BML lecture #1: Bayesics

http://github.com/rbardenet/bml-course

Rémi Bardenet

CNRS & CRIStAL, Univ. Lille, France

Outline

What comes to *your* mind when you hear "Bayesian ML"?

A quick motivating example before we go formal 1/2

- Let N individuals evolve from Susceptible to Infected to Recovered, $x_n(t) \in \{S, I, R\}$, $1 \leqslant n \leqslant N$, $t \in [0, T]$.
- Each susceptible individual n moves to R according to a Poisson process with intensity

$$\sum_{k : x_k(t) = I} \lambda_{nk}(\theta_{SI}).$$

- Each infected person recovers after a Gamma(a, b) time.
- This allows to express

$$p(x_1(t_{1,1}), \ldots, x_1(t_{1,T_1}), \cdots, x_n(t_{n,1}), \ldots, x_1(t_{n,T_n})|\theta).$$

  where $\theta = (\theta_{SI}, a, b)$.
- Now, consider $p(\theta|\text{data}) \propto p(\text{data}|\theta)p(\theta)$.

A quick motivating example before we go formal 2/2

- If asked to report an interval on a particular function of θ, say R_0, I would output a small interval I such that

$$\int_I p(\theta|\text{data})\,\mathrm{d}\theta \geqslant 0.95.$$

- If asked whether we should close universities, I would ask for
  - the cost α of closing unis when $R_0 < 1$,
  - the cost β of keeping unis open while $R_0 > 1$.

- Then I would recommend closing if and only if

$$p(R_0 > 1|\text{data}) > \frac{\alpha}{\alpha + \beta}.$$

- Additionally, I would check that the decision doesn't change if I change my prior $p(\theta)$ a little.

- If it did, then I would refine my likelihood and/or wait for more data.

Quotes from Gelman et al., 2013 on Bayesian methods

- *[...] practical methods for making inferences from data, using probability models for quantities we observe and for quantities about which we wish to learn.*

- *The essential characteristic of Bayesian methods is their explicit use of probability for quantifying uncertainty in inferences based on statistical data analysis.*

- *Three steps:*
  1. *Setting up a full probability model,*
  2. *Conditioning on observed data, calculating and interpreting the appropriate "posterior distribution",*
  3. *Evaluating the fit of the model and the implications of the resulting posterior distribution. In response, one can alter or expand the model and repeat the three steps.*

Notation that I will try to stick to

- $y_{1:n} = (y_1, \ldots, y_n) \in \mathcal{Y}^n$ denote observable data/labels.
- $x_{1:n} \in \mathcal{X}^n$ denote covariates/features/hidden states.
- $z_{1:n} \in \mathcal{Z}^n$ denote hidden variables.
- $\theta \in \Theta$ denote parameters.
- X denotes an $\mathcal{X}$-valued random variable. Lowercase x denotes either a point in $\mathcal{X}$ or an $\mathcal{X}$-valued random variable.

More notation

- Whenever it can easily be made formal, we write densities for our random variables and let the context indicate what is meant. So if $X \sim \mathcal{N}(0, \sigma^2)$, we write

$$\mathbb{E}h(X) = \int h(x) \frac{e^{-x^2/2\sigma^2}}{\sigma\sqrt{2\pi}} \mathrm{d}x = \int h(x)p(x)\mathrm{d}x.$$

Similarly, for $X \sim \mathcal{P}(\lambda)$, we write

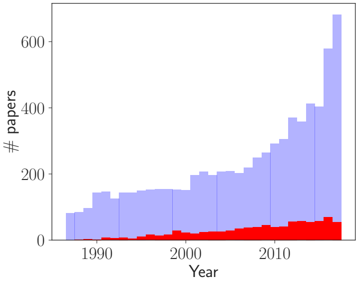
$$\mathbb{E}h(X) = \sum_{k=0}^{\infty} h(k)e^{-\lambda}\frac{\lambda^k}{k!} = \int h(x)p(x)\mathrm{d}x$$

- All pdfs are denoted by p, so that, e. g.

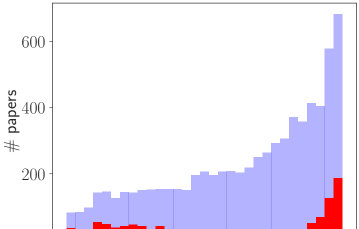
$$\begin{aligned}\mathbb{E}h(Y,\theta) &= \int h(y,\theta)p(y,\theta)\,\mathrm{d}y\mathrm{d}\theta \\ &= \int h(y,\theta)p(y,x,\theta)\,\mathrm{d}x\mathrm{d}y\mathrm{d}\theta \\ &= \int h(y,\theta)p(y,\theta|x)p(x)\,\mathrm{d}x\mathrm{d}y\mathrm{d}\theta\end{aligned}$$

Outline

Bayesian keywords in NeurIPS abstracts, up to 2016



(a) "Bayesian" at NeurIPS



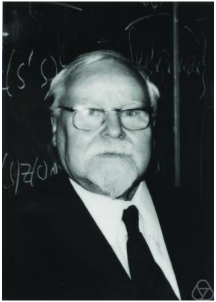
Topics automatically extracted from 1000+ “Bayesian” abstracts

model models data process latent Bayesian Dirichlet hierarchical nonparametric inference
features learn problem different knowledge learning image object example examples
method neural Bayesian using linear state based kernel approach model
belief propagation nodes local tree posterior node nbsp given algorithm
learning data Bayesian model training classification performance selection prediction sets
inference Monte Carlo Markov sampling variational time algorithm MCMC approximate
function optimization algorithm optimal learning problem gradient methods bounds state
learning networks variables structure network Bayesian EM paper distribution algorithm
Bayesian gaussian prior regression non estimation likelihood sparse parameters matrix
model information Bayesian human visual task probability sensory prior concept

Figure: Topics extracted by stochastic variational latent Dirichlet allocation, using scikit-learn (**sklearn11**).

Inference in regression models

Inference in regression models



Inference in regression models

Inference in regression models

Outline

Describing a decision problem under uncertainty

- A state space $\mathcal{S}$,
  Every quantity you need to consider to make your decision.
- Actions $\mathcal{A} \subset \mathcal{F}(\mathcal{S}, \mathcal{Z})$,
  Making a decision means picking one of the available actions.
- A reward space $\mathcal{Z}$,
  Encodes how you feel about having picked a particular action.
- A loss function $L : \mathcal{A} \times \mathcal{S} \rightarrow \mathbb{R}_+$.
  How much you would suffer from picking action a in state s.

Classification as a decision problem

- $\mathcal{S} = \mathcal{X}^n \times \mathcal{Y}^n \times \mathcal{X} \times \mathcal{Y}$, i.e. $s = (x_{1:n}, y_{1:n}, x, y)$.
- $\mathcal{Z} = \{0, 1\}$.
- $\mathcal{A} = \{a_g : s \mapsto 1_{y \neq g(x; x_{1:n}, y_{1:n})}, \quad g \in \mathcal{G}\}$.
- $L(a_g, s) = 1_{y \neq g(x; x_{1:n}, y_{1:n})}$.

PAC bounds; see e.g. (Shalev-Shwartz and Ben-David, 2014)

Let $(x_{1:n}, y_{1:n}) \sim \mathbb{P}^{\otimes n}$, and independently $(x, y) \sim \mathbb{P}$, we want an algorithm $g(\cdot; x_{1:n}, y_{1:n}) \in \mathcal{G}$ such that if $n \geqslant n(\delta, \varepsilon)$,

$$\mathbb{P}^{\otimes n}\left[\mathbb{E}_{(x,y)\sim\mathbb{P}} L(a_g, s) \leqslant \varepsilon\right] \geqslant 1 - \delta.$$

Regression as a decision problem

- $\mathcal{S} =$
- $\mathcal{Z} =$
- $\mathcal{A} =$
-

Estimation as a decision problem

- $\mathcal{S} =$
- $\mathcal{Z} =$
- $\mathcal{A} =$
-

Clustering as a decision problem

- $\mathcal{S} =$
- $\mathcal{Z} =$
- $\mathcal{A} =$
-

SEU is what defines the Bayesian approach

The subjective expected utility principle

1. Choose $\mathcal{S}, \mathcal{Z}, \mathcal{A}$ and a loss function $L(a, s)$,
2. Choose a distribution p over $\mathcal{S}$,
3. Take the the corresponding Bayes action

$$a^\star \in \arg\min_{a \in \mathcal{A}} \mathbb{E}_{s \sim p} L(a, s). \tag{1}$$

Corollary: minimize the posterior expected loss

Now partition $s = (s_{\text{obs}}, s_{\text{u}})$, then

$$a^\star \in \arg\min_{a \in \mathcal{A}} \mathbb{E}_{s_{\text{obs}}} \mathbb{E}_{s_{\text{u}} | s_{\text{obs}}} L(a, s).$$

In ML, $\mathcal{A} = \{a_g\}$, with $g = g(s_{\text{obs}})$, so that (1) is equivalent to

$$a^\star = \delta(s_{\text{obs}}) = \arg\min_{a \in \mathcal{A}} \mathbb{E}_{s_{\text{u}} | s_{\text{obs}}} L(a, s).$$

Outline

- PGMs (aka "Bayesian" networks) represent the dependencies in a joint distribution $p(y)$ by a directed graph $G = (E, V)$.
- Two important properties:

$$p(y) = \prod_{v \in V} p(y|y_{\mathrm{pa(v)}}) \qquad \text{and} \qquad y_v \perp y_{nd(v)} | y_{pa(v)}.$$

- Also good to know how to determine whether $A \perp B | C$; see (Murphy, 2012, Section 10.5).

Estimation as a decision problem: point estimates

Estimation as a decision problem: credible intervals

Choosing priors (see Exercises)

Classification as a decision problem

Regression as a decision problem 1/2

Dimensionality reduction as a decision problem

Clustering as a decision problem

Topic modelling as a decision problem

Image denoising as a decision problem

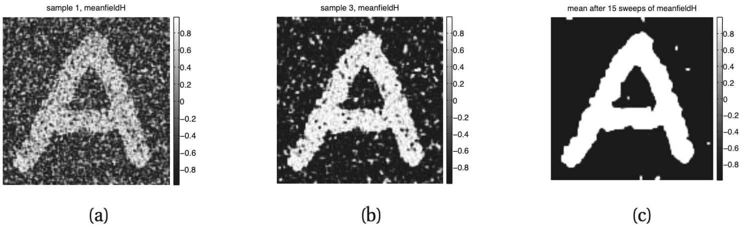


Figure: Taken from (Murphy, 2012, Chapter 21)

Outline

An issue (or is it?)

Depending on how they interpret and how they implement SEU, you will meet many types of Bayesians (46656, according to Good).

A few divisive questions

- Using data or the likelihood to choose your prior; see Lecture #5.
- Using MAP estimators for their computational tractability, like in inverse problems

$$\hat{x}_\lambda \in \arg\min \|y - Ax\| + \lambda\Omega(x).$$

- When and how should you revise your model (likelihood or prior)?
- MCMC vs variational Bayes (more in Lectures #2 and #3)

[1] A. Gelman et al. *Bayesian data analysis*. 3rd. CRC press, 2013.

[2] K. Murphy. *Machine learning: a probabilistic perspective*. MIT Press, 2012.

[3] S. Shalev-Shwartz and S. Ben-David. *Understanding machine learning: From theory to algorithms*. Cambridge university press, 2014.