ST790 — Fall 2022 Imprecise-Probabilistic Foundations of Statistics

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Week 11a

- Multinomial model
- Prediction of a categorical response
- A few different approaches¹
 - gBayes based on Walley's Imprecise Dirichlet Model
 - Denoeux's confidence-region-based belief function
 - my new prediction IM

...

¹Not an exhaustive list, e.g., conformal prediction can be applied here too

Multinomial model

• Consider a set of $K \ge 2$ categories

- could be ordered (e.g., small, medium, large)
- could be unordered (e.g., red, blue, green)
- Let X denote a random variable on $\mathbb{X} = \{1, 2, \dots, K\}$
- Distribution P of X determined by a probability vector

$$\theta_k = \mathsf{P}(X = k), \quad k = 1, \dots, K$$

All three are equivalent:

parameter space T for θ = (θ₁,...,θ_K)
 set of all probability distributions P for X
 probability simplex in R^K

Multinomial model, cont.

• Let
$$X^n = (X_1, \ldots, X_n)$$
 be iid copies of X

Likelihood function is

....

$$L_n(\theta) \propto \prod_{k=1}^{K} \theta_k^{N_k}, \quad N_k(X^n) = |\{i : X_i = k\}|$$

This likelihood is "nonparametric" by above equivalence
For inference on θ (equivalently, on P):

• maximum likelihood, $\hat{\theta}_k = N_k/n$

Bayes, e.g., with Dirichlet prior (below)

• Our goal here is predicting a new observation, X_{n+1}

Dirichlet distribution

- Dir_{\mathcal{K}}(β): continuous distribution on the simplex $\mathbb{T} \subset \mathbb{R}^{\mathcal{K}}$
- Density function,² depending on $\beta = (\beta_1, \dots, \beta_K)$,

$$artheta\mapsto c(eta)\prod_{k=1}^{\mathcal{K}}artheta_k^{eta_k-1},\quadartheta\in\mathbb{T}$$

It's the Bayesian conjugate prior for multinomial models³

• if $\Theta \sim \text{Dir}_{K}(\beta)$ • and $(X^{n} | \Theta = \theta) \stackrel{\text{iid}}{\sim} \text{Mult}_{K}(\theta)$ • then $(\Theta | X^{n} = x^{n}) \sim \text{Dir}_{K}(\beta + N(x^{n}))$ • and the predictive distribution is

$$\mathsf{P}(X_{n+1}=k\mid x^n)=\frac{\beta_k+N_k(x^n)}{\sum_{\kappa=1}^K\beta_\kappa+N_\kappa(x^n)},\quad k=1,\ldots,K$$

²https://en.wikipedia.org/wiki/Dirichlet_distribution ³This is the basis for Ferguson's Dirichlet process developments

Walley's imprecise Dirichlet model

- \blacksquare The Bayesian analysis above depends on the choice of β
- If information about β is available, then fine
- If not, then what? A "default" choice?
- Walley⁴ aimed to be more careful by allowing the Dirichlet prior to be *imprecise*, i.e., a set of Dirichlet priors
- Reparametrization of the Dirichlet model:
 - mean vector $t = (t_1, \ldots, t_K) \in \mathbb{T}$ and precision s > 0
 - then $\beta_k = st_k$, for $k = 1, \ldots, K$
- Walley proposed a prior credal set

$$\mathscr{C}(s) = \{\mathsf{Dir}_{\mathcal{K}}(s,t) : t \in \mathbb{T}\}$$

Almost vacuous...

⁴Walley (*JRSS-B* 1996), "Learning about a bag of marbles"

By the conjugacy result above, the posterior credal set is

$$\mathscr{C}(\mathbf{x}^n; \mathbf{s}) = \{ \mathsf{Dir}_{\mathcal{K}}(\mathbf{s} + n, t^n) : t_k^n = rac{\mathbf{s} t_k + N_k(\mathbf{x}^n)}{\mathbf{s} + n}, \ t \in \mathbb{T} \}$$

- This is a set of posterior distributions for Θ, so gBayes inference on Θ calculates lower/upper envelopes
- Our goal is prediction of X_{n+1}, and the above credal set for a collection of predictive distributions indexed by (s, xⁿ)
- Read off the lower/upper prediction probabilities:

$$\underline{\Pi}_{x^n,s}(A) = \frac{\sum_{k \in A} N_k(x^n)}{s+n}$$

$$\overline{\Pi}_{x^n,s}(A) = \frac{s + \sum_{k \in A} N_k(x^n)}{s+n}, \quad A \subseteq \mathbb{X}$$

Imprecision is controlled by the precision s

- large s means wider spacing between $\underline{\Pi}_{x^n,s}$ and $\overline{\Pi}_{x^n,s}$
- small s means narrower spacing
- can interpret s as a "learning rate"

Properties:

- super-simple to implement
- it's generalized Bayes, so entirely coherent
- output is a belief function in this case⁵

• both
$$\underline{\Pi}_{x^n,s}$$
 and $\overline{\Pi}_{x^n,s}$ converge to true P as $n \to \infty$

· · ·

 Walley considered the multinomial model specifically, but these ideas extend to other exponential families⁶

$${}^{5}m(\{k\}) = N_k/(n+s)$$
, for $k = 1, \dots, K$, and $m(\mathbb{X}) = s/(n+s)$
⁶e.g., Quaeghebeur & de Cooman (*ISIPTA* 2005)

Denoeux's belief function

- Thierry Denoeux is a leader in the belief function community, fundamental work on stat inference & ML
- A really nice paper⁷ of his is on the construction of a belief function for predicting X_{n+1} ~ Mult_K(·)
- Background:
 - I showed you Dempster's framework for K = 2 (binomial)
 - a belief function for prediction follows readily
 - computationally challenging for $K \ge 3...^8$
 - very recent work⁹ helps to overcome this challenge
- Denoeux's paper gives a relatively simple alternative to Dempster's approach for general K

⁹Jacob et al (*JASA* 2021)

⁷Denoeux (*IJAR* 2006)

⁸Dempster (Ann Math Stat 1966)

Denoeux's belief function, cont.

- Goal: a belief function <u>Π</u>_{Xⁿ} on X for predicting/quantifying uncertainty about the next observation X_{n+1}
- Lots of options, need some properties we want $\underline{\Pi}_{X^n}$ to satisfy
- Denoeux's two requirements:

R1 $\underline{\Pi}_{X^n}(A) \to \mathsf{P}(A)$ in P-probability, all $A \subseteq \mathbb{X}$, as $n \to \infty$ R2 For a given $\alpha \in (0, 1)$,

$$\mathsf{P}\{\underline{\Pi}_{X^n}(A) \leq \mathsf{P}(A) \text{ for all } A\} \geq 1 - \alpha$$

- Both are reasonable
- Superficially at least, R2 looks similar to validity, but it's actually very different; more later
- How to find $\underline{\Pi}_{X^n}$ that satisfies R1 and R2?

Denoeux's belief function, cont.

Recall:

- the multinomial parameter $\theta = (\theta_1, \dots, \theta_K)$
- equivalance between θ and P
- A $100(1-\alpha)$ % confidence region $C_{\alpha}(X^n)$ for θ satisfies

$$\mathsf{P}\{C_{\alpha}(X^{n}) \ni \theta\} \geq 1 - \alpha$$

For
$$C_{\alpha}(X^n)$$
, Denoeux recommends
 $C_{\alpha}(X^n) = [\theta_1^-, \theta_1^+] \times \cdots \times [\theta_K^-, \theta_K^+]$
where

$$\theta_k^{\pm} = \frac{a + 2N_k \pm \Delta_k^{1/2}}{2(n+a)}$$

• with a = qchisq(1 - lpha, df = 1) and

$$\Delta_k = a \Big\{ a + \frac{4N_k(n-N_k)}{n} \Big\}$$

Denoeux's belief function, cont.

Each θ in C_α(Xⁿ) corresponds to a probability dist on X
 Lower envelope defines a candidate solution

$$\underline{\Pi}^{\mathsf{tmp}}_{X^n}(A) = \max\Big\{\sum_{k\in A}\theta^-_k, 1-\sum_{k\not\in A}\theta^+_k\Big\}, \quad A\subseteq \mathbb{X}$$

- Properties:
 - easy to check R1, $n^{-1}N_k(X^n) \rightarrow \theta_k = P(X = k)$ ■ similarly for R2, i.e.,

 $\mathsf{P}\{\underline{\Pi}_{X^n}^{\mathsf{tmp}} \text{ lower-bounds } \mathsf{P}\} = \mathsf{P}\{C_{\alpha}(X^n) \ni \theta(\mathsf{P})\} \ge 1 - \alpha$

note that <u>Π</u>_{Xⁿ} depends on α...
 However, <u>Π</u>^{tmp}_{Xⁿ} isn't a belief function¹⁰ when K > 3

¹⁰But it is a 2-monotone capacity...

- Denoeux wants the output to be a belief function, so he needs to modify $\prod_{X^n}^{tmp}$ in a suitable way
- Natural idea: inner approximation of $\prod_{X^n}^{tmp}$ by a belief function
- This approximation is more complicated, requires optimization via solving a linear program
- Too messy to present here, but apparently easy to do
- Denoeux shows that the output, $\underline{\prod}_{X^n}$, of this optimization routine is a belief function and satisfies R1 and R2

Valid prediction IM

- In discrete settings, nonparametric = parametric
- Can do the IM stuff from before with multinomial modelIf I take a vacuous prior, then

$$\pi_{x^n}(\kappa) = \sup_{\theta} \mathsf{P}_{X^n, X_{n+1}|\theta} \{\eta(X^n, X_{n+1}) \le \eta(x^n, \kappa)\}$$

where

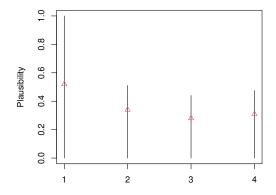
$$\eta(\mathbf{x}^{n},\kappa) = \frac{\sup_{\theta} \theta_{\kappa}^{N_{\kappa}+1} \prod_{k \neq \kappa} \theta_{k}^{N_{k}}}{\max_{\zeta} \sup_{\theta} \theta_{\zeta}^{N_{\zeta}+1} \prod_{k \neq \zeta} \theta_{k}^{N_{k}}}$$

Looks messier than it really is...

Illustration

Data from Denoeux's Example 1: $N(x^n) = (91, 49, 37, 43)$

Plot shows my mine and Denoeux's (\triangle) plausibility contour



Discussion

- Multinomial models are simple but represent an important class of problems — these are "discrete nonparametric"
- Walley's IDM is simple and powerful¹¹
- Denoeux's method is appealing:
 - very simple in the $K \in \{2,3\}$ cases
 - doable but more complicated in others
 - motivated by some performance-related criteria
 - ...
- Denoeux's R2 is not the same as "validity"
- I threw the IM solution together quickly and naively, would be interesting to explore this further...

¹¹Extensive literature on this covering pros and cons

Prediction with covariates

- regression
- classification
- Imprecise probabilistic methods

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