STSCI 4780/5780: The Dirichlet distribution and high-dimensional inference

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Agenda

- Multinomial distribution for categorical data
- The Dirichlet distribution—A PDF over PMFs
- Continuous parameter histograms—“categorical PDFs”
- Increasing dimension and the Dirichlet process
- “Curses” (and blessings) of high-dimensionality

Recap of beta-binomial inference

Setup

$\mathcal{C}$ specifies existence of two outcomes, S and F, in each of N cases or trials; for each case or trial, the probability for S is α; for 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 $p(\alpha|D,\mathcal{C})$

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

Posterior (using sequence, binomial, negative binomial data)

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

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*

I.e., draws from the posterior correspond to possible (p_0, p_1) PMFs

The beta-binomial conjugate model

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

$$
\begin{aligned}
p(\alpha|n, M') &\propto \mathrm{Beta}(\alpha|a, b) \times \mathrm{Binom}(n|\alpha, N) \\
&\propto \alpha^{a-1}(1-\alpha)^{b-1} \times \alpha^{n}(1-\alpha)^{N-n} \\
&\propto \alpha^{n+a-1}(1-\alpha)^{N-n+b-1}
\end{aligned}
$$

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

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

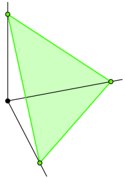
Conjugacy $\rightarrow$ it's easy to chain inferences from multiple experiments

Categorical data

D = Discrete outcomes from N observed trials, $o_1 o_2 o_3 \ldots o_N$:
Roles of a die: 321344622...
Customer choices: AAOBBOOO... (*A*pple, *B*anana, *O*range)

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



$K = 3$ case

Note that Bernoulli/binomial data corresponds to the $K = 2$ case

Sequence sampling dist'n/Likelihood function

$$
\begin{aligned}
p(D|\alpha, \mathcal{C}) &= p(o_1 = k_1|\alpha, \mathcal{C}) \times p(o_2 = k_2|\alpha, \mathcal{C}) \times \cdots \\
&= \prod_k \alpha_k^{n_k} \\
&\equiv \mathcal{L}(\alpha)
\end{aligned}
$$

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*:

$$
\begin{aligned}
p(D'|\alpha, \mathcal{C}) &= \frac{N!}{\prod_k n_k!} \prod_k \alpha_k^{n_k} \\
&\propto \mathcal{L}(\alpha)
\end{aligned}
$$

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:

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

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'):

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

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

Asymmetric parameterization

Note that we are treating the α_k parameters *asymmetrically*: we replace the α_K parameter with $1 - \sum_{k=1}^{K-1} \alpha_k$

This can make some inferences awkward (e.g., the posterior for α_K)

We could have instead used $(\alpha_2, \ldots, \alpha_K)$, with

$$\alpha_1 = \sum_{k=2}^{K} \alpha_k$$

or other similar choices

E.g., for the $K = 2$ Bernoulli case, with $\alpha = P(\text{success}|\mathcal{C})$, we found

$$p(\alpha|n, \mathcal{C}) \propto \alpha^n (1 - \alpha)^{N-n}$$

But we could have used $\beta = P(\text{failure}|\mathcal{C}) = 1 - \alpha$, which gives

$$p(\beta|n, \mathcal{C}) \propto \beta^{N-n} (1 - \beta)^n$$

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

- 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:

$$\begin{aligned} p(\alpha_K | \alpha_1, \ldots, \alpha_{K-1}, \ldots) &= \delta\left(\alpha_K - \left[1 - \sum_{k=1}^{K-1} \alpha_k\right]\right) \\ &= \delta\left(1 - \sum_{k=1}^{K} \alpha_k\right) \end{aligned}$$

Uniform prior—symmetric version

Earlier asymmetric prior PDF over $(K-1)$-D standard simplex:

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

with $1/C =$ "volume" of the $(K-1)$-D standard simplex

This can now be written as a K-D function:

$$p(\alpha|\mathcal{C}) = C \times \delta\left(1 - \sum_{k=1}^{K} \alpha_k\right)$$

with $\alpha_k \geq 0$; the δ function constrains the parameters to the simplex

Dirichlet dist'n posterior—symmetric version

Asymmetric posterior PDF over $(K-1)$-D standard simplex:

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

This can now be written as a K-D function:

$$p(\alpha|D, \mathcal{C}) \propto \left[\prod_{k=1}^{K} \alpha_k^{n_k}\right] \times \delta\left(1 - \sum_{k=1}^{K} \alpha_k\right)$$

with $\alpha_k \geq 0$

Normalization constants

$$\int_0^\infty d\alpha_1 \cdots \int_0^\infty d\alpha_K \; \alpha_1^{\kappa_1 - 1} \cdots \alpha_K^{\kappa_K - 1} \; \delta\left(a - \sum_k \alpha_k\right) = \frac{\Gamma(\kappa_1)\cdots\Gamma(\kappa_K)}{\Gamma(\kappa_0)} \; a^{\kappa_0 - 1}$$

with $\kappa_0 \equiv \sum_{k=1}^K \kappa_k$; this is the *Generalized beta integral*

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

Recall that, for integer n, $\Gamma(n+1) = n!$, and $\Gamma(1) = 1$

The volume of the standard K-simplex corresponds to $a = 1$, $\kappa_i = 1$:

$$\int_0^\infty d\alpha_1 \cdots \int_0^\infty d\alpha_K \; \delta\left(a - \sum_k \alpha_k\right) = \frac{1}{(K-1)!}$$

So the (normalized) uniform prior is (with $\alpha_k \geq 0$):

$$p(\alpha|\mathcal{C}) = (K-1)! \times \delta\left(1 - \sum_{k=1}^K \alpha_k\right)$$

Normalization constants...

Similarly, the normalized posterior is

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

For $K=2$ we recover beta posterior from Bernoulli/binomial cases, but in a symmetric form (with $\alpha_2 = 1-\alpha_1$)

Dirichlet distributions

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

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

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 $k = 1\ldots K$

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

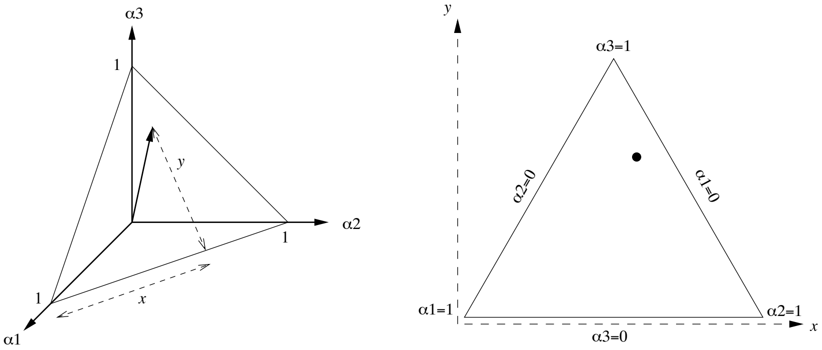
Marginal variances: $\mathrm{Var}(\alpha_k) = \frac{\kappa_i(\kappa_0-\kappa_i)}{\kappa_0^2(\kappa_0+1)}$

All covariances *negative* (necessarily!)

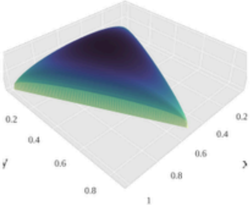
Special case: *Symmetric Dirichlet* with $\kappa_i = \kappa$

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

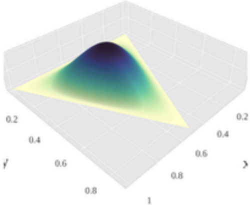
Simplex/ternary plots



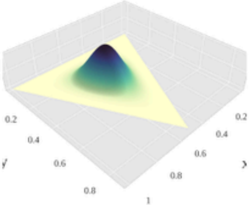
(1.3, 1.3, 1.3)



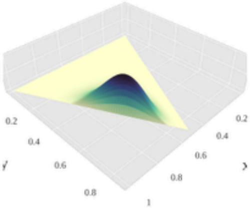
(3,3,3)



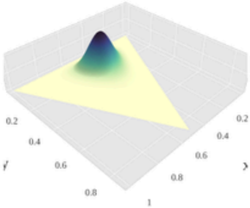
(7,7,7)



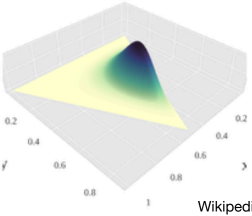
(2,6,11)



(14, 9, 5)



(6,2,6)



Wikipedia

Marginal PDF for one category

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

$$\begin{aligned}
p(\alpha_1|D,\mathcal{C}) &= \int d\alpha_2 \int d\alpha_3 \; p(\alpha|D,\mathcal{C}) \\
&= C\alpha_1^{n_1} \int d\alpha_2 \int d\alpha_3 \; \alpha_2^{n_2}\alpha_3^{n_3} \\
&\qquad \times\delta\left[(1-\alpha_1) - (\alpha_2+\alpha_3)\right] \\
&= C'\alpha_1^{n_1}(1-\alpha_1)^{n_2+n_3+1}; \quad \text{note } n_2+n_3 = N-n_1
\end{aligned}$$

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.

Marginal prior PDF for one category

Marginal prior PDF for α_1 with K categories:

$$
\begin{aligned}
p(\alpha_1|D,\mathcal{C}) &= C \int d\alpha_2 \cdots \int d\alpha_K \, \delta\left(1 - \sum_{k=1}^{K} \alpha_k\right) \\
&= C \int d\alpha_2 \cdots \int d\alpha_K \, \delta\left(1 - \alpha_1 - \sum_{k=2}^{K} \alpha_k\right) \\
&= C'(1-\alpha_1)^{K-2}; \quad \text{note } n_2 + n_3 = N - n_1
\end{aligned}
$$

For $K = 2$, we recover the uniform prior for α_1 that we used for Bernoulli/binomial inference

But when K is large, the uniform prior strongly prefers small values of α_k