BML lecture #1: Bayesics

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

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

Course outline

Outline

- 1 Introduction
- 2 A warmup: Estimation in regression models
- 3 ML as data-driven decision-making
- 4 Subjective expected utility
- 5 Specifying joint models
- 6 50 shades of Bayes

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A quick motivating example before we go formal 1/2

- Let N individuals evolve from Susceptible to Infected to Recovered, $x_n(t) \in \{S, I, R\}, 1 \le n \le N, t \in [0, T].$
- ► Each susceptible individual *n* moves to *I* 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

$$p(x_1(t_{1,1}), \dots, x_1(t_{1,T_1}), \dots, x_N(t_{N,1}), \dots, x_1(t_{N,T_N})|\theta).$$
 where $\theta = (\theta_{SI}, a, b).$

(031, 4, 5).

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 A on a particular function of θ , say $R_0 = h(\theta)$, I would report a small interval A such that

$$\int 1_{h(\theta)\in A} \, p(\theta|\mathsf{data}) \, \mathrm{d}\theta = p(h(\theta)\in A|\mathsf{data}) \geqslant 0.95.$$

- 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

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

- 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

- $y_{1:n} = (y_1, \dots, y_n) \in \mathcal{Y}^n$ denote observable data/labels.
- \triangleright $x_{1:n} \in \mathcal{X}^n$ denote covariates/features/hidden states.
- $ightharpoonup z_{1\cdot n}\in\mathcal{Z}^n$ denote hidden variables.
- ▶ θ ∈ Θ denote parameters.
- ightharpoonup 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

Nhenever 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

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

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

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

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

$$\mathbb{E}h(Y,\theta) = \int h(y,\theta)p(y,\theta) \,dyd\theta$$
$$= \int h(y,\theta)p(y,x,\theta) \,dxdyd\theta$$
$$= \int h(y,\theta)p(y,\theta|x)p(x) \,dxdyd\theta$$

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Describing a decision problem under uncertainty

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

Classification as a decision problem

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

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

- $ightharpoonup \mathcal{S} =$
- **▶** *Z* =
- ▶ A =

Estimation as a decision problem

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

Clustering as a decision problem

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

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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 S,
- 3 Take the the corresponding Bayes action

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

Corollary: minimize the posterior expected loss

Now partition $s = (s_{obs}, s_u)$, then

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

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

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

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A recap on probabilistic graphical models 1/2

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

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

A recap on probabilistic graphical models 2/2

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

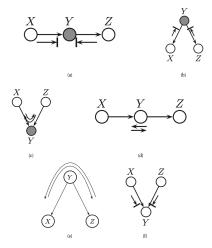


Figure 10.9 Bayes ball rules. A shaded node is one we condition on. If there is an arrow hitting a bar, it means the ball cannot pass through; otherwise the ball can pass through. Based on (Jordan 2007).

A recap on probabilistic graphical models 2/2

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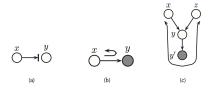


Figure 10.10 (a-b) Bayes ball boundary conditions. (c) Example of why we need boundary conditions. y' is an observed child of y, rendering y "effectively observed", so the ball bounces back up on its way from x to z.

A recap on probabilistic graphical models 2/2

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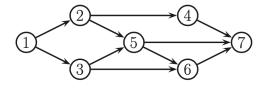


Figure 10.11 A DGM.

► Check that $x_2 \perp x_6 | x_5, x_1$, but that $x_2 \not\perp x_6 | x_5, x_1, x_7$.

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

Regression as a decision problem 2/2

Dimensionality reduction as a decision problem

Clustering as a decision problem

Topic modelling as a decision problem

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50 shades of Bayes

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)

References I

- [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.