Generalized Variational Inference (GVI)

Posterior beliefs with the rule of three

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1 The form of the Bayesian problem

Purpose of part 1: Motivate the rule of three

(1) Bayesian inference minimizes **losses**

(2) Bayesian inference **regularizes** with the prior

(3) Bayesian inference = **optimization** over **(sub)spaces of probability measures**

1.1 The Bayesian problem: Traditional perspective

Ingredients (for the simplest case) are:

- $n = n_1 + n_2$ observations $\boldsymbol{x} = (x_1, x_2, \ldots, x_{n_1+n_2})^T$,
- **prior** $\pi(\boldsymbol{\theta})$,
- **likelihoods** $\{p(x_i|\boldsymbol{\theta})\}_{i=1}^{n_1+n_2}$

Output = **posterior belief**:

$$q^*(\boldsymbol{\theta}) \propto \pi(\boldsymbol{\theta}) \prod_{i=1}^{n_1+n_2} p(x_i|\boldsymbol{\theta}) = \widetilde{\pi}(\boldsymbol{\theta}) \prod_{i=n_1+1}^{n_2} p(x_i|\boldsymbol{\theta}), \text{ for } \widetilde{\pi}(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta}) \prod_{i=1}^{n_1} p(x_i|\boldsymbol{\theta})$$

Inference interpretation = belief updates:

- likelihoods $\{p(x_i|\boldsymbol{\theta})\}_{i=1}^{n_1+n_2}$ update prior about $\boldsymbol{\theta}$
- Old posterior $\widetilde{\pi}(\boldsymbol{\theta})$ = new prior (**coherence**/**Bayesian additivity**)

1.2 The Bayesian problem: The optimization perspective

Zellner (1988) shows that the Bayes posterior $q^*(\boldsymbol{\theta})$ solves

$$q^*(\boldsymbol{\theta}) = \underset{q \in \mathcal{P}(\boldsymbol{\Theta})}{\arg\min} \left\{ \underbrace{\mathbb{E}_{q(\boldsymbol{\theta})}\left[\sum_{i=1}^{n} -\log(p(x_i|\boldsymbol{\theta}))\right]}_{\text{minimized by } q(\boldsymbol{\theta}) = \delta_{\hat{\boldsymbol{\theta}}_n}(\boldsymbol{\theta}),\ \hat{\boldsymbol{\theta}}_n = \text{MLE}} + \underbrace{\mathrm{KLD}\left(q||\pi\right)}_{\text{minimized by } q = \pi} \right\}, \quad (1)$$

Notation:

- $\mathcal{P}(\boldsymbol{\Theta})$ = all probability distributions on $\boldsymbol{\Theta}$
- KLD = Kullback-Leibler divergence = $\mathbb{E}_{q(\boldsymbol{\theta})}\left[\log q(\boldsymbol{\theta}) - \log \pi(\boldsymbol{\theta})\right]$

Inference interpretation = regularized loss-minimization:

- $-\log(p(x_i|\boldsymbol{\theta}))$ = **loss** of $\boldsymbol{\theta}$ for x_i
- Inference = regularizing MLE $\hat{\boldsymbol{\theta}}_n$ with $\mathrm{KLD}(q||\pi)$

1.3 The Bayesian problem: The loss-minimization perspective

Bissiri et al. (2016): Bayes posteriors $q^*(\boldsymbol{\theta})$ for general loss $\ell(\boldsymbol{\theta}, x_i)$:

$$q^*(\boldsymbol{\theta}) \propto \pi(\boldsymbol{\theta}) \exp\left\{-\sum_{i=1}^{n_1+n_2} \ell(\boldsymbol{\theta}, x_i)\right\} = \widetilde{\pi}(\boldsymbol{\theta}) \exp\left\{-\sum_{i=n_1+1}^{n_2} \ell(\boldsymbol{\theta}, x_i)\right\}$$

$$\text{for } \; \widetilde{\pi}(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta}) \exp\left\{-\sum_{i=1}^{n_1} \ell(\boldsymbol{\theta}, x_i)\right\}$$

Inference interpretation = belief updates:

- Again: losses $\{\ell(\boldsymbol{\theta}, x_i)\}_{i=1}^{n_1+n_2}$ update prior about $\boldsymbol{\theta}$
- Again: Old posterior $\widetilde{\pi}(\boldsymbol{\theta})$ = new prior (**coherence**)
- Difference: $\boldsymbol{\theta}$ arbitrary, e.g. $\ell(\boldsymbol{\theta}, x_i) = |x_i - \boldsymbol{\theta}|$ admissible

1.4 The Bayesian problem: The new perspective I/II

Easy to show: Zellner's representation valid for any $\ell(\boldsymbol{\theta}, x_i)$:

$$q^*(\boldsymbol{\theta}) = \underset{q \in \mathcal{P}(\boldsymbol{\Theta})}{\arg\min} \left\{ \underbrace{\mathbb{E}_{q(\boldsymbol{\theta})}\left[\sum_{i=1}^{n} \ell(\boldsymbol{\theta}, x_i)\right]}_{\text{minimized by } \delta_{\hat{\boldsymbol{\theta}}_n}(\boldsymbol{\theta})} + \underbrace{\mathrm{KLD}\left(q || \pi\right)}_{\text{minimized by } q = \pi} \right\}$$

Bissiri et al. (2016)'s generalization (preserves coherence):

- Replacing $-\log(p(x_i|\boldsymbol{\theta}))$ with other losses $\ell(\boldsymbol{\theta}, x_i)$

Two more generalizations (break coherence):

- Replacing $\mathcal{P}(\boldsymbol{\Theta})$ with $\mathcal{Q} \subset \mathcal{P}(\boldsymbol{\Theta})$ ($=$ **VI**)
- Replacing KLD with inference-problem specific regularizers

1.4 The Bayesian problem: The new perspective II/II

Our **generalized representation of Bayesian inference**:

$$q^*(\boldsymbol{\theta}) = \underset{q \in \Pi}{\arg\min} \left\{ \underbrace{\mathbb{E}_{q(\boldsymbol{\theta})}\left[\sum_{i=1}^{n} \ell(\boldsymbol{\theta}, x_i)\right]}_{\text{minimized by } \delta_{\hat{\boldsymbol{\theta}}_n}(\boldsymbol{\theta})} + \underbrace{D(q\|\pi)}_{\text{minimized by } q = \pi} \right\}$$

Notation:

- if $\boldsymbol{\Pi}$ = variational family, write $\mathcal{Q}$.
- $\ell_n(\boldsymbol{\theta}, \boldsymbol{x}) = \sum_{i=1}^{n} \ell(\boldsymbol{\theta}, x_i)$

Inference interpretation = regularized & constrained minimization:

- $\ell_n(\boldsymbol{\theta}, \boldsymbol{x})$ = **loss** of $\boldsymbol{\theta}$ to minimize
- **D** = **divergence**, acting as uncertainty quantifier/regularizer
- $\boldsymbol{\Pi}$ = set of **admissible posterior** beliefs
- **Inference** = constrained, regularized optimization

  $\Rightarrow$ **Shorthand Notation:** $P(\ell_n, D, \boldsymbol{\Pi})$

2 The form of the Generalized Bayesian problem

Purpose of part 2: Investigate $P(\ell_n, D, \Pi)$

(1) Interpretations & modularity of ℓ_n, D and Π?

(2) Is there an axiomatic justification?

(3) Which existing methods does this (not) encompass?

2.1 Generalized Bayesian problem: provable modularity

$$q^*(\boldsymbol{\theta}) = \underset{q \in \Pi}{\arg\min} \left\{ \underbrace{\mathbb{E}_{q(\boldsymbol{\theta})}\left[\sum_{i=1}^{n} \ell(\boldsymbol{\theta}, x_i)\right]}_{\text{minimized by } \delta_{\hat{\boldsymbol{\theta}}_n}(\boldsymbol{\theta})} + \underbrace{D\left(q \| \pi\right)}_{\text{minimized by } q = \pi} \right\}$$

Roles of ℓ_n, D, $\boldsymbol{\Pi}$::

- ℓ_n: which parameter $\boldsymbol{\theta}$ do we care about?
- **D**: How is uncertainty quantified/what does q^* look like?
- $\boldsymbol{\Pi}$: Which beliefs are allowed?

  $\Rightarrow$ (provable) modularity of $P(\ell_n, D, \boldsymbol{\Pi})$!

Theorem 1 (GVI modularity)

For Bayesian inference with $P(\ell_n, D, \boldsymbol{\Pi})$, making it robust to model misspecification amounts to changing ℓ_n. Conversely, adapting uncertainty quantification (fixing $\boldsymbol{\Pi}$, π, $\boldsymbol{\theta}^*$, $\hat{\boldsymbol{\theta}}_n$) amounts to changing D.

2.2 Generalized Bayesian problem: Axiomatic derivation I/II

Axiom 1 (Representation)

The posterior $q^* \in \mathcal{P}(\boldsymbol{\Theta})$ is constructed by solving an optimization problem over some space $\Pi \subseteq \mathcal{P}(\boldsymbol{\Theta})$. The optimization seeks to minimize exactly two criteria that do not interact:

(i) The in-sample loss $\sum_{i=1}^{n} \ell(\boldsymbol{\theta}, x_i)$ to be expected under $q^*(\boldsymbol{\theta})$.

(ii) The deviation from the prior $\pi(\boldsymbol{\theta})$ as measured by the magnitude of some statistical divergence D.

Axiom 2 (Information Equivalence)

Take any two constants $C, M \in \mathbb{R}_{>0}$ and let the posteriors $q_1^*, q_2^* \in \mathcal{P}(\boldsymbol{\Theta})$ be computed based on the same optimization problem, but with two different loss functions $\ell^{(1)}$ and $\ell^{(2)}$ as well as two different divergences $D^{(1)}, D^{(2)}$ so that $D^{(1)} = D^{(2)} + M$ and so that $\ell^{(1)} = \ell^{(2)} + C$. Then, $q_1^*(\boldsymbol{\theta}) = q_2^*(\boldsymbol{\theta})$ (almost everywhere).

2.2 Generalized Bayesian problem: Axiomatic derivation I/II

Axiom 3 (Generalized Likelihood Principle)

Suppose the posteriors $q_n^*, q_{n+m}^* \in \Pi$ are computed based on an optimization problem satisfying Axiom 1. Assume that the same optimization problem is used for both posteriors, except for a difference in the samples $x_{1:n}$ and $x_{1:n+m}$ and potentially different loss functions $\ell^{(1)}$ and $\ell^{(2)}$ that are used, respectively.

(i) Provided that there is an information difference between $x_{1:n}$ and $x_{1:n+m}$ for $m > 0$, the posteriors are different. In other words, $\sum_{i=1}^{n} \ell^{(1)}(\boldsymbol{\theta}, x_i) \neq \sum_{i=1}^{n+m} \ell^{(2)}(\boldsymbol{\theta}, x_i)$ implies that $q_n^* \neq q_{n+m}^*$, even if $\ell^{(1)} = \ell^{(2)}$.

(ii) Provided that there is a difference in the measure of information between $\ell^{(1)}$ and $\ell^{(2)}$, the posteriors are different. In other words, $\ell^{(1)} \neq \ell^{(2)}$ implies that $q_n^* \neq q_{n+m}^*$, even if $m = 0$ so that $x_{1:n} = x_{1:n+m}$.

2.2 Generalized Bayesian problem: Axiomatic derivation II/II

Theorem 2 (Form 1)

If Axiom 1 holds, $P(\ell_n, D, \Pi)$ has form $\arg\min_{q\in\Pi}\{L(q|\boldsymbol{x}, \ell_n, D)\}$ for $L(q|\boldsymbol{x}, \ell_n, D) = f\left(\mathbb{E}_{q(\boldsymbol{\theta})}[\boldsymbol{\ell}_n(\boldsymbol{\theta}, \boldsymbol{x})], D(q||\pi)\right)$, for some $f : \mathbb{R}^2 \to \mathbb{R}$.

Theorem 3 (Form 2)

For $P(\ell_n, D, \Pi)$ being $\arg\min_{q\in\Pi}\{L(q|\boldsymbol{x}, \ell_n, D)\}$ and $\circ$ an elementary operation on $\mathbb{R}$, $L(q|\boldsymbol{x}, \ell_n, D) = \mathbb{E}_{q(\boldsymbol{\theta})}[\ell_n(\boldsymbol{\theta}, \boldsymbol{x})] \circ D(q||\pi)$ satisfies Axioms 1, 2 and 3 only if $\circ = +$.

Implications/relevance:

- Bayesian inference = constrained, regularized optimization
- Objective only depends on $\mathbb{E}_{q(\boldsymbol{\theta})}[\boldsymbol{\ell}_n(\boldsymbol{\theta}, \boldsymbol{x})]$ and $D(q||\pi)$
- For elementary $f\left(\mathbb{E}_{q(\boldsymbol{\theta})}[\boldsymbol{\ell}_n(\boldsymbol{\theta}, \boldsymbol{x})], D(q||\pi)\right)$, f must be addition. (**Note:** Axiom 2 excludes most non-elementary f)

2.3 Generalized Bayesian problem & existing methods I/III

$$q^*(\boldsymbol{\theta}) = \underset{q \in \boldsymbol{\Pi}}{\arg\min} \left\{ \mathbb{E}_{q(\boldsymbol{\theta})} \left[\ell_n(\boldsymbol{\theta}, \boldsymbol{x}) \right] + D\left(q || \pi\right) \right\}$$

$P(\boldsymbol{\ell_n}, D, \boldsymbol{\Pi})$ covers & gives **insight** into existing methods, e.g.

- **Power Bayes**: $P(w\ell_n, D, \Pi) = P(\ell_n, \frac{1}{w}D, \Pi)$.
  ($\Longrightarrow$ w-power likelihood $= \frac{1}{w}\times$ **more trust in your prior**.)
- **Regularized Bayes**: Adding $\Phi(q(\boldsymbol{\theta}, \boldsymbol{x})) = \mathbb{E}_{q(\boldsymbol{\theta}, \boldsymbol{x})}\left[\phi(\boldsymbol{\theta}, \boldsymbol{x})\right]$ into the objective corresponds to $P\left(\ell_n + \phi, D, \Pi\right)$.
  ($\Longrightarrow$ RegBayes $=$ a form of **GVI** that changes ℓ_n)
- **PAC Bayes**: Operationalizes a variational inference procedure based on PAC-bounds whose complexity penalty is some $D \neq \mathrm{KLD}$ (e.g. Alquier and Guedj, 2018)

2.3 Generalized Bayesian problem & existing methods II/III

Method	$\ell(\boldsymbol{\theta}, x_i)$	D	Π
Standard Bayes	$-\log(p(\boldsymbol{\theta}\|x_i))$	KLD	$\mathcal{P}(\boldsymbol{\Theta})$
Generalized Bayes[1]	any ℓ	KLD	$\mathcal{P}(\boldsymbol{\Theta})$
Power Bayes[2]	$-\log(p(\boldsymbol{\theta}\|x_i))$	$\frac{1}{w}\text{KLD}$, $w > 1$	$\mathcal{P}(\boldsymbol{\Theta})$
Divergence Bayes[3]	divergence-based ℓ	KLD	$\mathcal{P}(\boldsymbol{\Theta})$
Standard VI	$\boldsymbol{-\log(p(\theta\|x_i))}$	**KLD**	$\mathcal{Q}$
Power VI[4]	$-\log(p(\boldsymbol{\theta}\|x_i))$	$\frac{1}{w}\text{KLD}$, $w > 1$	$\mathcal{Q}$
Regularized Bayes[5]	$-\log(p(\boldsymbol{\theta}\|x_i)) + \phi(\boldsymbol{\theta}, x_i)$	KLD	$\mathcal{Q}$
Gibbs VI[6]	any ℓ	KLD	$\mathcal{Q}$
Generalized VI	**any** $\boldsymbol{\ell}$	**any** $\boldsymbol{D}$	$\mathcal{Q}$

Table 1 – $P(\ell_n, D, Q)$ & existing methods. [1](Bissiri et al., 2016), [2](e.g. Holmes and Walker, 2017; Grünwald et al., 2017; Miller and Dunson, 2018), [3](e.g. Hooker and Vidyashankar, 2014; Ghosh and Basu, 2016; Futami et al., 2017; Jewson et al., 2018), [4](e.g. Yang et al., 2017; Huang et al., 2018) [5](Ganchev et al., 2010; Zhu et al., 2014), [6](Alquier et al., 2016; Futami et al., 2017)

2.3 Generalized Bayesian problem & existing methods II/III

$$
\begin{tikzcd}[column sep=huge, row sep=large]
\begin{matrix}\text{Rule of Three} \\ P(\ell, D, \Pi)\end{matrix} \arrow[r, "\begin{matrix} D = \mathrm{KLD} \\ \Pi = \mathcal{P}(\Theta) \end{matrix}"] \arrow[d, "\Pi = \mathcal{Q} \subset \mathcal{P}(\Theta)"] & \begin{matrix}\text{PAC/Gibbs Bayes} \\ P(\ell, \mathrm{KLD}, \mathcal{P}(\Theta))\end{matrix} \arrow[r, "\ell = -\log p(\cdot|\theta)"] \arrow[d, "\Pi = \mathcal{Q} \subset \mathcal{P}(\Theta)"] & \begin{matrix}\text{Standard Bayes} \\ P(-\log p(\cdot|\theta), \mathrm{KLD}, \mathcal{P}(\Theta))\end{matrix} \arrow[d, "\Pi = \mathcal{Q} \subset \mathcal{P}(\Theta)"] \\
\begin{matrix}\textbf{Generalized VI} \\ P(\ell, D, \mathcal{Q})\end{matrix} \arrow[r, "D = \mathrm{KLD}"'] & \begin{matrix}\text{Gibbs VI} \\ P(\ell, \mathrm{KLD}, \mathcal{Q})\end{matrix} \arrow[r, "\ell = -\log p(\cdot|\theta)"'] & \begin{matrix}\textbf{Standard VI} \\ P(-\log p(\cdot|\theta), \mathrm{KLD}, \mathcal{Q})\end{matrix}
\end{tikzcd}
$$

Figure 1 – A taxonomy of some important belief distributions as special cases.

2.3 Generalized Bayesian problem & existing methods III/III

Not everything fits $P(\ell_n, D, \mathbf{\Pi})$:

(1) **Laplace approximations** (e.g., INLA)

(2) **Divergence-Variational inference (DVI)**: VI based on discrepancy $D \neq \text{KLD}$ (locally) solving $q^* = \arg\min_{q \in \mathcal{Q}} D(q \| \widetilde{q})$ for $\widetilde{q} =$ standard Bayesian posterior, e.g.

$D =$ Rényi's α-divergence (Li and Turner, 2016; Saha et al., 2017)

$D =$ χ-divergence (Dieng et al., 2017)

$D =$ operators (Ranganath et al., 2016)

$D =$ scaled AB-divergence (Regli and Silva, 2018)

$D =$ Wasserstein distance (Ambrogioni et al., 2018)

...

(3) **Expectation Propagation (EP)** (Minka, 2001; Opper and Winther, 2000) and its variants (e.g. Hernández-Lobato et al., 2016).
Note: Particular type of **DVI**, with $D =$ (local) reverse KLD

3 Reinterpreting VI

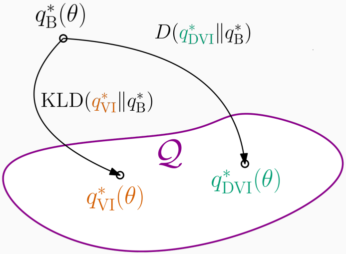
Purpose of part 3: Motivating **GVI**

(1) **Standard VI**: Optimality & reinterpretation

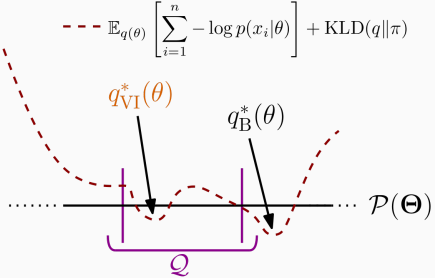
(2) **DVI**: "suboptimal" methods with better posteriors

(3) **GVI**: A modular alternative to **DVI**

Relationship between VI, GVI, DVI and exact inference?



(a) DVI (projection-centric) interpretation of **VI**



(b) GVI (= optimization-centric) Interpretation of **VI**

3.1 Optimality & reinterpretation of standard VI II/V

Standard VI: $q^*_{\mathrm{VI}} = \arg\min_{q \in \mathcal{Q}} \mathrm{KLD}(q \| q^*_B)$, q^*_B solves $P(\ell_n, \mathbf{KLD}, \mathcal{P}(\Theta))$

$$\mathrm{KLD}(q||q^*_B) =$$

$$\underbrace{\mathbb{E}_{q(\boldsymbol{\theta})}\left[\log\left(\frac{q(\boldsymbol{\theta})}{\exp\left\{-\sum_{i=1}^n \ell(\boldsymbol{\theta}, x_i)\right\}\pi(\boldsymbol{\theta})}\right)\right]}_{\text{(Generalized) ELBO}} + \underbrace{\log\left(\int_{\boldsymbol{\theta}} \exp\left\{-\sum_{i=1}^n \ell(\boldsymbol{\theta}, x_i)\right\}\pi(\boldsymbol{\theta})d\boldsymbol{\theta}\right)}_{\text{Generalized 'log evidence'}}$$

Inference = minimizing ELBO, which you can rewrite as

$$\mathrm{ELBO}(q) = \mathbb{E}_{q(\boldsymbol{\theta})}\left[\sum_{i=1}^n \ell(\boldsymbol{\theta}, x_i)\right] + \mathrm{KLD}(q||\pi). \tag{2}$$

...which is exactly the objective of $P(\ell_n, \mathbf{KLD}, \mathcal{Q})$

In other words, $P(\ell_n, \mathbf{KLD}, \mathcal{Q})$ $(= \mathrm{ELBO})$ is

$$q^*_{\mathrm{VI}}(\boldsymbol{\theta}) = \underset{q \in \mathcal{Q}}{\arg\min} \left\{ \mathbb{E}_{q(\boldsymbol{\theta})} \left[\ell_n(\boldsymbol{\theta}, \boldsymbol{x}) \right] + \mathrm{KLD}\left(q || \pi \right) \right\},$$

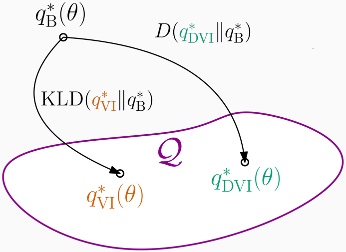
the $\mathcal{Q}$-constrained relaxation of $P(\ell_n, \mathbf{KLD}, \mathcal{P}(\boldsymbol{\Theta}))$, whose objective is

$$q^*_B(\boldsymbol{\theta}) = \underset{q \in \mathcal{P}(\boldsymbol{\Theta})}{\arg\min} \left\{ \mathbb{E}_{q(\boldsymbol{\theta})} \left[\ell_n(\boldsymbol{\theta}, \boldsymbol{x}) \right] + \mathrm{KLD}\left(q || \pi \right) \right\},$$

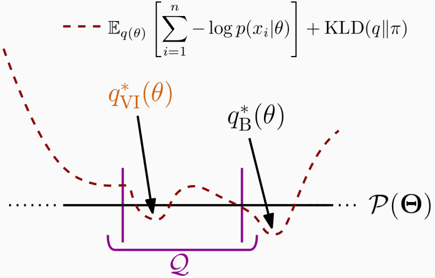
(which is the exact Bayesian objective).

$\Rightarrow$ Reinterpretation of **standard VI** as **Constrained optimization**!

3.1 Optimality & reinterpretation of standard VI IV/V



(a) **DVI** (projection-centric) interpretation of **VI**



(b) **GVI** (= optimization-centric) Interpretation of **VI**

Consequence I/II: VI-optimality

Theorem 4 (VI optimality)

For exact and coherent Bayesian posteriors solving $P(\ell_n, \mathrm{KLD}, \mathcal{P}(\Theta))$ and a fixed variational family $\mathcal{Q}$, standard **VI** produces the uniquely optimal $\mathcal{Q}$-constrained approximation to $P(\ell_n, \mathrm{KLD}, \mathcal{P}(\Theta))$ Having decided on approximating the Bayesian posterior with some $q \in \mathcal{Q}$, **VI** provides the uniquely optimal solution.

Consequences II/II: **DVI**-suboptimality. **Three** big disadvantages:

(1) If $F \neq \mathrm{KLD}$, **DVI** violates Axioms 1–3.

(2) **DVI** conflates ℓ_n and D (i.e., modularity of $P(\ell_n, D, \mathbf{\Pi})$ lost).

(3) Last Thm: **DVI** gives worse $\mathcal{Q}$-constrained posterior than standard **VI** (*relative to the standard Bayesian problem* $P(\ell_n, \mathrm{KLD}, \mathcal{P}(\mathbf{\Theta}))$)

Objection! **DVI** often produces better posteriors than **standard VI**!

3.2 Why does DVI produce better posteriors? II/II

Seeming contradiction:

(1) **VI** is the best approximation to the *standard* Bayesian posterior

(2) **DVI** often outperforms **VI** (e.g., on test scores)

Resolution:

> **DVI** outperforms **VI** by implicitly **defining a new, non-standard Bayesian problem***

$\Longrightarrow$ Inspires **Generalized Variational Inference (GVI)**

***non-standard Bayesian problem** = problem defining a belief distribution that can be understood as updating a prior belief with some data, but which is **not** obtained by Bayes' rule

3.3 Towards GVI I/II

GVI = combining advantages of **VI** and **DVI**:

(1) Has form $P(\ell_n, D, \mathcal{Q})$ Like **VI** i.e.

  (i) satisfies Axioms 1–3;

  (ii) provably interpretable modularity (**loss, uncertainty quantifier, admissible posteriors**

(2) Derives different & more appropriate posteriors like **DVI** but

  (i) without conflating ℓ_n and D

  (ii) with **explicit** rather than **implicit** changes .

Definition 1 (GVI)

Any Bayesian inference method solving $P(\ell_n, D, \mathcal{Q})$ with admissible choices ℓ_n, D and $\mathcal{Q}$ is a Generalized Variational Inference (**GVI**) method (and satisfies Axioms 1–3 by definition).

Illustration: DVI aims for D, but changes ℓ_n – GVI doesn't

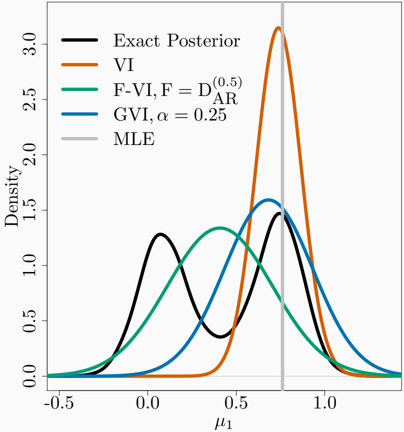


Figure 4 – **Exact**, VI, DVI ($F = D_{AR}^{(0.5)}$) and $P(\ell_n, D_{AR}^{(\alpha)}, \mathcal{Q})$ based GVI marginals of the location in a 2 component mixture model. Respecting ℓ_n, VI and GVI provide uncertainty quantification around the most likely value $\widehat{\boldsymbol{\theta}}_n$ via D. In contrast, DVI implicitly changes the loss and has a mode at the locally most *unlikely* value of $\boldsymbol{\theta}$.

4 GVI: What does it do?

Purpose of part 4: Exploring **GVI**'s relationship to M-open world & study three use cases

(1) Embed **GVI** into the M-open world

(2) Robust alternatives to $\ell(\boldsymbol{\theta}, x_i) = -\log(p(x_i|\boldsymbol{\theta}))$

(3) Prior-robust uncertainty quantification and adjusting marginal variances via D

4.1 M-open vs M-closed inference

M-closed view: Model and prior are correct, i.e.

$$\exists \boldsymbol{\theta}^* \in \boldsymbol{\Theta} \text{ s.t. } x_i \sim p(x_i|\boldsymbol{\theta}^*)$$

Q: Why do purist Bayesians love **exact** inference (MCMC, SMC, ...)?
A: With M-closed view, can focus on computation of Bayes posterior

$$q^*(\boldsymbol{\theta}) \propto \prod_{i=1}^{n} p(x_i|\boldsymbol{\theta})\pi(\boldsymbol{\theta}) \quad = \text{solution of } P\left(\sum_{i=1}^{n} -\log p(x_i|\boldsymbol{\theta}), D, \mathcal{P}(\boldsymbol{\Theta})\right)$$

M-open view: Model and prior are **not** correct, i.e.

$$\nexists \boldsymbol{\theta}^* \in \boldsymbol{\Theta} \text{ s.t. } x_i \sim p(x_i|\boldsymbol{\theta}^*)$$

Traditional stats: Devise better models until they are 'close enough'
$\Longrightarrow$ Focus on inference still useful!
Modern stats/ML: Use some black box model (BNN, DGP, ...)
$\Longrightarrow$ Do we even want standard posterior!?

4.1 Consequences for inference

Conclusion 1: If your model is pretty good, use exact inference or **VI**.
Conclusion 2: If **DVI** works better than **VI**, your model is not great.
Conclusion 3: If you know why model isn't great, address it with **GVI**.

M-closed assumptions are very far from the truth sometimes:

- Time Series/on-line inference:
  - (i) Stationarity
  - (ii) Short-term memory
  - (iii) Noise level constant/non-erratic
- Bayesian Neural Networks (BNNs):
  - (i) There is a true weight parameter $\boldsymbol{\theta}^*$ indexing the network
  - (ii) All priors on the thousands of entries of $\boldsymbol{\theta}$ is well-specified
- (Deep) Gaussian Processes (DGPs):
  - (i) (Conditionally on latent space) correct likelihood is specified
  - (ii) DGP prior and kernel choice generate correct latent spaces

$\Longrightarrow$ Clearly, **M-open** world more appropriate $\Longrightarrow$ **GVI**

GVI modularity: The loss ℓ_n

Q1: Why use $\ell_n(\boldsymbol{\theta}, \boldsymbol{x}) = \sum_{i=1}^n -\log(p(x_i|\boldsymbol{\theta}))$?
A: Assuming that the true data-generating mechanism is $\boldsymbol{x} \sim g$,

$$\arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} -\log(p(x_i|\boldsymbol{\theta})) \approx \arg\min_{\boldsymbol{\theta}} \mathbb{E}_g\left[-\log(p(\boldsymbol{x}|\boldsymbol{\theta}))\right]$$
$$= \arg\min_{\boldsymbol{\theta}} \mathbb{E}_g\left[-\log\left(p(\boldsymbol{x}|\boldsymbol{\theta})\right) + \log(g(\boldsymbol{x}))\right] = \arg\min_{\boldsymbol{\theta}} \mathrm{KLD}(g\|p(\cdot|\boldsymbol{\theta}))$$

Interpretation: $\boldsymbol{-\log\left(p(x_i|\theta)\right)}$ = targeting KLD-minimizing $p(\cdot|\boldsymbol{\theta})$

Q2: Are there other $\boldsymbol{\mathcal{L}^D(p(x_i|\theta))}$ for divergence $\boldsymbol{D}$?
A: Yes! (e.g. Jewson et al., 2018; Futami et al., 2017; Ghosh and Basu, 2016; Hooker and Vidyashankar, 2014)

4.2 GVI: The losses II/III

Q3: Why use other $\mathcal{L}^{D}(p(x_i|\theta))$?
A: Robustness (for D = a robust divergence) [log/KLD non-robust!]

Robustness recipe: $\alpha/\beta/\gamma$-divergences using generalized log functions
E.g.: β indexes β-divergence ($D_B^{(\beta)}$) via

$$\log_\beta(x) = \frac{1}{(\beta-1)\beta}\left[\beta x^{\beta-1} - (\beta-1)x^{\beta}\right]$$
$$D_B^{(\beta)}(g||p(\cdot|\boldsymbol{\theta})) = \mathbb{E}_g\left[\log_\beta(p(\boldsymbol{x}|\boldsymbol{\theta})) - \log_\beta(g(\boldsymbol{x}))\right]$$

Note 1: $D_B^{(\beta)} \to \mathrm{KLD}$ as $\beta \to 1$!
Note 2: Admits $D_B^{(\beta)}$-targeting loss as

$$\mathcal{L}_p^{\beta}(\theta, x_i) = -\frac{1}{\beta-1}p(x_i|\boldsymbol{\theta})^{\beta-1} + \frac{I_{p,\beta}(\boldsymbol{\theta})}{\beta}, \quad I_{p,c}(\boldsymbol{\theta}) = \int p(x|\boldsymbol{\theta})^c dx$$

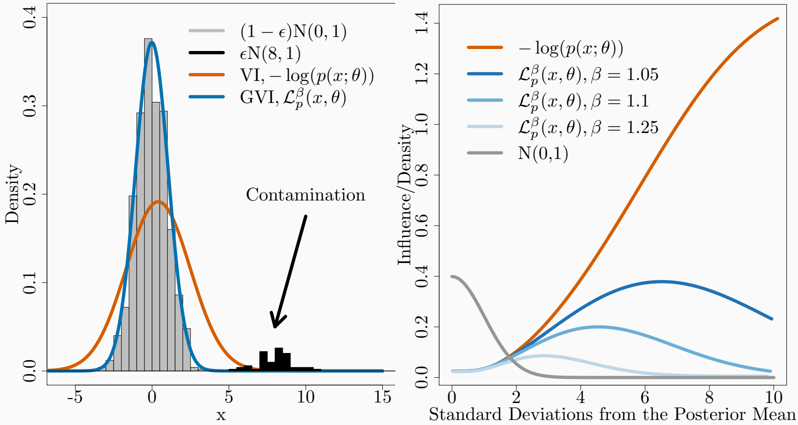


Figure 5 – Left: Robustness against model misspecification. Depicted are posterior predictives under $\varepsilon = 5\%$ outlier contamination using **VI** and $P(\sum_{i=1}^n \mathcal{L}_p^\beta(\boldsymbol{\theta}, x_i), \mathrm{KLD}, \mathcal{Q})$, $\beta = 1.5$. **Right:** From Knoblauch et al. (2018). Influence of x_i on exact posteriors for different losses.

GVI modularity: The uncertainty quantifier D

Q: Which VI drawbacks can be addressed via D?

A: Any **uncertainty quantification** properties, e.g.

- Over-concentration (= underestimating marginal variances)
- Sensitivity to badly specified priors
- ...

Example 1: GVI can fix over-concentrated posteriors

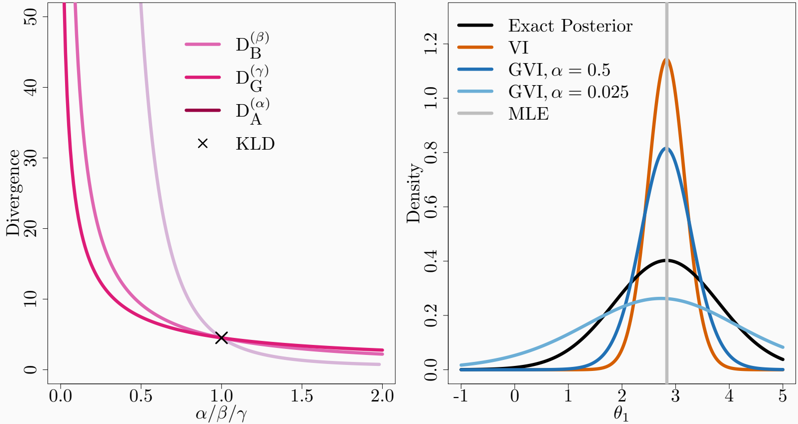


Figure 6 – Left: Magnitude of the penalty incurred by $D(q||\pi)$ for different uncertainty quantifiers D and fixed densities π, q. **Right**: Using $D_{AR}^{(\alpha)}$ with different choices of α to "customize" uncertainty.

Example 2: Avoiding prior sensitivity

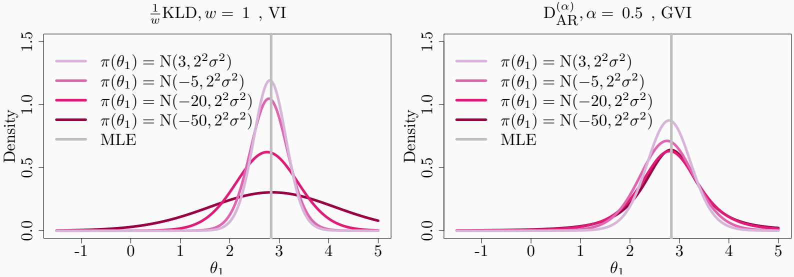


Figure 7 – Prior sensitivity with **VI** (**left**) vs. prior robustness with **GVI** (**right**). Priors are more badly specified for **darker** shades.

4.4 GVI: Three use cases

Summary: **GVI** is natural in the M-open (i.e. real) world. Applications include

(1) Robustness to model misspecification ($=$ adapting ℓ_n)

(2) "Customized" marginal variances ($=$ adapting D)

(3) Prior robustness ($=$ adapting D)

Purpose of part 5: GVI inference & experiments

(1) How/when can we "black box" **GVI**?

(2) A case study in robustness with Bayesian On-line Changepoint Detection

(3) **DVI** vs **GVI** & changes in D (on Bayesian Neural Nets)

(4) **VI** vs **GVI** & changes in ℓ_n (on Deep Gaussian Processes)

Setup: $\mathcal{Q} = \{q(\boldsymbol{\theta}|\boldsymbol{\kappa}) : \boldsymbol{\kappa} \in K\}$ variational family s.t.

(i) one can sample $\boldsymbol{\theta}^{(1:S)} \sim q(\boldsymbol{\theta}|\boldsymbol{\kappa})$;

(ii) derivative $\nabla_{\boldsymbol{\kappa}} \log(q(\boldsymbol{\theta}|\boldsymbol{\kappa}))$ exists.

Case 1: Closed form for $\nabla_{\boldsymbol{\kappa}} D(q||\pi)$ $\rightarrow$ unbiased estimate:

$$\nabla_{\boldsymbol{\kappa}} \hat{L}(q|\ell_n, D) = \frac{1}{S} \sum_{s=1}^{S} \left\{ \ell_n(\boldsymbol{\theta}^{(s)}, \boldsymbol{x}) \cdot \nabla_{\boldsymbol{\kappa}} \log(q(\boldsymbol{\theta}^{(s)}|\boldsymbol{\kappa})) \right\} + \nabla_{\boldsymbol{\kappa}} D(q||\pi)$$

Thm. 7: Closed forms for most $\alpha/\beta/\gamma$- & Rényi-divergence.

Case 2: $D(q||\pi) = \mathbb{E}_q[\ell^D_{\boldsymbol{\kappa},\pi}(\boldsymbol{\theta})]$ (e.g., f-divs) $\rightarrow$ unbiased estimate:

$$\nabla_{\boldsymbol{\kappa}} \hat{L}(q|\ell_n, D) = \frac{1}{S} \sum_{s=1}^{S} \left\{ \left[\ell_n(\boldsymbol{\theta}^{(s)}, \boldsymbol{x}) + \ell^D_{\boldsymbol{\kappa},\pi}(\boldsymbol{\theta}^{(s)}) \right] \cdot \nabla_{\boldsymbol{\kappa}} \log(q(\boldsymbol{\theta}^{(s)}|\boldsymbol{\kappa})) + \nabla_{\boldsymbol{\kappa}} \ell^D_{\boldsymbol{\kappa},\pi}(\boldsymbol{\theta}^{(s)}) \right\}.$$

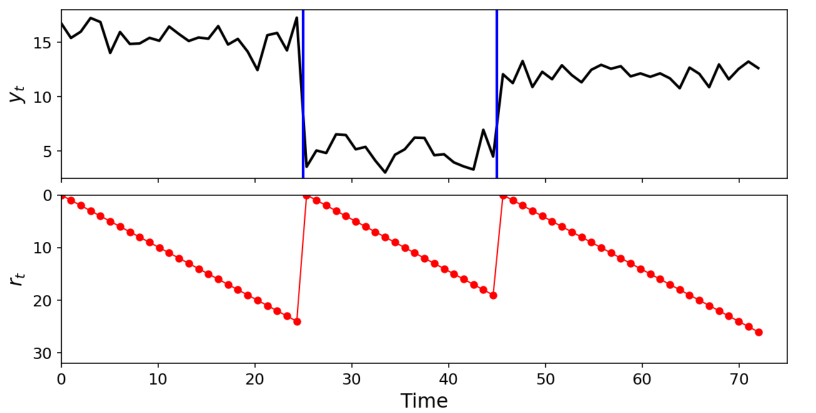
5.2 Standard BOCPD I/XI

Idea due to Adams and MacKay (2007) and Fearnhead and Liu (2007):

(1) Define **Run-length at** $t = r_t \iff$ there was a CP at time $t - r_t$.

(2) **Inference on last CP** via $p(r_t|y_{1:t})$ rather than on *all* CPs

(3) Resulting complexity: $\mathcal{O}(t)$ **rather than** $\mathcal{O}(\prod_{i=1}^{t} i)$.



5.2 BOCPD + model selection (Knoblauch and Damoulas, 2018) II/XI

Idea: Multiple models, different between segments
New Random Variable: m_t, the model at time t

$$r_t|r_{t-1} \sim H(r_t, r_{t-1}) \quad \text{[conditional \textbf{CP} prior]} \tag{3a}$$

$$m_t|m_{t-1}, r_t \sim q(m_t|m_{t-1}, r_t) \quad \text{[conditional \textbf{model} prior]} \tag{3b}$$

$$\boldsymbol{\theta}_m|m_t \sim \pi_{m_t}(\boldsymbol{\theta}_{m_t}) \quad \text{[parameter prior]} \tag{3c}$$

$$\boldsymbol{y}_t|m_t, \boldsymbol{\theta}_{m_t} \sim f_{m_t}(\boldsymbol{y}_t|\boldsymbol{\theta}_{m_t}) \quad \text{[\textbf{observation} density]} \tag{3d}$$

where $q(m_t|m_{t-1}, r_t) = \mathbb{1}_{\{r_t>0\}}\delta(m_{t-1}) + \mathbb{1}_{\{r_t=0\}}q(m_t)$.

Recursion:

$$p(\boldsymbol{y}_1, r_1 = 0, m_1) = q(m_1)\int_{\Theta_{m_1}} f_{m_1}(\boldsymbol{y}_1|\boldsymbol{\theta}_{m_1})\pi_{m_1}(\boldsymbol{\theta}_{m_1})d\boldsymbol{\theta}_{m_1} = q(m_1)f_{m_1}(\boldsymbol{y}_1|\boldsymbol{y}_0)$$

$$p(\boldsymbol{y}_{1:t}, r_t, m_t) = \sum_{m_{t-1}, r_{t-1}} \Big\{ f_{m_t}(\boldsymbol{y}_t|\boldsymbol{y}_{1:(t-1)}, r_{t-1})q(m_t|\boldsymbol{y}_{1:(t-1)}, r_{t-1}, m_{t-1}) H(r_t, r_{t-1})p(\boldsymbol{y}_{1:(t-1)}, r_{t-1}, m_{t-1}) \Big\}$$

5.2 Standard BOCPD with model selection III/XI

$$p(\boldsymbol{y}_{1:t}, r_t, m_t) = \sum_{m_{t-1}, r_{t-1}} \Big\{ f_{m_t}(\boldsymbol{y}_t | \boldsymbol{y}_{1:(t-1)}, r_{t-1}) q(m_t | \boldsymbol{y}_{1:(t-1)}, r_{t-1}, m_{t-1}) \\ H(r_t, r_{t-1}) p(\boldsymbol{y}_{1:(t-1)}, r_{t-1}, m_{t-1}) \Big\}$$

Inference:

(1) Evidence: $p(\boldsymbol{y}_{1:t}) = \sum_{r_t, m_t} p(\boldsymbol{y}_{1:t}, r_t, m_t)$

(2) run-length & model posterior: $p(r_t, m_t | \boldsymbol{y}_{1:t}) = p(\boldsymbol{y}_{1:t}, r_t, m_t) / p(\boldsymbol{y}_{1:t})$

(3) Prediction: $p(\boldsymbol{y}_{t+1} | \boldsymbol{y}_{1:t}) = \sum_{r_t, m_t} f_{m_t}(\boldsymbol{y}_{t+1} | \boldsymbol{y}_{1:t}, r_t) p(r_t, m_t | \boldsymbol{y}_{1:t})$

(4) Run-length marginal posterior: $p(r_t | \boldsymbol{y}_{1:t}) = \sum_{m_t} p(r_t, m_t | \boldsymbol{y}_{1:t})$

(5) Model marginal posterior: $p(m_t | \boldsymbol{y}_{1:t}) = \sum_{r_t} p(r_t, m_t | \boldsymbol{y}_{1:t})$.

(6) MAP segmentation:
$MAP_t = \max_{r,t} \{ MAP_{t-r-1} \cdot p(r_t = r, m_t = m | \boldsymbol{y}_{1:t}) \}$

Last plot: Clear that model selection non-robust! Why?

- On-line processing
- Moderate/high dimensions for $\boldsymbol{y}_t$

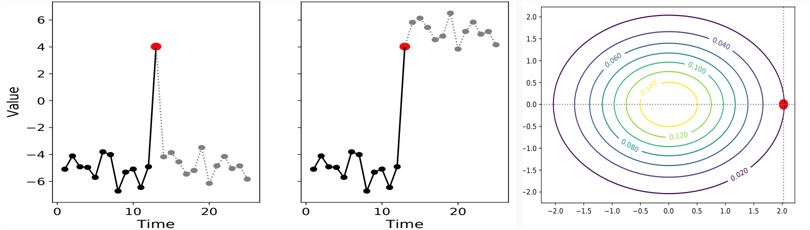
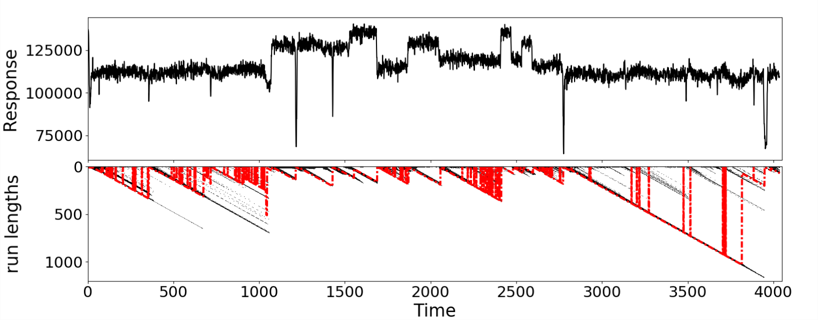


Figure 8 – Left, Center: Price for on-line processing is that outliers are confused with changepoings. **Right:** Multivariate densities become very small even if outliers occur only in a single dimension.

5.2 Issue: Outliers & misspecification V/X



Five Autoregressive processes with two CPs

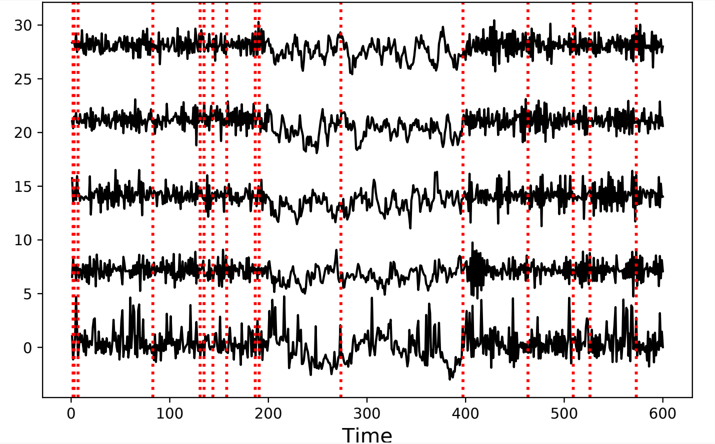
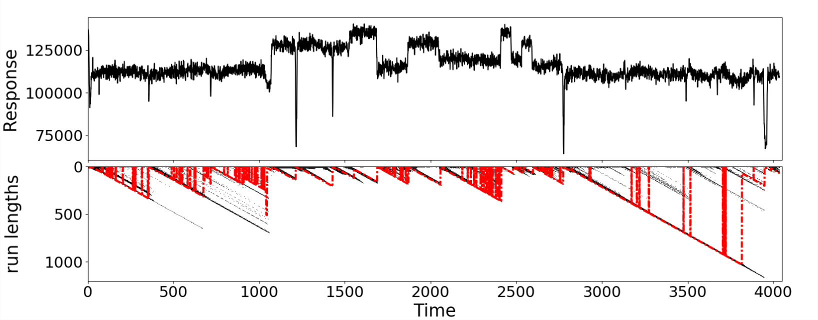


Figure 9 – Maximum A Posteriori (MAP) CPs of standard BOCPD shown as dashed vertical lines. True CPs at $t = 200, 400$.

5.2 Fix: Adapt loss (Knoblauch et al., 2018) VII/XI



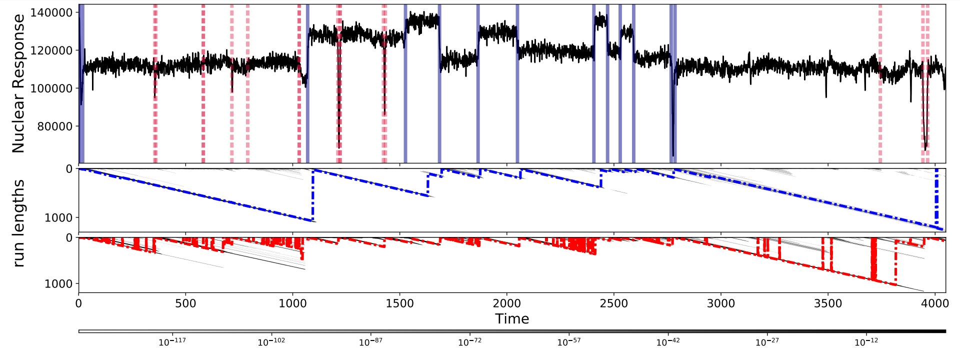


Figure 10 – Robust segmentation and run-length distribution and **additionally found CPs with non-robust run-length distribution**

[$\text{FDR}: > 99\% \Longrightarrow 8\%$ and reduction in MSE (MAE) by 10% (6%)]

Five Autoregressive processes with two CPs

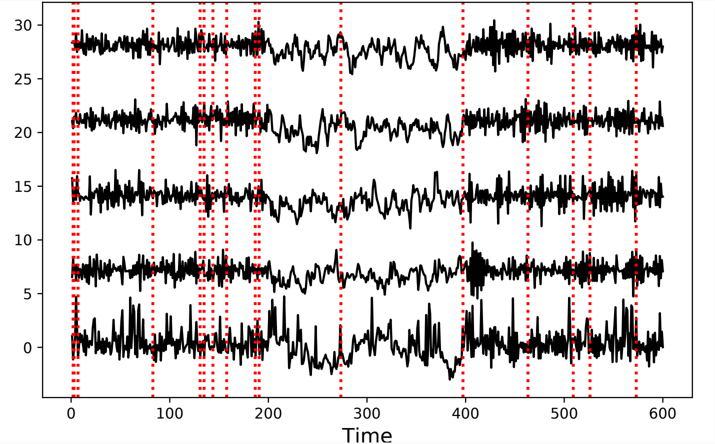


Figure 11 – Maximum A Posteriori (MAP) CPs of standard BOCPD shown as dashed vertical lines. True CPs at $t = 200, 400$.

Five Autoregressive processes with two CPs

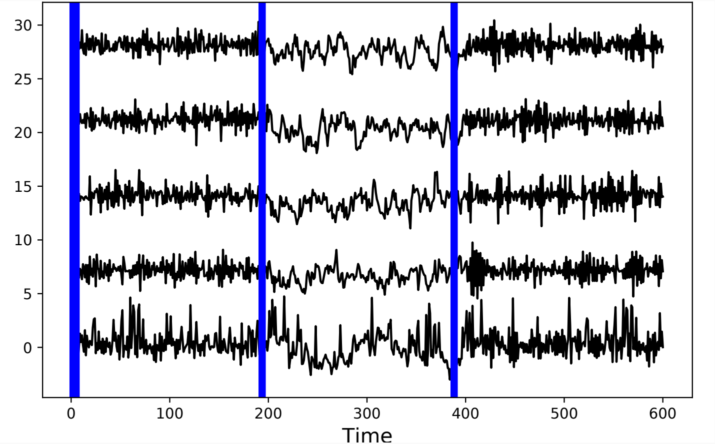


Figure 12 – Maximum A Posteriori (MAP) CPs of **robust** BOCPD shown as solid vertical lines. True CPs at $t = 200, 400$.

5.2 Fix: Robustness by adapting the loss XI/XI

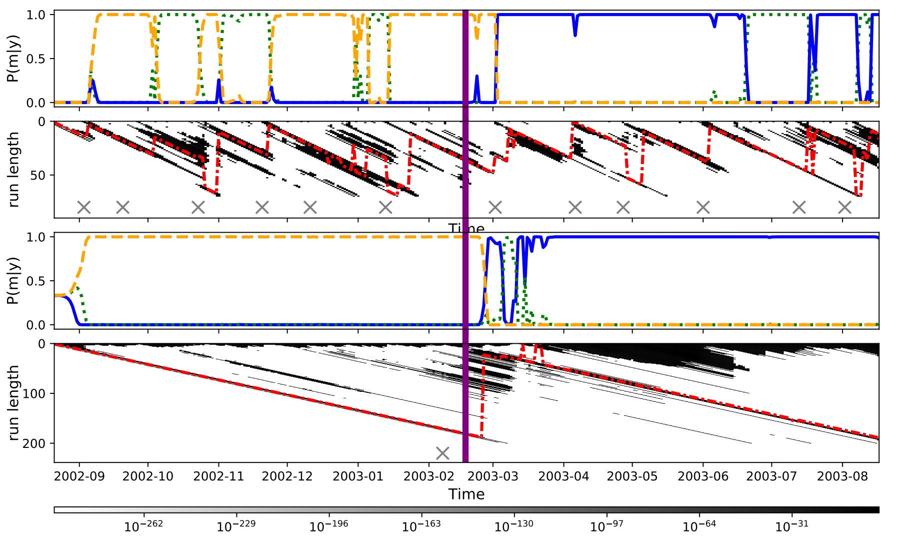


Figure 13 – Top & bottom two panels: standard & robust BOCPD.

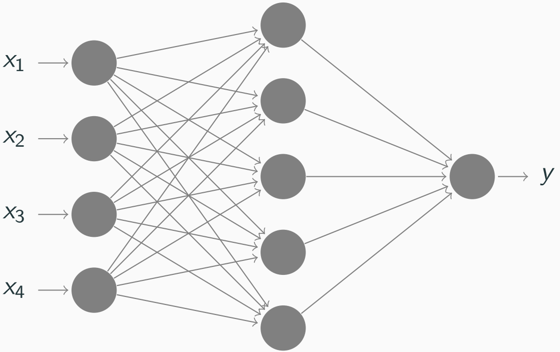
5.3 Experiments with Bayesian Neural Nets (BNNs) I/IV

BNNs are intractable Bayesian regression models with

$$y|\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{y}; F_{\boldsymbol{\theta}}(\boldsymbol{x}), \sigma^2),$$

with $F_{\boldsymbol{\theta}}(\boldsymbol{x})$ defining a non-linear transform of $\boldsymbol{x}$ parameterized by $\boldsymbol{\theta}$.
(**Note:** Our experiments use one hidden layer with 50 ReLu neurons.)

$F_{\boldsymbol{\theta}}(\boldsymbol{x})$



5.3 Experiments with Bayesian Neural Nets (BNNs) II/IV

Methods: Comparison of black box approximate Bayesian methods:

- **VI**
- **DVI** based on $F = D_{AR}^{(\alpha)}$ (Li and Turner, 2016)
- **DVI** based on $F = D_{A}^{(\alpha)}$ (Hernández-Lobato et al., 2016)
- **GVI** with $D = D_{AR}^{(\alpha)}$.

Note: Everything run with settings of Li and Turner (2016) and Hernández-Lobato et al. (2016)

- Variational family $\mathcal{Q}$: A fully factorized normal
- Optimization of σ^2 (i.e., point estimation akin to type-II ML)
- ADAM (Kingma and Ba, 2014) with default settings and 500 epochs
- 50 Random splits with 90:10 training:test ratio
- benchmark UCI (Lichman et al., 2013) datasets

...

5.3 Experiments with Bayesian Neural Nets (BNNs) III/IV

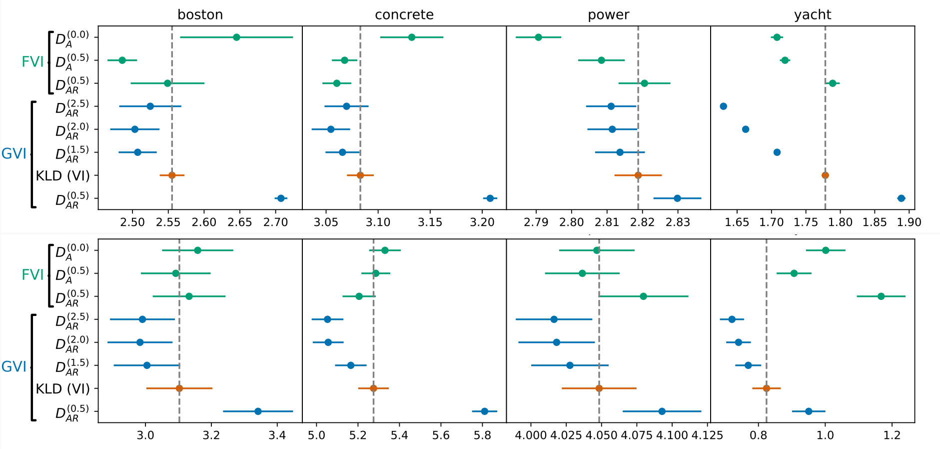


Figure 14 – Performance on BNNs: **DVI**, **GVI** with $D = D_{AR}^{(\alpha)}$, and **VI**. **Top**: Negative test log likelihoods. **Bottom row**: Test RMSE.

Observation: **GVI** outperforms **VI** for **over-concentrated** posteriors (i.e. $\alpha > 1$)! So how does **under-concentrated** **DVI** outperform **VI**?!?

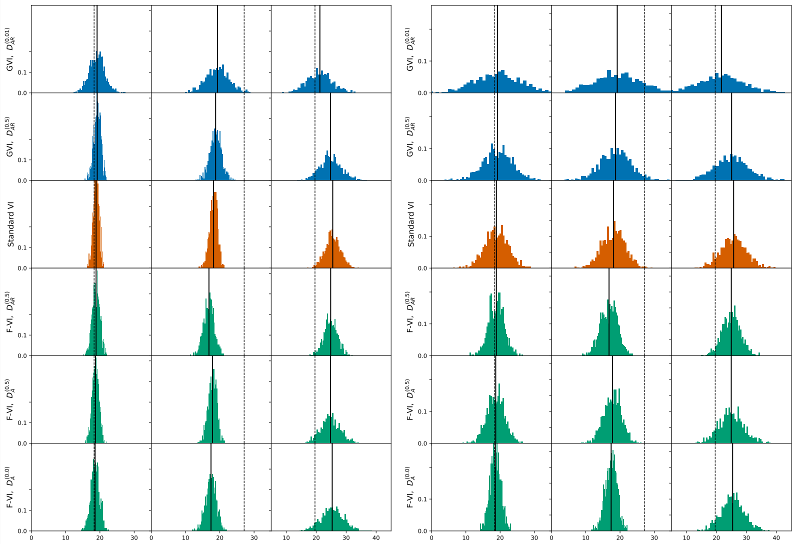


Figure 15 – Left: Parameter posteriors (**DVI** as expected). **Right:** Posterior predictives (**DVI not** as expected)

5.3 Experiments with Bayesian Neural Nets (BNNs) V/V

Q: Why does this happen for **DVI** and not for **GVI**?!

A: **DVI** does not distinguish uncertainty quantification & loss!

DVI objective: σ^2 affects **target (!)**

$$\widehat{\sigma}^2, q^*(\boldsymbol{\theta}|\widehat{\sigma}^2, \boldsymbol{\kappa}) = \arg\min_{\sigma^2} \left\{ \arg\min_{q \in \mathcal{Q}} F\left(q(\boldsymbol{\theta}|\sigma^2, \boldsymbol{\kappa}) \| \underbrace{\widetilde{q}(\boldsymbol{\theta}|\sigma^2, \boldsymbol{x}, \boldsymbol{y})}_{\text{i.e., } \widetilde{q} = \widetilde{q}^{\sigma}} \right) \right\}$$

$\Rightarrow$ optimizing for $\sigma^2 =$ **changing the target $\widetilde{\boldsymbol{q}}^{\boldsymbol{\sigma}}$**!

GVI objective: σ^2 indexes the **loss** only

$$\widehat{\sigma}^2, q^*(\boldsymbol{\theta}|\widehat{\sigma}^2, \boldsymbol{x}, \boldsymbol{y}) = \arg\min_{\sigma^2} \left\{ \arg\min_{q \in \mathcal{Q}} \left\{ \mathbb{E}_q \left[\underbrace{\boldsymbol{\ell_n(\theta, x|y, \sigma^2)}}_{\text{i.e., } \ell_n = \ell_n^{\sigma}} \right] + D(q\|\pi) \right\} \right\}$$

$\Rightarrow$ optimizing for $\sigma^2 =$ finding **optimal loss $\boldsymbol{\ell_n^{\sigma}}$**

5.4 Experiments with Deep Gaussian Processes (DGPs) I/II

Principal idea: Use the BNN architecture with GP priors on $F_{\boldsymbol{\theta}}(\cdot)$:

$$
\begin{aligned}
y|\boldsymbol{F}^L &\sim p\left(y\middle|\ \boldsymbol{F}^L\right) \\
\boldsymbol{F}^L|\boldsymbol{F}^{L-1} &\sim \mathrm{GP}\left(\mu^L(\boldsymbol{F}^{L-1}), \mathsf{K}^L(\boldsymbol{F}^{L-1}, \boldsymbol{F}^{L-1})\right) \\
\boldsymbol{F}^{L-1}|\boldsymbol{F}^{L-2} &\sim \mathrm{GP}\left(\mu^{L-1}(\boldsymbol{F}^{L-2}), \mathsf{K}^{L-1}(\boldsymbol{F}^{L-2}, \boldsymbol{F}^{L-2})\right) \\
&\dots \\
\boldsymbol{F}^1|\boldsymbol{x} &\sim \mathrm{GP}\left(\mu^1(\boldsymbol{x}), \mathsf{K}^1(\boldsymbol{x}, \boldsymbol{x})\right),
\end{aligned}
$$

Methods: Comparison of black box approximate Bayesian methods:

- State of the art **VI** (Salimbeni and Deisenroth, 2017) (comprehensively beat competing **DVI** methods (Bui et al., 2016))
- **GVI** with $\ell_n = \sum_{i=1}^n \mathcal{L}_p^{\gamma}(\boldsymbol{\theta}, x_i)$.

Note: Everything run with settings of Salimbeni and Deisenroth (2017)

[Derivations for **DGP-GVI**: `https://arxiv.org/abs/1904.02303`.]

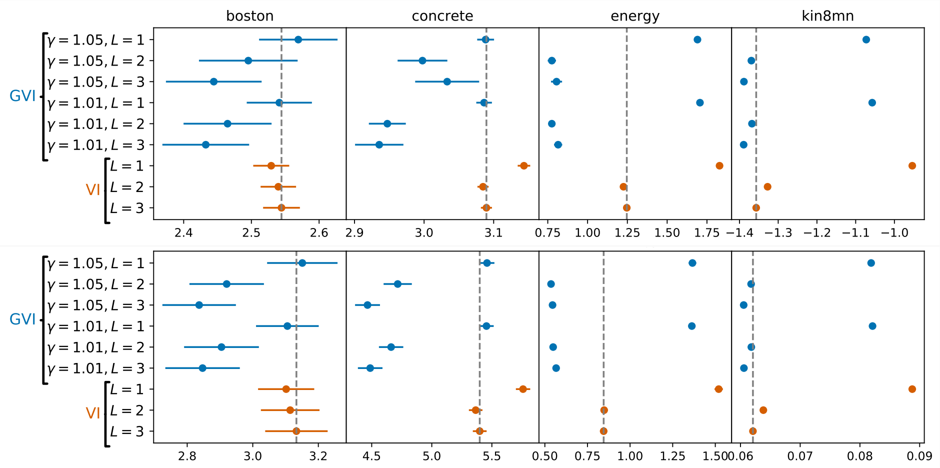


Figure 16 – DGP performance with L layers, **GVI** with & **VI**. **Top row**: Negative test log likelihoods. **Bottom row**: Test RMSE.

Summary & Conclusion

Summary:

Part 1: Ways to look at Bayesian inference: belief updates (about arbitrary parameters) & optimization over $\mathcal{P}(\boldsymbol{\Theta})$

Part 2: Bayesian inference as a modular & interpretable triplet $P(\ell_n, D, \boldsymbol{\Pi})$: **loss**, **uncertainty quantifier** & **admissible posteriors**.

Part 3: Fallout of $P(\ell_n, D, \boldsymbol{\Pi})$: **VI** optimality & **DVI** suboptimality $\rightarrow$ **GVI**

Part 4: Some of **GVI**'s use cases: Robust losses, alternative ways of quantifying uncertainty. Also: its upper bound interpretation

Part 5: Black box methods with **GVI** & empirical performance.

Main Conclusions:

(I) **GVI**: **principled & explicit** design of $\mathcal{Q}$-constrained posteriors

(II) **GVI**: **tackles drawbacks of VI** (e.g., robustness, marginals)

(III) **GVI**: **State of the art** $\mathcal{Q}$-constrained posteriors **on BNNs & DGPs**

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4.2 GVI: Choosing loss hyperparameters

$$\mathcal{L}_p^{\beta}(\boldsymbol{\theta}, x_i) = -\frac{1}{\beta - 1} p(x_i|\boldsymbol{\theta})^{\beta-1} + \frac{I_{p,\beta}(\boldsymbol{\theta})}{\beta}$$

$$\mathcal{L}_p^{\gamma}(\boldsymbol{\theta}, x_i) = -\frac{1}{\gamma - 1} p(x_i|\boldsymbol{\theta})^{\gamma-1} \frac{\gamma}{I_{p,\gamma}(\boldsymbol{\theta})^{\frac{\gamma-1}{\gamma}}}$$

$$I_{p,c}(\boldsymbol{\theta}) = \int p(x|\boldsymbol{\theta})^c dx$$

where $I_{p,c}(\boldsymbol{\theta}) = \int p(x|\boldsymbol{\theta})^c dx$.

Note 1: $\mathcal{L}_p^{\gamma}(\boldsymbol{\theta}, x_i)$ multiplicative & always $< 0 \rightarrow$ store as log!
Note 2: Conditional independence $\neq$ additive for $\mathcal{L}_p^{\beta}(\boldsymbol{\theta}, x_i), \mathcal{L}_p^{\gamma}(\boldsymbol{\theta}, x_i)$
Note 3: In practice, usually best to choose $\beta/\gamma = 1 + \varepsilon$ for some small ε

Appendix: Choosing hyperparameters

Q: Any principled way of choosing hyperparameters?

A: Very much unsolved problem, solutions so far:

- D: brute force (CV) (Regli and Silva, 2018) [slow/expensive]
- ℓ_n: Via *points of highest influence* (Knoblauch et al., 2018)
- ℓ_n: on-line updates using loss-minimization (Knoblauch et al., 2018)

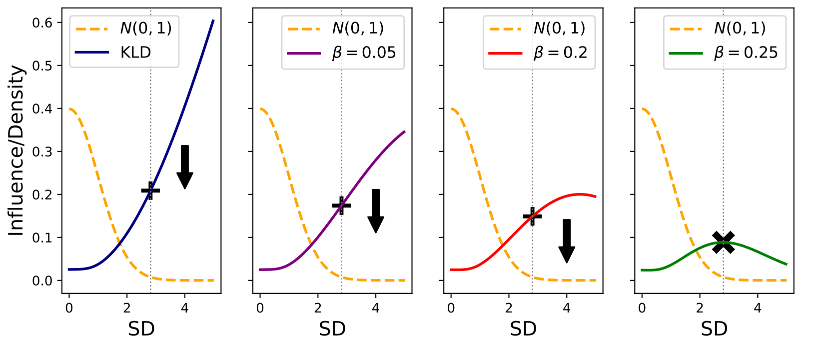


Figure 17 – Illustration of the initialization procedure using *points of highest influence* logic, from left to right.

Appendix: Choosing D for conservative marginals I/II

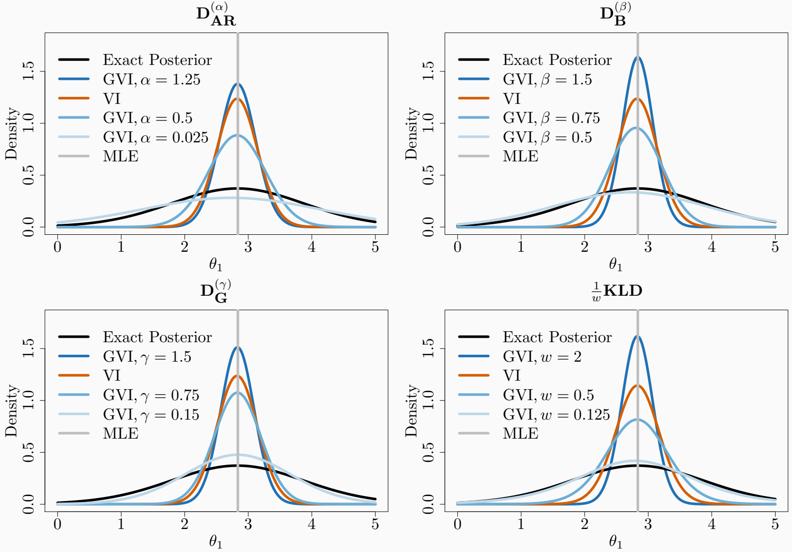


Figure 18 – Marginal VI and GVI posterior for a Bayesian linear model under the $D_{AR}^{(\alpha)}$, $D_{B}^{(\beta)}$, $D_{G}^{(\gamma)}$ and $\frac{1}{w}\mathrm{KLD}$ uncertainty quantifier for different values of the divergence hyperparameters.

Appendix: Choosing D for conservative marginals II/II

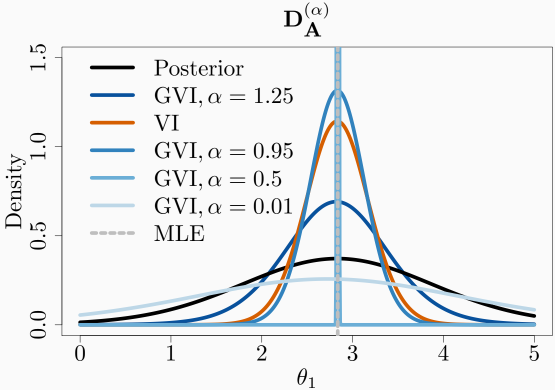


Figure 19 – Marginal **VI** and **GVI** posterior for a Bayesian linear model under the $D_A^{(\alpha)}$ uncertainty quantifier. The boundedness of the $D_A^{(\alpha)}$ causes **GVI** to severely over-concentrate if α is not carefully specified.

Appendix: Choosing D for prior robustness I/IV

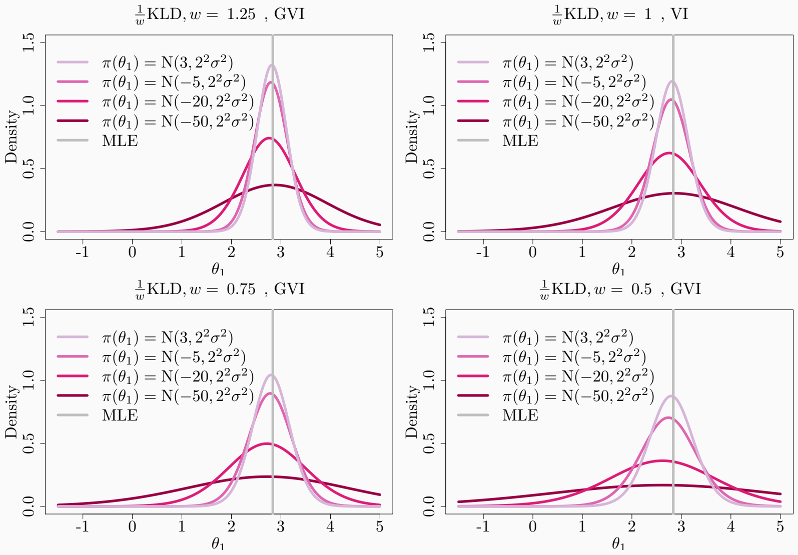


Figure 20 – Marginal **VI** and **GVI** posterior for a Bayesian linear model under different priors, using $D = \frac{1}{w}\mathrm{KLD}$ as the uncertainty quantifier.

Appendix: Choosing D for prior robustness II/IV

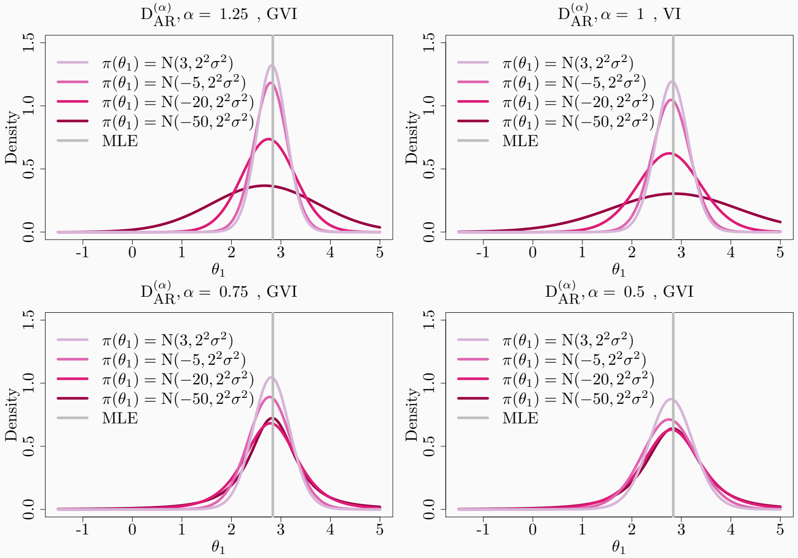


Figure 21 – Marginal **VI** and **GVI** posterior for a Bayesian linear model under different priors, using $D = D_{AR}^{(\alpha)}$ as the uncertainty quantifier.

Appendix: Choosing D for prior robustness III/IV

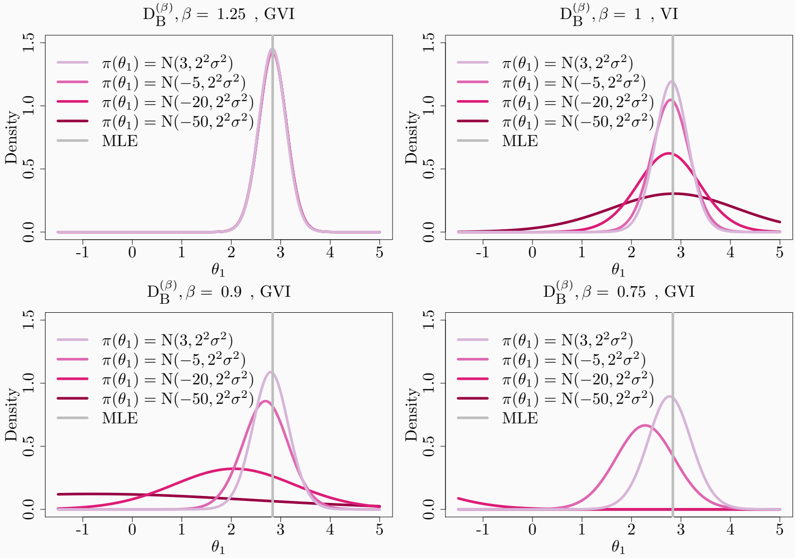


Figure 22 – Marginal **VI** and **GVI** posterior for a Bayesian linear model under different priors, using $D = D_B^{(\beta)}$ as the uncertainty quantifier.

Appendix: Choosing D for prior robustness IV/IV

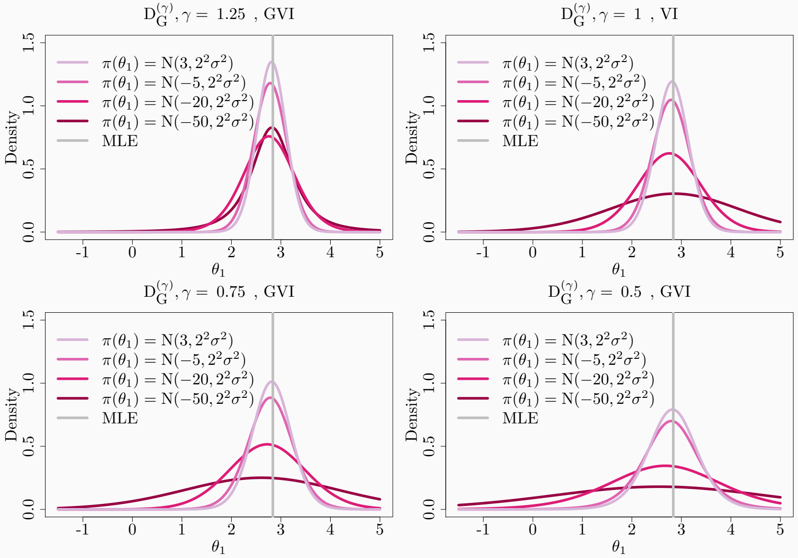


Figure 23 – Marginal **VI** and **GVI** posterior for a Bayesian linear model under different priors, using $D = D_G^{(\gamma)}$ as the uncertainty quantifier.

Appendix: GVI lower bound interpretation I/II

Question: VI is also interpretable as optimizing a lower bound on the evidence! Is there anything comparable for GVI?

Answer: Yes, e.g. for $D_B^{(\beta)}$, $D_G^{(\gamma)}$, $D_{AR}^{(\alpha)}$: Consider *generalized* evidence:

Recall: Generalized Bayes posterior (Bissiri et al., 2016) is

$$q^*_{\ell_n}(\boldsymbol{\theta}) \propto \pi(\boldsymbol{\theta}) \exp\{-\ell_n(\boldsymbol{\theta}, \boldsymbol{x})\} \quad \text{and so } p_{\ell_n}(\boldsymbol{x}) = \int_{\boldsymbol{\Theta}} q^*_{\ell_n}(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

GVI's objectives $L(q|\boldsymbol{x}, D, \ell_n)$ will optimize

$$L(q|\boldsymbol{x}, D, \ell_n) \geq g^D(\underbrace{-\log p_{f^D(\ell_n)}(\boldsymbol{x})}_{\substack{\text{negative log evidence;} \\ f^D(\ell_n) \text{ maps } \ell_n \text{ into a new loss}}}) + \underbrace{T^D(q)}_{\text{Approximate target}}$$

(**Note**: VI is special case where this holds with *equality* (so that the approximate target is the exact target) and where $g^{\mathrm{KLD}}(x) = x$, $L(q|\boldsymbol{x}, D, \ell_n) = \mathrm{ELBO}(q)$, $T^{\mathrm{KLD}}(q) = \mathrm{KLD}(q||q^*_{\ell_n})$, $f^{\mathrm{KLD}}(\ell_n) = \ell_n$.)

Appendix: GVI lower bound interpretation II/II

GVI's objectives $L(q|\boldsymbol{x}, D, \ell_n)$ will optimize

$$L(q|\boldsymbol{x}, D, \ell_n) \geq g^D\Big(\underbrace{-\log p_{f^D(\ell_n)}(\boldsymbol{x})}_{\substack{\text{negative log evidence;} \\ f^D(\ell_n) \text{ maps } \ell_n \text{ into a new loss}}} \Big) + \underbrace{T^D(q)}_{\text{Approximate target}}$$

Example: Rényi's α-divergence ($D_{AR}^{(\alpha)}$) for $\alpha > 1$ gives

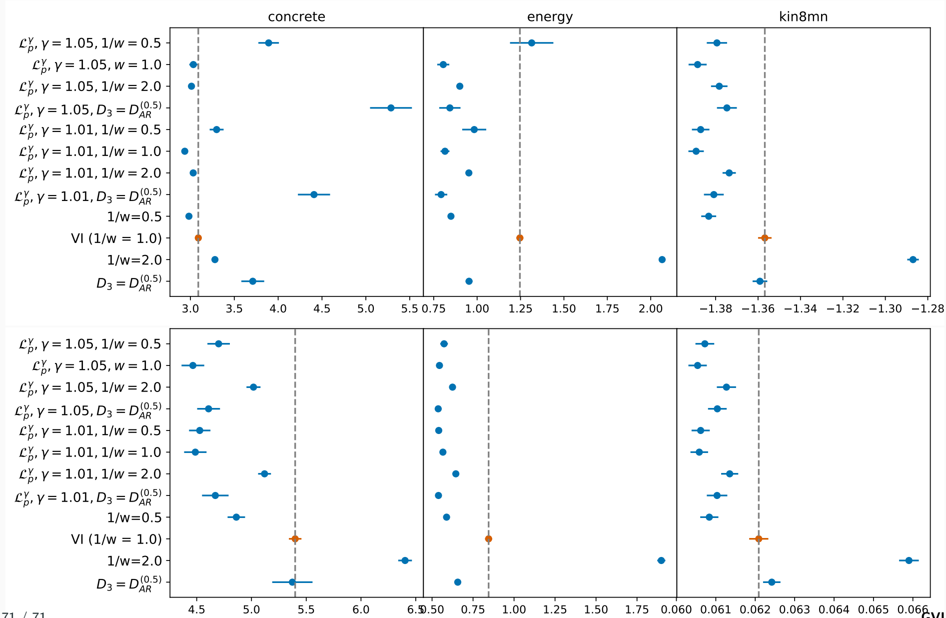
$$g^{D_{AR}^{(\alpha)}}(x) = \tfrac{1}{\alpha}x,$$
$$f^{D_{AR}^{(\alpha)}}(\ell_n) = \alpha\ell_n,$$
$$T_{D_{AR}^{(\alpha)}}(q) = \tfrac{1}{\alpha}\mathrm{KLD}(q||q^*_{\alpha\ell_n}),$$

so putting it together one finds that for $D = D_{AR}^{(\alpha)}$ with $\alpha > 1$,

$$L(q|\boldsymbol{x}, D, \ell_n) \geq -\frac{1}{\alpha}\log p_{\alpha\ell_n}(\boldsymbol{x}) + \frac{1}{\alpha}\mathrm{KLD}(q||q^*_{\alpha\ell_n})$$

(Which is just a $\frac{1}{\alpha}$-scaled version of the ELBO for the loss $\alpha\ell_n$!)

5.4 Experiments with Deep Gaussian Processes (DGPs) III/IV



GVI