Estadística bayesiana y aplicaciones en ciencia de datos

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2 Dirichlet process: the canonical BNP prior





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2 Dirichlet process: the canonical BNP prior



Random phenomena drive many aspects of this world













The Bayesian approach to statistical induction

Random phenomena

The Bayesian approach to statistical induction



The Bayesian approach to statistical induction



The basic probabilistic setup

- $(\Omega, \mathcal{A}, \mathbb{P})$: Probability space
 - $\triangleright \ \Omega$ –sample space. Set of all possible outcomes
 - $\triangleright \mathcal{A} \sigma$ -field. Collection of subsets of Ω with all events of interest
 - ▷ $\mathbb{P} : \mathcal{A} \mapsto [0, 1]$ –*Probability measure*. Mathematically coherent measure to quantify all *events* $A \in \mathcal{A}$
- Features of interest can be translated into "numeric" quantities via
 ▷ (X, X)-valued functions, X : Ω → X. random variables (r.v.'s)
 Given a r.v. X, the set function defined by

$$\mathsf{P}_X(B) = \mathbb{P}(X^{-1}(B)), \quad \text{for all } B \in \mathcal{X}$$
(1)

is termed the *distribution or law* of the random variable X.

 \triangleright When $\mathbb{X} = \mathbb{R}$ and $B = (-\infty, x]$ we write

 $\mathsf{F}_X(x) = \mathsf{P}_X((-\infty, x]) = \mathbb{P}(X \le x) \quad o \text{ the } (cdf) \text{ of } X$

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Ex. toss a coin

$$\Omega = \{\text{head}, \text{tail}\} = \{\omega_1, \omega_2\} = \{0, 1\}$$
$$\mathcal{A} = \{\Omega, \{0\}, \{1\}, \emptyset\}$$

Let X the r.v. that assigns 1 if the outcome is tail and 0 otherwise, i.e. $\mathsf{P}_X(\{1\}) = \mathbb{P}(X(\omega_1) = 1)$ with $\mathbb{X} = \{0, 1\}$

• For such quantity, we might assign a value $\theta \in [0, 1]$, i.e.

 $\mathsf{P}_X(\{1\}) = \theta$

 \Rightarrow Uncertainty about X is transferred to the *parameter* of interest θ .

How can we improve our knowledge about θ in the presence of observations from the random phenomena?

- Availability of more info about a random phenomenon
 - \Rightarrow better uncertainty quantification
 - \Rightarrow better statistical induction
- Realizations of a given phenomenon encoded via r.v.'s {X_i}_{i∈I}
 ▷ Logical/physical independence ≠ stochastic independence

so $\mathbb{P}(X_{n+1} \in B \mid X_1, \dots, X_n) = \mathbb{P}(X_{n+1} \in B)$ not always a good idea!

▷ Statistical learning requires stochastic dependence !

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• Symmetry/Stability principles in the law modelling $\{X_i\}$'s are fundamental for statistical induction

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- Major symmetries used in statistics
 - ▷ IID r.v.'s: physical & stochastic independence (rare in real apps!)
 - ▷ Exchangeability: physical indep. + sampling order invariace!
 - ▷ Stationarity: Uncertainty is not "time" invariant
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Exchangeable sequences

A finite sequence of r.v.'s, $\{X_n\}_{i=1}^n$, is said to be *finite exchangeable* if, for any permutation π of $(1, \ldots, n)$

$$(X_1,\ldots,X_n) \stackrel{\mathrm{d}}{=} (X_{\pi(1)},\ldots,X_{\pi(n)})$$

An infinite sequence $\{X_n\}_{i=1}^{\infty}$ is said to be *exchangeable* if every subcollection is exchangeable.

- \approx Distributional invariance under sampling order
- ▷ What can we say about the law of an exchangeable sequence
- \triangleright B. de Finetti's representation characterises exchangeable sequences

• B. de Finetti 1931: A seq. of binary r.v.'s $\{X_i\}_{i=1}^{\infty}$, e.g. with values in $\mathbb{X} = \{0, 1\}$, is exchangeable iff there exists a dist. q on [0, 1]

$$\mathbb{P}(X_1 = x_1, \dots, X_n = x_n) = \int_{[0,1]} \theta^{s_n} (1-\theta)^{n-s_n} \mathsf{q}(\mathrm{d}\theta)$$

where $s_n := \sum_{i=1}^n x_i$.

• $q(\cdot)$ is the distribution of $\lim_{n\to\infty} \frac{s_n}{n}$

• Conditional independence

$$\mathbb{P}(X_1 = x_1, \dots, X_n = x_n \mid \theta) = \prod_{i=1}^n \mathbb{P}(X_i = x_i \mid \theta) = \theta^{s_n} (1-\theta)^{n-s_n}$$

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Example: $\{X_i\}_{i=1}^{\infty}$ be Bernoulli r.v.'s

Two different Bernoulli exchangeable laws by two different persons

$$\mathbb{P}(x_1, \dots, x_n) = \frac{12}{s_n + 2} \frac{1}{\binom{n+4}{s_n + 2}} \text{ and } \mathbb{P}(x_1, \dots, x_n) = \frac{1}{[n+1]\binom{n}{s_n}},$$

- ▷ These persons believe that $\mathbb{P}(X_1 = 1) = 0.4 \& \mathbb{P}(X_1 = 1) = 0.5$ resp.
- ▷ Both believe that $\Theta := \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} X_i$ exists & $\mathbb{P}(X_1 = 1 \mid \Theta = \theta) = \theta$
- ▷ Since $\mathbb{P}(X_1 = 1) = \mathbb{E}(\Theta)$ they must have different values for $\mathbb{E}(\Theta)$
- ▷ Assume we observe the result of n = 20 given by 14 "1s" and 6 "0s".

$$\mathbb{P}[X_{21} \mid x_1, \dots, x_{20}] = 0.64$$
 and $\mathbb{P}[X_{21} \mid x_1, \dots, x_{20}] = 0.68.$

• Regardless of the prior mean on Θ , they should modify their opinion about the prop. of 1's!

• Consequence due to exchangeability, regardless of frequencies being interpreted as probabilities.

Schervish, 1995.

If X is a r.v. on $\mathbb{X} = \{1, 2\}$ with prob. p_1 and $p_2 = 1 - p_1$ assigned to each element of X. That is $\{X \mid p_1, p_2\} \sim \text{Bernoulli}(p_1, p_2)$

• Each value of $\mathbf{p} = (p_1, p_2)$ defines probability measure on X

• $q = \mathsf{Be}(\alpha_1, \alpha_2)$ defines a probability measure on

 $\mathcal{P}_{\mathbb{X}} := \{ \text{Space of prob. measures on } \mathbb{X} \} = \{ (p_1, p_2); p_i \ge 0 \text{ y } p_1 + p_2 = 1 \}$

$$\Rightarrow p_1 \mid X^{(n)} \sim \mathsf{Be}\left(\alpha_1 + \sum_{i=1}^n \delta_{X_i}(\{1\}), \alpha_2 + \sum_{i=1}^n \delta_{X_i}(\{2\})\right)$$

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Prior to posterior effect



Exchangeable sequences: general X

 \bullet Let $\mathcal{P}_{\mathbb{X}}$ be the space of all probability measures on (\mathbb{X},\mathcal{X})

A seq. $\{X_i\}_{i=1}^{\infty}$ is exchangeable iff there exists Q on $\mathcal{P}_{\mathbb{X}}$ such that

$$\mathbb{P}(X_1 \in A_1, \dots, X_n \in A_n) = \int_{\mathcal{P}_{\mathbf{X}}} \prod_{i=1}^n \mathbb{P}(A_i) \mathbb{Q}(d\mathbb{P}), \quad \forall n \ge 1 \text{ and } A_i \in \mathcal{X}$$

Alternatively: $X_i \mid \mathsf{P} \stackrel{\text{iid}}{\sim} \mathsf{P}$ and $\mathsf{P} \sim \mathsf{Q}$ (conditionally iid).

Hewitt and Savage 1955

- ▷ If $P_n(A) := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}(A)$ denotes the empirical dist. hence, **Q** is the dist. of the RPM **P**, where $\mathbb{P}[P_n \Rightarrow \mathsf{P}] = 1$ (**P** ~ **Q**)
- \triangleright **Q** is unique
- ▷ "The unknown", P, that allows us to disaggregate the elements of $X^{(\infty)}$ as a conditional iid sample, is random.

Statistical induction

Consequences of de Finetti's representation

• There is a clear bijection between the law of $\{X_i\}_{i=1}^{\infty}$ and Q

- Pick $\mathbb{Q} \Rightarrow$ we have a law for $\{X_i\}_{i=1}^{\infty}$
- Pick a law for $\{X_i\}_{i=1}^{\infty} \Rightarrow$ there exist a unique Q
 - i.e. $\mathsf{P}[X_{n+1} \in A \mid X^{(n)}] = \mathbb{E}_{\mathsf{Q}_{X^{(n)}}}[\mathsf{P}(A)]$ characterizes Q with $\mathsf{Q}_{X^{(n)}}(B) := \mathbb{P}(\mathsf{P} \in B \mid X^{(n)}),$
- However, any $\mathsf{P} \in \mathcal{P}_{\mathbb{X}}$ can be seen as the limit of P_n !
- Bayesian interpretation:
 - ${\sf Q}$ takes the interpretation of prior distributions on ${\sf P}$

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i.e. P[X_{n+1} ∈ A | X⁽ⁿ⁾] = E_{Q_X(n)} [P(A)] characterizes Q with Q_{X⁽ⁿ⁾}(B) := P(P ∈ B | X⁽ⁿ⁾),

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de Finetti and the Bayesian approach

The law of the exchangeable r.v's (and thus Q) is characterized by the conditional probabilities (or predictive distributions)

$$\mathbb{P}\left[X_{n+1} \in A_{n+1} \mid X_1 \in A_1, \dots, X_n \in A_n\right] = \frac{\mathsf{E}_{\mathsf{Q}}\left[\prod_{i=1}^{n+1} \mathsf{P}(A_i)\right]}{\mathsf{E}_{\mathsf{Q}}\left[\prod_{i=1}^{n} \mathsf{P}(A_i)\right]}$$

 $= \mathsf{E}_{\mathsf{Q}_{X^{(n)}}}\left[\mathsf{P}(A_{n+1})\right]$

for all n > 1, with $P_0 := \mathbb{P}[X_1 \in A_1] = \mathsf{E}_{\mathsf{Q}}[\mathsf{P}(A_1)]$ and where

$$\mathsf{Q}_{X^{(n)}}(\mathrm{d}\mathsf{P}) = \frac{\prod\limits_{i=1}^{n}\mathsf{P}(A_i)\,\mathsf{Q}(\mathrm{d}\mathsf{P})}{\mathsf{E}_{\mathsf{Q}}\left[\prod\limits_{i=1}^{n}\mathsf{P}(A_i)\right]}, \quad (\text{dominated case})$$

the posterior distribution of P given $X^{(n)} := (X_1, \ldots, X_n)$

Exchangeability: statistical learning for physically independent observations

Random phenomena encoded in X-valued $\{X_i\}_{i=1}^{\infty}$ exchangeable sequence driven by $\mathsf{P} \sim \mathsf{Q}$

•
$$\mathbb{Q}(\cdot) = \delta_{q_{\theta}}(\cdot) \Rightarrow X_{i}$$
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 $\mathcal{P}_{\mathbb{X}}:$ Space of all distributions on \mathbb{X}

Exchangeability: statistical learning for physically independent observations

Random phenomena encoded in X-valued $\{X_i\}_{i=1}^{\infty}$ exchangeable sequence driven by $\mathsf{P} \sim \mathsf{Q}$

• $Q(\mathcal{F}_{\Theta}) = 1 \Rightarrow$ Parametric family

Epistemic uncertainty

$$\mathbb{P}(X_1 \in A_1, \dots, X_n \in A_n) = \int_{\mathcal{F}_{\Theta}} \prod_{i=1}^n \underbrace{\mathcal{F}_{\theta}(A_i)}_{\text{Bandom}} \widetilde{\pi_{\theta}(d\theta)}$$

uncertainty via param. model



 $\mathcal{P}_{\mathbb{X}}$: Space of all distributions on \mathbb{X}

Exchangeability: statistical learning for physically independent observations

Random phenomena encoded in X-valued $\{X_i\}_{i=1}^{\infty}$ exchangeable sequence driven by $\mathsf{P} \sim \mathsf{Q}$

• $Q(P: d(P, \eta) < \varepsilon) > 0, \ \forall \ \eta \in \mathcal{P}_X \ y \ \varepsilon > 0 \Rightarrow BNP$

$$\mathbb{P}(X_1 \in A_1, \dots, X_n \in A_n) = \int_{\mathcal{P}_{\mathbf{X}}} \prod_{i=1}^n \underbrace{\mathbb{P}(A_i) \, \mathbb{Q}(d\mathbb{P})}_{i=1}$$

Random and epistemic uncertainties in one stroke!



 $\mathcal{P}_{\mathbb{X}}$: Space of all distributions on \mathbb{X} ... or other infinite dimensional sub-spaces of interest, $\mathcal{P}^{d}_{\mathbb{X}}$, $\mathcal{P}^{c}_{\mathbb{X}}$, etc.

Bayesian nonparametrics

What happens if X is of an infinite nature?

- \triangleright We could $\mathcal{P}_{\mathbb{X}}|_{\mathcal{F}_{\Theta}}$, but doesn't resolve the "random uncertainty"
- ▷ We want models Q giving positive prob. to all elements of $\mathcal{P}_{\mathbf{X}}$, or at least some infinite subset, e.g. set of densities, cdf's, etc.
- > de Finetti's representation Th. for general X gives an answer...
- ▷ Remember: $\{X_i\}_{i=n}^{\infty}$ exchangeable is driven by P ~ Q

How to construct suitable models for Q (nonparametric priors!)?

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How to construct suitable models for Q (nonparametric priors!)?

The Dirichlet distribution

Let
$$Z_i \stackrel{\text{iid}}{\sim} \mathsf{Ga}(\alpha_i, 1), i = 1, \dots, m \text{ and } \mathbf{W} := (W_1, \dots, W_m) \text{ with}$$

$$W_i = \frac{Z_i}{\sum_{i=1}^m Z_i}, \ i = 1, \dots, m \quad \Rightarrow \mathbf{W} \sim \text{Dirichlet}(\alpha_1, \dots, \alpha_m)$$

and is independent of $Z := \sum_{i=1}^{m} Z_i \sim \mathsf{Ga}(\sum_{i=1}^{m} \alpha_i, 1)$ with density

$$f(\mathbf{w}) = \frac{\Gamma\left(\sum_{i=1}^{m} \alpha_i\right)}{\prod_{i=1}^{m} \Gamma(\alpha_i)} \prod_{i=1}^{m-1} w_i^{\alpha_i - 1} \left(1 - \sum_{i=1}^{n-1} w_i\right)^{\alpha_m - 1} \mathbb{I}_{\Delta_{m-1}}(\mathbf{w}),$$

where $\Delta_{m-1} := \left\{ (w_1, \dots, w_{m-1}) : w_i \ge 0, \sum_{i=1}^{m-1} w_i \le 1 \right\}$

Properties of Dirichlet distribution

Moments Let $\alpha := \sum_{i=1}^{m} \alpha_i$ and $p_i := \alpha_i / \alpha$ hence • $\mathsf{E}[w_i] = p_i$ • Var $[w_i] = \frac{p_i(1-p_i)}{\alpha+1}$ • Corr $[w_i, w_j] = -\frac{p_i p_j}{2^{i+1}}$ Addition property If $W \sim \text{Dirichlet}(\alpha_1, \alpha_2, \ldots, \alpha_m)$ then i) For any partition A_1, \ldots, A_k of $\{1, \ldots, n\}$, the vector

 $\left(\sum_{i\in A_1} w_i, \sum_{i\in A_2} w_i, \dots, \sum_{i\in A_k} w_i\right) \sim \text{Dirichlet}(\alpha'_1, \dots, \alpha'_k)$

where $\alpha'_i := \sum_{j \in A_i} \alpha_j$

0.2

0.4-3 x/

0.6-

0.8

1

$$\alpha_{1} = \alpha_{2} = \alpha_{3} = 0.2 \qquad \alpha_{1} = \alpha_{2} = \alpha_{3} = 1 \qquad \alpha_{1} = \alpha_{2} = \alpha_{3} = 5$$





0.8

1

Ferguson 1973: The canonical example

• Via infinite dimensional distributions with pre-scribed fdds

Let $\alpha > 0$ a non-atomic finite measure on a Polish space $(\mathbb{X}, \mathcal{X})$. A $\mathcal{P}_{\mathbb{X}}$ -valued RPM, P , is said to have a Dirichlet process (\mathcal{D}_{α}) distribution, if for all measurable partition (B_1, \ldots, B_k) de \mathbb{X}

$$(\mathsf{P}(B_1),\ldots,\mathsf{P}(B_k)) \sim \operatorname{Dir}(\alpha(B_1),\ldots,\alpha(B_k))$$

• Ferguson 73' proved that the Dirichlet dist. is projective and therefore Daniel-Kolmogorov's existence theorem ensures the existence of \mathcal{D}_{α} . Namely, a stochastic process indexed on \mathcal{X} .

The Dirichlet process \mathcal{D}_{α} : The canonical example

Extending the finite-dim properties to the infinite-dim object it can be seen that if $X_i \stackrel{\text{iid}}{\sim} \mathsf{P}$ and $\mathsf{P} \sim \mathcal{D}_{\alpha}$ then

• $P_0(B) := \mathsf{E}_{\mathcal{D}_\alpha}[\mathsf{P}] = \frac{\alpha(B)}{\theta}$ for $B \in \mathcal{X}$ and where $\theta := \alpha(\mathbb{X})$

•
$$\operatorname{Var}_{\mathcal{D}_{\alpha}}[\mathsf{P}(B)] = \frac{P_0(B)(1-P_0(B))}{\theta+1}$$

•
$$\operatorname{Cov}(\mathsf{P}(B_1), \mathsf{P}(B_2)) = \frac{P_0(B_1 \cap B_2) - P_0(B_1)P_0(B_2)}{\theta + 1}$$

If $X_i | \mathsf{P} \stackrel{\text{iid}}{\sim} \mathsf{P} \text{ y } \mathsf{P} \sim \mathcal{D}_{\theta P_0}$, then $X_i \sim P_0, \forall i = 1, 2, \dots$

 $\mathsf{P} \mid X_1, \dots, X_n \sim \mathcal{D}_{\theta P_0 + n P_n}$ (conjugacy)

$$\mathsf{E}[\mathsf{P} \mid X_1, \dots, X_n] = \frac{\theta}{\theta + n} P_0 + \frac{n}{\theta + n} \sum_{i=1}^n \frac{\delta_{X_i}}{n}, \quad (\text{Bayes estimator})$$

Ferguson (1973)

${\it 2}$ Specification of Q via predictive distributions.

• Q can be characterized by its predictive dist. (Bayes estimator)

$$\mathbb{P}(X_{n+1} \in A \mid X_1, \dots, X_n) = \mathbb{E}\left[\mathbb{P}(A) \mid X_1, \dots, X_n\right] = \frac{\alpha_n(A)}{\alpha_n(\mathbb{X})}$$

with $\alpha_n(\cdot) = \alpha(\cdot) + \sum_{i=1}^n \delta_{X_i}(A)$. In other terms

$$\mathbb{P}[X_{n+1} \in \cdot \mid X^{(n)}] = \underbrace{\frac{\theta}{\theta+n}}_{\mathbb{P}[X_{n+1} = \text{``new''} \mid X^{(n)}]} \underbrace{\frac{\theta}{P_0(\cdot)}}_{\mathbb{P}[X_{n+1} = \text{``old''} \mid X^{(n)}]} \underbrace{\frac{\theta}{\sum_{i=1}^n \delta_{X_i}}}_{i=1}(\cdot),$$

Q is a DP iff the predictive is a linear combination of P₀ and the empirical measure

Regazzini (1978); Lo (1991)

Dirichlet process prior 0000000

The Dirichlet process \mathcal{D}_{α} : Pólya urn representation

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Blackwell and MacQueen 73' observed that when $n \to \infty$

$$\frac{\alpha_n()}{\alpha_n(\mathbb{X})} \stackrel{\text{a.s.}}{\to} \mathsf{P}, \qquad \text{with} \qquad \mathsf{P} \sim \mathcal{D}_{\alpha}$$

 \rightarrow Very appealing for MCMC implementations \rightarrow A direct consequence is that

$$\mathbb{P}(X_i = X_j) = \frac{1}{\theta + 1} > 0, \qquad i \neq j$$

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