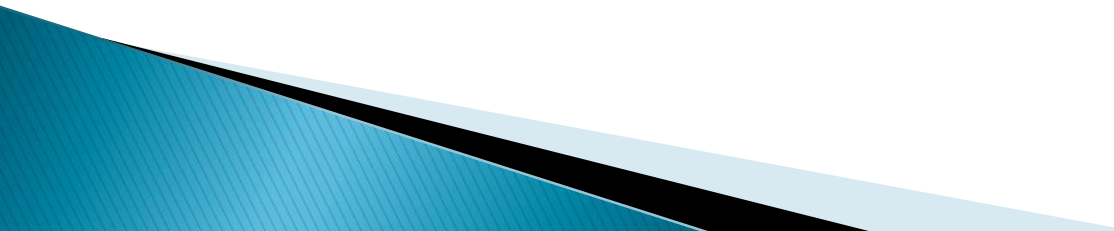


# GOFer

## Online Goodness-of-Fit Testing

- ▶ No knowledge of R required
  - ▶ Can handle continuous or binned data
  - ▶ Can handle model specified via expression (density) or via bin probabilities
  - ▶ Model expressions can be specified via R or C++
  - ▶ Finds a variety of standard tests (Chisquare variants and EDF tests)
  - ▶ Allows for “optimal” binning
- 

# How to run App

- ▶ App is online at <https://drrolke.shinyapps.io/GOFer/>
  - ▶ You can install all you need to run the app on your computer in less than 10 minutes. To see how go here <http://academic.uprm.edu/wrolke/GOFer/>
  - ▶ Page also has detailed explanations on how to use app.
- 

# GOFer

For a detailed explanation of the app go [here](#)

Run MC!

Data is ...

Continuous

Model is ...

Continuous

MC runs

1000

Sample size is ..

fixed

Source of Data?

Use Included Examples

Select Data Set

Uniform y=1

Left End Point

0

Right End Point

1

Choose Probability Model to Test

Enter R expression for density

Enter R expression for density and hit Go

1

Go

Select EDF Tests

- ☒ Kolmogorov-Smirnov
- ☒ Anderson-Darling
- ☒ Cramer-vonMises

Select Chi Square Tests

- ☒ Pearson  $\chi^2$
- ☐  $\chi^2 \lambda, p$
- ☐  $\chi^2 \lambda, m$

Number of Bins (0=Default Formula)

0

Type of bins

Equal Probability

Type I error rate for envelope test

$\alpha = 5\%$

Do you want to find the Power of the Tests?

No

## Choose Probability Model to Test

## Enter R expression for density and hit Go

Go

Enter R expression for density

$\exp(-x)$

## Select EDF Tests

- ☒ Kolmogorov-Smirnov
- ☒ Anderson-Darling
- ☒ Cramer-vonMises

## Select Chi Square Tests

- ☒ Pearson  $\chi^2$
- ☐  $\chi^2 \lambda, p$
- ☐  $\chi^2 \lambda, m$

## Number of Bins (0=Default Formula)

0

## Type of bins

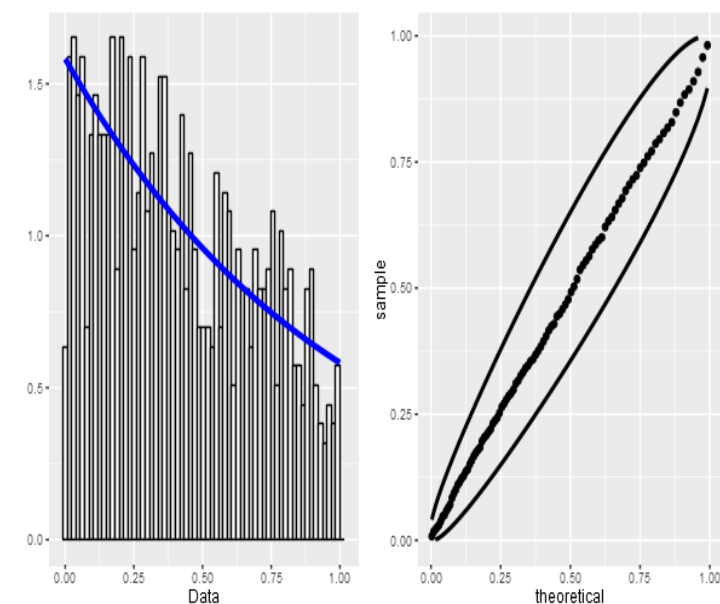
Equal Probability

## Type I error rate for envelope test

$\alpha = 5\%$

## Do you want to find the Power of the Tests?

No



| Result of GOF Tests                  |                   |             |
|--------------------------------------|-------------------|-------------|
| Chi Square Tests. Number of bins: 32 |                   |             |
| Method                               | Bin Type          | p-value     |
| Pearson $\chi^2$                     | Equal Probability | $p = 0.561$ |
| EDF Type Tests                       |                   |             |
| Kolmogorov-Smirnov                   |                   | $p = 0.825$ |
| Anderson-Darling                     |                   | $p = 0.593$ |
| Cramer-vonMises                      |                   | $p = 0.966$ |

Choose Probability Model to Test

Enter R expression for density

exp(-x)

Go

Select EDF Tests

☒ Kolmogorov-Smirnov

☒ Anderson-Darling

☒ Cramer-vonMises

Select Chi Square Tests

☒ Pearson  $\chi^2$

☐  $\chi^2 \lambda, p$

☐  $\chi^2 \lambda, m$

Number of Bins (0=Default Formula)

0

Type of bins

Equal Probability

Type I error rate for envelope test

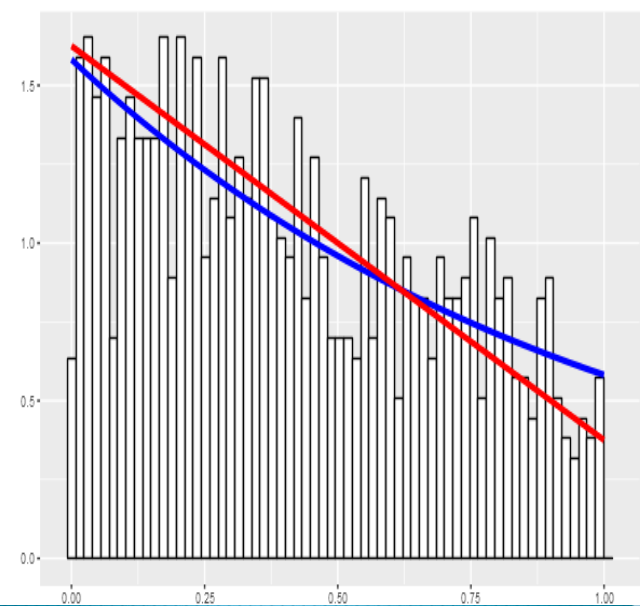
$\alpha = 5\%$

Do you want to find the Power of the Tests?

Yes

Enter R expression for alternative density

1-x/1.3



| Result of GOF Tests                  |                   |           |
|--------------------------------------|-------------------|-----------|
| Chi Square Tests. Number of bins: 32 |                   |           |
| Method                               | Bin Type          | p-value   |
| Pearson $\chi^2$                     | Equal Probability | p = 0.561 |
| EDF Type Tests                       |                   |           |
| Kolmogorov-Smirnov                   |                   | p = 0.825 |
| Anderson-Darling                     |                   | p = 0.593 |
| Cramer-vonMises                      |                   | p = 0.966 |

| Power of the Tests |                   |        |
|--------------------|-------------------|--------|
| $\chi^2$ Tests     |                   |        |
| Method             | Bin Type          | Power  |
| Pearson $\chi^2$   | Equal Probability | 27.9 % |
| EDF Type Tests     |                   |        |
| Kolmogorov-Smirnov |                   | 61.3 % |
| Anderson-Darling   |                   | 69.4 % |
| Cramer-vonMises    |                   | 59 %   |

# File Upload

R

```
Density
exp(-param[1]*x)
Distribution
1-exp(-param[1]*x)
Alternative
1-x/5
Estimator
xbar<-mean(x)
new<-param[1]
repeat {
  old<-new
  new<-old-(1/old-xbar-exp(-old)/(1-
exp(-old)))/(-1/old^2+exp(-old)/(1-exp(-
old))^2)
  if(abs(old-new)<0.0001) break
}
return(new)
```

C++

```
Density
for(int i=0;i<n;++i) y[i] = exp(-
param[0]*x[i]);
Distribution
for(int i=0;i<n;++i) y[i] = 1.0-exp(-
param[0]*x[i]);
Alternative
for(int i=0;i<n;++i) y[i] = 1.0-x[i]/5.0;
Estimator
double pold,pnew,xbar;
xbar=0;
for(int i=0;i<n;++i) xbar+=x[i];
xbar=xbar/n;
pnew=param[0];
while(abs(pold-pnew)>0.0001) {
  pold=pnew;
  pnew=pold-(1.0/pold-xbar-exp(-
pold)/(1.0-exp(-pold)))/(-
1.0/(pold*pold)+exp(-pold)/(1.0-exp(-
pold))/(1.0-exp(-pold)));
}
p[0]=pnew;
```

Thanks!