Bayesian inverse problems II: Bayes' Theorem and Well-posedness

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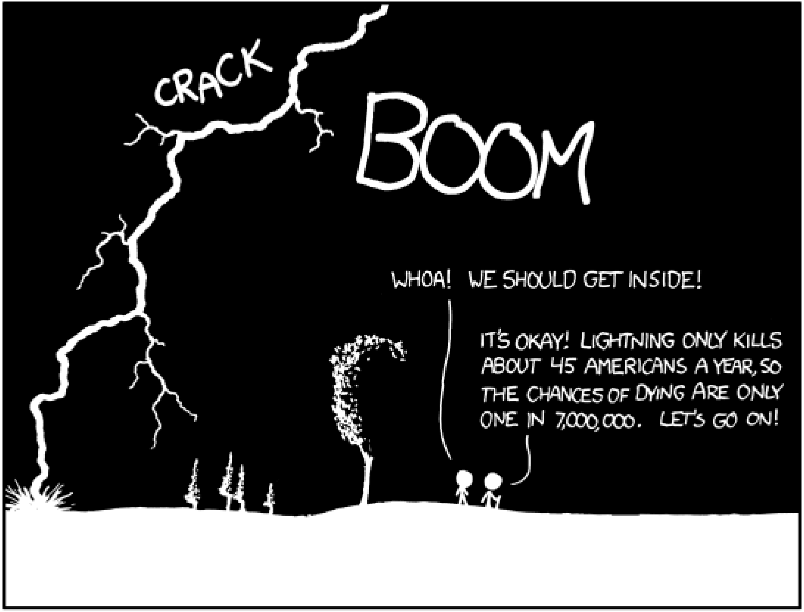
Outline



THE ANNUAL DEATH RATE AMONG PEOPLE WHO KNOW THAT STATISTIC IS ONE IN SIX.

What has happened so far...

Consider the inverse problem of the form

$$\mathcal{A}(f^*) + e = g,$$

where $f^* \in X$ is the unknown parameter/signal/image, $g \in Y$ is observed data, e is noise, and $\mathcal{A} : X \to Y$ is a linear or non-linear operator.

- we model f^* and e as random variables $F \sim \mu_{\text{prior}}$ and $E \sim \mu_{\text{noise}}$, respectively, to especially represent our reasonable expectation about f^*
- Bayesian idea: obtain the reasonable expectation that incorporates the observation, given by the so-called posterior:

$$\mathbb{P}(F \in \cdot | \mathcal{A}(F) + E = g)$$

- Representing conditional distributions is a bit tough, conditional densities are nice though!
- We have generalised the setting a bit, by defining a more general problem:
  - $F : \Omega \to X$, $G : \Omega \to Y$ are (dependent) random variables.
  - Given that we observe $G = g$, find F.

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Recap and outlook

Introducing Bayes' Theorem

- Bayes' Theorem will give us a strategy to obtain the posterior density
- More than anything, it is an inversion formula, it let's us flip a conditional density:

$$\pi_{F|G=g} \overset{\leftarrow}{\rightarrow} \pi_{G|F=f}$$

- so, we first need to access $\pi_{G|F=f}$
  - we refer to $L(g|f) := \pi_{G|F=f}(g)$ as (data) likelihood of g given f
  - it describes how well the parameter f describes the data g (or, how likely is the data f if the chosen parameter is g?)
  - the observed data is a sample from the data generating distribution

$$g \sim L(\cdot|f^*).$$

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Likelihoods in inverse problems

In our example with additive noise,

$$\mathcal{A}(F) + E = g,$$

with $Y := \mathbb{R}^d$ and $E \sim \mathrm{N}(0, \Gamma)$, we have

$$L(f|g) \propto \exp\left(-\frac{1}{2}\|\Gamma^{-1/2}(\mathcal{A}(f) - g)\|^2\right)$$

Observations:

- Considering this likelihood, we retrieve the classical least-squares formulation of an inverse problem when applying maximum likelihood estimation
- in statistics, we call a statistical model parametric if $X \subseteq \mathbb{R}^n$; our theory works for fairly general 'parameters' $f \in X$ that I will continue to call so.
- If Y is infinite-dimensional the definition of a likelihood is a bit tougher, as there is no Lebesgue measure. If applicable (non-trivial!), the Cameron–Martin Theorem can be used to obtain a likelihood

Bayes' Theorem.

Having understood likelihoods, we can now move on to Bayes' Theorem:

Bayes' Theorem.

Let π_{prior} be the density of the prior with respect to our reference measure ν_X. If $L(g|\cdot) \in \mathbf{L}^1(X, \mu_{\mathrm{prior}}; \mathbb{R})$ and $L(g|\cdot) > 0$ for $g \in Y$ $\mathbb{P}(G \in \cdot)$-a.s., we have

$$Z(g) := \int_X L(g|f) \mathrm{d}\mu_{\mathrm{prior}}(f) \in (0, \infty)$$

and μ_{post} has a density with respect to ν_X, which is given by

$$\pi_{\mathrm{post}} = \frac{L(g|\cdot)\pi_{\mathrm{prior}}}{Z(g)} \qquad (\nu_X\text{-a.e.}),$$

for $g \in Y$, $\mathbb{P}(G \in \cdot)$-a.s..

Bayes' Theorem.

Sketch of a proof.

1. $Z(g)$ is an integral of a function that is positive everywhere. Thus, $Z(g) > 0$.
2. We can write
$$\pi_{\text{post}} = \pi_{F|G=g} = \frac{\pi_{F,G}(\cdot, g)}{\pi_G(g)},$$
if $\pi_G(g) > 0$. From the definition of the converse
$$L(\cdot|f) = \pi_{G|F=f} = \frac{\pi_{F,G}(f, \cdot)}{\pi_F(f)}, \text{ where } \pi_F = \pi_{\text{prior}}$$
and some algebra we obtain
$$\pi_{F,G}(f, g) = L(g|f)\pi_{\text{prior}}(f) \text{ and, by the first step: } \pi_G(g) = Z(g) > 0.$$
Thus, Bayes' Theorem is true. □

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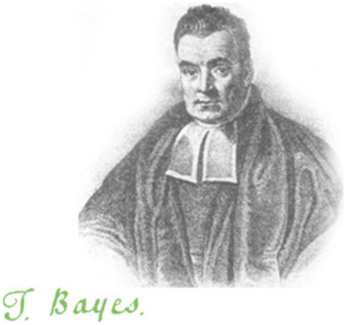
Bayes'(?) theorem



ce qui est le principe énoncé ci-dessus, lorsque toutes les causes sont *à priori* également possibles. Si cela n'est pas, en nommant p la probabilité *à priori* de la cause que nous venons de considérer; on aura $E = Hp$; et en suivant le raisonnement précédent, on trouvera

$$P = \frac{Hp}{S.Hp};$$

ce qui donne les probabilités des diverses causes, lorsqu'elles ne sont pas toutes, également possibles *à priori*.

Pour appliquer le principe précédent à un exemple, supposons qu'une urne renferme trois boules dont chacune ne puisse être que,

Figure: Left: Maybe Bayes. Right: Certainly not Bayes [[Laplace 1812]].

Bayesian inverse problem

Bayesian inverse problem: Given likelihood $L : Y \times X \to \mathbb{R}$ measurable and μ_{prior} that satisfy Bayes' theorem.

$$\text{Find: } \mu_{\text{post}} \text{ with } \nu_X\text{-density } \pi_{\text{post}} = \frac{L(g|\cdot)\pi_{\text{prior}}}{Z(g)} \qquad (\nu_X\text{-a.e.}) \qquad \text{(BIP)}$$

for any data set $g \in Y$.

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- Is (BIP) well-posed?

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- Is (BIP) well-posed?

Outline

When is a (BIP) well-posed?

[Dashti, Stuart 2017: **The Bayesian Approach to Inverse Problems.** In Ghanem, Higdon, Owhadi (editors): Handbook of Uncertainty Quantification, 311–428.] [Engel, Hafemeyer, Münch, Schaden 2019: **An application of sparse measure valued Bayesian inversion to acoustic sound source identification.** Inverse Probl. 35(7)] [Ernst, Sprungk, Starkloff 2015: **Analysis of the Ensemble and Polynomial Chaos Kalman Filters in Bayesian Inverse Problems.** SIAM/ASA JUQ 3(1):823–851.] [Dolera, Mainini 2019: **On uniform continuity of posterior distributions.** Stat Probabil Lett (in Press)] [Hosseini 2017: **Well-Posed Bayesian Inverse Problems with Infinitely Divisible and Heavy-Tailed Prior Measures.** SIAM/ASA JUQ 5(1):1024–1060.] [Hosseini, Nigam 2017: **Well-Posed Bayesian Inverse Problems: Priors with Exponential Tails.** SIAM/ASA JUQ 5(1):436–465,] [Iglesias, Lin, Stuart 2014: **Well-posed Bayesian geometric inverse problems arising in subsurface flow.** Inverse Probl., 30(11):114001.] [Iglesias, Lu, Stuart 2016: **A Bayesian level set method for geometric inverse problems.** Interfaces and Free Boundaries 18:181–217.] [Kahle, Lam, JL, Ullmann 2019: **Bayesian parameter identification in Cahn–Hilliard models for biological growth**. SIAM/ASA JUQ 7(2):526-552.] [JL 2020: **On the Well-posedness of Bayesian Inverse Problems,**. SIAM/ASA JUQ 8(1):451-482.] [JL 2023: **Bayesian Inverse Problems are Usually Well-posedness**. SIAM Rev. 65(3):831-865.] [JL, Eisenberger, Ullmann 2019: **Fast Sampling of parameterised Gaussian random fields**. Comput. Methods in Appl. Mech. Engrg. 348:978-1012.] [Sprungk 2019: **On the Local Lipschitz Robustness of Bayesian Inverse Problems.** arXiv:1906.07120] [Stuart 2010: **Inverse problems: a Bayesian perspective.** Acta Numerica 19:451-559.] [Sullivan 2017: **Well-posed Bayesian inverse problems and heavy-tailed stable quasi-Banach space priors.** Inverse Probl. Imaging 11(5):857–874.],...

When is a (BIP) well-posed?

How do we define well-posedness?

Definition. [JL; 2020, 2023]

Given a metric space of probability measures (P, d). (BIP) is (P, d)-well-posed, if

(1) $\mu_{\mathrm{post}} \in \mathrm{P}$ exists

(2) μ_{post} is unique

(3) μ_{post} is stable, i.e.

$$\forall g \in Y, \varepsilon > 0 \ \exists \delta > 0 : d(\mu_{\mathrm{post}}(\cdot|g)), \mu_{\mathrm{post}}(\cdot|g')) \leq \varepsilon \quad (\|g - g'\|_Y \leq \delta)$$

(continuity in (P, d))

Thus, we need to choose an appropriate metric space (P, d) on which we measure continuity.

(P, d)?

[JL; 2020, 2023]

$(\mathrm{Prob}(X), d_{\mathrm{TV}})$-well-posed $\quad :\Leftrightarrow$: total variation well-posed

$$d_{\mathrm{TV}}(\mu, \mu') = \sup_{A \in \mathcal{B}X} |\mu(A) - \mu'(A)|, \quad \mu, \mu' \in \mathrm{Prob}(X) := \{\mu : \mu \text{ is probability distribution on } (X, \mathcal{B}X)\}$$

$(\mathrm{Prob}(X, \mu_{\mathrm{prior}}), \mathrm{d}_{\mathrm{Hel}})$-well-posed $\quad :\Leftrightarrow$: Hellinger well-posed

$(\mathrm{Prob}(X), d_{\mathrm{Prok}})$-well-posed $\quad :\Leftrightarrow$: weakly well-posed

(P, d)?

[JL; 2020, 2023]

$(\mathrm{Prob}(X), d_{\mathrm{TV}})$-well-posed $\quad :\Leftrightarrow$: total variation well-posed

$(\mathrm{Prob}(X, \mu_{\mathrm{prior}}), \mathrm{d}_{\mathrm{Hel}})$-well-posed $\quad :\Leftrightarrow$: Hellinger well-posed

$$\mathrm{d}_{\mathrm{Hel}}(\mu, \mu') = \sqrt{\frac{1}{2} \int \left(\sqrt{\frac{\mathrm{d}\mu}{\mathrm{d}\mu_{\mathrm{prior}}}} - \sqrt{\frac{\mathrm{d}\mu'}{\mathrm{d}\mu_{\mathrm{prior}}}} \right)^2 \mathrm{d}\mu_{\mathrm{prior}}},$$

$$\mu, \mu' \in \mathrm{Prob}(X, \mu_{\mathrm{prior}}) := \{\mu \in \mathrm{Prob}(X) : \mu \ll \mu_{\mathrm{prior}}\}$$

$(\mathrm{Prob}(X), d_{\mathrm{Prok}})$-well-posed $\quad :\Leftrightarrow$: weakly well-posed

(P, d)?

[JL; 2020, 2023]

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$(\mathrm{Prob}(X), d_{\mathrm{Prok}})$-well-posed $\quad :\Leftrightarrow$ weakly well-posed

d_{Prok} metrises weak convergence, i.e. $d_{\mathrm{Prok}}(\mu, \mu') \to 0$

$$\Leftrightarrow \forall Q \text{ continuous, bounded: } \int_X Q(f)\mu(\mathrm{d}f) \to \int_X Q(f)\mu'(\mathrm{d}f) \qquad \mu, \mu' \in \mathrm{Prob}(X)$$

Main result

Theorem. [JL; 2020, 2023]

Let $\mu_{\text{prior}} \in \mathrm{Prob}(X)$. BIP is weakly, Hellinger, and total variation well-posed, if (W1)-(W4) are satisfied for $f \in X$ (μ_{prior}-a.s.) and $g \in Y$.

(W1) $L(\cdot|f)$ is a strictly positive probability density function,

(W2) $L(g|\cdot) \in \mathbf{L}^1(X, \mu_{\text{prior}})$,

(W3) $k \in \mathbf{L}^1(X, \mu_{\text{prior}})$ exists such that $L(g'|\cdot) \leq k$ for all $g' \in Y$.

(W4) $L(\cdot|f)$ is continuous.

- we can also show continuity in Wasserstein(p) distance and the Kullback–Leibler divergence, but need additional assumptions

Discussion

[JL; 2020, 2023]

(W1) $L(\cdot|f)$ is a strictly positive probability density function,

- $L(\cdot|f)$ is typically by definition of the inverse problem a probability density function
- $L > 0$: no data-parameter combinations are impossible

(W2) $L(g|\cdot) \in \mathbf{L}^1(X, \mu_{\text{prior}})$,

- Implied by (W3)

(W3) $g \in \mathbf{L}^1(X, \mu_{\text{prior}})$ exists such that $L(g'|\cdot) \leq k$ for all $g' \in Y$.

- Often satisfied by choosing g constant

(W4) $L(\cdot|f)$ is continuous.

- Simple continuity statement, in g, not f

Discussion

Assume, we have a finite number of observations, i.e. $g \in Y := \mathbb{R}^{N_{\mathrm{obs}}}$, to identify the parameter $f^* \in X$, with

$$g := \mathcal{A}(f^*) + e,$$

where the noise $E \sim \mathrm{N}(0, \Gamma)$, with $\Gamma > 0$, and $\mathcal{A} : X \to Y$ is some measurable function

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Corollary. [JL; 2020, 2023]

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Discussion

- Corollary can be generalised to infinite-dimensional data spaces and other noise models
  - infinite-dimensional case requires boundedness assumptions on $\mathcal{A}$
  - continuity and boundedness of the noise density function
- Assumptions (W1)-(W4) only imply continuity of the posterior, not more than that. Other works, [Stuart 2010], [Dashti+Stuart 2017], [Sprungk 2020],... show Lipschitz continuity and also other stability criteria under considerably stronger assumptions
- Well-posedness does not imply that the chosen model is sensible
  - additionally, we should look at the small noise/large data limit [Nickl 2023]
  - those are similar to the $\delta \downarrow 0$ in the variational approach to inverse problems and give results like

$$\mu_{\text{post}} \to \delta(\cdot - f^*) \qquad \text{('posterior consistency')}$$

or, even better,

$$\mu_{\text{post}} \approx \mathrm{N}(f^*, N_{\text{obs}}^{-1}\mathcal{I}^{-1}) \qquad \text{('Bernstein – von Mises Theorem').}$$

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Point estimators

It is nice to have a posterior measure, in practice, however

- that is usually computationally complicated
- not always practical

Obvious question: Can we find some point estimator (e.g. a value in X) that uses the Bayesian framework?

- posterior mean
- maximum-a-posteriori (MAP) estimator

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Posterior mean

Given that it exists, we can use the mean of the posterior as a point estimator

$$f_{\mathrm{Bayes}}(g) = \int_X f \, \mu_{\mathrm{post}}(\mathrm{d}f) = \mathbb{E}_{\mathrm{post}}[F],$$

which is also called 'Bayes estimator'.

Posterior mean

Why is that a good idea? (Assume μ_{post} has finite second moment)

- The Bayes estimator is the best function in $\mathcal{L}^2(Y;X)$ to describe the mapping from G to F, i.e. it solves

$$f_{\text{Bayes}} = \operatorname{argmin}_{k \in \mathcal{L}^2(Y;X)} \int \|f - k(g)\|_X^2 \mathbb{P}((F,G) \in (\mathrm{d}f, \mathrm{d}g))$$

- Hellinger well-posedness will imply well-posedness of the posterior mean with the same modulus of continuity!

Why is using bad idea?

- You usually need to approximate μ_{post} to obtain f_{Bayes}...
- It often has a smoothing effect that is

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Maximum-a-posteriori (MAP)

Idea: Maximum likelihoods (=the maximum of the likelihood) are good estimators, how about the maximum of the posterior density?

Let's assume for a moment that $X := \mathbb{R}^n$ and our prior/posterior has a Lebesgue density. Then, finding the maximum of π_{post} is identical to finding:

$$f_{\text{MAP}} \in \operatorname{argmin}_{f \in X} - \log \pi_{\text{post}}(f|g) = \operatorname{argmin}_{f \in X} - \log L(g|f) - \log \pi_{\text{prior}}(f) + \log Z(g)$$
$$= \operatorname{argmin}_{f \in X} \underbrace{- \log L(g|f)}_{\text{data misfit}} \underbrace{- \log \pi_{\text{prior}}(f)}_{\text{regulariser}},$$

which is exactly equivalent to a regularised variational problem.

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Idea: Maximum likelihoods (=the maximum of the likelihood) are good estimators, how about the maximum of the posterior density?

Let's assume for a moment that $X := \mathbb{R}^n$ and our prior/posterior has a Lebesgue density. Then, finding the maximum of π_{post} is identical to finding:

$$\begin{aligned} f_{\text{MAP}} \in \operatorname{argmin}_{f \in X} - \log \pi_{\text{post}}(f|g) &= \operatorname{argmin}_{f \in X} - \log L(g|f) - \log \pi_{\text{prior}}(f) + \log Z(g) \\ &= \operatorname{argmin}_{f \in X} \underbrace{- \log L(g|f)}_{\text{data misfit}} - \underbrace{\log \pi_{\text{prior}}(f)}_{\text{regulariser}}, \end{aligned}$$

which is exactly equivalent to a regularised variational problem.

Maximum-a-posteriori (MAP)

This equivalence of MAP and regularised variational approach is considerably more complicated if X is infinite-dimensional

- there is not really a natural reference density, so that way of defining it doesn't work.
- people define the MAP via the Onsager-Machlup functional
  - Essentially, finding the point around which the posterior assigns maximum probability
- the equivalence to variational problems is still mostly correct [Helin+Burger 2015]

Maximum-a-posteriori (MAP)

Why is using f_{MAP} a good idea?

- Getting the MAP is only an optimisation problem! Very cheap!
- Properties tend to be better for pure reconstruction

Why is using f_{MAP} a bad idea?

- Well-posedness not automatic!

Recap and outlook

Recap

Bayes' Theorem

Well-posedness of Bayesian inverse problems

Bayesian point estimators

Outlook

Recap and outlook

Recap.

- Bayes' formula allows us to obtain the posterior from prior and likelihood
- Bayesian inverse problems are usually well-posed

Outlook.

- The posterior is a conditional distribution. How can we get the its density?
- What is a good prior?
- Which properties does the posterior have?