Transport Reversible Jump Proposals

Laurence Davies[1,3] **Robert Salomone**[2,3] **Matthew Sutton**[1,3] **Christopher Drovandi**[1,3]
[1] School of Mathematical Sciences, Queensland University of Technology
[2] School of Computer Science, Queensland University of Technology
[3] Centre for Data Science, Queensland University of Technology

Abstract

Reversible jump Markov chain Monte Carlo (RJMCMC) proposals that achieve reasonable acceptance rates and mixing are notoriously difficult to design in most applications. Inspired by recent advances in deep neural network-based normalizing flows and density estimation, we demonstrate an approach to enhance the efficiency of RJMCMC sampling by performing transdimensional jumps involving reference distributions. In contrast to other RJMCMC proposals, the proposed method is the first to apply a non-linear transport-based approach to construct efficient proposals between models with complicated dependency structures. It is shown that, in the setting where exact transports are used, our RJMCMC proposals have the desirable property that the acceptance probability depends only on the model probabilities. Numerical experiments demonstrate the efficacy of the approach.

1. Introduction

The problem of interest is sampling from a probability distribution π with support

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

where $\mathcal{K}$ is a discrete *index* set, and $\Theta_k \subseteq \mathbb{R}^{n_k}$, where the n_k may differ, and hence $\mathcal{X}$ is a *transdimensional* space. The choice of notation Θ_k is made as the problem typically arises in Bayesian model selection, where such sets correspond to the space of model *parameters*, and $k \in \mathcal{K}$ is a *model index* or indicator. The reversible jump Markov chain Monte Carlo (RJMCMC) algorithm, formally introduced by Green (1995), generalizes the Metropolis–Hastings (Hastings, 1970) algorithm via the introduction of user-specified diffeomorphisms[1] $h_{k,k'} : \Theta_k \times \mathcal{U}_k \to \Theta_{k'} \times \mathcal{U}_{k'}$ where $\mathcal{U}_k, \mathcal{U}_{k'}$ are (possibly empty) sets chosen to ensure dimensions are matched. Due to this additional complexity, RJMCMC proposals that perform well in practice are generally challenging to design.

RJMCMC methods are a frequently revisited research topic for which many approaches exist. Brooks et al. (2003) outline several approaches to improve the efficiency of jump proposals on various problem types, including variable selection and nested models. Green and Mira (2001) identify the efficiency issues associated with naïve transdimensional proposals between non-overlapping targets and propose a delayed-rejection auxiliary-proposal mechanism. Al-Awadhi et al. (2004) employ an auxiliary target density instead of an auxiliary proposal. Hastie (2005) proposes an approach for (potentially) multi-modal conditional target densities, achieved by fitting a Gaussian mixture model to each individual conditional target, and using a shift and whitening transformation corresponding to a randomly selected mixture component. Fan et al. (2008) propose a conditional factorization of a differentiable target density to sequentially construct a proposal density. Karagiannis and Andrieu (2013) propose the construction of a Markov chain through a geometrically annealed sequence of intermediate distributions between models to encourage higher acceptance rates between model jumps. Farr et al. (2015) propose a KD-tree approximation of the target density for auxiliary variable draws to improve the efficiency of RJMCMC proposals. Gagnon (2021) uses the locally-informed MCMC approach for discrete spaces developed by Zanella (2020) to improve the exploration efficiency of the model space when global jump proposals are unavailable. However, there appears to be no *general* strategy for the design of across-model proposals that is widely applicable, theoretically justified, and of practical use.

The use of measure transport to enhance sampling methods is an area of recent interest. First formalized and demonstrated in Parno and Marzouk (2018), where *approx-*

[1] bijective functions that are differentiable and have a differentiable inverse

imate TMs are used for accelerating MCMC. The form of the approximate transports as applied to MCMC sampling is described in general terms, but their choice of transports uses systems of orthogonal multivariate polynomials. The use of approximate TMs to enhance sampling methods includes mapping a deterministic step within sequential Monte Carlo (Arbel et al., 2021); the transformation of a continuous target distribution to an easier-to-sample distribution via a map learned using stochastic variational inference (Hoffman et al., 2018); and the use of approximate TMs for the construction of independence proposals in an adaptive MCMC algorithm (Gabrié et al., 2022).

However, despite the considerable promise of incorporating approximate TMs into sampling methodology, to our knowledge such ideas have not been considered in the *transdimensional* sampling setting. Such an omission is somewhat surprising, as RJMCMC samplers are constructed using a form of invertible maps involving distributions, and hence it would intuitively appear natural that distributional transport could feature in a useful capacity. This work aims to develop such an approach and to demonstrate its benefits.

Contribution. The primary contributions of this work are as follows:

I. A new class of RJMCMC proposals for across-model moves, called *transport reversible jump* (TRJ) proposals are developed. In the idealised case where exact transports are used, the proposals are shown to have a desirable property (Proposition 1).
II. A numerical study on challenging examples demonstrating the efficacy of the proposed approach in the setting where *approximate* transport maps are used is conducted.
III. A modified version of the model probability estimator of Bartolucci et al. (2006) is considered as a way to assess the quality of across-model proposals, and as an example use of effective TRJ proposals in the setting where one has samples from each conditional target.
IV. An alternative "all-in-one" approach to training approximate TMs is developed, which involves combining a saturated state space formulation of the target distribution with *conditional* TMs, is explored.

Structure of this Article The remainder of this article is structured as follows: Section 2 discusses the required background concepts regarding RJMCMC, transport maps, and flow-based models. Section 3 introduces a general strategy for using transport maps within RJMCMC and discusses its properties. Section 4 conducts a numerical study to demonstrate the efficacy of the strategy in the case where *approximate* transports are used. Section 5 explores an alternative "all-in-one" approach to training transport maps, and provides an associated numerical example. Section 6 concludes the paper.

Notation. For a function T and distribution ν, $T\sharp\nu$ denotes the *pushforward* of ν under T. That is, if $\boldsymbol{Z} \sim \nu$, then $T\sharp\nu$ is the probability distribution of $T(\boldsymbol{Z})$. For a univariate probability distribution ν, define $\otimes_n \nu$ as $\underbrace{\nu \otimes \cdots \otimes \nu}_{n \text{ times}}$. Throughout, univariate functions are to be interpreted as applied element-wise when provided with a vector as input. The symbol $\odot$ denotes the Hadamard (element-wise) product. The univariate standard normal probability density function is denoted as ϕ, ϕ_d is the d-dimensional multivariate standard normal probability density function, and $\phi_{\boldsymbol{\Sigma}_d}$ is the d-dimensional multivariate normal probability density function centered at $\mathbf{0}_d$ with covariance $\boldsymbol{\Sigma}_d$. For a function $f : \mathbb{R}^n \to \mathbb{R}^n$, the notation $|J_f(\boldsymbol{\theta})|$ denotes the absolute value of the determinant of the Jacobian matrix of f evaluated at some $\boldsymbol{\theta} \in \mathbb{R}^n$. For distributions π defined on sets of the form in (1), we write π_k for the distribution conditional on k, and $\pi(k)$ for its k-marginal distribution.

2. Background

2.1 Reversible Jump Markov Chain Monte Carlo

For a distribution π defined on a space of the form in (1), with associated probability density function $\pi(\boldsymbol{x})$, the standard method to construct a π-invariant Metropolis–Hastings kernel (and thus an associated Markov chain Monte Carlo sampler) is the *reversible jump* approach introduced in the seminal work by Green (1995). The proposal mechanism is constructed to take $\boldsymbol{x} = (k, \boldsymbol{\theta}_k)$ to $\boldsymbol{x}' = (k', \boldsymbol{\theta}'_{k'})$ where the dimensions of $\boldsymbol{\theta}_k$ and $\boldsymbol{\theta}'_{k'}$ are n_k and $n_{k'}$, respectively. The approach employs *dimension matching*, introducing auxiliary random variables $\boldsymbol{u}_k \sim g_{k,k'}$ and $\boldsymbol{u}'_{k'} \sim g_{k',k}$ of dimensions w_k and $w_{k'}$, which are arbitrary provided that $n_k + w_k = n_{k'} + w_{k'}$. A proposal is then made using these auxiliary random variables and a chosen diffeomorphism $h_{k,k'}$ defined so that $(\boldsymbol{\theta}'_{k'}, \boldsymbol{u}'_{k'}) = h_{k,k'}(\boldsymbol{\theta}_k, \boldsymbol{u}_k)$. A discrete proposal distribution j_k is also specified for each $k \in \mathcal{K}$, where $j_k(k')$ defines the probability of proposing to model k' from model k. More generally, the distributions j_k may also depend on $\boldsymbol{\theta}_k$, but we do not consider this case. With the above formulation of the proposal, the RJMCMC acceptance probability is

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

2.2 Transport Maps and Flow-Based Models

Consider two random vectors $\boldsymbol{\theta} \sim \mu_{\boldsymbol{\theta}}$ and $\boldsymbol{Z} \sim \mu_{\boldsymbol{Z}}$, such that their distributions $\mu_{\boldsymbol{\theta}}$ and $\mu_{\boldsymbol{Z}}$ are absolutely continuous with respect to n-dimensional Lebesgue measure. A function $T : \mathbb{R}^n \to \mathbb{R}^n$ is called a *transport map* (TM) from $\mu_{\boldsymbol{\theta}}$ to $\mu_{\boldsymbol{Z}}$ if $\mu_{\boldsymbol{Z}} = T\sharp\mu_{\boldsymbol{\theta}}$. In this setting, we refer to $\mu_{\boldsymbol{\theta}}$ as the *target* distribution and $\mu_{\boldsymbol{Z}}$ as the *reference* distribution. Transport maps between two prescribed distributions

are known to exist under mild conditions (see e.g., Parno and Marzouk (2018) and references therein).

One strategy for obtaining approximate TMs from samples of a target π is via density estimation with a family of distributions arising from transformations. Let $\{T_{\boldsymbol{\psi}}\}$ be a family of diffeomorphisms parameterized by $\boldsymbol{\psi} \in \Psi$ with domain on the support of some arbitrary *base* distribution $\mu_{\boldsymbol{z}}$. Then, for fixed $\boldsymbol{\psi}$, the probability density function of the random vector $\boldsymbol{\zeta} = T_{\boldsymbol{\psi}}(\boldsymbol{Z})$ is

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

An approximate TM from $\mu_{\boldsymbol{z}}$ to some prescribed target distribution π can be learned as a result of fitting a model of the above form to samples from π by minimizing KL divergence between the model and an empirical distribution of possibly-approximate samples from π, which is equivalent to maximum likelihood estimation.

Families of distributions arising from the specification of highly flexible and scalable $\{T_{\boldsymbol{\psi}}\}$ have been an area of intense recent interest in the machine learning literature, often referred to as *flow-based models*, with the families $\{T_{\boldsymbol{\psi}}\}$ often referred to as *flows* or *normalizing flows* (NF). A general class of transform are *autoregressive flows*, briefly described as follows. Let $\tau(\cdot; \boldsymbol{\omega})$, called the *transformer*, be a univariate diffeomorphism parametrized by $\boldsymbol{\omega} \in \boldsymbol{\Omega}$, where $\boldsymbol{\Omega}$ is the set of admissible parameters. Then, the transformation is defined elementwise via

$$T(\boldsymbol{Z})_i = \tau(Z_i; \boldsymbol{c}_i(\boldsymbol{z}_{<i}; \boldsymbol{\psi})), \quad i = 1, \ldots, n, \quad (4)$$

where the functions $\{\boldsymbol{c}_i : \mathbb{R}^{i-1} \to \boldsymbol{\Omega}\}$ are called the *conditioners*. In practice, the $\{\boldsymbol{c}_i\}$ are each individually subsets of the output of a single neural network that takes $\boldsymbol{Z}$ as input and is designed to respect the autoregressive structure. When fitting approximate transports to samples in our experiments in Section 4, for additional flexibility the flow-based model used is one that arises from *several* chained transformations of the form in (4), each with different parameters, and where the conditioner is a piecewise function involving monotonic rational-quadratic splines (Durkan et al., 2019). For further details and a comprehensive overview of other flows, see Papamakarios et al. (2021).

3. Transport Reversible Jump Proposals

We introduce a special form of general proposal between two models, corresponding to indices k and k'. Let ν be some *univariate* reference distribution, and let $\{T_k : \mathbb{R}^{n_k} \to \mathcal{Z}^{n_k}\}$ be a collection of diffeomorphisms such that $T_k \sharp \pi_k \approx \otimes_{n_k} \nu$, $k \in \mathcal{K}$, i.e., T_k is an approximate TM from the conditional target corresponding to index k, to an appropriately-dimensioned product of independent reference distributions. Similarly, T_k^{-1} is an approximate TM *from* the reference to the conditional target for index k. The general idea of the proposal scheme from model k to model k' is to first apply the transformation that would (approximately) transport π_k to its product reference, drawing auxiliary variables (if proposing to a higher-dimensional model), optionally applying a product reference measure preserving diffeomorphism, discarding auxiliary variables (if proposing to a lower dimensional model), and then applying the transformation that would (approximately) transport the augmented vector to the new conditional target. Figure 1 illustrates this idea from jumps between targets of one and two dimensions.

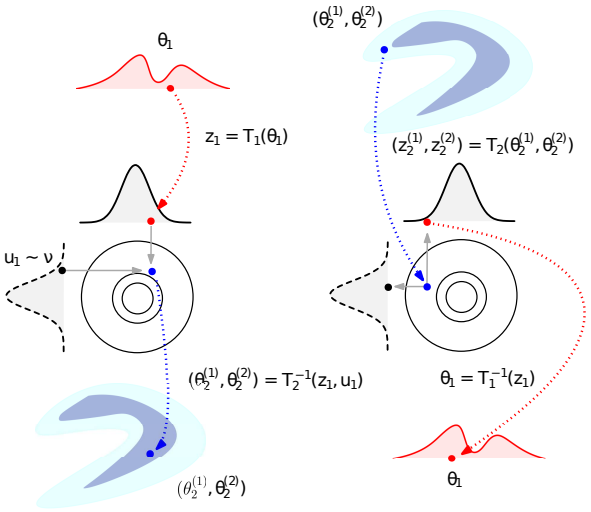

Figure 1: Illustration of the proposal class. Here, the reference ν is Gaussian. The diffeomorphisms ($\bar{h}$) on the reference distributions simply concatenate or extract coordinates as required.

Formally, we first restrict the dimension of proposed auxiliary variables $\boldsymbol{u}$ (if any) to w_k, which is defined to be the dimension difference between $\boldsymbol{\theta}_k$ and $\boldsymbol{\theta}'_{k'}$, i.e., $n_k + w_k = n_{k'}$. Then, assuming $w_k \geq 0$ (a jump is proposed to a model of equal or higher dimension), the proposal is obtained via

$$\begin{aligned} \boldsymbol{z}_k &= T_k(\boldsymbol{\theta}_k), \\ \boldsymbol{z}_{k'} &= \bar{h}_{k,k'}(\boldsymbol{z}_k, \boldsymbol{u}_k), \quad \text{where } \boldsymbol{u}_k \sim \otimes_{w_k} \nu, \\ \boldsymbol{\theta}'_{k'} &= T_{k'}^{-1}(\boldsymbol{z}_{k'}), \end{aligned} \quad (5)$$

where each $\bar{h}_{k,k'} : \mathbb{R}^{n_k} \times \mathbb{R}^{w_k} \to \mathbb{R}^{n_{k'}}$, is a diffeomorphism that both satisfies the pushforward-invariance condition

$$\bar{h}_{k,k'} \sharp \otimes_{\max\{n_k, n'_k\}} \nu = \otimes_{\max\{n_k, n'_k\}} \nu, \quad (6)$$

and is volume-preserving (i.e.,absolute value of the Jacobian determinant is always equal to one). The default choice is to set each $\bar{h}_{k,k'}$ equal to the identity (resulting in

just concatenation of the two inputs), but other choices are possible. For example, as $\otimes_{\max\{n_k,n'_k\}}\nu$ is exchangeable, permutations are also suitable. Proposal moves to lower dimensions are similar to those in (5), but as opposed to drawing auxiliary variables, the variables are discarded. The procedure of using our TRJ proposals within RJMCMC is given in Algorithm 1.

The following proposition provides a formal justification for the proposed approach, showing that when exact transports are used, (2) reduces to a form depending only on the marginal posterior model probabilities (i.e., there is a marginalizing effect).

Proposition 1. *Suppose that RJMCMC proposals are of the form described in (5), and for each $k \in \mathcal{K}$, satisfy $T_k \sharp \pi_k = \otimes_{n_k}\nu$. Then, (2) reduces to*

$$\alpha(\boldsymbol{x}, \boldsymbol{x}') = 1 \wedge \frac{\pi(k')}{\pi(k)} \frac{j_{k'}(k)}{j_k(k')}. \tag{7}$$

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

$$\pi(k')j_{k'}(k) = \pi(k)j_k(k'), \quad \forall k, k' \in \mathcal{K}, \tag{8}$$

leads to a rejection-free proposal.

A natural choice when allowing *global* moves, i.e., $j_k(k') > 0$ for all $k, k' \in \mathcal{K}$ that solves the above detailed balance condition (8) is simply to choose $j_k(k') = \pi(k')$ for all $\forall k \in \mathcal{K}$. Of course, in practice the marginal probabilities $\pi(k)$ are typically unknown. However, the above observation is potentially instructive as to what a good choice may be if some approximation of model probabilities is available.

Transdimensional RJMCMC proposals that employ *exact* transport maps to and from a reference distribution result in the same acceptance probabilities as performing *marginal* MCMC on the model indicator space, and thus are in some sense an optimal proposal for general RJMCMC settings.

4. Numerical Experiments

For all experiments, we use masked autoregressive transforms with rational quadratic splines (RQMA) (Durkan et al., 2020). Prior to the RQMA transforms, a fixed (i.e., non-trainable) element-wise standardization is applied, which we find has a positive effect on the speed and stability of training. The performance of transdimensional proposals is benchmarked in two different ways in our expeiments that follow.

Model Probability (Running Estimates) One way to benchmark the performance of an RJMCMC chain is to visualise the running estimates of the marginal probability of a given k as the RJMCMC chain progresses. On average, a chain that mixes more rapidly is expected to produce more accurate results with fewer iterations.

Modified Bartolucci Estimator To assess the effect of different transdimensional proposals alone (as opposed to in combination with within-model moves), we employ the Bayes factor bridge-sampling estimator of Bartolucci et al. (2006, Eq.16). The estimator relies on constructing a Rao-Blackwellized bridge sampling estimator on a special collection of augmented targets. An advantage of the approach is that it can be computed from stored values from the RJMCMC run. Specifically, the Bayes factor $B_{k,k'}$ (ratio of marginal likelihoods) is estimated via

$$\hat{B}_{k,k'} = \frac{N_{k'}^{-1}\sum_{i=1}^{N_{k'}} \alpha'_i}{N_k^{-1}\sum_{i=1}^{N_k} \alpha_i}, \tag{9}$$

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. The α and α' terms are simply the acceptance probabilities corresponding to those proposals, respectively. Rather than use the output of an RJMCMC run, a straightforward alternative when one has samples from the individual conditionals π_k and $\pi_{k'}$ (not necessarily obtained via RJMCMC) is the following. First, for each sample from model k and k', make one proposal of RJMCMC (inclusive of the random choice of model to jump to). Then, compute the estimator (9) using the acceptance probabilities corresponding to those proposals which propose a change in model. In the special case when prior model probabilities are uniform, it is straightforward to convert estimators of Bayes factors to estimators of model probabilities (Bartolucci et al., 2006) via

$$\hat{\pi}(k) = \hat{B}_{j,k}^{-1}\left(1 + \sum_{i \in \mathcal{K}\setminus\{j\}} \hat{B}_{i,j}\right)^{-1}, \tag{10}$$

for arbitrary $j \in \mathcal{K}$. In the sequel, the combination of multiple estimators of the form (9) within (10) is referred to as the *modified Bartolucci estimator* (MBE) of model probabilities. We expect the MBE to exhibit the lowest variance for the best across-model proposal type when computed using the same input set of samples from all models (as well as the same model jump probabilities $\{j_k\}$).

4.1 Illustrative Example

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

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

Algorithm 1: TRJ: Transport Reversible Jump MCMC

input : $\boldsymbol{x} = (k, \boldsymbol{\theta}_k), \{T_k\}, \pi, \{j_k\}, \nu, \{P_k(\boldsymbol{\theta}, d\boldsymbol{\theta}')\}$ such that each P_k is π_k-reversible.

Draw $k' \sim j_k$

if $k' = k$ **then**

  Draw $\boldsymbol{\theta}'_k \sim P_k(\boldsymbol{\theta}_k, d\boldsymbol{\theta}'_k)$ and **return** $(k, \boldsymbol{\theta}'_k)$

else

  $\boldsymbol{z}_k \leftarrow T_k(\boldsymbol{\theta}_k)$

  if $n_{k'} > n_k$ **then**

    $w_k \leftarrow n_{k'} - n_k$

    Draw $\boldsymbol{u} \sim \otimes_{w_k} \nu$

    $g_u \leftarrow (\otimes_{w_k} \nu)(\boldsymbol{u})$, $g'_u \leftarrow 1$

    $\boldsymbol{z}_{k'} \leftarrow \bar{h}_{k,k'}(\boldsymbol{z}_k, \boldsymbol{u})$

  else if $n_{k'} < n_k$ **then**

    $w_{k'} \leftarrow n_k - n_{k'}$

    $(\boldsymbol{z}_{k'}, \boldsymbol{u}) \leftarrow \bar{h}^{-1}_{k,k'}(\boldsymbol{z}_k)$

    $g_u \leftarrow 1$, $g'_u \leftarrow (\otimes_{w_{k'}} \nu)(\boldsymbol{u})$

  else

    $\boldsymbol{z}_{k'} \leftarrow \bar{h}^{-1}_{k,k'}(\boldsymbol{z}_k)$

    $g_u \leftarrow 1$, $g'_u \leftarrow 1$

  $\boldsymbol{\theta}'_{k'} \leftarrow T^{-1}_{k'}(\boldsymbol{z}_{k'})$

  $\boldsymbol{x}' \leftarrow (k', \boldsymbol{\theta}'_{k'})$

  $\alpha \leftarrow 1 \wedge \frac{\pi(\boldsymbol{x}')}{\pi(\boldsymbol{x})} \frac{j_{k'}(k)}{j_k(k')} \frac{g'_u}{g_u} \left| J_{T_k}(\boldsymbol{\theta}_k) \right| \left| J_{T_{k'}}(\boldsymbol{\theta}'_{k'}) \right|^{-1}$

  Draw $V \sim \mathcal{U}(0,1)$

  if $\alpha > V$ **then return** $\boldsymbol{x}'$

  else return $\boldsymbol{x}$

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

$$T(\boldsymbol{Z}) = S_{\boldsymbol{\epsilon},\boldsymbol{\delta}}(\mathrm{L}\boldsymbol{Z}), \tag{11}$$

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

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

where $S^{-1}_{\boldsymbol{\epsilon},\boldsymbol{\delta}}(\cdot) = \sinh(\boldsymbol{\delta} \odot \sinh^{-1}(\cdot) - \boldsymbol{\epsilon})$. We consider a transdimensional target consisting of 2 models of dimension $n_1 = 1$ and $n_2 = 2$. We assign a probability of $1/4$ for model $k = 1$ with parameters $\boldsymbol{\theta}_1 = (\theta_1^{(1)})$ and model probability of $3/4$ for $k = 2$ with parameters $\boldsymbol{\theta}_2 = (\theta_2^{(1)}, \theta_2^{(2)})$. The target of interest for this example is

$$\pi(k, \boldsymbol{\theta}_k) = \begin{cases} \frac{1}{4} p_{\epsilon_1,\delta_1,1}(\boldsymbol{\theta}_1), & k = 1, \\ \frac{3}{4} p_{\boldsymbol{\epsilon}_2,\boldsymbol{\delta}_2,\mathrm{L}}(\boldsymbol{\theta}_2), & k = 2, \end{cases} \tag{12}$$

where

$$\begin{aligned} &\epsilon_1 = -2, \qquad \delta_1 = 1, \\ &\boldsymbol{\epsilon}_2 = (1.5, -2), \quad \text{and} \quad \boldsymbol{\delta}_2 = (1, 1.5), \end{aligned} \tag{13}$$

and L is a lower-triangular matrix such that

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

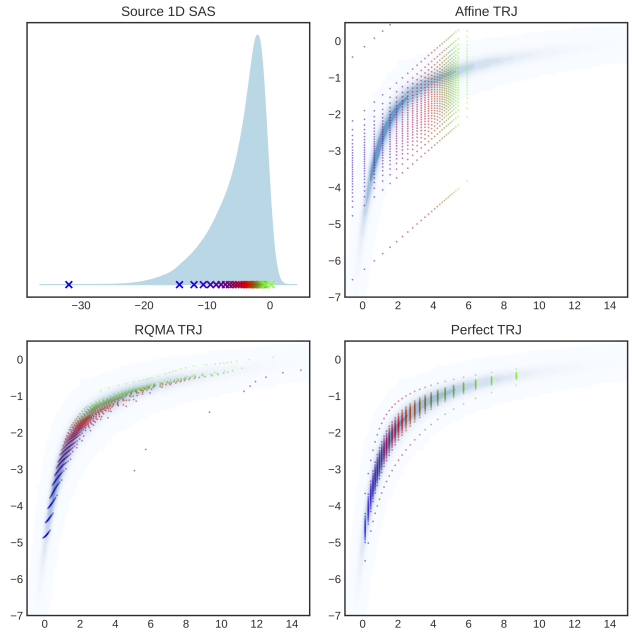

Figure 2: Systematic draws from conditional target $\pi(x_1|k=1)$ defined in (12) are transported from $(1, \theta_1) \in \mathcal{K} \times \mathbb{R}^1$ (*top left*) to $(2, (\theta_1, \theta_2)) \in \mathcal{K} \times \mathbb{R}^2$ via proposals using: (1) approximate affine (*top right*), (2) approximate RQMA-NF (*bottom left*), and (3) perfect (*bottom right*) TMs. The auxilliary variables in the proposals are also drawn systematically (30 for each point in the source distribution).

By construction, for a reference distribution chosen to be a multidimensional standard Gaussian of appropriate dimension, the exact transport is given by the function

$$T^{-1}(\cdot) = \mathrm{L}^{-1} S^{-1}_{\boldsymbol{\epsilon},\boldsymbol{\delta}}(\cdot). \tag{14}$$

Here, the choice of $j_k(k') = \frac{1}{4}\mathbb{I}_{\{k'=1\}} + \frac{3}{4}\mathbb{I}_{\{k'=2\}}$, for $k \in \{1, 2\}$, i.e., the mixture weights, correspond to a rejection-free proposal when the above are used.

In this example, for each individual k-conditional target, a training set and an independent test set of samples are drawn via exact sampling. RQMA-based NFs are fit to the conditional targets using the training set. Proposals are compared using the test set. The performance of RQMA-NF TRJ proposals is assessed via comparison to a TRJ proposal that uses a simple affine whitening transformation based on the estimated first two moments of the training set.

Figure 2 depicts a visualization of the proposal distributions (including those obtained using the exact transport map), and Figure 3 visualizes the running estimate of

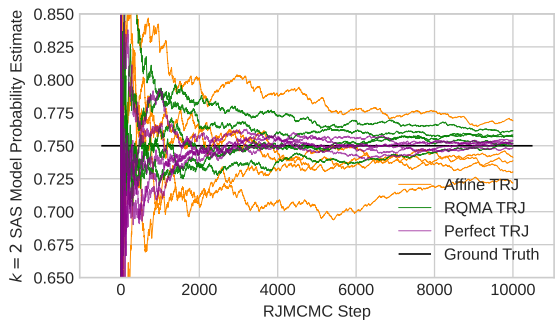

Figure 3: Running estimates of the model probabilities for the $k = 2$ component of the Sinh-Arcsinh target (12). Proposal are all Algorithm 1 with input approximate TMs (1) Affine, (2) RQMA-NF, (3) Perfect (14). Ten chains on each proposal type are depicted, where alternating within-model proposals are a simple normal random walk.

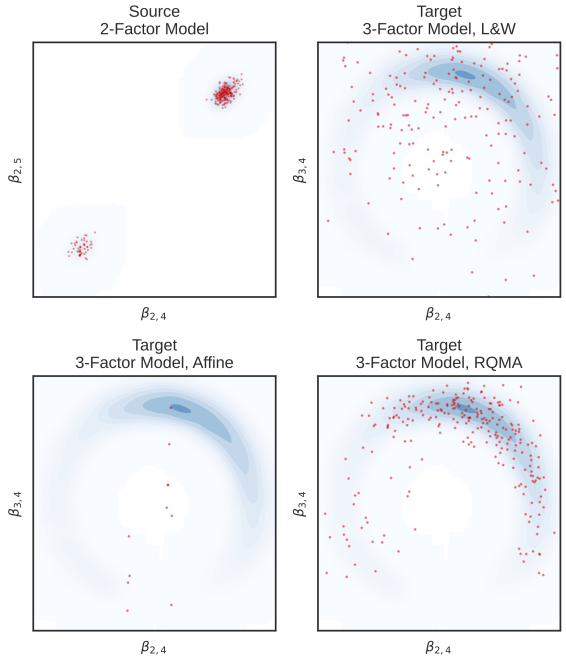

Figure 4: A visualization (using selected bivariate plots) of the proposal from points on the 2-factor model (*top-left*) to proposed points on the 3-factor model for each proposal type: Lopes and West (2004) independence RJMCMC proposal (*top right*); TRJ with Affine map (*bottom left*); TRJ with RQMA-NF map (*bottom right*).

model probabilities for each proposal type, where $j_k(k')$ is set to the mixture weights as above.

4.2 Bayesian Factor Analysis Example

Here we consider the factor analysis (FA) model from Lopes and West (2004) (also treated in South et al. (2019)). Factor analysis assumes the model $\boldsymbol{Y} \sim \mathcal{N}(\boldsymbol{0}_6, \boldsymbol{\Sigma})$ where the covariance takes the form $\boldsymbol{\beta}_k\boldsymbol{\beta}_k^\top + \boldsymbol{\Lambda}$, where 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, and the total number of parameters is $6(k+1) - k(k-1)/2$. We model monthly exchange rates of six currencies relative to the British pound, spanning January 1975 to December 1986 (West and Harrison, 1997) as 143 realisations, denoted as $\boldsymbol{y}_i \in \mathbb{R}^6$ for $i = 1, ..., 143$, of the random vector $\boldsymbol{Y}$. For this example, we are interested in $k = 2$ or 3 factors, producing parameter spaces of dimension 17 and 21, respectively. Following Lopes and West (2004), for each $\boldsymbol{\beta}_k = [\beta_{ij}]$ with $i = 1, \ldots, 6$, $j = 1, \ldots, k$, the priors are

$$\begin{aligned} \beta_{ij} &\sim \mathcal{N}(0, 1), \quad i < j \\ \beta_{ii} &\sim \mathcal{N}_+(0, 1), \\ \Lambda_{ii} &\sim \mathcal{IG}(1.1, 0.05), \end{aligned} \tag{15}$$

where $\mathcal{N}_+$ denotes the (positive) half-normal distribution and $\mathcal{IG}$ the inverse gamma distribution. We are interested in the posterior probability of $\boldsymbol{\theta}_k = (\boldsymbol{\beta}_k, \boldsymbol{\Lambda})$ for $k = 2$ or 3 factors. Via Bayes' Theorem the posterior is

$$\pi(k, \boldsymbol{\theta}_k|\boldsymbol{y}) \propto p(k)p(\boldsymbol{\beta}_k|k)p(\boldsymbol{\Lambda}) \prod_{i=1}^{143} \phi_{\boldsymbol{\beta}\boldsymbol{\beta}^\top + \boldsymbol{\Lambda}}(\boldsymbol{y}_i), \tag{16}$$

where $\boldsymbol{y} = (\boldsymbol{y}_1, ..., \boldsymbol{y}_{143})$. The proposals used in this study are the original RJMCMC proposal from Lopes and West (2004), and two instances of Algorithm 1 that use approximate affine and RQMA-NF TMs respectively trained on samples from the conditional target distributions. The form of the Lopes and West (2004) RJMCMC proposal is an independence proposal trained on the conditional posterior of each model. We 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 $q_k(\boldsymbol{\theta}_k) = q_k(\boldsymbol{\beta}_k) \prod_{i=1}^6 q_k(\Lambda_{ii})$, 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.

To obtain training and test sets of samples from (16), we use the No-U-Turn Sampler (NUTS) (Hoffman and Gelman, 2014) as implemented in PyMC (Salvatier et al., 2016) for the 3-factor model and static sequential Monte Carlo (SMC) (Del Moral et al., 2006) for the 2-factor model where the target (16) is annealed from the prior (15) to define the sequence of distributions. Training and test sets were sampled in independent runs, with the size of each set being either $N = 2000$ or $N = 16000$. This was performed ten times. Subsequently, TRJ proposals were constructed using an approximate TM trained on each training set, and independence proposals were trained on the same. This was performed one hundred times. Each proposal was then used to perform one run of the MBE estimator.

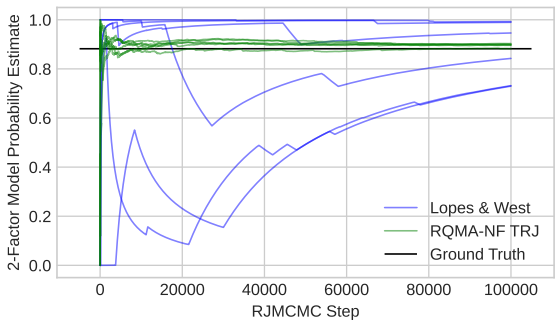

Figure 5: Running estimates of the model probabilities for the 2-factor model. Proposal types are the Lopes and West (2004) independence proposal and the RQMA-NF proposal using Algorithm 1. Six chains on each proposal type are depicted, where alternating within-model proposals are not shown.

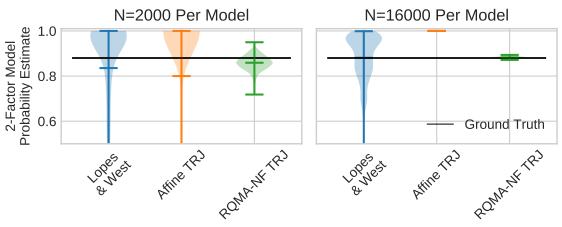

Figure 6: Violin plot (based on the example in Section 4.2) showing the variability of the 2-factor model probability estimates in the case where only the 2-factor and 3-factor models are compared. Model probability estimates are obtained via the MBE. Ground truth is estimated via extended individual SMC runs ($N = 5 \cdot 10^4$).

Figure 5 visualizes a comparison of the running estimate of the 2-factor posterior model probability for RJMCMC chains that use the independence proposal and the RQMA-NF TRJ proposal against the ground truth value of 0.88. Each chain was run for $200,000$ steps alternating between RJMCMC and within-model normal random walk proposals (the latter steps removed for visualization). Figure 6 visualizes the variability of model probability estimates from application of the MBE method.

Numerical examples demonstrate a clear benefit to using transport RJMCMC proposals in cases where the transport maps are *approximate*, which is typically the best one can hope for in practice.

5. Conditional Transport Proposals

So far, we have introduced a proposition for rejection-free RJMCMC moves based on perfect TMs and model probabilities, and an approach to approximate both of the unknown quantities. However, there is one clear drawback to this approach: larger model spaces, such as those encountered in variable selection problems, would still require k *individual* approximate TMs to be trained. This section explores how to overcome the above problem so one can obtain the approximate TMs by training a *single* conditional NF, and modifying the sampling problem appropriately via a *saturated space* approach. It also provides a numerical variable selection example as a proof of concept for the approach.

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

$$\tilde{\pi}(\tilde{\boldsymbol{x}}) = \pi(\boldsymbol{x})(\otimes_{n_{\max}-n_k}\nu)(\boldsymbol{u}_{\backsim k}), \tag{17}$$

where $\tilde{\boldsymbol{x}} = (k, \boldsymbol{\theta}, \boldsymbol{u}_{\backsim k})$, and "$\backsim k$" identifies that the auxiliary variable is of dimension $n_{\max} - n_k$. 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 (5) are constructed as $(\boldsymbol{\theta}'_{k'}, \boldsymbol{u}_{\backsim k'}) = c_{k'}^{-1} \circ \tilde{T}^{-1}(\cdot|k') \circ \tilde{T}(\cdot|k) \circ c_k(\boldsymbol{\theta}_k, \boldsymbol{u}_{\backsim k})$, where $k' \sim j_k$, and c_k is simply concatenation. The above yields Algorithm 2.

Algorithm 2: CTRJ: Conditional Transport RJMCMC

input : $\tilde{\boldsymbol{x}} = (k, \boldsymbol{\theta}_k, \boldsymbol{u}_{\backsim k}), \tilde{T}, \tilde{\pi}, \{j_k\}, \nu, \{P_k(\boldsymbol{\theta}, d\boldsymbol{\theta}')\}$
Draw $k' \sim j_k$
if $k' = k$ **then**
  Draw $\boldsymbol{\theta}'_k \sim P_k(\boldsymbol{\theta}_k, d\boldsymbol{\theta}'_k)$
  return $(k, \boldsymbol{\theta}'_k, \boldsymbol{u}_{\backsim k})$
else

$$\begin{aligned}
\boldsymbol{\xi}_k &\leftarrow c_{k,k'}(\boldsymbol{\theta}_k, \boldsymbol{u}_{\backsim k}) \\
\boldsymbol{z} &\leftarrow \tilde{T}(\boldsymbol{\xi}_k|k) \\
\boldsymbol{\xi}_{k'} &\leftarrow \tilde{T}^{-1}(\boldsymbol{z}|k') \\
(\boldsymbol{\theta}'_{k'}, \boldsymbol{u}_{\backsim k'}) &\leftarrow c_{k',k}^{-1}(\boldsymbol{\xi}_{k'}) \\
\tilde{\boldsymbol{x}}' &\leftarrow (k', \boldsymbol{\theta}'_{k'}, \boldsymbol{u}_{\backsim k'}) \\
\alpha &\leftarrow 1 \wedge \frac{\tilde{\pi}(\tilde{\boldsymbol{x}}')}{\tilde{\pi}(\tilde{\boldsymbol{x}})} \frac{j_{k'}(k)}{j_k(k')} \left|J_{\tilde{T}}(\boldsymbol{\theta}_k|k)\right| \left|J_{\tilde{T}}(\boldsymbol{\theta}'_{k'}|k')\right|^{-1}
\end{aligned}$$

  Draw $V \sim \mathcal{U}(0,1)$
  if $\alpha > V$ **then return** $\tilde{\boldsymbol{x}}'$
  else return $\tilde{\boldsymbol{x}}$

5.1 Block Variable Selection in Robust Regression Example

For this example, we seek a challenging Bayesian model choice problem where conventional methods do not perform well. We are interested in realizations of a random response variable Y through a linear combination of pre-

dictor variables X_1, X_2, X_3 in a regression model

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

where $\boldsymbol{\beta} = (\beta_0, ..., \beta_3)$ is the vector of unknown regression parameters. We model the residual error term as a mixture between standard normal variable and a normal variable with a large variance. To ease the exposition, we adjust the notation slightly to accommodate the Bayesian variable selection literature. Let k be an indicator vector where the ith position of k equals 1 if the variable β_i variable is included in model k and 0 otherwise — e.g. the model indexed by $k = (1, 0, 1, 1)$ corresponds to the model with parameters $\boldsymbol{\theta}_k = (\beta_0, \beta_2, \beta_3)$. We consider model-space cardinality of 4 composed of all models of the form $k = (1, k_1, k_2, k_2)$ where $k_i \in \{0, 1\}$ for $i = 1, 2$. These models will include or exclude the parameters β_2 and β_3 jointly as commonly considered in group variable selection (e.g. Xu and Ghosh (2015)).

The prior distributions are specified as

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

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

We consider simulated data consisting of 80 observations. The covariates of the model were simulated independently from a standard normal distribution. The data was simulated from the model $k = (1, 1, 0, 0)$ where the first half was generated using $\boldsymbol{\theta}_k = (1, 1)$ and the second half was simulated using $\boldsymbol{\theta}_k = (6, 1)$ and the residuals were simulated from a normal distribution with mean zero and variance 25. We made this choice to induce challenging multimodal features in the resulting posterior. See the supplementary materials for visualisations of the pathological posterior behaviour.

The design of each proposal is as follows. The "standard" proposal adopts the *independent auxiliary variable* method of Brooks et al. (2003), which is equivalent to using the augmented target (17) where ν is the prior distribution for β_i, i.e. $\mathcal{N}(0, 10^2)$. The standard proposals are deterministic in the sense that no auxiliary variables are drawn, but rather the i^{th} block of parameters is reinstated when $k_i = 1$. The TRJ affine and RQMA-NF proposals apply Algorithm 1 with approximate affine and RQMA-NF TMs respectively trained on samples from the conditional target distributions. The CTRJ proposal adopts the augmented target (17) where ν is set to the reference univariate density as described in Section 5, and proceeds as per Algorithm 2. The empirical performance of each proposal is examined for training and test sets of various sizes for each conditional target distribution. The Bayes Factors are estimated via application of the MBE. Figure 7 visualizes the variability of the $k = (1, 1, 1, 1)$ model probability estimate using the same approach as in Section 4.2, but with conditional posteriors of sizes $N = 2 \times 1000$ and $N = 2 \times 8000$ sampled from a single SMC pass before being split evenly into training and test sets, and using one MBE pass per training/test set for a total of 80 sets.

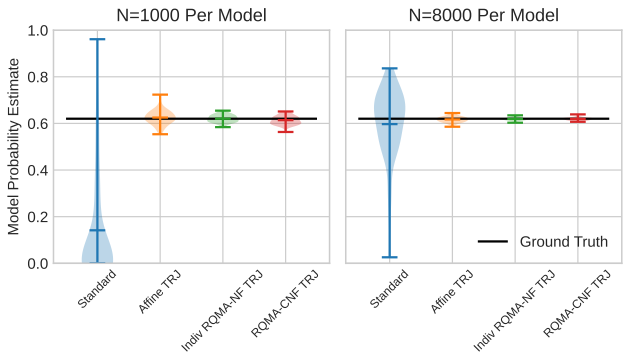

Figure 7: Violin plot (from the example in Section 5.1) showing the variability of the $k = (1, 1, 1, 1)$ model probability estimate for each proposal type using the Bartolucci Estimator vs ground truth individual SMC ($N = 5 \cdot 10^4$). Each model posterior was sampled using individual SMC samplers of $N = 1000, 8000$ particles with a random walk kernel for a total of 80 passes.

6. Discussion

The work introduces a method to design across-model RJMCMC proposals using ideas from measure transport. The approach was shown to have desirable properties in the case where exact TMs are used, while still providing good performance in the case where the TMs are approximate. Although some form of initial effort to obtain samples from each conditional target are somewhat common when calibrating proposals (e.g., as in Lopes and West (2004); Hastie (2005)), this is still a weakness of TRJ proposals, along with the required effort in training of the maps. The use of conditional NFs may mitigate the latter somewhat, but a promising avenue for future research would be some form of amortized approach in model spaces where there is some shared structure (and thus perhaps samples from only *some* models would suffice). Moreover, the effort may be justified in settings where likelihoods are particularly expensive, gradient-based methods are unavailable (e.g., implicit models), or else the gain in performance appropriately justifies the effort in obtaining the approximate TMs.

Finally, while we mainly introduced the MBE to benchmark cross-model proposal quality, the results seem promising and it may be interesting to explore its use in lieu of standard RJMCMC if efforts to obtain approximate TMs have already occurred.

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Supplementary Materials

A. Proof of Proposition 1

Proof. **(Proposition 1)** Here, we employ the shorthand notation $\nu_n := \otimes_n \nu$ and $\nu_n(\cdot) := (\otimes_n \nu)(\cdot)$ for measure and probability density functions, respectively. For a diffeomorphism $(\boldsymbol{\theta}'_{k'}, \boldsymbol{u}_{k'}) = h_{k,k'}(\boldsymbol{\theta}_k, \boldsymbol{u}_k)$, auxiliary variables $\boldsymbol{u}_k \sim g_{k,k'}$, $\boldsymbol{u}_{k'} \sim g_{k',k}$ of respective dimensions w_k and $w_{k'}$, if the dimension matching requirement $n_{k'} + w_{k'} = n_k + w_k$ is satisfied, then the standard choice (Green, 1995) for the acceptance probability that satisfies detailed balance is

$$\alpha(\boldsymbol{x}, \boldsymbol{x}') = 1 \wedge \frac{\pi(\boldsymbol{x}')j_{k'}(k)g_{k',k}(\boldsymbol{u}_{k'})}{\pi(\boldsymbol{x})j_k(k')g_{k,k'}(\boldsymbol{u}_k)}|J_{h_{k,k'}}(\boldsymbol{\theta}_k, \boldsymbol{u}_k)|. \tag{19}$$

First, consider the case that $n_{k'} > n_k$. The proposed move from index k to k' is

$$\boldsymbol{\theta}'_{k'} = h_{k,k'}(\boldsymbol{\theta}_k, \boldsymbol{u}_k) = T_{k'}^{-1}(\bar{h}_{k,k'}(T_k(\boldsymbol{\theta}_k), \boldsymbol{u}_k)), \quad \text{where } \boldsymbol{u}_k \sim \nu_{w_k}. \tag{20}$$

In this setting, we have $\boldsymbol{u}_{k'} = \emptyset$, $w_{k'} = 0$, and $g_{k,k'} = \nu_{w_k}$. Note that $g_{k,k'} = \nu_0$ (i.e., an "empty" distribution), so $g_{k',k}(\boldsymbol{u}_{k'}) = 1$. Further, the dimension-matching requirement reduces to $n_{k'} = n_k + w_k$. Using the properties that $|J_{f_1 \circ f_2}| = |J_{f_1}| \cdot |J_{f_2}|$ and $|J_{f^{-1}}| = |J_f|^{-1}$, along with the assumption that $\bar{h}_{k,k'}$ is a volume-preserving map, i.e., $|J_{\bar{h}_{k,k'}}| = 1$, we have that

$$|J_{h_{k,k'}}(\boldsymbol{\theta}'_{k'}, \boldsymbol{u}_{k'})| = |J_{T_k}(\boldsymbol{\theta}_k)| \cdot |J_{\bar{h}_{k,k'}}(T_k(\boldsymbol{\theta}'_{k'}), \boldsymbol{u}_{k'})| \cdot |J_{T_{k'}}(\boldsymbol{\theta}'_{k'})|^{-1} = \frac{|J_{T_k}(\boldsymbol{\theta}_k)|}{|J_{T_{k'}}(\boldsymbol{\theta}'_{k'})|}. \tag{21}$$

Making the above substitutions into (19), and employing the conditional factorization identity $\pi(\boldsymbol{x}) = \pi(k)\pi_k(\boldsymbol{\theta}_k)$ to both $\pi(\boldsymbol{x})$ and $\pi(\boldsymbol{x}')$ yields

$$\alpha(\boldsymbol{x}, \boldsymbol{x}') = 1 \wedge \frac{j_{k'}(k)\pi(k')}{j_k(k')\pi(k)} \left(\frac{\pi_{k'}(\boldsymbol{\theta}'_{k'})|J_{T_k}(\boldsymbol{\theta}_k)|}{\nu_{w_k}(\boldsymbol{u}_k)\pi_k(\boldsymbol{\theta}_k)|J_{T_{k'}}(\boldsymbol{\theta}'_{k'})|} \right). \tag{22}$$

Hence, showing that the bracketed term above must always be equal to one establishes the desired result. To accomplish this, we make use of several identities. First, note that by hypothesis, T_k and $T_{k'}$ are diffeomorphic and satisfy $T_k \sharp \pi_k = \nu_{n_k}$ and $T_{k'} \sharp \pi_{k'} = \nu_{n_{k'}}$. Thus, by the standard change of variables theorem, we obtain the identities

$$\pi_k(\boldsymbol{\theta}_k) = \nu_{n_k}(T_k(\boldsymbol{\theta}_k))|J_{T_k}(\boldsymbol{\theta}_k)|, \quad \text{and} \quad \pi_{k'}(\boldsymbol{\theta}'_{k'}) = \nu_{n_{k'}}(T_{k'}(\boldsymbol{\theta}'_{k'}))|J_{T_{k'}}(\boldsymbol{\theta}'_{k'})|. \tag{23}$$

Next, by hypothesis $\bar{h}_{k,k'} \sharp \nu_{n_k+w_k} = \nu_{n_k+w_k}$, and since $\bar{h}_{k,k'}$ is a volume-preserving diffeomorphism we obtain

$$\nu_{n'_k}(\boldsymbol{z}) = \nu_{n'_k}(\bar{h}_{k,k'}^{-1}(\boldsymbol{z})). \tag{24}$$

Finally, observe

$$\bar{h}_{k,k'}^{-1} \circ T_k(\boldsymbol{\theta}'_{k'}) \underbrace{=}_{(20)} \bar{h}_{k,k'}^{-1} \circ T_{k'} \circ T_{k'}^{-1} \circ \bar{h}_{k,k'}(T_k(\boldsymbol{\theta}_k), \boldsymbol{u}_k) = (T_k(\boldsymbol{\theta}_k), \boldsymbol{u}_k), \tag{25}$$

where the final equality above uses associativity of function composition. Using the above identities, and that $\nu_{n_{k'}} = \nu_{n_k+w_k}$, we obtain

$$\frac{\pi_{k'}(\boldsymbol{\theta}'_{k'})|J_{T_k}(\boldsymbol{\theta}_k)|}{\nu_{w_k}(\boldsymbol{u}_k)\pi_k(\boldsymbol{\theta}_k)|J_{T_{k'}}(\boldsymbol{\theta}_{k'})|} \underbrace{=}_{(23)} \frac{\nu_{n'_k}(T_{k'}(\boldsymbol{\theta}'_k))}{\nu_{n_k+w_k}(T_k(\boldsymbol{\theta}_k), \boldsymbol{u}_k)} \underbrace{=}_{(24)} \frac{\nu_{n'_k}(\bar{h}_{k,k'}^{-1}(T_{k'}(\boldsymbol{\theta}'_{k'})))}{\nu_{n_k+w_k}(T_k(\boldsymbol{\theta}_k), \boldsymbol{u}_k)} \underbrace{=}_{(25)} \frac{\nu_{n_k+w_k}(T_k(\boldsymbol{\theta}_k), \boldsymbol{u}_k)}{\nu_{n_k+w_k}(T_k(\boldsymbol{\theta}_k), \boldsymbol{u}_k)} = 1,$$

and the result is established for the stated case. The result is established for the case $n_k = n_{k'}$ by repeating the above argument but setting $\nu_{w_k}(\cdot) = 1$ because $w_k = 0$ in that case. Similarly, for the case where $n_{k'} < n_k$, repeat the above argument by applying the reverse move (replacing $h_{k,k'}$ with $h_{k',k} := h_{k,k'}^{-1}$), and using $\bar{h}_{k',k}^{-1} \sharp \nu_{n_k+w_k} = \nu_{n_k+w_k}$. □

B. Normalizing Flow Configuration

This section gives details regarding the flows used in the experiments. Write $h : \mathbb{R}^n \to [0,1]^n$ to denote the sigmoid function (applied element-wise). Define

$$s(\boldsymbol{z}; \boldsymbol{a}, \boldsymbol{b}) = \boldsymbol{b} \odot (\boldsymbol{z} - \boldsymbol{a}), \quad \boldsymbol{a} \in \mathbb{R}^n, \boldsymbol{b} \in \mathbb{R}^n_+. \tag{26}$$

The flow-based models used are of the form

$$T = h^{-1} \circ F \circ h \circ s,$$

where $F : [0,1]^n \to [0,1]^n$ is the composition of three (3) *masked autoregressive rational quadratic spline* transforms, implemented in the Python package nflows. Parameters used for each of the three transforms were 10 bins (corresponding to 11 "knot" points), the autoregressive neural networks used in each transform had two hidden layers, each with $32 \times n$ hidden features. A Stochastic Gradient Descent (SGD) algorithm is used to train the parameters of the sequence of transforms F. The transform s is fixed at the beginning of training and remains so during training, with the values of $\boldsymbol{a}$ and $\boldsymbol{b}$ taken to be the marginal means and reciprocal standard deviations of the data (samples), respectively, from a given π_k. It is beneficial to fix s as described above as it essentially standardizes the data prior to model training.

B.1 Conditional Normalizing Flow

The conditional approach uses the conditional transform

$$\tilde{T}(\,\cdot\,|k) = h^{-1} \circ F(\,\cdot\,|k) \circ h \circ s(\,\cdot\,|k).$$

Above, $F(\cdot; k)$ is has the same parameters and setup as F in the non-conditional case, with the distinct difference that it now takes as additional input a context (conditioning) variable k. Additionally, the CNF base distribution is now a *conditional* base — an independent Gaussian whose mean and scale parameters are determined via a context k (implemented as *ConditionalDiagonalNormal* in nflows).

Finally, $s(\cdot|k)$ is a *conditional standardization* that takes into account the known distribution of the auxiliary variables as well as when they feature for different models. Note that under the augmented target distribution, conditional on $k \in \mathcal{K}$, $\boldsymbol{\theta}_k$ is distributed according to the conditional target π_k, and the auxiliary variables $\boldsymbol{u}_{\backsim k}$ are distributed according to $\nu_{n_{\max}-n_k}$. Rather than simply standardize the auxilliary variables (which are known to be marginally distributed according to ν) for each model, it is often straightforward to apply a perfect *Gaussianizing* transform. Write F_ν for the cumulative density function (cdf) of the reference distribution ν, and Φ^{-1} for the inverse cdf of the univariate standard normal distribution (i.e., the probit function). The generalization of the standardizing transform to the saturated state space (defined for output i) is then

$$s(\boldsymbol{v}|k; \{\boldsymbol{a}_k, \boldsymbol{b}_k\}_{k\in\mathcal{K}})_i = \begin{cases} b_{ki}(v_i - a_{ki}), & v_i \text{ is } \textit{not} \text{ an auxilliary variable for model } k, \\ \Phi^{-1} \circ F_\nu(v_i), & \text{otherwise.} \end{cases} \tag{27}$$

Similar to the unconditional case, the vectors $\boldsymbol{b}_k$ and $\boldsymbol{a}_k$ are fixed to be the reciprocal standard deviation and mean vectors of the data (samples) from each π_k. Optionally, one can set $\boldsymbol{a}_k = \boldsymbol{a}$ and $\boldsymbol{b}_k = \boldsymbol{b}$ for all k using the same quantities obtained from pooling the samples (this is the approach implemented). In the considered example, the reference distribution ν was taken to be a standard Gaussian, and thus the second case above reduces simply to returning v_i. We highlight that the check for which case to apply in the function above is implemented via a *masking* function that, for input $k \in \mathcal{K}, i \in \{1, \ldots, n_{\max}\}$, returns one if the condition is satisfied, and zero otherwise.

C. Block Variable Selection Example

Figure 8 depicts the distributions for each conditional target in the example. Note that each is multi-modal. However, there are overlaps in some regions of high probability mass, which could possibly assist the performance of the CTRJ proposal. Figure 9 is an extended version of Figure 7 in the main paper, showing results of the Bartolucci estimator across varying number of samples N for each of the four estimated model probabilities.

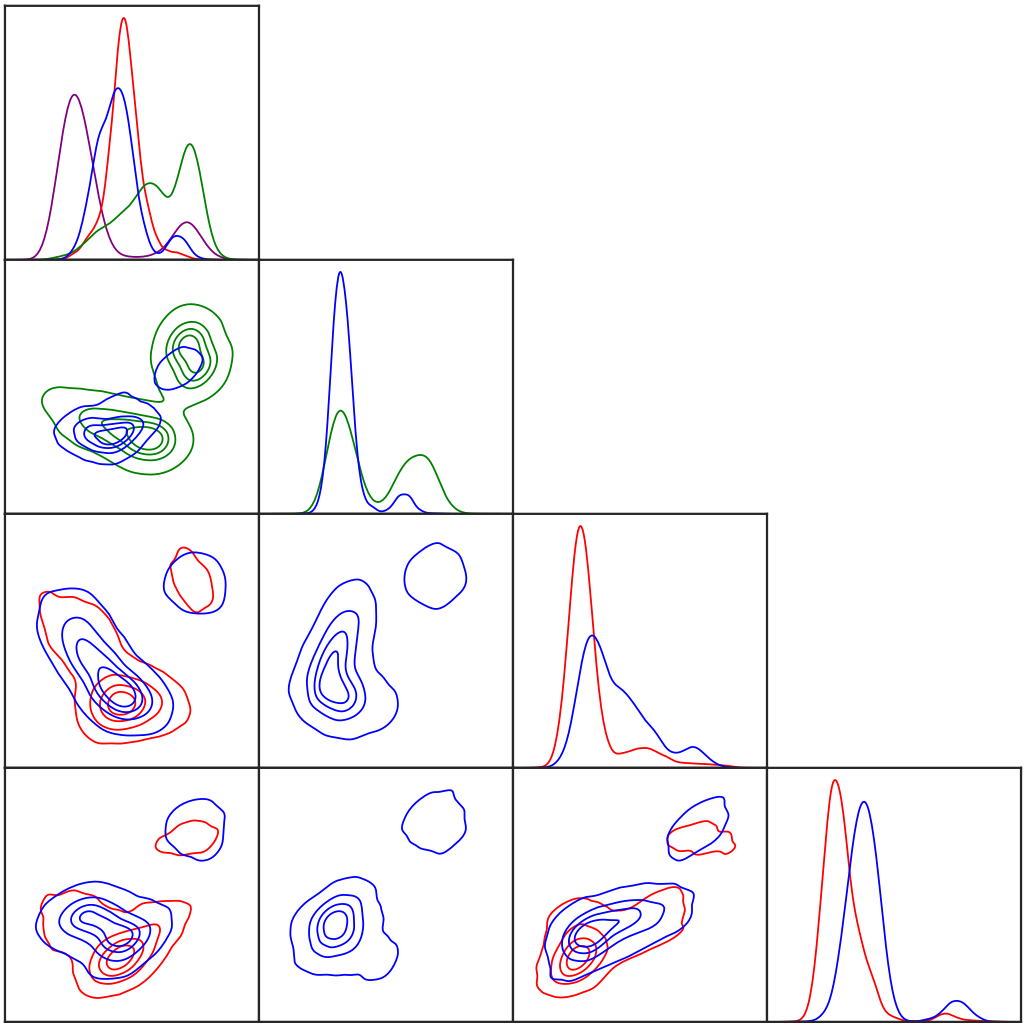

Figure 8: Pairwise plot of the conditional bivariate posterior densities in the Bayesian variable selection example. All four models feature: $k = (1, 0, 0, 0)$ (*Purple*) , $k = (1, 1, 0, 0)$ (*Green*), $k = (1, 0, 1, 1)$ (*Red*), and $k = (1, 1, 1, 1)$ (*Blue*).

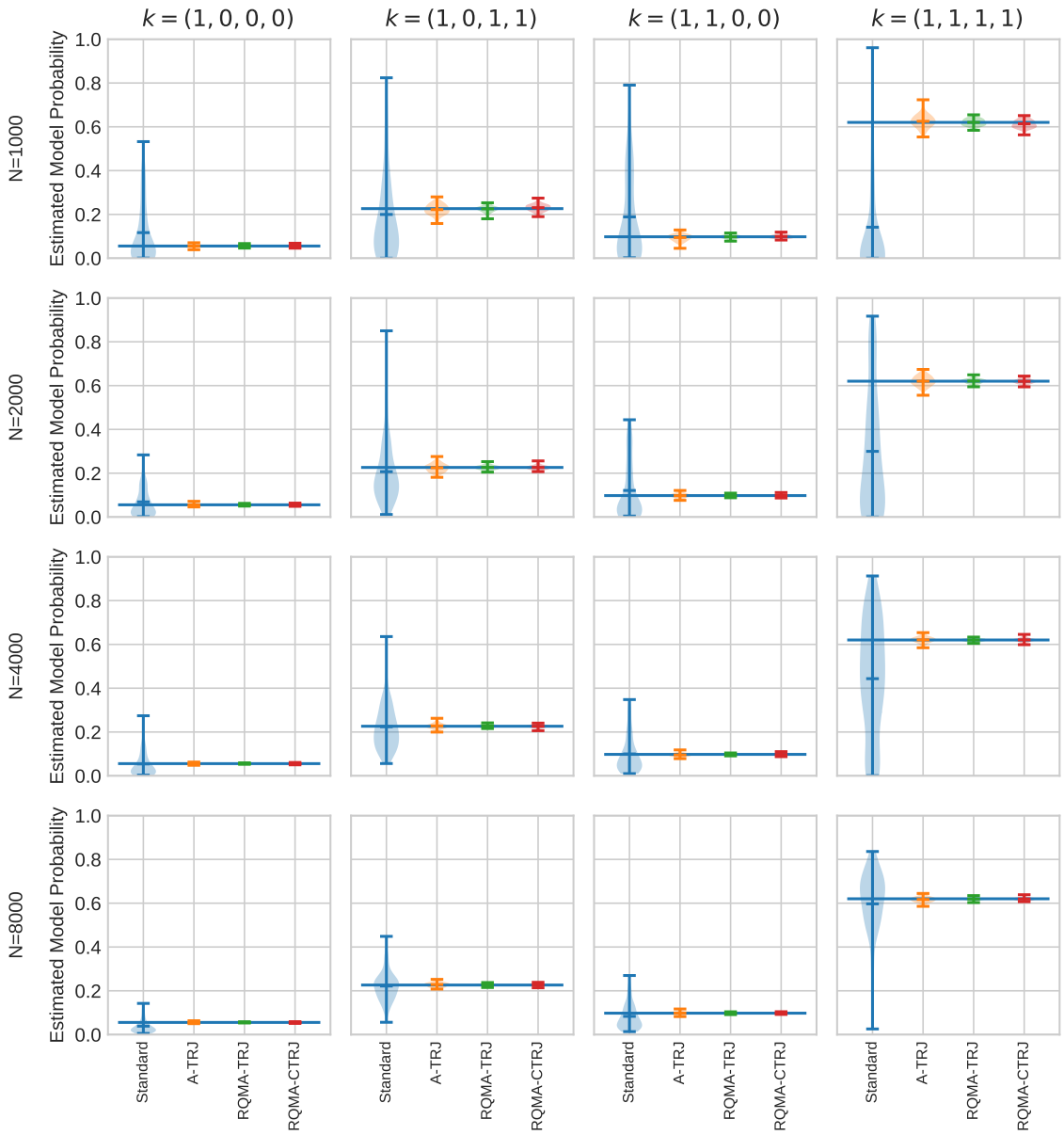

Figure 9: Violin plot showing variability of each proposal type using the Modified Bartolucci Estimator for the Bayesian variable selection example. To obtain samples to train the approximate transport maps, each model posterior was sampled using individual SMC samplers of $N = 1000, \ldots, 8000$ particles with a random walk kernel. Horizontal lines indicate ground-truth values obtained using large-sample runs of individual SMC ($N = 5 \cdot 10^4$).