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: $H_0 : \boldsymbol{\theta} \in \boldsymbol{\Theta}_0$

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 $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$, 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 $\sqrt{n}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) \xrightarrow{\mathrm{d}} \mathrm{N}(\mathbf{0}, \boldsymbol{\mathcal{I}}^{-1}(\boldsymbol{\theta}^*))$ and simply uses the standard tools for the normal distribution to carry out inference
- **Proposition:** If regularity conditions (A)-(D)[1] hold,

$$(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \boldsymbol{\mathcal{I}}_n(\boldsymbol{\theta}^*)(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) \xrightarrow{\mathrm{d}} \chi^2_d$$

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

[1] If one assumes (A)-(C) only, the result still holds, but for the consistent sequence of roots (which may or may not be the MLE); this applies to all of the theorems in this lecture

Which information?

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

$$(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \boldsymbol{\mathscr{I}}_n(\boldsymbol{\theta}^*)(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) \xrightarrow{\mathrm{d}} \chi^2_d$$

$$(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \boldsymbol{\mathscr{I}}_n(\hat{\boldsymbol{\theta}})(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) \xrightarrow{\mathrm{d}} \chi^2_d$$

$$(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \boldsymbol{\mathcal{I}}_n(\boldsymbol{\theta}^*)(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) \xrightarrow{\mathrm{d}} \chi^2_d$$

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$$(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^\top \mathbf{V}_n(\hat{\boldsymbol{\theta}})(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*) \xrightarrow{\mathrm{d}} \chi^2_d,$$

  where $\mathbf{V}_n(\boldsymbol{\theta}) = \sum_i \mathbf{u}_i(\boldsymbol{\theta})\mathbf{u}_i(\boldsymbol{\theta})^\top$
- In practice, Wald approaches typically use $\boldsymbol{\mathcal{I}}_n(\hat{\boldsymbol{\theta}})$ or $\boldsymbol{\mathscr{I}}_n(\hat{\boldsymbol{\theta}})$

Nuisance parameters

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

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

  where $\boldsymbol{\mathscr{V}}_{11} = \boldsymbol{\mathscr{I}}^{11}$ is the (1,1) block of the inverse of $\boldsymbol{\mathscr{I}}(\boldsymbol{\theta}^*)$
- Again, recall that $\boldsymbol{\mathscr{V}}_{11}^{-1} = \boldsymbol{\mathscr{I}}_{11} - \boldsymbol{\mathscr{I}}_{12}\boldsymbol{\mathscr{I}}_{22}^{-1}\boldsymbol{\mathscr{I}}_{21}$, so that $\boldsymbol{\mathscr{V}}_{11}^{-1} \preceq \boldsymbol{\mathscr{I}}_{11}$ and $\boldsymbol{\mathscr{V}}_{11} \succeq \boldsymbol{\mathscr{I}}_{11}^{-1}$; 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:

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

  is an approximate $1-\alpha$ confidence interval for θ_j
- Again, this is *not* the same thing as

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

  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 around the score vector
- **Proposition:** If (A)-(C)[2] hold,

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

- Again, we can replace $\boldsymbol{\mathcal{I}}_n(\boldsymbol{\theta}^*)$ with any estimator $\hat{\boldsymbol{\mathcal{I}}}_n$ such that $\frac{1}{n}\hat{\boldsymbol{\mathcal{I}}}_n \xrightarrow{\text{P}} \boldsymbol{\mathcal{I}}(\boldsymbol{\theta}^*)$; score approaches typically use $\boldsymbol{\mathcal{I}}_n(\boldsymbol{\theta}_0)$ or $\boldsymbol{\mathcal{I}}_n(\boldsymbol{\theta}_0)$
- In principle, this can be inverted to find a confidence region, but in practice, doing so is usually not straightforward

[2] Don't need (D) here since the MLE doesn't appear

Nuisance parameters

- What about testing $H_0 : \boldsymbol{\theta}_1 = \boldsymbol{\theta}_0$?
- This is less straightforward than the Wald case
- We need to evaluate the score and information, but for what value of $\boldsymbol{\theta}$?
- Setting $\boldsymbol{\theta}_1 = \boldsymbol{\theta}_0$ seems obvious, but for $\boldsymbol{\theta}_2$, 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 $\hat{\boldsymbol{\theta}}_2(\boldsymbol{\theta}_0)$ as the value of $\boldsymbol{\theta}_2$ that maximizes $L(\boldsymbol{\theta})$ under the restriction that $\boldsymbol{\theta}_1 = \boldsymbol{\theta}_0$, with $\hat{\boldsymbol{\theta}}_0 = (\boldsymbol{\theta}_0, \hat{\boldsymbol{\theta}}_2(\boldsymbol{\theta}_0))$
- The following lemma will prove useful to us (its proof is essentially identical to the case for the unrestricted MLE $\hat{\boldsymbol{\theta}}$)
- **Lemma:** If (A)-(D) hold and $\boldsymbol{\theta}_0 = \boldsymbol{\theta}_1^*$, then

$$\sqrt{n}(\hat{\boldsymbol{\theta}}_2(\boldsymbol{\theta}_0) - \boldsymbol{\theta}_2^*) \xrightarrow{\mathrm{d}} \mathrm{N}(\mathbf{0}, \boldsymbol{\mathcal{I}}_{22}^{-1});$$

  note that here we *do* have convergence to $\boldsymbol{\mathcal{I}}_{22}^{-1}$, not $\boldsymbol{\mathcal{V}}_{22}$, as under H_0, we are not affected by uncertainty regarding $\boldsymbol{\theta}_1$
- Note that this only works if H_0 is true: if it isn't, $\hat{\boldsymbol{\theta}}_2(\boldsymbol{\theta}_0)$ may converge to something very different from $\boldsymbol{\theta}_2^*$

Score test with nuisance parameters

- **Theorem:** If (A)-(D) hold and $\boldsymbol{\theta}_0 = \boldsymbol{\theta}_1^*$, then

$$\mathbf{u}_1(\hat{\boldsymbol{\theta}}_0)^\top \boldsymbol{\mathscr{V}}_{11}^n(\hat{\boldsymbol{\theta}}_0)\mathbf{u}_1(\hat{\boldsymbol{\theta}}_0) \xrightarrow{\mathrm{d}} \chi^2_r,$$

  where $\boldsymbol{\mathscr{V}}^n = \boldsymbol{\mathscr{I}}_n^{-1}$
- In the special case where the parameter of interest is θ_j, we have $u_j(\hat{\boldsymbol{\theta}}_0)\sqrt{\mathscr{V}_{jj}^n(\hat{\boldsymbol{\theta}}_0)} \dot{\sim} \mathrm{N}(0,1)$
- 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 $\hat{\boldsymbol{\theta}}_2(\theta_0)$

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 $\mathbf{y} \sim \mathrm{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$; 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 $z_j \sim \mathrm{N}(0, 1)$ under the null hypothesis

Example: Linear regression (cont'd)

- In particular, note that the "expensive" part of this calculation, $\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top$, 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

Wald vs. Score: Univariate with nuisance parameters

- Comparing their univariate forms, the Wald test depends only on the MLE:

$$W_n = \frac{(\hat{\theta}_j - \theta_0)^2}{\mathcal{V}_{jj}^n(\hat{\boldsymbol{\theta}})}$$

- Meanwhile, the score test depends only on the restricted MLE:

$$S_n = u_j(\hat{\boldsymbol{\theta}}_0)^2 \, \mathcal{V}_{jj}^n(\hat{\boldsymbol{\theta}}_0)$$

  (both W_n and S_n follow approximate χ_1^2 distributions under the null)
- Note that $\mathcal{V}_{jj}^n$ shows up in different places for each test: $\boldsymbol{\mathcal{I}}$ is the variance of the score, but $\boldsymbol{\mathcal{I}}^{-1}$ is the variance of the MLE (with proper $\sqrt{n}$ scaling)

Likelihood ratio approach

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

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

- 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)-(D) hold and $\boldsymbol{\theta}_0 = \boldsymbol{\theta}_1^*$, then

$$2 \log \frac{L(\hat{\boldsymbol{\theta}})}{L(\hat{\boldsymbol{\theta}}_0)} \xrightarrow{\mathrm{d}} \chi^2_r$$

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

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,

$$\mathbf{u} = \begin{bmatrix} n \log \beta - n\psi_0(\alpha) + \sum \log x_i \\ n\alpha/\beta - \sum x_i \end{bmatrix}$$

$$\boldsymbol{\mathcal{I}}_n = \begin{bmatrix} n\psi_1(\alpha) & -n/\beta \\ -n/\beta & n\alpha/\beta^2 \end{bmatrix}$$

- 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 $\boldsymbol{\mathcal{I}}_n^{-1}(\hat{\boldsymbol{\theta}})$ corresponding to β is 0.118, so an approximate 95% confidence interval is given by

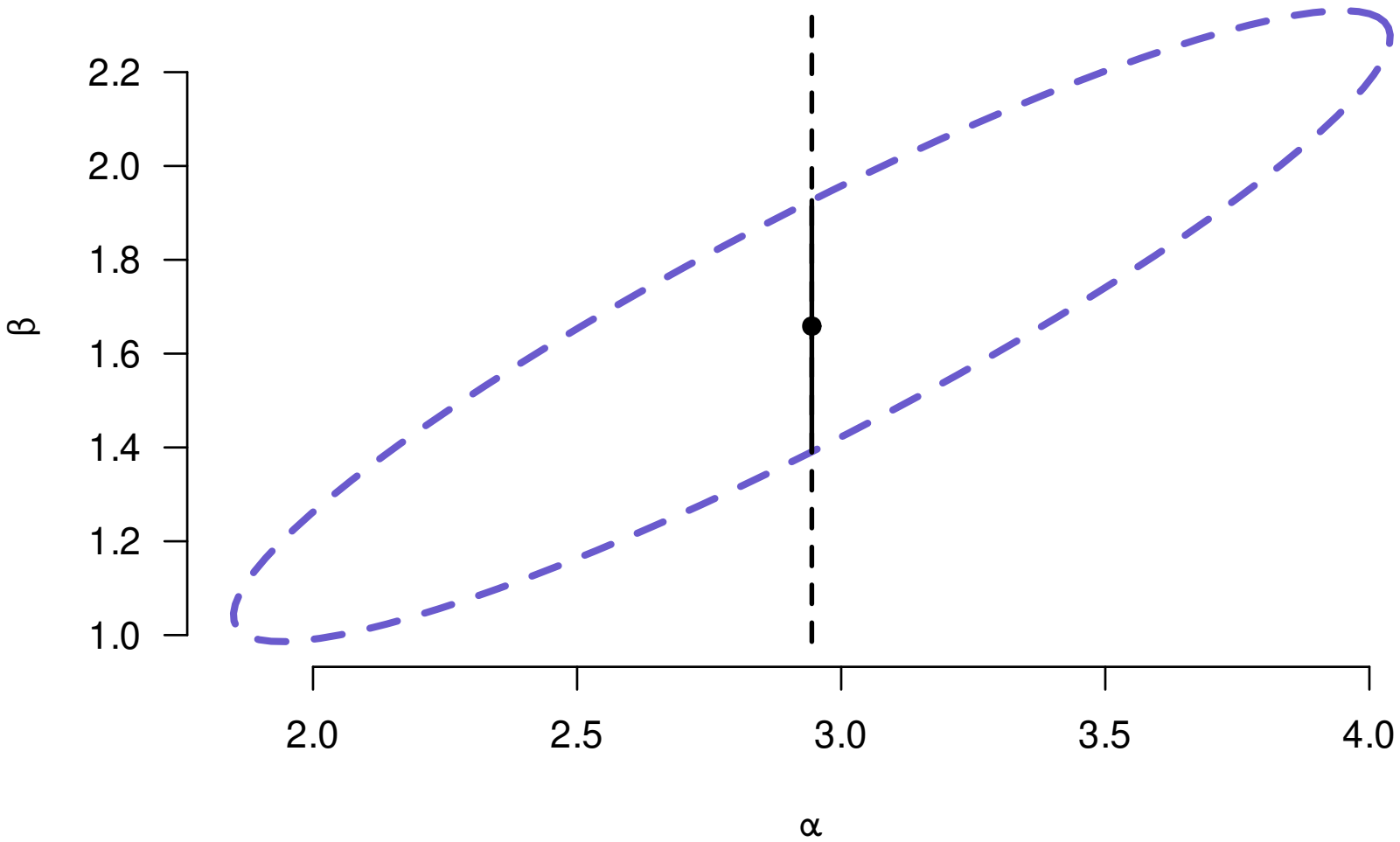
$$\hat{\theta}_2 \pm z_{0.975}\sqrt{\mathcal{V}_{22}^n(\hat{\boldsymbol{\theta}})} = (0.99, 2.33)$$

- Note that this is much wider than the incorrect interval we get from just inverting $\mathcal{I}_{22}^n(\hat{\boldsymbol{\theta}})$:

$$\hat{\theta}_2 \pm \frac{z_{0.975}}{\sqrt{\mathcal{I}_{22}^n(\hat{\boldsymbol{\theta}})}} = (1.39, 1.93);$$

  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 95% confidence interval, then, can be found by finding the two solutions of

$$u_2(\hat{\alpha}(\beta), \beta)^2 \mathscr{V}_{22}^n(\hat{\alpha}(\beta), \beta) = \chi^2_{1,0.95}$$

- 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)

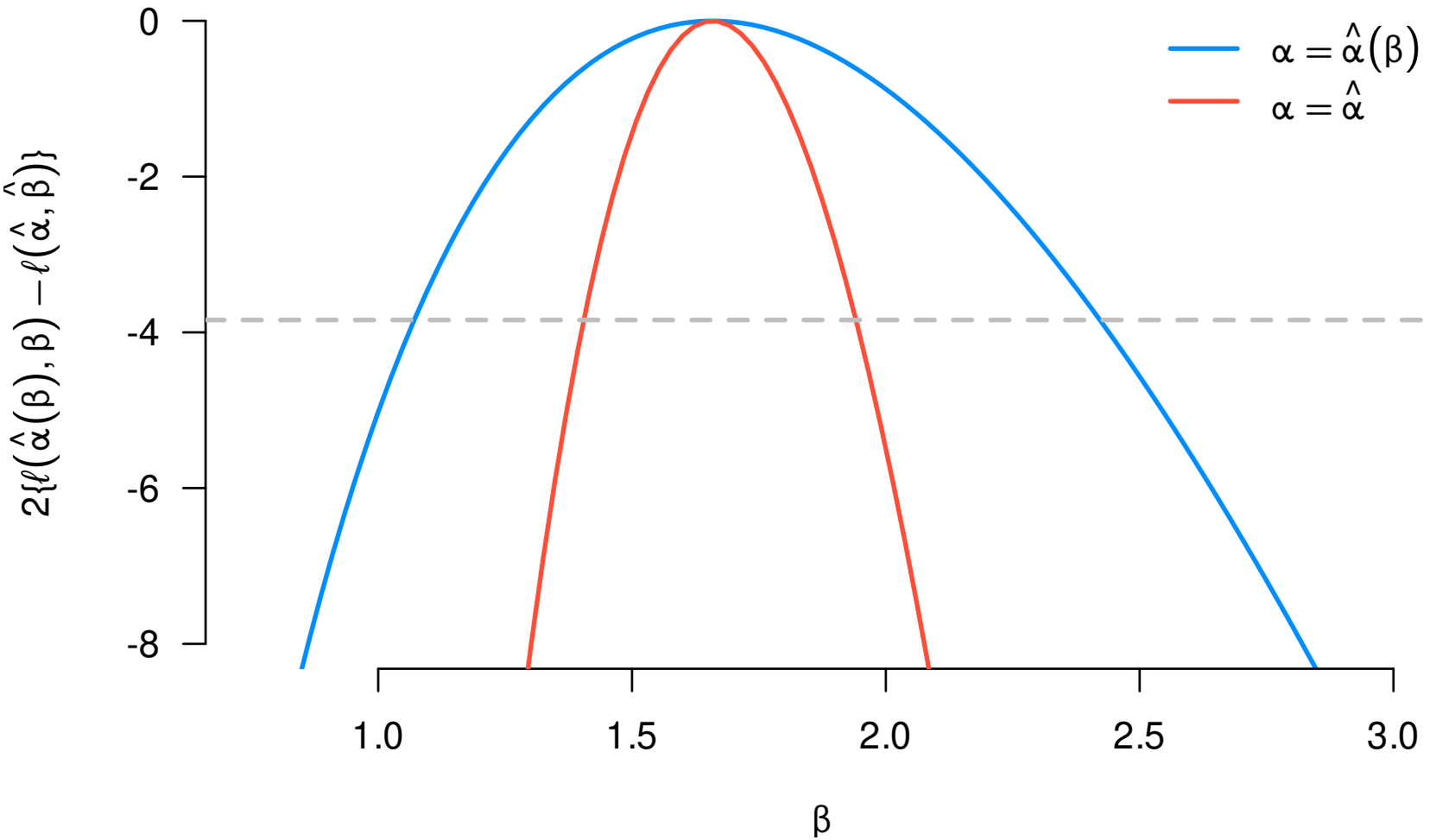
Likelihood ratio

- Similarly, finding the endpoints of the 95% likelihood ratio confidence interval involves finding the roots of

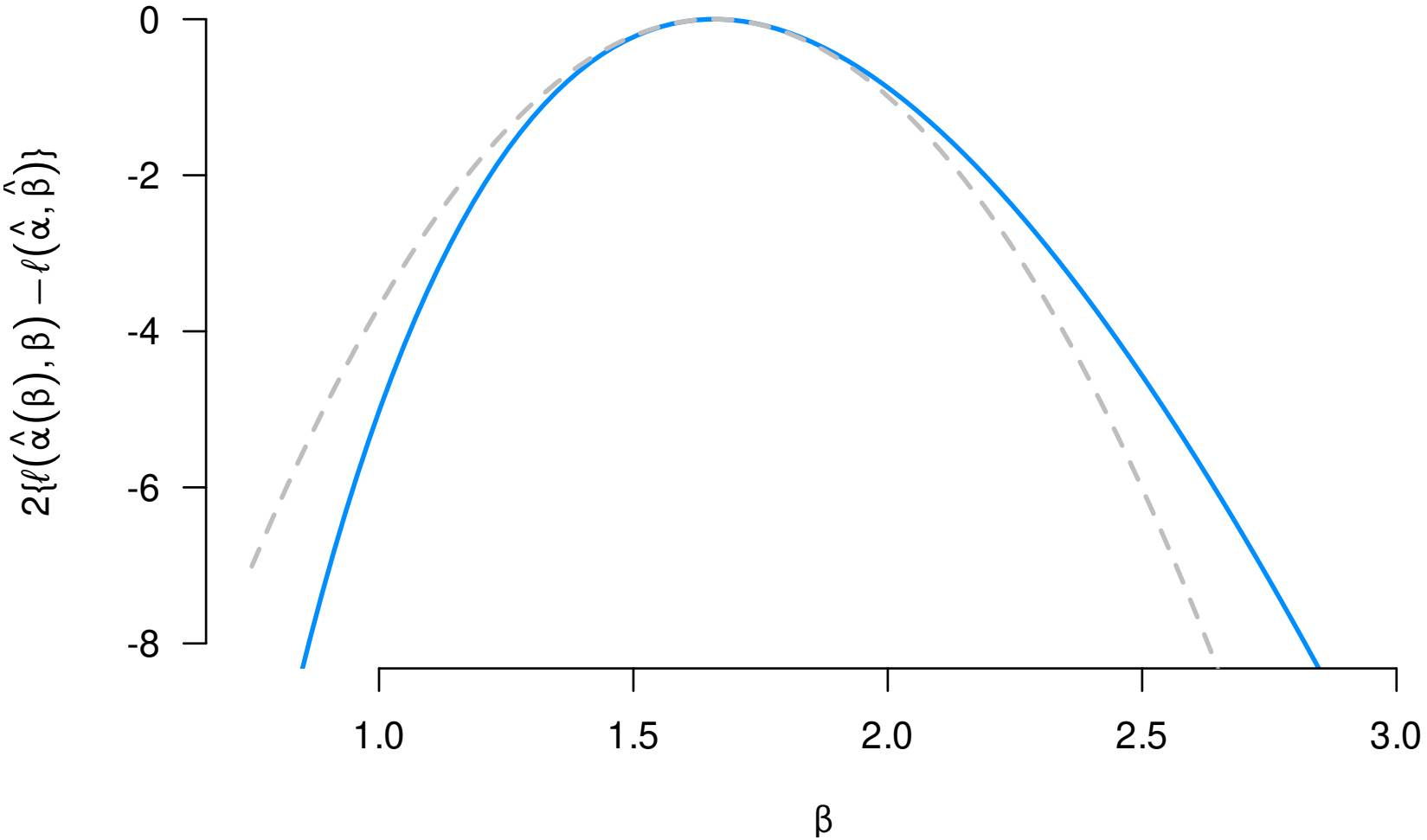
$$2\{\ell(\hat{\alpha}, \hat{\beta}) - \ell(\hat{\alpha}(\beta), \beta)\} = \chi^2_{1,0.95}$$

- This yields the interval (1.07, 2.42)

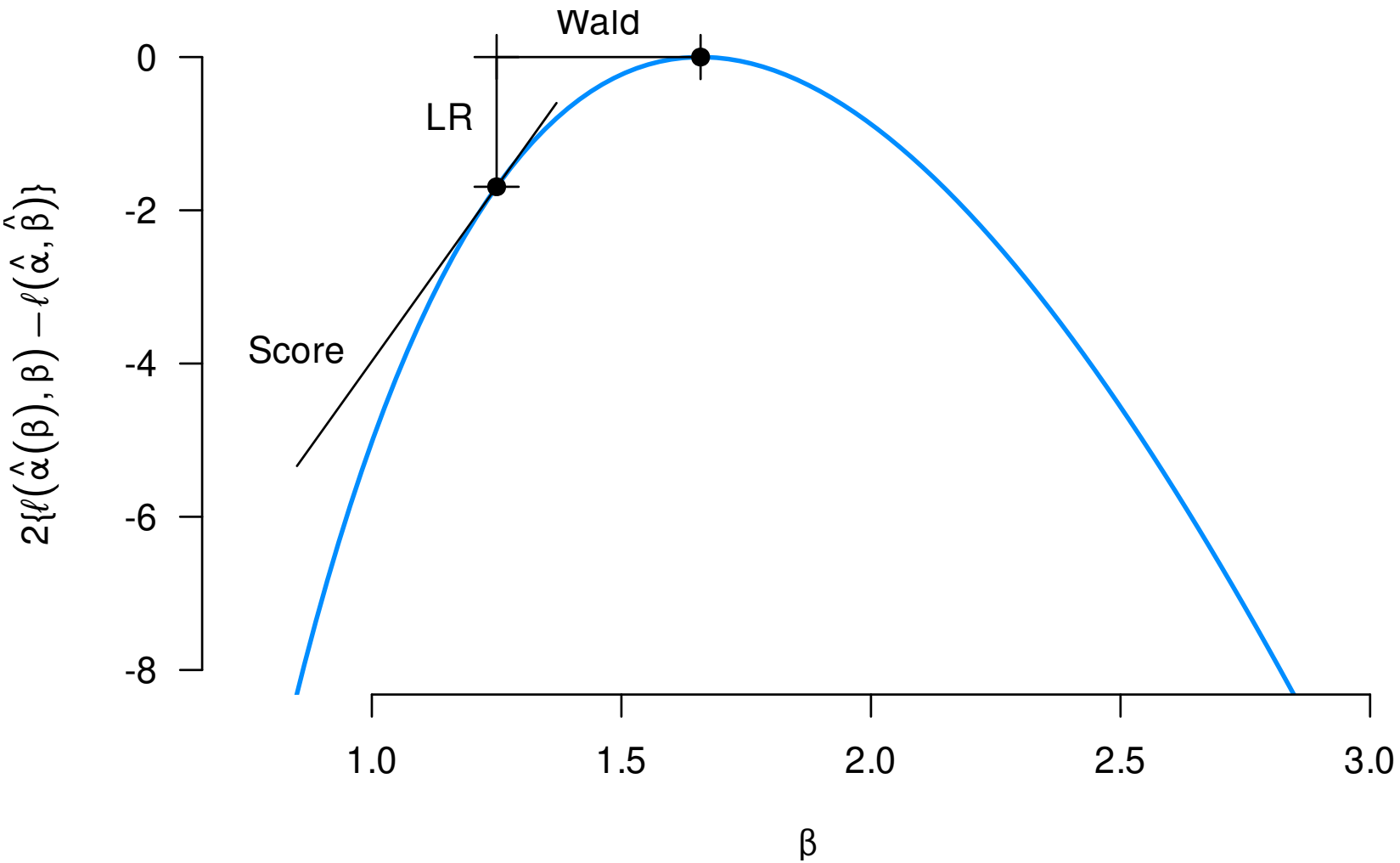
Likelihood ratio plot



Quadratic approximation



Visualization of all three methods



Final remarks

- Under H_0, 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,

$$\mathrm{LR}_n = W_n + o_p(1)$$
$$\mathrm{LR}_n = S_n + o_p(1);$$

  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 approximate inference

Superiority of the likelihood ratio approach

- The likelihood ratio approach tends to be the most accurate of the three; this has been shown in many theoretical and simulation studies
- The Wald approach depends on the parameterization (e.g., θ vs. $\log \theta$): it works well only if we happen to choose a parameterization in which ℓ is nearly quadratic
- In a sense, the LR approach finds this parameterization automatically
- The score test is less affected by parameterization, but like the Wald test, it relies only on local information (slope and curvature) at a single point; the LR test compares the log-likelihood itself at two points