A Brief Introduction to Bayesian Inference

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CG168 notes

A brief review of *discrete* probability theory

- Ω is the set of all *elementary events* (c.f. interpretations in logic)
- If $\omega \in \Omega$, then $P(\omega)$ is the probability of event ω
 - $P(\omega) \ge 0$
 - $\sum_{\omega \in \Omega} \mathbf{P}(\omega) = 1$
- A *random variable* X is a function from Ω to some set of values X
 - If \mathcal{X} is countable then X is a *discrete* random variable
 - If *X* is continuous then *X* is a *continuous* random variable
- If *x* is a possible value for *X*, then

$$P(X = x) = \sum_{\substack{\omega \in \Omega \\ X(\omega) = x}} P(\omega)$$

Independence and conditional distributions

- Two RVs *X* and *Y* are *independent* iff P(X, Y) = P(X)P(Y)
- The *conditional distribution* of Y given X is:

$$P(Y|X) = \frac{P(Y,X)}{P(X)}$$

so *X* and *Y* are independent iff P(Y|X) = P(Y) (here and below I assume strictly positive distributions)

• We can decompose the joint distribution of a sequence of RVs into a product of conditionals:

 $P(X_1,...,X_n) = P(X_1)P(X_2|X_1)P(X_3|X_2,X_1)...P(X_n|X_{n-1},...,X_1)$

i.e., the probability of generating X_1, \ldots, X_n "at once" is the same as generating them one at a time if each X_i is conditioned on the X_1, \ldots, X_{i-1} that preceded it

Conditional distributions

• It's always possible to factor any distribution over $X = (X_1, ..., X_n)$ into a product of conditionals

$$\mathbf{P}(\mathbf{X}) = \prod_{i=1}^{n} \mathbf{P}(X_i | X_1, \dots, X_{i-1})$$

• But in many interesting cases, *X_i* depends only on a subset of *X*₁,..., *X_{i-1}*, i.e.,

$$\mathbf{P}(\boldsymbol{X}) = \prod_{i} \mathbf{P}(X_{i} | \boldsymbol{X}_{\mathsf{Pa}(i)})$$

where $Pa(i) \subseteq \{1, ..., i-1\}$ and $X_S = \{X_j : j \in S\}$

- X and Y are *conditionally independent* given Z iff P(X, Y|Z) = P(X|Z) P(Y|Z) or equivalently, P(X|Y,Z) = P(X|Z)
- Note: the "parents" Pa(*i*) of *X_i* depend on the order in which the variables are enumerated!



• A Bayes net is a graphical depiction of a factorization of a probability distribution into products of conditional distributions

$$\mathbf{P}(\mathbf{X}) = \prod_{i} \mathbf{P}(X_i | \mathbf{X}_{\mathsf{Pa}(i)})$$

A Bayes net has a node for each variable X_i and an arc from X_j to X_i iff j ∈ Pa(i)

Bayes rule

• Bayes theorem:

$$P(Y|X) = \frac{P(X|Y) P(Y)}{P(X)}$$

- Bayes inversion: swap direction of arcs in Bayes net
- Interpreted as a recipe for "belief updating":

$$\underbrace{\frac{P(\mathsf{Hypothesis}|\mathsf{Data})}_{\mathsf{Posterior}} \propto \underbrace{\frac{P(\mathsf{Data}|\mathsf{Hypothesis})}_{\mathsf{Likelihood}} \underbrace{\frac{P(\mathsf{Hypothesis})}_{\mathsf{Prior}}}$$

• The normalizing constant (which you have to divide Likelihood times Prior by) is:

$$P(\mathsf{Data}) \ = \ \sum_{\mathsf{Hypothesis'}} P(\mathsf{Data}|\mathsf{Hypothesis'}) \ P(\mathsf{Hypothesis'})$$

which is the probability of generating the data under *any* hypothesis

Iterated Bayesian belief updating

• Suppose the data consists of 2 components $D = (D_1, D_2)$, and P(H) is our prior over hypotheses H

$$P(H|D_1, D_2) \propto P(D_1, D_2|H) P(H)$$

$$\propto P(D_2|H, D_1) P(H|D_1)$$

- This means the following are equivalent:
 - ► update the prior P(H) treating (D₁, D₂) as a single observation
 - update the prior P(H) wrt the first observation D₁ producing posterior P(H|D₁) ∝ P(D₁|H) P(H), which serves as the prior for the second observation D₂

Incremental Bayesian belief updating

- Consider a "two-part" data set (d₁, d₂). We show posterior obtained by Bayesian belief updating on (d₁, d₂) together is same as posterior obtained by updating on d₁ and then updating on d₂.
- Bayesian belief updating on both (d_1, d_2) using prior P(H) P(H|d_1, d_2) \propto P(d_1, d_2|H) P(H) = P(d_1, d_2, H)
- Incremental Bayesian belief updating
 - Bayesian belief updating on d_1 using prior P(H)

 $\mathbf{P}(H|d_1) \propto \mathbf{P}(d_1|H) \mathbf{P}(H) = \mathbf{P}(d_1, H)$

• Bayesian belief updating on d_2 using prior $P(H|d_1)$

$$P(H|d_1, d_2) \propto P(d_2|H, d_1) P(H|d_1)$$

$$\propto P(d_2|H, d_1) P(H, d_1)$$

$$= P(d_2, d_1, H)$$

"Distributed according to" notation

- A *probability distribution F* is a non-negative function from some set \mathcal{X} whose values sum (integrate) to 1
- A random variable *X* is *distributed according* to a distribution *F*, or more simply, *X* has distribution *F*, written *X* ~ *F*, iff:

$$P(X = x) = F(x)$$
 for all x

(This is for discrete RVs).

• You'll sometimes see the notion

$$X \mid Y \sim F$$

which means "X is generated conditional on Y with distribution F" (where F usually depends on Y)

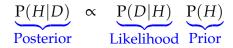


Dirichlet priors for categorical and multinomial distributions

Comparing discrete and continuous hypotheses

Continuous hypothesis spaces

• Bayes rule is the same when *H* ranges over a continuous space *except* that P(*H*) and P(*H*|*D*) are *continuous functions* of *H*



• The normalizing constant is:

$$\mathbf{P}(D) = \int \mathbf{P}(D|H') \mathbf{P}(H') \, dH'$$

- Some of the approaches you can take:
 - Monte Carlo sampling procedures (which we'll talk about later)
 - ► Choose P(H) so that P(H|D) is easy to calculate ⇒ use a prior *conjugate* to the likelihood

Categorical distributions

- A *categorical distribution* has a finite set of outcomes 1, ..., *m*
- A categorical distribution is parameterized by a vector $\boldsymbol{\theta} = (\theta_1, \dots, \theta_m)$, where $P(X = j | \boldsymbol{\theta}) = \theta_j$ (so $\sum_{j=1}^m \theta_j = 1$)
 - Example: An *m*-sided die, where θ_i = prob. of face *j*
- Suppose $X = (X_1, ..., X_n)$ and each $X_i | \theta \sim \text{CATEGORICAL}(\theta)$. Then:

$$P(\boldsymbol{X}|\boldsymbol{\theta}) = \prod_{i=1}^{n} CATEGORICAL(X_i; \boldsymbol{\theta}) = \prod_{j=1}^{m} \theta_j^{N_j}$$

where N_j is the number of times *j* occurs in **X**.

• Goal of next few slides: compute $P(\theta|X)$

Multinomial distributions

- Suppose X_i ~ CATEGORICAL(θ) for i = 1,..., n, and N_j is the number of times j occurs in X
- Then $N|n, \theta \sim MULTI(\theta, n)$, and

$$\mathbf{P}(\boldsymbol{N}|n,\boldsymbol{\theta}) = \frac{n!}{\prod_{j=1}^{m} N_j!} \prod_{j=1}^{m} \theta_j^{N_j}$$

where $n! / \prod_{j=1}^{m} N_j!$ is the number of sequences of values with occurence counts *N*

• The vector *N* is known as a *sufficient statistic* for *θ* because it supplies as much information about *θ* as the original sequence *X* does.

Dirichlet distributions

• *Dirichlet distributions* are probability distributions over multinomial parameter vectors

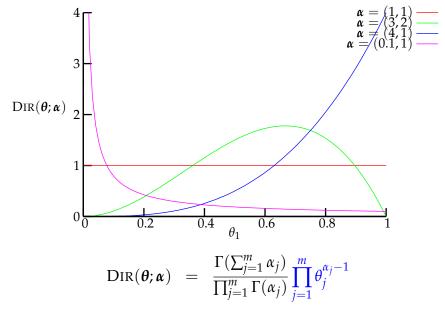
• called *Beta distributions* when m = 2

Parameterized by a vector *α* = (*α*₁,..., *α*_m) where *α*_j > 0 that determines the shape of the distribution

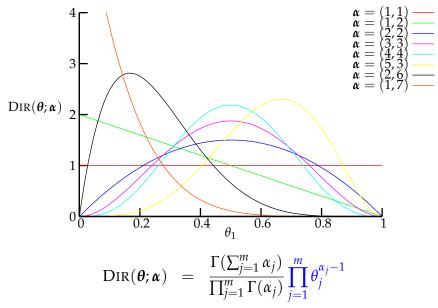
$$DIR(\boldsymbol{\theta}; \boldsymbol{\alpha}) = \frac{1}{C(\boldsymbol{\alpha})} \prod_{j=1}^{m} \theta_{j}^{\alpha_{j}-1}$$
$$C(\boldsymbol{\alpha}) = \int \prod_{j=1}^{m} \theta_{j}^{\alpha_{j}-1} d\boldsymbol{\theta} = \frac{\prod_{j=1}^{m} \Gamma(\alpha_{j})}{\Gamma(\sum_{j=1}^{m} \alpha_{j})}$$

- Γ is a generalization of the factorial function
- $\Gamma(k) = (k 1)!$ for positive integer *k*
- $\Gamma(x) = (x-1)\Gamma(x-1)$ for all x

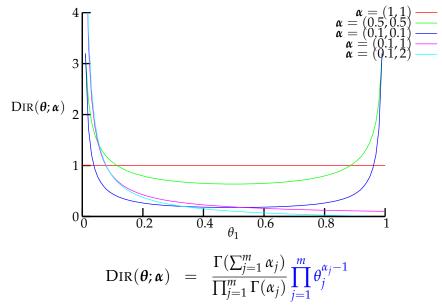
Plots of the Dirichlet distribution



Plots of the Dirichlet distribution (2)



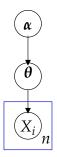
Plots of the Dirichlet distribution (3)



Dirichlet distributions as priors for θ

• Generative model:

• We can depict this as a Bayes net using *plates*, which indicate *replication*



Inference for θ with Dirichlet priors

- Data $X = (X_1, ..., X_n)$ generated i.i.d. from CATEGORICAL(θ)
- Prior is DIR(*α*). By Bayes Rule, posterior is:

$$P(\boldsymbol{\theta}|\boldsymbol{X}) \propto P(\boldsymbol{X}|\boldsymbol{\theta}) P(\boldsymbol{\theta})$$
$$\propto \left(\prod_{j=1}^{m} \theta_{j}^{N_{j}}\right) \left(\prod_{j=1}^{m} \theta_{j}^{\alpha_{j}-1}\right)$$
$$= \prod_{j=1}^{m} \theta_{j}^{N_{j}+\alpha_{j}-1}, \text{ so}$$
$$P(\boldsymbol{\theta}|\boldsymbol{X}) = DIR(\boldsymbol{N}+\boldsymbol{\alpha})$$

- So if prior is Dirichlet with parameters α , posterior is Dirichlet with parameters $N + \alpha$
- ⇒ can regard Dirichlet parameters α as "pseudo-counts" from "pseudo-data"

Point estimates from Bayesian posteriors

- A "true" Bayesian prefers to use the full P(*H*|*D*), but sometimes we have to choose a "best" hypothesis
- The Maximum a posteriori (MAP) or posterior mode is

$$\widehat{H} = \operatorname{argmax}_{H} \operatorname{P}(H|D) = \operatorname{argmax}_{H} \operatorname{P}(D|H) \operatorname{P}(H)$$

• The *expected value* $E_P[X]$ of X under distribution P is:

$$\mathbf{E}_{\mathbf{P}}[\mathbf{X}] = \int x \, \mathbf{P}(\mathbf{X} = x) \, dx$$

The expected value is a kind of average, weighted by P(X). The *expected value* $E[\theta]$ of θ is an estimate of θ .

The posterior mode of a Dirichlet

• The Maximum a posteriori (MAP) or posterior mode is

$$\widehat{H} = \operatorname{argmax}_{H} \operatorname{P}(H|D) = \operatorname{argmax}_{H} \operatorname{P}(D|H) \operatorname{P}(H)$$

• For Dirichlets with parameters *a*, the MAP estimate is:

$$\hat{\theta}_j = \frac{\alpha_j - 1}{\sum_{j'=1}^m (\alpha_{j'} - 1)}$$

so if the posterior is $DIR(N + \alpha)$, the MAP estimate for θ is:

$$\hat{ heta}_{j} = rac{N_{j} + lpha_{j} - 1}{n + \sum_{j'=1}^{m} (lpha_{j'} - 1)}$$

• If $\alpha = 1$ then $\hat{\theta}_j = N_j/n$, which is also the *maximum likelihood estimate* (MLE) for θ

The expected value of θ for a Dirichlet

• The *expected value* $E_P[X]$ of X under distribution P is:

$$\mathbf{E}_{\mathbf{P}}[X] = \int x \, \mathbf{P}(X=x) \, dx$$

• For Dirichlets with parameters α , the expected value of θ_i is:

$$\mathbf{E}_{\mathrm{DIR}(\boldsymbol{\alpha})}[\theta_j] = \frac{\alpha_j}{\sum_{j'=1}^m \alpha_{j'}}$$

• Thus if the posterior is $DIR(N + \alpha)$, the expected value of θ_i is:

$$\mathbf{E}_{\mathrm{DIR}(\mathbf{N}+\boldsymbol{\alpha})}[\theta_j] = \frac{N_j + \alpha_j}{n + \sum_{j'=1}^m \alpha_{j'}}$$

• E[*θ*] *smooths* or *regularizes* the MLE by adding pseudo-counts *α* to *N*

Sampling from a Dirichlet

$$\boldsymbol{\theta} \mid \boldsymbol{\alpha} \sim \operatorname{DIR}(\boldsymbol{\alpha}) \quad \text{iff} \quad \operatorname{P}(\boldsymbol{\theta} \mid \boldsymbol{\alpha}) = \frac{1}{C(\boldsymbol{\alpha})} \prod_{j=1}^{m} \theta_{j}^{\alpha_{j}-1}, \text{ where:}$$

 $C(\boldsymbol{\alpha}) = \frac{\prod_{j=1}^{m} \Gamma(\alpha_{j})}{\Gamma(\sum_{j=1}^{m} \alpha_{j})}$

- There are several algorithms for producing samples from DIR(*α*). A simple one relies on the following result:
- If $V_k \sim \text{GAMMA}(\alpha_k)$ and $\theta_k = V_k / (\sum_{k'=1}^m V_{k'})$, then $\theta \sim \text{DIR}(\alpha)$
- This leads to the following algorithm for producing a sample *θ* from DIR(*α*)
 - Sample v_k from GAMMA(α_k) for k = 1, ..., m

• Set
$$\theta_k = v_k / (\sum_{k'=1}^m v_{k'})$$

Conjugate priors

• If prior is $DIR(\alpha)$ and likelihood is i.i.d. $CATEGORICAL(\theta)$, then posterior is $DIR(N + \alpha)$

 \Rightarrow prior parameters α specify "pseudo-observations"

- A class C of prior distributions P(H) is *conjugate* to a class of likelihood functions P(D|H) iff the posterior P(H|D) is also a member of C
- In general, conjugate priors encode "pseudo-observations"
 - ► the difference between prior P(*H*) and posterior P(*H*|*D*) are the observations in *D*
 - but P(H|D) belongs to same family as P(H), and can serve as prior for inferences about more data D'
 - \Rightarrow must be possible to encode observations *D* using parameters of prior
- In general, the likelihood functions that have conjugate priors belong to the *exponential family*

Outline

Dirichlet priors for categorical and multinomial distributions

Comparing discrete and continuous hypotheses

Categorical and continuous hypotheses about coin flips

- Data: A sequence of coin flips $X = (X_1, \ldots, X_n)$
- Hypothesis h_1 : *X* is generated from a fair coin, i.e., $\theta_H = 0.5$
- Hypothesis h_2 : X is generated from a biased coin with unknown bias, i.e., $\theta_H \sim \text{DIR}(\alpha)$

$$\mathbf{P}(H|\mathbf{X}) = \mathbf{P}(\mathbf{X}|H) \mathbf{P}(H)$$

- Assume $P(h_1) = P(h_2) = 0.5$
- $P(X|h_1) = 2^{-n}$, but *what is* $P(X|h_2)$?
- P(X|h₂) is the probability of generating θ from DIR(α) and then generating X from CATEGORICAL(θ). But we don't care about the value of θ, so we *marginalize* or *integrate out* θ

$$P(\boldsymbol{X}|\boldsymbol{\alpha},h_2) = \int P(\boldsymbol{X},\boldsymbol{\theta}|\boldsymbol{\alpha}) d\boldsymbol{\theta}$$

Posterior with Dirichlet priors

• *Integrate out* θ to calculate posterior probability of *X*

$$P(\mathbf{X}|\boldsymbol{\alpha}) = \int P(\mathbf{X},\boldsymbol{\theta}|\boldsymbol{\alpha}) d\boldsymbol{\theta} = \int P(\mathbf{X}|\boldsymbol{\theta}) P(\boldsymbol{\theta}|\boldsymbol{\alpha}) d\boldsymbol{\theta}$$

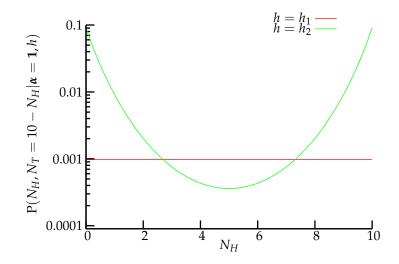
$$= \int \left(\prod_{j=1}^{m} \theta_{j}^{N_{j}}\right) \left(\frac{1}{C(\boldsymbol{\alpha})} \prod_{j=1}^{m} \theta_{j}^{\alpha_{j}-1}\right) d\boldsymbol{\theta}$$

$$= \frac{1}{C(\boldsymbol{\alpha})} \int \prod_{j=1}^{m} \theta_{j}^{N_{j}+\alpha_{j}-1} d\boldsymbol{\theta}$$

$$= \frac{C(\mathbf{N}+\boldsymbol{\alpha})}{C(\boldsymbol{\alpha})}, \text{ where } C(\boldsymbol{\alpha}) = \frac{\prod_{j=1}^{m} \Gamma(\alpha_{j})}{\Gamma(\sum_{j=1}^{m} \alpha_{j})}$$

 Collapsed Gibbs samplers and the Chinese Restaurant Process rely on this result

Posteriors under h_1 and h_2



Understanding the posterior

$$P(X|\alpha) = \frac{C(N+\alpha)}{C(\alpha)} \text{ where } C(\alpha) = \frac{\prod_{j=1}^{m} \Gamma(\alpha_j)}{\Gamma(\alpha_{\bullet})} \text{ and } \alpha_{\bullet} = \sum_{j=1}^{m} \alpha_j$$

$$P(X|\alpha) = \left(\frac{\prod_{j=1}^{m} \Gamma(N_j + \alpha_j)}{\Gamma(n + \alpha_{\bullet})}\right) \left(\frac{\Gamma(\alpha_{\bullet})}{\prod_{j=1}^{m} \Gamma(\alpha_j)}\right)$$

$$= \left(\prod_{j=1}^{m} \frac{\Gamma(N_j + \alpha_j)}{\Gamma(\alpha_j)}\right) \left(\frac{\Gamma(\alpha_{\bullet})}{\Gamma(n + \alpha_{\bullet})}\right)$$

$$= \frac{\alpha_1}{\alpha_{\bullet}} \times \frac{\alpha_1 + 1}{\alpha_{\bullet} + 1} \times \ldots \times \frac{\alpha_1 + N_1 - 1}{\alpha_{\bullet} + N_1 - 1}$$

$$\times \frac{\alpha_2}{\alpha_{\bullet} + N_1} \times \frac{\alpha_2 + 1}{\alpha_{\bullet} + N_1 + 1} \times \ldots \times \frac{\alpha_2 + N_2 - 1}{\alpha_{\bullet} + N_1 + N_2 - 1}$$

$$\times \ldots$$

$$\times \frac{\alpha_m}{\alpha_{\bullet} + n - N_m - 1} \times \frac{\alpha_m + 1}{\alpha_{\bullet} + n - N_m} \times \ldots \times \frac{\alpha_m + N_m - 1}{\alpha_{\bullet} + n - 1}$$

Exchangability

- The individual X_i in a Dirichlet-multinomial distribution $P(X|\alpha) = C(N + \alpha)/C(\alpha)$ are *not independent*
 - the probability of X_i depends on X_1, \ldots, X_{i-1}

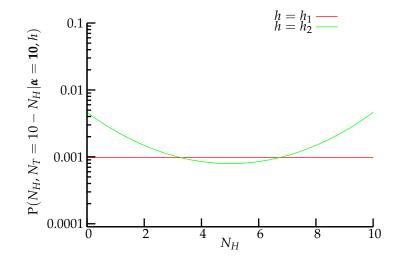
$$P(X_n = k | X_1, \dots, X_{n-1}, \boldsymbol{\alpha}) = \frac{P(X_1, \dots, X_n | \boldsymbol{\alpha})}{P(X_1, \dots, X_{n-1} | \boldsymbol{\alpha})}$$
$$= \frac{\alpha_k + N_k(X_1, \dots, X_{n-1})}{\alpha_{\bullet} + n - 1}$$

- but X_1, \ldots, X_n are *exchangable*
 - $P(X|\alpha)$ depends only on *N*
 - \Rightarrow doesn't depend on *the order* in which the *X* occur
- A distribution over a sequence of random variables is *exchangable* iff *the probability of all permutations of the random variables are equal*

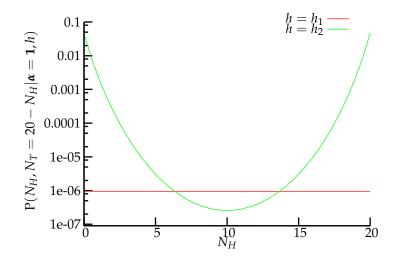
Summary so far

- Bayesian inference can compare models of *differing complexity* (assuming we can *calculate posterior probability*)
 - ▶ Hypothesis *h*¹ has no free parameters
 - Hypothesis h_2 has one free parameter θ_H
- *Bayesian Occam's Razor:* "A more complex hypothesis is only prefered if its greater complexity consistently provides a better account of the data"
- But: h_1 makes every sequence equally likely. h_2 seems to *dislike* $\theta_H \approx 0.5$ What's going on here?

Posteriors with $n = 10, \alpha = 10$



Posteriors with $n = 20, \alpha = 1$



Dirichlet-Multinomial distributions

- Only one sequence of 10 heads out of 10 coin flips
- but 252 different sequences of 5 heads out of 10 coin flips
- Each particular sequence of 5 heads out of 10 flips is unlikely, but there are so many of them that *the group is very likely*
- The number of ways of picking *N* outcomes out of *n* trials is:

$$\frac{n!}{\prod_{j=1}^m N_j!}$$

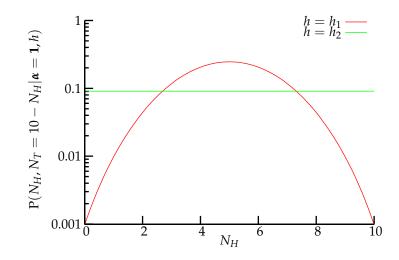
• The probability of observing N given θ is:

$$\mathbf{P}(\boldsymbol{N}|\boldsymbol{\theta}) = \frac{n}{\prod_{j=1}^{m} N_j!} \prod_{j=1}^{m} \theta_j^{N_j}$$

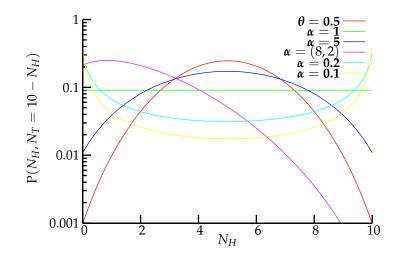
• The probability of observing *N* given α is:

$$\mathbf{P}(\mathbf{N}|\boldsymbol{\alpha}) = \frac{n}{\prod_{j=1}^{m} N_j!} \frac{C(\mathbf{N}+\boldsymbol{\alpha})}{C(\boldsymbol{\alpha})}$$

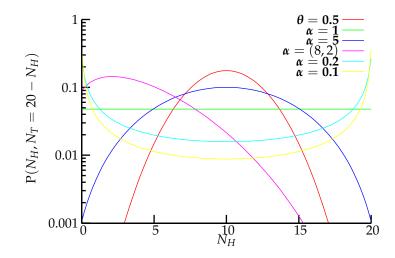
Dirichlet-**multinomial** posteriors with $n = 10, \alpha = 1$



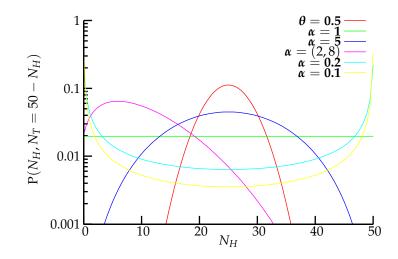
Dirichlet-**multinomial** posteriors with n = 10, varying α



Dirichlet-**multinomial** posteriors with n = 20, varying α



Dirichlet-**multinomial** posteriors with n = 50, varying α



Entropy vs. "rich get richer"

• Notation: If $X = (X_1, ..., X_n)$, then $X_{-j} = (X_1, ..., X_{j-1}, X_{j+1}, ..., X_n)$

$$P(X_n = k | \boldsymbol{\alpha}, \boldsymbol{X}_{-n}) = \frac{N_k(\boldsymbol{X}_{-n}) + \alpha_k}{\alpha_{\bullet} + n - 1}$$

- The probability of generating an outcome is proportional to the number of times it has been seen before (including prior)
- ⇒ Next outcome is most likely to be most frequently generated previous outcome ⇒ *sparse outcomes*
 - But there are far fewer sparse outcomes than non-sparse outcomes ⇒ entropy "prefers" non-sparse outcomes
 - If α > 1 then most likely outcomes are not sparse i.e., entropy is stronger than prior
 - If α < 1 then most likely outcomes are sparse i.e., prior is stronger than entropy