Γ-convergence of Onsager–Machlup functionals and MAP estimation in non-parametric Bayesian inverse problems

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Motivation

- In applications such as the Bayesian approach to inverse problems and the analysis of transitions of dynamical systems, it is often desirable to summarise a complicated probability measure μ on a high-dimensional space X by a single point $x^\star \in X$ — a "point of maximum probability under μ".

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What does "point of maximum probability under μ" even mean when μ is a measure on a metric space X, with no uniform reference measure etc.?

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Challenge II — Stability

Are such points stable under perturbations of μ, or perturbations of problem data determining μ (changes of prior, likelihood, data, discretisation. . .)?

Some notation

- Throughout, X will be a separable metric space— occasionally something better, such as a separable Banach or Hilbert space.
- $B_r(x) := \{y \in X \mid d(x, y) \leqslant r\}$ denotes the closed ball of radius $r \geqslant 0$ centred on $x \in X$.
- $\mathcal{P}(X)$ denotes the set of all probability measures on the Borel σ-algebra of X.
- (Separability ensures that every $\mu \in \mathcal{P}(X)$ has a non-empty support, i.e. there is some $x \in X$ with $\mu(B_r(x)) > 0$ for every $r > 0$, and so $M_r := \sup_{x \in X} \mu(B_r(x)) > 0$.)
- Given a positive sequence $\gamma = (\gamma_k)_{k \in \mathbb{N}}$, we have the corresponding weighted ℓ^p norm and weighted ℓ^p space:

$$\|h\|_{\ell^p_\gamma} := \big\|(h_k/\gamma_k)_{k \in \mathbb{N}}\big\|_{\ell^p},$$
$$\ell^p_\gamma := \big\{h \in \mathbb{R}^{\mathbb{N}} \big| (h_k/\gamma_k)_{k \in \mathbb{N}} \in \ell^p\big\}.$$

Well-posedness of (Bayesian) inverse problems

- In an **inverse problem** we recover a parameter $u \in X$ from observed data $y \in Y$. Such problems are usually ill posed: the recovered $u^y \in X$ depends sensitively on y, and this sensitivity is worse the "nicer" the forward map $u \mapsto y$ is (and this is why inverse problems need to be regularised).
- In a **Bayesian inverse problem (BIP)**, the recovery of u from y is expressed in the form of a posterior probability distribution $\mu^y \in \mathcal{P}(X)$.
- BIPs *are* well posed (Stuart, 2010; ...; Sprungk, 2020). The posterior μ^y is a stable function of the problem setup — the prior distribution $\mu_0 \in \mathcal{P}(X)$, the observed data $y \in Y$, and the likelihood model $\ell \colon X \to \mathcal{P}(Y)$ — with respect to e.g. the Hellinger, Kullback–Leibler, or Wasserstein distances on $\mathcal{P}(X)$, e.g.

$$\mathrm{KL}(\mu^y \| \mu^{y+\delta y}) \lesssim \|\delta y\| \quad \text{(for fixed } \ell \text{ and } \mu_0\text{)}.$$

- Are the MAP estimators, the "most likely points under μ^y", also stable?

Similarity of modes $\not\Rightarrow$ similarity of measures

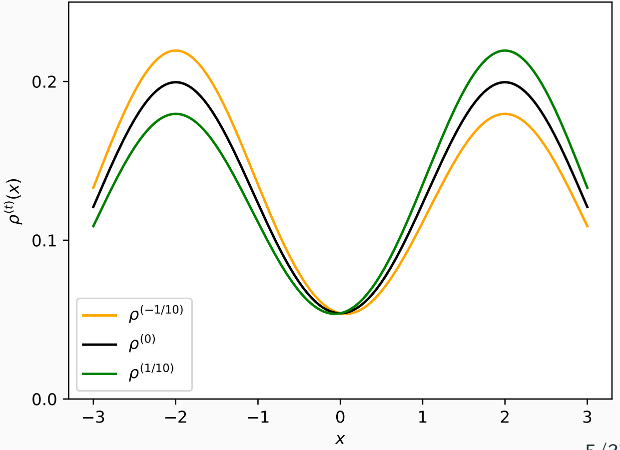
- Unfortunately, closeness of probability measures and closeness of their modes are "orthogonal" questions, even using a strong distance on $\mathcal{P}(X)$ like Kullback–Leibler.
- This is the case even for probability measures on $\mathbb{R}$ with continuous Lebesgue densities, for which a mode is easily defined as a maximiser of the density.
- Obviously, two measures can have very similar (or even the same) modes and yet be very different as measures, e.g. $\mathcal{N}(0, 1)$ and $\mathcal{N}(0, 10^6)$ or $\mu(E) = \int_E \max(0, 1 - |x|)\, \mathrm{d}x$!
- Perhaps if a sequence of probability measures converges "strongly enough", then their modes will also converge?
- Unfortunately, this is not the case.

Similarity of measures $\not\Rightarrow$ similarity of modes

Consider, for $t \in \mathbb{R}$, $\mu^{(t)} \in \mathcal{P}(\mathbb{R})$ with Lebesgue density

$$\rho^{(t)}(x) := \frac{(1+t)\exp(-\frac{1}{2}(x-r)^2) + (1-t)\exp(-\frac{1}{2}(x+r)^2)}{2\sqrt{2\pi}}.$$

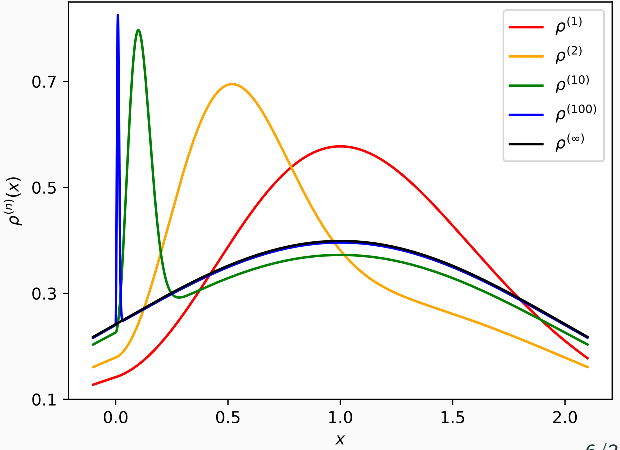
- For $t > 0$ and for $r > 0$ large enough, $\rho^{(\pm t)}$ has a unique maximiser at $x^\star_{\pm t} \approx \pm r$.
- $\mathrm{KL}(\mu^{(t)} \| \mu^{(-t)}) \approx Ct^2$, and yet their modes are order 1 apart.
- This isn't too bad: The *cluster points* of the modes of $\mu^{(t)}$ as $t \to 0$ form the modes of $\mu^{(0)}$.



Consider, for $n \in \mathbb{N}$, $\mu^{(n)} \in \mathcal{P}(\mathbb{R})$ with Lebesgue density

$$\rho^{(n)}(x) := \frac{\exp\left(-\frac{1}{2}(x-1)^2\right) + \mathbb{1}[x \geqslant 0] 4n^2x^2 \exp(-n^2x^2)}{\sqrt{2\pi} + \sqrt{\pi}/n}$$

- Each $\rho^{(n)}$ has a unique maximiser at $x_n^\star \approx \frac{1}{n}$.
- Pointwise, $\rho^{(n)} \to \rho^{(\infty)}$, the density of $\mu^{(\infty)} = \mathcal{N}(1, 1)$.
- $\mathrm{KL}(\mu^{(\infty)} \| \mu^{(n)}) \approx \frac{1}{n}$
- But the maximiser of $\rho^{(\infty)}$ is at $x_\infty^\star = 1 \neq \lim_{n\to\infty} x_n^\star$!



Ouch.

A role for Γ-convergence

- Evidently, these densities are not converging the "the right way", and even "strong" distances on $\mathcal{P}(X)$ like Kullback–Leibler are not the right notion of convergence.
- Modes are characterised as maximisers of the density — or minimisers of the negative log-density.
- The well-established notion of Γ-convergence from the calculus of variations (De Giorgi and Franzoni, 1975), which aims to give conditions for convergence of minimisers of minimisation problems, would seem to be a natural thing to try.
- (And it would be nice not to have to talk about densities, because not every measure has one...)

Overview

1. Modes, MAP estimators, and Onsager–Machlup functionals
2. Γ-convergence: A capsule summary
3. Γ-convergence of OM functionals
4. Bayesian inverse problems
5. MAP estimation for BIPs
6. Closing remarks

Modes, MAP estimators, and Onsager–Machlup functionals

Defining a mode of a measure. 1: Strong modes

- There is no such thing as a "Lebesgue-like" uniform reference measure λ on an infinite-dimensional space X (Sudakov, 1959), so we can't define a mode of μ as a maximiser of the density $\frac{\mathrm{d}\mu}{\mathrm{d}\lambda}$.
- Over the last decade, it has become common to define modes directly using the masses of metric balls in the small-radius limit (Dashti et al., 2013; Helin and Burger, 2015; Clason et al., 2019).

Definition 1 (after Dashti et al. (2013))

A **strong mode** of $\mu \in \mathcal{P}(X)$ is any $x^\star \in X$ such that

$$\lim_{r \to 0} \frac{\mu(B_r(x^\star))}{M_r} = 1,$$

where $B_r(x) := \{x' \in X \mid d(x, x') \leqslant r\}$ and $M_r := \sup_{x \in X} \mu(B_r(x))$.

Defining a mode of a measure. 2: Weak modes

Note that $\mu(B_r(x^\star)) \,/\, M_r \in [0, 1]$, so

$$\begin{aligned} x^\star \text{ is a strong mode} \iff & \lim_{r \to 0} \frac{\mu(B_r(x^\star))}{M_r} = 1 \\ \iff & \liminf_{r \to 0} \frac{\mu(B_r(x^\star))}{M_r} \geqslant 1 \\ \iff & \limsup_{r \to 0} \frac{M_r}{\mu(B_r(x^\star))} \leqslant 1. \end{aligned}$$

This motivates another definition:

Definition 2 (after Helin and Burger (2015))

A **global weak mode** of $\mu \in \mathcal{P}(X)$ is any $x^\star \in X$ such that

$$\limsup_{r \to 0} \frac{\mu(B_r(x'))}{\mu(B_r(x^\star))} \leqslant 1 \text{ for all } x' \in X.$$

Defining a mode of a measure. 3: Minimisers of OM functionals

Definition 3

An **Onsager–Machlup (OM) functional** for $\mu \in \mathcal{P}(X)$ is a function $I_\mu \colon E \to \mathbb{R}$ with

$$\lim_{r \to 0} \frac{\mu(B_r(x))}{\mu(B_r(y))} = \frac{\exp(-I_\mu(x))}{\exp(-I_\mu(y))} \text{ for all } x, y \in E.$$

We call $E \subseteq X$ the **domain** of the OM functional.

- OM functionals are at most unique up to addition of constants — this aspect requires some care, which this presentation will neglect!
- If $\mu \in \mathcal{P}(\mathbb{R}^d)$ has Lebesgue density ρ, then $I_\mu := -\log \rho$ is an OM functional for μ.
- Any measure admits an OM functional if E is small enough.
- Can measures on "large" spaces have OM functionals with large E?
- Are minimisers of I_μ "most probable points" under μ? (Cf. Dürr and Bach (1978).)

The Gaussian OM functional

- The prime example of an OM functional is the OM functional of a centred Gaussian measure $\mu = \mathcal{N}(0, C)$ on a separable Hilbert space X.
- Here, for simplicity, we assume that the covariance operator $C \colon X \to X$,

$$\langle u, Cv \rangle := \int_X \langle u, x \rangle \langle v, x \rangle \, \mu(\mathrm{d}x)$$

  which is always symmetric and positive semi-definite, is actually positive definite.
- In this case, μ has the OM functional $I_\mu \colon H(\mu) := \operatorname{ran} C^{1/2} \to \mathbb{R}$

$$I_\mu(u) = \frac{1}{2} \| C^{-1/2} u \|^2 \text{ for } u \in H(\mu).$$

- Furthermore, one can show that, for $u \notin H(\mu)$, $\lim_{r \to 0} \frac{\mu(B_r(u))}{\mu(B_r(0))} = 0$, so we can sensibly think of I_μ as taking the value $+\infty$ there.

A new-ish formal property

We formalise a property used implicitly in e.g. Dashti et al. (2013):

Definition 4

We will say that **property** $M(\mu, E)$ holds for $\mu \in \mathcal{P}(X)$ and $E \subseteq X$ if, for some $x^\star \in E$,

$$x \in X \setminus E \implies \lim_{r \to 0} \frac{\mu(B_r(x))}{\mu(B_r(x^\star))} = 0.$$

- Property $M(\mu, E)$ always holds if E is large enough.
- Property $M(\mu, E)$ does not say that $\mu(X \setminus E) = 0$!
- Property $M(\mu, E)$ does say that points outside E cannot qualify as modes of μ.
- Standard example: a Gaussian measure $\mu = \mathcal{N}(0, C)$ on an infinite-dimensional Hilbert space X with infinite-dimensional **Cameron–Martin space** $H(\mu) :=$ **ran** $C^{1/2}$ satisfies property $M(\mu, H(\mu))$ and yet has $\mu(H(\mu)) = 0$.

OM functionals, property M, and modes

- Property $M(\mu, E)$ says that $+\infty$ is a sensible value for the OM functional outside E — as opposed to the mass ratio oscillating so badly that **the limit does not exist** at all, cf. Lambley (2022).
- This being the case, the next result should be no surprise:

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- Property $M(\mu, E)$ says that $+\infty$ is a sensible value for the OM functional outside E — as opposed to the mass ratio oscillating so badly that **the limit does not exist** at all, cf. Lambley (2022).
- This being the case, the next result should be no surprise:

Lemma 5 (Ayanbayev et al., 2022a, Prop. 4.1)

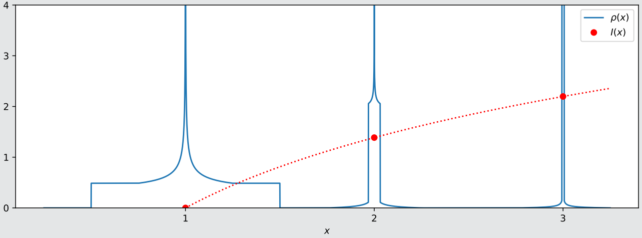
Let μ have OM functional $I_\mu \colon E \to \mathbb{R}$ and satisfy property $M(\mu, E)$. Set $I_\mu(x) := +\infty$ for $x \notin E$. Then the global weak modes of μ are precisely the global minimisers of $I_\mu \colon X \to \overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$.

- This result gives a rigorous meaning to the claim of Dürr and Bach (1978) that OM minimisers should be seen as "most likely points" in the sense of global weak modes.
- Unfortunately, it is **not** generally true that strong modes are OM-minimisers, even when such minimisers exist and property M holds!

Example 6

Let $\mu \in \mathcal{P}(\mathbb{R})$ have Lebesgue density $\rho := \frac{24}{5\pi^2} \sum_{k\in\mathbb{N}} \rho_k$, where

$$\rho_0(x) := \tfrac{1}{4}\left(|x|^{-1/2} - 2\right) \mathbb{1}_{[-\frac{1}{4},\frac{1}{4}]\setminus\{0\}}(x), \qquad \rho_k(x) := \frac{\rho_0(x-k)}{k^2} + k^2\, \mathbb{1}_{\left[-\frac{1}{2k^4},\frac{1}{2k^4}\right]}(x-k).$$



The measure μ has OM functional $I_\mu(x) = 2\log x$ for $x \in E = \mathbb{N}$, this domain cannot be extended, and property $M(\mu, \mathbb{N})$ holds. However, μ has a global weak mode at 1, and this minimises I_μ, but it is not a strong mode.

Γ-convergence: A capsule summary

Γ-convergence

- Γ-convergence, originating with De Giorgi and Franzoni (1975), is a principal example of a kind of variational convergence for functionals $F_n \colon X \to \overline{\mathbb{R}}$.
- The idea, under suitable assumptions, is to have a notion of convergence for functionals so that

$$F_n \xrightarrow[n\to\infty]{\Gamma} F \implies \operatorname*{arg\,min}_X F_n \xrightarrow[n\to\infty]{} \operatorname*{arg\,min}_X F.$$

  i.e. the minimisers of F_n converge to the minimisers of F.
- Γ-convergence, and related notions such as Mosco convergence, have met great success in the study of optimisation problems in general and the calculus of variations in particular.

Definition 7

Given extended-real-valued functions $F_n, F\colon X \to \overline{\mathbb{R}}$, we say that F_n **Γ-converges** to F, written $F_n \xrightarrow[n\to\infty]{\Gamma} F$, if, for every $x \in X$,

- (Γ-lim inf inequality) for every sequence $(x_n)_{n\in\mathbb{N}}$ converging to x,

$$F(x) \leqslant \liminf_{n\to\infty} F_n(x_n);$$

- (Γ-lim sup inequality) and there exists a "recovery sequence" $(x_n)_{n\in\mathbb{N}}$ converging to x such that

$$F(x) \geqslant \limsup_{n\to\infty} F_n(x_n).$$

Pointwise, continuous, uniform and Γ-convergence

Definition 8

For $F_n, F \colon X \to \overline{\mathbb{R}}$ as before, we say that F_n **converges continuously** to F if, for every $x \in X$ and every neighbourhood V of $F(x)$ in $\overline{\mathbb{R}}$, there exists $N \in \mathbb{N}$ and $r > 0$ such that

$$(n \geqslant N \text{ and } d(x', x) < r) \implies F_n(x') \in V.$$

$$F_n \xrightarrow[n\to\infty]{\text{unif}} F \xRightarrow{\text{if } F \text{ continuous}} F_n \xrightarrow[n\to\infty]{\text{cts}} F \Longrightarrow F_n \xrightarrow[n\to\infty]{\Gamma} F$$

$$F_n \xrightarrow[n\to\infty]{\text{cts}} F \Longrightarrow F_n \xrightarrow[n\to\infty]{\text{pt}} F$$

$$F_n \xrightarrow[n\to\infty]{\Gamma} F \quad \not\Downarrow \;\; \not\Uparrow \quad F_n \xrightarrow[n\to\infty]{\text{pt}} F$$

$$\left(F_n \xrightarrow[n\to\infty]{\Gamma} F \text{ and } F_n \xrightarrow[n\to\infty]{\text{pt}} G \right) \implies F \leqslant G.$$

$$\left(F_n \xrightarrow[n\to\infty]{\text{cts}} F \text{ and } G_n \xrightarrow[n\to\infty]{\Gamma} G \right) \implies F_n + G_n \xrightarrow[n\to\infty]{\Gamma} F + G.$$

The fundamental theorem of Γ-convergence

Definition 9

We say that $(F_n)_{n\in\mathbb{N}}$ is **equicoercive** if for all $t \in \mathbb{R}$, there exists a compact $K_t \subseteq X$ such that, for all $n \in \mathbb{N}$, $F_n^{-1}([-\infty, t]) \subseteq K_t$.

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Theorem 10 (Fundamental theorem of Γ-convergence; Braides, 2006, Theorem 2.10)

Suppose that $F_n, F\colon X \to \overline{\mathbb{R}}$ are such that $F_n \xrightarrow[n\to\infty]{\Gamma} F$ and $(F_n)_{n\in\mathbb{N}}$ is equicoercive. Then

- *F has a minimum value and $\min_X F = \lim_{n\to\infty} \inf_X F_n$;*
- *if $(x_n)_{n\in\mathbb{N}}$ is a precompact sequence such that $\lim_{n\to\infty} F_n(x_n) = \min_X F$, then every limit of a convergent subsequence of $(x_n)_{n\in\mathbb{N}}$ is a minimiser of F; and*
- *if each F_n has a minimiser $x_n^\star$, then every convergent subsequence of $(x_n^\star)_{n\in\mathbb{N}}$ has as its limit a minimiser of F.*

(The hypotheses of the fundamental theorem can be relaxed somewhat to use only "equi-mild coercivity".)

Γ-convergence of OM functionals

Γ-convergence of OM functionals and convergence of modes

We're in a position to state our first theorem, and it comes almost for free...

Theorem 11 (Γ-convergence and equicoercivity imply convergence of modes; Ayanbayev et al. (2022a, Theorem 4.2))

For $n \in \mathbb{N} \cup \{\infty\}$, let $\mu^{(n)} \in \mathcal{P}(X)$ have OM functional $I_{\mu^{(n)}} \colon E^{(n)} \to \mathbb{R}$ and satisfy property $M(\mu^{(n)}, E^{(n)})$; extend each $I_{\mu^{(n)}}$ to take the value $+\infty$ on $X \setminus E^{(n)}$. Suppose that the sequence $(I_{\mu^{(n)}})_{n \in \mathbb{N}}$ is equicoercive and Γ-converges to $I_{\mu^{(\infty)}}$. Then, if $u^{(n)}$ is a global weak mode of $\mu^{(n)}$, $n \in \mathbb{N}$, every convergent subsequence of $(u^{(n)})_{n \in \mathbb{N}}$ has as its limit a global weak mode of $\mu^{(\infty)}$.

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Proof.

The global weak modes are exactly the minimisers of the extended OM functionals, and the rest follows from the fundamental theorem of Γ-convergence. □

Γ-convergence of OM functionals and convergence of modes

- The pathological examples of non-convergent modes given earlier fall outside the realm of Theorem 11: the negative log-densities involved converge pointwise but not uniformly, and indeed do not Γ-converge.
- Theorem 11 is very general, and there is no free lunch: one does need to verify equicoercivity and Γ-convergence for the application at hand.
- Let's examine the Γ-convergence and equicoercivity of the OM functionals of measures that are often used as priors in BIPs, even though their modes are quite obvious.
- This only *looks* like a trivial exercise: Γ-convergence and equicoercivity of posterior OM functionals — i.e. for reweightings of these priors — and hence convergence of MAP estimators, will follow later.

Skip discussion of pseudoinverse square roots ▶

A digression on pseudoinverses and pseudoinverse square roots

- "Everyone knows" that the OM functional of a Gaussian measure is one half the square of its Cameron–Martin norm.
- To make this statement precise, we need to be precise about the inverse square root of its (possibly indefinite) covariance operator.

Definition 12

For a bounded linear operator A between Hilbert spaces X and Y, the **Moore–Penrose pseudoinverse** $A^\dagger$ of A is the unique extension of $(A|_{(\ker A)^\perp})^{-1}$ to a (generally unbounded) linear operator $A^\dagger \colon \operatorname{ran} A \oplus (\operatorname{ran} A)^\perp \to X$ subject to the restriction that $\ker A^\dagger = (\operatorname{ran} A)^\perp$.

For $y \in \operatorname{ran} A \oplus (\operatorname{ran} A)^\perp$,

$$A^\dagger y = \arg\min \big\{ \|x\|_X \big| x \text{ minimises } \|Ax - y\| \big\}.$$

In particular, for $y \in \operatorname{ran} A$, $A^\dagger y$ is the minimum-norm solution of $Ax = y$.

Definition 13

For a compact SPSD operator $C = \sum_{n\in\mathbb{N}} \sigma_n^2 e_n \otimes e_n$ on a Hilbert space X, $(e_n)_{n\in\mathbb{N}}$ being an orthonormal system in X and $\sigma_n \geqslant 0$ for each $n \in \mathbb{N}$, we denote the SPSD operator square root of C by $C^{1/2}$ and furthermore set

$$C^{\dagger/2} := (C^{1/2})^{\dagger} = \sum_{n\in\mathbb{N}\,:\,\sigma_n\neq 0} \sigma_n^{-1} e_n \otimes e_n.$$

Note that $(C^{\dagger})^{1/2}$ can differ from $(C^{1/2})^{\dagger}$ since it may have a smaller domain.

OM functionals for Gaussian measures

Lemma 14 (Ayanbayev et al., 2022a, Cor. 5.4)

The extended OM functional of $\mu = \mathcal{N}(m, C)$ *on a separable Hilbert space* X *is* $I_\mu \colon X \to \overline{\mathbb{R}}$,

$$I_\mu(u) := \begin{cases} \frac{1}{2}\left\| C^{\dagger/2}(u - m) \right\|_X^2 & \text{for } u - m \in H(\mu) = \operatorname{ran} C^{1/2}, \\ +\infty & \text{otherwise,} \end{cases}$$

and property $M(\mu, m + H(\mu))$ *holds.*

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and property $M(\mu, m + H(\mu))$ *holds.*

Theorem 15 (Γ-convergence and equicoercivity of Gaussian OM functionals; Ayanbayev et al., 2022a, Thm. 5.5)

Let X *be a separable Hilbert space and* $\mu^{(n)} = \mathcal{N}(m^{(n)}, C^{(n)})$, *for* $n \in \mathbb{N} \cup \{\infty\}$, *be Gaussian measures on* X. *Then*

$$\left.\begin{array}{c} \left\| m^{(n)} - m^{(\infty)} \right\|_X \to 0 \text{ and} \\ \left\| C^{(n)} - C^{(\infty)} \right\|_{\mathrm{op}} \to 0 \end{array}\right\} \implies \left\{ \begin{array}{c} I_{\mu^{(n)}} \xrightarrow[n\to\infty]{\Gamma} I_{\mu^{(\infty)}} \text{ and} \\ (I_{\mu^{(n)}})_{n\in\mathbb{N}} \text{ is equicoercive.} \end{array}\right.$$

Besov measures

- **Besov priors** (Lassas et al., 2009; Dashti et al., 2012; Agapiou et al., 2018) have been advocated as an extension of Gaussian priors for BIPs.
- Besov priors have two key parameters: **"smoothness"** $s \in \mathbb{R}$ and **"integrability"** $p \geqslant 1$; for historical reasons to do with connections to PDE theory, there is also a "spatial dimension" $d \in \mathbb{N}$ and the quantity s/d occurs often.
- The case $p = 2$ corresponds to Gaussian distributions.
- The case $p = 1$ has been studied for its sparsifying / edge-preserving properties (contrast with TV regularisation, Lassas and Siltanen (2004)).
- Just to simplify the notation, this talk will concentrate on the case $p = 1$ and study stability w.r.t. smoothness s, but our results do cover general p and a large class of more general product priors and their perturbations (Ayanbayev et al., 2022b).

Besov-1 measures

- Let $s \in \mathbb{R}$, $d \in \mathbb{N}$, $\eta > 0$, $t := s - d(1+\eta)$.
- The parameter s is thought of as a "smoothness parameter" and d as a "spatial dimension". The parameter t is "a bit less smooth" than s.
- Define $\gamma_0 := 1$ and $\gamma, \delta \in \mathbb{R}^{\mathbb{N}}$ by

$$\gamma_k := k^{1-s/d-1/2}, \qquad \delta_k := k^{1-t/d-1/2} = k^{2+\eta-s/d-1/2}, \qquad k \in \mathbb{N},$$

and let $\mu_k \in \mathcal{P}(\mathbb{R})$ for $k \in \mathbb{N} \cup \{0\}$ have the Lebesgue density

$$\frac{\mathrm{d}\mu_k}{\mathrm{d}u}(u) = \frac{1}{2\gamma_k^{-1}} \exp(-|u/\gamma_k|).$$

Definition 16 (Sequence space Besov measures and Besov spaces)

We call $\mu := \bigotimes_{k\in\mathbb{N}} \mu_k$ a (**sequence space**) **Besov measure** on $\mathbb{R}^{\mathbb{N}}$ and write $B_1^s := \mu$. The corresponding **Besov space** is the weighted sequence space $(X_1^s, \|\cdot\|_{X_1^s}) := (\ell_\gamma^1, \|\cdot\|_{\ell_\gamma^1})$, i.e.

$$\|h\|_{X_1^s} := \sum_{k\in\mathbb{N}} k^{s/d-1/2}|h_k|$$

Besov-1 measures

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- One can perform the same construction in any separable Hilbert space instead of $\ell^2 \subset \mathbb{R}^{\mathbb{N}}$, considering random expansion w.r.t. a countable complete orthonormal basis.
- In the case of $L^2(\mathbb{T}^d;\mathbb{R})$ with the Fourier basis, X_1^s is the Besov space B_{11}^s (hence the name).

OM functionals for Besov-1 measures

- One thinks of B_1^s as having a formal Lebesgue density proportional to $\exp(-\| \cdot \|_{X_1^s})$ in the same way that $\mathcal{N}(0, C)$ has a formal density proportional to $\exp(-\frac{1}{2}\| C^{-1/2} \cdot \|^2)$.
- But is this actually true on the level of OM functionals?

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- But is this actually true on the level of OM functionals?

Lemma 17 (Support of a Besov-1 measure; Ayanbayev et al., 2022a, Lem. 5.10)

Let $\mu = B_1^s$ be the Besov measure defined above and $X = X_1^t = \ell_\delta^1$. Then $\mu(X) = 1$.

Proposition 18 (OM functional of a Besov-1 measure; Ayanbayev et al., 2022a, Prop. 5.11)

Let $\mu = B_1^s$ on the space $X = X_1^t = \ell_\delta^1$. Then property $M(\mu, X_1^s)$ is satisfied and the OM functional $I_\mu \colon X_1^t \to \overline{\mathbb{R}}$ of μ is given by

$$I_\mu(u) = \begin{cases} \|u\|_{X_1^s} & \text{for } u \in X_1^s, \\ \infty & \text{otherwise.} \end{cases}$$

OM functionals for Besov-1 measures

Theorem 19 (Γ-convergence and equicoercivity of Besov-1 OM functionals; Ayanbayev et al., 2022a, Thm. 5.13)

Let $\mu^{(n)} := B_1^{s^{(n)}}$, $n \in \mathbb{N} \cup \{+\infty\}$, be centered Besov measures such that $s^{(n)} \to s^{(\infty)}$. Then there exists $n_0 \in \mathbb{N}$ such that, for each $n \geqslant n_0$, $\mu^{(n)}(\ell^1_{\delta(\infty)}) = 1$ and we therefore consider these measures on $X = X_1^{t(\infty)} = \ell^1_{\delta(\infty)}$ (after dropping the first $n_0 - 1$ measures). Then the associated OM functionals $I_{\mu^{(n)}} = \| \cdot \|_{X_1^{s^{(n)}}} : X \to \overline{\mathbb{R}}$, $n \geqslant n_0$, are equicoercive and

$$I_{\mu^{(n)}} \xrightarrow[n \to \infty]{\Gamma} I_{\mu^{(\infty)}}.$$

- For emphasis: each of the measures $B_1^{s^{(n)}}$ is centred, with the origin being both the mean and the mode. Convergence of modes is therefore trivial.
- However, Γ-convergence of the OM functionals is not trivial — it is essential for the study of Γ-convergence of posterior OM functionals in the next step.

A sketch of some generalisations

- Besov-p measures with $1 \leqslant p \leqslant 2$ and mean $m \in X$
  - Infinite product of marginal densities $\propto \exp(-|\frac{u_k - m_k}{\gamma_k}|^p)$
  - OM functional is $\|u - m\|_{X_p^s}^p$ on $m + X_p^t$, with property $M(\mu, m + X_p^s)$. ✓
  - Γ-convergence and equicoercivity with respect to mean and smoothness. ✓
- Cauchy measures
  - Countable products of marginal densities $\propto \left(1 + |\frac{u_k - m_k}{\gamma_k}|\right)^{-1}$.
  - OM functional is $\sum_k \log(1 + \gamma_k^{-2}(u_k - m_k))$ with property $M(\mu, m + \ell_\gamma^2)$. ✓
  - Γ-convergence and equicoercivity with respect to location and scale parameters. ✓
- General scaled product measures
  - Countable products of marginal densities $\rho_k(u_u) \propto \rho_0\left(\frac{u_k - m_k}{\gamma_k}\right)$, with ρ_0 a "nice" reference density on $\mathbb{R}$
  - OM functional is more or less what it should be (lower bound is relatively straightforward, upper bound only in some cases, maximal domain and property M are also tricky. . .) ≈ ✓
  - Γ-convergence and equicoercivity with respect to location and scale parameters. ✓

Bayesian inverse problems

Bayesian inverse problems

- An inverse problem consists of the recovery of an unknown u from related observational data y. In the Bayesian approach to inverse problems (Kaipio and Somersalo, 2005; Stuart, 2010), these two objects are treated as coupled random variables $\boldsymbol{u}$ and $\boldsymbol{y}$ that take values in spaces X and Y respectively.
- A priori knowledge about $\boldsymbol{u}$ is represented by a prior probability measure $\mu_0 \in \mathcal{P}(X)$ and one is given access to a realisation y of $\boldsymbol{y}$. One also posits a likelihood model $\ell \colon X \to \mathcal{P}(Y)$.
- The solution of the BIP is, by definition, the posterior probability measure $\mu^y \in \mathcal{P}(X)$, i.e. the conditional distribution of $\boldsymbol{u}$ given that $\boldsymbol{y} = y$, or the disintegration of the joint distribution $\mu(\mathrm{d}u, \mathrm{d}y) \propto \mu_0(\mathrm{d}u)\ell(\mathrm{d}y|u)$ of $(\boldsymbol{u}, \boldsymbol{y})$ along the y-fibre (Chang and Pollard, 1997).

Bayesian inverse problems

- For simplicity, focus on the case that μ^y has a density with respect to μ_0 of the form

$$\mu^y(\mathrm{d}u) \propto \exp(-\Phi(u; y))\, \mu_0(\mathrm{d}u).$$

- The potential $\Phi \colon X \times Y \to \mathbb{R}$ encodes both the idealised relationship between the unknown and the data and statistical assumptions about any observational noise.
- Textbook example: X is a separable Hilbert or Banach space of functions, $Y = \mathbb{R}^J$ for some $J \in \mathbb{N}$, and that $\boldsymbol{y} = \mathcal{O}(\boldsymbol{u}) + \boldsymbol{\eta}$ for some deterministic observation map $\mathcal{O} \colon X \to Y$ and additive non-degenerate Gaussian noise $\boldsymbol{\eta} \sim \mathcal{N}(0, C_{\boldsymbol{\eta}})$ that is a priori independent of $\boldsymbol{u}$, in which case Φ is the familiar quadratic misfit

$$\Phi(u; y) = \frac{1}{2} \left\| C_{\boldsymbol{\eta}}^{-1/2} (y - \mathcal{O}(u)) \right\|^2.$$

Bayesian inverse problems

- So, on a hand-wavy level, the posterior $\mu^y(\mathrm{d}u) \propto \exp(-\Phi(u; y))\,\mu_0(\mathrm{d}u)$ has a "negative log-Lebesgue density"

$$-\log \rho^y(u) = \underbrace{\Phi(u; y)}_{\text{misfit}} \underbrace{- \log \rho_0(u)}_{\text{regularisation}}.$$

- In the case of a Gaussian prior $\mu_0 = \mathcal{N}(m_0, C_0)$, this is Tikhonov–Philips regularisation:

$$-\log \rho^y(u) = \Phi(u; y) + \frac{1}{2}\langle u, C_0^{-1} u\rangle.$$

- This is the connection between the Bayesian viewpoint and the regularised optimisation viewpoint on inverse problems:
  Minimisers of the posterior "negative log-Lebesgue density" ought to be regarded as "most probable points for μ^y".

MAP estimation for BIPs

Consequences for MAP estimation in BIPs

- In view of the earlier discussion, we can be more rigorous in our statements about MAP estimators.
- We want to be able to define “MAP estimator” to mean “global weak mode of the posterior”. . .

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  ...that the OM functional of the posterior is Φ plus the OM functional of the prior...
  ...and that the MAP estimators are stable under suitable continuous convergence / Γ-convergence / equicoercivity assumptions on Φ and I_{μ_0}.
- And this is indeed what we can show!

Skip the formal statement of the theorem ▶

Transfer of property M, Γ-convergence, equicoercivity, etc.

Theorem 20 (Ayanbayev et al. (2022a, Theorem 6.1))

For each $n \in \mathbb{N} \cup \{\infty\}$, let $\mu_0^{(n)} \in \mathcal{P}(X)$ and let $\Phi^{(n)} \colon X \to \mathbb{R}$ be locally uniformly continuous. Suppose that, for each $n \in \mathbb{N} \cup \{\infty\}$

$$\mu^{(n)}(\mathrm{d}x) := \frac{1}{Z^{(n)}} e^{-\Phi^{(n)}(x)} \, \mu_0^{(n)}(\mathrm{d}x), \qquad Z^{(n)} := \int_X e^{-\Phi^{(n)}(x)} \, \mu_0^{(n)}(\mathrm{d}x) \in (0, \infty),$$

and each $\mu_0^{(n)}$ has an OM functional $I_{\mu_0^{(n)}} \colon E^{(n)} \to \mathbb{R}$. Then:

1. *Each $\mu^{(n)}$ has $I_{\mu^{(n)}} := \Phi^{(n)} + I_{\mu_0^{(n)}} \colon E^{(n)} \to \mathbb{R}$ as an OM functional.*
2. *Suppose that property $M(\mu_0^{(n)}, E^{(n)})$ holds. Then property $M(\mu^{(n)}, E^{(n)})$ also holds, and the global weak modes of $\mu_0^{(n)}$ (resp. of $\mu^{(n)}$) are the global minimisers of the extended OM functional $I_{\mu_0^{(n)}} \colon X \to \overline{\mathbb{R}}$ (resp. of $I_{\mu^{(n)}} \colon X \to \overline{\mathbb{R}}$).*
3. *If $I_{\mu_0^{(n)}} \xrightarrow[n\to\infty]{\Gamma} I_{\mu_0^{(\infty)}}$ and $\Phi^{(n)} \xrightarrow[n\to\infty]{\text{cts}} \Phi^{(\infty)}$ as $n \to \infty$, then $I_{\mu^{(n)}} \xrightarrow[n\to\infty]{\Gamma} I_{\mu^{(\infty)}}$.*

Transfer of property M, Γ-convergence, equicoercivity, etc.

Theorem 20 (Ayanbayev et al. (2022a, Theorem 6.1))

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and each $\mu_0^{(n)}$ has an OM functional $I_{\mu_0^{(n)}} \colon E^{(n)} \to \mathbb{R}$. Then:

4. *If $(I_{\mu_0^{(n)}})_{n \in \mathbb{N}}$ is equicoercive and the functions $\Phi^{(n)}$ are uniformly bounded from below by some constant $M \in \mathbb{R}$, then $(I_{\mu^{(n)}})_{n \in \mathbb{N}}$ is also equicoercive with respect to the same representatives of $I_{\mu^{(n)}}$ as for the Γ-convergence.*
5. *Under the assumptions of parts 2–4, the cluster points as $n \to \infty$ of the global weak modes of the posteriors $\mu^{(n)}$ are the global weak modes of the limiting posterior $\mu^{(\infty)}$.*

Consequences for BIPs

Consider a BIP with prior μ_0, potential Φ bounded below, and observed data y, each of which may now be approximated. In addition to the assumptions of Theorem 20, assume for simplicity that I_{μ_0} is lower semicontinuous, so that it equals its own Γ-limit.

- If the potential Φ and prior μ_0 are held constant and we examine the posterior $\mu^{(n)}$ associated to data $y^{(n)}$, then

$$\Phi(\,\cdot\,; y^{(n)}) \xrightarrow[n\to\infty]{\text{cts}} \Phi(\,\cdot\,; y) \implies \begin{cases} I_{\mu^{(n)}} \xrightarrow[n\to\infty]{\Gamma} I_{\mu} \text{ and} \\ (I_{\mu^{(n)}})_{n\in\mathbb{N}} \text{ is equicoercive} \end{cases}$$

$$\implies \text{convergence of MAP estimators (up to subsequences)}$$

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- If the data y and potential Φ are held constant and we examine the posterior $\mu^{(n)}$ associated to prior $\mu_0^{(n)}$, then

$$\left.\begin{array}{c} I_{\mu_0^{(n)}} \xrightarrow[n\to\infty]{\Gamma} I_{\mu_0} \text{ and} \\ (I_{\mu_0^{(n)}})_{n\in\mathbb{N}} \text{ is equicoercive} \end{array}\right\} \implies \left\{\begin{array}{c} I_{\mu^{(n)}} \xrightarrow[n\to\infty]{\Gamma} I_{\mu} \text{ and} \\ (I_{\mu^{(n)}})_{n\in\mathbb{N}} \text{ is equicoercive} \end{array}\right.$$

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Consequences for BIPs

Consider a BIP with prior μ_0, potential Φ bounded below, and observed data y, each of which may now be approximated. In addition to the assumptions of Theorem 20, assume for simplicity that I_{μ_0} is lower semicontinuous, so that it equals its own Γ-limit.

- Finally, if the data and prior are held constant and we examine the posterior $\mu^{(n)}$ associated to the potential $\Phi^{(n)}$, then

$$\Phi^{(n)}(\cdot\,;y) \xrightarrow[n\to\infty]{\text{cts}} \Phi(\cdot\,;y) \implies \begin{cases} I_{\mu^{(n)}} \xrightarrow[n\to\infty]{\Gamma} I_\mu \text{ and} \\ (I_{\mu^{(n)}})_{n\in\mathbb{N}} \text{ is equicoercive} \end{cases}$$

$$\implies \text{convergence of MAP estimators (up to subsequences)}$$

In particular, this holds when the approximate misfit/potential $\Phi^{(n)}$ arises through projection, e.g. Galerkin discretisation.

Closing remarks

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- We have established a stability theory for non-parametric MAP estimators by focussing on global weak modes, which are characterised as minimisers of extended Onsager–Machlup functionals, and then studying the variational Γ-convergence of these functionals.
- Our analysis encompasses Bayesian posteriors associated to Gaussian, Besov, and Cauchy priors and reveals simple sufficient conditions for stability of MAP estimators (continuous convergence of log-likelihoods, Γ-convergence and equicoercivity of prior OM functionals).
- These conditions could be added to the now-standard conditions for stability of the BIP à la Stuart (2010) to ensure stability of *both* the BIP and the MAP estimation problem. (There are hypotheses that imply both BIP stability and MAP stability, but the BIP and MAP stability assumptions are generally independent.)
- Open problems / avenues for further work:
  - Unfortunately Γ-convergence + equicoercivity alone cannot deliver a convergence rate for the modes!
  - Other classes of priors, e.g. hierarchical and deep priors, priors on non-linear spaces such as shape spaces, etc.

Thank You!

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