Advances in EM-test for Finite Mixture Models

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International Workshop on Perspectives on High-dimensional Data Analysis

OUTLINE

- **1** FINITE MIXTURE MODELS
 - Genetic Example
 - Finite mixture models
- 2 Hypothesis test
 - Test of homogeneity
 - Advances toward realistic solution
- 3 EM-TEST
 - Further advances
 - Limiting distribution

A GENETIC EXAMPLE: TRAIT

- Geneticists often study Sodium-lithium countertransport (SLC) activity in red blood cells, since it
 - relates to blood pressure and the prevalence of hypertension;
 - is relatively easier to study than blood pressure.
- A search of "Sodium-lithium countertransport" shows up 12,400 results. The leading one is cited 676 times.

- One genetic hypothesis is that the SLC activity is determined by a simple model of inheritance compatible with the action of a single gene with two alleles.
- Each observation (of SLC value) was composed of the sum of the effect of a genetic component and a normally distributed fluctuation
- Thus, a general population may be divided into three subpopulations:
 - (1) those has two copies of the allele that elevates the SLC activity;
 - (2) those have one copy; and (3) those have 0 copies
- Hence, a random sample from the population should behave as a finite mixture of up to three components.

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HETEROGENEITY LEADS TO MIXTURE MODEL

- There are two competing genetic models: simple dominance model and additive model.
 - If one allele is dominant, then the data are a random sample from a two-component normal mixture model;
 - If the genetic effect is additive, then the data are a random sample from a three-component normal mixture model.

The data will be shown in the next slide.

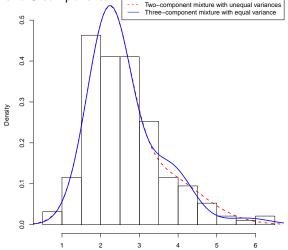
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SLC DATA

FIGURE: Histogram of 190 SLC measurements and suggestive normal mixture models with 2 and 3 components.



READING FROM THE HISTOGRAM AND FITS

- It is not apparent whether a 2-component or a 3-component model is the "correct model".
- A rigorous statistical analysis would be helpful to shed light to the preference of the two competing models.
- One may take model selection approach, diagnostic approach and so on to answer this question.
- A statistical hypothesis test is likely the most desired approach.

Density function of a finite mixture

- Let $\{f(x;\theta):\theta\in\Theta\}$ be a parametric distribution family where Θ is parameter space for θ .
- A finite mixture model is a class of distributions with density function in the form of

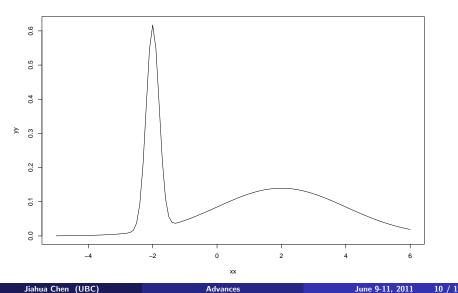
$$f(x; \Psi) = \sum_{h=1}^{m} \alpha_h f(x; \theta_h).$$

- $f(x;\theta)$: kernel/component density function.
- m: order of the finite mixture model.
- θ_h : the parameter of the hth sub-population.
- α_h : the proportion of the hth sub-population.

MIXING DISTRIBUTION

- One may put all parameters into a mixing distribution:
 - $\Psi(\theta) = \sum_{h=1}^{m} \alpha_h I(\theta_h \leq \theta)$.
 - $\Psi(\theta)$ is a distribution on Θ with m support points.

DENSITY FUNCTION OF A 2-COMPONENT NORMAL **MIXTURE**



Incomplete data structure

- A random variable X from a finite mixture model can be regarded as generated in two steps.
 - In the first step, a value of θ is generated from the mixing distribution Ψ .
 - When Ψ is discrete, this θ is labelled by h, the hth subpopulation.
 - Given θ_h , X is a random outcome from sub-population $f(x; \theta_h)$.
- Thus, the data from mixture models are "by definite" incomplete observations.

GENETIC EXAMPLE AND THE MIXTURE MODEL

- An individual can have genotypes AA, Aa or aa.
- The SLC activity level of a randomly selected individual has density function

$$f(x; \Psi) = \sum_{h \in \{AA, Aa, aa\}} \alpha_h \phi(x; \mu_h, \sigma_h^2).$$

where $\phi(x; \mu_h, \sigma_h^2)$ is the normal density with mean μ_h and variance σ_h^2 .

 The genotype of the sample individual is generally unknown, particularly in this case.

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GENETIC QUESTION IN STATISTICAL TERMINOLOGY

- Ignore some details, the statistical problem on the existence of a major gene is to test the null hypothesis of m=1 against m>1.
 - This is homogeneity test.
- To determine whether the major gene (allele) is additive or dominate, the statistical problem is to test the null hypothesis of m=2 against m = 3.
 - This is to test the order of the mixture model.

- Given an iid sample X_1, \ldots, X_n from a two-component mixture,
- the log-likelihood function of the mixing distribution is given by

$$\ell_n(\alpha_1, \alpha_2, \theta_1, \theta_2) = \sum_i \log \{\alpha_1 f(x_i; \theta_1) + \alpha_2 f(x_i; \theta_2)\}.$$

- Is the underlying population in fact homogeneous?
- That is, does $\theta_1 = \theta_2$?

LIKELIHOOD RATIO TEST (LRT) FOR HOMOGENEITY

• The standard approach is to compute likelihood ratio test statistic:

$$R_n = 2\{\sup \ell_n(\alpha_1, \alpha_2, \theta_1, \theta_2) - \sup \ell_n(\alpha_1, \alpha_2, \theta, \theta)\}.$$

- Reject H_0 if R_n is larger than some threshold value.
- It only leaves a technical issue of computing the proper threshold value.

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THE TECHNICAL ISSUE IS CHALLENGING

- For regular models, R_n has an asymptotic chisquared distribution under the null hypothesis.
- Chisquared distributions are well documented and easily computed numerically.
- Hence, a proper threshold value can be easily determined based on chisquared distribution for hypothesis testing under regular models.

FINITE MIXTURE MODEL IS NOT REGULAR

- Use $\alpha_1 f(x; \theta_1) + \alpha_2 f(x; \theta_2)$ for illustration:
 - When $\alpha_1 = 0$, any θ_1 value parameterizes the same distribution. There is a loss of identifiability (type I).
 - When $\theta_1 = \theta_2$, any (α_1, α_2) parameterize the same distribution. There is again a loss of identifiability (type II).
 - The null model is not an interior point in the set of alternative models.
- All of these violate the "regularity conditions" for "good behaviors" of classical likelihood approaches.

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SURPRISES ON LRT, I

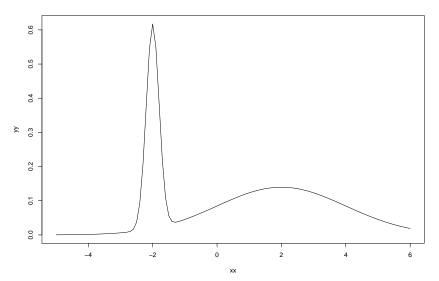
- Researchers/geneticists believed the limiting distribution of R_n is still chisquare, except the degree of freedom needs more research.
- However.
 - For $(1 \alpha)N(0, 1) + \alpha N(\theta, 1)$ and when $\Theta = R$ Hartigan (1985) found that $R_n \to \infty$ as $n \to \infty$.
 - If the LRT statistics R_n is used, no finite threshold value is appropriate from asymptotic point of view.

SURPRISES ON LRT, II

- For $(1 \alpha)N(\mu_1, \sigma_1^2) + \alpha N(\mu_2, \sigma_2^2)$, the likelihood function is unbounded (based on an iid sample).
- See the plot of the density function of the two-component normal mixture model again.

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Density function of a 2-component normal mixture



Breakthroughs starts from a Binomial mixture

 Suppose we have iid observations from a 2-component binomial distribution:

$$\alpha_1 \text{Bin}(m, \theta_1) + \alpha_2 \text{Bin}(m, \theta_2).$$

- Using parameter transformation and for homogeneity test, Chernoff and Lander (1995) obtained limiting distributions of the LRT statistics R_n .
 - This is the first result without requiring "separation condition" $|\theta_1 \theta_2| > \epsilon$.

- The limiting distribution of R_n was derived without separation condition by many authors soon after.
 - key conditions include
 - (1) Θ is compact,
 - (2) $E\{f(X;\theta)/f(X;\theta_0)\}^2 < \infty$ for any $\theta \in \Theta$.
 - drawbacks of the limiting distribution include
 - (1) being a functional of Gaussian process,
 - (2) dependent on Θ and θ_0 .
- So what? the limiting distribution is not too useful for determining the threshold value.

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A MEANINGFUL STEP TOWARD A STATISTICAL SOLUTION

Let

$$p\ell_n(\alpha_1,\alpha_2,\theta_1,\theta_2) = \ell_n(\alpha_1,\alpha_2,\theta_1,\theta_2) + C\log\{4\alpha_1\alpha_2\}.$$

Similar to usual LRT, define

$$\tilde{R}_n = 2\{\max_{H_1} p\ell_n(\alpha_1, \alpha_2, \theta_1, \theta_2) - \max_{H_0} p\ell_n(\alpha_1, \alpha_2, \theta_1, \theta_2)\}.$$

• Chen (1995, CJS) shows that the limiting distribution of \tilde{R}_n is $0.5\chi_0^2 + 0.5\chi_1^2$.

WHAT IS THE SIGNIFICANCE?

- The modified likelihood ratio statistic \tilde{R}_n is an asymptotic pivot: its distribution does not depend the null distribution.
- The quantiles of $0.5\chi_0^2 + 0.5\chi_1^2$ (rather than a functional of a Gaussian process) can be easily computed.
- Significance of this result: practically the first implementable likelihood-based homogeneity test.

Why properties make $p\ell_n$ work?

- The first helpful property is that ℓ_n is bounded under binomial mixture model.
- The second helpful property is $C \log\{4\alpha_1\alpha_2\} \to -\infty$ as $\alpha_1\alpha_2 \to 0$.
 - Thus, $p\ell_n$ does not attain its maximum at small $\alpha_1\alpha_2$.
- Because of these, the \tilde{R}_n is practically confined on $\alpha_1 \in [\epsilon, 1-\epsilon]$.
- On $[\epsilon, 1-\epsilon]$, the mixture model is almost "regular" which leads a simple limiting behavior.

Advance to homogeneity test to non-binomial mixtures

- The idea works for general homogeneity tests if ℓ_n is stochastically bounded.
- Boundedness comes under key conditions:
 - (1) Θ is compact,
 - (2) $E\{f(X;\theta)/f(X;\theta_0)\}^2 < \infty$ for any $\theta \in \Theta$.

Modified likelihood ratio test

- As long as (1) and (2) hold, the MLRT idea works and the limiting distributions are useful in applications:
 - Chen, Chen and Kalbfleisch (2001, JRSS, B) give the result for general homogeneity tests.
 - Chen, Chen and Kalbfleisch (2004, JRSS, B) succeed at finding the limiting distribution of \tilde{R}_n for testing m=2 against some m>2.
- ullet Regretfully, these results are obtained when Θ is compact and is one-dim.

SOMETHING NEW IS STILL DESIRABLE

- Neither Chen, et al. (2001, 2004) is applicable to the genetic problem on SLC activity data because:
 - its $\theta = (\mu, \sigma)$ is 2-dimensional.
 - under normal mixture models, condition $E\{f(X;\theta)/f(X;\theta_0)\}^2 < \infty$ is not satisfied for all θ .
- Moving MLRT forward is vital. How?

An insight to the test of homogeneity, I

- Suppose the data are from a homogeneous model $f(x; \theta_0)$ and we want to examine the possibility that the actual model is a mixture with m = 2.
- Both LRT and MLRT let $f(x; \theta_0)$ compete against all potential models with m = 2.

An insight to the test of homogeneity, II

• In particular, a model such as

$$(1-\epsilon)f(x;\theta_0)+\epsilon f(x;\theta)$$

is a competitor.

- ullet Without compact assumption on Θ , there are "too many" competitors.
- A competitor with θ -value such that

$$E\{f(X;\theta)/f(X;\theta_0)\}^2 = \infty$$

30 / 1

has, in addition, unfair advantage!

They explain the two undesirable conditions behind LRT and MLRT.

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EM-TEST FOR HOMOGENEITY TEST, I

- The key behind EM-test is to initially confine the range of H_a .
- Here is a simplified illustration:
 - initially test $H_0: f(x;\theta)$ against $H_a': 0.30f(x;\theta_1) + 0.70f(x;\theta_2)$.
 - Under H_0 , this R_n has a simple $0.5\chi_0^2 + 0.5\chi_1^2$ limiting distribution.
- This test is not sensible, because the actual distribution of the data could be $0.45f(x; \theta_1) + 0.55f(x; \theta_2)$.

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EM-TEST FOR HOMOGENEITY TEST, II

- If the sample is from H_0 , both $0.45f(x; \theta_1) + 0.55f(x; \theta_2)$ and $0.30f(x; \theta_1) + 0.70f(x; \theta_2)$ will fit data well.
- If the sample is from $0.45f(x;\theta_1) + 0.55f(x;\theta_2)$, fitting $0.30f(x;\theta_1) + 0.70f(x;\theta_2)$ should leave a lot of room for further improvement.

EM-TEST FOR HOMOGENEITY TEST, III

- Thus, whether the data is from H_0 or not can be judged on how big a room there still is for improvement from the initially fit of a restrictive model $0.30f(x; \theta_1) + 0.70f(x; \theta_2)$.
- Our additional trick: use EM-iteration to improve the initial fit gradually.
- If a fixed number of EM-iteration increases the value of R_n substantially, H_0 is rejected.
- Further enhancement: use multiple initial fits $\beta f(x; \theta_1) + (1 - \beta) f(x; \theta_2)$, such as $\beta \in \{0.1, 0.3, 0.5\}$.

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THE EM-TEST STATISTIC FOR HOMOGENEITY

- Find the MLE of θ under the null hypothesis $\hat{\theta}_0$.
- Define two intervals $I_1=(-\infty,\hat{\theta}_0)$ and $I_2=[\hat{\theta}_0,\infty)$.
- Find $\hat{\theta}_1 \in I_1$ and $\hat{\theta}_2 \in I_2$ that maximizes $p\ell_n(0.3, 0.7, \theta_1, \theta_2)$.
- Let $(\alpha_1, \alpha_2, \theta_1, \theta_2)^{(0)} = (0.3, 0.7, \hat{\theta}_1, \hat{\theta}_2)$
- Perform EM-iteration *k* times.
- Define

$$EM_n^{(k)}(0.3) = 2\{p\ell_n((\alpha_1, \alpha_2, \theta_1, \theta_2)^{(K)}) - p\ell_n(0.5, 0.5, \hat{\theta}_0, \hat{\theta}_0)\}.$$

• Finally, let $EM_n^{(k)} = \max\{EM_n^{(k)}(0.1), EM_n^{(k)}(0.3), EM_n^{(k)}(0.5)\}.$

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UGLY DEFINITION, BEAUTIFUL LIMITING DISTRIBUTION

THEOREM (LI, CHEN AND MARRIOTT, 2008, BIOMETRIKA)

- Given a random sample of size *n* from $\alpha_1 f(x; \theta_1) + \alpha_2 f(x; \theta_2)$.
- Assume that $f(x; \theta)$ is smooth enough, makes the mixture model identifiable, and so on.
- Under the null distribution $f(x; \theta_0)$, and for any fixed finite k, $EM_n^{(k)} \rightarrow 0.5\chi_0^2 + 0.5\chi_1^2$ in distribution as $n \rightarrow \infty$.
- This result is obtained without $E\{f(X;\theta)/f(X;\theta_0)\}^2 < \infty$ nor compact Θ .
- Yet it is still for one-dim θ , and for homogeneity test only.
- We cannot stop at this point!

35 / 1

EM-TEST FOR $H_0: m = m_0$

- From homogeneity test to H_0 : $m=m_0$ can be technical challenging.
- Li and Chen (2010, JASA) employed some special tricks to ensure the success of generalizing the result.

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Define EM-test for $H_0: m = m_0$, I

- Consider the case when θ is one-dim, and an iid sample is given.
- We first obtain the "MLE" $\hat{\Psi}_0$ under the null hypothesis (maximizing $p\ell_n$).
- Let $\hat{\theta}_{i0}$, $j=1,2,\ldots,m_0$ be estimated value of sub-population parameters.
- Let I_i 's be the interval that contain $\hat{\theta}_{i0}$ and partition Θ evenly.

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Define EM-test for $H_0: m = m_0$, II

• We define a specific class of order- $2m_0$ mixture models

$$\Omega_{2m_0} = \{ \sum_{j=1}^{m_0} \{ \beta_j f(x; \theta_{j1}) + (1 - \beta_j) f(x; \theta_{j2}) \} : \theta_j \in I_j \}.$$

where $\beta_j \in \{0.1, 0.3, 0.5\}.$

- Next, we find a $\hat{\Psi}^{(0)} \in \Omega_{2m_0}$ that maximizes $\ell_n(\Psi)$.
- Last, use EM-iteration to improve the fit of $\hat{\Psi}^{(k)}$.
- Multiple initial β_j will be used.

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38 / 1

Define EM-test for $H_0: m = m_0$, III

• After a pre-chosen iterations k = K, the EM-statistic is

$$M_n^{(K)} = 2\{\ell_n(\Psi^{(K)}) - \ell_n(\hat{\Psi}_0)\}$$

(take the largest out of multiple initial β).

• The EM-test rejects $H_0: m = m_0$ in favour of $m > m_0$ if $M_n^{(K)}$ exceeds some threshold value.

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"Tricks" in this EM-test

- We confined the initial alternative to Ω_{2m_0} .
 - It prevents wild models from being fitted.
- For each sub-population fitted under null model, we examine its possibility to be split into two sub-subpopulations.
 - We have a sub-homogeneity test within each initially fitted sub-population.
 - If these initial subpopulations spread out far away from each other, the limiting distribution would be a convolution of m_0 0.5 χ_0^2 + 0.5 χ_1^2 .

EM-TEST: LIMITING DISTRIBUTION (1)

THEOREM 2

Under some regularity conditions on $f(x; \theta)$ and penalty function $p(\beta)$, and assume $0.5 \in B$ (set of initial values),

$$EM_n^{(K)} o \sup_{\mathbf{v} \geq 0} (2\mathbf{v}^{\tau}\mathbf{w} - \mathbf{v}^{\tau}\Omega\mathbf{v}) = \sum_{h=0}^{m_0} a_h \chi_h^2$$

for some $a_h \ge 0$ and $\sum_{h=0}^{m_0} a_h = 1$, under Ψ_0 and fixed K.

- $\mathbf{w} = (w_1, \dots, w_{m_0})^{\tau}$: a 0-mean multivariate normal random vector with correlation matrix $\Omega = (\omega_{ii})$.
- $\mathbf{v} = (v_1, \dots, v_{m_0})^{\tau}$ and $\{\mathbf{v} \ge 0\} = \{v_1 \ge 0, \dots, v_{m_0} \ge 0\}.$
- The weights (a_0, \ldots, a_{m_0}) depend on Ω .
- Ω can be calculated based on Ψ_0 or $\hat{\Psi}_0$.

EM-TEST: LIMITING DISTRIBUTION (2)

THEOREM 2 (CONTINUED)

In particular,

- ① when $m_0 = 1$, $a_0 = a_1 = 0.5$;
- ② when $m_0=2$, $a_0=(\pi-\arccos\omega_{12})/(2\pi)$, $a_1=0.5$, and $a_0+a_2=0.5$;
- **3** when $m_0 = 3$, $a_0 + a_2 = a_1 + a_3 = 0.5$ and

$$a_0 = (2\pi - \arccos \omega_{12} - \arccos \omega_{13} - \arccos \omega_{23})/(4\pi),$$

 $a_1 = (3\pi - \arccos \omega_{12:3} - \arccos \omega_{13:2} - \arccos \omega_{23:1})/(4\pi),$

where

$$\omega_{ij:k} = \frac{(\omega_{ij} - \omega_{ik}\omega_{jk})}{\sqrt{(1 - \omega_{ik}^2)(1 - \omega_{jk}^2)}}.$$

42 / 1

FURTHER PROGRESS IS DESIRED

- The previous result of Li and Chen (2010, JASA) succeeded at testing hypothesis of $H_0: m=m_0$ against $H_a: m>m_0$.
- Yet the result is only applicable for one-dim Θ .
- The suggested model for SLC data is a finite normal mixture. Its $\theta = (\mu, \sigma^2)$ is 2-dimensional.
- Keep working!

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EM-TEST FOR NORMAL MIXTURE MODEL

- While the result of Li and Chen (2010, JASA) is not applicable, the EM-test principle is.
- Chen and Li (2009, AOS) worked out EM-test for homogeneity under finite normal mixture models.
- Surprisingly, the limiting distributions of $EM_n^{(k)}$ (defined similarly) are very simple and beautiful.

EM-TEST FOR HOMOGENEITY WITH EQUAL-VARIANCE ASSUMPTION

THEOREM 3

Suppose the penalty function $p(\cdot)$ introduced in $p\ell_n$ satisfies some conditions.

The initial set of value B contains 0.5.

The alternative H_a is under equal-variance assumption.

Then under the homogeneous null distribution $N(\theta_0, \sigma_0^2)$ and for any finite K, as $n \to \infty$,

$$\Pr(EM_n^{(K)} \le x) \to F(x - \Delta)\{0.5 + 0.5F(x)\},\$$

where F(x) is the cumulative density function (cdf) of the χ^2_1 and

$$\Delta = 2 \max_{\alpha_i \neq 0.5} \{ p(\alpha_j) - p(0.5) \}.$$

EM-TEST FOR HOMOGENEITY WITHOUT EQUAL-VARIANCE ASSUMPTION

THEOREM 4

Suppose the penalty function $p(\cdot)$ introduced in $p\ell_n$ satisfies some conditions.

The initial set of value B contains 0.5.

The alternative H_a is any two component normal mixture.

Under the homogeneous null distribution $N(\theta_0, \sigma_0^2)$ and for any finite K, as $n \to \infty$,

$$EM_n^{(K)} \rightarrow \chi_2^2$$
.

- The results in Chen and Li (2009) is designed for finite normal mixture models. Hence model-wise, the method is applicable.
- A simple application shows the homogeneity assumption is rejected soundly.
- We are more interested in checking whether $H_0: m=2$ will be rejected in favour of $H_a: m>2$.
- Charge forward further!

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EM-TEST ON THE ORDER OF FINITE NORMAL MIXTURE MODEL

THEOREM 5 (CHEN, LI AND FU, SUBMITTED)

Assume the same conditions on penalty functions placed in $p\ell_n$.

The initial set of value B contains 0.5.

Under the null distribution $f(x; \Psi_0)$ of order m_0 , and for any fixed finite K, as $n \to \infty$,

$$EM_n^{(K)} \rightarrow \chi^2_{2m_0}$$
.

- We have not worked on the case when σ_i are equal;
- ullet The statistic is defined similarly but needed special care on $p\ell_n$.
- The method is fully applicable to the SLC data analysis.

BACK TO SLC DATA, NULL-FIT

- We test the hypothesis of H_0 : m = 2 against H_a : m = 3.
- The best null model divides the population into two sub-populations with proportions: 65.4% and 34.6%.
- The fitted means and variances of two sub-populations are:

	mean	variance	proportion
Comp 1	2.194	0.557	65.4%
Comp 2	3.457	1.081	34.6%

BACK TO SLC DATA, CONCLUSION

- Whether or not we reject H_0 : m=2 in favor of H_a : m=3 depends on how much better higher order models can fit the data.
- This question of "how much better" is answered through EM-statistics: we find

$$EM_n^{(1)} = 4.597$$
, $EM_n^{(2)} = 4.639$, $EM_n^{(3)} = 4.659$.

- So when H_0 is true, EM-statistic can attain or exceed the above level with probability 33%.
- That is, such better fits as measured by EM-statistic can be easily explained by random fluctuation. Hence, H_0 is not rejected.

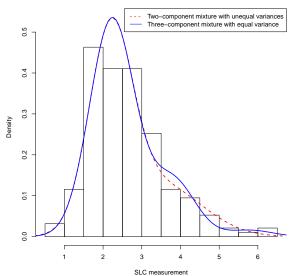
Jiahua Chen (UBC) Advances June 9-11, 2011

50 / 1

- Roeder (1994) uses diagnostic tool and finds a 3-component model is favoured.
- The diagnostic tool requires equal-component-variance assumption which is unfortunate.
 - A formal test can be easily deviced to show that the equal-variance assumption is not plausible.
- Her conclusion can be read as: if component variances must be equal, then one needs a 3-component model to describe the data properly.
- We believe that the EM-test is superior when applied to this and many other real data examples.

SLC DATA AGAIN

FIGURE: SLC and 2/3-component normal mixture models again.



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Thank you

Questions are welcome