Bayesian model comparison with data-driven priors

Learned proximal nested sampling

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Goal

Bayesian parameter estimation and model selection
for inverse imaging problems...

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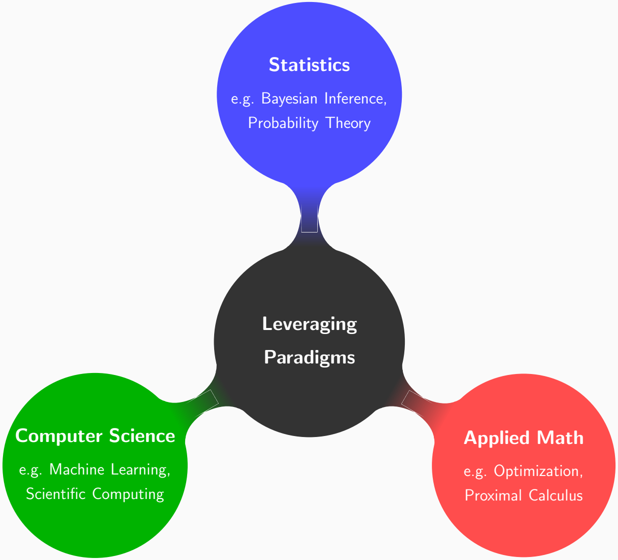
with data-driven priors (learned regularisation).

Questions that can be addressed by model selection

- What is the best forward model?
- (How set regularisation strength?)
- What is the best learned data-driven prior (regulariser)?
- What is the best training data-set?
- ...

Address these questions using the data itself... not by, *e.g.*, cross-validation.

Leveraging paradigms



Outline

1. Nested sampling
2. Proximal nested sampling
3. Learned data-driven priors

Nested sampling

Bayesian inference: parameter estimation

First, let's set the notation (and colour code)...

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Bayes' theorem

$$\underbrace{p(\theta \mid \mathbf{y}, M)}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{y} \mid \theta, M)}^{\text{likelihood}} \; \overbrace{p(\theta \mid M)}^{\text{prior}}}{\underbrace{p(\mathbf{y} \mid M)}_{\text{evidence}}} = \frac{\overbrace{\mathcal{L}(\theta)}^{\text{likelihood}} \; \overbrace{\pi(\theta)}^{\text{prior}}}{\underbrace{z}_{\text{evidence}}},$$

for parameters θ, model M and observed data $\mathbf{y}$.

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for parameters θ, model M and observed data $\mathbf{y}$.

For **parameter estimation**, typically draw samples from the posterior by *Markov chain Monte Carlo (MCMC)* sampling.

Bayesian inference: model selection

By Bayes' theorem for model M_j:

$$p(M_j \mid \boldsymbol{y}) = \frac{p(\boldsymbol{y} \mid M_j) p(M_j)}{\sum_j p(\boldsymbol{y} \mid M_j) p(M_j)} \, .$$

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For **model selection**, consider posterior model odds:

$$\underbrace{\frac{p(M_1 \mid \boldsymbol{y})}{p(M_2 \mid \boldsymbol{y})}}_{\text{posterior odds}} = \underbrace{\frac{p(\boldsymbol{y} \mid M_1)}{p(\boldsymbol{y} \mid M_2)}}_{\text{Bayes factor}} \times \underbrace{\frac{p(M_1)}{p(M_2)}}_{\text{prior odds}} .$$

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Must compute the **Bayesian model evidence** or **marginal likelihood** given by the normalising constant

$$z = p(\mathbf{y} \mid M) = \int \mathrm{d}\theta \, \mathcal{L}(\theta) \, \pi(\theta) .$$

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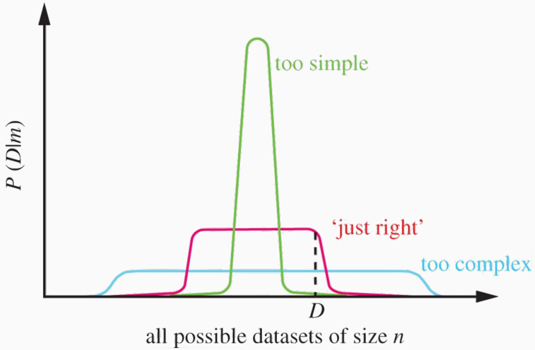
$\rightarrow$ Extremely challenging computational problem in high-dimensions.

The marginal likelihood **naturally incorporates Occam's razor**, trading off model complexity and goodness of fit.

- In Bayesian formalism models specified as probability distributions over datasets.
- Each model has limited "probability budget".
- Complex models can represent a wide range of datasets well, but spreads predictive probability.
- In doing so, marginal likelihood of complex models penalised if complexity not required.



Ghahramani (2013); MacKay (1991)

On priors

- Physics-informed priors
  e.g. mass constrained to be positive
- Uninformative prior
  e.g. objective Bayes, invariance to symmetry transformations
- **Informative priors**
  e.g. regularize by imposing sparsity in dictionary
- Data-informed priors
  e.g. prior $\sim$ old data, likelihood $\sim$ new data, posterior $\sim$ old and new data
- **Data-driven priors**
  e.g. empirical Bayes (estimate prior from data), learn by machine learning (generative models)

Nested sampling: reparameterising the likelihood

Nested sampling is ingenious approach to evaluate the marginal likelihood (Skilling 2006).

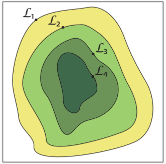
Consider $\Omega_{L^*} = \{x | \mathcal{L}(x) \geq L^*\}$, which groups the parameter space Ω into a series of **nested subspaces**.

Define the prior volume ξ within Ω_{L^*} by $\xi(L^*) = \int_{\Omega_{L^*}} \pi(x) \mathrm{d}x$.

The marginal likelihood integral can then be rewritten as

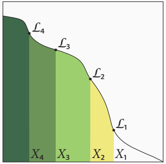
$$z = \int_0^1 \mathcal{L}(\xi) \mathrm{d}\xi,$$

which is a **one-dimensional integral** over the prior volume ξ.



Feroz *et al.* (2013)

Nested subspaces



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Reparameterised likelihood

Require strategy to compute likelihood level-sets (iso-contours) L_i and corresponding prior volumes $0 < \xi_i \leq 1$.

Nested sampling (Skilling 2006)

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5. Repeat 2–5.

Nested sampling: evidence estimation and posterior inference

Given the sequence of decreasing prior volumes $\{\xi_i\}_{i=0}^{N}$ and corresponding likelihoods $L_i = \mathcal{L}(\xi_i)$, the **marginal likelihood** can be computed numerically using standard quadrature:

$$z = \sum_{i=1}^{N} L_i w_i \ ,$$

for quadrature weight w_i (e.g. the trapezium rule with $w_i = (\xi_{i-1} + \xi_{i+1})/2$).

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Posterior inferences can also be computed by assigning importances weights

$$p_i = \frac{L_i w_i}{z} \ .$$

Nested sampling: challenge

Recall: to compute the marginal likelihood by nested sampling require strategy to generate likelihoods L_i and associated prior volumes ξ_i.

Crux: **sample from the prior, subject to the likelihood level-set constraint**, *i.e.* sample from the prior $\pi(\boldsymbol{x})$, such that $\mathcal{L}(\boldsymbol{x}) > L^*$.

This is the main difficulty in applying nested sampling to high-dimensional problems.

Proximal nested sampling

Exploit common structure

Many high-dimensional inverse problems are **log-convex**, *e.g.* inverse imaging problems with Gaussian data fidelity and sparsity-promoting prior.

Exploit structure (log convexity) of the problem.

$\Rightarrow$ Proximal nested sampling (Cai, McEwen & Pereyra 2022; arXiv:2106.03646)

Constrained sampling formulation

Consider case where likelihood and prior of the form

$$\mathcal{L}(x) \propto \exp(-g(x)), \qquad \pi(x) \propto \exp(-f(x)),$$

Likelihood | Prior

where g is convex lower semicontinuous function (prior need not be log-convex).

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Let $\iota_{L^*}(x)$ and $\chi_{L^*}(x)$ be the indicator and characteristic functions:

$$\iota_{L^*}(x) = \begin{cases} 1, & \mathcal{L}(x) > L^*, \\ 0, & \text{otherwise}, \end{cases} \quad \text{and} \quad \chi_{L^*}(x) = \begin{cases} 0, & \mathcal{L}(x) > L^*, \\ +\infty, & \text{otherwise}. \end{cases} \tag{1}$$

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Let $\pi_{L^*}(x) = \pi(x)\iota_{L^*}(x)$ represent prior distribution with hard likelihood constraint.

Equivalently, $-\log \pi_{L^*}(x) = -\log \pi(x) + \chi_{\mathcal{B}_\tau}(x)$, $\mathcal{B}_\tau := \{x \mid -\log \mathcal{L}(x) < \tau\}$, $\tau = -\log L^*$.

MCMC sampling with Langevin dynamics

Require MCMC sampling strategy that can scale to **high-dimensions**.

If target distribution $p(x)$ is differentiable can adopt **Langevin dynamics**.

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Langevin diffusion process $\boldsymbol{x}(t)$, with $p(\boldsymbol{x})$ as stationary distribution:

$$\mathrm{d}\boldsymbol{x}(t) = \frac{1}{2}\nabla \log p\big(\boldsymbol{x}(t)\big)\,\mathrm{d}t + \mathrm{d}\boldsymbol{w}(t),$$

where $\boldsymbol{w}$ is Brownian motion.

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Langevin diffusion process $x(t)$, with $p(x)$ as stationary distribution:

$$\mathrm{d}x(t) = \frac{1}{2} \underbrace{\nabla \log p\big(x(t)\big)}_{\text{Gradient}} \mathrm{d}t + \mathrm{d}w(t),$$

where w is Brownian motion.

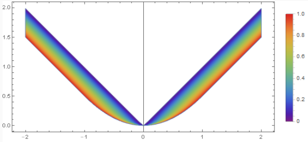
Need gradients so **not directly applicable** $\Rightarrow$ adopt Morea-Yosida approximation.

Moreau-Yosida approximation

Morea-Yosida (M-Y) approximation

The Morea-Yosida approximation of a convex function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is given by the **infimal convolution**:

$$f^{\lambda}(x) = \inf_{u \in \mathbb{R}^N} f(u) + \frac{\|u - x\|^2}{2\lambda}$$



M-Y envelope of $|x|$ for varying λ.

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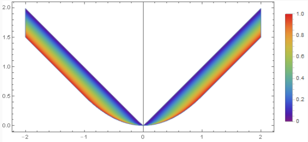

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Important **properties** of $f^\lambda(x)$:

1. As $\lambda \rightarrow 0, f^\lambda(x) \rightarrow f(x)$
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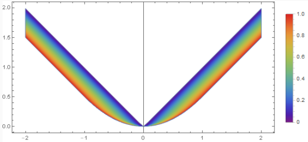

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- **Regularise** non-differentiable function (e.g. likelihood level-set constraint!)
- **Compute gradient** by prox.
- Leverage **gradient-based Bayesian computation**.

Proximal nested sampling

Proximal nested sampling (Cai, McEwen & Pereyra 2021; arXiv:2106.03646)

- Constrained sampling formulation
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- Moreau-Yosida approximation of constraint (and any non-differentiable prior)

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Proximal nested sampling Markov chain:

$$x^{(k+1)} = x^{(k)} + \frac{\delta}{2}\nabla \log \pi(x^{(k)}) - \frac{\delta}{2\lambda}\left[x^{(k)} - \text{prox}_{\chi_{\mathcal{B}_\tau}}(x^{(k)})\right] + \sqrt{\delta} w^{(k+1)} .$$

Proximal nested sampling intuition

Recall proximal nested sampling Markov chain (from previous slide):

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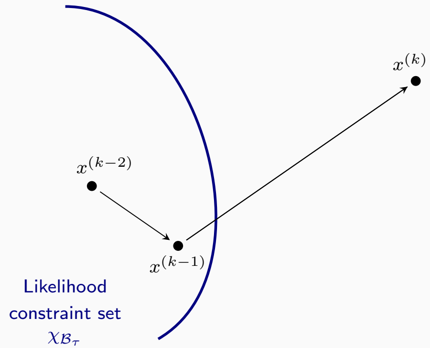

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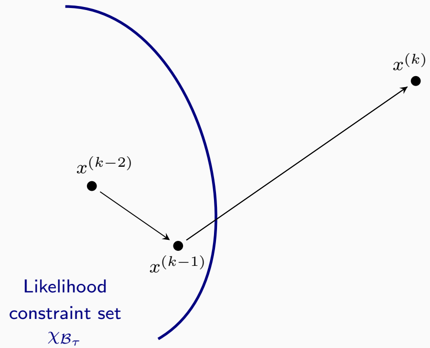

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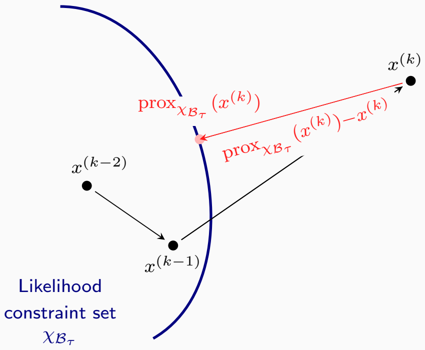

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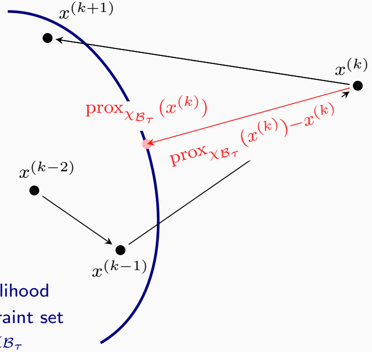

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For sparsity-promoting **non-differentiable priors** $f(x)$ (e.g. $-\log \pi(x) = \|\Psi^\dagger x\|_1$), can also make Moreau-Yosida approximation $f^\lambda(x)$ and leverage prox to compute gradient ∇f^λ:

$$x^{(k+1)} = x^{(k)} - \frac{\delta}{2\lambda}\left[x^{(k)} - \text{prox}^{\lambda}_{-\log \pi}(x^{(k)})\right] - \frac{\delta}{2\lambda}\left[x^{(k)} - \text{prox}_{\chi_{\mathcal{B}_\tau}}(x^{(k)})\right] + \sqrt{\delta}\, w^{(k+1)} .$$

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Explicit forms of proximal nested sampling

Must compute the proximity operators.

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Consider common imaging problem as example:

$$-\log \pi(x) = \left\|\Psi^\dagger x\right\|_1 + \text{const.}$$

Prior

$$\text{prox}^{\lambda}_{-\log \pi}(x) = x + \Psi\left(\text{soft}_{\lambda\mu}(\Psi^\dagger x') - \Psi^\dagger x\right),$$

Explicit forms of proximal nested sampling

Must compute the proximity operators.

Consider common imaging problem as example:

$$-\log \mathcal{L}(x) = \|y - \boldsymbol{\Phi} x\|_2^2 + \text{const.}$$

Likelihood

$$-\log \pi(x) = \|\Psi^\dagger x\|_1 + \text{const.}$$

Prior

Straightforward when $\boldsymbol{\Phi}$ is identity.

Otherwise express as equivalent saddle-point problem and solve using primal-dual method.

$$\text{prox}^{\lambda}_{-\log \pi}(x) = x + \Psi\left(\text{soft}_{\lambda\mu}(\Psi^\dagger x') - \Psi^\dagger x\right),$$

Computing proximal operator for likelihood

Prox for the likelihood is equivalent to the saddle-point problem:

$$\min_{x \in \mathbb{R}^d} \max_{z \in \mathbb{C}^K} \left\{ z^\dagger \Phi x - \chi^*_{\mathcal{B}'_{\tau'}}(z) + \|x - x'\|_2^2 / 2 \right\}.$$

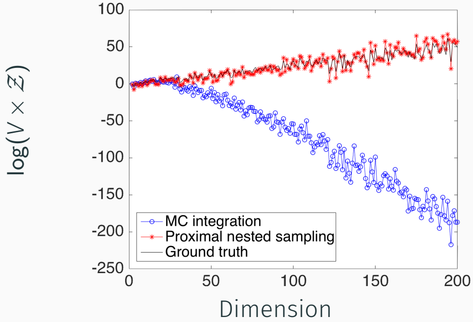
Solve iteratively by primal dual method:

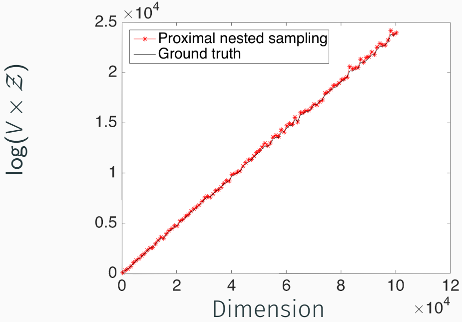
1. $z^{(i+1)} = z^{(i)} + \delta_1 \Phi \bar{x}^{(i)} - \mathrm{prox}_{\chi_{\mathcal{B}'_{\tau'}}}(z^{(i)} + \delta_1 \Phi \bar{x}^{(i)})$,

   where $\mathrm{prox}_{\chi_{\mathcal{B}'_{\tau'}}}(z) = \mathrm{proj}_{\mathcal{B}'_{\tau'}}(z) = \begin{cases} z, & \text{if } z \in \mathcal{B}'_{\tau'}, \\ \frac{z-y}{\|z-y\|_2}\sqrt{2\tau\sigma^2} + y, & \text{otherwise.} \end{cases}$

2. $x^{(i+1)} = (x' + x^{(i)} - \delta_2 \Phi^\dagger z^{(i+1)})/2$
3. $\bar{x}^{(i+1)} = x^{(i+1)} + \delta_3 (x^{(i+1)} - x^{(i)})$

Validation on Gaussian problem





Comparison of proximal nested sampling (red), naive MC integration (blue) and ground truth (black).

Also validated in 10^6 **dimensions**.

Truth: 2.3850×10^5 Proximal nested sampling: $(2.3851 \pm 0.0002) \times 10^5$

Denoising wavelet dictionary experiment

Clean image

Noisy image

$\Psi = I$

$\Psi = \text{DB2}$

$\Psi = \text{DB8}$

Denoising wavelet dictionary experiment

Prior	$\log z$	RMSE (Requires ground truth)
$\Psi = I$	-6.54×10^4	41.07
$\Psi = \text{DB2}$	-3.06×10^4	14.29
$\Psi = \text{DB8}$	-3.09×10^4	14.51

Evidence computed by proximal nested sampling correctly compares wavelet dictionaries.

Learned data-driven priors

Empirical Bayes: deep data-driven priors

Handcrafted priors (e.g. promoting sparsity in a wavelet basis) are **not expressive enough**.

Consider **empirical Bayes** approach with **data-driven priors** learned from training data.

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Aim: integrate learned deep data-driven priors into proximal nested sampling.

Proximal nested sampling requires only likelihood to be convex, so **prior can be arbitrarily complex** (e.g. deep learned model).

Proximal nested sampling with data driven-priors for physical scientists
(McEwen, Liaudat, Price, Cai & Pereyra 2023; arXiv:2307.00056)

Tobias Liaudat

Henry Aldridge

Matt Price

Xiaohao Cai

Marcelo Pereyra

Tweedie's formula

Tweedie's formula (Robins 1956)

Consider noisy observations $x \sim \mathcal{N}(z, \sigma^2 I)$ of z sampled from some underlying prior.

Tweedie's formula gives the posterior expectation of z given x as

$$\mathbb{E}(z \,|\, x) = x + \sigma^2 \nabla \log p(x),$$

where $p(x)$ is the marginal distribution of x.

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$$\mathbb{E}(z \mid x) = x + \sigma^2 \nabla \log p(x),$$

where $p(x)$ is the marginal distribution of x.

- Can be interpreted as a denoising strategy.
- Can be used to relate a denoiser (potentially a trained deep neural network) to the score $\nabla \log p(x)$.

Learning score of regularised prior

No guarantee that data-driven prior is well-suited for gradient-based Bayesian computation, *e.g.* it may not be differentiable.

⇒ Consider **regularised prior** defined by Gaussian smoothing:

$$\pi_\epsilon(x) = (2\pi\epsilon)^{-d/2} \int \mathrm{d}x' \, \exp(-\|x - x'\|_2^2/(2\epsilon)) \, \pi(x').$$

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Consider **learned denoiser** D_ϵ trained to recover x from noisy observations $x_\epsilon \sim \mathcal{N}(x, \epsilon I)$.

By Tweedie's formula the score of the regualised prior related to the learned denoiser by

$$\nabla \log \pi_\epsilon(x) = \epsilon^{-1}(D_\epsilon(x) - x).$$

Proximal nested sampling with learned data-driven priors

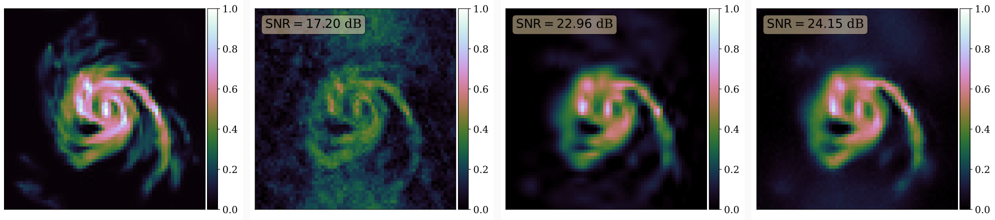
Substituting the denoiser $\nabla \log \pi_\epsilon(x) = \epsilon^{-1}(D_\epsilon(x) - x)$ into the proximal nested sampling Markov chain update:

$$x^{(k+1)} = x^{(k)} - \frac{\delta}{2\epsilon}\left[x^{(k)} - D_\epsilon(x^{(k)})\right] - \frac{\delta}{2\lambda}\left[x^{(k)} - \text{prox}_{\chi_{\mathcal{B}_\tau}}(x^{(k)})\right] + \sqrt{\delta}w^{(k+1)} \, .$$

Hand-crafted vs data-driven priors

Consider simple radio interferometric imaging inverse problem with:

- ▷ **hand-crafted prior** based on sparsity-promoting wavelet representation;
- ▷ **data-driven prior** based on a deep convolutional neural network (Ryu et al. 2019).



Ground truth | Backprojected (17.2dB) | Hand-crafted prior (23.0dB) | Data-driven prior (24.2dB)

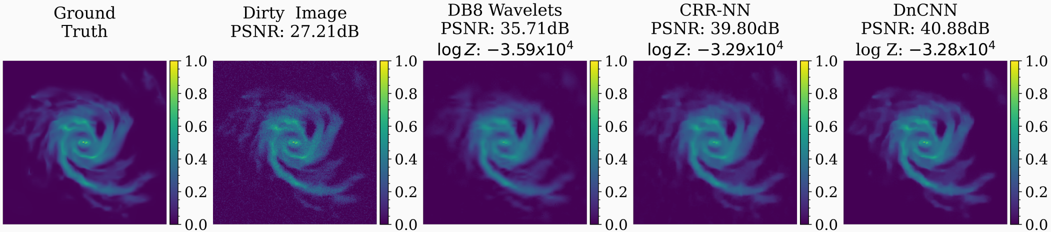
Which model best?

- ▷ SNR ⇒ **data-driven priors best** but require ground-truth;
- ▷ Bayesian evidence ⇒ **data-driven priors best** (no ground-truth knowledge).

Hand-crafted vs data-driven priors

Consider simple Galaxy denoising inverse problem with:

- **hand-crafted prior** based on sparsity-promoting wavelet representation;
- **data-driven priors** based on deep neural networks (Goujon et al. 2023, Ryu et al. 2019).



Which model best?

- SNR $\Rightarrow$ **data-driven priors best** but require ground-truth;
- Bayesian evidence $\Rightarrow$ **data-driven priors best** (no ground-truth knowledge).

Summary

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- **Proximal nested sampling** (arXiv:2106.03646) framework scales to **high-dimensions**, opening up Bayesian model comparison for, e.g., imaging problems.
- Constrained to **log-convex likelihoods**, which are ubiquitous in imaging sciences.
- Prior not constrained to be log-convex so can be a deep neural network.
- **Learned proximal nested sampling** (arXiv:2307.00056) approach to support **data-driven priors**.
- **Future work**:
  - More extensive experiments to showcase use
  - Remove convexity constraint
  - More expressive data-driven priors (*e.g.* denoising diffusion models)

Extra Slides

Alternatives to marginal likelihood

- **Posterior predictive checks**
  - ✔ Fine for model consistency checks
  - ✖ Not suitable for model comparison
    - Does not guarantee Bayesian consistency
    - Does not penalise model complexity

- **Bayesian leave one out (LOO) cross validation**
  - ✔ Fine for validation
  - ✖ Not suitable for model comparison
    - Does not guarantee Bayesian consistency
    - Does not penalise model complexity

- **Bayesian model complexity and dimensionality**
  - ✔ Only weakly dependent on prior through posterior

- **Bayesian suspicious** for testing for tensions between datasets
  - ✔ Only weakly dependent on prior through posterior

Nested sampling: estimating enclosed prior volume stochastically

Enclosed prior volume decreases exponentially at each step: $\xi_{i+1} = t_{i+1}\xi_i$.

Shrinkage ratio can be estimated stochastically since $\mathbb{E}(\log t) = -1/N_{\text{live}}$.

The enclosed prior volume can then be estimated by

$$\xi_{i+1} = \exp(-i/N_{\text{live}}) \; .$$