Statistical Theory for Data Science

STA2212H S LEC9101

Week 5

February 3 2026

Today

1. Recap: Formal theory of testing
2. Some examples
3. Goodness-of-fit tests
4. Diagnostic testing

Recap: Formal theory of testing

- null and alternative hypotheses: H_0 and H_1
- type 1 and type 2 error: probability of a wrong conclusion

  reject H_0 when true; do not reject H_0 when false
- rejection region, critical region, define a subset of the sample space
- either through an indicator (test) function or more usually as $\{\boldsymbol{x} : t(\boldsymbol{x}) > c\}$

  $t(\cdot), c$ to be determined
- for parametric model, with $H_0 : \theta \in \Theta_0, H_1 : \theta \in \Theta_1$ power function $\beta(\theta) = \mathrm{pr}_\theta(\boldsymbol{X} \in R)$
- size of the test $\alpha = \sup_{\Theta_0} \beta(\theta)$

- p-value = $\inf\{\alpha : T(\boldsymbol{X}) \in R\} = \sup_{\Theta_0} \mathrm{pr}_\theta\{T(\boldsymbol{X}) \geq T(\boldsymbol{x})\}$
- simple H_0 specifies distribution of $T(\boldsymbol{X})$; composite H_0 does not

Recap: Neyman-Pearson lemma

AoS Thm 10.30, MS Thm 7.2

- for testing simple H_0 against simple H_1
- test statistic

$$T = \frac{L(\theta_1; \boldsymbol{x})}{L(\theta_0; \boldsymbol{x})} = \frac{f(\boldsymbol{x}; \theta_1)}{f(\boldsymbol{x}; \theta_0)}$$

- critical region

$$\{\boldsymbol{x} : t(\boldsymbol{x}) \geq k\}$$

- Choose $k = k_\alpha$ to satisfy

$$\mathrm{pr}_{H_0}(T \geq k_\alpha) = \alpha$$

- This test is a most powerful test of H_0 against H_1 at level α

A neatly-typed proof (from SM 7.3)

Let R be the rejection region for the test based on $T = f_1(\boldsymbol{x})/f_0(\boldsymbol{x})$

$$R = \{\boldsymbol{x} : T(\boldsymbol{x}) \geq k_\alpha\}$$

Let R' be some other rejection region also of size α $\leq \alpha$

$$\alpha = \int_R f_0(\boldsymbol{x})d\boldsymbol{x} = \int_{R'} f_0(\boldsymbol{x})d\boldsymbol{x}$$

$$\int_{R-R'} f_0(\boldsymbol{x})d\boldsymbol{x} = \int_{R'-R} f_0(\boldsymbol{x})d\boldsymbol{x}$$

On LHS $f_1(\boldsymbol{x}) \geq k_\alpha f_0(\boldsymbol{x})$. $R - R' \subset R$

On RHS $f_1(\boldsymbol{x}) < k_\alpha f_0(\boldsymbol{x})$. $R' - R \subset R^c$

$$\int_{R-R'} f_1(\boldsymbol{x})d\boldsymbol{x} \geq \int_{R'-R} f_1(\boldsymbol{x})d\boldsymbol{x}$$

Add integral over intersection $R \cap R'$

A neatly-typed proof (from MS)

Let $\phi(\boldsymbol{x})$ be the test function for the test based on T.
Let $\psi(\boldsymbol{x})$ be any other function that maps $\boldsymbol{x}$ to $[0, 1]$.
If

$$\mathrm{E}_{H_0}\{\psi(\boldsymbol{X})\} \leq \mathrm{E}_{H_0}\{\phi(\boldsymbol{X})\} = \alpha$$

then it must follow that

$$\mathrm{E}_{H_1}\{\psi(\boldsymbol{X})\} \leq \mathrm{E}_{H_1}\{\phi(\boldsymbol{X})\}$$

Proof: $\forall\, \boldsymbol{x}$,

$$\psi(\boldsymbol{x})\{f_1(\boldsymbol{x}) - kf_0(\boldsymbol{x})\} \leq \phi(\boldsymbol{x})\{f_1(\boldsymbol{x}) - kf_0(\boldsymbol{x})\}$$

Integrate and re-arrange terms to get the result

Hypothesis tests and significance tests

- Hypothesis tests typically means:
  - H_0, H_1
  - critical/rejection region $R \subset \mathcal{X}$,
  - level α, power $1 - \beta$
  - conclusion: "reject H_0 at level α" or "do not reject H_0 at level α"
  - planning: maximize power for some relevant alternative

minimize type II error

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  - planning: maximize power for some relevant alternative — minimize type II error

- Significance tests typically means:
  - H_0,
  - test statistic T
  - observed value t^{obs},
  - p-value $p^{obs} = \Pr(T \geq t^{obs}; H_0)$
  - alternative hypothesis often only implicit — large T points to alternative

Choosing test statistics

1. Optimal choice – Neyman-Pearson lemma — Might be UMP
2. Pragmatic choice – pivotal quantity — exact or approximate
3. Pragmatic choice – nonparametric test statistics

(a) Need to know distribution of test statistic under H_0

(b) Test statistic should be large when H_0 is not true — in probability

(c) Test statistic should have maximum/good power to detect departures from H_0

Example 1: N-P lemma

- $f(\boldsymbol{x};\theta) = \prod_{i=1}^{n} h(x_i)\exp\{\theta s(x_i) - A(\theta)\}, \quad s, \theta \in \mathbb{R}, \qquad H_0 : \theta = \theta_0, H_1 : \theta = \theta_1 > \theta_0$
- MP test of H_0 vs H_1 has critical region

$$R = \{\boldsymbol{x} : \frac{f(\boldsymbol{x};\theta_1)}{f(\boldsymbol{x};\theta_0)} > k\}$$

- UMP against H_0': $R = \{s > c_\alpha\}$

Example 2: approximate pivotal quantities

- Wald test: AoS Def 10.3
- Score test:
- Likelihood ratio test: AoS §10.6

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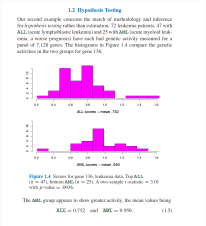
Example 2: two-sample t-test

AoS Ex.10.8

- model
- null and alternative hypothesis
- rejection region
- test statistics and critical value
- type I and type II error



1.2 Hypothesis Testing

Our second example concerns the search of methodology and inference for *hypothesis testing* rather than estimation: 72 leukemia patients, 47 with ALL (acute lymphoblastic leukemia) and 25 with AML (acute myeloid leukemia, a worse prognosis) have each had genetic activity measured for a panel of 7,128 genes. The histograms in Figure 1.4 compare the genetic activities in the two groups for gene 136.

Figure 1.4 Scores for gene 136, leukemia data. Top ALL ($n = 47$), bottom AML ($n = 25$). A two-sample t statistic $= 3.01$ with p-value $= .0026$.

The AML group appears to show greater activity, the mean values being

$$\text{ALL} = 0.752 \quad \text{and} \quad \text{AML} = 0.950. \tag{1.5}$$

```
library("tidyverse")
leukemia_big<- read.csv
       ("http://web.stanford.edu/~hastie/CASI_files/DATA/leukemia_big.csv")
leukemia_big[136,] %>% select(starts_with("ALL")) %>% as.numeric() -> all136
leukemia_big[136,] %>% select(starts_with("AML")) %>% as.numeric() -> aml136
t.test(all136,aml136, var.equal = TRUE)
##
Two Sample t-test

data:  all136 and aml136
t = -3.014, df = 70, p-value = 0.003589
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 -0.32817995 -0.06680742
sample estimates:
```

A word on the *t*-test

```
## Default S3 method:
t.test(x, y = NULL,
       alternative = c("two.sided", "less", "greater"),
       mu = 0, paired = FALSE, var.equal = FALSE,
       conf.level = 0.95, ...)

       > t.test(x= oneline[1,one], y= oneline[1,two], var.equal=T)
       t = -3.014, df = 70, p-value = 0.003589

       > t.test(x= oneline[1,one], y= oneline[1,two])
       t = -3.1323, df = 54.667, p-value = 0.002786

       > pt(-3.1323, df=54.667) #[1] 0.001392839
       > pt(-3.014, df=70)  # [1] 0.001794297
```

Example 3: Permutation test

EH 4.4, AoS 10.5

leukemia data (EH): $X_1, \ldots, X_{47}$; $Y_1, \ldots, Y_{25}$

AoS Ex. 10.20

```
oneline
          ALL    ALL.1     ALL.2     ALL.3     ALL.4     ALL.5     ALL.6     ALL.7
136 0.9186952 1.634002 0.4595867 0.6379664 0.3440379 0.8614784 0.5132176 0.9790902
        ALL.8     ALL.9    ALL.10    ALL.11  ALL.12    ALL.13    ALL.14    ALL.15   ALL.16
136 0.2105782 0.8016072 0.6006949 0.3614374 1.04632 0.9697635 0.4873159 0.4976364 1.101717
       ALL.17   ALL.18   ALL.19       AML     AML.1     AML.2     AML.3     AML.4     AML.5
136 0.8563937 0.661415 0.817711 0.7671718 0.9793741 1.425479 1.074389 0.9839282 0.9859271
        AML.6     AML.7    AML.8     AML.9   AML.10    AML.11    AML.12   AML.13    AML.20
136 0.3247027 0.7110302 1.09625 0.9675151 0.975123 0.7775957 0.9472205 1.261352 0.5679544
       ALL.21    ALL.22    ALL.23    ALL.24    ALL.25    ALL.26   ALL.27    ALL.28
136 0.8462901 0.8838616 0.7239931 0.7327029 0.7823618 0.5435396 0.832537 0.5527333
       ALL.29    ALL.30    ALL.31    ALL.32   ALL.33    ALL.34    ALL.35    ALL.36
136 0.7327029 0.5510955 0.8214005 0.6418498 0.720798 0.5830999 0.7657568 0.5262976
      ALL.37    ALL.38    ALL.39   ALL.40    ALL.41    ALL.42    ALL.43    ALL.44
136 1.466999 0.5445589 0.5725049 1.362768 0.8533535 0.8132982 0.8538596 0.5689876
       ALL.45   ALL.46    AML.14    AML.15   AML.16   AML.17    AML.18    AML.19   AML.20
136 0.6930355 1.067526 0.9677959 0.9338141 1.138926 1.161753 0.6242354 0.6590103 1.215186
       AML.21   AML.22   AML.23    AML.24
136 0.9340861 1.310376 0.771426 0.7556606
```

$H_0 : F_X = F_Y$ H_1 $T = T(\boldsymbol{X}, \boldsymbol{Y}) =$

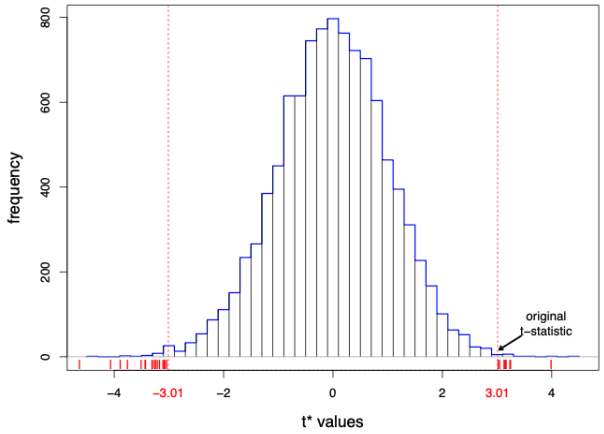


Figure 4.3 10,000 permutation t^*-values for testing **ALL** vs **AML**, for gene 136 in the **leukemia** data of Figure 1.3. Of these, 26 t^*-values (red ticks) exceeded in absolute value the observed t-statistic 3.01, giving permutation significance level 0.0026.

- $X_1, \ldots, X_n$ i.i.d.
- $H_0 : X_i \sim f(x; \theta)$; $H_1 : X_i$ has an arbitrary distribution
- Define k sets $I_1, \ldots, I_k$ s.t. could be intervals

$$\mathrm{pr}(X_i \in \cup_{j=1}^{k} I_j\} = 1$$

- Define

$$Y_j = \sum_{i=1}^{n} 1\{X_i \in I_j\}$$

number of obs in category j

Goodness of fit tests

- $X_1, \ldots, X_n$ i.i.d.
- $H_0 : X_i \sim f(x; \theta)$; $H_1 : X_i$ has an arbitrary distribution
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- Define

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number of obs in category j

- $Y = (Y_1, \ldots, Y_k) \sim Mult_k(n; p)$
- $\mathrm{pr}(Y_1 = y_1, \ldots, Y_k = y_k; p) =$
- $H_0 : p = p(\theta)$; $H_1 : p$ arbitrary

Multinomial goodness of fit tests

AoS 10.8; SM 7.3.1

- log-likelihood function

- generalized likelihood ratio test

- log-likelihood function

- generalized likelihood ratio test

- Theorem 10.22: Under H_0 $p = \dim(\theta)$

$$W = 2\sum_{j=1}^{k} Y_j \log\left(\frac{Y_j}{np_j(\tilde{\theta})}\right) \xrightarrow{d} \chi^2_{k-1-p}$$

- log-likelihood function

- generalized likelihood ratio test

- Theorem 10.22: Under H_0 $p = \dim(\theta)$

$$W = 2\sum_{j=1}^{k} Y_j \log\left(\frac{Y_j}{np_j(\tilde{\theta})}\right) \xrightarrow{d} \chi^2_{k-1-p}$$

- Theorem 10.29 Under H_0

$$Q = \sum_{j=1}^{k} \frac{\{Y_j - np_j(\tilde{\theta})\}^2}{np_j(\tilde{\theta})} \xrightarrow{d} \chi^2_{k-1-p}$$

Table 9.1 *Frequency of goals in First Division matches and "expected" frequency under Poisson model in Example 9.2*

Goals	0	1	2	3	4	≥ 5
Frequency	252	344	180	104	28	16
Expected	248.9	326.5	214.1	93.6	30.7	10.2

$$p_0(\lambda) = 1 - \sum_{j=0}^{4} p_j(\lambda); \quad p_j(\lambda) = e^{-\lambda}\lambda^j/j!, \quad \tilde{\lambda} = 1.3118$$

$$Q = 11.09; \quad W = 10.87; \quad \mathrm{pr}(\chi^2_4 > [11.09, 10.87]) = [0.026, 0.028]$$

		Antigen 'B'		
		Absent	Present	Total
Antigen 'A'	Absent	'O': 202	'B': 35	237
	Present	'A': 179	'AB': 6	185
Total		381	41	422

Table 4.3 Blood groups in England (Taylor and Prior, 1938). The upper part of the table shows a cross-classification of 422 persons by presence or absence of antigens 'A' and 'B', giving the groups 'A', 'B', 'AB', 'O' of the human blood group system. The lower part shows genotypes and corresponding probabilities under one- and two-locus models. See Example 4.38 for details.

	Two-locus model		One-locus model	
Group	Genotype	Probability	Genotype	Probability
'A'	$(AA;bb),(Aa;bb)$	$\alpha(1-\beta)$	$(AA),(AO)$	$\lambda_A^2+2\lambda_A\lambda_O$
'B'	$(aa;BB),(aa;Bb)$	$(1-\alpha)\beta$	$(BB),(BO)$	$\lambda_B^2+2\lambda_B\lambda_O$
'AB'	$(AA;BB),(Aa;BB),$ $(AA;Bb),(Aa;Bb)$	$\alpha\beta$	(AB)	$2\lambda_A\lambda_B$
'O'	$(aa;bb)$	$(1-\alpha)(1-\beta)$	(OO)	λ_O^2

$Q = 15.73; W = 17.66$ (two-locus)

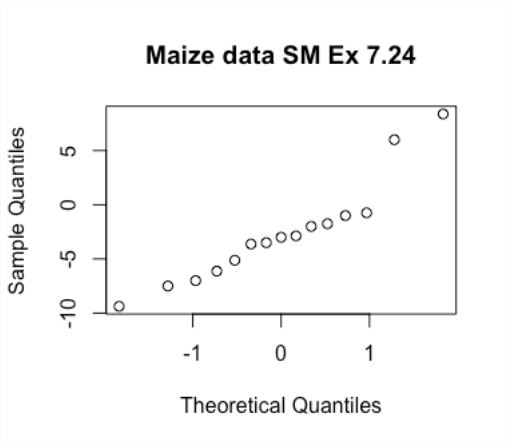
$p < 10^{-5}$

$Q = 2.82; W = 3.17$ (single locus)

$p = 0.09; 0.07$

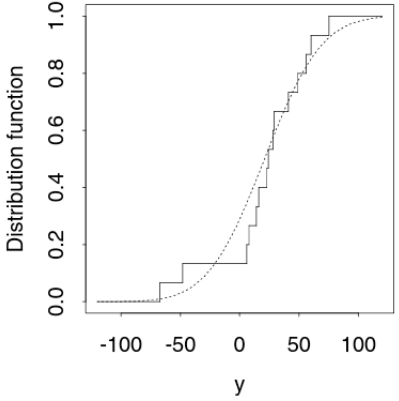
Smooth goodness-of-fit tests

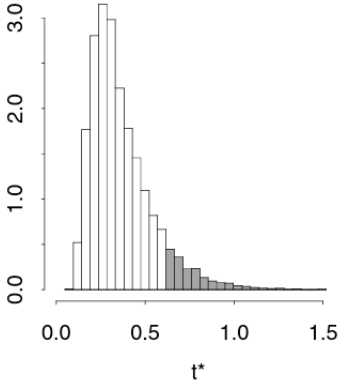
MS 9, SM p.327-9




```
library(SMPracticals)
data(darwin)
cross <- seq(1,30,by=2)
self <- cross+1
diffs <- darwin[self,4]-darwin[cross,4]
qqnorm(diffs)
```

Figure 7.5 Analysis of maize data. Left: empirical distribution function for height differences, with fitted normal distribution (dots). Right: null density of Anderson–Darling statistic T for normal samples of size $n = 15$ with location and scale estimated. The shaded part of the histogram shows values of T^* in excess of the observed value t_{obs}.





SM Example 7.24 testing $N(\mu, \sigma^2)$ distribution

Smooth goodness-of-fit tests

- $X_1, \ldots, X_n \quad i.i.d. \quad F(\cdot); \quad H_0 : F = F_0$ cumulative d.f.
- $\widehat{F}_n(t) = \frac{1}{n} \sum_{i=1}^{n} 1\{X_i \leq t\}$

- three test statistics:
  1. $\sup_t |\widehat{F}_n(t) - F_0(t)|$
  2. $\int \{\widehat{F}_n(t) - F_0(t)\}^2 dF_0(t)$
  3. $\int \frac{\{\widehat{F}_n(t) - F_0(t)\}^2}{F_0(t)\{1 - F_0(t)\}} dF_0(t)$

- SM Example 7.24 testing $N(\mu, \sigma^2)$ distribution
- SM Example 7.23; 6.14 testing $U(0, 1)$ distribution

Smooth goodness-of-fit tests

- Special case $H_0 : F(t) = F_0(t) = t$ $\quad X_i \sim U(0,1)$
- Recall

$$E_0\{\widehat{F}_n(t)\} = F_0(t) = t, \quad \text{var}\{\widehat{F}_n(t)\} = t(1-t)/n$$

- What about distribution of

$\sup_t |\widehat{F}_n(t) - t|$ $\qquad$ $\int \{\widehat{F}_n(t) - t\}^2 dt$ $\qquad$ $\int \dfrac{\{\widehat{F}_n(t) - t\}^2}{F_0(t)\{1-t\}} dt$

- need joint density of $\widehat{F}_n(t)\ \forall\ t$

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$\sup_t |\widehat{F}_n(t) - t|$ $\int \{\widehat{F}_n(t) - t\}^2 dt$ $\int \frac{\{\widehat{F}_n(t) - t\}^2}{F_0(t)\{1-t\}} dt$

- need joint density of $\widehat{F}_n(t)\ \forall\ t$
- define stochastic process $B_n(t) = \sqrt{n}(\widehat{F}_n(t) - t)$
- vector $(B_n(t_1), \ldots, B_n(t_k)) \xrightarrow{d} N_k(0, C), \quad C_{ij} = \min(t_i, t_j) - t_i t_j$ MS 9.3
- a Brownian bridge is a continuous function on $(0,1)$
  with all finite-dimensional distributions as above

Smooth goodness-of-fit tests

- Kolmogorov-Smirnov test

$$K_n = \sup_{0 \leq t \leq 1} |B_n(t)|$$

- Cramer-vonMises test

$$W_n^2 = \int_0^1 B_n^2(t) dt$$

- Anderson-Darling test

$$A_n^2 = \int_0^1 \frac{B_n^2(t)}{t(1-t)} dt$$

Smooth goodness-of-fit tests

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- limit theorems

$$K_n \xrightarrow{d} K, \qquad W_n^2 \xrightarrow{d} \sum_{j=1}^{\infty} \frac{Z_j^2}{j^2 \pi^2}, \qquad A_n^2 \xrightarrow{d} \sum_{j=1}^{\infty} \frac{Z_j^2}{j(j+1)}$$

$$\mathrm{pr}(K > x) = 2 \sum_{j=1}^{\infty} (-1)^{j+1} \exp(-2j^2 x^2)$$

1. Hypothesis testing

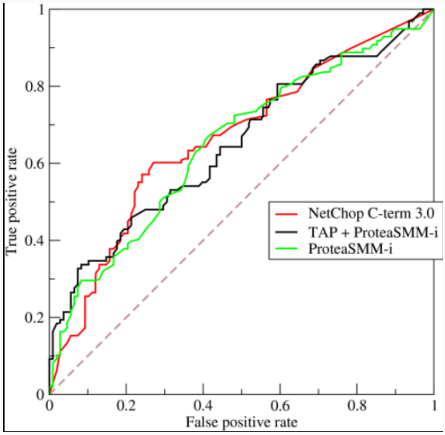
AoS Table 10.1

		H_0 not rejected	H_0 rejected
truth	H_0 true		type 1 error
	H_1 true	type 2 error	

2. Diagnostic testing

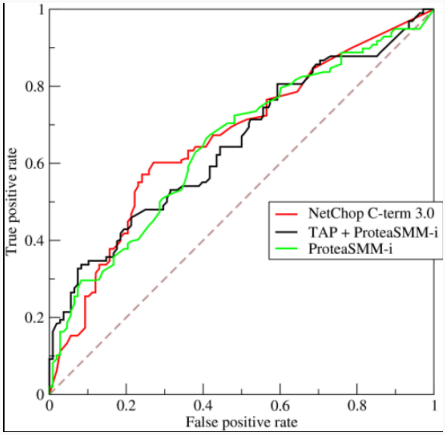
link

		test negative	test positive	
truth	C19 neg	TN	FP	N
	C19 pos	FN	TP	P



True positive rate =
sensitivity =
TP/P

False positive rate =
1− specificity =
$1 - TN/N$



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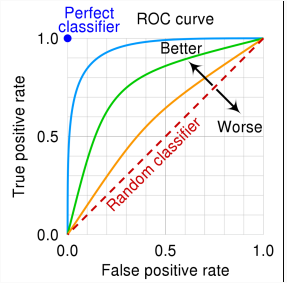

Rapid flow test, care home link

		test negative	test positive	
truth	C19 neg	114,993	101	115,094
	C19 pos	371	128	499

Sensitivity = TP/P = 128/499 = 0.257
Specificity = TN/N = 114,993/115094 =0.999

Cochrane review

meta-analysis

“consistently high specificities”

“sensitivity varied widely: average sensitivities by brand ranged from 34.3% to 91.3% ”