STSCI 4780: Continuous parameter estimation, cont'd

Tom Loredo, CCAPS & SDS, Cornell University

2020-02-06

Plan

Inference with discrete spaces

- Lec03: Binary hypothesis space (C, \overline{C}) , binary data (+, -)
- **Lec04:** Larger discrete hypothesis space (doors, α_i), discrete data from *multiple* binary outcomes

Inference with continuous spaces

- PDFs vs. PMFs
- Bernoulli trials with continous parameter space
- Multinomial distribution: Multiple, discrete outcomes (categorical data)
- Poisson distribution: Inferring rates from count data over intervals

Recap

- PMFs on discrete spaces, PDFs on continuous spaces
- BT holds for PDFs ($d\theta$'s cancel)
- Estimating the outcome probability, α , for binary outcomes

Setup

 ${\cal C}$ specifies existence of two outcomes, ${\cal S}$ and ${\cal F}$, in each of ${\cal N}$ cases or trials; for each case or trial, the probability for ${\cal S}$ is α ; for ${\cal F}$ it is $(1-\alpha)$

The trial probabilities are *IID* (independent and identically distributed)

 H_i = Statements about α , the probability for success on the next trial \rightarrow seek $p(\alpha|D,C)$

Adopt a *flat/uniform prior* as a default expression of initial ignorance about α — two motivations

Posterior (using sequence, binomial, negative binomial data)

$$p(\alpha|D,C) = \frac{(N+1)!}{n!(N-n)!}\alpha^n(1-\alpha)^{N-n}$$

A Beta distribution.

Beta distribution (in general)

A two-parameter family of distributions for a quantity α in the unit interval [0,1]:

$$p(\alpha|a,b) = \frac{1}{B(a,b)} \alpha^{a-1} (1-\alpha)^{b-1}$$

A PDF over possible 2-outcome PMFs

The beta-binomial conjugate model

Generalize from the flat prior to a $Beta(\alpha|a,b)$ prior for α

$$p(\alpha|n, M') \propto \operatorname{Beta}(\alpha|a, b) \times \operatorname{Binom}(n|\alpha, N)$$

 $\propto \alpha^{a-1} (1-\alpha)^{b-1} \times \alpha^{n} (1-\alpha)^{N-n}$
 $\propto \alpha^{n+a-1} (1-\alpha)^{N-n+b-1}$

 \Rightarrow the posterior is Beta($\alpha | n + a, N - n + b$)

When the prior and likelihood are such that the posterior is in the same family as the prior, the prior and likelihood are a *conjugate* pair

A Beta prior is a conjugate prior for the Bernoulli process, binomial, and negative binomial sampling distributions

Conjugacy \rightarrow it's easy to chain inferences from multiple experiments

Probability & frequency

Recall $\hat{\alpha}=\frac{n}{N}$, the *relative frequency* of successes; also $\sigma_{\alpha}\approx\frac{\sqrt{n}}{N}$ for $N,n\gg 1$

Frequencies arise when modeling repeated trials, or repeated sampling from a population or ensemble.

Finite-sample frequencies are observables

- When available, can be used to infer probabilities for next trial
- When unavailable, can be predicted

Bayesian/Frequentist relationships

- Relationships between probability and frequency
- Long-run performance of Bayesian procedures in IID settings (no accumulation of information)

Probability & frequency in IID settings

Frequency from probability

Bernoulli's (weak) law of large numbers: In repeated IID trials, given $P(\text{success}|...) = \alpha$, predict

$$rac{ extit{n}_{ ext{success}}}{ extit{N}_{ ext{total}}}
ightarrow lpha \quad ext{as} \quad extit{N}_{ ext{total}}
ightarrow \infty$$

"Bernoulli's swindle" — B. argued this justified estimating a next-trial probability with a (finite-sample) frequency

Probability from frequency

Bayes's "An Essay Towards Solving a Problem in the Doctrine of Chances" \rightarrow First use of Bayes's theorem:

Probability for success in next trial of IID sequence:

$$\mathbb{E}(lpha)
ightarrow rac{n_{
m success}}{N_{
m total}} \quad {
m as} \quad N_{
m total}
ightarrow \infty$$

If P(success|...) does not change from sample to sample, it may be estimated using relative frequency data

Categorical data

 $D = \text{Discrete outcomes from } N \text{ observed trials, } o_1 o_2 o_3 \dots o_N$:

Roles of a die: 321344622...

Customer choices: AAOBBOOO... (Apple, Banana, Orange)

 $\mathcal{C} = \text{Each outcome in one of } K \text{ categories; parameters } \alpha \equiv \{\alpha_k\} \text{ such that } P(o_i = k | \alpha, \dots, \mathcal{C}) = \alpha_k \text{ (categorical distribution)}$

Constraint: $\sum_k \alpha_k = 1$; equivalently $\alpha_K = 1 - \sum_{k=1}^{K-1} \alpha_k$ I.e., the K-dimensional α must lie on the (K-1)-dimensional standard simplex:



Sequence sampling dist'n/Likelihood function

$$p(D|\alpha, C) = p(o_1 = k_1|\alpha, C) \times p(o_2 = k_2|\alpha, C) \times \cdots$$

$$= \prod_k \alpha_k^{n_k}$$

$$\equiv \mathcal{L}(\alpha)$$

The counts (frequencies) are sufficient statistics

Count data sampling dist'n/Likelihood function

Take $D' = \{n_k\}$ (e.g., histogram); then the sampling PMF is a *multinomial dist'n*:

$$p(D'|\alpha, \mathcal{C}) = \frac{N!}{\prod_{k} n_{k}!} \prod_{k} \alpha_{k}^{n_{k}}$$

$$\propto \mathcal{L}(\alpha)$$

The factor $N!/\prod_k n_k!$ counts the number of sequences having the stated numbers of outcomes in each category

Uniform prior

Prior PDF over (K-1)-D standard simplex:

$$p(\alpha_1, \dots, \alpha_{K-1} | \mathcal{C}) = \begin{cases} \mathcal{C} & \text{for } 0 \leq \alpha_k \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

with 1/C= "volume" of the (K-1)-D standard simplex satisfying the normalization constraint (one of the boundaries of the K-D corner simplex in the full α space)

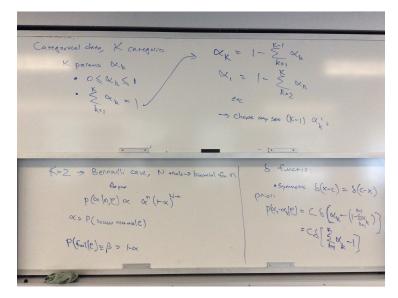
Posterior

Posterior PDF over (K-1)-D standard simplex (using either D or D'):

$$\begin{split} p(\alpha_1, \dots, \alpha_{K-1} | D, \mathcal{C}) &\propto \\ &\left\{ \begin{bmatrix} \prod_{k=1}^{K-1} \alpha_k^{n_k} \end{bmatrix} \left(1 - \sum_{k=1}^{K-1} \alpha_k \right)^{n_K} & \text{for } 0 \leq \alpha_k \leq 1 \\ 0 & \text{otherwise} \\ \end{bmatrix} \end{split}$$

This has the form of a *Dirichlet dist'n* (the multivariate generalization of the beta dist'n)

Note that we are treating the α_k parameters asymmetrically, which can make some inferences awkward (e.g., the posterior for α_K)



Symmetrical treatment with delta functions

Write a PDF over a (K-1)-D standard simplex as a K-D function *constrained* to lie on the (K-1)-D simplex:

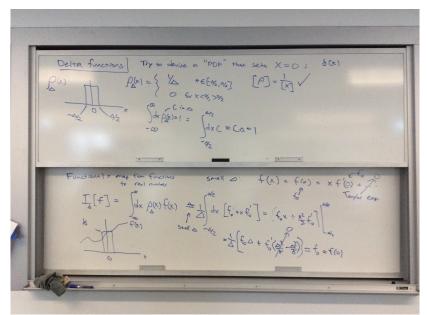
$$p(\alpha_1,\ldots,\alpha_K|\ldots) = p(\alpha_1,\ldots,\alpha_{K-1}|\ldots) \times p(\alpha_K|\alpha_1,\ldots,\alpha_{K-1},\ldots)$$

where $p(\alpha_K | \alpha_1, \dots, \alpha_{K-1}, \dots)$:

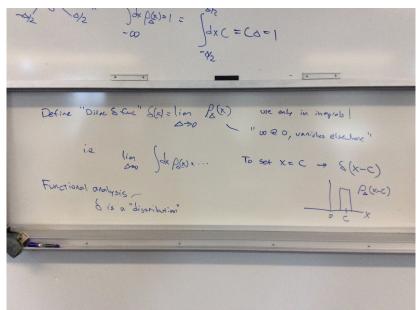
- Must set $\alpha_K = 1 \sum_{k=1}^{K-1} \alpha_k$
- Must be a proper PDF (normalized!)

The Dirac delta function, $\delta(x)$, can accomplish this

Delta function development, whiteboards 1 & 2



Delta function development, whiteboard 3



Normalization constant

Generalized beta integral:

$$\int_{0}^{\infty} d\alpha_{1} \cdots \int_{0}^{\infty} d\alpha_{K} \ \alpha_{1}^{\kappa_{1}-1} \cdots \alpha_{K}^{\kappa_{K}-1} \ \delta \left(\mathbf{a} - \sum_{k} \alpha_{k} \right) = \frac{\Gamma(\kappa_{1}) \cdots \Gamma(\kappa_{K})}{\Gamma(\kappa_{0})} \ \mathbf{a}^{\kappa_{0}-1}$$

with $\kappa_0 \equiv \sum_{k=1}^K \kappa_k$

With a = 1 this is also known as the multinomial beta function

$$\Rightarrow p(\alpha|D,C) = \frac{(N+K-1)!}{n_1!\cdots n_K!} \left[\prod_k \alpha_k^{n_k}\right] \delta\left(1-\sum_k \alpha_k\right)$$

For K = 2 we recover beta posterior from Bernoulli/binomial cases

Marginal PDF for one category

Consider K = 3, but suppose we are interested only in α_1 :

$$p(\alpha_{1}|D,C) = \int d\alpha_{2} \int d\alpha_{3} \ p(\alpha|D,C)$$

$$= C\alpha_{1}^{n_{1}} \int d\alpha_{2} \int d\alpha_{3} \ \alpha_{2}^{n_{2}} \alpha_{3}^{n_{3}}$$

$$\times \delta \left[(1 - \alpha_{1}) - (\alpha_{2} + \alpha_{3}) \right]$$

$$= C'\alpha_{1}^{n_{1}} (1 - \alpha_{1})^{n_{2} + n_{3} + 1}; \text{ note } n_{2} + n_{3} = N - n_{1}$$

The marginal for a single category is a beta PDF, almost as if the data from the other categories were pooled—but not quite.

For the K=3 case, there's an $N-n_1+1$ exponent, instead of the $N-n_1$ we might expect from pooling the data. This hints at a problem with the uniform prior we adopted; see Lab04 and Assignment03.

Dirichlet distributions

A family of "PDFs for PMFs," i.e., densities over possible categorical or multinomial distributions:

$$\operatorname{Dir}(\alpha|\kappa_1,\ldots,\kappa_K) = \frac{\Gamma(\kappa_0)}{\Gamma(\kappa_1)\cdots\Gamma(\kappa_K)} \left[\prod_{k=1}^K \alpha_k^{\kappa_k-1}\right] \delta\left(1 - \sum_{k=1}^K \alpha_k\right)$$

with $\kappa_0 = \sum_k \kappa_k$; the κ_k are concentration parameters

Mode: $\hat{\alpha}_k = \frac{\kappa_k - 1}{\kappa_0 - K}$ for $k = 1 \dots K$

Marginal means: $\mathbb{E}(\alpha_k) = \frac{\kappa_k}{\kappa_0}$

Marginal variances: $Var(\alpha_k) = \frac{\kappa_i(\kappa_0 - \kappa_i)}{\kappa_0^2(\kappa_0 + 1)}$

All covariances *negative* (necessarily!)

Special case: *Symmetric Dirichlet* with $\kappa_i = \kappa$

Dirichlet distribution priors are *conjugate priors* for categorical and multinomial likelihood functions

Simplex/ternary plots

