Score and information

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Introduction

- In our previous lecture, we saw how likelihood-based inference works for exponential families
- Starting today, we are going to adopt a more general outlook on likelihood, and not make any specific assumptions about its form
- As we remarked at the outset of the course, the likelihood function is minimal sufficient
- This means that the *entire function* is the object that contains the information necessary for objective inference

Maximum likelihood estimation

- However, a number is of course much simpler and easier to communicate and manipulate than an entire function, so it is desirable to summarize and simplify the likelihood
- The single most important information about the likelihood is surely the value at which it is maximized
- The *maximum likelihood estimator*, $\hat{\boldsymbol{\theta}}$, of a parameter $\boldsymbol{\theta}$, given observed data $\mathbf{x}$, is

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} L(\boldsymbol{\theta}|\mathbf{x}).$$

- This was Fisher's original motivation for the likelihood (in his later years, however, he came to realize that likelihood was more than merely a device for producing point estimates)

Curvature

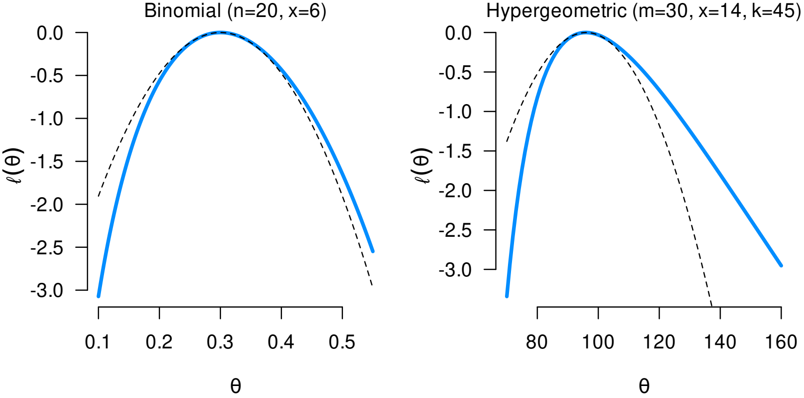
- A single number is not enough to represent a function
- However, if the likelihood function is approximately quadratic, then two numbers are enough to represent it: the location of its maximum and its curvature at the maximum
- Specifically, what I mean by this is that any quadratic function can be written

  $$f(x) = c(x - m)^2 + \text{Const},$$

  where c is the curvature and m the location of its maximum; the constant is irrelevant given our earlier remarks about how likelihood comparisons are only meaningful in the relative sense

Quadratic approximation: Illustration

The likelihood itself does not tend to be quadratic, but the *log-likelihood* does; from our first lecture:



Remarks

- Log is a monotone function, so the value of θ that maximizes the log-likelihood also maximizes the likelihood
- Even good approximations break down for $\boldsymbol{\theta}$ far from $\hat{\boldsymbol{\theta}}$: regularity is a local phenomenon
- As we will be referring to it often, we will use the symbol ℓ to denote the log-likelihood: $\ell(\boldsymbol{\theta}) = \log L(\boldsymbol{\theta})$
- The situation is similar in multiple dimensions; any quadratic function can be written

$$f(\mathbf{x}) = (\mathbf{x} - \mathbf{m})^\top \mathbf{C}(\mathbf{x} - \mathbf{m}) + \text{Const};$$

we now require a $d \times 1$ vector $\mathbf{m}$ to denote the location of the maximum and a $d \times d$ matrix $\mathbf{C}$ to describe the curvature

Regularity

- Likelihood functions that can be adequately represented by a quadratic approximation are called *regular*[1]
- Conditions that ensure the validity of the approximation are called *regularity conditions*
- We will discuss regularity conditions in detail later; for now, we will just assume that the likelihood is regular

[1]When we say that the likelihood has a quadratic approximation, what we really mean of course is that the log-likelihood has a quadratic approximation

The score statistic

- The derivative of the log-likelihood is a critical quantity for describing this quadratic approximation
- The quantity is so important that it is given its own name in statistics, the *score*, and often denoted $\mathbf{u}$:

$$\mathbf{u}(\boldsymbol{\theta}) = \nabla \ell(\boldsymbol{\theta}|\mathbf{x})$$

- Note that
  - $\mathbf{u}$ is a function of θ
  - For any given $\boldsymbol{\theta}$, $\mathbf{u}(\boldsymbol{\theta})$ is a random variable, as it depends on the data $\mathbf{x}$; usually suppressed in notation
  - For independent observations, the score of the entire sample is the sum of the scores for the individual observations:

$$\mathbf{u}(\boldsymbol{\theta}) = \sum_i \mathbf{u}_i(\boldsymbol{\theta})$$

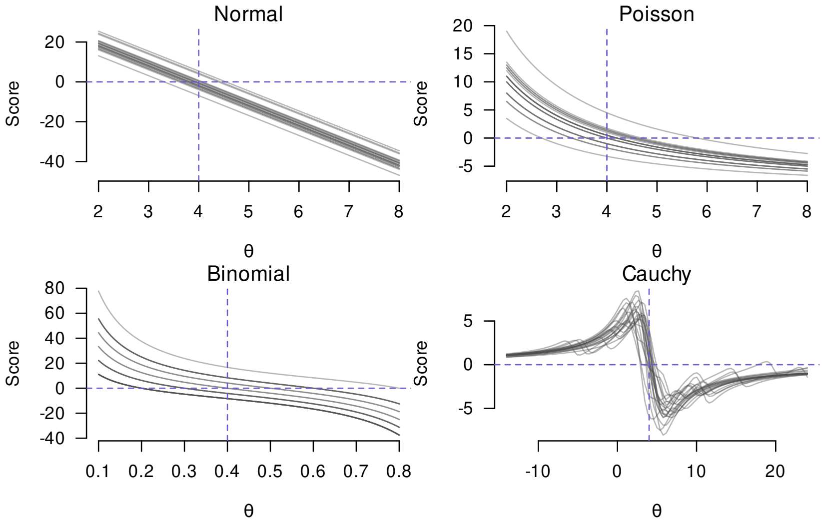
Score equations

- If the likelihood is regular, we can find $\hat{\boldsymbol{\theta}}$ by setting the gradient equal to zero; the MLE is the solution to the equation(s)

$$\mathbf{u}(\boldsymbol{\theta}) = \mathbf{0};$$

  this system of equations is known as the *score equation(s)* or sometimes the *likelihood equation(s)*
- For example, suppose we have $X_i \overset{\text{iid}}{\sim} \mathrm{N}(\theta, \sigma^2)$ with σ^2 known
  - $U_i(\theta) = (X_i - \theta)/\sigma^2$
  - $U(\theta) = \sum_i (X_i - \theta)/\sigma^2$
  - $U(\hat{\theta}) = 0 \implies \hat{\theta} = \bar{x}$

Illustration (vertical line at θ^*)



Information

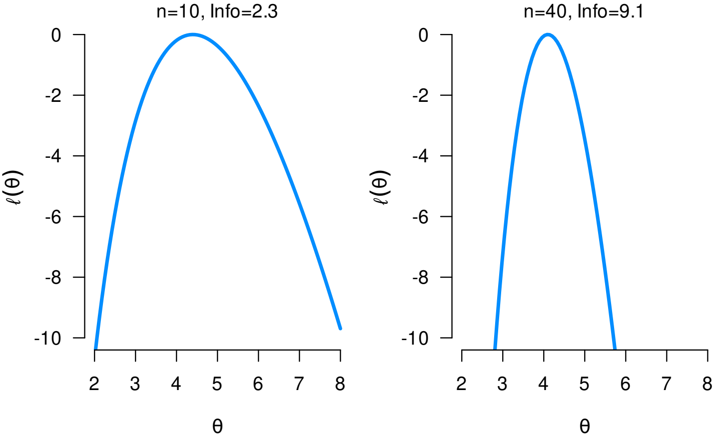
- Meanwhile, the curvature is given by the second derivative
- This quantity is called the *information*,

$$\boldsymbol{\mathcal{I}}_n(\boldsymbol{\theta}) = -\nabla^2 \ell(\boldsymbol{\theta});$$

  the negative sign arises because the curvature at the maximum is negative
- The name "information" is an apt description: the larger the curvature, the sharper (less flat) the peak, so the less uncertainty we have about $\boldsymbol{\theta}$

Information: Illustration

Random sample from the Poisson distribution:



Information: Example

- As an analytic example, let's return to the situation with $X_i \overset{\text{iid}}{\sim} \mathrm{N}(\theta, \sigma^2)$ and σ^2 known
  - $\mathcal{I}_i(\theta) = 1/\sigma^2$
  - $\mathcal{I}_n(\theta) = n/\sigma^2$
- Note that
  - For independent samples, the total information is the sum of the information obtained from each observation
  - Noisier data $\implies$ less information
- In general, the information depends on both X and θ (the normal is a special case); we'll return to this point later

Information: Another example

- As another example, suppose there are 5 observations taken from a $\mathrm{N}(\theta, 1)$ distribution, but we observe only the maximum $x_{(5)} = 3.5$
- Here, it is not clear how we would find the MLE, score, and information analytically, but we can use numerical procedures to optimize and calculate derivatives
- In this case, the information is 2.4, implying that knowing the maximum of 5 observations is worth 2.4 observations – better than a single observation, but not as good as having all 5 observations

Normal likelihood

- From an inferential standpoint, we can view this quadratic approximation as a normal approximation, as a quadratic log-likelihood corresponds to the Gaussian distribution
- As we mentioned in our first class, connecting likelihood to probability is challenging in general; however, it is easy in the case of the normal distribution
- For an iid sample from a $\mathrm{N}(\theta, \sigma^2)$ distribution (assuming σ^2 known; we'll consider the multiparameter case next), the likelihood is

$$
\begin{aligned}
L(\theta) &\propto \exp\left\{-\frac{1}{2\sigma^2}\sum_i (x_i - \theta)^2\right\} \\
&\propto \exp\left\{-\frac{n}{2\sigma^2}(\bar{x} - \theta)^2\right\}
\end{aligned}
$$

Likelihood ratios

- The likelihood ratio, then, is simply

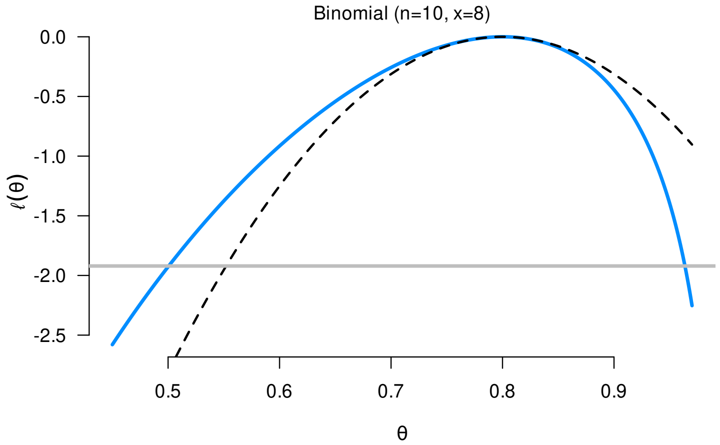
$$\log \frac{L(\theta)}{L(\hat{\theta})} = -\frac{n}{2\sigma^2}(\bar{x} - \theta)^2$$

- Furthermore, letting θ^* denote the true value of θ, we know that $(\bar{x} - \theta^*)/(\sigma/\sqrt{n}) \sim \mathrm{N}(0, 1)$, so

$$2 \log \frac{L(\hat{\theta})}{L(\theta^*)} \sim \chi^2_1$$

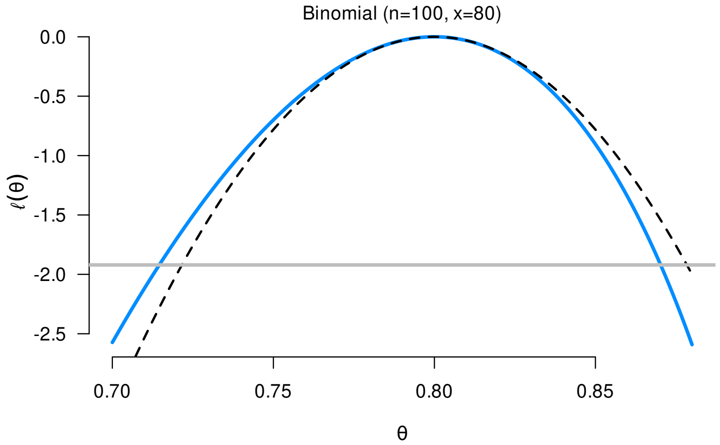
- In other words, if we want a 95% confidence interval, we should set $c = \exp\{-\frac{1}{2}\chi^2_{1,(.95)}\} \approx 0.15$

Binomial illustration (n=10, $\theta = 0.8$)



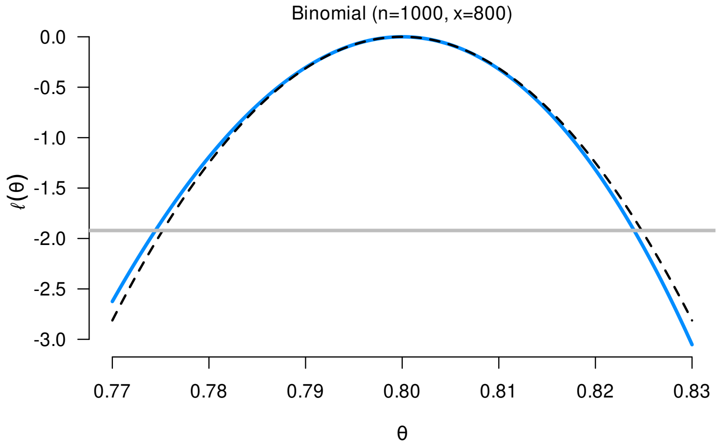
Actual coverage (simulation): 88.3%

Binomial illustration (n=100, $\theta = 0.8$)



Actual coverage (simulation): 93.2%

Binomial illustration (n=1000, $\theta = 0.8$)



Actual coverage (simulation): 94.9%

Multiparameter case

- Similarly, for the multivariate normal (assuming a nonsingular variance),

$$\log \frac{L(\boldsymbol{\theta})}{L(\hat{\boldsymbol{\theta}})} = -\tfrac{1}{2}(\bar{\mathbf{x}} - \boldsymbol{\theta})^\top \boldsymbol{\Sigma}^{-1}(\bar{\mathbf{x}} - \boldsymbol{\theta}),$$

  so the likelihood interval $\{\boldsymbol{\theta} : L(\boldsymbol{\theta})/L(\hat{\boldsymbol{\theta}}) \geq c\}$ has probability $\mathbb{P}(\chi^2_d \leq -2\log c)$ of containing $\boldsymbol{\theta}^*$
- Note that the presence of multiple parameters changes the probability calibration; for example, with $d = 5$
  - $c = 0.15$ now provides only a 0.42 probability of containing θ^*
  - We now need $c = 0.004$ to attain 95% coverage

"Pure" likelihood for multiparameter problems?

- The interval $\{\theta : L(\theta)/L(\hat{\theta}) \geq c\}$ is based purely on likelihood; as we remarked in our first lecture, the interval itself is neither Bayesian nor frequentist – those paradigms arise only in attempting to assign this interval a probability
- Is a "pure" likelihood approach possible in the multiparameter case (i.e., without the frequentist χ^2 calculations to guide us)?
- Suppose the (relative) likelihood of each parameter is (approximately) independent so that, for example, if $L(\theta_1) = 0.2$ and $L(\theta_2) = 0.2$, then $L(\boldsymbol{\theta}) = 0.2^2 = 0.04$
- Using $c = 0.15$ leads to something of a contradiction: θ_1 and θ_2 are both "likely", but somehow the pair (θ_1, θ_2) is "unlikely"

"Pure" likelihood for the multiparameter case

- An obvious solution is to use c^d: now if $L(\boldsymbol{\theta}) < 0.15^2$, then we must have $L(\theta_1) < 0.15$ or $L(\theta_2) < 0.15$
- Furthermore, we can write $\{\boldsymbol{\theta} : L(\boldsymbol{\theta})/L(\hat{\boldsymbol{\theta}}) < c^d\}$ as

$$2\ell(\boldsymbol{\theta}) - 2\ell(\hat{\boldsymbol{\theta}}) < 2d \log c,$$

  or, using the specific value $c = e^{-1}$,

$$-2\ell(\hat{\boldsymbol{\theta}}) + 2d < -2\ell(\boldsymbol{\theta})$$

- We have arrived at AIC: $\hat{\boldsymbol{\theta}}$ is an attractive model, despite adding d parameters, if the above inequality holds

Properties of the score: Introduction

- Earlier, we defined the score as the random function $\mathbf{u}(\boldsymbol{\theta}) = \nabla \ell(\boldsymbol{\theta}|\mathbf{x})$
- With some mild conditions, the random variable $\mathbf{u}(\boldsymbol{\theta}^*)$ turns out to have some rather elegant properties
- These properties are at the core of proving many important results about likelihood theory

Expectation

- We saw earlier that $\mathbf{u}(\boldsymbol{\theta}^*)$ tends to vary randomly about zero; let us now formalize this observation
- **Theorem:** Suppose the likelihood allows its gradient to be passed under the integral sign. Then $\mathbb{E}\mathbf{u}(\boldsymbol{\theta}^*) = \mathbf{0}$.
- A derivative is a type of limit, so whether or not it can be passed under the integral sign is governed by the dominated convergence theorem (we'll go into more details next lecture)
- Note that this is an *identity*, not an asymptotic relationship

Variance of the score

- Under similar conditions involving the second derivative, we also have a nice result involving the variance: namely, that the variance of the score is the expected information
- The variance of the score is called the *Fisher information*, which we will denote $\mathscr{I}$: $\mathscr{I}(\boldsymbol{\theta}) = \mathbb{V}\mathbf{u}(\boldsymbol{\theta}|X)$; its connection with our previous definition of information is made clear in the following theorem
- **Theorem:** Suppose the likelihood allows its Hessian to be passed under the integral sign. Then $\mathscr{I}(\boldsymbol{\theta}^*) = \mathbb{E}\mathcal{I}(\boldsymbol{\theta}^*|X)$.
- This requires the same sort of smoothness conditions as before, except now applied to the second derivatives

Remarks

- Recall that the information $\boldsymbol{\mathcal{I}}(\boldsymbol{\theta}) = -\nabla^2 \ell(\boldsymbol{\theta})$ depends on the data X
- By taking an expected value, we are essentially averaging over different data sets that could occur, weighted by their probability
- To distinguish between the two, the information using the observed data is called the *observed information*
- Note: Keep in mind that that $\boldsymbol{\mathcal{I}}$ is random, while $\boldsymbol{\mathscr{I}}$ is fixed

Notation

Notation to distinguish between all these information variants is not universal, but here is what I'll use in this class:

- $\mathcal{I}_i$ is the observed information for observation i
- $\mathscr{I}$ is Fisher information for observation i (for iid data, this will be the same for every observation, hence no i subscript)
- $\mathcal{I}_n$ is the observed information for the full sample
- $\mathscr{I}_n$ is the Fisher information for the full sample; if the data are iid then

$$\mathbb{E}\mathcal{I}_n = n\mathscr{I} = \mathscr{I}_n$$

- $\mathbf{I}$ is the identity matrix

Distribution

- Furthermore, since $\mathbf{u}(\boldsymbol{\theta}|\mathbf{x}) = \sum_i \mathbf{u}(\boldsymbol{\theta}|x_i)$, we can apply the central limit theorem to see that

$$\sqrt{n}\{\bar{\mathbf{u}}(\boldsymbol{\theta}^*) - \mathbb{E}\mathbf{u}(\boldsymbol{\theta}^*)\} \xrightarrow{\mathrm{d}} \mathrm{N}(\mathbf{0}, \boldsymbol{\mathscr{I}}(\boldsymbol{\theta}^*)),$$

or

$$\frac{\mathbf{u}(\boldsymbol{\theta}^*)}{\sqrt{n}} \xrightarrow{\mathrm{d}} \mathrm{N}(\mathbf{0}, \boldsymbol{\mathscr{I}}(\boldsymbol{\theta}^*))$$

- Showing that the maximum likelihood estimators, on the other hand, are asymptotically normal (thereby justifying our earlier normal-based inferential procedures) involves a bit more work (we'll take up this question in a later lecture)

Observed vs expected information

- Earlier, we discussed the idea that the width of confidence intervals depends on the information
- We've now introduced two kinds of information; which should we use for inferential purposes?
- Broadly speaking, either one is fine: by the WLLN, $\frac{1}{n}\boldsymbol{\mathcal{I}}(\boldsymbol{\theta}) \xrightarrow{\text{P}} \boldsymbol{\mathscr{I}}(\boldsymbol{\theta})$, so we have both

$$\boldsymbol{\mathscr{I}}_n(\boldsymbol{\theta}^*)^{-1/2}\mathbf{u}(\boldsymbol{\theta}^*) \xrightarrow{\text{d}} \text{N}(\mathbf{0}, \mathbf{I})$$

and

$$\boldsymbol{\mathcal{I}}_n(\boldsymbol{\theta}^*)^{-1/2}\mathbf{u}(\boldsymbol{\theta}^*) \xrightarrow{\text{d}} \text{N}(\mathbf{0}, \mathbf{I})$$

assuming $\boldsymbol{\mathscr{I}}$ and $\boldsymbol{\mathcal{I}}$ are positive definite

Observed vs expected information (cont'd)

- In practice as well, the difference between the two is typically not very important or noticeable
- However, they aren't the same . . . surely one tends to be better than the other?
- I'll present some advantages of both observed and expected information, but remember that they are far more alike than they are different

Advantages of Fisher information

The Fisher information has two major advantages

- Smoothness and stability
  - Especially when n is small, the observed information can be noisy, whereas its expectation is more unstable
  - Fisher information is particularly attractive for software to avoid numerical issues
- Mathematical tractability
  - In many models, the Fisher information is easy to derive and results in a great deal of cancellation, leading to much simpler formulas

Advantages of observed information

To illustrate the advantages of observed information, let's consider $T_i \overset{\text{iid}}{\sim} \text{Exp}(\theta)$ subject to right censoring, where the observed information is d/θ^2 while the expected information is $\mathbb{E}d/\theta^2$, with d the number of uncensored events

- *Always available:* Fisher information can be impractical / impossible to calculate
- *Relevance:* Suppose we observed more events than expected… is it really relevant that we could have obtained a sample with less information?
- *Accuracy:* In general, theoretical analysis and simulation studies indicate that observed information results in more accurate inference (Efron and Hinkley, 1978)