Goodness of Fit hypothesis testing:

Pearson's chi-square test

Did you know that M&M's® Milk Chocolate Candies are supposed to come in the following percentages: 24% blue, 20% orange, 16% green, 14% yellow, 13% red, 13% brown?

http://www.scientificameriken.com/candy5.asp

"To our surprise M&Ms met our demand to review their procedures in determining candy ratios. It is, however, noted that the figures presented in their email differ from the information provided from their website (http://us.mms.com/us/about/products/milkchocolate/). An email was sent back informing them of this fact. To which M&Ms corrected themselves with one last email:

In response to your email regarding M&M'S CHOCOLATE CANDIES

Thank you for your email.
On average, our new mix of colors for M&M'S® Chocolate Candies is:

M&M'S® Milk Chocolate: 24% blue, 20% orange, 16% green, 14% yellow, 13% red, 13% brown.

M&M'S® Peanut: 23% blue, 23% orange, 15% green, 15% yellow, 12% red, 12% brown.

M&M'S® Kids MINIS®: 25% blue, 25% orange, 12% green, 13% yellow, 12% red, 13% brown.

M&M'S® Crispy: 17% blue, 16% orange, 16% green, 17% yellow, 17% red, 17% brown.

M&M'S® Peanut Butter and Almond: 20% blue, 20% orange, 20% green, 20% yellow, 10% red, 10% brown.

Have a great day!

Your Friends at Masterfoods USA
A Division of Mars, Incorporated

How to accept or reject the null hypothesis that these probabilities are correct from a finite sample?

Pearson chi^2 Goodness of Fit Test

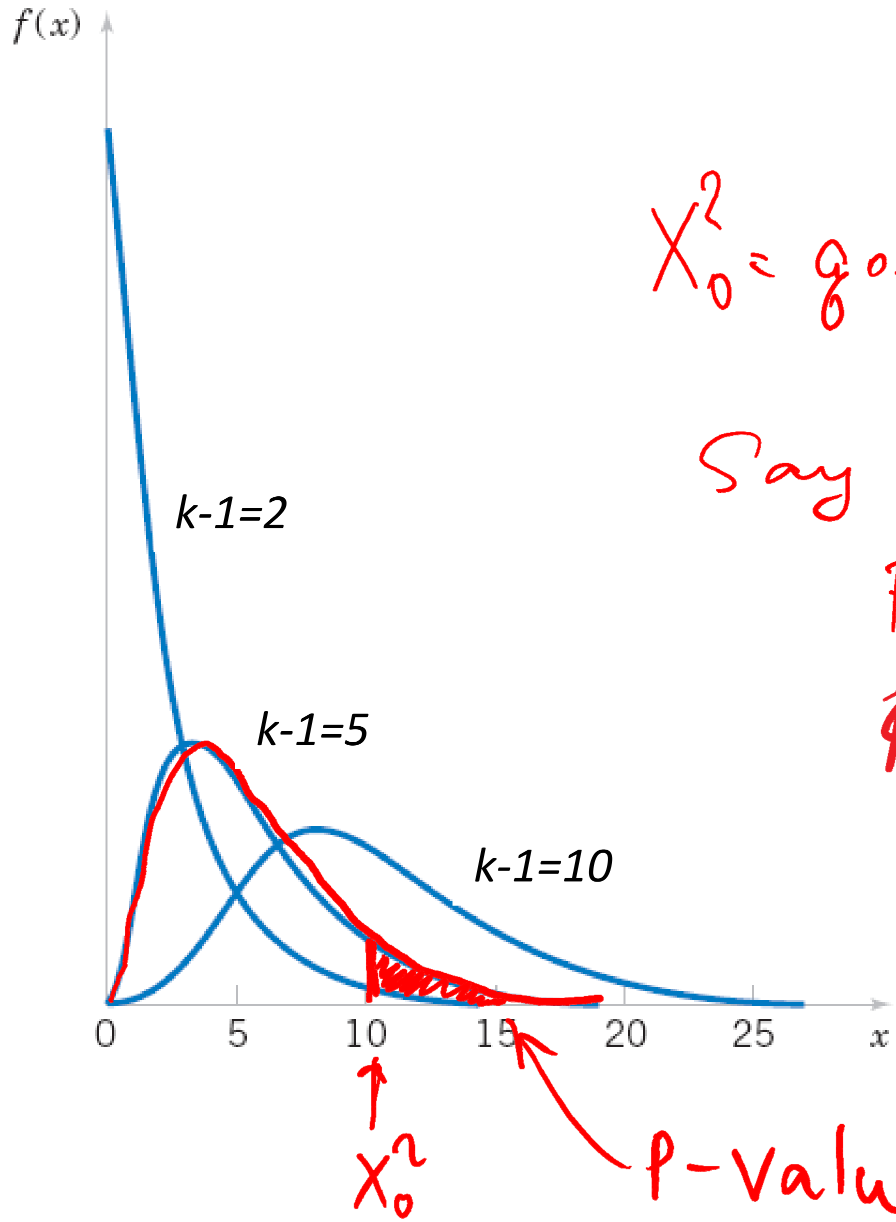
- Assume there is a sample of size *n* from a population with *k* classes (e.g. 6 M&M colors)
- Null hypothesis H_0: class *i* has frequency f_i in the population
- Alternative hypothesis H_1: some population frequencies are inconsistent with f_i
- Let O_i be the observed number of sample elements in the *i*th class and $E_i = n\, f_i$ be the expected number of sample elements in the *i*th class.
- Group any bin with E_i <3 with
  a) if numerical value of i is important, group it with its neighbor (k=i-1 or k=i+1) which has the smallest E_k until E_{group} >=3;
  b) If numerical value of i is irrelevant, group together all E_i <3 bins until E_{group} >=3
- The test statistic is

$$X_0^2 = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i} \qquad (9\text{-}47)$$

P-value is calculated based on the chi-square distribution with k-1 degrees of freedom:

P-value = Prob(H_0 is correct) =1-CDF_chi-squared(X_0^2, *k-1*)

chi[2] Goodness of Fit Test
is a ***one-sided*** hypothesis



$$X_0^2 = gof = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i}$$

Say $X_0^2 = 10$

For M&M

$k = 6 \rightarrow k-1 = 5$

p-value that null hypothesis is correct

M&M group exercise

- DO NOT EAT CANDY BEFORE COUNTING IS FINISHED! THEN, **PLEASE, DO**.
- We will be testing three null hypotheses one after another:
  - M&M official data: 24% blue, 20% orange, 16% green, 14% yellow, 13% red, 13% brown
  - Website (fan collected) data from http://joshmadison.com/2007/12/02/mms-color-distribution-analysis: 18.36% blue, 20.76% orange, 18.44% green, 14.08% yellow, 14.20% red, 14.16% brown
  - Uniform distribution: 1/6~16.67% of each candy color
- You will estimate P-values for each one of these null hypotheses
- Hints: O_i – is the observed # of candies of color i; calculate the expected # E_i=(# candies in your sample)*f_i

Use **1-chi2cdf(X0squared, 5)** for P-value

$$X_0^2 = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i}$$

M&M matlab exercise

- **observed=mm_table(group,:); group % use when analyzing one group**
- **f_mm=[0.24,0.2,0.16, 0.14, 0.13,0.13];**
- **f_u=1./6.*ones(1,6);**
- **f_website=[18,21,18,14,14,14,14];**
- **f_website=f_website./sum(f_website);**
- **%p_website=[0.1836, 0.2076, 0.1844, 0.1408, 0.1420, 0.1416]**
- **%p_u=[0.1500, 0.2200, 0.2100, 0.1200, 0.1600, 0.1500];**
- **n=sum(observed)**
- **expected_u=n.*f_u;**
- **expected_mm=n.*f_mm;**
- **expected_website=n.*f_website;**
- **gf_mm=0; gf_u=0; gf_website=0;**
- **for m=1:6;**
- **gf_mm=gf_mm+(observed(m)...**
- **-expected_mm(m)).^2./expected_mm(m);**
- **gf_u=gf_u+(observed(m)-expected_u(m)).^2./expected_u(m);**
- **gf_website=gf_website+(observed(m)...**
- **-expected_website(m)).^2./expected_website(m);**
- **end;**
- **disp('goodness of fit of MM ='); disp(num2str(gf_mm));**
- **disp('p-value of MM ='); disp(num2str(1-chi2cdf(gf_mm,5))); disp(' ');**
- **disp('goodness of fit of website ='); disp(num2str(gf_website));**
- **disp('p-value of MM ='); disp(num2str(1-chi2cdf(gf_website,5))); disp(' ');**
- **disp('goodness of fit of uniform ='); disp(num2str(gf_u));**
- **disp('p-value of uniform='); disp(num2str(1-chi2cdf(gf_u,5)));**

Statistical tests of independence

How to **test the hypothesis** if multiple sample are drawn from the same population?

- Table: samples (Student groups) – rows, classes (M&M colors) – columns
- Test if color fractions are **independent** from group
- ***P(Group 1 and Color = green) = P(Group 1)*P(Color green)***
- Compute for all groups/colors 6*4=24 in our case

  $E_{green}(group\ 1) = n_{tot} * (group1/n_{tot}) * (green/n_{tot})$
- $\chi^2 = \sum_{groups\ \&\ colors}^{n_{tot}} \frac{(O_{color}(group) - E_{color}(group))^2}{E_{color}(group)}$
- # degrees of freedom=(colors-1)*(groups-1)

- M&M exercise Spring 2024
- Was the M&M box from Costco well mixed? Let's compare the first two groups' data

Title	Blue	Orang	Greer	Yellov	Red	Brow	Sampl	Origir
group 1	29	22	34	45	41	14	185	Costco
group 2	30	28	25	43	44	27	197	Costco
all Costco	59	50	59	88	85	41	382	
							0	
group 3	44	30	52	10	50	27	213	Schnucl
group 4	53	31	58	17	41	30	230	Schnucl
all Schnuc	97	61	110	27	91	57	443	

- Using $\chi^2 = \sum_{groups\ \&\ colors}^{24} \frac{(O_{color}(group) - E_{color}(group))^2}{E_{color}(group)}$

with # degrees of freedom (colors-1)*(groups-1)

Find P-value of null hypothesis H_0 that samples are independent from each other

Was the Costco box well mixed?

- `clear mm_table`
- `mm_table=mm_table_all(1:2,:);`
- `ngroups=2;`
- `ncolors=6;`
- `sumt=sum(sum(mm_table))`
- `sum_color=sum(mm_table, 1)`
- `sum_group=sum(mm_table, 2)`
- `mm_exp=kron(sum_group,sum_color)./sumt`
- `gof=sum(sum((mm_table-mm_exp).^2./mm_exp))`
- `P_value_gof=1-chi2cdf(gof, (ngroups-1)*(ncolors-1))`
- `%gof = 6.0121; P_value_gof = 0.3050`
- The null model that samples are independent is **not rejected → The Costco box was well mixed!**

Batch effect

Does color composition vary between Costco and Schnucks

- Costco: 59 50 59 88 85 41
- Schnucks: 97 61 110 27 91 57
- Test if they are significantly different from each other:
- Same statistical independence test: ngroups=2; ncolors=6;
- Results:

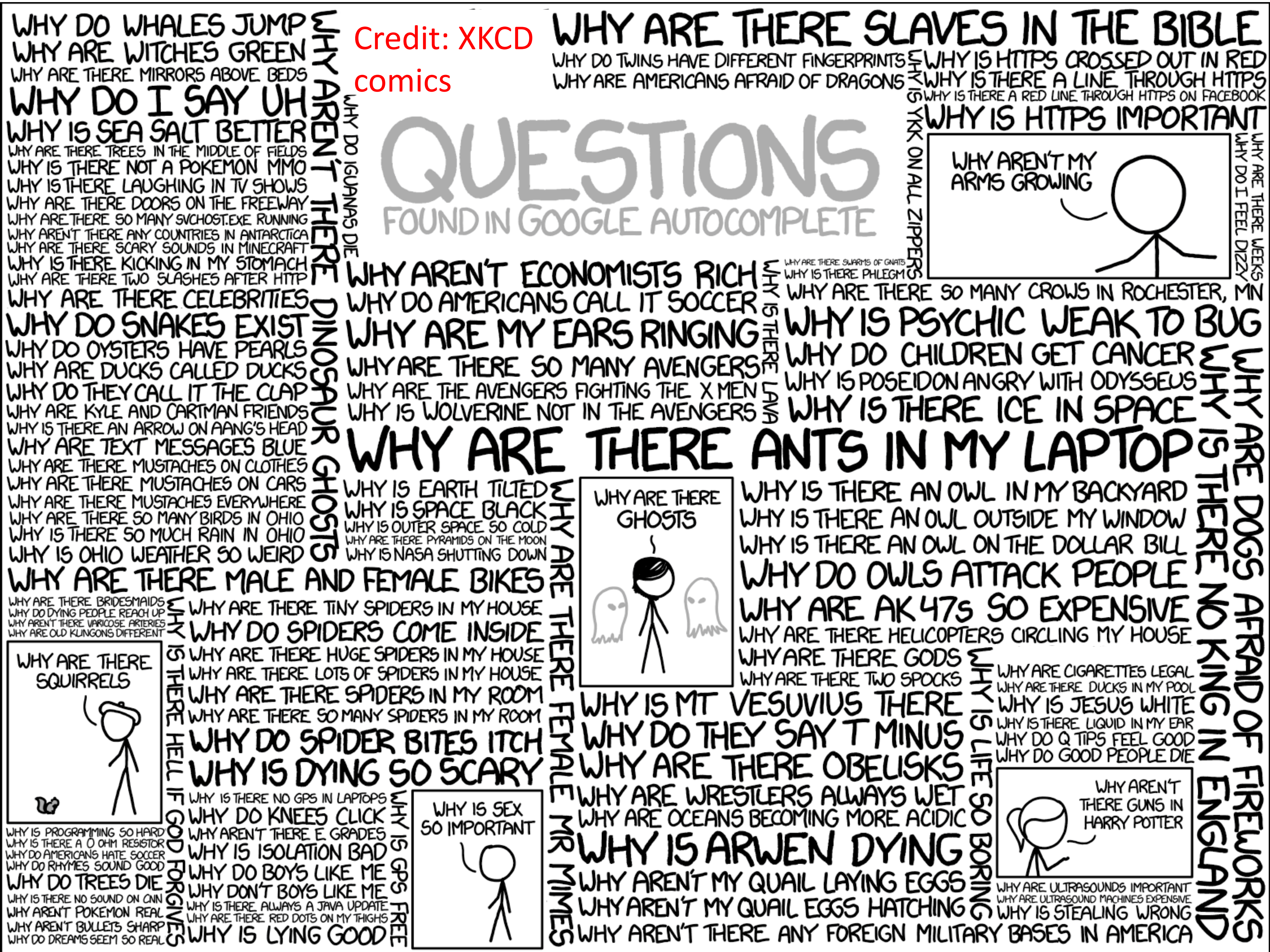
  Goodness of Fit = 56.7101

  P-value = 5.8028e-11
- Batch effect is highly statistically significant! Costco and Schnucks do nor represent the same population

Do Costco (groups 1 and 2) and Schnucks (groups 3 and 4) data come from the same population (factory?)

- `clear mm_table`
- `mm_table(1,:)=sum(mm_table_all(1:2,:));`
- `mm_table(2,:)=sum(mm_table_all(3:4,:));`
- `ngroups=2;`
- `ncolors=6;`
- `sumt=sum(sum(mm_table))`
- `sum_color=sum(mm_table, 1)`
- `sum_group=sum(mm_table, 2)`
- `mm_exp=kron(sum_group,sum_color)./sumt`
- `gof=sum(sum((mm_table-mm_exp).^2./mm_exp))`
- `P_value_gof=1-chi2cdf(gof, (ngroups-1)*(ncolors-1))`
- **`% Goodness of Fit = 56.7101`**
- **`% P-value = 5.8028e-11`**
- The null model that samples are independent is **rejected**
- **Costco and Schnucks get candy from different factories**

Credit: XKCD comics



Goodness of fit with a PDF defined by m parameters

- As before: k classes (e.g. M&M colors)
- Use parameter estimators to find the best parameters for the fit
  - Method of moments
  - MLE: method of maximum likelihood
- Use chi-squared distribution with k-1-m degrees of freedom
- As before: if E_i <3, group it together with another group and reduce k by 1

$$X_0^2 = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i} \qquad (9\text{-}47)$$

9-7 Testing for Goodness of Fit

Example 9-12

EXAMPLE 9-12 Printed Circuit Board Defects

Poisson Distribution

The number of defects in printed circuit boards is hypothesized to follow a Poisson distribution. A random sample of $n = 60$ printed boards has been collected, and the following number of defects observed.

Number of Defects	Observed Frequency
0	32
1	15
2	9
3	4

9-7 Testing for Goodness of Fit

Example 9-12

The mean of the assumed Poisson distribution in this example is unknown and must be estimated from the sample data. The estimate of the mean number of defects per board is the sample average, that is, $(32 \cdot 0 + 15 \cdot 1 + 9 \cdot 2 + 4 \cdot 3)/60 = 0.75$. From the Poisson distribution with parameter 0.75, we may compute p_i, the theoretical, hypothesized probability associated with the ith class interval. Since each class interval corresponds to a particular number of defects, we may find the p_i as follows:

$$p_1 = P(X = 0) = \frac{e^{-0.75}(0.75)^0}{0!} = 0.472$$

$$p_2 = P(X = 1) = \frac{e^{-0.75}(0.75)^1}{1!} = 0.354$$

$$p_3 = P(X = 2) = \frac{e^{-0.75}(0.75)^2}{2!} = 0.133$$

$$p_4 = P(X \geq 3) = 1 - (p_1 + p_2 + p_3) = 0.041$$

9-7 Testing for Goodness of Fit

Example 9-12

The expected frequencies are computed by multiplying the sample size $n = 60$ times the probabilities p_i. That is, $E_i = np_i$. The expected frequencies follow:

Number of Defects	Probability	Expected Frequency
0	0.472	28.32
1	0.354	21.24
2	0.133	7.98
3 (or more)	0.041	2.46

9-7 Testing for Goodness of Fit

Example 9-12

Since the expected frequency in the last cell is less than 3, we combine the last two cells:

Number of Defects	Observed Frequency	Expected Frequency
0	32	28.32
1	15	21.24
2 (or more)	13	10.44

The chi-square test statistic in Equation 9-47 will have $k - p - 1 = 3 - 1 - 1 = 1$ degree of freedom, because the mean of the Poisson distribution was estimated from the data.

9-7 Testing for Goodness of Fit

Example 9-12

The seven-step hypothesis-testing procedure may now be applied, using $\alpha = 0.05$, as follows:

1. **Parameter of interest:** The variable of interest is the form of the distribution of defects in printed circuit boards.
2. **Null hypothesis:** H_0: The form of the distribution of defects is Poisson.
3. **Alternative hypothesis:** H_1: The form of the distribution of defects is not Poisson.
4. **Test statistic:** The test statistic is

$$\chi_0^2 = \sum_{i=1}^{k} \frac{(o_i - E_i)^2}{E_i}$$

9-7 Testing for Goodness of Fit

Example 9-12

5. **Reject H_0 if:** Reject H_0 if the *P*-value is less than 0.05.

6. **Computations:**

$$\chi_0^2 = \frac{(32 - 28.32)^2}{28.32} + \frac{(15 - 21.24)^2}{21.24} + \frac{(13 - 10.44)^2}{10.44} = 2.94$$

7. **Conclusions:** We find from Appendix Table III that $\chi^2_{0.10,1} = 2.71$ and $\chi^2_{0.05,1} = 3.84$. Because $\chi_0^2 = 2.94$ lies between these values, we conclude that the *P*-value is between 0.05 and 0.10. Therefore, since the *P*-value exceeds 0.05 we are unable to reject the null hypothesis that the distribution of defects in printed circuit boards is Poisson. The exact *P*-value computed from Minitab is 0.0864.

Credit: XKCD comics