MEM6810 Engineering Systems Modeling and Simulation 工程系统建模与仿真

Theory

Lecture 5: Input Modeling

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- The quality of outputs is no better than the quality of inputs.
 - "Garbage in, garbage out."
- "All models are wrong, but some are useful." George Box.
 - There is no "true" model for any stochastic input.
 - The best we can do is to obtain an approximation that yields reasonable and useful results.



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 - can capture the physical properties of the system;
 - can be easily tuned to the situation at hand;
 - can be efficiently generated with certain random variate generation technique.
- Input modeling is sometimes more of an art than an engineering.
 - It nearly always requires the analysts to use their judgment as well as to apply appropriate statistical tools.
 - Since there is no "true" model, it is sensible to run the simulation with several plausible input models to see if the conclusions are robust or highly sensitive to the choices.



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- If the fit is not good, select another candidate and go to Step 3, or use an empirical distribution.



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- People often have the **false** impression that data are readily available, but it is one of the most *challenging* task in solving a real problem.
- Never trust data blindly!
 - A common mistake is to simply throw data into a software and ask for a "best" fit model.
 - Always take into account under what context (e.g., time, potential influence of other factors) the data was collected.



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- "dirty" (containing errors);
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- Sometimes the effort or cost to transform data into a usable form, or "clean" data, can be as significant as that required to obtain them.



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- Check for autocorrelation.
- Collect input data, not output data.

- Example: customer arrival times and service times are input, whereas waiting times are output.



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- Do not ignore the physical characteristics of the process when selecting distributions.
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 - Is it bounded or is there no natural bound?
- There are literally hundreds of probability distributions that have been created; many were created with some specific physical process in mind.



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empirical distribution: Often used when no theoretical distribution seems appropriate.

The CDF of the empirical distribution (empirical CDF) is defined as

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The empirical CDF is a right-continuous step function.

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- *Example 1*: the times between the arrivals from a large population of potential customers who act independently.

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• Weibull: Models the time to failure for components.

- Note: the failure rate can be increasing, decreasing, or constant (reduce 1/2) to exponential distribution).

- Continuous Distributions:
 - Erlang: Models the time that can be viewed as the sum of several exponentially distributed times.
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 Note: can be shifted away from 0 by adding a constant; can cover a range different from [0, 1] by multiplying by a constant.
- triangular: Models a process for which only the minimum, most likely, and maximum values of the distribution are known.
 Example: only the minimum, most likely, and maximum time required to test a product are known.

- Useful in determining the shape of the distribution from which the data have been sampled:
 - **Histogram** describes frequency or relative frequency (i.e., ratio) of (usually continuous) data in different ranges.
 - **Bar chart** (or bar graph) describes frequency or relative frequency of data among discrete categories.



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- For continuous data:
 - Histogram corresponds to the pdf of a theoretical distribution.
 - In terms of the shape, not the exact value![†]
- For discrete data:
 - Usually use bar chart instead of histogram.
 - Bar chart corresponds to the pmf of a theoretical distribution.
 - In terms of both the *shape* and *value* (if the bar chart uses relative frequency).



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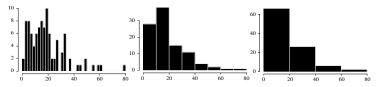


Figure: Ragged, Appropriate and Coarse Histograms (from Banks et al. (2010))



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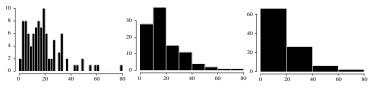


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• Choosing the number of intervals approximately equal to the square root of the sample size often works well in practice (Hines et al. 2002).

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- After a family of distributions has been selected, the next step is to determine the parameters of the distribution that can "best" fit the data.
 - Called distribution fitting, or parameter estimation.
- There are many different approaches and we discuss two simple ones:
 - method of moments (MoM)
 - maximum likelihood estimation (MLE)



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- Suppose the considered distribution family has *s* unknown parameters.
 - **1** Analytically compute $\mathbb{E}[X^1], \ldots, \mathbb{E}[X^s]$, as functions of those parameters.
 - Note: the moments of common distributions are well-known.
 - **2** Compute m_1, \ldots, m_s from the data.
 - **3** Solve $\mathbb{E}[X^k] = m_k$, $k = 1, \dots, s$, for s unknown parameters.

 Example 1: Suppose X₁,..., X_n are iid from Gamma(α, λ) (in shape & rate parametrization).

• Recall: $f(x) = \frac{\lambda^{\alpha}}{\Gamma(\alpha)} x^{\alpha-1} e^{-\lambda x}$, $\mathbb{E}[X] = \alpha/\lambda$, $\operatorname{Var}(X) = \alpha/\lambda^2$. Estimate α and λ using MoM.



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<u>Solution</u>. The first two moments are

$$\mathbb{E}[X] = \alpha/\lambda = m_1,$$

$$\mathbb{E}[X^2] = \operatorname{Var}(X) + (\mathbb{E}[X])^2 = (\alpha + \alpha^2)/\lambda^2 = m_2.$$

Solving two equations yields MoM estimators

$$\widehat{\alpha} = \frac{m_1^2}{m_2 - m_1^2}, \quad \widehat{\lambda} = \frac{m_1}{m_2 - m_1^2}.$$



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So the MoM estimator of λ is $\widehat{\lambda} = \frac{1}{m_1} = \frac{n}{X_1 + \dots + X_n}$.



• Example 3: Suppose X_1, \ldots, X_n are iid from $\mathcal{N}(\mu, \sigma^2)$. Estimate μ and σ^2 using MoM.



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$$\hat{\mu} = m_1, \quad \hat{\sigma}^2 = m_2 - m_1^2.$$
Remark: $\hat{\mu} = \frac{\sum_{i=1}^n X_i}{n}$, and
$$\hat{\sigma}^2 = \frac{X_1^2 + \dots + X_n^2}{n} - \bar{X}^2 = \frac{\sum_{i=1}^n X_i^2 - n\bar{X}^2}{n}$$

$$= \frac{\sum_{i=1}^n (X_i - \bar{X})^2}{n}. \quad \text{(why?)}$$

 Many common distributions have no more than 2 parameters: Ber(p), B(n, p), NB(r, p), Geo(p), Pois(λ), Unif[a, b], Exp(λ), Erl(k, λ), Gamma(α, λ), Beta(α, β), Weibull(α, β), N(μ, σ²), t_p, χ²_p.



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- Instead of using MoM, another convenient way to estimate the parameters is using sample mean \bar{X} and sample variance S^2 :

$$\bar{X} = \frac{\sum_{i=1}^{n} X_i}{n} = m_1,$$

$$S^2 = \frac{\sum_{i=1}^{n} (X_i - \bar{X})^2}{n-1} = \frac{\sum_{i=1}^{n} X_i^2 - n\bar{X}^2}{n-1} = \frac{n}{n-1} (m_2 - m_1^2),$$

to solve $\mathbb{E}[X]=\bar{X},$ and $\mathrm{Var}(X)=S^2$ (if necessary).



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• Note 1: Purpose of n-1 in S^2 is to ensure $\mathbb{E}[S^2] = \operatorname{Var}(X)$.

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• Note 1: Purpose of n-1 in S^2 is to ensure $\mathbb{E}[S^2] = \operatorname{Var}(X)$.

• Note 2: In original MoM, we solve $Var(X) = m_2 - m_1^2$.

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- Sometimes, both MoM and MLE yield the same estimator.



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- Remarks:
 - If X_1, \ldots, X_n haven't been observed, $\lambda^* = n/(X_1 + \cdots + X_n)$.
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For discrete distributions, replace the pdf with pmf. → Fill L #

Introduction

2 Data Collection

- 3 Identifying Distribution
 ▶ Physical Basis of Distributions
 ▶ Histogram and Bar Chart
- 4 Distribution Fitting
 ▶ Method of Moments
 ▶ A Simple Variation of MoM
 ▶ Maximum Likelihood Estimation

5 Goodness of Fit

- Graphical Methods
- Statistical Tests
- Remarks

6 An Illustrative Example



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- Try more than one plot/test before making conclusion.



• Compare the shape of **histogram** or **bar chart** of data against the fitted pdf or pmf.

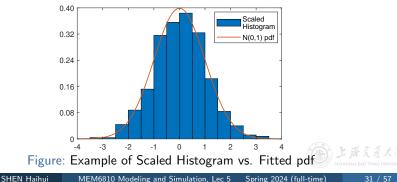


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(cc) BY-SA

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- The q-quantile of X is that value γ such that $\mathbb{P}(X \leq \gamma) = F(\gamma) = q$, for 0 < q < 1. When F(x) has an inverse, we can write $\gamma = F^{-1}(q)$.
 - Median: 50% quantile.
 - In financial risk management, quantile of the profit-and-loss of a portfolio is also called Value-at-Risk (VaR).



- To make Q-Q plots, given the data $\{x_1, \ldots, x_n\}$ and the fitted distribution with CDF F(x):
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 - If the data is indeed generated from distribution F(x), then

$$y_j \approx F^{-1} \Big(\frac{j - 0.5}{n} \Big),$$

so the plot will be approximately a straight line with slop 1.



► Graphical Methods

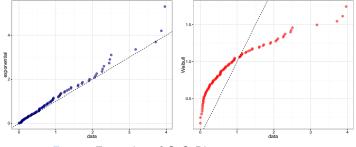


Figure: Examples of Q-Q Plot (from ZHANG Xiaowei)



► Graphical Methods

Goodness of Fit

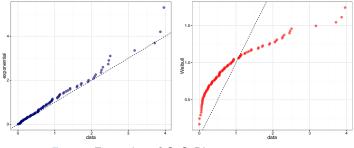


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- The observed values will never fall exactly on a straight line
- The ordered values are not independent because they are ranked. Hence, if one point lies above the line, it is likely that the next one will too.
- The values at the extremes have a much higher variance than those in the middle. So greater discrepancies can be acceptable at the extremes; linearity in the middle is much more important.

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Decision Truth	reject H_0	fail to reject H_0
H_0 is true	type I error	correct
H_1 is true	correct	type II error

- A hypothesis test only directly controls the type I error.
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- We will reject H_0 if
 - p-value is smaller than some specified α , or, equivalently,
 - the computed test statistic falls in certain range (called *rejection region*), which is determined by α .

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 - If the likelihood is very small (i.e., *p*-value is very small), then H_0 is unlikely to be true (reject H_0);
 - otherwise, there is no enough evidence to reject H_0 (fail to reject H_0).



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$$= n \times \mathbb{P}(a_{i-1} \le X < a_i)$$

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 $E_i :=$ **expected** number of points in $[a_{i-1}, a_i)$ for fitted dist. = $n \times \mathbb{P}(a_{i-1} < X < a_i)$

$$= n \int_{a_{i-1}}^{a_i} f(x) \mathrm{d}x \quad \text{or} \quad n \sum_{a_{i-1} \leq x_j < a_i} p(x_j).$$

3 Compute the test statistic $R \coloneqq \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i}$.



- The chi-square test (χ² test, 卡方检验) is a more formal comparison of a histogram with the fitted pdf f(x) or pmf p(x).
- The procedure of chi-square test:
 - First divide the entire range of the fitted distribution into k adjacent intervals, [a₀, a₁), [a₁, a₂), ..., [a_{k-1}, a_k).
 - 2 Define
 - $O_i \coloneqq \mathbf{actual}$ number of data points in $[a_{i-1}, a_i)$,
 - $E_i \coloneqq \mathbf{expected}$ number of points in $[a_{i-1}, a_i)$ for fitted dist.

$$= n \times \mathbb{P}(a_{i-1} \le X < a_i)$$

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3 Compute the test statistic $R \coloneqq \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i}$.

• Reject H_0 if R is too large.

– Reason: A large value of ${\cal R}$ indicates a poor fit, whereas a small value indicates a good fit.

- Question: How large is too large? (i.e., what is the rejection region?)

- View the test statistic *R* as a random variable.
 - Since we assume the collected data is one observed random sample from some unknown distribution, if we conduct the study multiple times, the values of the statistics will be different because the collected data will be different.
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- For the fitted distribution, suppose $s \ge 0$ parameters are unknown and estimated via MLE.
- If H_0 is true, then R approximately follows the chi-square distribution with k s 1 degrees of freedom (i.e., χ^2_{k-s-1} distribution) when sample size n is large.

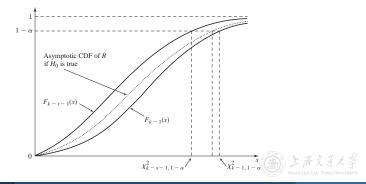
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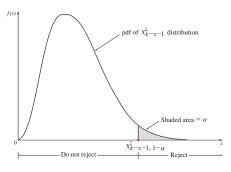
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 - It can be applied to any hypothesized distribution, which makes it widely used.
- Disadvantage of chi-square test:
 - It is valid only in an asymptotic sense (large n).
 - **Major drawback**: The validity and power of chi-square test are affected by the number and size of the chosen intervals, while there is no clear prescription for such selection.



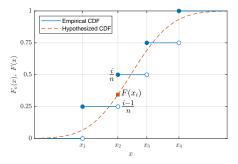
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- In the absence of a definitive guideline for choosing the intervals, it's usually recommended to make E_i equal (or approximately equal) and no less than 5, for all intervals.



 The Kolmogorov-Smirnov test (K-S test, 柯尔莫哥洛夫– 斯米尔诺夫检验) formally compares the empirical CDF F_n(x) with the CDF of the hypothesized distribution, F(x).

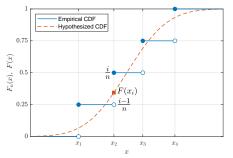


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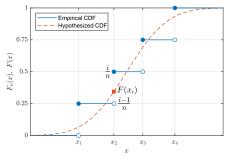


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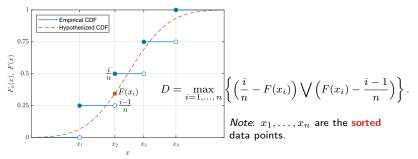
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- For current data at hand, we have already observed the value of D, which is denoted as d. **Reject** H_0 if
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 - Numerical tables and accurate approximation are available.
- If F(x) is CDF of distribution such as normal, exponential, or Weibull, and parameters are estimated via MLE (except for normal σ², which is estimated by S²):
 - Given H_0 is true, the distribution of D depends on F(x), and it is complicated.
 - Approximations and numerical tables are available.



Goodness of Fit

Statistical Tests

- Advantage of K-S test:
 - It does not require us to group the data in any way, so no information is lost and no troublesome selection is faced.
 - It is valid (exactly) for any sample size, whereas chi-square test is valid only in an asymptotic sense.
 - It tends to be more powerful than chi-square test.
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 - When applicable, its computation of *p*-value and rejection region is usually complicated.
- K-S test is relatively more convenient to be used in a case where the hypothesized distribution is continuous and no parameter is estimated. For example:
 - Test random number generators.
 - Test a Poisson process (more details later).

- Comments on *p*-value:
 - *p*-value can be viewed as a measure of fit: a large *p*-value tends to indicate a good fit, while a small *p*-value suggests a poor fit.
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 - **However**, *p*-value is just a summary measure. It says little or nothing about where the lack of fit occurs (body? left tail? right tail?).
 - Different statistical tests may give different *p*-values.
 - Whether or not you reject H_0 also depends on the significance level α chosen by yourself.



- Comments on general goodness-of-fit tests:
 - If very little data are available, then a goodness-of-fit test is unlikely to reject any candidate distribution.
 - No enough evidence to reject H_0 .
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• Do not have blind faith in goodness-of-fit tests!

- Failing to reject a candidate distribution should be taken as only **one piece of evidence** in favor of that choice.

– Rejecting a candidate distribution should be taken as only **one piece of evidence** against the choice.



- Graphical Methods vs. Statistical Tests
 - Graphical methods *qualitatively* measure the fitting goodness, while statistical tests *quantitatively* measure the fitting goodness.
 - Statistical tests measure the lack of fit by summary statistics, while graphical methods show where the lack of fit occurs (body, left tail, right tail) and allow users to decide whether it is important.
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- Always combine statistical test results with graphical analysis.
- When no model fits the data satisfactorily, we may end up with the empirical distribution.



Goodness of Fit

- ► Remarks
- Many softwares do have a "best fit" option (or button).
 - It recommends the "best" distribution in its library based on summary measure like the *p*-value (and perhaps other factors such as discrete or continuous, bounded or unbounded).



Goodness of Fit

- Many softwares do have a "best fit" option (or button).
 - It recommends the "best" distribution in its library based on summary measure like the *p*-value (and perhaps other factors such as discrete or continuous, bounded or unbounded).
- Always keep the following in mind when using such an option:
 - The software might know nothing about the physical basis of the data.
 - Automated best-fit procedures tend to choose the more flexible distributions (gamma over Erlang, Weibull over exponential).
 - But, close conformance to the data does not always lead to the most appropriate input model (overfitting).
 - The limitation of summary measure like *p*-value.
 - View the automated distribution selection as one suggestion, inspect it using graphical methods, and remember that *the final choice is yours*.

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- All the graphical methods and statistical tests can be used to check the uniformity of a random number generator (RNG).
 - Generate a sequences of numbers (as many as you want) using the RNG.
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 - Suppose we observe an arrival process for a time interval [0, T], where T is a constant decided before we start our observation.
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- Given N(T) = n, the n arrival times S_1, \ldots, S_n have the same distribution as n independent RVs from Unif(0, T) that are sorted,

Introduction

2 Data Collection

- 3 Identifying Distribution
 ▶ Physical Basis of Distributions
 ▶ Histogram and Bar Chart
- 4 Distribution Fitting
 ▶ Method of Moments
 ▶ A Simple Variation of MoM
 ▶ Maximum Likelihood Estimation

5 Goodness of Fit

- ► Graphical Methods
- Statistical Tests
- Remarks

6 An Illustrative Example



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• Suppose we want to build a statistical model for the life time (i.e., time to failure) of a electronic component at 1.5 times the nominal voltage.



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Data Collection.

• Perform life tests on a random sample (n = 50) of electronic components and record their lifetime, in days:

79.919	3.081	0.062	1.961	5.845
3.027	6.505	0.021	0.013	0.123
6.769	59.899	1.192	34.760	5.009
18.387	0.141	43.565	24.420	0.433
144.695	2.663	17.967	0.091	9.003
0.941	0.878	3.371	2.157	7.579
0.624	5.380	3.148	7.078	23.960
0.590	1.928	0.300	0.002	0.543
7.004	31.764	1.005	1.147	0.219
3.217	14.382	1.008	2.336	4.562



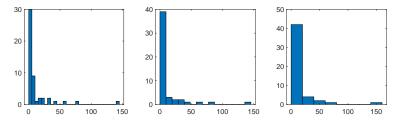
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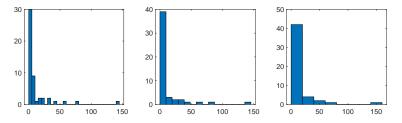
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• We decide to first try exponential distribution family $Exp(\lambda)$.

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3 Distribution Fitting.

- Recall Example 2, MoM (or its variation) and MLE yield the same estimator for λ , which is $\hat{\lambda} = \frac{n}{X_1 + \dots + X_n}$.
- Plug the data in, and the estimate of λ is 0.084.

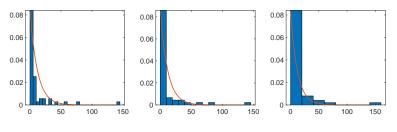


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Goodness of Fit.

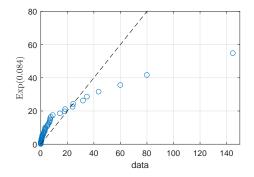
• Scaled histogram vs. pdf of Exp(0.084).





4 Goodness of Fit.

• Q-Q plot.





- Goodness of Fit.
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Class Interval	Observed Frequency O _i	Expected Frequency E_i	$\frac{(O_i-E_i)^2}{E_i}$
[0, 1.590)	19	6.25	26.01
[1.590, 3.425)	10	6.25	2.25
[3.425, 5.595)	3	6.25	0.81
[5.595, 8.252)	6	6.25	0.01
[8.252, 11.677)	1	6.25	4.41
[11.677, 16.503)	1	6.25	4.41
[16.503, 24.755)	4	6.25	0.81
[24.755, ∞)	6	6.25	0.01
	50	50	39.6

Choose intervals (make E_i equal).



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Choose intervals (make E_i equal).

Number of intervals is k = 8. Compute test statistic $r = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i} = 39.6$.



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Number of intervals is k = 8. Compute test statistic $r = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i} = 39.6$. Note that $R \sim \chi^2_{k-s-1}$ distribution $= \chi^2_6$ distribution. So, *p*-value $= \mathbb{P}(R \ge r) = \mathbb{P}(R \ge 39.6) = 5 \times 10^{-7}$.



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• Chi-square test (H_0 : The data come from Exp(0.084)). Number of estimated parameters is s = 1.

Class Interval	Observed Frequency O _i	Expected Frequency E _i	$\frac{(O_i - E_i)^2}{E_i}$
[0, 1.590)	19	6.25	26.01
[1.590, 3.425)	10	6.25	2.25
[3.425, 5.595)	3	6.25	0.81
[5.595, 8.252)	6	6.25	0.01
[8.252, 11.677)	1	6.25	4.41
[11.677, 16.503)	1	6.25	4.41
[16.503, 24.755)	4	6.25	0.81
[24.755, ∞)	6	6.25	0.01
	50	50	39.6

Choose intervals (make E_i equal).

Number of intervals is k = 8. Compute test statistic $r = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i} = 39.6$. Note that $R \sim \chi^2_{k-s-1}$ distribution $= \chi^2_6$ distribution. So, *p*-value $= \mathbb{P}(R \ge r) = \mathbb{P}(R \ge 39.6) = 5 \times 10^{-7}$. Hence, at almost any practical level of significance, e.g., $\alpha = 0.05, \ \alpha = 0.01$, we will reject H_0 .