Bayesian inference in imaging inverse problems - Part 1

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- 3 Bayesian computation based on SDEs and proximal optimisation
- 4 Empirical Bayes MAP estimation with unknown regularisation parameters
- 5 Conclusion

Forward imaging problem



True scene



Imaging device



Observed image

Inverse imaging problem



True scene



Imaging device



Observed image



Restored image

- We are interested in an unknown image $x^* \in \mathbb{R}^d$.
- We measure $y \in Y$, related to x^* by some mathematical model.
- For example, in many imaging problems

$$y = Ax^* + w,$$

for some operator A that is poorly conditioned or rank deficient, and an unknown perturbation or "noise" w.

• The recovery of x^* from y is usually not well posed. Additional information is required in order to deliver meaningful solutions.

- There are three main mathematical and computational frameworks for inference in imaging inverse problems:
 - Mathematical analysis
 - 2 Bayesian statistics.
 - Machine learning.
- These frameworks have complementary strengths and weaknesses.
- Our aim is to develop a unifying framework of theory, methods, and algorithms that inherits the benefits of each approach.

- Model x^{*} as a realisation of a r.v. x on R^d. Use the distribution of x to regularise the problem and promote expected properties.
- The observation y is a realisation of a r.v. $(y|x = x^*)$.
- Inferences about x^{*} from y are derived from the joint distribution of (x, y) specified via the decomposition p(x, y) = p(y|x)p(x).

The Bayesian framework

The decomposition p(x, y) = p(y|x)p(x) has two key ingredients:

The likelihood function: the conditional distribution p(y|x) that models the data observation process (forward model).

The prior function: the marginal distribution $p(x) = \int p(x, y) dy$ that models our knowledge about the solution x.

For example, for y = Ax + w, with $w \sim \mathcal{N}(0, \sigma^2 \mathbb{I})$, we have

$$y \sim \mathcal{N}(Ax, \sigma^2 \mathbb{I}),$$

or equivalently

$$p(y|x) \propto \exp\{-\|y - Ax\|_2^2/2\sigma^2\}.$$

Prior distribution

For this tutorial, we assume a prior distribution of the form:

$$p(x) = \frac{1}{Z(\theta)} e^{-\theta^{\mathsf{T}} \psi(x)} \mathbf{1}_{\Omega}(x),$$

for some statistic $\psi : \mathbb{R}^d \to \mathbb{R}^m$, $\theta \in \mathbb{R}^m$, and constraint set $\Omega \subset \mathbb{R}^d$.

Often ψ and Ω are convex on \mathbb{R}^d and p(x) is log-concave.

The normalising constant $Z(\theta)$ is given by

$$Z(\theta) = \int_{\Omega} \mathrm{e}^{-\theta^{\mathsf{T}}\psi(x)} \mathrm{d}x,$$

so $\int_{\Omega} p(x) dx = 1$. This will play a key role in model selection techniques.

The statistic ψ can be assumption-driven (e.g., a sparsity promoting norm), purely data-driven, or a combination of both.

We base our inferences on the posterior distribution p(x|y).

We derive p(x|y) from the likelihood p(y|x) and the prior p(x) by using

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$

where $p(y) = \int p(y|x)p(x)dx$ measures model-fit-to-data.

The conditional p(x|y) models our beliefs about x after observing y = y. In this first tutorial, we consider that p(x|y) is log-concave; i.e.,

$$p(x|y) = \exp\left\{-\phi(x)\right\} / \int \exp\left\{-\phi(x)\right\} dx,$$

where $\phi(x)$ is a convex function on \mathbb{R}^d .

Illustrative example: astronomical image reconstruction

Recover $x \in \mathbb{R}^d$ from low-dimensional degraded observation

 $y = M\mathcal{F}x + w,$

where \mathcal{F} is the continuous Fourier transform, $M \in \mathbb{C}^{m \times d}$ is a measurement operator, Ψ is a wavelet basis, and $w \sim \mathcal{N}(0, \sigma^2 \mathbb{I}_m)$. We use the model

$$p(x|y) \propto \exp\left(-\|y - M\mathcal{F}x\|^2/2\sigma^2 - \theta\|\Psi x\|_1\right) \mathbf{1}_{\mathbb{R}^n_+}(x). \tag{1}$$



Figure: Radio-interferometric measurements of the W28 supernova.

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The predominant Bayesian approach in imaging is MAP estimation

$$\hat{x}_{MAP} = \operatorname*{argmax}_{x \in \mathbb{R}^d} p(x|y),$$

=
$$\operatorname*{argmin}_{x \in \mathbb{R}^d} \phi(x).$$
 (2)

When p(x|y) is log-concave, \hat{x}_{MAP} is a convex optimisation problem. We are usually able to solve convex problems very efficiently (see Chambolle and Pock (2016)).

See, e.g., Chambolle and Pock (2016) for more details.

MAP estimation by proximal optimisation

To compute \hat{x}_{MAP} we could use a proximal splitting algorithm. Let

$$f(x) = \|y - M\mathcal{F}x\|^2/2\sigma^2, \quad \text{and} \quad g(x) = \theta \|\Psi x\|_1 + -\log \mathbf{1}_{\mathbb{R}^n_+}(x),$$

where f and g are l.s.c. convex on \mathbb{R}^d , and f is L_f -Lipschitz differentiable.

For example, we could use a proximal gradient iteration

$$x^{m+1} = \operatorname{prox}_{g}^{L_{f}^{-1}} \{ x^{m} + L_{f}^{-1} \nabla f(x^{m}) \},$$

converges to \hat{x}_{MAP} at rate O(1/m), with poss. acceleration to $O(1/m^2)$.

Definition For $\lambda > 0$, the λ -proximal operator of a convex l.s.c. function g is defined as (Moreau, 1962)

$$\operatorname{prox}_{g}^{\lambda}(x) \triangleq \operatorname{argmin}_{u \in \mathbb{R}^{\mathbb{N}}} g(u) + \frac{1}{2\lambda} ||u - x||^{2}.$$

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 $p(x|y) \propto \exp\left(-\|y - M\mathcal{F}x\|^2/2\sigma^2 - \theta\|\Psi x\|_1\right) \mathbf{1}_{\mathbb{R}^n_+}(x). \tag{3}$



Figure: Radio-interferometric image reconstruction of the W28 supernova.

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- Modern convex optimisation can compute \hat{x} very efficiently...
- With parallelised and distributed algorithms...
- With theoretical convergence guarantees..
- And GPU implementations...
- With data-driven flavours based on input convex neural networks..
- Also non-convex extensions...

So the problem is quite solved, right?

Not really...



Elephant 1: what is the uncertainty about \hat{x} ?



How confident are we about all these structures in the image? What is the error in their intensity, position, spectral properties? Using \hat{x}_{MAP} to derive physical quantities? what error bars should we put...

Illustrative example: magnetic resonance imaging

We use very similar techniques to produce magnetic resonance images...



Ŷ



 \hat{x} (zoom)

Figure: Magnetic resonance imaging of brain lession.

How can we quantify our uncertainty about the brain lesion in the image?

Illustrative example: magnetic resonance imaging

What about this other solution to the problem, with no lesion?



 \hat{x}'



 \hat{x}' (zoom)

Figure: Magnetic resonance imaging of brain lession.

Do we have any arguments to reject this solution?

Another example related to sparse super-resolution in live-cell microscopy



Figure: Live-cell microscopy data (Zhu et al., 2012).

The image is sharpened to enhance molecule position measurements, but what is the precision of the procedure?

Two imaging scientists often formulate different models/cost functions to recover \boldsymbol{x}

$$\hat{x}_{1} = \underset{x \in \mathbb{R}^{d}}{\operatorname{argmin}} \|y - A_{1}x\|_{2}^{2} + \theta_{1}h_{1}(x),$$

$$\hat{x}_{2} = \underset{x \in \mathbb{R}^{d}}{\operatorname{argmin}} \|y - A_{2}x\|_{2}^{2} + \theta_{2}h_{2}(x),$$
(4)

How can we compare them without ground truth available?

Can we use several models simultaneously?

Some of the model parameters might also be unknown; e.g., $\theta \in \mathbb{R}^+$ in

$$\hat{x}_1 = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \|y - A_1 x\|_2^2 + \frac{\theta}{h_1}(x).$$
(5)

Then θ parametrises a class of models for $y \to x$.

How can we select θ without using ground truth?

Could we use all models simultaneously?

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Given the following elements defining a decision problem:

- $\bullet \quad \text{Decision space } \Delta$
- **②** Loss function $L(\delta, x) : \Delta \times \mathbb{R}^d \to \mathbb{R}$ quantifying the loss (or profit) related to taking action $\delta \in \Delta$ when the truth is $x \in \mathbb{R}^d$.
- **③** A model p(x) representing probabilities for x.

What is the optimal decision $\delta^* \in \Delta$ when x is unknown?

Given the following elements defining a decision problem:

- Decision space Δ
- ② Loss function $L(\delta, x) : \Delta \times \mathbb{R}^d \to \mathbb{R}$ quantifying the loss (or profit) related to taking action $\delta \in \Delta$ when the truth is $x \in \mathbb{R}^d$.
- **③** A probability model p(x) representing knowledge about x.

According to Bayesian decision theory (Robert, 2001), the optimal decision under uncertainty is

$$\delta^* = \operatorname*{argmin}_{\delta \in \Delta} \mathrm{E}\{L(\delta, \mathbf{x}) | y\} = \operatorname*{argmin}_{\delta \in \Delta} \int L(\delta, x) p(x) \mathrm{d}x.$$

Bayesian point estimators arise from the decision "what point $\hat{x} \in \mathbb{R}^d$ summarises x|y best?". The optimal decision under uncertainty is

$$\hat{x}_{L} = \operatorname*{argmin}_{u \in \mathbb{R}^{d}} \mathrm{E}\{L(u, \mathbf{x}) | y\} = \operatorname*{argmin}_{u \in \mathbb{R}^{d}} \int L(u, x) p(x|y) \mathrm{d}x$$

where the loss L(u, x) measures the "dissimilarity" between u and x.

General desiderata:

•
$$L(u,x) \ge 0, \forall u, x \in \mathbb{R}^d$$
,

$$L(u,x) = 0 \iff u = x,$$

Solution L strictly convex w.r.t. its first argument (for estimator uniqueness).

Example: the squared Euclidean distance $L(u, x) = ||u - x||^2$ defines the so-called minimum mean squared error estimator.

$$\hat{x}_{MMSE} = \underset{u \in \mathbb{R}^d}{\operatorname{argmin}} \int \|u - x\|_2^2 p(x|y) dx.$$

By differentiating w.r.t. to u and equating to zero we obtain that

$$\int (\hat{x}_{MMSE} - x) p(x|y) dx = 0 \implies \hat{x}_{MMSE} \int p(x|y) dx = \int x p(x|y) dx,$$

hence $\hat{x}_{MMSE} = \mathbb{E}\{x|y\}$ (recall that $\int p(x|y)dx = 1$).

What about the MAP estimator?

Assume that $p(x|y) \propto \exp\{-\phi_y(x)\}$ is log-concave, i.e., ϕ_y convex on \mathbb{R}^d .

The Bayesian estimator that minimises the Bregman divergence loss $L(u,x) = D_{\phi}(u,x) \triangleq \phi(u) - \phi(x) - \nabla \phi(x)(u-x)$, is the MAP estimator

$$\hat{x}_{L} = \underset{u \in \mathbb{R}^{d}}{\operatorname{argmin}} \operatorname{E}\{L(u, \mathbf{x})|y\} = \underset{u \in \mathbb{R}^{d}}{\operatorname{argmin}} \int D_{\phi}(u, x)p(x|y)dx$$
$$= \underset{x \in \mathbb{R}^{d}}{\operatorname{argmin}} p(x|y),$$
$$= \underset{x \in \mathbb{R}^{d}}{\operatorname{argmin}} -\phi_{y}(x),$$
$$= \hat{x}_{MAP}$$
(6)

Interestingly, the "dual" estimator is \hat{x}_{MMSE} , i.e.,

$$\hat{x}_{L} = \underset{u \in \mathbb{R}^{d}}{\operatorname{argmin}} \operatorname{E}\{L(x, \underline{x})|y\} = \underset{u \in \mathbb{R}^{d}}{\operatorname{argmin}} \int D_{\phi}(x, u) p(x|y) \mathrm{d}x$$

$$= \hat{x}_{MMSE}$$
(7)

See Pereyra (2019) for proof and details.

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Where does the posterior probability mass of x lie?

A set C_{α} is a posterior credible region of confidence level $(1 - \alpha)$ % if

$$\mathbf{P}\left[\mathbf{x}\in C_{\alpha}|\boldsymbol{y}\right]=1-\alpha.$$

For any $\alpha \in (0, 1)$ there are infinitely many regions of the parameter space that verify this property.

The *highest posterior density* (HPD) region is decision-theoretically optimal in a compactness sense

 $C_{\alpha}^{*} = \{x : \phi(x) \leq \gamma_{\alpha}\}$

with $\gamma_{\alpha} \in \mathbb{R}$ chosen such that $\int_{C_{\alpha}^{*}} p(x|y) dx = 1 - \alpha$ holds.

Hypothesis test split the solution space in two meaningful regions, e.g.,

$$H_0: x \in \mathcal{S}$$
$$H_1: x \notin \mathcal{S}$$

where $S \subset \mathbb{R}^d$ contains all solutions with some characteristic of interest.

We can then assess the degree of support for H_0 vs. H_1 by computing

$$P(H_0|y) = \int_{\mathcal{S}} p(x|y) dx, \quad P(H_1|y) = 1 - P(H_0|y).$$

We can also reject H_0 in favour of H_1 with significance $\alpha \in [0,1]$ if

 $\mathsf{P}(\mathrm{H}_0|y) \leq \alpha.$

The Bayesian framework provides theory for comparing models objectively.

Given K alternative models $\{\mathcal{M}_j\}_{j=1}^K$ with posterior densities

$$\mathcal{M}_j: \quad p_j(x|y) = p_j(y|x)p_j(x))/p_j(y),$$

we compute the (marginal) posterior probability of each model, i.e.,

$$p(\mathcal{M}_j|y) \propto p(y|\mathcal{M}_j)p(\mathcal{M}_j)$$
(8)

where $p(y|\mathcal{M}_j) \triangleq p_j(y) = \int p_j(y|x)p_j(x)dx$ measures model-fit-to-data.

We then select for our inferences the "best" model, i.e.,

$$\mathcal{M}^* = \operatorname*{argmax}_{j \in \{1, \dots, K\}} p(\mathcal{M}_j | y).$$

Alternatively, given a continuous class of models $\{\mathcal{M}_{\theta}, \theta \in \theta\}$ with

$$\mathcal{M}_{\boldsymbol{\theta}}: \quad p(\boldsymbol{x}|\boldsymbol{y},\boldsymbol{\theta}) = \frac{p(\boldsymbol{y}|\boldsymbol{x},\boldsymbol{\theta})p(\boldsymbol{x}|\boldsymbol{\theta})}{p(\boldsymbol{y}|\boldsymbol{\theta})},$$

we compute the (marginal) posterior

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}$$
(9)

where $p(y|\theta) = \int p(y|x,\theta)p(x|\theta)dx$ measures model-fit-to-data.

We then calibrate our model with the "best" value of θ , i.e.,

$$\hat{\theta}_{MAP} = \underset{\theta \in \Theta}{\operatorname{argmax}} p(\theta|y).$$

We can also use all models simultaneously!

Given K alternative models $\{\mathcal{M}_j\}_{j=1}^K$ with posterior densities

$$\mathcal{M}_j: \quad p_j(x|y) = p_j(y|x)p_j(x))/p_j(y),$$

we marginalise w.r.t. the model selector j, i.e.,

$$p(x|y) = \sum_{j=1}^{K} p(x, \mathcal{M}_j|y) = \sum_{j=1}^{K} \frac{p(x|y, \mathcal{M}_j)p(\mathcal{M}_j|y)}{(\mathcal{M}_j|y)}$$
(10)

where the posterior probabilities $p(\mathcal{M}_j|y)$ control the relative importance of each model.

Similarly, given a continuous class of models $\{\mathcal{M}_{\theta}, \theta \in \Theta\}$ with

$$\mathcal{M}_{\boldsymbol{\theta}}: \quad p(\boldsymbol{x}|\boldsymbol{y},\boldsymbol{\theta}) = \frac{p(\boldsymbol{y}|\boldsymbol{x},\boldsymbol{\theta})p(\boldsymbol{x}|\boldsymbol{\theta})}{p(\boldsymbol{y}|\boldsymbol{\theta})},$$

and a prior $p(\theta)$, we marginalise θ

$$p(x|y) = \int_{\Theta} p(x,\theta|y) d\theta,$$
$$= \int_{\Theta} p(x|y,\theta) p(\theta|y) d\theta$$

where again $p(\theta|y)$ controls the relative contribution of each model.

Log-concave priors regularise the inverse problem by promoting solutions for which $\psi(x)$ is close to its expectation $E(\psi|\theta)$, controlled by $\theta \in \mathbb{R}^p$.

Formally, when ψ is convex we have concentration of probability mass on the typical set (see Bobkov and Madiman (2011))

$$\mathbf{P}\{\|\psi(\mathbf{x}) - \mathbf{E}(\psi|\theta)\| > \eta|\theta\} < 3\exp\{-\eta^2 d/16\}, \quad \forall \eta \in (0,2)$$
(11)

Moreover, by differentiating $Z(\theta)$ and using Leibniz integral rule

$$E(\psi(\mathbf{x})|\theta) = \int_{\Omega} \psi(x) p(x) dx = -\nabla_{\theta} \log Z(\theta),$$
(12)

hence $p(x|\theta)$ softly constrains $\psi(x) \approx -\nabla_{\theta} \log Z(\theta)$ when *d* is large.

 $Z(\theta)$ is strongly log-concave, hence $\nabla_{\theta} \log Z(\theta)$ spans \mathbb{R}^{p} (think duality).

For example, priors of the form

$$p(x) \propto \mathrm{e}^{-\theta \|Bx\|_{\dagger}},$$

for some basis or dictionary $W \in \mathbb{R}^{d imes p}$ and norm $\| \cdot \|_{\dagger}$, are encoding

$$\mathrm{E}(\|B\mathbf{x}\|_{\dagger}|\theta) = \frac{d}{\theta}.$$

See Pereyra et al. (2015); Fernandez-Vidal and Pereyra (2018) for more details and other examples.
- The Bayesian statistical paradigm provides a power mathematical framework to solve imaging problems...
- It allows deriving optimal estimators for x..
- As well as quantifying the uncertainty in the solutions delivered...
- It supports hypothesis tests to inform decisions and conclusions...
- And allows operating with partially unknown models...
- And with several competing models...

So the problem is quite solved, right?

Not really...



How do we compute all these probabilities?

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Monte Carlo integration

Given a set of samples X_1, \ldots, X_M distributed according to p(x|y), we approximate posterior expectations and probabilities

$$\frac{1}{M}\sum_{m=1}^M h(X_m) \to \mathrm{E}\{h(\mathbf{x})|y\}, \quad \text{as } M \to \infty$$

Markov chain Monte Carlo:

Construct a Markov kernel $X_{m+1}|X_m \sim K(\cdot|X_m)$ such that the Markov chain X_1, \ldots, X_M has p(x|y) as stationary distribution.

MCMC simulation in high-dimensional spaces is very challenging.

Suppose for now that $p(x|y) \in C^1$. Then, we can generate samples by mimicking a Langevin diffusion process that converges to p(x|y) as $t \to \infty$,

$$\boldsymbol{X}: \quad \mathrm{d}\boldsymbol{X}_t = \nabla \log p\left(\boldsymbol{X}_t | y\right) \mathrm{d}t + \sqrt{2} \mathrm{d}W_t, \quad 0 \leq t \leq T, \quad \boldsymbol{X}(0) = x_0.$$

where W is the Brownian motion on \mathbb{R}^d .

Because solving X_t exactly is generally not possible, we use an Euler Maruyama approximation and obtain the "unadjusted Langevin algorithm"

ULA:
$$X_{m+1} = X_m + \delta \nabla \log p(X_m|y) + \sqrt{2\delta}Z_{m+1}, \quad Z_{m+1} \sim \mathcal{N}(0, \mathbb{I}_n)$$

ULA is remarkably efficient when p(x|y) is sufficiently regular.

Unfortunately, imaging models often violate these regularity conditions.

Without loss of generality, suppose that

$$p(x|y) \propto \exp\left\{-f(x) - g(x)\right\}$$
(13)

where f(x) and g(x) are l.s.c. convex functions from $\mathbb{R}^d \to (-\infty, +\infty]$, f is L_f -Lipschitz differentiable, and $g \notin C^1$.

For example,

$$f(x) = \frac{1}{2\sigma^2} \|y - Ax\|_2^2, \quad g(x) = \alpha \|Bx\|_{\dagger} + \mathbf{1}_{\mathcal{S}}(x),$$

for some linear operators A, B, norm $\|\cdot\|_{\dagger}$, and convex set S. Unfortunately, such non-models are beyond the scope of ULA.

Idea: Regularise p(x|y) to enable efficient Langevin sampling.

Moreau-Yoshida approximation of p(x|y) (Pereyra, 2015):

Let $\lambda > 0$. We propose to approximate p(x|y) with the density

$$p_{\lambda}(x|y) = \frac{\exp[-f(x) - g_{\lambda}(x)]}{\int_{\mathbb{R}^d} \exp[-f(x) - g_{\lambda}(x)] dx},$$

where g_{λ} is the Moreau-Yoshida envelope of g given by

$$g_{\lambda}(x) = \inf_{u \in \mathbb{R}^d} \{g(u) + (2\lambda)^{-1} \|u - x\|_2^2\},\$$

and where λ controls the approximation error involved.

Moreau-Yoshida approximations

Key properties (Pereyra, 2015; Durmus et al., 2018):

- **(**) $\forall \lambda > 0$, p_{λ} defines a proper density of a probability measure on \mathbb{R}^d .
- Onvexity and differentiability:
 - p_{λ} is log-concave on \mathbb{R}^d .
 - $p_{\lambda} \in \mathcal{C}^1$ even if p not differentiable, with

 $\nabla \log p_{\lambda}(x|y) = -\nabla f(x) + \{\operatorname{prox}_{g}^{\lambda}(x) - x\}/\lambda,$

and $\operatorname{prox}_{g}^{\lambda}(x) = \operatorname{argmin}_{u \in \mathbb{R}^{\mathbb{N}}} g(u) + \frac{1}{2\lambda} ||u - x||^{2}$.

• $\nabla \log p_{\lambda}$ is Lipchitz continuous with constant $L \leq L_f + \lambda^{-1}$.

Solution Approximation error between $p_{\lambda}(x|y)$ and p(x|y):

- $\lim_{\lambda \to 0} \|p_{\lambda} p\|_{TV} = 0.$
- If g is L_g -Lipchitz, then $||p_{\lambda} p||_{TV} \le \lambda L_g^2$.

Examples of Moreau-Yoshida approximations:



Figure: True densities (solid blue) and approximations (dashed red).

We approximate \boldsymbol{X} with the "regularised" auxiliary Langevin diffusion

$$\boldsymbol{X}^{\lambda}: \quad \mathrm{d} \boldsymbol{X}^{\lambda}_t = \nabla \log \boldsymbol{p}_{\lambda} \left(\boldsymbol{X}^{\lambda}_t | \boldsymbol{y} \right) \mathrm{d} t + \sqrt{2} \mathrm{d} W_t, \quad 0 \leq t \leq T, \quad \boldsymbol{X}^{\lambda}(0) = x_0,$$

which targets $p_{\lambda}(x|y)$. Remark: we can make \mathbf{X}^{λ} arbitrarily close to \mathbf{X} .

Finally, an Euler Maruyama discretisation of \pmb{X}^{λ} leads to the (Moreau-Yoshida regularised) proximal ULA

 $MYULA: \quad X_{m+1} = (1 - \frac{\delta}{\lambda})X_m - \delta \nabla f\{X_m\} + \frac{\delta}{\lambda} \operatorname{prox}_g^{\lambda}\{X_m\} + \sqrt{2\delta}Z_{m+1},$

where we used that $\nabla g_{\lambda}(x) = \{x - \operatorname{prox}_{g}^{\lambda}(x)\}/\lambda$.

Non-asymptotic estimation error bound

Theorem 3.1 (Durmus et al. (2018))

Let $\delta_{\lambda}^{max} = (L_1 + 1/\lambda)^{-1}$. Assume that g is Lipchitz continuous. Then, there exist $\delta_{\epsilon} \in (0, \delta_{\lambda}^{max}]$ and $M_{\epsilon} \in \mathbb{N}$ such that $\forall \delta < \delta_{\epsilon}$ and $\forall M \ge M_{\epsilon}$

$$\|\delta_{x_0} Q_{\delta}^M - p\|_{TV} < \epsilon + \lambda L_g^2,$$

where Q_{δ}^{M} is the kernel assoc. with *M* iterations of MYULA with step δ .

Note 1: δ_{ϵ} and M_{ϵ} are explicit and tractable. If f + g is strongly convex outside some ball, then M_{ϵ} scales with order $\mathcal{O}(d \log(d))$. See Durmus et al. (2018) for other convergence results.

Illustrative example 1

Three toy models:



Figure: True densities (blue) and MC approximations (red histogram).

Illustrative example 2: radio-interferometric imaging

Astro-imaging experiment with redundant wavelet frame (Cai et al., 2017).



 $\hat{x}_{penMLE}(y)$



 $\hat{x}_{penMLE}(y)$



 $\hat{x}_{MMSE} = \mathrm{E}(x|y)$



 $\hat{x}_{MMSE} = \mathrm{E}(x|y)$



credible intervals (scale 10×10)



credible intervals (scale 10×10)

3C2888 and M31 radio galaxies (size 256×256 pixels).

Bayesian Uncertainty quantification

Where does the posterior probability mass of x lie?

• A set C_{α} is a posterior credible region of confidence level $(1 - \alpha)$ % if

$$\mathbf{P}\left[\mathbf{x}\in C_{\alpha}|y\right]=1-\alpha.$$

• The *highest posterior density* (HPD) region is decision-theoretically optimal (Robert, 2001)

$$C^*_{\alpha} = \{x : \phi(x) \le \gamma_{\alpha}\}$$

with $\gamma_{\alpha} \in \mathbb{R}$ chosen such that $\int_{C_{\alpha}^{*}} p(x|y) dx = 1 - \alpha$ holds.

- Given a set of samples X_1, \ldots, X_M distributed according to p(x|y), we can estimate γ_{α} from (sample) quantiles of $\phi(X_1), \ldots, \phi(X_M)$.
- Alternatively, we can compute a bound $\gamma_{\alpha} \leq \tilde{\gamma}_{\alpha}(\hat{x}_{MAP})$ analytically by using probability concentration results. See Pereyra (2016).

Bayesian Uncertainty quantification

Bayesian hypothesis test for specific image structures (e.g., lesions)

- $\mathrm{H}_{0}: \mathrm{The}\ \mathrm{structure}\ \mathrm{of}\ \mathrm{interest}\ \mathrm{is}\ \mathrm{ABSENT}\ \mathrm{in}\ \mathrm{the}\ \mathrm{true}\ \mathrm{image}$
- $\mathrm{H}_{1}:$ The structure of interest is PRESENT in the true image

The null hypothesis H_0 is rejected with significance α if

 $\mathsf{P}(\mathrm{H}_0|y) \leq \alpha.$

Theorem (Repetti et al., 2018)

Let S denote the region of \mathbb{R}^d associated with H_0 , containing all images without the structure of interest. Then

 $\mathcal{S} \cap \mathcal{C}_{\alpha} = \emptyset \implies \mathsf{P}(H_0|y) \leq \alpha$.

If in addition S is convex, then checking $S \cap C_{\alpha} = \emptyset$ is a convex problem

$$\min_{\bar{x},\underline{x}\in\mathbb{R}^d}\|\bar{x}-\underline{x}\|_2^2 \quad \text{s.t.} \quad \bar{x}\in\mathcal{C}_\alpha\,, \quad \underline{x}\in\mathcal{S}\,.$$

Uncertainty quantification in MRI imaging



MRI experiment: test images $\bar{x} = \underline{x}$, hence we fail to reject H_0 and conclude that there is little evidence to support the observed structure.

Uncertainty quantification in MRI imaging



MRI experiment: test images $\bar{x} \neq \underline{x}$, hence we reject H_0 and conclude that there is significant evidence in favour of the observed structure.

Uncertainty quantification in radio-interferometric imaging

Quantification of minimum energy of different energy structures, at level $(1 - \alpha) = 0.99$, as the number of measurements $T = \dim(y)/2$ increases.



Figure: Analysis of 3 structures in the W28 supernova RI image.

Note: energy ratio calculated as

$$\rho_{\alpha} = \frac{\|\bar{x} - \underline{x}\|_2}{\|x_{MAP} - \tilde{x}_{MAP}\|_2}$$

where \bar{x}, \underline{x} are computed with $\alpha = 0.01$, and \tilde{x}_{MAP} is a modified version of x_{MAP} where the structure of interest has been carefully removed from the image.

M. Pereyra

The Bayesian framework provides theory for comparing models objectively.

Given K alternative models $\{\mathcal{M}_j\}_{j=1}^K$ with posterior densities

$$\mathcal{M}_j: \quad p_j(x|y) = p_j(y|x)p_j(x))/p_j(y),$$

we compute the (marginal) posterior probability of each model, i.e.,

$$p(\mathcal{M}_j|y) \propto p(y|\mathcal{M}_j)p(\mathcal{M}_j)$$
(14)

where $p(y|\mathcal{M}_j) \triangleq p_j(y) = \int p_j(y|x)p_j(x)dx$ measures model-fit-to-data.

We then select for our inferences the "best" model, i.e.,

$$\mathcal{M}^* = \operatorname*{argmax}_{j \in \{1, \dots, K\}} p(\mathcal{M}_j | y).$$

Experiment setup

We degrade the Boat image of size 256×256 pixels with a 5×5 uniform blur operator A^* and Gaussian noise $w \sim \mathcal{N}(0, \sigma^2 \mathbb{I}_N)$ with $\sigma = 0.5$.

$$y = A^* x + w$$

We consider four alternative models to estimate x, given by

$$\mathcal{M}_j: \quad p_j(x|y) \propto \exp\left[-(\|y - A_j x\|^2 / 2\sigma^2) - \beta_j \phi_j(x)\right]$$
(15)

with fixed hyper-parameters σ and β , and where:

- \mathcal{M}_1 : A_1 is the correct blur operator and $\phi_j(x) = TV(x)$.
- \mathcal{M}_2 : A_2 is a mildly misspecified blur operator and $\phi_j(x) = TV(x)$.
- \mathcal{M}_3 : A_3 is the correct blur operator and $\phi_j(x) = \|\Psi x\|_1$.
- \mathcal{M}_4 : A_4 is a mildly misspecified blur operator and $\phi_j(x) = ||\Psi x||_1$.

where Ψ is a wavelet frame and $TV(x) = \|\nabla_d x\|_{1-2}$ is the total-variation pseudo-norm. The β_j are adjusted automatically (see model calibration).

To perform model selection we use MYULA to approximate the posterior probabilities $p(M_j|y)$ for j = 1, 2, 3, 4 by Monte Carlo integration.

For each model we generate $n = 10^5$ samples $\{X_k^j\}_{k=1}^n \sim p(x|y, \mathcal{M}_j)$ and use the truncated harmonic mean estimator

$$p(y|\mathcal{M}_j) \approx \left(\sum_{k=1}^n \frac{\mathbf{1}_{\mathcal{S}^{\star}}(X_k^M)}{p(X_k^M, y|\mathcal{M}_j)}\right)^{-1} \operatorname{vol}(\mathcal{S}^{\star}), \quad j = \{1, 2, 3, 4\}$$
(16)

where S^* is a union of HPDs of $p(x|y, \mathcal{M}_j)$, also estimated from $\{X_k^j\}_{k=1}^n$. Computing time approx. 30 minutes per model.

MYULA can also be used within a nested sampling scheme that provides a faster and more reliable estimation of $p(y|\mathcal{M}_i)$. See Cai et al. (2022).

Numerical results

We obtain that $p(\mathcal{M}_1|y) \approx 0.68$ and $p(\mathcal{M}_3|y) \approx 0.27$ with the correct blur are the best models, $p(\mathcal{M}_2|y) < 0.05$ and $p(\mathcal{M}_4|y) < 0.01$ perform poorly.



Figure: MAP estimation results for the Boat image deblurring experiment. (Note: error w.r.t. "exact" probabilities from Px-MALA approx. 0.5%.)

MYULA and Px-MALA efficiency comparison:



Figure: (a) Convergence of the chains to the typical set of x|y under model \mathcal{M}_1 , (b) chain autocorrelation function (ACF).)

- ULA samplers are based on a simple Euler-Maruyama approximation of the Langevin diffusion that behaves similarly to gradient descent optimisation.
- These samplers are useful for introducing ideas, however, they have been superseded by accelerated samplers, see, e.g., Pereyra et al. (2020).

1 Bayesian modelling in imaging inverse problems

2 Bayesian inference

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5 Conclusion

Problem statement

Consider the class of Bayesian models

$$p(x|y,\theta) = \frac{p(y|x)p(x|\theta)}{p(y|\theta)},$$

parametrised by a regularisation parameter $\theta \in \Theta$. For example,

$$p(x|\theta) = \frac{1}{Z(\theta)} \exp \left\{-\frac{\theta}{\psi(x)}\right\}, \quad p(y|x) \propto \exp \left\{-f_y(x)\right\},$$

with f_y and ψ convex l.s.c. functions, and f_y *L*-Lipschitz differentiable.

We assume that $p(x|\theta)$ is proper, i.e.,

$$Z(\theta) = \int_{\mathbb{R}^d} \exp\left\{-\theta\psi(x)\right\} \mathrm{d}x < \infty,$$

with $Z(\theta)$ unknown and generally intractable.

M. Pereyra

Recall that when θ is fixed, the posterior $p(x|y,\theta)$ is log-concave and

$$\hat{x}_{MAP} = \operatorname*{argmin}_{x \in \mathbb{R}^d} f_y(x) + \frac{\theta}{\psi}(x)$$

is a convex optimisation problem that can be often solved efficiently.

For example, one can consider the proximal gradient algorithm

$$x^{m+1} = \operatorname{prox}_{\psi}^{L^{-1}} \{ x^m + L^{-1} \nabla f_y(x^m) \}$$

to iteratively compute \hat{x}_{MAP} .

However, θ is often unknown, significantly complicating the problem.

We have two option to tackle $\theta.$ We first consider an empirical Bayes approach based on the MLE

$$\begin{split} \hat{\theta} &= \operatorname*{argmax}_{\theta \in \Theta} p(y|\theta) , \\ &= \operatorname*{argmax}_{\theta \in \Theta} \int_{\mathbb{R}^d} p(y, x|\theta) \mathrm{d}x , \end{split}$$

which we solve efficiently by using a stochastic gradient algorithm driven by two proximal MCMC kernels (see Fernandez-Vidal and Pereyra (2018)).

Given $\hat{\theta}$, we then straightforwardly compute

$$\hat{x}_{MAP} = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} f_y(x) + \hat{\theta} \psi(x) .$$
(17)

Assume that Θ is convex, and that $\hat{\theta}$ is the only root of $\nabla_{\theta} \log p(y|\theta)$ in Θ . Then $\hat{\theta}$ is also the unique solution of the fixed-point equation

$$\theta = P_{\Theta} \left[\theta + \delta \nabla_{\theta} \log p(y|\theta) \right] \,.$$

where P_{Θ} is the projection operator on Θ and $\delta > 0$.

If $\nabla \log p(y|\theta)$ was tractable, we could compute $\hat{\theta}$ iteratively by using

$$\theta^{(t+1)} = P_{\Theta} \left[\theta^{(t)} + \delta_t \nabla_{\theta} \log p(y|\theta^{(t)}) \right],$$

with sequence $\delta_t = \alpha t^{-\beta}$, $\alpha > 0$, $\beta \in [1/2, 1]$.

However, $\nabla \log p(y|\theta)$ is "doubly" intractable...

Stochastic projected gradient algorithm

To circumvent the intractability of $\nabla_{\theta} \log p(y|\theta)$ we use Fisher's identity

$$\begin{aligned} \nabla_{\theta} \log p(y|\theta) &= \mathrm{E}_{\mathbf{x}|y,\theta} \{ \nabla_{\theta} \log p(\mathbf{x}, y|\theta) \} \,, \\ &= -\mathrm{E}_{\mathbf{x}|y,\theta} \{ \psi(\mathbf{x}) + \nabla_{\theta} \log Z(\theta) \} \,, \end{aligned}$$

together with the identity

$$\nabla_{\theta} \log Z(\theta) = - \mathbf{E}_{\mathbf{x}|\theta} \{ \psi(\mathbf{x}) \},\$$

to obtain $\nabla_{\theta} \log p(y|\theta) = E_{x|\theta} \{\psi(x)\} - E_{x|y,\theta} \{\psi(x)\}.$

This leads to the equivalent fixed-point equation

$$\theta = P_{\Theta} \left(\theta + \delta \mathbf{E}_{\mathbf{x}|\theta} \{ \psi(\mathbf{x}) \} - \delta \mathbf{E}_{\mathbf{x}|\mathbf{y},\theta} \{ \psi(\mathbf{x}) \} \right), \tag{18}$$

which we solve by using a stochastic approximation algorithm.

M. Pereyra

SAPG algorithm driven by MCMC kernels

Initialisation $x^{(0)}, u^{(0)} \in \mathbb{R}^d, \theta^{(0)} \in \Theta, \delta_t = \delta_0 t^{-0.8}$.

for t = 0 to n

- 1. MCMC update $x^{(t+1)} \sim M_{x|y,\theta^{(t)}}(\cdot|x^{(t)})$ targeting $p(x|y,\theta^{(t)})$
- 2. MCMC update $u^{(t+1)} \sim K_{x|\theta^{(t)}}(\cdot|u^{(t)})$ targeting $p(x|\theta^{(t)})$
- 3. Stoch. grad. update

$$\theta^{(t+1)} = P_{\Theta}\left[\theta^{(t)} + \delta_t \psi(u^{(t+1)}) - \delta_t \psi(x^{(t+1)})\right].$$

end for

Output The iterates $\theta^{(t)} \rightarrow \hat{\theta}$ as $n \rightarrow \infty$.

SAPG algorithm driven MCMC kernels

Initialisation $x^{(0)}$, $u^{(0)} \in \mathbb{R}^d$, $\theta^{(0)} \in \Theta$, $\delta_t = \delta_0 t^{-0.8}$, $\lambda = 1/L$, $\gamma = 1/4L$. for t = 0 to n

1. Coupled Proximal MCMC updates: generate $z^{(t+1)} \sim \mathcal{N}(0, \mathbb{I}_d)$

$$\begin{aligned} x^{(t+1)} &= \left(1 - \frac{\gamma}{\lambda}\right) x^{(t)} - \gamma \nabla f_y\left(x^{(t)}\right) + \frac{\gamma}{\lambda} \operatorname{prox}_{\psi}^{\theta\lambda}\left(x^{(t)}\right) + \sqrt{2\gamma} z^{(t+1)} \,, \\ u^{(t+1)} &= \left(1 - \frac{\gamma}{\lambda}\right) u^{(t)} + \frac{\gamma}{\lambda} \operatorname{prox}_{\psi}^{\theta\lambda}\left(u^{(t)}\right) + \sqrt{2\gamma} z^{(t+1)} \,, \end{aligned}$$

2. Stochastic gradient update

$$\theta^{(t+1)} = P_{\Theta} \left[\theta^{(t)} + \delta_t \psi(u^{(t+1)}) - \delta_t \psi(x^{(t+1)}) \right].$$

end for

Output Averaged estimator $\bar{\theta} = n^{-1} \sum_{t=1}^{n} \theta^{(t+1)}$ converges approx. to $\hat{\theta}$.

Illustrative example: hyperspectral unmixing

• We seek to recover fractional abundances x from the mixed noisy spectral signatures y measured for every pixel.



Empirical Bayesian MAP estimation

We consider the prior of lordache et al. (IEEE TGRS, 2012)

$$p(x|\theta) \propto \exp\{\theta_{TV} TV(x) + \theta_{L1} \|x\|_1\} \quad \text{s.t.} x \ge 0,$$

and use the SAPG scheme to estimate θ_{TV} and θ_{L1} by MMLE.



Figure: Evolution of the iterates associated to θ_{TV} and θ_{L1} .

Given $\hat{\theta}_{TV}$ and $\hat{\theta}_{L1}$, we compute the MAP solution by using the convex optimisation algorithm SUNSAL:



MAP estimates of fractional abundances for 5 end members

Option 2: hierarchical Bayesian inference also allows estimating x without specifying the value of θ .

We incorporate θ to the model by assigning it an hyper-prior $p(\theta)$.

The extended model is

$$p(x,\theta|y) = p(y|x)p(x|\theta)p(\theta)/p(y),$$

$$\propto \frac{\exp\{-f_y(x) - \theta\psi(x) - \log p(\theta)\}}{Z(\theta)},$$
(19)

but $Z(\theta) = \int_{\mathbb{R}^d} \exp\{-\theta\psi(x)\} dx$ is typically <u>intractable</u>!

If we had access to $Z(\theta)$ we could either estimate x and θ jointly, or alternatively marginalise θ followed by MAP inference on x.
Idea: Use MYULA to estimate $E[\psi(\mathbf{x})|\theta]$ over a θ -grid, and then approximate $\log Z(\theta)$ by using the identity $\frac{d}{d\theta} \log Z(\theta) = E[\psi(\mathbf{x})|\theta]$.



Figure: Monte Carlo approximations of $E[\psi(\mathbf{x})|\theta]/d$ Vs θ for 4 widely used prior distributions and for $\theta \in [10^{-3}, 10^2]$. Surprise: they all coincide!

Definition[*k*-homogeneity] The regulariser ψ is a *k*-homogeneous function if $\exists k \in \mathbb{R}^+$ such that

$$\psi(\eta x) = \eta^{k} \psi(x), \quad \forall x \in \mathbb{R}^{d}, \forall \eta > 0.$$
(20)

Theorem[Pereyra et al. (2015)] Suppose that ψ , the sufficient statistic of $p(x|\theta)$, is k-homogenous. Then the normalisation factor has the form $Z(\theta) = Z(1)\theta^{-d/k},$

with (generally intractable) constant Z(1) independent of θ .

Note: This result holds for all norms (e.g., ℓ_1 , ℓ_2 , total-variation, nuclear, etc.), composite norms (e.g., $\ell_1 - \ell_2$), and compositions of norms with linear operators (e.g., analysis terms of the form $\|\Psi x\|_1$)!

Marginal maximum-a-posteriori estimation of x

Knowledge of $Z(\theta)$ enables (for example) marginal MAP estimation of x

$$\hat{x}_{MAP}^{\dagger} = \underset{x \in \mathbb{R}^{d}}{\operatorname{argmax}} \int_{0}^{\infty} p(x, \theta | y) d\theta,$$

$$= \underset{x \in \mathbb{R}^{d}}{\operatorname{argmin}} f_{y}(x) + (d/k + \alpha) \log\{\psi(x) + \beta\},$$
(21)

where we have used the hyper-prior $\theta \sim \text{Gamma}(\alpha, \beta)$.

We can compute \hat{x}^{\dagger} efficiently by *majorisation-minimisation* optimisation

$$x^{(t)} = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} f_y(x) + \theta^{(t-1)} \psi(x),$$

$$\theta^{(t)} = \frac{d/k + \alpha}{\psi(x^{(t)}) + \beta}.$$
(22)

which is also an *expectation-maximisation* algorithm.

We use the hyperspectral unmixing example to develop an intuition for the strengths and drawbacks of the EB and HB approaches.



EB performs remarkably well in low SNR (high noise) regimes, close to the oracle performance. The benefits of HB kick-in in high SNR regimes.

Illustrative example: image deconvolution with a TV prior

	SNR=20dB		SNR=30		SNR=40	
	MSE	Time (min)	MSE	Time (min)	MSE	Time (min)
Best	23.29		21.39		19.06	
Emp. Bayes	23.50	0.86	21.46	0.85	19.24	0.85
Hier. Bayes	25.07	0.58	22.84	1.27	19.84	3.27
Disc. Princp.	23.73		21.87		19.78	
SUGAR	24.44	3.92	24.24	4.50	24.21	4.81





Denoising with Total Generalized Variation

We consider $TGV_{\theta}^{2}(u) = \inf_{v \in BD(\Omega)} \theta_{1} \int_{\Omega} |\nabla u - v| + \theta_{2} \int_{\Omega} |\varepsilon(v)|$ with k = 2.



Figure: Goldhill image (Original-Degraded-Estimated MAP), SNR=12dB.

Denoising with Total Generalized Variation



Evolution of θ through iterations starting from different initial values:



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5 Conclusion

- There are three main frameworks to solve imaging inverse problems mathematical analysis, Bayesian statistics, and machine learning with complementary strengths and drawbacks.
- This tutorial focused on Bayesian imaging methods that leverage a range of ideas and techniques from mathematical analysis to perform computations efficiently.
- We explored integrating modern stochastic and optimisation approaches to construct proximal MCMC methods and stochastic proximal gradient algorithms.
- The tutorials of tomorrow will focus on methods at that also incorporate a significant machine learning component.

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