

Transport Reversible Jump Proposals - Follow Along!



Figure: (a) Website (b) Preprint (c) Slides

Transport Reversible Jump Proposals

Using Normalizing Flows

L. Davies¹ R. Salomone² M. Sutton¹ C. Drovandi¹

¹School of Mathematical Sciences
Queensland University of Technology

²School of Computer Science
Queensland University of Technology

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Table of Contents

- 1 Motivation and Background
- 2 Transport Reversible Jump Proposals
- 3 Illustrative Example
- 4 Testing Proposal Performance
- 5 Numerical Example - Bayesian Factor Analysis
- 6 Conditional Transport Proposals
- 7 Discussion

Table of Contents

- 1 Motivation and Background
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- 3 Illustrative Example
- 4 Testing Proposal Performance
- 5 Numerical Example - Bayesian Factor Analysis
- 6 Conditional Transport Proposals
- 7 Discussion

Problem: Sampling a Transdimensional Space

The problem of interest is sampling probability distribution π on

$$\mathcal{X} = \bigcup_{k \in \mathcal{K}} (\{k\} \times \Theta_k), \quad (1)$$

with *Parameters* $\theta_k \in \Theta_k \subseteq \mathbb{R}^{n_k}$ and *Model index* (or indicator) $k \in \mathcal{K}$. We want to make inference on the joint distribution (or conditional factorization)

$$\pi(k, \theta_k) = \pi(k) \pi(\theta_k | k).$$

When data \mathbf{y} is introduced this is $\pi(k, \theta_k | \mathbf{y}) = \pi(k | \mathbf{y}) \pi(\theta_k | k, \mathbf{y})$.

Notation. Denote $\mathbf{x} = (k, \theta_k)$, ϕ_n is n-dimensional standard normal, ϕ_{Σ_n} is an n-dimensional normal with mean $\mathbf{0}$ and Σ_n covariance, $|J_f(\theta)|$ denotes absolute determinant of Jacobian matrix of function $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$, and $\otimes_n \nu$ is $\underbrace{\nu \otimes \cdots \otimes \nu}_{n \text{ times}}$ for a distribution ν .

Reversible Jump Markov Chain Monte Carlo

We want to propose from point \mathbf{x} to point \mathbf{x}' , noting $\boldsymbol{\theta}_k, \boldsymbol{\theta}_{k'}$ have dimensions $n_k, n_{k'}$ respectively.

- Require dimensions match: introduce auxiliary variables $\mathbf{u}_k \in \mathcal{U}_{k,k'} \subseteq \mathbb{R}^{w_k}$ and $\mathbf{u}_{k'} \in \mathcal{U}_{k',k} \subseteq \mathbb{R}^{w_{k'}}$ such that $n_k + w_k = n_{k'} + w_{k'}$.
- **Choose** a diffeomorphism e. $\boldsymbol{\theta}_{k'}, \mathbf{v} = h_{k,k'}(\boldsymbol{\theta}_k, \mathbf{u})$.

A (simplified) RJMCMC Algorithm when $n_{k'} > n_k$ is:

- 1 Propose model index $k' \sim j_k(\cdot)$
- 2 Propose auxiliary variables $\mathbf{u}_k \sim g_{k,k'}(\cdot)$
- 3 Accept with probability

$$\alpha(\mathbf{x}, \mathbf{x}') = 1 \wedge \frac{\pi(\mathbf{x}') j_{k'}(k) g_{k',k}(\mathbf{u}'_{k'})}{\pi(\mathbf{x}) j_k(k') g_{k,k'}(\mathbf{u}_k)} |J_{h_{k,k'}}(\boldsymbol{\theta}_k, \mathbf{u}_k)|. \quad (2)$$

Transport Maps and Normalizing Flows

Consider random vectors $\theta \sim \mu_\theta$, $Z \sim \mu_z$, s.t. their distributions μ_θ , μ_z are absolutely continuous w.r.t. the n -dimensional Lebesgue measure.

Transport Map (TM)

A function $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is called a *transport map* from μ_θ to μ_z if $\mu_z = T_\# \mu_\theta$.

Normalizing Flows (NF) and Flow-Based Models

Let $\{T_\psi\}$ be a $\psi \in \Psi$ -parameterized family of diffeomorphisms with domain on the support of some arbitrary *base* distribution μ_z . Then, for fixed ψ , the PDF of the random vector $\zeta = T_\psi(Z)$ is

$$\mu_\zeta(\zeta; \psi) = \mu_z(T_\psi^{-1}(\zeta)) |J_{T_\psi^{-1}}(\zeta)|, \quad \zeta \in \mathbb{R}^n. \quad (3)$$

Distributions μ_ζ are *flow-based models*, where $\{T_\psi\}$ are the *normalizing flows*.

With finite samples $s \sim \pi$, we obtain an *approximate* TM \hat{T} via density estimation, minimising the KLD from $\{s\}$ to μ_ζ .

Table of Contents

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- 3 Illustrative Example
- 4 Testing Proposal Performance
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Then, a transdimensional proposal

where $n_{k'} > n_k$ is

$$\begin{aligned} \mathbf{z}_k &\leftarrow T_k(\boldsymbol{\theta}_k), \\ \mathbf{z}'_{k'} &\leftarrow \bar{h}_{k,k'}(\mathbf{z}_k, \mathbf{u}_k), \\ \boldsymbol{\theta}_{k'} &\leftarrow T_{k'}^{-1}(\mathbf{z}'_{k'}), \end{aligned} \quad (4)$$

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For each model $k \in \mathcal{M}$:

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where $\bar{h}_{k,k'}$ is a *volume-preserving* diffeomorphism on $\otimes_{n_k} \nu$.

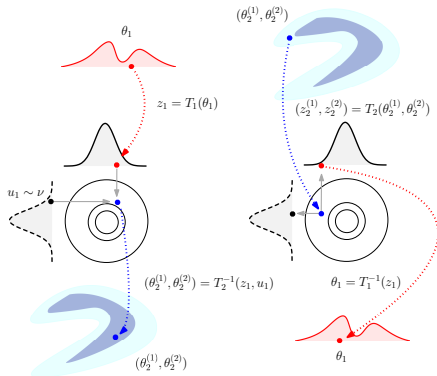


Figure: Illustration of the proposal class. Here, the reference ν is Gaussian. The diffeomorphisms (\bar{h}) on the reference distributions simply concatenate or extract coordinates as required.

Proposition: RJMCMC with Exact TMs

Proposition 1

Suppose that RJMCMC proposals are of the form described in (4), and for each $k \in \mathcal{K}$, satisfy $T_k \# \pi_k = \otimes_{n_k} \nu$. Then, (2) reduces to

$$\alpha(\mathbf{x}, \mathbf{x}') = 1 \wedge \frac{\pi(k')}{\pi(k)} \frac{j_{k'}(k)}{j_k(k')}. \quad (5)$$

Corollary

Provided the conditions of Proposition 1 are satisfied, choosing $\{j_k\}$ such that

$$\pi(k') j_{k'}(k) = \pi(k) j_k(k'), \quad \forall k, k' \in \mathcal{K}, \quad (6)$$

leads to a rejection-free proposal.

Table of Contents

- 1 Motivation and Background
- 2 Transport Reversible Jump Proposals
- 3 Illustrative Example**
- 4 Testing Proposal Performance
- 5 Numerical Example - Bayesian Factor Analysis
- 6 Conditional Transport Proposals
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Sinh Arcsinh 1D 2D Example

As an illustrative example with known TMs, we use the (element-wise) inverse sinh-arcsinh transformation of [Jones and Pewsey, 2009]

$$S_{\epsilon, \delta}(\cdot) = \sinh(\delta^{-1} \odot (\sinh^{-1}(\cdot) + \epsilon)),$$

where $\epsilon \in \mathbb{R}^n$, $\delta \in \mathbb{R}_+^n$. For an $n \times n$ matrix L , define a transform $T(\mathbf{Z})$ where

$$T(\mathbf{Z}) = S_{\epsilon, \delta}(L\mathbf{Z}), \quad (7)$$

and $\mathbf{Z} \sim \mathcal{N}(\mathbf{0}_n, I_{n \times n})$. The probability density function for the transformed variable $\boldsymbol{\theta} = T(\mathbf{Z})$ is

$$p_{\epsilon, \delta, L}(\boldsymbol{\theta}) = \phi_{LL^\top} \left(S_{\epsilon, \delta}^{-1}(\boldsymbol{\theta}) \right) |J_{S_{\epsilon, \delta}^{-1}}(\boldsymbol{\theta})|,$$

where $S_{\epsilon, \delta}^{-1}(\cdot) = \sinh(\delta \odot \sinh^{-1}(\cdot) - \epsilon)$.

Sinh Arcsinh 1D 2D Example

The target of interest for this example, where $\boldsymbol{\theta}_1 = (\theta_1^{(1)})$ and $\boldsymbol{\theta}_2 = (\theta_2^{(1)}, \theta_2^{(2)})$, is

$$\pi(k, \boldsymbol{\theta}_k) = \begin{cases} \frac{1}{4} p_{\epsilon_1, \delta_1, 1}(\boldsymbol{\theta}_1), & k = 1, \\ \frac{3}{4} p_{\epsilon_2, \delta_2, L}(\boldsymbol{\theta}_2), & k = 2, \end{cases} \quad (8)$$

where

$$\begin{aligned} \epsilon_1 &= -2, & \delta_1 &= 1, \\ \epsilon_2 &= (1.5, -2), & \text{and } \delta_2 &= (1, 1.5), \end{aligned} \quad (9)$$

and L is a lower-triangular matrix such that

$$LL^\top = \begin{bmatrix} 1 & 0.99 \\ 0.99 & 1 \end{bmatrix}.$$

By construction, for chosen reference distributions ϕ_n , $n_k = k$, the exact transport is given by the function

$$T^{-1}(\cdot) = L^{-1} S_{\epsilon, \delta}^{-1}(\cdot). \quad (10)$$

Example: Sinh Arcsinh Target with Transport RJ Proposal

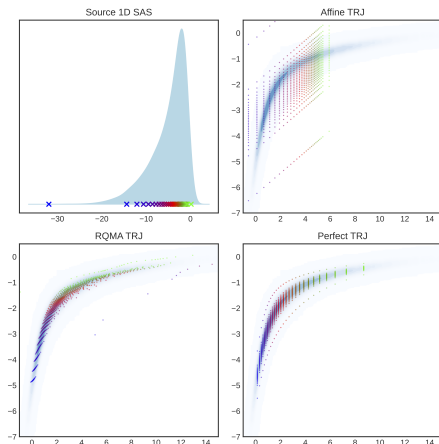
Systematic draws from conditional target $\pi(x_1 | k = 1)$ of (8) are transported from $(1, \theta_1) \in \mathcal{K} \times \mathbb{R}^1$ (top left) to $(2, (\theta_1, \theta_2)) \in \mathcal{K} \times \mathbb{R}^2$ via TRJ proposals using:

Top right Approximate affine,

Bottom left Approx RQMA-NF,

Bottom right Perfect TM.

The auxiliary variables in the proposals are also drawn systematically (30 for each point in the source distribution).



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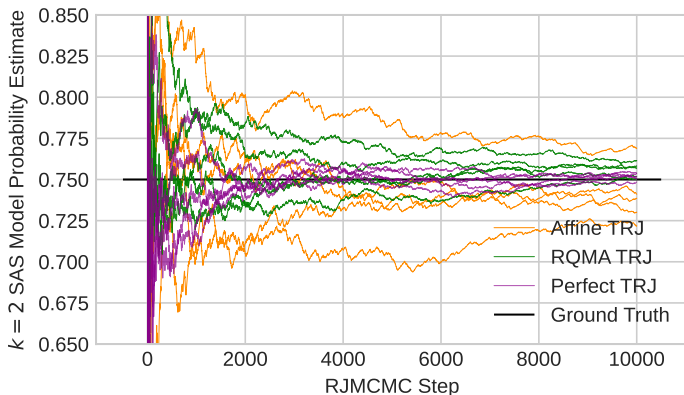


Figure: Running estimates of the model probabilities for the $k = 2$ component of the Sinh-Arcsinh target. Proposal are all TRJ with input TMs (1) Affine, (2) RQMA-NF, (3) Perfect. Ten chains on each proposal type are depicted, where alternating within-model proposals are a simple normal random walk.

Table of Contents

- 1 Motivation and Background
- 2 Transport Reversible Jump Proposals
- 3 Illustrative Example
- 4 Testing Proposal Performance**
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Modified Bartolucci Bridge Sampling Estimator

For an RJMCMC chain, [Bartolucci et al., 2006] showed that the Bayes factor $B_{k,k'}$ (ratio of marginal likelihoods) is estimated via

$$\hat{B}_{k,k'} = \frac{N_{k'}^{-1} \sum_{i=1}^{N_{k'}} \alpha'_i}{N_k^{-1} \sum_{i=1}^{N_k} \alpha_i}, \quad (11)$$

where $N_{k'}$ and N_k are the number of proposed moves from model k' to k , and from k to k' , respectively in the run of the chain.

In the special case when prior model probabilities are uniform, convert estimators of Bayes factors to estimators of model probabilities [Bartolucci et al., 2006,] via

$$\hat{\pi}(k) = \hat{B}_{j,k}^{-1} \left(1 + \sum_{i \in \mathcal{K} \setminus \{j\}} \hat{B}_{i,j} \right)^{-1}, \text{ for arbitrary } j \in \mathcal{K}. \quad (12)$$

The **Modified Bartolucci Estimator** (MBE) simply adopts the above for proposals from *samples* of the conditional targets.

Table of Contents

- 1 Motivation and Background
- 2 Transport Reversible Jump Proposals
- 3 Illustrative Example
- 4 Testing Proposal Performance
- 5 Numerical Example - Bayesian Factor Analysis**
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- 7 Discussion

Bayesian Factor Analysis

We model monthly exchange rates of six currencies relative to the British pound, spanning January 1975 to December 1986

[West and Harrison, 1997,], denoted as $\mathbf{y}_i \in \mathbb{R}^6$ for $i = 1, \dots, 143$, of the random vector \mathbf{Y} .

We assume $\mathbf{Y} \sim \mathcal{N}(\mathbf{0}_6, \Sigma)$, where

- $\Sigma = \beta_k \beta_k^\top + \Lambda$,
- Λ is a 6×6 positive diagonal matrix,
- β_k is a $6 \times k$ lower-triangular matrix with a positive diagonal,
- k is the number of factors, θ_k dimension $6(k+1) - k(k-1)/2$.

Bayesian Factor Analysis: Model Configuration

Following [Lopes and West, 2004], for each $\beta_k = [\beta_{ij}]$ with $i = 1, \dots, 6$, $j = 1, \dots, k$, the priors are

$$\begin{aligned}\beta_{ij} &\sim \mathcal{N}(0, 1), \quad i < j \\ \beta_{ii} &\sim \mathcal{N}_+(0, 1), \\ \Lambda_{ii} &\sim \mathcal{IG}(1.1, 0.05),\end{aligned}\tag{13}$$

We are interested in the posterior probability of $\theta_k = (\beta_k, \Lambda)$ for $k = 2$ or 3 factors, with θ_k dimensions 17 and 21 respectively. Via Bayes' Theorem the posterior is

$$\pi(k, \theta_k | \mathbf{y}) \propto p(k) p(\beta_k | k) p(\Lambda) \prod_{i=1}^{143} \phi_{\beta\beta^\top + \Lambda}(\mathbf{y}_i),\tag{14}$$

where $\mathbf{y} = (\mathbf{y}_1, \dots, \mathbf{y}_{143})$.

Bayesian Factor Analysis: Proposal Design

Original [Lopes and West, 2004] Independence Proposal

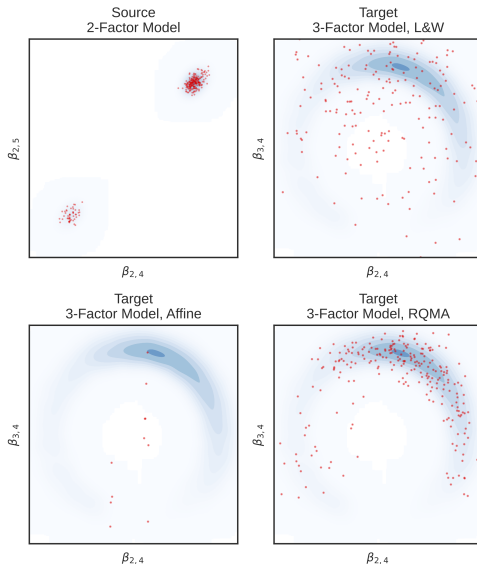
Write μ_{β_k} , B_k as the posterior mean and covariance of β_k . Denoting $\theta_k = (\beta_k, \Lambda)$, the independence proposal is

$$q_k(\theta_k) = q_k(\beta_k) \prod_{i=1}^6 q_k(\Lambda_{ii}), \quad (15)$$

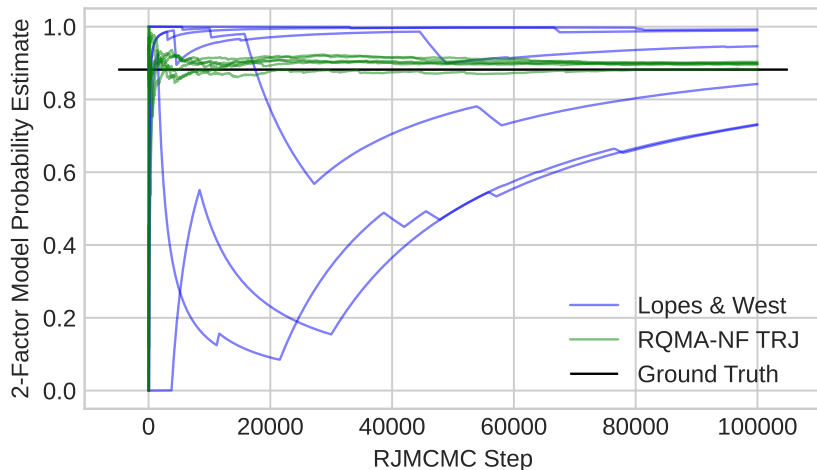
where for $k \in \mathcal{K}$, $q_k(\beta_k) = \mathcal{N}(\mu_{\beta_k}, 2B_k)$, and $q_k(\Lambda_{ii}) = \mathcal{IG}(18, 18v_{k,i}^2)$ where $v_{k,i}^2$ is the approximate conditional posterior mode of Λ_{ii} given k .

We compare the [Lopes and West, 2004] proposal to Affine and RQMA-NF TRJ trained on finite draws $s \sim \pi(\theta_k|k)$ obtained via HMC-NUTS (for $k = 3$) and SMC (for $k = 2$).

Bayesian Factor Analysis: Proposal Comparison



Bayesian Factor Analysis: Running Estimates from RJMCMC Chain



Bayesian Factor Analysis: MBE Study

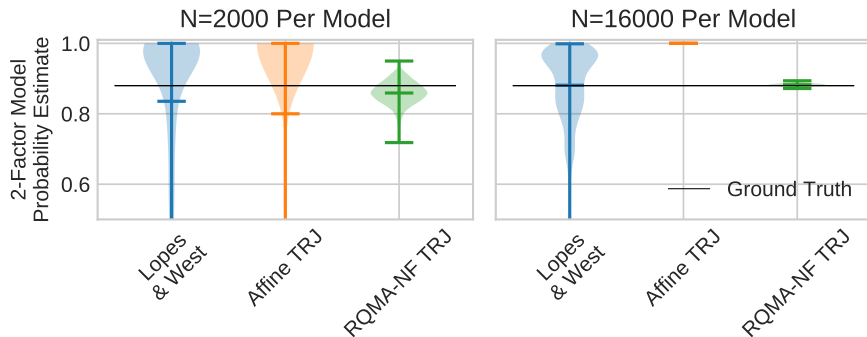


Figure: Violin plot showing the variability of the 2-factor model probability estimates in the case where only the 2-factor and 3-factor models are compared. Model probability estimates are obtained via the MBE. Ground truth is estimated via extended individual SMC runs ($N = 5 \cdot 10^4$).

Table of Contents

- 1 Motivation and Background
- 2 Transport Reversible Jump Proposals
- 3 Illustrative Example
- 4 Testing Proposal Performance
- 5 Numerical Example - Bayesian Factor Analysis
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Using One Transport (to rule them all)

Problem: Currently, we need to train an approximate TM for each model $k \in K$.

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Problem: Currently, we need to train an approximate TM for each model $k \in K$.

Solution: Re-frame target so that a *conditional* approximate TM can be used.

Conditional Transport Reversible Jump Proposals

The dimension-saturation approach, originally formalized in [Brooks et al., 2003], is an equivalent formulation of RJMCMC that involves an augmented target. Writing the maximum model dimension as n_{\max} (assumed to be finite) and recalling that $\mathbf{x} = (\boldsymbol{\theta}_k, k)$, we define our augmented target to be

$$\tilde{\pi}(\tilde{\mathbf{x}}) = \pi(\mathbf{x})(\otimes_{n_{\max}-n_k} \nu)(\mathbf{u}_{\smile k}), \quad (16)$$

where $\tilde{\mathbf{x}} = (k, \boldsymbol{\theta}, \mathbf{u}_{\smile k})$, and “ $\smile k$ ” identifies that the auxiliary variable is of dimension $n_{\max} - n_k$. In this setting, one can obtain approximate TMs by training a single conditional NF with the conditioning vector being the model index $k \in \mathcal{K}$. The associated proposals analogous to those in (4) are constructed as

$$(\boldsymbol{\theta}'_{k'}, \mathbf{u}_{\smile k'}) = c_{k'}^{-1} \circ \tilde{T}^{-1}(\cdot | k') \circ \tilde{T}(\cdot | k) \circ c_k(\boldsymbol{\theta}_k, \mathbf{u}_{\smile k}), \quad (17)$$

where $k' \sim j_k$, and c_k is simply concatenation.

Example: Block Variable Selection in Robust Regression

We are interested in realizations of a random response variable Y through a linear combination of predictor variables X_1, X_2, X_3 and $\beta = (\beta_0, \dots, \beta_3)$ parameters in a regression model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \epsilon,$$

We model the residual error term as a mixture between standard normal variable and a normal variable with a large variance. Use the notation for the model space $k = (1, k_1, k_2, k_2)$ where $k_i \in \{0, 1\}$ for $i = 1, 2$. The prior distributions are specified as

$$\begin{aligned} k_i &\sim \text{Bernoulli}(1/2), \quad i \in \{1, 2\}, \quad \text{and} \\ \beta_i &\sim \mathcal{N}(0, 10^2), \quad i \in \{0, 1, 2, 3\}. \end{aligned} \tag{18}$$

The target π is then the posterior distribution over the set of models and regression coefficients defined using Bayes' Theorem.

Example: Block Variable Selection in Robust Regression

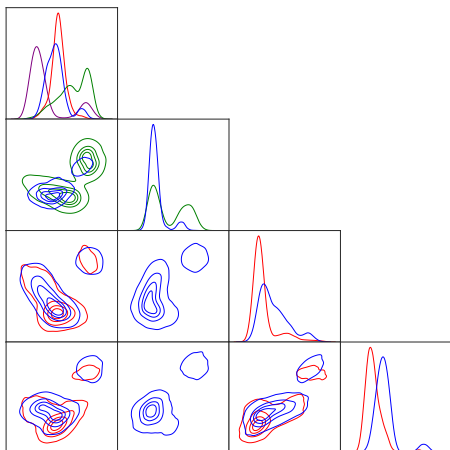


Figure: Pairwise plot of the conditional bivariate posterior densities in the Bayesian variable selection example. All four models feature: $k = (1, 0, 0, 0)$ (Purple), $k = (1, 1, 0, 0)$ (Green), $k = (1, 0, 1, 1)$ (Red), and $k = (1, 1, 1, 1)$ (Blue).

Example: Block Variable Selection in Robust Regression

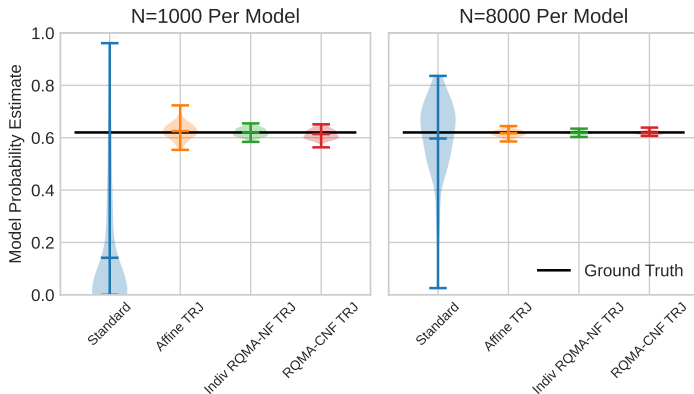


Figure: Violin plot showing the variability of the $k = (1, 1, 1, 1)$ model probability estimate for each proposal type using the MBE vs ground truth individual SMC ($N = 5 \cdot 10^4$). Individual SMC with $N = 1000, 8000$ particles sampled conditional targets split into training/test samples for a total of 80 passes.

Table of Contents

- 1 Motivation and Background
- 2 Transport Reversible Jump Proposals
- 3 Illustrative Example
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- We have introduced the idea of using a conditional normalizing flow to reduce training time. This would be useful for large model spaces!
- Efforts are justified in expensive-likelihood scenarios.
- Finally, whilst the MBE benchmark was used to assess cross-model proposal quality, the results seem promising and justify further investigation in lieu of standard RJMCMC.

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