

Score, Wald, and Likelihood Ratio

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Introduction

- We've now covered the most important theoretical properties of the MLE: it is consistent, asymptotically normal, and efficient
- Today, we turn our attention to a different problem: likelihood-based inference
- Specifically, we will go beyond the likelihood as a mechanism for simply producing point estimates and look at how we can use the likelihood function to construct (frequentist) confidence intervals and carry out hypothesis tests

The holy trinity

- There are three widely used approaches for carrying out likelihood-based inference:
 - Wald (Abraham Wald)
 - Score (C.R. Rao)
 - Likelihood ratio (Jerzy Neyman / Egon Pearson / Samuel Wilks)
- We'll be discussing all three approaches, and considering two different scenarios:
 - Simple null hypotheses: $H_0 : \boldsymbol{\theta} = \boldsymbol{\theta}_0$
 - Composite null hypotheses: $H_0 : \boldsymbol{\theta} \in \Theta_0$

Nuisance parameters

- The second case is particularly important in the multivariate setting, as we are usually interested in testing something like $H_0 : \theta_j = 0$, which means $H_0 : \boldsymbol{\theta} \in \{\boldsymbol{\theta} : \theta_j = 0\}$
- So, to be more specific, we won't necessarily consider composite null hypotheses in their full generality, but rather focus on the setting where $\boldsymbol{\theta}$ can be divided into parameters of interest, $\boldsymbol{\theta}_1$, and nuisance parameters, $\boldsymbol{\theta}_2$, with $\boldsymbol{\theta} = (\boldsymbol{\theta}_1^\top \boldsymbol{\theta}_2^\top)^\top$, with r denoting the length of $\boldsymbol{\theta}_1$ and $d - r$ the length of $\boldsymbol{\theta}_2$
- Our composite tests, then, will be of the form $H_0 : \boldsymbol{\theta}_1 = \boldsymbol{\theta}_0$, with $\boldsymbol{\theta}_2$ left unspecified by the null hypothesis
- (I'm describing these ideas in terms of tests, but everything applies to confidence intervals as well)

Wald approach

- The Wald approach is perhaps the simplest to understand
- It is based on the result that $\sqrt{n}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) \xrightarrow{d} N(\mathbf{0}, \mathcal{F}_1^{-1}(\boldsymbol{\theta}^*))$ and simply uses the standard tools for the normal distribution to carry out inference
- **Proposition:** If consistency assumptions (A)-(C) hold,

$$(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \mathcal{F}(\boldsymbol{\theta}^*) (\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) \xrightarrow{d} \chi_d^2$$

- This can be inverted to find confidence regions for $\boldsymbol{\theta}$

Which information?

- As alluded to previously, we could use either the Fisher or expected information here and the result would still hold
- In fact, we have even more choices; all of the following hold:

$$\begin{aligned}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \mathcal{F}(\boldsymbol{\theta}^*)(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) &\xrightarrow{d} \chi_d^2 \\(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \mathcal{F}(\hat{\boldsymbol{\theta}})(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) &\xrightarrow{d} \chi_d^2 \\(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \mathcal{I}(\boldsymbol{\theta}^*)(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) &\xrightarrow{d} \chi_d^2 \\(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \mathcal{I}(\hat{\boldsymbol{\theta}})(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) &\xrightarrow{d} \chi_d^2 \\(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \mathbf{V}(\hat{\boldsymbol{\theta}})(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) &\xrightarrow{d} \chi_d^2,\end{aligned}$$

where $\mathbf{V}(\boldsymbol{\theta}) = \sum_i \mathbf{u}_i(\boldsymbol{\theta})\mathbf{u}_i(\boldsymbol{\theta})^\top$

- In practice, Wald approaches typically use $\mathcal{I}(\hat{\boldsymbol{\theta}})$

Nuisance parameters

- Testing $H_0 : \boldsymbol{\theta}_1 = \boldsymbol{\theta}_0$ is also rather straightforward with the Wald approach
- **Proposition:** If (A)-(C) hold and $\boldsymbol{\theta}_0 = \boldsymbol{\theta}_1^*$ (i.e., if H_0 is true), then

$$\sqrt{n}(\hat{\boldsymbol{\theta}}_1 - \boldsymbol{\theta}_0) \xrightarrow{d} N(\mathbf{0}, \mathcal{V}_{11}^1),$$

where $\mathcal{V}_{11}^1 = \mathcal{I}_1^{11}$ is the (1,1) block of the inverse of \mathcal{I}_1

- Again, recall that $\mathcal{V}_{11}^{-1} = \mathcal{I}_{11} - \mathcal{I}_{12}\mathcal{I}_{22}^{-1}\mathcal{I}_{21}$, so that $\mathcal{V}_{11}^{-1} \preceq \mathcal{I}_{11}$ and $\mathcal{V}_{11} \succeq \mathcal{I}_{11}^{-1}$; the presence of unknown nuisance parameters increases the variance of our estimator

Wald confidence intervals

- If our parameter of interest is a scalar, then we have simple closed-form expressions for confidence intervals:

$$\hat{\theta}_j \pm z_{1-\alpha/2} \sqrt{\mathcal{V}_{jj}(\hat{\theta})}$$

is an approximate $1 - \alpha$ confidence interval for θ_j

- Again, this is *not* the same thing as

$$\hat{\theta}_j \pm \frac{z_{1-\alpha/2}}{\sqrt{\mathcal{I}_{jj}(\hat{\theta})}};$$

this second approach is incorrect, as it fails to account for the impact of nuisance parameters and produces confidence intervals that are too narrow

Remarks on the Wald approach

- The ease with which confidence intervals can be constructed is the primary advantage of the Wald approach
- As we will see, confidence intervals are considerably more cumbersome in the score and likelihood ratio approaches
- The primary disadvantage of the Wald approach is that it tends to provide the least accurate approximation of the three approaches

Score approach: Simple null

- Next, let's consider the score approach
- As the name implies, this method revolves entirely around consideration of the score vector
- **Proposition:** If (A)-(C) hold,

$$\mathbf{u}(\boldsymbol{\theta}^*)^\top \mathcal{I}^{-1}(\boldsymbol{\theta}^*) \mathbf{u}(\boldsymbol{\theta}^*) \xrightarrow{d} \chi_d^2$$

- Again, we can use any consistent estimator of $\mathcal{I}_1(\boldsymbol{\theta}^*)$ in place of the Fisher information; score approaches typically use $\mathcal{I}(\boldsymbol{\theta}_0)$
- In principle, this can be inverted to find a confidence region, but in practice, doing so is usually not straightforward

Nuisance parameters

- What about testing $H_0 : \theta_1 = \theta_0$?
- This is less straightforward than the Wald case
- We need to evaluate the score and information, but for what value of θ ?
- Setting $\theta_1 = \theta_0$ seems obvious, but for θ_2 , we are going to have to maximize the likelihood under the restriction imposed by H_0

Restricted MLEs

- Specifically, let us define the restricted, or constrained, MLE $\hat{\theta}_2(\theta_0)$ as the value of θ_2 that maximizes $L(\theta)$ under the restriction that $\theta_1 = \theta_0$, with $\hat{\theta}_0 = (\theta_0^\top \hat{\theta}_2(\theta_0)^\top)^\top$
- The following lemma will prove useful to us (its proof is essentially identical to the case for the unrestricted MLE $\hat{\theta}$)
- **Lemma:** If (A)-(C) hold and $\theta_0 = \theta_1^*$, then

$$\sqrt{n}(\hat{\theta}_2(\theta_0) - \theta_2^*) \xrightarrow{d} N(\mathbf{0}, \mathcal{I}_{22}^{-1});$$

note that here we *do* have convergence to \mathcal{I}_{22}^{-1} , not \mathcal{V}_{22} , as under H_0 , we are not affected by uncertainty regarding θ_1

- Not that this only works if H_0 is true: if it isn't, $\hat{\theta}_2(\theta_0)$ may converge to something very different from θ_2^*

Score test with nuisance parameters

- **Theorem:** If (A)-(C) hold and $\theta_0 = \theta_1^*$, then

$$\mathbf{u}_1(\hat{\theta}_0)^\top \mathcal{V}_{11}(\hat{\theta}_0) \mathbf{u}_1(\hat{\theta}_0) \xrightarrow{d} \chi_r^2$$

- In the special case where the parameter of interest is θ_j , we have $u_j(\hat{\theta}_0) \sqrt{\mathcal{V}_{jj}(\hat{\theta}_0)} \sim N(0, 1)$
- Unfortunately, inverting this test to obtain a confidence interval is not trivial, as every time we change θ_0 , we would need to re-solve for $\hat{\theta}_2(\theta_0)$

Remarks on the score approach

- The difficulty of obtaining confidence intervals is the biggest drawback of the score approach
- Conversely, it is often the easiest test to carry out, which is its biggest advantage
- In particular, we don't even need to solve for the MLE in order to carry out the test

Example: Linear regression

- For example, consider the linear regression model $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$; for the purposes of this exercise, we'll treat σ^2 as known
- Suppose we have fit a baseline model involving a number of covariates that we know we want to adjust for, and are considering including an additional predictor \mathbf{x}_j in the model
- The score test $H_0 : \beta_j = 0$ is

$$z_j = \frac{\mathbf{x}_j^\top \mathbf{r}}{\sigma \sqrt{\mathbf{x}_j^\top \mathbf{x}_j - \mathbf{x}_j^\top \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{x}_j}},$$

where \mathbf{r} is the vector of residuals from the baseline fit and $z_j \sim N(0, 1)$ under the null hypothesis

Example: Linear regression

- In particular, note that the “expensive” part of this calculation, $\mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}$, only needs to be computed once, and the rest of the calculations are simple
- This makes score tests very attractive if you are, say, carrying out a genetic association study in which you want to adjust for some baseline characteristics such as age, sex, etc., then test for associations between a clinical outcome and hundreds of thousands of genetic markers
- To apply the Wald or likelihood ratio tests, we would need to fit hundreds of thousands of models; the score tests involve dramatically less computational burden

Likelihood ratio approach

- Finally, let's consider the likelihood ratio approach
- **Theorem:** If (A)-(C) hold, then

$$2 \log \frac{L(\hat{\boldsymbol{\theta}})}{L(\boldsymbol{\theta}^*)} \xrightarrow{d} \chi_d^2$$

- Note that the likelihood ratio test does not involve calculating any derivatives (score or information), only the likelihood function itself

LRT with nuisance parameters

- Like the score test, when nuisance parameters are involved we must solve for restricted MLEs
- **Theorem (Wilks):** If (A)-(C) hold and $\theta_0 = \theta_1^*$, then

$$2 \log \frac{L(\hat{\theta})}{L(\hat{\theta}_0)} \xrightarrow{d} \chi_r^2$$

- Again, this can be inverted to find confidence intervals for θ_j (a root-finding problem), but this involves repeatedly re-solving for $\hat{\theta}_0$

Example: Gamma distribution

- As an example of how all these tests work, let's apply them to the gamma distribution
- As you have already derived on assignment 6,

$$\mathbf{u} = \begin{bmatrix} n \log \beta - n\psi_0(\alpha) + \sum \log x_i \\ n\alpha/\beta - \sum x_i \end{bmatrix}$$
$$\mathcal{I} = \begin{bmatrix} n\psi_1(\alpha) & -n/\beta \\ -n/\beta & n\alpha/\beta^2 \end{bmatrix}$$

- Let's derive confidence intervals for the rate parameter β (you may recall that $\beta^* = 1$ and $\hat{\beta} = 1.66$)

Wald approach

- First, the Wald approach
- The diagonal element of \mathcal{I}^{-1} corresponding to β is 0.118, so an approximate 95% confidence interval is given by

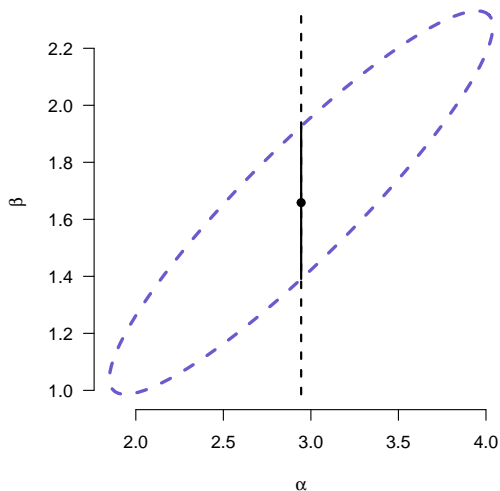
$$\hat{\theta}_j \pm z_{1-\alpha/2} \sqrt{\mathcal{V}_{jj}(\hat{\theta})} = (0.99, 2.33)$$

- Note that this is much wider than the incorrect interval we get from just inverting \mathcal{I}_{jj} :

$$\hat{\theta}_j \pm \frac{z_{1-\alpha/2}}{\sqrt{\mathcal{I}_{jj}(\hat{\theta})}} = (1.39, 1.93);$$

as we have said several times, this second interval does not account for uncertainty in α

Wald: Correct and incorrect intervals



Score

- Obtaining score intervals for β is considerably more computer-intensive, as we must repeatedly solve for $\hat{\alpha}(\beta)$, the MLE of α under the constraint that the rate is equal to β
- The endpoints of the confidence interval, then, can be found by finding the two solutions of

$$u_j(\hat{\alpha}(\beta), \beta)^2 \mathcal{V}_{jj}(\hat{\alpha}(\beta), \beta) = \chi_{1,1-\alpha}^2$$

- This yields the confidence interval (0.99, 2.33); not identical to the Wald interval, but equal up to 2 decimal places
- Again, failing to account for uncertainty by using the MLE $\hat{\alpha}$ instead of the restricted MLE $\hat{\alpha}(\beta)$ produces an interval that is much too narrow: (1.39, 1.93)

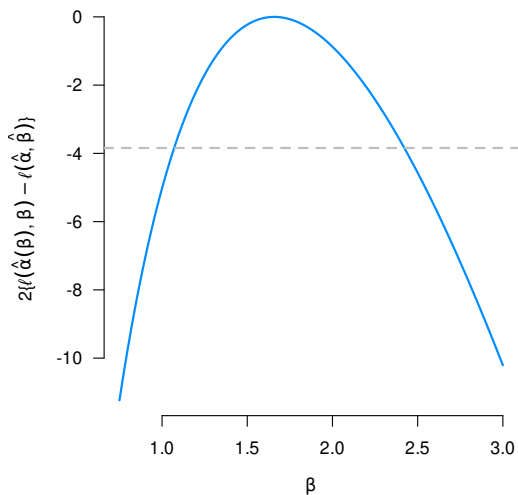
Likelihood ratio

- Similarly, finding the endpoints of the likelihood ratio confidence interval involves finding the roots of

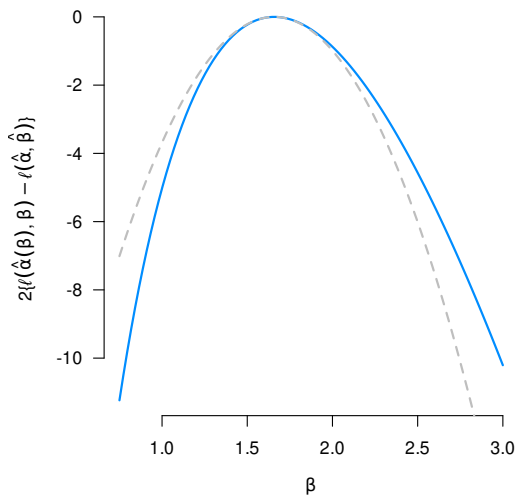
$$2\{\ell(\hat{\alpha}, \hat{\beta}) - \ell(\hat{\alpha}(\beta), \beta)\} = \chi_{1,1-\alpha}^2$$

- This yields the interval (1.07, 2.42)

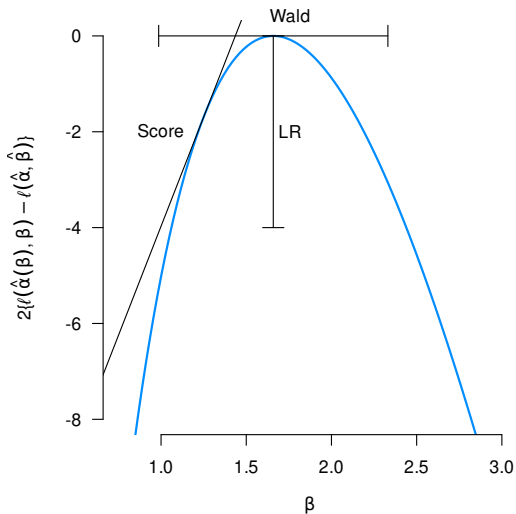
Likelihood ratio plot



Quadratic approximation



Visualization of all three methods



Final remarks

- All three approaches are asymptotically equivalent; letting W_n denote the Wald test statistic, S_n the score test statistic, and LR_n the likelihood ratio test statistic,

$$LR_n = W_n + o_p(1)$$

$$LR_n = S_n + o_p(1),$$

and indeed, all three approaches are potentially useful and widely used, depending on the context

- However, this potentially gives the wrong impression that all three approaches are equally accurate in terms of approximation inference

Superiority of the likelihood ratio approach

- This is not true – the likelihood ratio approach is the most accurate of the three approaches
- This has been shown repeatedly in many theoretical and simulation studies, but it is also intuitive
- The Score and Wald approaches depend on derivatives, and thus, can change substantially if we reparameterize the model (e.g., if we consider $\theta = \log \lambda$)
- In other words, the best-case scenario for Score and Wald is that we find a normalizing transformation, in which case the results are simply equivalent to the LR
- Conversely, Score and Wald can be much worse approximations than LR if we choose a bad transformation