Transport Reversible Jump Proposals

Using Normalising Flows

L. Davies[1] R. Salomone[2] M. Sutton[1] C. Drovandi[1]

[1]School of Mathematical Sciences
Queensland University of Technology

[2]School of Computer Science
Queensland University of Technology

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Problem: Sampling a Transdimensional Space

The problem of intrest is sampling probability distribution π on

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

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

$$\pi(k, \boldsymbol{\theta}_k) = \pi(k)\pi(\boldsymbol{\theta}_k | k).$$

When data $\boldsymbol{y}$ is introduced this is $\pi(k, \boldsymbol{\theta}_k | \boldsymbol{y}) = \pi(k|\boldsymbol{y})\pi(\boldsymbol{\theta}_k | k, \boldsymbol{y})$.
Notation. Denote $\boldsymbol{x} = (k, \boldsymbol{\theta}_k)$, ϕ_n is n-dimensional standard normal, $\phi_{\boldsymbol{\Sigma}_n}$ is an n-dimensional normal with mean $\mathbf{0}$ and $\boldsymbol{\Sigma}_n$ covariance, $|J_f(\boldsymbol{\theta})|$ denotes absolute determinant of Jacobian matrix of function $f : \mathbb{R}^n \to \mathbb{R}^n$, 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 $\boldsymbol{x}$ to point $\boldsymbol{x}'$, noting $\boldsymbol{\theta}_k$, $\boldsymbol{\theta}_{k'}$ have dimensions n_k, $n_{k'}$ respectively.

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

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

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

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

Transport Maps and Normalizing Flows

Consider random vectors $\boldsymbol{\theta} \sim \mu_{\boldsymbol{\theta}}$, $\boldsymbol{Z} \sim \mu_{\boldsymbol{z}}$, s.t. their distributions $\mu_{\boldsymbol{\theta}}$, $\mu_{\boldsymbol{z}}$ are absolutely continuous w.r.t. the n-dimensional Lebesgue measure.

Transport Map (TM)

A function $T : \mathbb{R}^n \to \mathbb{R}^n$ is called a *transport map* from $\mu_{\boldsymbol{\theta}}$ to $\mu_{\boldsymbol{z}}$ if $\mu_{\boldsymbol{z}} = T\sharp\mu_{\boldsymbol{\theta}}$.

Normalizing Flows (NF) and Flow-Based Models

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

$$\mu_{\boldsymbol{\zeta}}(\boldsymbol{\zeta}; \boldsymbol{\psi}) = \mu_{\boldsymbol{z}}(T_{\boldsymbol{\psi}}^{-1}(\boldsymbol{\zeta}))|J_{T_{\boldsymbol{\psi}}^{-1}}(\boldsymbol{\zeta})|, \ \boldsymbol{\zeta} \in R^n. \tag{3}$$

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

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

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Then, a transdimensional proposal where $n_{k'} > n_k$ is

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

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

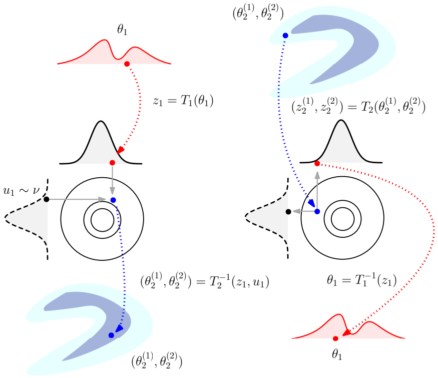

Figure: Illustration of the proposal class. Here, the reference ν is Gaussian. The diffeomorphisms ($\bar{h}$) on the reference distributions simply concatenate or extract coordinates as required.

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 $T_k \sharp \pi_k = \otimes_{n_k} \nu$. Then, (2) reduces to

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

Corollary

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

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

leads to a rejection-free proposal.

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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]

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

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

$$T(\boldsymbol{Z}) = S_{\boldsymbol{\epsilon},\boldsymbol{\delta}}(L\boldsymbol{Z}), \tag{7}$$

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

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

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

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

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

where

$$\begin{aligned} \epsilon_1 &= -2, & \delta_1 &= 1, \\ \boldsymbol{\epsilon}_2 &= (1.5, -2), \quad \text{and} & \boldsymbol{\delta}_2 &= (1, 1.5), \end{aligned} \tag{9}$$

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

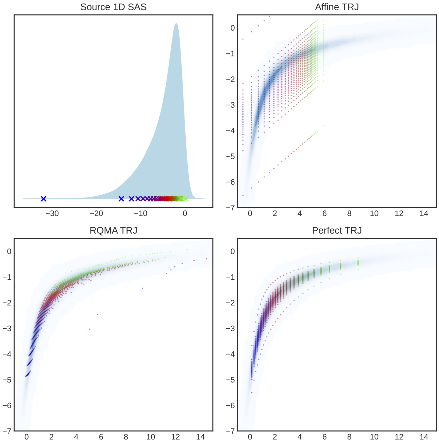
$$T^{-1}(\cdot) = L^{-1} S^{-1}_{\boldsymbol{\epsilon}, \boldsymbol{\delta}}(\cdot). \tag{10}$$

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



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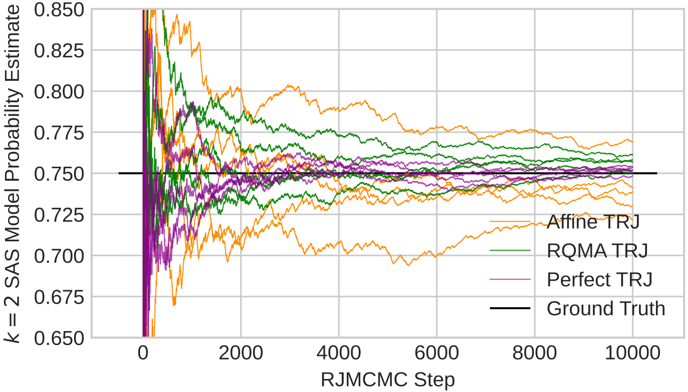

Figure: Running estimates of the model probabilities for the $k = 2$ component of the Sinh-Arcsinh target. Proposal are all TRJ with input TMs (1) Affine, (2) RQMA-NF, (3) Perfect. Ten chains on each proposal type are depicted, where alternating within-model proposals are a simple normal random walk.

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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

$$\hat{B}_{k,k'} = \frac{N_{k'}^{-1} \sum_{i=1}^{N_{k'}} \alpha_i'}{N_k^{-1} \sum_{i=1}^{N_k} \alpha_i}, \tag{11}$$

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

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

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

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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 $\boldsymbol{y}_i \in \mathbb{R}^6$ for $i = 1, ..., 143$, of the random vector $\boldsymbol{Y}$.

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

- $\boldsymbol{\Sigma} = \boldsymbol{\beta}_k \boldsymbol{\beta}_k^\top + \boldsymbol{\Lambda}$,
- Λ is a 6×6 positive diagonal matrix,
- $\boldsymbol{\beta}_k$ is a $6 \times k$ lower-triangular matrix with a positive diagonal,
- k is the number of factors, $\boldsymbol{\theta}_k$ dimension $6(k+1) - k(k-1)/2$.

Bayesian Factor Analysis: Model Configuration

Following [Lopes and West, 2004], for each $\boldsymbol{\beta}_k = [\beta_{ij}]$ with $i = 1, \ldots, 6$, $j = 1, \ldots, k$, 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 $\boldsymbol{\theta}_k = (\boldsymbol{\beta}_k, \boldsymbol{\Lambda})$ for $k = 2$ or 3 factors, with $\boldsymbol{\theta}_k$ dimensions 17 and 21 respectively. Via Bayes' Theorem the posterior is

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

where $\boldsymbol{y} = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_{143})$.

Bayesian Factor Analysis: Proposal Design

Original [Lopes and West, 2004] Independence Proposal

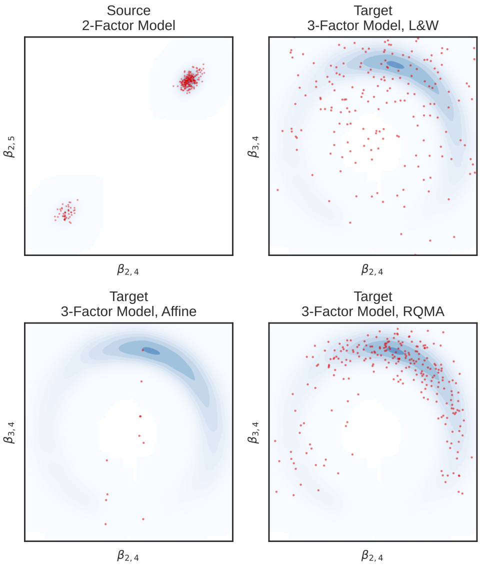
Write $\boldsymbol{\mu}_{\boldsymbol{\beta}_k}$, $\boldsymbol{B}_k$ as the posterior mean and covariance of $\boldsymbol{\beta}_k$. Denoting $\boldsymbol{\theta}_k = (\boldsymbol{\beta}_k, \boldsymbol{\Lambda})$, the independence proposal is

$$q_k(\boldsymbol{\theta}_k) = q_k(\boldsymbol{\beta}_k) \prod_{i=1}^{6} q_k(\Lambda_{ii}), \tag{15}$$

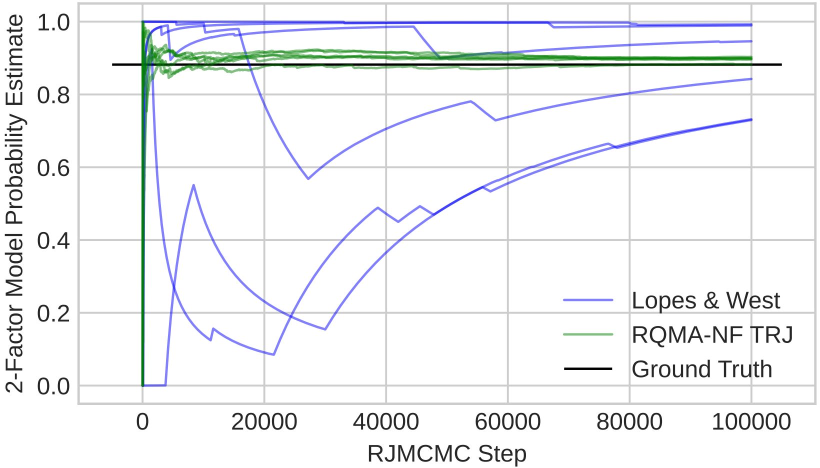
where for $k \in \mathcal{K}$, $q_k(\boldsymbol{\beta}_k) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\beta}_k}, 2\boldsymbol{B}_k)$, and $q_k(\Lambda_{ii}) = \mathcal{IG}(18, 18\upsilon_{k,i}^2)$ where $\upsilon_{k,i}^2$ is the approximate conditional posterior mode of Λ_{ii} given k.

We compare the [Lopes and West, 2004] proposal to Affine and RQMA-NF TRJ trained on finite draws $\boldsymbol{s} \sim \pi(\boldsymbol{\theta}_k|k)$ 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

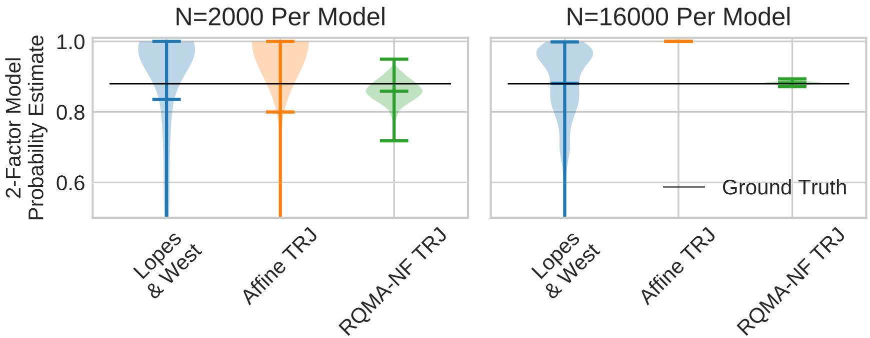


Figure: Violin plot showing the variability of the 2-factor model probability estimates in the case where only the 2-factor and 3-factor models are compared. Model probability estimates are obtained via the MBE. Ground truth is estimated via extended individual SMC runs ($N = 5 \cdot 10^4$).

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

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 $\boldsymbol{x} = (\boldsymbol{\theta}_k, k)$, we define our augmented target to be

$$\tilde{\pi}(\tilde{\boldsymbol{x}}) = \pi(\boldsymbol{x})(\otimes_{n_{\max}-n_k}\nu)(\boldsymbol{u}_{\backsim k}), \tag{16}$$

where $\tilde{\boldsymbol{x}} = (k, \boldsymbol{\theta}, \boldsymbol{u}_{\backsim k})$, and "$\backsim k$" identifies that the auxiliary variable is of dimension $n_{\max} - n_k$.

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 $\boldsymbol{\beta} = (\beta_0, ..., \beta_3)$ 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

$$\begin{aligned} &k_i \sim \text{Bernoulli}(1/2),\ i \in \{1, 2\}, \quad \text{and} \\ &\beta_i \sim \mathcal{N}(0, 10^2),\ i \in \{0, 1, 2, 3\}. \end{aligned} \tag{17}$$

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

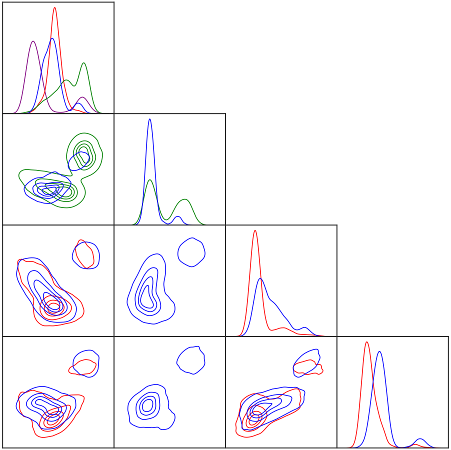

Figure: Pairwise plot of the conditional bivariate posterior densities in the Bayesian variable selection example. All four models feature: $k = (1, 0, 0, 0)$ (*Purple*) , $k = (1, 1, 0, 0)$ (*Green*), $k = (1, 0, 1, 1)$ (*Red*), and $k = (1, 1, 1, 1)$ (*Blue*).

Example: Block Variable Selection in Robust Regression

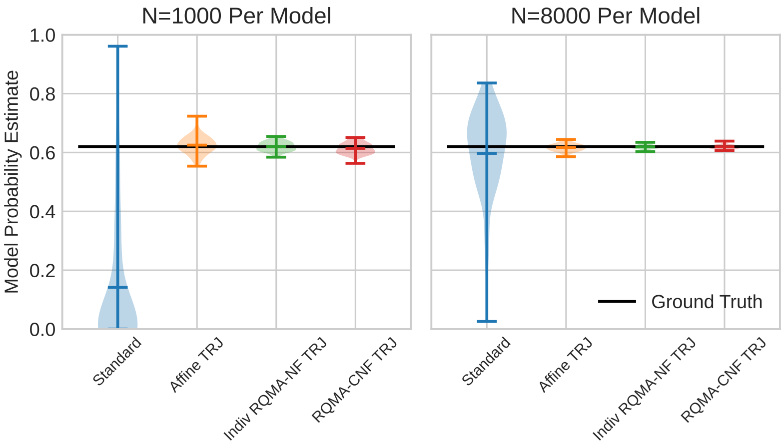

Figure: Violin plot showing the variability of the $k = (1, 1, 1, 1)$ model probability estimate for each proposal type using the MBE vs ground truth individual SMC ($N = 5 \cdot 10^4$). Individual SMC with $N = 1000, 8000$ particles sampled conditional targets split into training/test samples for a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

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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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