An open-sourced comprehensive Monte-Carlo-aided educational toolkit for statistics

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Summary

This paper introduces a Monte Carlo-based educational toolkit for probability and statistics-related courses. We have published it as an open-sourced project to benefit a broad range of peer researchers and educators. The toolkit provides an empirical way to solve complex probability problems. It can intuitively illustrate the specific distribution that a particular experiment or test statistic follows. It contains three modules. (1) The "experiments" module provides simulations for classical numeric or probability problems, e.g., Buffon's needle puzzle and the locker problem. (2) The "distributions" module uses simulations to generate common distributions, e.g., Benford, Poisson, and Zipf. (3) The "samplings" module illustrates the sampling distributions of hypothesis test statistics, e.g., the chi-squared statistic in Pearson's GOF test and the F statistic in ANOVA. This toolkit provides an empirical and intuitive alternative to formal math proofs for complex probability problems. Until now, it has been used in higher education courses for three years and was positively reviewed by both peer educators and undergraduate students. In the next development milestone, we will (1) extend API to support more experiments and sampling distributions, and (2) provide a dedicated cross-platform desktop or web GUI (based on tk-inter or Flask) to make the toolkit more user-friendly.

Statement of need

The Monte Carlo (MC) method is a powerful computer-simulated technique to study probability problems and complex systems. Based on LLN (Law of Large Numbers), MC can provide a convincing approximation for theoretical solutions, i.e., the observed frequency will asymptotically approach its theoretical probability($f \rightarrow p$). The early idea of using LLN can be traced back to the 18th century when French scientist Buffon proposed his famous needle problem. Since the 20th century, digital computers have made the MC method much more helpful and popular. MC has been used in many theoretical research and engineering domains, e.g., optics (Sharma et al., 2019; Zou et al., 2017), radiation research (Chiriotti et al., 2017), nuclear physics (Guifeng et al., 2019), medicine (Teles et al., 2016), materials science (Fazio et al., 2018; Zuo et al., 2021), quality management (Bedelean, 2018), supply chain (Elsayed et al., 2022), software engineering (Horcas et al., 2021), etc.

As higher education teachers, we found the MC method a powerful and promising didactic tool. This paper introduces an MC-aided educational toolkit for probability and statistics-related courses and studies. The project was initiated in 2019 and is now published as an open-source Python package(mc-tk). Highlights of the toolkit functionality include: (1) It provides an intuitive and versatile complement to theoretical math proofs. For example, it may be challenging to prove why the statistic used in a particular test follows a specific sampling

distribution. Meanwhile, we can run MC simulations and plot the frequency histogram of the statistic to verify whether it is close to the theoretical distribution. This provides an easier and more intuitive alternative. (2) It includes historical and real-life experiments. For example, the package offers MC experiments for Buffon's needle problem, Galton board, the locker puzzle, Benford's law, etc. The rich case library has proved to be very helpful in statistical education. (3) Side-by-side visual comparison between empirical and theoretical distributions/results. (4) Flexible and tunable. The package follows the OOP (object-oriented programming) design allowing users to set many experiment-specific parameters in the derivative classes. This helps study asymptotic distributions or limits. For example, the locker puzzle allows users to increase the prisoner number and test its limit (when $n \to \infty$). In the survival game experiment, users can set the per-round survival rate p to a very low value to get the asymptotic exponential distribution. The CLT (central limit theorem) class allows users to change the underlying distribution (e.g., uniform, Bernoulli, exponential) and the sample size to verify the theorem.

Until now, the toolkit has been used in the probability and statistics course and was well received by teachers and students. The following manuscript will provide details on the software functionality.

Overview

The following table provides an overview of the toolkit's API (application programming interface). The toolkit is organized into three modules. The first module offers simulations for solving classical numeric or probability problems, e.g., Buffon's needle problem, the locker puzzle, etc. The second module provides simulated experiments to generate simulations for commonly used distributions, e.g., a sudden death game that produces the exponential distribution and the paper clip experiment that generates the Zipf distribution. For each MC experiment, both the observed histogram and theoretical density function are provided for comparison. The third module illustrates the sampling distribution of popular hypothesis test statistics. e.g., the χ^2 statistic in Pearson's chi-squared GOF test, ANOVA's F statistic, etc.

Module	Class	Description
mc.experiments	Pi	Perform Buffon's needle experiment to estimate π.
	Parcel	Simulate a bi-directional parcel passing game.
	Dices	Estimate the probabilities of various dice combinations.
	Prisoners	The famous locker puzzle(100-prisoner quiz). The asymptotic_analysis() function will demonstrate that the survival chance limit is $1 - \ln(2)$ when *n* approaches $+\infty$.
	Galton_Board	Use the classic Galton board experiment to produce a binomial distribution.
	Paper_Clips	Use the paper clip experiment to create a Zipf distribution.
	Sudden_Death	This class simulates a sudden death game to make the exponential distribution.
mc.distributions	Poisson	This class will demonstrate that Poisson is a limit distribution of *b(n,p)* when *n* is large and *p* is small.
	Benford	Verify Benford's law using real-life datasets, including the stock market data, international trade data, and the Fibonacci series.

Module	Class	Description
mc.experiments	Clt	Using various underlying distributions to verify the central limit theorem. This class provides the following underlying distributions: "uniform" - a uniform distribution U(-1,1); "expon" - an exponential distribution Expon(1); "poisson" - Poisson distribution $\pi(1)$; "coin" - Bernoulli distribution with $p = 0.5$; "tampered_coin" - PMF:{0:0.2,1:0.8}, i.e., head more likely than tail; "dice" - PMF:{1:1/6,2:1/6,3:1/6,4:1/6,5:1/6,6:1/6}; "tampered_dice" - PMF: {1:0.1,2:0.1,3:0.1,4:0.1,5:0.1,6:0.5}, i.e., 6 is more likely.
	T_Test	This class constructs an r.v. (random variable) following the t distribution.
	Chisq_Gof_Test	Verify the statistic used in Pearson's Chi-Square Goodness-of-Fit test follows the χ^2 distribution.
	Fk_Test	Verify the Fligner-Killeen Test statistic(FK) follows the χ^2 distribution.
	Bartlett_Test	Verify that Bartlett's test statistic follows the χ^2 distribution.
	Anova	Verify the statistic of ANOVA follows the F distribution.
	Kw_Test	Verify the Kruskal-Wallis test statistic (H) is a χ^2 r.v.
	Sign_Test	For the sign test (medium test), verify its N- and N+ statistics follow b(n,1/2).
	Cochrane_Q_Test	Verify the statistic T in the Cochrane-Q test follows the χ^2 distribution.
	Median_Test	Verify the statistic MT in the Median test follows the χ^2 distribution.
	Hotelling_T2_Test	Verify the T^2 statistic from two multivariate Gaussian populations follows the Hotelling's T^2 distribution.

Illustrative Examples

This section will showcase some classes provided by the software.

Classes for Classical MC Experiments

The "experiments" module provides MC simulation for classical probability problems, such as Buffon's needle experiment, the bi-directional game, the dice game, the locker puzzle, the Galton board experiment, the survival game, and the paper clip experiment. Here, we will demonstrate the locker puzzle.

The Locker Puzzle

The "hundred-prisoner puzzle" or "the locker puzzle" was first addressed by Danish scientist Peter Bro Miltersen (Gál & Miltersen, 2007; Warshauer & Curtin, 2006). In this puzzle, there are 100 lockers containing No.1 to No.100. In each round, one prisoner will open 50 lockers. The game will continue if his/her number is found inside any of the opened lockers. Otherwise, the game is over, and all prisoners will be executed. The prisoners cannot communicate with each other during the game. What are the best strategy and the highest survival probability?

With no strategy (becomes a repeated Bernoulli experiment), the survival probability will be $(\frac{1}{2})^{100}$, which is virtually 0. According to the authors, the best strategy is the "circular chain," i.e., the prisoner first opens the locker of their number then opens the locker whose number is inside the last locker. With this strategy, the survival probability equals the probability of

87 creating circular chains no longer than 50. This probability is: $p = 1 - \frac{1}{100!} \sum_{l=51}^{100} \left(\frac{1}{l} \times 100! \right) =$

88 $1 - \sum_{l=51}^{100} \frac{1}{l} = 1 - 0.688 = 0.312$. Furthermore, if we increase the total prisoner number, we

89 can prove that this probability will converge to $1 - ln2$ (0.307).

90 The Prisoners class simulates this experiment, and users can get the survival chance plot
91 against different prisoner numbers(Figure 1).

```
Prisoners(n=100,N=2000).run()
    # n : the number of prisoners.
    # N : how many MC experiments to run.
    result : p = 0.3116

Prisoners.asymptotic_analysis(ns=[250,500,750,1000,1250,1500,1750,2000],
                              repeat=10, SD=1,N = 1000)
    # ns : prisoner numbers to be tested.
    # repeat : repeat multiple times to calculate the SD (standard deviation).
    # SD : how many SD (standard deviation) to show in the error bar chart.
    # N : the number of MC experiments performed for each n.
```
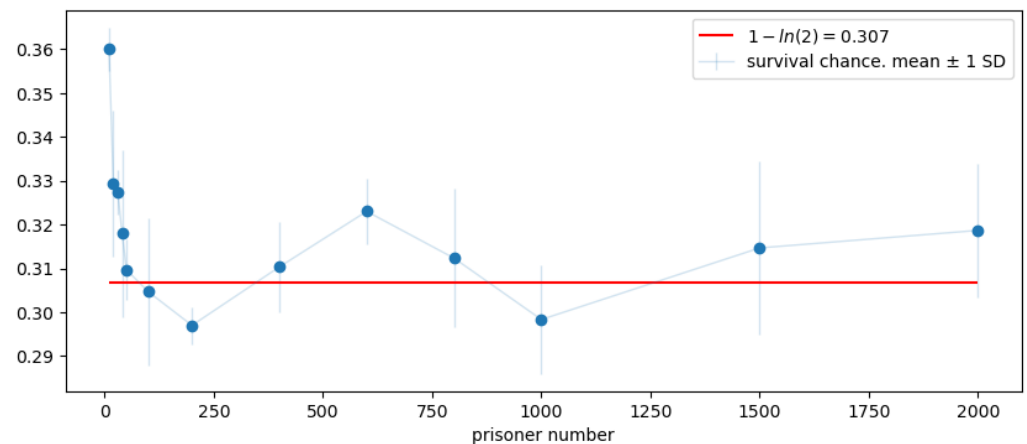

Figure 1: Survival chance against prisoner number (n). When n is large enough, this chance will approach $1 - ln2$.

Classes for Common Distributions

93 The "distributions" module provides MC experiments to generate specific distributions (e.g.,
94 Poisson distribution and Benford distribution) and compare the observed MC results with the
95 PDF/PMF of the theoretical distribution side-by-side. Here, we will demonstrate the Benford
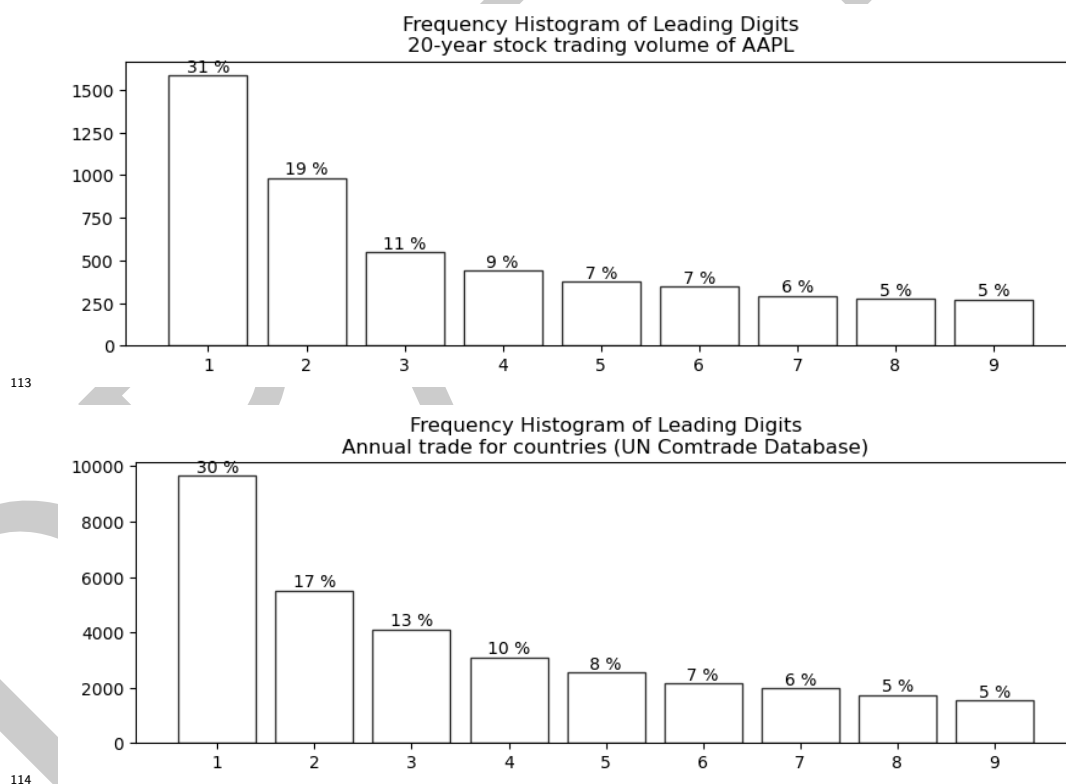96 distribution.

Benford Distribution

98 The Benford law, a.k.a. the Newcomb-Benford law or the first-digit law, describes the PMF of
99 leading digits in many real-life financial and social data (Cerioli et al., 2019). In essence, the
100 natural or social processes that follow the power laws (very common) often demonstrate this
101 distribution. Financial audits often use it to check faked or manipulated data. The Benford
102 PMF is as follows.

leading digit	1	2	3	4	5	6	7	8	9
p	30.1%	17.6%	12.5%	9.7%	7.9%	6.7%	5.8%	5.1%	4.6%

The Benford class provides three examples to verify the Benford law (Figure 2). The first example uses the 20-year trading volume data of AAPL (Apple Inc.). The second example uses the United Nations' international trading data. The last example uses the Fibonacci series.

```
Benford(data='stock',N=1000).run()
    # data : data set to be used.
    #  'stock' - use 20-year stock trading volume data of Apple Inc. (AAPL)
    #  'trade' - use annual trade data from various countries.
    #           https://comtrade.un.org/data/mbs
    #  'fibonacci' - use the top-N fibonacci series.
    # N : how many MC experiments to run.
```

According to Figure 2, all the examples fit well against the theoretical Benford distribution. We can use the Fibonacci series to explain the Benford law intuitively. The Fibonacci sequence represents how a population (e.g., rabbits) grows in a resource-unlimited environment. At a steady breeding speed, it takes much longer time to increase the population from 100 to 200 (need to increase by 100) than from 90 to 100 (only need to increase by 10). It also takes longer time than 200 to 300 because the population has grown bigger in the latter case. Therefore, it stays longer at smaller leading digits than the bigger ones.
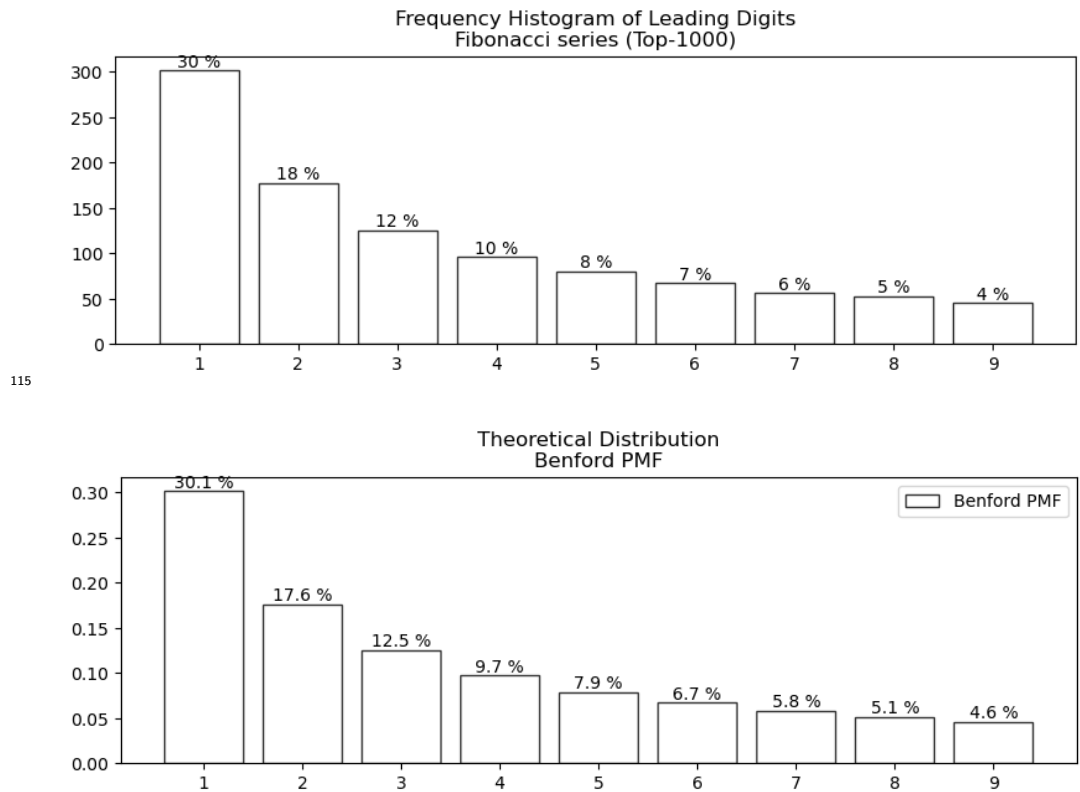
Figure 2: Verify the Benford law using two real-life datasets and the Fibonacci series.

Classes for Sampling Distributions

The "samplings" module provides classes to verify the sampling of common hypothesis testing statistics, including the student's t test, Pearson's Chi-Squared Goodness-of-Fit(GOF) test, ANOVA(analysis of variance) test, the Kruskal-Wallis test, the Fligner-Killeen test, Bartlett's test, the sign test, the Cochran's Q test and the Hotelling's T^2 test. It also contains a class to demonstrate the Central Limit Theorem (CLT). In each class, we construct the test statistics and compare them with the theoretical sampling distributions. Here we present GOF test, ANOVA test and the Hotelling's T^2 test as examples.

Pearson's Chi-Square Goodness-of-Fit Test

Pearson's Chi-Square Goodness-of-Fit (GOF) test uses the following statistic.

$$\chi^2 = \sum_{j=1}^{k} \frac{(f_j - np_j)^2}{np_j} \sim \chi^2(k-1)$$

When n is large enough ($n \geq 50$), χ^2 will follow the $\chi^2(k-1)$ distribution. As Pearson's chi-square GOF test is non-parametric, there is no restriction on the population distribution. The Chisq_Gof_Test class provides two population distributions. (1) The first is the Galton board (use the binominal population, Figure 3). (2) The second is the dice game (use the uniform PMF, Figure 4). In both cases, the statistic histogram from the MC experiment is very close to the theoretical $\chi^2(k-1)$ distribution.

```
Chisq_Gof_Stat(underlying_dist='binom',k=8,sample_size=100,N=10000).run()
        # underlying_dist : what kind of population dist to use. By default,
        #                    we use binom, i.e., the Galton board.
```

```
#     'binom'/'galton' – the population is binom.
#     'dice' – 6 * 1/6.
# k : classes in the PMF.
# N : how many MC experiments to run.
```
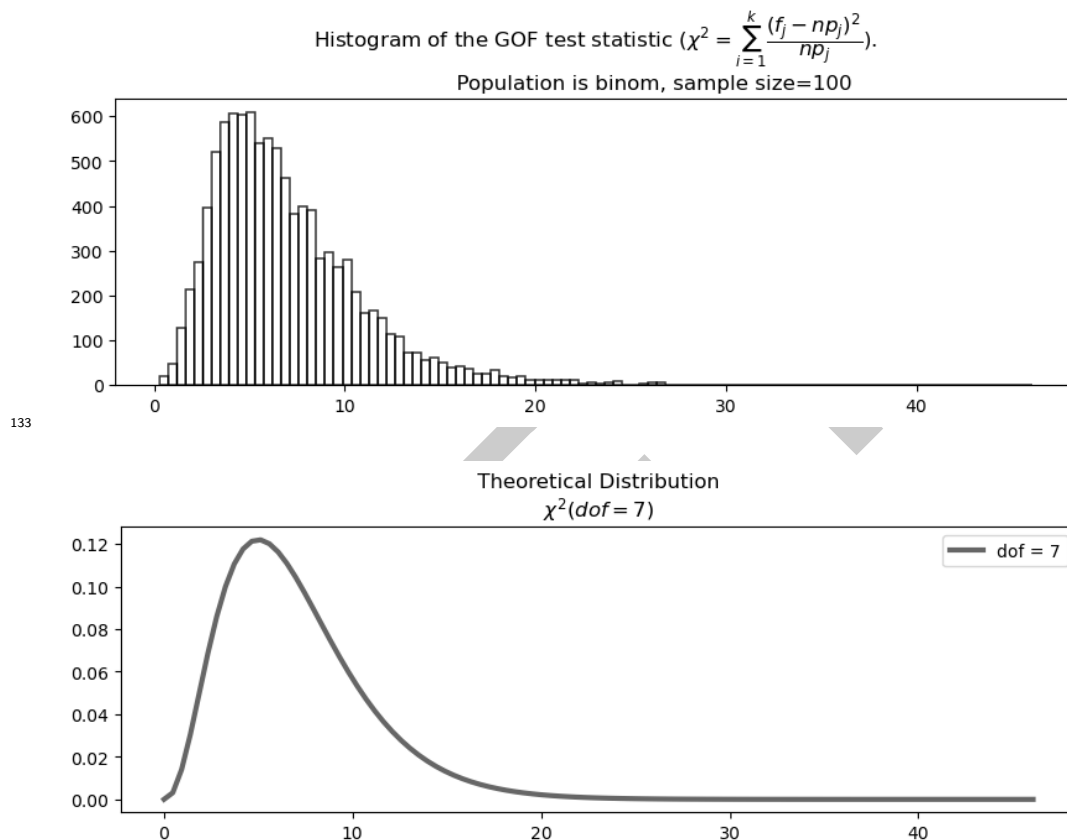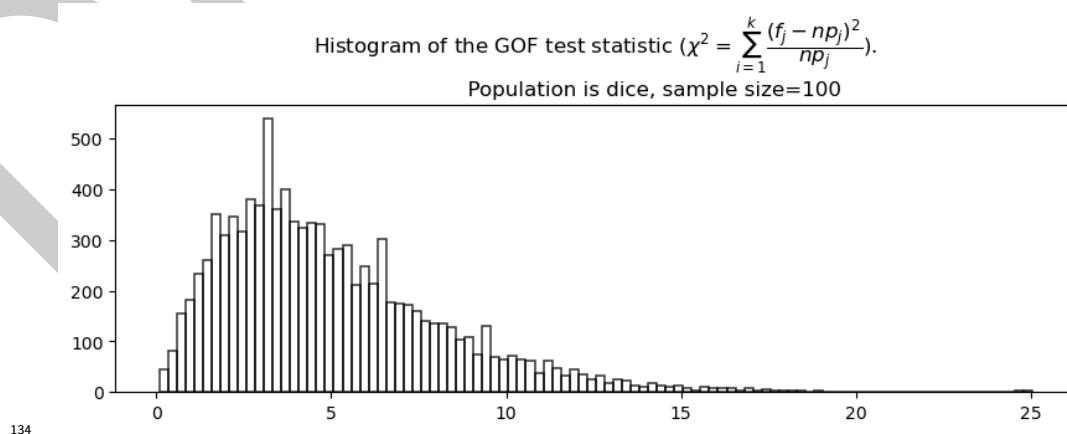
Histogram of the GOF test statistic ($\chi^2 = \sum_{i=1}^{k} \frac{(f_j - np_j)^2}{np_j}$).
Population is binom, sample size=100

Theoretical Distribution
$\chi^2(dof = 7)$

Figure 3: Use the Galton Board game to verify the statistic in Pearson's chi-square GOF test.

Histogram of the GOF test statistic ($\chi^2 = \sum_{i=1}^{k} \frac{(f_j - np_j)^2}{np_j}$).
Population is dice, sample size=100

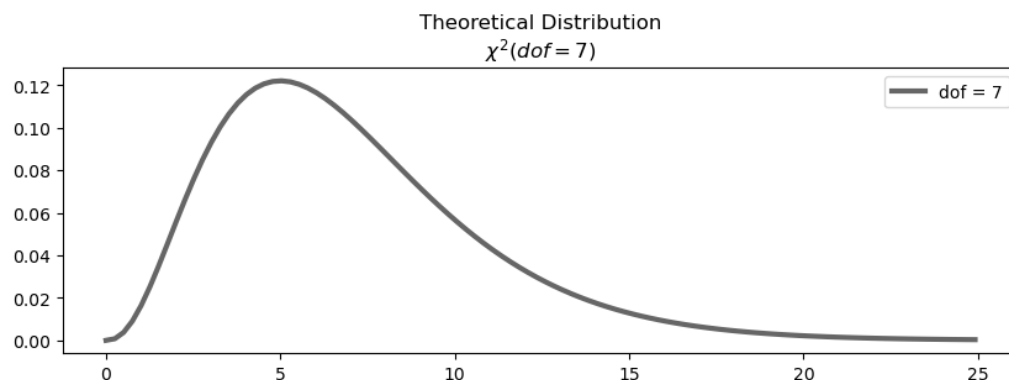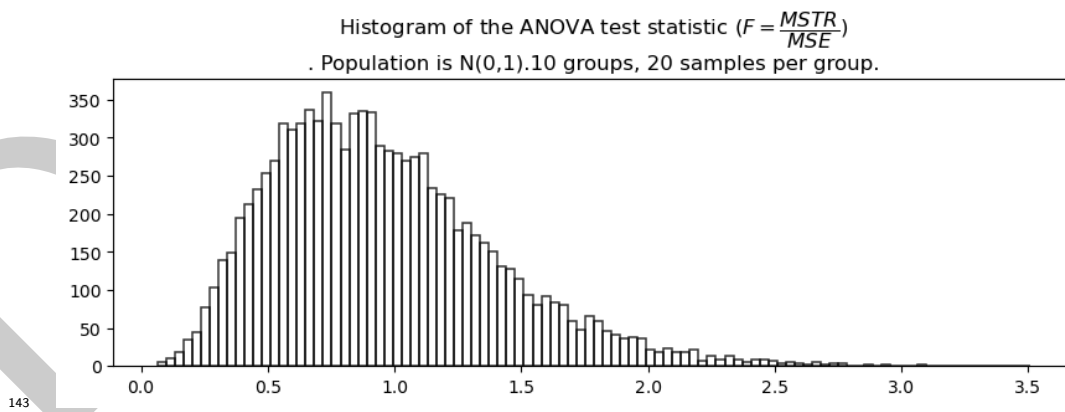Theoretical Distribution
$\chi^2(dof = 7)$

Figure 4: Use the dice game to verify the statistic in Pearson's chi-square GOF test.

ANOVA

ANOVA (analysis of variance) is a parametric mean test for multiple groups. Its null hypothesis H_0 is: $\mu_1 = \mu_2 = ... = \mu_k$. ANOVA constructs the test statistic by splitting the total variance into treatment (between-class difference, MSTR) and noise (within-class variance, MSE). When H_0 is true, the ratio of MSTR and MSE will follow the F distribution, i.e., $F = \frac{MSTR}{MSE} \sim F(k-1, n-1)$.

The Anova class will calculate the histogram of the F statistic observed from a multi-group normal sample (Figure 5).

```
Anova(k=10,n=10,N=10000).run()
    # k : the number of classes/groups.
    # n : the sample size in each class/group. The total sample size is [k]*[n].
    # N : how many MC experiments to run.
```
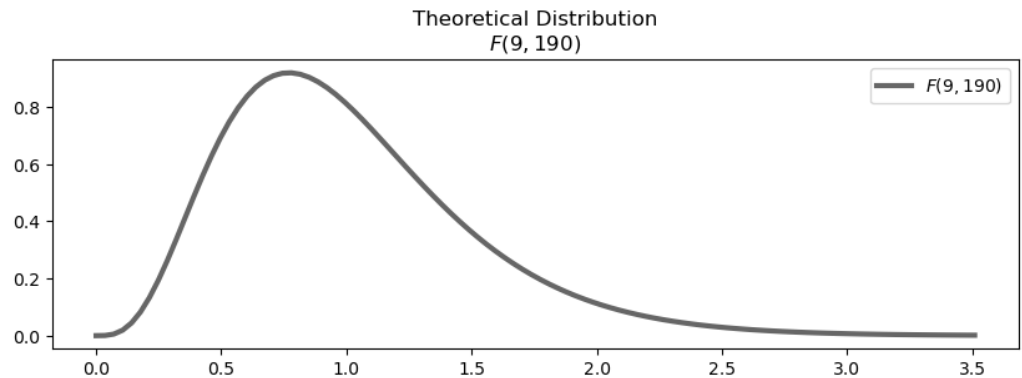
Histogram of the ANOVA test statistic ($F = \frac{MSTR}{MSE}$)
. Population is N(0,1).10 groups, 20 samples per group.

Theoretical Distribution
$F(9, 190)$

Figure 5: Use MC to verify the ANOVA test statistic follows the F distribution.
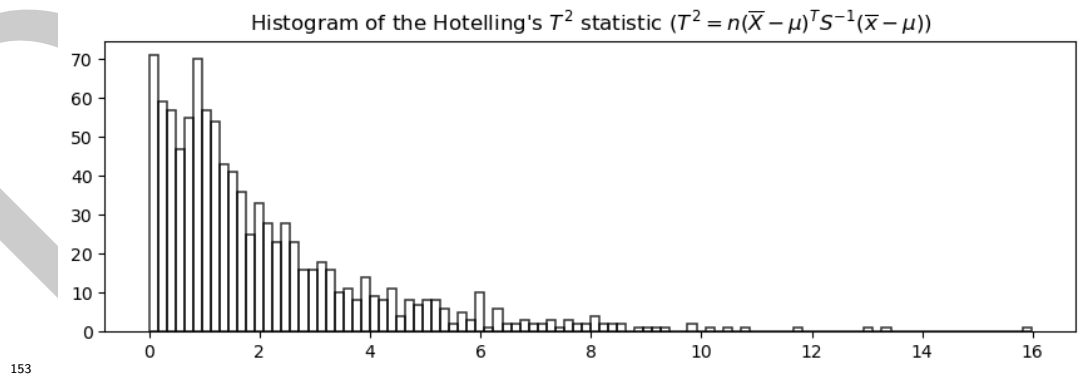
Hotelling's T^2 Test

The Hotelling's T^2 test compares the mean of two multivariate populations. Suppose we have two groups of samples from $N(\mu_1, \sum)$ and $N(\mu_2, \sum)$. They share the same covariance matrix $\sum$. The null hypothesis is $H_0 : \mu_1 = \mu_2$ and the test statistic is:

$$T^2 = n(\overline{x} - \mu)^T S^{-1}(\overline{x} - \mu)$$

$S = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \overline{x})(x_i - \overline{x})^T$ is the grand covariance matrix.

If the dimensionality $k = 1$, Hotelling's T^2 degenerates into the t distribution. When $k \geq 2$, it is a multivariate generalization of the t distribution. The Hotelling_T2_Test class verifies the T^2 sampling distribution (Figure 6).

```
Hotelling_T2_Test(n=50,k=2,N=1000).run()
    # n : the sample size in each class.
    # k : data dimension.
    # N : how many MC experiments to run.
```
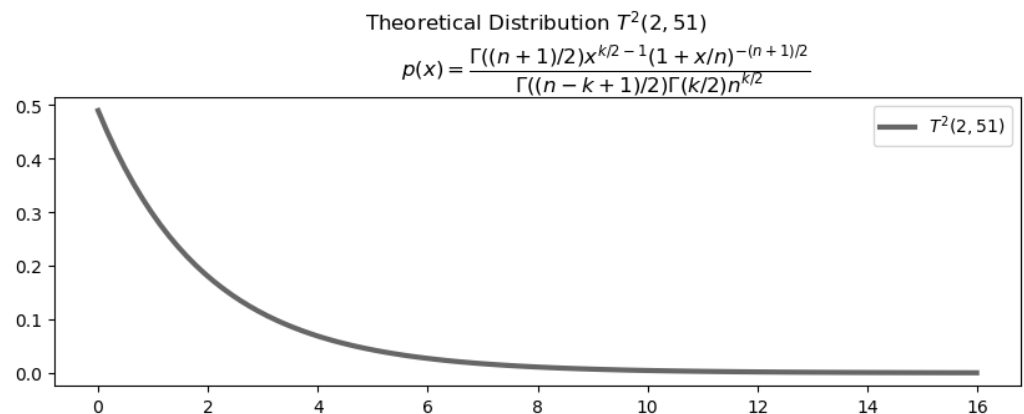

Histogram of the Hotelling's T^2 statistic ($T^2 = n(\overline{X} - \mu)^T S^{-1}(\overline{x} - \mu)$)

Theoretical Distribution $T^2(2, 51)$

$$p(x) = \frac{\Gamma((n+1)/2)x^{k/2-1}(1+x/n)^{-(n+1)/2}}{\Gamma((n-k+1)/2)\Gamma(k/2)n^{k/2}}$$

Figure 6: The T^2 statistic of Hotelling's test.

Acknowledgment

Data Availability Statement

The source code is hosted on GitHub: https://github.com/zhangys11/mc.

License: Apache License 2.0

The CodeOcean reproducible Capsule is published at: https://doi.org/10.24433/CO.4921884.v2.

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