Bayesian philosophy, noninformative priors, exchangeability

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Outline

- Bayesian vs. frequentist
- Uninformative priors
- Exchangeability, de Finetti's theorem

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- Frequentist: θ is some fixed parameter, no randomness
 - We want to estimate it from observations

$$\boldsymbol{\theta}_{ML} = \operatorname*{argmax}_{\boldsymbol{\theta}} \sum_{i=1}^{N} \log p(\mathbf{x}_i | \boldsymbol{\theta})$$

- How to quantify your uncertainty?
 - confidence level, note that $heta_{ML}$ is a R.V., but $oldsymbol{ heta}$ is not.

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$$p(\boldsymbol{\theta}|\mathcal{D}) \propto p(\boldsymbol{\theta}) \prod_{i=1}^{N} p(\mathbf{x}_i|\boldsymbol{\theta})$$

– How to quantify your uncertainty?

Posterior distribution!
$$p(\boldsymbol{\theta}|\mathcal{D})$$

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 - \Box We can make probabilistic statements about $oldsymbol{ heta}$ (mean, variance, quantiles, etc.).
 - ☐ We can make Bayesian prediction that integrates all the possible outcomes

$$p(\mathbf{x}^*|\mathbf{x}_1,\ldots,\mathbf{x}_N) = \int p(\mathbf{x}^*|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{x}_1,\ldots,\mathbf{x}_N)$$
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- Is Bayesian analysis subjective?
 - Not necessary: Bayesian provides a convenient way to incorporate subjective believes (important for AI!) But it can also uses uninformative priors (this is objective Bayesian!)
 - Frequentist models make assumptions, too!
 - Whether using frequent or Bayesian models, always check
 the assumptions you make

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- In many cases, we have little idea of what form the distribution should take
- Though conjugate priors are computationally nice, objective Bayesians instead prefer priors which has little influence on the posterior distribution. Such a prior is called an uninformative prior.
- Let the data speak for themselves

What priors do you have immediately in mind?

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Uniform distribution!

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Uniform distribution!

Now that I do not know which parameter is more likely to be sampled, let us just assume the chances are equal!

Uninformative priors

Uniform distribution

For finite states:
$$p(\lambda) = 1/K$$

For finite interval:
$$p(\lambda) = 1/(b-a)$$

Uninformative priors

Uniform distribution

What about unbounded domains? $\lambda \in \mathbb{R}$

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Uninformative priors

Uniform distribution

What about unbounded domains? $\lambda \in \mathbb{R}$

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This is an *improper* prior, because normalization diverges We can still use it as long as the posterior is *proper*

Uninformative priors

Problem of uniform distribution: transformation invariance

$$p(\lambda) \propto {\rm const}$$

$$\lambda = \eta^2$$

Uninformative priors

Problem of uniform distribution: transformation invariance

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$$\lambda = \eta^2$$

$$p_{\eta}(\eta) = p_{\lambda}(\lambda) \left| \frac{\mathrm{d}\lambda}{\mathrm{d}\eta} \right| = p_{\lambda}(\eta^2) 2\eta \propto \eta$$

Uninformative priors

Problem of uniform distribution: transformation invariance

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When we do variable transformations, the prior is no longer uninformative!

Uninformative priors

Let us take translation invariance into account

If the likelihood takes the form

$$p(x|\lambda) = f(x - \lambda)$$

Let us take translation invariance into account

If the likelihood takes the form

$$p(x|\lambda) = f(x - \lambda)$$

 λ is *location* parameter, and the density exhibits *shift invariance*

$$\hat{x} = x + c$$
 $\hat{\lambda} = \lambda + c$

$$p(\hat{x}|\hat{\lambda}) = f(\hat{x} - \hat{\lambda})$$

Uninformative priors

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$$\int_{A}^{B} p(\lambda) d\lambda = \int_{A+c}^{B+c} p(\lambda) d\lambda$$

$$\int_{A}^{B} p(\lambda) d\lambda = \int_{A+c}^{B+c} p(\lambda) d\lambda = \int_{A}^{B} p(\lambda + c) d\lambda$$
$$p(\lambda) = p(\lambda + c)$$
$$p(\lambda) \propto \text{const}$$

Uninformative priors

Example: for a Gaussian likelihood

$$p(x|\mu) = \mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

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shift invariance density

Conjugate prior

$$p(\mu|\alpha, v^2) = N(\mu|\alpha, v^2) = \frac{1}{\sqrt{2\pi}v} \exp\left(-\frac{1}{2v^2}(\mu - \alpha)^2\right)$$

$$p(\mathbf{x}|\lambda)$$

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$$p(\mu) \propto \text{const}$$

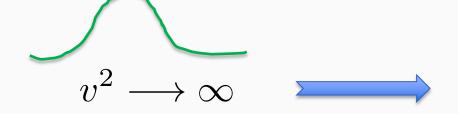
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 σ is *scale* parameter, and the density exhibits *scale invariance*

$$\widehat{x} = cx$$
 $\widehat{\sigma} = c\sigma$

$$p(\widehat{x}|\widehat{\sigma}) = \frac{1}{\widehat{\sigma}} f\left(\frac{\widehat{x}}{\widehat{\sigma}}\right) \qquad \text{Verify it by yourself}$$

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- How, consider an arbitrary interval [A, B], the prior should assign equal mass over an arbitrary scaled interval [A/c, B/c]

$$\int_{A}^{B} p(\sigma) d\sigma = \int_{A/c}^{B/c} p(\sigma) d\sigma$$

$$\int_{A}^{B} p(\sigma) d\sigma = \int_{A/c}^{B/c} p(\sigma) d\sigma = \int_{A}^{B} p\left(\frac{1}{c}\sigma\right) \frac{1}{c} d\sigma$$

$$p(\sigma) = p\left(\frac{1}{c}\sigma\right) \frac{1}{c}$$

$$p(\sigma) \propto 1/\sigma$$

Example: for a Gaussian likelihood

$$p(x|\sigma) = \mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma} \exp\left(-\frac{1}{2} \left[\frac{x-\mu}{\sigma}\right]^2\right)$$

Uninformative prior
$$p(\sigma) \propto 1/\sigma \qquad \xrightarrow{\lambda = 1/\sigma^2} \qquad p(\lambda) \propto 1/\lambda$$

Conjugate prior

$$p(\lambda|a,b) = \operatorname{Gam}(\lambda|a,b) \propto \lambda^{a-1} \exp(-b\lambda)$$

$$a = 0, b = 0$$
 $p(\lambda) \propto 1/\lambda$

Jeffreys priors

$$\pi_J(oldsymbol{ heta}) \propto |I(oldsymbol{ heta})|^{rac{1}{2}}$$

Fisher information
$$I(\theta) = -\mathbb{E}_{\theta} \left[\frac{d^2 \log p(X|\theta)}{d\theta^2} \right]$$

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Expectation w.r.t $p(X|\theta)$

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Fisher information

$$I(\theta) = -\mathbb{E}_{\theta} \left[\frac{d^2 \log p(X|\theta)}{d\theta^2} \right] \quad \text{Note, for vector case, it becomes the Hessian}$$
 Expectation w.r.t
$$p(X|\theta)$$

Binomial likelihood

$$X \sim \text{Bin}(n,\theta), 0 \le \theta \le 1$$

$$p(x|\theta) = \binom{n}{x} \theta^x (1-\theta)^{n-x}$$

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$$p(x|\theta) = \binom{n}{x} \theta^x (1 - \theta)^{n - x}$$

Let's construct a Jeffreys prior over θ

$$\log p(x|\theta) = x \log \theta + (n-x) \log(1-\theta)$$

$$\frac{d}{d\theta} \log p(x|\theta) = \frac{x}{\theta} - \frac{n-x}{1-\theta}$$

$$\frac{d^2}{d\theta^2} \log p(x|\theta) = -\frac{x}{\theta^2} - \frac{n-x}{(1-\theta)^2}$$

$$\frac{d^2}{d\theta^2}\log p(x|\theta) = -\frac{x}{\theta^2} - \frac{n-x}{(1-\theta)^2}$$



$$\mathbb{E}[x] = n\theta$$

$$I(\theta) = -\mathbb{E}_{\theta} \left[\frac{d^2 \log p(x|\theta)}{d\theta^2} \right]$$

$$= \frac{n\theta}{\theta^2} + \frac{n - n\theta}{(1 - \theta)^2}$$

$$= \frac{n}{\theta} + \frac{n}{1 - \theta}$$

$$\pi_J(\theta) = I(\theta)^{\frac{1}{2}} \propto \theta^{-\frac{1}{2}} (1 - \theta)^{-\frac{1}{2}}$$

$$= \frac{n}{\theta} + \frac{n}{1 - \theta}$$
Beta(\frac{1}{2}, \frac{1}{2})

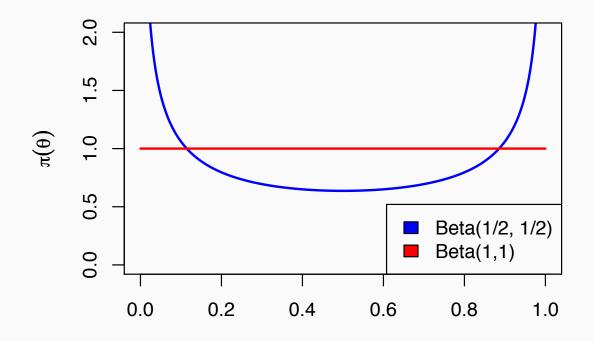
$$\pi_J(\theta) = I(\theta)^{\frac{1}{2}} \propto \theta^{-\frac{1}{2}} (1-\theta)^{-\frac{1}{2}}$$

 $\operatorname{Beta}(\frac{1}{2},\frac{1}{2})$

Binomial likelihood

$$X \sim \text{Bin}(n,\theta), 0 \le \theta \le 1$$

$$p(x|\theta) = \binom{n}{x} \theta^x (1-\theta)^{n-x}$$



θ

Data takes least effect

$$\theta = \frac{1}{2}$$

Data takes greatest effect

$$\theta = 0 \text{ or } 1$$

Prior is consistent with the data effect!

Let us consider a general translation

$$\phi = h(\theta)$$

$$P(\theta) = P(\theta). \mid \theta$$

What is the Jeffreys prior over ϕ ?

$$\pi_J(\phi) \propto |\mathbf{I}(\phi)|^{\frac{1}{2}}$$

Use Chain rule

$$\mathbf{I}(\phi) = -\mathbb{E}\left[\frac{\mathrm{d}^2 \log p(X|\phi)}{\mathrm{d}\phi^2}\right]$$

$$= -\mathbb{E}\left[\frac{\mathrm{d}^2 \log p(X|\theta)}{\mathrm{d}\theta^2}\right] \left(\frac{\mathrm{d}\theta}{\mathrm{d}\phi}\right)^2 + \mathbb{E}\frac{\mathrm{d} \log p(X|\theta)}{\mathrm{d}\theta} \frac{\mathrm{d}^2\theta}{\mathrm{d}\phi^2}\right]$$

$$\frac{d^{2} \log P(x|\phi)}{d\phi} = \frac{d \log P(x|\phi)}{d\phi}$$

$$= \frac{d \log P(x|\phi)}{d\phi} = \frac{d \log P(x|\phi)}{d\phi}$$

We know
$$\mathbb{E}\left[\frac{\mathrm{d}\log p\left(X|\theta\right)}{\mathrm{d}\theta}\right]=0 \quad \text{Why?}$$

Thy?
$$\frac{\sqrt{p(x|\theta)}}{\sqrt{d\theta}} \propto x$$

$$\forall \theta, \int p(X|\theta) dX = 1$$

$$\frac{d^{1} P(x|\theta)}{d\theta} = \frac{1}{P(x|\theta)} \frac{d^{1} P(x|\theta)}{d\theta}$$

$$Q = \frac{\mathrm{d}}{\mathrm{d}\theta} \int p(X|\theta) dX$$

$$= \int \frac{\mathrm{d}p(X|\theta)}{\mathrm{d}\theta} \left[\frac{p(X|\theta)}{p(X|\theta)} \right] dX$$

$$= \int \left[\frac{\mathrm{d}p(X|\theta)}{\mathrm{d}\theta} \frac{1}{p(X|\theta)} \right] p(X|\theta) dX$$

$$= \int \left[\frac{\mathrm{d}\log p(X|\theta)}{\mathrm{d}\theta} \right] p(X|\theta) dX$$

$$= \mathbb{E}\left[\frac{\mathrm{d}\log p(X|\theta)}{\mathrm{d}\theta} \right]$$

$$\mathbf{I}(\phi) = -\mathbb{E}\left[\frac{\mathrm{d}^{2}\log p\left(X|\theta\right)}{\mathrm{d}\theta^{2}}\right] \left(\frac{\mathrm{d}\theta}{\mathrm{d}\phi}\right)^{2} + \frac{\mathrm{d}\log p\left(X|\theta\right)}{\mathrm{d}\theta} \left(\frac{\mathrm{d}^{2}\theta}{\mathrm{d}\phi^{2}}\right)$$

$$\mathbf{I}(\theta) = \mathbf{I}(\theta)\left(\frac{\mathrm{d}\theta}{\mathrm{d}\phi}\right)^{2} \qquad p(\theta) \neq \gamma_{1}(\phi)$$

$$\uparrow (\phi) \neq \gamma_{2}(\phi) \neq \gamma_{3}(\phi) = \sqrt{\mathbf{I}(\phi)} \left|\frac{\mathrm{d}\theta}{\mathrm{d}\phi}\right|$$

$$\uparrow (\phi) \neq \gamma_{3}(\phi) \neq \gamma_{4}(\phi) \neq \gamma_{5}(\phi)$$

$$\sqrt{\mathbf{I}(\phi)} = \sqrt{\mathbf{I}(\theta)} \left| \frac{\mathrm{d}\theta}{\mathrm{d}\phi} \right|$$

Now, we can see

When we directly construct Jeffreys prior

$$\pi_J(\phi) \propto \sqrt{\mathbf{I}(\phi)}$$
 The same!

When we derive the prior via variable transformation

$$\pi_J(\phi) \propto \sqrt{\mathbf{I}(h^{-1}(\phi))} \left| \frac{\mathrm{d}\theta}{\mathrm{d}\phi} \right| = \sqrt{\mathbf{I}(\theta)} \left| \frac{\mathrm{d}\theta}{\mathrm{d}\phi} \right|^{-1}$$

Now we can show, for a Gaussian likelihood

$$p(x|\underline{\mu}, \underline{\sigma}) = \mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

$$\pi_J(\mu) \propto \underline{1}$$
 $\pi_J(\sigma) \propto \underline{\frac{1}{\sigma}}$



Jeffreys prior

- Usually not conjugate
 - If you choose Jeffreys prior over μ, σ for a Gaussian likelihood

The posterior of μ will be a student t distribution

 Works well for single parameter, but not for models with multidimensional parameters (e.g., poor convergence properties, not very reasonable estimates)

Reference priors

- formalize what exactly we mean by an "uninformative prior": a function that maximizes some measure of distance or divergence between the posterior and prior, as data observations are made.
- A commonly used divergence is KL divergence

$$KL(p(\theta|t)||p(\theta)) = \int p(\theta|t) \log \frac{p(\theta|t)}{p(\theta)} d\theta$$

Reference priors

 We choose the prior that maximizes the expected KL divergence between the posterior and the prior

$$I(\Theta, \overline{T}) = \int p(t) \int p(\theta|t) \log \frac{p(\theta|t)}{p(\theta)} d\theta dt$$

$$= \int \int p(\theta,t) \log \frac{p(\theta,t)}{p(\theta)p(t)} d\theta dt$$

$$p^*(\theta) = \arg \max_{p(\theta)} I(\Theta,T) \quad \text{Mutual information}$$

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Bayesian vs. Frequentist

- Given a distribution $p(x|\theta)$ governed by θ
- Frequentist: I believe $\underline{\theta}$ is objective constant, I need to estimate it from IID samples $\underline{x_1, \dots, x_N}$
- Bayesian: I believe θ is some latent random variable it was first sampled from a prior distribution $p(\theta)$, then given θ , we sample the observations x_1, \ldots, x_N

Bayesian vs. Frequentist

• Bayesian: I believe θ is some latent random variable — it was first sampled from a prior distribution $p(\theta)$, then given θ , we sample the observations x_1, \ldots, x_N

 Although it sounds a philosophical choice, can we justify Bayesian modeling with some mathematical evidence?

Exchangeability

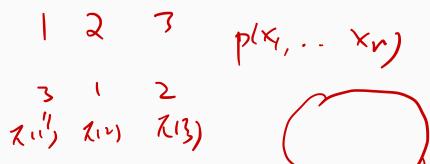
• Most statistical analysis are based on IID observations x_1, \ldots, x_N

$$p(X_1 = x_1, \dots, X_N = x_N) = \prod_{n=1}^N p(X_n = x_n)$$

 While the assumption is convenient, it may not be reasonable in many problems: weather conditions, stock prices, precipitation, disease rate, ...

Exchangeability is a much weaker assumption

Exchangeability



• Finite exchangeability: Given N random variables, and arbitrary permutation $\pi(1),\dots,\pi(N)$

$$X_1, \dots, X_N \stackrel{d}{=} X_{\pi(1)}, \dots, X_{\pi(N)}$$



 $\forall x_1, \dots, x_N$ in the domain

$$p(X_1=\underline{x}_1,\ldots,\underline{X}_N=\underline{x}_N)=p(X_1=\underline{x}_{\pi(1)},\ldots,X_N=x_{\pi(N)})$$

e.g.
$$\begin{cases} p(X_1=1,X_2=2,X_3=3)=p(X_1=2,X_2=3,X_3=1)\\ =p(X_1=3,X_2=1,X_3=2)=\ldots \end{cases}$$

Exchangeability – infinite sequence

• An infinite sequence of random variables $\{X_i\}_{i=1}^{\infty}$ is exchangeable if $\forall n=1,2,\ldots$

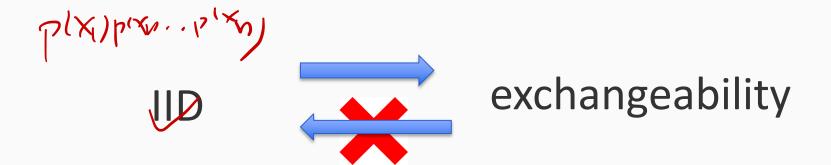
$$X_1, ..., X_n \stackrel{d}{=} X_{\pi(1)}, ..., X_{\pi(n)}, \quad \forall \pi \in S(n),$$

where S(n) are all possible permutations over the first n variables

Exchangeability

Essentially assume the symmetry of the density

$$p(X_1 = x_1, \dots, X_N = x_N) = p(X_1 = x_{\pi(1)}, \dots, X_N = x_{\pi(N)})$$



$$p(X_1 = rainy, X_2 = dry) = p(X_1 = dry, X_2 = rainy)$$

$$p(X_1 = rainy) \cdot p(X_2 = dry)$$

$$p(X_1 = rainy) \cdot p(X_2 = dry)$$
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Exchangeability - one specific example

Polya's Urn

- Given an urn with B_0 black and W_0 white balls, draw balls with the following procedure
 - (1) Draw a ball at random from the urn and note its color
 - (2) If the ball is black then $X_i = 1$; otherwise $X_i = 0$
 - (3) i = i + 1
 - (4) Place a balls of the same color in the urn

a=1)

• (5) Goto (1)

Exchangeability - one specific example

Polya's Urn

- Given an urn with B₀ black and W₀ white balls, draw balls with the following procedure
 - (1) Draw a ball at random from the urn and note its color

•
$$(3) i = i + 1$$

$$(5) \text{ Goto (1)}$$

$$p(1,1,0,1) = \frac{B_0}{B_0 + W_0} \times \frac{B_0 + a - 1}{B_0 + W_0 + a - 1} \times \frac{W_0}{B_0 + W_0 + 2a - 2} \times \frac{B_0 + 2a - 2}{B_0 + W_0 + 3a - 3}$$

$$p(1,0,1,1) = \frac{B_0}{B_0 + W_0} \times \frac{W_0}{B_0 + W_0 + a - 1} \times \frac{B_0 + a - 1}{B_0 + W_0 + 2a - 2} \times \frac{B_0 + 2a - 2}{B_0 + W_0 + 3a - 3}$$

De Finetti's theorem

(de Finetti 1931) A binary sequence $\{X_i\}_{i=1}^{\infty}$ is <u>exchangeable</u> iff there exists a distribution function F on [0, 1] such that for all n,

$$p(x_1,\ldots,x_n)=\int_0^1\underline{\theta^{t_n}(1-\theta)^{n-t_n}}dF(\theta),$$

where $p(x_1, ..., x_n) = P(X_1 = x_1, ..., X_n = x_n)$ and $t_n = \sum_{i=1}^n x_i$.

- $p(\theta)\mathrm{d}\theta$
- 1. There is a latent random variable θ
- 2. It has a prior distribution

df(0)

De Finetti's theorem

It further holds that \underline{F} is the distribution function of the limiting frequency:

$$\overline{X} = \lim_{n \to \infty} \sum_{i} X_{i}/n, \quad P(Y \le y) = F(y)$$

and the Bernoulli distribution is obtained by conditioning with $Y = \theta$:

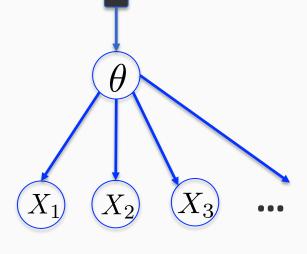
$$P(X_1 = x_1, \dots, X_n = x_n \mid Y = \theta) = \underbrace{\theta^{t_n}(1 - \theta)^{n-t_n}}_{P(\theta)}.$$

De Finetti's theorem – the underlying sampling process

• If our binary observations $\{X_i\}_{i=1}^{\infty}$ are exchangeable, it implies a hierarchical sampling process:

$$\theta \sim p(\theta)$$

Conditional independent
$$X_1, X_2, \dots | \theta \sim \prod_{i=1}^{\infty} p(X_i | \theta)$$



This justifies Bayesian modeling --- prior distribution objectively exists!

Exchangeability

- Very widely used assumption in Bayesian modeling
- More flexible than IID, but is also restrictive
- Some classical/popular models

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Lloyd, J., Orbanz, P., Ghahramani, Z., & Roy, D. M. (2012). Random function priors for exchangeable arrays with applications to graphs and relational data. In *Advances in Neural Information Processing Systems* (pp. 998-1006).

What you need to know

- Bayesian vs. Frequentist
- What is uninformative prior
- What are shift invariance, scale invariance in likelihood? How to derive the corresponding uninformative prior?
- What is Jeffery's prior? Arbitrary translation invariance
- Exchangeability
- De-Finette theorem (how does it justify Bayesian)s