Machine learning assisted Bayesian evidence computation

The *learnt* harmonic mean estimator

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Outline

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Bayesian inference
Parameter estimation

Bayes' theorem

$$\underbrace{\mathsf{P}(\theta \,|\, \boldsymbol{y}, M)}_{\text{posterior}} = \frac{\overbrace{\mathsf{P}(\boldsymbol{y} \,|\, \theta, M)}^{\text{likelihood}} \; \overbrace{\mathsf{P}(\theta \,|\, M)}^{\text{prior}}}{\underbrace{\mathsf{P}(\boldsymbol{y} \,|\, M)}_{\text{constant}}},$$

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

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Shorthand notation:

$$\underbrace{\mathrm{P}(\theta \mid \boldsymbol{y})}_{\text{posterior}} = \frac{\overbrace{\mathcal{L}(\theta)}^{\text{likelihood}} \; \overbrace{\pi(\theta)}^{\text{prior}}}{\underbrace{z}_{\text{constant}}},$$

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

Bayesian inference

Model selection

For **model selection**, consider the posterior model probabilities:

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$\rightarrow$ **Challenging computational problem in high-dimensions.**

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→ **Challenging computational problem in high-dimensions.**

Variety of powerful methods exist but often place restrictions on sampling method and struggle to push to high dimensional settings.

Desirable properties for Bayesian evidence estimators

Seek estimator that is:

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Harmonic mean estimator has potential to meet these criteria but has serious shortcomings as originally posed.

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Harmonic mean relationship (Newton & Raftery 1994)

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Very simple approach but **can fail catastrophically** (Neal 1994).

Original harmonic mean estimator

Importance sampling interpretation

Alternative derivation of harmonic mean relationship:

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Importance sampling interpretation:

- Importance **sampling target distribution is prior** $\pi(\theta)$.
- Importance **sampling density is posterior** $\mathsf{P}(\theta \,|\, \boldsymbol{y})$.

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Not the case when importance sampling density is the posterior and the target is the prior.

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where $\mathrm{P}(\Omega)$ is the prior probability of the posterior simulation support $\Omega \subset \Theta$.

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Mitigates simulation pseudo bias but does not eliminate.

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Importance sampling derivation:

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$\rightarrow$ **How set importance sampling target distribution $\varphi(\theta)$?**

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(resulting estimator has zero variance).

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Recall:

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But clearly **not feasible** since requires knowledge of the evidence z (recall the target must be normalised) $\rightarrow$ **requires problem to have been solved already!**

Learnt harmonic mean estimator

Learn an approximation of the optimal target distribution:

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Also develop strategy to estimate the variance of the estimator, its variance, and other sanity checks.

Learnt harmonic mean estimator

Learning the target distribution

Consider a **variety of machine learning approaches**:

- Uniform hyper-ellipsoid
- Kernel Density Estimation (KDE)
- Modified Gaussian mixture model (MGMM)

Modify learning objective function to include **variance penalty and regularisation**.

Solve by bespoke **mini-batch stochastic gradient descent**.

Cross-validation to select machine learning approach and hyperparameters.

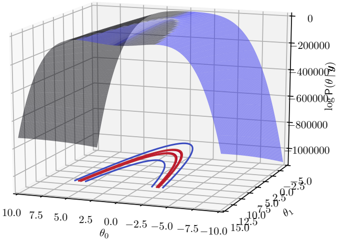
Outline

Rosenbrock example

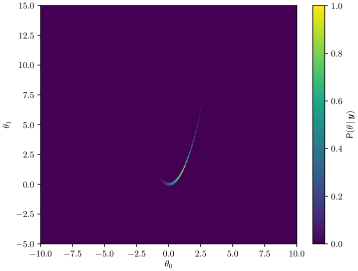
Posterior

Rosenbrock function is the classical example of a **pronounced thin curving degeneracy**, with likelihood defined by

$$f(\theta) = \sum_{i=1}^{n-1} \left[(a - \theta_i)^2 + b(\theta_{i+1} - \theta_i^2)^2 \right] , \qquad \log(\mathcal{L}(\theta)) = -f(\theta) \, .$$



(a) Log-Posterior



(b) Posterior

Figure: Rosenbrock posterior evaluated on grid.

Rosenbrock example

MCMC sampling and learning the target distribution φ

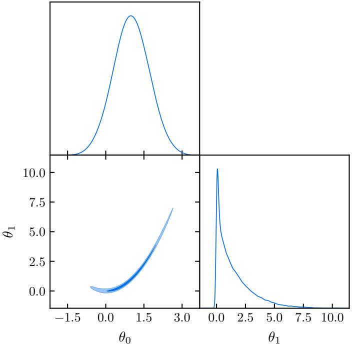


Figure: Posterior recovered by MCMC sampling.

Rosenbrock example

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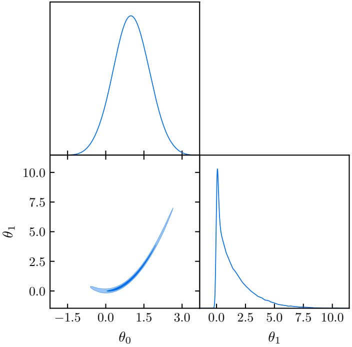

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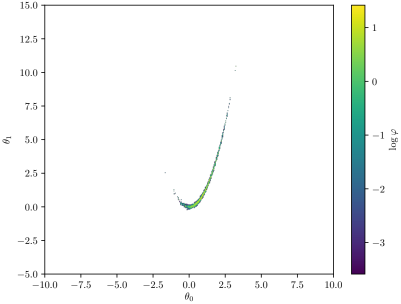
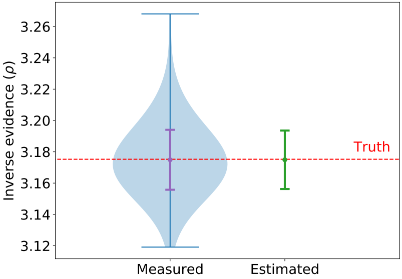


Figure: Learnt target distribution φ (by KDE).

Rosenbrock example

Accuracy of learnt harmonic mean estimator

- Compare to Monte Carlo simulations, repeating entire analysis.
- Also estimate the variance of the estimator and its variance.



(a) Inverse evidence

Figure: Accuracy of learnt harmonic mean estimator for Rosenbrock example.

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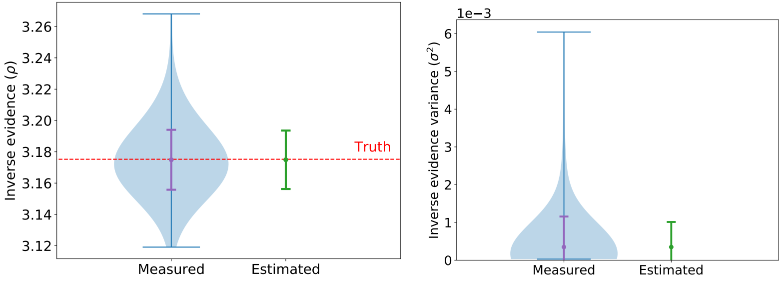

(a) Inverse evidence **(b) Variance of inverse evidence**

Figure: Accuracy of learnt harmonic mean estimator for Rosenbrock example.

Normal-Gamma example

Model

Pathological example (Friel & Wyse 2012) where original harmonic mean estimator fails.

Normal-Gamma example
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Data model:

$$y_i \sim \mathrm{N}(\mu, \tau^{-1})$$

Prior model:

$$\text{Mean: } \mu \sim \mathrm{N}\big(\mu_0, (\tau_0 \tau)^{-1}\big)$$
$$\text{Precision: } \tau \sim \mathrm{Ga}(a_0, b_0)$$

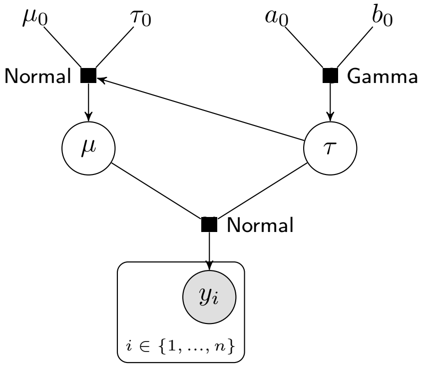

Figure: Graph of hierarchical Bayesian model of Normal-Gamma example.

Normal-Gamma example

Analytic evidence

Analytic evidence:

$$z = (2\pi)^{-n/2} \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}} \left(\frac{\tau_0}{\tau_n} \right)^{1/2}$$

where

$$\tau_n = \tau_0 + n \, , \quad a_n = a_0 + n/2 \, , \quad b_n = b_0 + \frac{1}{2} \sum_{i=1}^{n} (y_i - \bar{y})^2 + \frac{\tau_0 n (\bar{y} - \mu_0)^2}{2(\tau_0 + n)} \, .$$

Normal-Gamma example

Accuracy of learnt harmonic mean estimator and sensitivity to prior

Table: Analytic and estimated evidence for various prior sizes τ_0.

Prior size τ_0	10^{-4}	10^{-3}	10^{-2}	10^{-1}	10^{0}
Analytic $\log(z)$	-160.3888	-159.2375	-158.0863	-156.9359	-155.7935
Estimated $\log(\hat{z})$	-160.3883	-159.2370	-158.0851	-156.9359	-155.7921
Error (learnt harmonic mean)	-0.0005	-0.0005	-0.0012	0.0000	-0.0014
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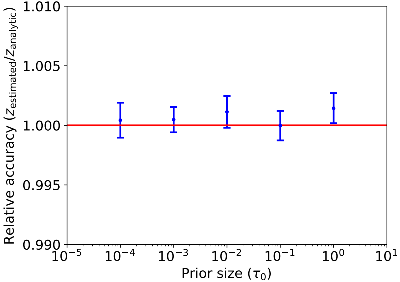

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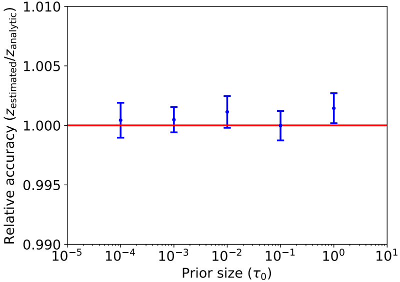

Figure: Accuracy for various prior sizes τ_0.

Non-nested linear regression: Radiata pine example
Data

Radiata pine data-set has become **classical benchmark** for evaluating evidence estimators:

- maximum compression strength parallel to grain y_i,
- density x_i,
- density adjust for resin content z_i,

for $i \in \{1, \ldots, n\}$ where $n = 42$ specimens.

Is density or resin-adjusted density a better predictor of compression strength?

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Models

Gaussian linear models:

$$M_1: \quad y_i = \alpha + \boxed{\beta(x_i - \bar{x})} + \epsilon_i \,, \quad \epsilon_i \sim \mathsf{N}(0, \tau^{-1}) \,.$$

Density

$$M_2: \quad y_i = \gamma + \boxed{\delta(z_i - \bar{z})} + \eta_i \,, \quad \eta_i \sim \mathsf{N}(0, \lambda^{-1}) \,.$$

Resin-adjusted density

Priors for model 1 (similar for model 2):

$$\alpha \sim \mathsf{N}\big(\mu_\alpha, (r_0\tau)^{-1}\big) \,,$$
$$\beta \sim \mathsf{N}\big(\mu_\beta, (s_0\tau)^{-1}\big) \,,$$
$$\tau \sim \mathsf{Ga}(a_0, b_0) \,,$$

($\mu_\alpha = 3000$, $\mu_\beta = 185$, $r_0 = 0.06$, $s_0 = 6$, $a_0 = 3$, $b_0 = 2 \times 300^2$).

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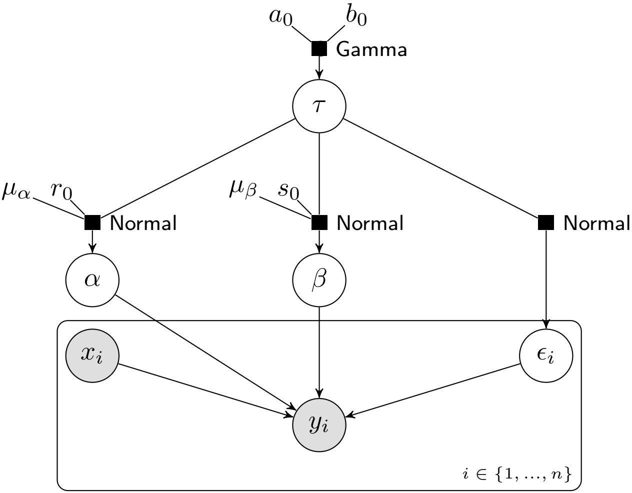

Figure: Graph of hierarchical Bayesian model for Radiata pine example (for model 1; model 2 is similar).

Non-nested linear regression: Radiata pine example

Analytic evidence

Analytic evidence:

$$z = \pi^{-n/2} b_0^{a_0} \frac{\Gamma(a_0 + n/2)}{\Gamma(a_0)} \frac{|Q_0|^{1/2}}{|M|^{1/2}} \left(\boldsymbol{y}^\mathsf{T}\boldsymbol{y} + \boldsymbol{\mu_0}^\mathsf{T} Q_0 \boldsymbol{\mu_0} - \boldsymbol{\nu_0}^\mathsf{T} M \boldsymbol{\nu_0} + 2b_0\right)^{-a_0-n/2}$$

where $\boldsymbol{\mu_0} = (\mu_\alpha, \mu_\beta)^\mathsf{T}$, $Q_0 = \text{diag}(r_0, s_0)$, and $M = X^\mathsf{T} X + Q_0$.

Non-nested linear regression: Radiata pine example

Accuracy of learnt harmonic mean estimator

Table: Analytic and estimated evidence.

	Model M_1 $\log(z_1)$	Model M_2 $\log(z_2)$	$\log \textsf{BF}_{21}$ $= \log(z_2) - \log(z_1)$
Analytic	-310.12833	-301.70460	8.42368
Estimated	-310.12839	-301.70489	8.42350
Error (learnt harmonic mean)	0.00006	0.00029	0.00018
Error (original harmonic mean)*	–	–	0.17372

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Outline

Code
Python package: harmonic

Harmonic python package implementing *learnt* harmonic mean estimator.

User-facing features:

- **Ease of use** (modular python package).
- Follow **software engineering best-practice** (*e.g.* well documented, extensive test suite, CI).
- Cython for **speed**.
- **Flexible** choice of sampler (we use **emcee**).
- Bespoke integrated **cross-validation** to select machine learning algorithm and hyperparameters.

Under the hood:

- Bespoke objective functions with **variance penalty** and **regularisation**.
- Solve by bespoke **mini-batch stochastic gradient descent**.

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```
# Compute evidence
evidence = harmonic.Evidence(chains_test.nchains, model)
evidence.add_chains(chains_test)
ln_evidence, ln_evidence_std = evidence.compute_ln_evidence()
```

Summary and future work

Problems of harmonic mean estimator can be fixed by re-targeting.

Apply machine learning to approximate optimal importance sampling target.

$\Rightarrow$ ***Learnt* harmonic mean estimator**

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- Apply to more examples and push to higher dimensions.
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