Multiple Solutions to the Likelihood Equations in the Behrens-Fisher Problem

Mathias Drton
Department of Statistics, University of Chicago, 5734 S. University Avenue, Chicago, Illinois 60637, U.S.A.
Email: drton@galton.uchicago.edu

Abstract

The Behrens-Fisher problem concerns testing the equality of the means of two normal populations with possibly different variances. The null hypothesis in this problem induces a statistical model for which the likelihood function may have more than one local maximum. We show that such multimodality contradicts the null hypothesis in the sense that if this hypothesis is true then the probability of multimodality converges to zero when both sample sizes tend to infinity. Additional results include a finite-sample bound on the probability of multimodality under the null and asymptotics for the probability of multimodality under the alternative.

Keywords: Algebraic statistics; Discriminant; Heteroscedasticity; Maximum likelihood estimation; Two-sample t-test.

1 Introduction

The Behrens-Fisher problem is concerned with testing

$$H_0 : \mu_X = \mu_Y \quad \text{vs.} \quad H_1 : \mu_X \neq \mu_Y,$$

where $\mu_X$ and $\mu_Y$ are the means of two normal populations with possibly different variances $\sigma^2_X$ and $\sigma^2_Y$. An interesting aspect of the problem is that the likelihood equations for the model induced by $H_0$ may have more than one solution. In fact, with probability one, there will be either one or three solutions with the two cases corresponding to one or two local maxima of the likelihood function. According to simulations of Sugiura and Gupta (1987), three solutions to the likelihood equations occur infrequently if the observations are drawn

*This material is based upon work supported by the National Science Foundation under Grant No. 0505612.
from a distribution in $H_0$. In this note we provide an explanation for this rare occurrence of multiple solutions by proving that under $H_0$ the probability of this event converges to zero when $n$ and $m$ tend to infinity (Corollary 3). This and more general large-sample results about the probability of multiple solutions (Proposition 2 and Theorem 6) are based on two observations. First, solving the likelihood equations amounts to solving one cubic polynomial equation. Second, the number of real roots of a cubic can be determined using the cubic discriminant. The discriminant criterion also allows us to derive a finite-sample bound on the null probability of multiple solutions to the likelihood equations (Proposition 1).

While arguments can be given for using a likelihood ratio-based test instead of Welch’s approximate $t$-test in the Behrens-Fisher problem (Jensen, 1992), the latter test is widely used in practice and avoids maximization of the likelihood function under the null hypothesis. In that sense the practical implications of our study are perhaps not immediate. However, in more general models involving heteroscedastic structures statistical practice often relies on likelihood ratio tests that do require solving the maximization problem. Our results provide geometric intuition about this problem in the simple univariate Behrens-Fisher model (Figure 1), for which it holds, rather reassuringly, that the likelihood function for the null model is asymptotically unimodal if the model is correctly specified. It would be interesting to obtain generalizations of this fact for other, more complicated models.

2 Solving the likelihood equations

We start out by deriving a convenient form of the likelihood equations for the three-parameter model induced by the null hypothesis in the Behrens-Fisher problem.

2.1 A cubic equation

Let $X_1, \ldots, X_n \sim N(\mu_X, \sigma^2_X)$ and $Y_1, \ldots, Y_m \sim N(\mu_Y, \sigma^2_Y)$ be two independent normal samples. Under the null hypothesis $H_0$, $\mu_X$ is equal to $\mu_Y$ and we denote this common mean by $\mu$. The log-likelihood function for the null model can be written as

$$
\ell(\mu, \sigma^2_X, \sigma^2_Y) = -\frac{n + m}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2_X) - \frac{m}{2} \log(\sigma^2_Y) - \frac{n}{2} \left[ \frac{\sigma^2_X}{\sigma^2_X} + \frac{(\bar{X} - \mu)^2}{\sigma^2_X} \right] - \frac{m}{2} \left[ \frac{\sigma^2_Y}{\sigma^2_Y} + \frac{(\bar{Y} - \mu)^2}{\sigma^2_Y} \right].
$$

Here, $\bar{X}$ and $\bar{Y}$ are the two sample means, and

$$
\hat{\sigma}^2_X = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})^2
$$

is the empirical variance for the first sample; the second empirical variance $\hat{\sigma}^2_Y$ is defined analogously. If $\min(n, m) \geq 2$, then both $\hat{\sigma}^2_X$ and $\hat{\sigma}^2_Y$ are positive with probability one. This sample size condition will be assumed throughout.
The partial derivatives of the log-likelihood function are

\[
\frac{\partial \ell}{\partial \mu} = \frac{n(\bar{X} - \mu)}{\sigma^2_X} + \frac{m(\bar{Y} - \mu)}{\sigma^2_Y}
\]

and

\[
\frac{\partial \ell}{\partial \sigma^2_X} = -\frac{n}{2\sigma^2_X} + \frac{n[\hat{\sigma}^2_X + (\bar{X} - \mu)^2]}{2\sigma^4_X};
\]

the partial derivative for \( \sigma^2_Y \) is analogous. Let \( r_n = n/m \). Then the likelihood equations obtained by setting the three partial derivatives to zero are equivalent to the polynomial equations

\[
r_n(\bar{X} - \mu)\sigma^2_Y + (\bar{Y} - \mu)\sigma^2_X = 0, \quad (2.1)
\]

\[
\sigma^2_X = (\bar{X} - \mu)^2 + \hat{\sigma}^2_X, \quad (2.2)
\]

\[
\sigma^2_Y = (\bar{Y} - \mu)^2 + \hat{\sigma}^2_Y. \quad (2.3)
\]

Here, equivalence means that the two solution sets are almost surely equal. Plugging the expressions for \( \sigma^2_X \) and \( \sigma^2_Y \) from (2.2) and (2.3) into (2.1) yields the cubic equation

\[
f(\mu) = a_3\mu^3 + a_2\mu^2 + a_1\mu + a_0 = 0 \quad (2.4)
\]

with

\[
a_3 = 1 + r_n,
\]

\[
a_2 = -(2\bar{X} + \bar{Y}) - r_n(2\bar{Y} + \bar{X}),
\]

\[
a_1 = \bar{X}^2 + 2(1 + r_n)\bar{X}\bar{Y} + r_n\bar{Y}^2 + \hat{\sigma}^2_X + r_n\hat{\sigma}^2_Y, \quad \text{and}
\]

\[
a_0 = -\bar{X}^2\bar{Y} - r_n\bar{Y}^2\bar{X} - \hat{\sigma}^2_X\bar{Y} - r_n\hat{\sigma}^2_Y\bar{X}.
\]

Hence, the maximum likelihood estimator \( \hat{\mu} \) can be computed in closed form by solving the univariate cubic equation (2.4). We remark that the manipulations leading to the polynomial equations (2.2), (2.3) and (2.4) form a trivial case of a computation of a lexicographic Gröbner basis (Pachter and Sturmfels, 2005, p. 86).

### 2.2 The discriminant

A quadratic polynomial \( a_2x^2 + a_1x + a_0 \) in the indeterminate \( x \) may have no, one, or two (distinct) real roots. Which one of the three cases applies is determined by the sign of the discriminant \( a_1^2 - 4a_0a_2 \). In the Behrens-Fisher problem we are led to the cubic polynomial \( f \) in (2.4). A cubic always has at least one real root, and so we would like to know whether it has one, two, or three real roots. This can again be decided based on the sign of the discriminant, which for the cubic takes the form

\[
\Delta = a_1^2a_2^3 - 4a_0a_2^3 - 4a_1^3a_3 + 18a_0a_1a_2a_3 - 27a_0^2a_2^2.
\]
If $\Delta > 0$ then $f$ has three distinct real roots. If $\Delta < 0$ then $f$ has a unique real root and two complex ones. If $\Delta = 0$, then $f$ may have one real root of multiplicity three or two distinct real roots of which one has multiplicity two. These and more general results on discriminants can be found for example in Basu et al. (2003, §4.1-2).

The coefficients $a_0$, $a_1$ and $a_2$ of $f$ in (2.4) are random variables with a continuous distribution and $a_3$ is a constant. Consequently, $\Delta$ is also a continuous random variable such that the event $\{\Delta = 0\}$ occurs with probability zero. In other words the Behrens-Fisher likelihood equations almost surely have one or three real solutions.

The discriminant $\Delta$ is a homogeneous polynomial of degree 6 in $\bar{X}$, $\bar{Y}$, $\hat{\sigma}_X$ and $\hat{\sigma}_Y$, and depends on $\bar{X}$ and $\bar{Y}$ only through their difference. However, with probability one, the sign of $\Delta$ depends only on $r_n$ and the two ratios $\hat{\gamma} = \hat{\sigma}_X/\hat{\sigma}_Y$ and $\hat{\delta} = (\bar{X} - \bar{Y})/\hat{\sigma}_Y$. This follows because $\Delta = \hat{\sigma}_Y^6 \cdot D$ with

$$D = \hat{\delta}^6 r_n^2 - 2\hat{\delta}^4 \left[\hat{\gamma}^2 (2 + 2r_n - r_n^2) + (2r_n^3 + 2r_n^4 - r_n^2)\right]$$

$$- \hat{\delta}^2 \left[\hat{\gamma}^4 (8 + 8r_n - r_n^2) + (8r_n^4 + 8r_n^3 - r_n^2) - 2\hat{\gamma}^2 (10r_n + 19r_n^2 + 10r_n^3)\right]$$

$$- 4(1 + r_n)(r_n + \hat{\gamma}^2)^3.$$  \hspace{1cm} (2.5)

While $\Delta$ (and $D$) remain unchanged if $n$ and $m$ are replaced by $\bar{n}$ and $\bar{m}$ with $r_n = n/m = \bar{n}/\bar{m} = \bar{r}_n$, such a change of sample sizes affects the sampling distribution of $\Delta$ (and $D$) and thus the probability of multiple solutions to the likelihood equations. We remark that instead of working with $\hat{\delta}$ one could work with the more symmetric quantities

$$\frac{\bar{X} - \bar{Y}}{\sqrt{\hat{\sigma}_X^2 + \hat{\sigma}_Y^2}} = \hat{\delta} \cdot \frac{1}{\sqrt{\hat{\gamma}^2 + 1}}$$

or

$$\frac{\bar{X} - \bar{Y}}{\sqrt{\hat{\sigma}_X^2 + r_n\hat{\sigma}_Y^2}} = \hat{\delta} \cdot \frac{1}{\sqrt{\hat{\gamma}^2 + r_n}}.$$  

However, such a substitution would lead to an increased degree in the analog of (2.5) such that we keep working with $\hat{\delta}$ in the sequel.

For any given value of $r_n$, the polynomial $D = D_{r_n}$ in the indeterminates $\hat{\gamma}$ and $\hat{\delta}$ defines an algebraic curve. Figure 1 shows two examples of these curves over the statistically relevant region with $\hat{\gamma} > 0$. By symmetry, the curve for $r_n = 1$ has four cusp points at $(\hat{\gamma}, \hat{\delta}) = (\pm 1, \pm 2)$; the cusps for $r_n = 4$ are at $(\hat{\gamma}, \hat{\delta}) = (\pm \sqrt{27}/2, \pm \sqrt{25}/2)$. In general, the four cusps have coordinates

$$\hat{\gamma} = \pm \frac{(2r_n + 1)\sqrt{(r_n + 2)r_n(2r_n + 1)}}{(r_n + 2)^2},$$

$$\hat{\delta} = \pm \frac{3(1 + r_n)\sqrt{3(r_n + 2)r_n}}{(r_n + 2)^2}.  \hspace{1cm} (2.6)$$
Figure 1: Algebraic curve defined by the polynomial $D_{r_n}$ that is derived from the discriminant: (a) $r_n = 1$ and (b) $r_n = 4$. In each plot, points $(\gamma, \delta)$ between the two curves correspond to a unique real root to the Behrens-Fisher likelihood equations. Points above and below the curves correspond to three distinct real roots.

The curve has two asymptotes, namely, $r_n \hat{\delta} = \pm 2\sqrt{1 + r_n \hat{\gamma}}$.

The two respective branches of the curves in Figure (a) enclose the region $\{D < 0\}$, which contains the (horizontal) $\hat{\gamma}$-axis. Over this region the discriminant $\Delta$ is negative and the Behrens-Fisher likelihood equations have a unique real root. Clearly, neither the region $\{D < 0\}$ nor the region $\{D > 0\}$ need to be convex. When fixing $\hat{\gamma}$ and increasing $\hat{\delta}$ then $D$ will eventually remain positive because the leading term of $D$, when viewed as a univariate polynomial in $\hat{\delta}$, is $r_n^2 \hat{\delta}^6$ with $r_n^2 > 0$. This means that bimodal likelihood functions arise when the difference between the means $\bar{X}$ and $\bar{Y}$ of the two samples is large compared to the empirical variances $\hat{\sigma}_X^2$ and $\hat{\sigma}_Y^2$. However, as can be seen in Figure (b) with $r_n = 4$, there may exist values of $\hat{\gamma}$ such that the values of $\hat{\delta}$ corresponding to unimodal likelihood functions do not form an interval.

2.3 Finite-sample bound

A finite-sample study of the probability of one versus three solutions to the Behrens-Fisher likelihood equations seems difficult. However, under the null hypothesis, we can give a very simple bound.

**Proposition 1.** Let the random variable $T$ have a $t$-distribution with $m - 1$ degrees of freedom. Let $\gamma = \sigma_X / \sigma_Y$. If the null hypothesis $H_0$ is true, i.e., if $\mu_X = \mu_Y$, then the probability of three distinct real solutions to the Behrens-Fisher likelihood equations is smaller than

$$P \left( |T| > \sqrt{m - 1} \cdot \frac{3(1 + r_n)r_n\sqrt{3(r_n + 2)}}{(r_n + 2)^2 \sqrt{\gamma^2 + r_n}} \right).$$
Proof. Three solutions occur if $(\hat{\gamma}, \hat{\delta})$ falls in the region \( \{D > 0\} \). This region is strictly contained in the region of pairs $(\hat{\gamma}, \hat{\delta})$ that have $|\hat{\delta}| > c_n$ with

$$c_n = \frac{3(1 + r_n)\sqrt{3(r_n + 2)r_n}}{(r_n + 2)^2};$$

compare Figure 1 and (2.6). Hence, $P(D > 0)$ is smaller than $P(|\hat{\delta}| > c_n)$. Under $H_0$,

$$\frac{\sigma_Y}{\sqrt{m/(m-1) \cdot \sqrt{\frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}}} \cdot \hat{\delta}}$$

is distributed according to the t-distribution with $m - 1$ degrees of freedom. Expressing the event \( \{|\hat{\delta}| > c_n\} \) in terms of this t-random variable yields the claim.

Suppose, for example, that the samples are of equal size with the standard deviation $\sigma_X$ being half the standard deviation $\sigma_Y$, i.e., $r_n = 1$ and $\gamma = 1/2$. Then, by Proposition 1, the probability of three distinct real solutions to the Behrens-Fisher likelihood equations is smaller than 0.023 if $n = m = 5$, 0.00045 if $n = m = 10$ and 0.00001 if $n = m = 15$. Hence, despite its crude nature, the bound informs us that the probabilities are small. Monte Carlo simulations suggest that the three considered probabilities are in fact a factor 10 or more smaller than the stated bounds.

3 Large-sample results

We begin our study of the large-sample behaviour of the likelihood equations with the case when the discriminant converges almost surely to a non-zero limit.

**Proposition 2.** Suppose $\min(n, m) \to \infty$ such that $r_n = n/m \to r \in (0, \infty)$. Let $\delta = (\mu_X - \mu_Y)/\sigma_Y$ and $\gamma = \sigma_X/\sigma_Y$. Define $D_r(\gamma, \delta)$ to be the quantity obtained from $D$ in (2.5) by replacing $r_n$ by $r$ and $(\hat{\gamma}, \hat{\delta})$ by $(\gamma, \delta)$.

(i) If $D_r(\gamma, \delta) < 0$, then the probability that the Behrens-Fisher likelihood equations have exactly one real solution converges to one.

(ii) If $D_r(\gamma, \delta) > 0$, then the probability that the Behrens-Fisher likelihood equations have three distinct real solutions converges to one.

**Proof.** The polynomial $D$ is a continuous function of $\bar{X}, \bar{Y}, \hat{\sigma}_X^2$ and $\hat{\sigma}_Y^2$. Applying laws of large numbers to the four random variables, we find that $D_{r_n}(\hat{\gamma}, \hat{\delta})$ converges almost surely to $D_r(\gamma, \delta)$. In case (i), $D_r(\gamma, \delta)$ is negative, and thus $P(D_{r_n}(\hat{\gamma}, \hat{\delta}) < 0)$ converges to one, which implies the claim. Case (ii) is analogous.

The next result is a corollary to both Propositions 1 and 2.
Corollary 3. Suppose $H_0$ is true, i.e., $\mu_X = \mu_Y = \mu$. If $\min(n, m) \to \infty$ and $r_n = n/m \to r \in (0, \infty)$, then the probability that the Behrens-Fisher likelihood equations have exactly one real solution converges to one.

Proof. If $\mu_X = \mu_Y$, then $\delta = 0$ and the claim follows from Proposition 2 because $D_r(\gamma, 0) = -4(1 + r)(r + \gamma^2)^3$ is negative.

Proposition 2 does not apply to the situation when $D_r$ is zero. However, these critical cases can be studied using asymptotics similar to those encountered with likelihood ratio tests. The resulting asymptotic probabilities will depend on whether or not the point $(\gamma, \delta)$ forms a singular point of the curve defined by the vanishing of $D_r$.

Definition 4. Let $h$ be a polynomial in the ring of polynomials in the indeterminates $x_1$ and $x_2$ with real coefficients. Let $V(h)$ be the algebraic curve $\{x \in \mathbb{R}^2 \mid h(x) = 0\}$. A point $x \in V(h)$ is a singular point if the gradient $\nabla h(x)$ is zero.

Our curve of interest, $V(D_r)$, has four singular points whose coordinates were given in (2.6); recall Figure 1. All other points on $V(D_r)$ are non-singular.

We will show that the critical behaviour of the number of real roots to the Behrens-Fisher likelihood equations is determined by the local geometry of the curve $V(D_r)$ at the true parameter values $(\gamma, \delta)$. This geometry is captured in the tangent cone.

Definition 5. The tangent cone of $V \subseteq \mathbb{R}^2$ at $x \in \mathbb{R}^2$ is the set of vectors that are limits of sequences $\alpha_n(x_n - x)$, where $\alpha_n$ are positive reals and $x_n \in V$ converge to $x$.

The tangent cone, which is a closed set, is indeed a cone. This means that if $\tau$ is in the tangent cone then so is the half-ray $\{\lambda \tau \mid \lambda \geq 0\}$.

Theorem 6. Suppose that $\min(n, m) \to \infty$ and $r_n = r + o(1/\sqrt{n})$. Let $\gamma > 0$.

(i) If $(\gamma, \delta)$ is a non-singular point of the curve $V(D_r)$, then the probability of exactly one real solution as well as the probability of three distinct real solutions to the Behrens-Fisher likelihood equations converge to $1/2$.

(ii) If $(\gamma, \delta)$ is one of two singular points of the curve $V(D_r)$ that have $\gamma > 0$, then the probability of exactly one real solution converges to one.

Proof. We first show that the asymptotic probability can be obtained from a distance between a normal random point and a tangent cone. Different types of tangent cones will then be shown to lead to results (i) and (ii).

Let $W(D_{r_n})$ be the set of points $(\hat{\gamma}, \hat{\delta}) \in (0, \infty) \times \mathbb{R}$ such that $D_{r_n}(\hat{\gamma}, \hat{\delta}) \leq 0$. Let

$$
\lambda_n = n \cdot \min_{(\hat{\gamma}, \hat{\delta}) \in W(D_{r_n})} (\hat{\gamma} - \tilde{\gamma})^2 + (\hat{\delta} - \tilde{\delta})^2
$$

be the squared and scaled distance between the random point $(\hat{\gamma}, \hat{\delta})$ and $W(D_{r_n})$. In Figure 1 the set $W(D_{r_n})$ corresponds to the region between and including the two curve branches.
The Behrens-Fisher likelihood equations have three distinct real solutions if and only if $D_{rn}(\hat{\gamma}, \hat{\delta}) > 0$ if and only if $\lambda_n > 0$.

By the central limit theorem and the delta method, the two random variables $A_n = \sqrt{n}(\hat{\gamma} - \gamma)$ and $B_n = \sqrt{n}(\hat{\delta} - \delta)$ converge jointly to a centered bivariate normal distribution $N_2(0, \Sigma)$. In order to make use of this convergence, we rewrite

$$\lambda_n = \min_{(\bar{\gamma}, \bar{\delta}) \in W(D_{rn})} \left[ A_n - \sqrt{n}(\hat{\gamma} - \gamma) \right]^2 + \left[ B_n - \sqrt{n}(\hat{\delta} - \delta) \right]^2.$$

The limits, for $n \to \infty$, of convergent sequences of the form $\sqrt{n}[(\bar{\gamma}_n, \bar{\delta}_n) - (\gamma, \delta)]$ with $(\bar{\gamma}_n, \bar{\delta}_n) \in W(D_{rn})$ form the tangent cone $T(\gamma, \delta)$ of the set $W(D_r)$ at $(\gamma, \delta)$. It thus follows from van der Vaart (1998, Lemma 7.13) that as $n$ tends to infinity, the random distance $\lambda_n$ converges in distribution to the distance

$$\lambda_\infty = \min_{(\bar{\gamma}, \bar{\delta}) \in T(\gamma, \delta)} (Z_1 - \bar{\gamma})^2 + (Z_2 - \bar{\delta})^2,$$

between the normal random vector $Z = (Z_1, Z_2) \sim N_2(0, \Sigma)$ and $T(\gamma, \delta)$.

**Case (i):** If $(\gamma, \delta)$ is a non-singular point of $V(D_r)$, then $T(\gamma, \delta)$ is a half-space $H$ comprising all points on and to one side of a line through the origin. The normal vector of this line is given by the gradient $\nabla D_r(\gamma, \delta)$. The probability $P(\lambda_\infty > 0) = P(\Sigma^{-1/2}Z \in \Sigma^{-1/2}H)$ is equal to 1/2 because $\Sigma^{-1/2}Z \sim N_2(0, I)$ is standard normal and because $\Sigma^{-1/2}H$ is still a half-space with the origin on its boundary. Since $P(D_{rn}(\hat{\gamma}, \hat{\delta}) > 0) = P(\lambda_n > 0)$ converges to $P(\lambda_\infty > 0)$ we have established claim (i).

**Case (ii):** If $(\gamma, \delta)$ is a singular point, then $T(\gamma, \delta)$ is all of $\mathbb{R}^2$; compare Figure 1. Thus $P(\lambda_\infty > 0) = 0$, which implies claim (ii).

For the curious reader, we remark that the tangent cone to the curve $V(D_r)$ at its singular point $(\gamma, \delta)$ with $\gamma, \delta > 0$ is the half-ray of points $(\gamma, \delta)$ with $\delta \geq 0$ and $\gamma \sqrt{3(2r + 1)} = \delta(r - 1)$. If $r = 1$, then this half-ray is the non-negative $\delta$-axis. The half-ray has positive slope if $r > 1$. The slope is negative if $r < 1$.

We conclude by illustrating the results obtained in this section in Figure 2 which shows simulations on the probability of three distinct real roots to the Behrens-Fisher likelihood equations. This figure addresses the case $\gamma = r = 1$ in which $\delta = \mu_X - \mu_Y$. The simulations confirm Theorem 6(ii) because the probability of three distinct real roots appears to converge to zero if $\delta = 2$ and $(\gamma, \delta) = (1, 2)$ is a singularity of $V(D_1)$.

**References**

Basu, S., Pollack, R., Roy, M.-F., 2003. *Algorithms in Real Algebraic Geometry*, Berlin: Springer-Verlag.

Jensen, J. L., 1992. The modified signed likelihood statistic and saddlepoint approximations. *Biometrika* 79, 693-703.
Figure 2: Simulations for the probability of three distinct real roots to the Behrens-Fisher likelihood equations ($\sigma^2_X = \sigma^2_Y = 1$). The steeper curve corresponds to $n = m = 1000$; the other to $n = m = 15$.

Pachter, L., and Sturmfels, B., 2005. Algebraic Statistics for Computational Biology, Cambridge: Cambridge University Press.
Sugiura, N., and Gupta, A. K., 1987. Maximum likelihood estimates for Behrens-Fisher problem, Journal of the Japan Statistical Society, 17, 55–60.
van der Vaart, A. W., 1998. Asymptotic Statistics, Cambridge: Cambridge University Press.