Math in Transdimensional Bayesian Inversions: a Rigorous Formulation

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1 Classical, Isotropic Transdimensional Inversion

The proposed algorithm aims to find

$$\underbrace{p(\mathbf{m} \mid \mathbf{d}_{obs})}_{\text{posterior}} \propto \underbrace{p(\mathbf{d}_{obs} \mid \mathbf{m})}_{\text{likelihood}} \times \underbrace{p(\mathbf{m})}_{\text{prior}}, \tag{1}$$

by means of a reversible-jump Markov chain Monte Carlo sampling.

1.1 Free parameters

For simplicity, assume the data variance is known, i.e. the $n \times n$ matrix $\mathbf{C}_e$ can be computed before the inversion. Then, following *Bodin et al.* [2012], we only have three free parameters in the inversion; these are

1. number of layers k;
2. isotropic velocity $\mathbf{v}$, corresponding to V_S, of the k Voronoi cells;
3. position (depth) $\mathbf{c}$ of the k Voronoi cells.

1.2 Likelihood: $p(\mathbf{d}_{obs} \mid \mathbf{m})$

The general formula for the likelihood reads

$$p(\mathbf{d}_{obs} \mid \mathbf{m}) = \frac{1}{\sqrt{(2\pi)^n \, |\mathbf{C}_e|}} \exp\left\{ \frac{-\mathbf{\Phi}(\mathbf{m})}{2} \right\}, \tag{2}$$

where $\mathbf{\Phi}(\mathbf{m}) = (\mathbf{g}(\mathbf{m}) - \mathbf{d}_{obs})^T \cdot \mathbf{C}_e^{-1} \cdot (\mathbf{g}(\mathbf{m}) - \mathbf{d}_{obs})$ denotes the misfit between the observed ($\mathbf{d}_{obs}$) and modeled ($\mathbf{g}(\mathbf{m})$) data, and T transposition. As we will see in the following, since $\mathbf{C}_e$ is fixed, the multiplicative factor on the left of the exponential will cancel out.

1.3 Prior probability: $p(\mathbf{m})$

The prior probability

$$p(\mathbf{m}) = p(\mathbf{c}, \mathbf{v} \mid k)\ p(k), \tag{3}$$

is a function of the number of layers k. Assuming $\mathbf{c}$ and $\mathbf{v}$ are independent from each other, we can write

$$p(\mathbf{v} \mid k) = \prod_{i=1}^{k} p(v_i|k), \tag{4}$$

and the Dirichlet distribution as prior for the thicknesses

$$p(\mathbf{c} \mid k) = p(h_1, ..., h_k) = \frac{1}{B(\alpha)} \frac{1}{\Delta z} \prod_{i=1}^{k} h_i^{\alpha_i - 1}, \tag{5}$$

where h_i denotes the thickness of the ith Voronoi cell, $\Delta z = z_{max} - z_{min}$, and α denotes the concentration parameters in the Dirichlet distribution, and

$$B(y_1, ..., y_k) = \frac{\prod_{i=1}^{k} \Gamma(y_i)}{\Gamma(\sum_{i=1}^{k} y_i)} \tag{6}$$

Similar to expression (4), the prior probability of having k layers

$$p(k) = \frac{1}{\Delta k}, \tag{7}$$

where $\Delta k = k_{max} - k_{min}$.

1.4 Acceptance probability: $\alpha(\mathbf{m}' \mid \mathbf{m})$

In the inverse problem described thus far, a given model $\mathbf{m}'$ is preferred over the current model $\mathbf{m}$ if and only if its acceptance probability $\alpha(\mathbf{m}' \mid \mathbf{m}) \geq r$, where $0 \leq r < 1$ denotes a random number. It has been shown [*Green*, 2003] that the chain of sampled models will converge to the transdimensional posterior distribution $p(\mathbf{m} \mid \mathbf{d}_{obs})$ if

$$\alpha(\mathbf{m}' \mid \mathbf{m}) = \min\left[1, \underbrace{\frac{p(\mathbf{m}')}{p(\mathbf{m})}}_{\text{Prior ratio}} \underbrace{\frac{p(\mathbf{d}_{obs} \mid \mathbf{m}')}{p(\mathbf{d}_{obs} \mid \mathbf{m})}}_{\text{Likelihood ratio}} \underbrace{\frac{q(\mathbf{m} \mid \mathbf{m}')}{q(\mathbf{m}' \mid \mathbf{m})}}_{\text{Proposal ratio}}\right]. \tag{8}$$

It is the purpose of the following sections to robustly define each ratio in the right-hand side (RHS) of equation (8), so as to compute $\alpha(\mathbf{m}' \mid \mathbf{m})$ accurately at each iteration of the transdimensional inversion.

1.5 Perturbations

In general, a new model is proposed based on a random perturbation of the current model. Since we are considering only three free parameters (i.e. k, $\mathbf{c}$, and $\mathbf{v}$), the proposed model can be obtained based on four different kinds of perturbations:

1. **Change in velocity**. The velocity v_i corresponding to a Voronoi cell is randomly changed to a new value v_i' according to a Gaussian probability distribution centered

onto v_i, i.e. the proposal probability distribution

$$q_1(v_i' \mid v_i) = \frac{1}{\theta_1\sqrt{2\pi}}\exp\left\{-\frac{(v_i' - v_i)^2}{2\theta_1^2}\right\}, \tag{9}$$

where the standard deviation of the Gaussian θ_1 should be chosen a priori and can be dependent on depth of the Voronoi cell. And

$$v_i' = v_i + u, \tag{10}$$

with u being a random deviate from the normal distribution $\mathcal{N}(0, \theta_1)$.

2. **Change in position (depth)**. The position c_i of a Voronoi cell is randomly changed to a new value c_i' according to a Gaussian probability distribution centered onto c_i, i.e.

$$q_2(c_i' \mid c_i) = \frac{1}{\theta_2\sqrt{2\pi}}\exp\left\{-\frac{(c_i' - c_i)^2}{2\theta_2^2}\right\}, \tag{11}$$

where the standard deviation of the Gaussian θ_2 is chosen a priori and can be depth dependent.

3. **Birth**. A new Voronoi cell is created by choosing randomly its position from the range (z_{min}, z_{max}). Similar to expression (9) a velocity v_{k+1}' is assigned to the new Voronoi cell by sampling the Gaussian distribution

$$q_3(v_{k+1}' \mid v_i) = \frac{1}{\theta_3\sqrt{2\pi}}\exp\left\{-\frac{\left(v_{k+1}' - v_i\right)^2}{2\theta_3^2}\right\}, \tag{12}$$

where, once again, θ_3 should be chosen a priori.

4. **Death**. Remove one layer by drawing a random integer between 0 and k.

2 Cases for acceptance probability

The above four perturbation types have different prior and proposal ratios reported below. In the RHS of equation (8), one term does not depend on the type of perturbations is the ratio between the likelihood of the proposed model and that of the current model, and reads

$$\begin{aligned}\frac{p\left(\mathbf{d}_{obs} \mid \mathbf{m}'\right)}{p\left(\mathbf{d}_{obs} \mid \mathbf{m}\right)} &= \frac{\exp\left\{\frac{-\boldsymbol{\Phi}(\mathbf{m}')}{2}\right\}}{\sqrt{(2\pi)^n\left|\mathbf{C}_e\right|}}\frac{\sqrt{(2\pi)^n\left|\mathbf{C}_e\right|}}{\exp\left\{\frac{-\boldsymbol{\Phi}(\mathbf{m})}{2}\right\}} \\ &= \exp\left\{-\frac{\boldsymbol{\Phi}(\mathbf{m}') - \boldsymbol{\Phi}(\mathbf{m})}{2}\right\}.\end{aligned} \tag{13}$$

The rest to evaluate is the product of prior ratio and proposal ratio

$$\frac{p(m')}{p(m)}\frac{q(m \mid m')}{q(m' \mid m)} \tag{14}$$

We will expand equation (14) below on the basis of the following:

1. For proposal distribution:

$$q(\mathbf{m} \mid \mathbf{m}') = q(\mathbf{c} \mid \mathbf{m}')q(\mathbf{v} \mid \mathbf{m}') \tag{15}$$

2. For prior distribution, expanding equation (3):

$$p(\mathbf{m}) = p(\mathbf{c} \mid k)p(\mathbf{v} \mid k)p(\mathbf{k}) \tag{16}$$

   where $p(\mathbf{c})$ is dependent on the types of perturbation, $p(\mathbf{v})$ is dependent on the perturbation types and the prior distribution for the model parameters, and $p(\mathbf{k}) = \frac{1}{\Delta k}$.

3. When a model parameter follows the depth-dependent uniform distribution as prior,

$$p(\mathbf{v} \mid k) = \prod_{i=1}^{k} \frac{1}{\Delta v_i} \tag{17}$$

4. When a model parameter follows the depth-dependent Gaussian distribution as prior,

$$p(\mathbf{v} \mid k) = \prod_{i=1}^{k} \frac{1}{\sigma_i\sqrt{2\pi}} \exp\Big\{-\frac{1}{2}(\frac{v_i - \mu_i}{\sigma_i})^2\Big\} \tag{18}$$

Therefore, we will discuss the prior and proposal ratio based on the four different perturbation types. Under each perturbation type, we discuss the proposal ratio $\frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})}$, the depth part of prior ratio $\frac{p(\mathbf{c}'|k)}{p(\mathbf{c}|k)}$; the parameter part of prior ratio $\frac{p(\mathbf{v}'|k)}{p(\mathbf{v}|k)}$ for each of the three subcases: uniform distribution parameter, Gaussian distribution parameter, and a more generic case where there are multiple uniform and Gaussian parameters.

2.1 Perturbation type 1: change in velocity

2.1.1 Proposal ratio $\frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})}$

When there is a change in the velocity, the calculation of the ratios at the RHS of equation (8) is straightforward. There is no change in the parameterization, and the proposal perturbations have symmetrical distributions [*Bodin et al.*, 2012], i.e.

$$q_1(v_i' \mid v_i) = q_1(v_i \mid v_i'), \tag{19}$$

Therefore,

$$\frac{q(\mathbf{m} \mid \mathbf{m}')}{q(\mathbf{m}' \mid \mathbf{m})} = \frac{q(\mathbf{v} \mid \mathbf{v}')}{q(\mathbf{v}' \mid \mathbf{v})} = 1 \tag{20}$$

2.1.2 Prior ratio (depth part): $\frac{p(\mathbf{c}'|k)}{p(\mathbf{c}|k)}$

When the change is in the parameter value instead of depth, the prior probability on the depth part doesn't change, i.e.

$$p(\mathbf{c}' \mid k) = p(\mathbf{c} \mid k) \tag{21}$$

Therefore,

$$\frac{p(\mathbf{c}' \mid k)}{p(\mathbf{c} \mid k)} = 1 \tag{22}$$

2.1.3 Prior ratio (parameter part): $\frac{p(\mathbf{v}'|k)}{p(\mathbf{v}|k)}$

1. **Single uniform parameter**. Assuming the velocity is perturbed at the qth Voronoi cell,

$$\frac{p(\mathbf{v}' \mid k)}{p(\mathbf{v} \mid k)} = 1 \tag{23}$$

2. **Single Gaussian parameter**.

$$\frac{p(\mathbf{v}' \mid k)}{p(\mathbf{v} \mid k)} = \exp\left\{\frac{(v_q - \mu_q)^2 - (v_q' - \mu_q)^2}{2\sigma_q^2}\right\} \tag{24}$$

3. **Multiple uniform and Gaussian parameters**. Refer to equation (23) when the perturbed parameter is a depth-dependent uniform parameter, and to equation (24) when it's a depth-dependent Gaussian parameter.

2.2 Perturbation type 2: change in position

2.2.1 Proposal ratio $\frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})}$

When there is a change in the Voronoi site position, we calculate the ratio based on equation (11),

$$\frac{q(\mathbf{m} \mid \mathbf{m}')}{q(\mathbf{m}' \mid \mathbf{m})} = \frac{q(\mathbf{c} \mid \mathbf{c}')}{q(\mathbf{c}' \mid \mathbf{c})} = \frac{\theta_2}{\theta_2'}\exp\left\{\frac{(\theta_2^2 - \theta_2'^2)(c - c')^2}{2\theta_2'^2\theta_2^2}\right\} \tag{25}$$

2.2.2 Prior ratio (depth part): $\frac{p(\mathbf{c}'|k)}{p(\mathbf{c}|k)}$

$$\frac{p(\mathbf{c}' \mid k)}{p(\mathbf{c} \mid k)} = \frac{\Gamma(\alpha_q)\Gamma(\sum_{i=1}^k \alpha_i')}{\Gamma(\alpha_q')\Gamma(\sum_{i=1}^k \alpha_i)} \prod_{\substack{i \\ h_i \neq h_i'}} \frac{h_i'^{\alpha_i'-1}}{h_i^{\alpha_i-1}} \tag{26}$$

When $\alpha = 1$, given that $p(\mathbf{c} \mid k) = k!\frac{1}{\Delta z}$,

$$\frac{p(\mathbf{c}' \mid k)}{p(\mathbf{c} \mid k)} = 1 \tag{27}$$

2.2.3 Prior ratio (parameter part): $\frac{p(\mathbf{v}'|k)}{p(\mathbf{v}|k)}$

1. **Single uniform parameter**.

$$\frac{p(\mathbf{v}' \mid k)}{p(\mathbf{v} \mid k)} = \frac{\Delta v_q}{\Delta v_q'} \tag{28}$$

2. **Single Gaussian parameter**.

$$\frac{p(\mathbf{v}' \mid k)}{p(\mathbf{v} \mid k)} = \frac{\sigma_q}{\sigma_q'}\exp\left\{\frac{\sigma_q'^2(v_q - \mu_q)^2 - \sigma_q^2(v_q - \mu_q')^2}{2\sigma_q^2\sigma_q'^2}\right\} \tag{29}$$

3. **Multiple uniform and Gaussian parameters**.

$$\frac{p(\mathbf{v}' \mid k)}{p(\mathbf{v} \mid k)} = (\prod_{j=1}^{N} \frac{\Delta v_{jq}}{\Delta v'_{jq}})(\prod_{j=1}^{M} \frac{\sigma_{jq}}{\sigma'_{jq}} \exp\{\frac{\sigma'^2_{jq}(v_{jq} - \mu_{jq})^2 - \sigma^2_{jq}(v_{jq} - \mu'_q)^2}{2\sigma^2_q \sigma'^2_q}\}) \tag{30}$$

2.3 Perturbation type 3: Birth

2.3.1 Proposal ratio $\frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})}$

Based on the following equations,

$$\begin{aligned} q(\mathbf{c} \mid \mathbf{m}') &= \frac{1}{k+1}, \\ q(\mathbf{v} \mid \mathbf{m}') &= 1, \\ q(\mathbf{c}' \mid \mathbf{m}) &= \frac{1}{\Delta z}, \\ q(\mathbf{v}' \mid \mathbf{m}) &= \frac{1}{\theta'^2_3 \sqrt{2\pi}} \exp\left\{ - \frac{(v'_{new} - v_{new})^2}{2\theta'^2_3} \right\}, \end{aligned} \tag{31}$$

where v_{new} is the velocity for the new Voronoi cell before value perturbation, and v'_{new} is the perturbed value for the new location. We then simplify the proposal ratio,

$$\begin{aligned} \frac{q(\mathbf{m} \mid \mathbf{m}')}{q(\mathbf{m}' \mid \mathbf{m})} &= \frac{q(\mathbf{c} \mid \mathbf{m}')q(\mathbf{v} \mid \mathbf{m}')}{q(\mathbf{c}' \mid \mathbf{m})q(\mathbf{v}' \mid \mathbf{m})} \\ &= \frac{\Delta z \theta^2_3 \sqrt{2\pi}}{(k+1) \cdot \exp\left\{ - \frac{(v'_{new} - v_{new})^2}{2\theta'^2_3} \right\}} \end{aligned} \tag{32}$$

2.3.2 Prior ratio (depth part): $\frac{p(\mathbf{c}'|k)}{p(\mathbf{c}|k)}$

$$\frac{p(\mathbf{c}' \mid k+1)}{p(\mathbf{c} \mid k)} = \frac{\Gamma(\sum_{i=1}^{k+1} \alpha'_i) h'^{\alpha'_{new}-1}_{new}}{\Gamma(\sum_{i=1}^{k} \alpha_i)\Gamma(\alpha'_{new})\Delta z} \prod_{\substack{i \\ h_i \neq h'_i}} \frac{h'^{\alpha'_i - 1}_i}{h^{\alpha_i - 1}_i} \tag{33}$$

For the case when $\alpha = 1$,

$$\frac{p(\mathbf{c}' \mid k)}{p(\mathbf{c} \mid k)} = \frac{k+1}{\Delta z} \tag{34}$$

2.3.3 Prior ratio (parameter part): $\frac{p(\mathbf{v}'|k)}{p(\mathbf{v}|k)}$

1. **Single uniform parameter**.

$$\frac{p(\mathbf{v}' \mid k+1)}{p(\mathbf{v} \mid k)} = \frac{1}{\Delta v_{new}} \tag{35}$$

2. **Single Gaussian parameter**.

$$\frac{p(\mathbf{v}' \mid k+1)}{p(\mathbf{v} \mid k)} = \frac{1}{\sigma_{new}\sqrt{2\pi}} \exp\{-\frac{(v_{new} - \mu_{new})^2}{2\sigma_{new}}\} \tag{36}$$

3. **Multiple uniform and Gaussian parameters**.

$$\frac{p(\mathbf{v}' \mid k+1)}{p(\mathbf{v} \mid k)} = TODO \tag{37}$$

2.4 Perturbation type 4: Death

2.4.1 Proposal ratio $\frac{q(\mathbf{m}|\mathbf{m}')}{q(\mathbf{m}'|\mathbf{m})}$

For this last category of random perturbation, we can simply take the reciprocals of the RHS in equation (32),

$$\frac{q(\mathbf{m} \mid \mathbf{m}')}{q(\mathbf{m}' \mid \mathbf{m})} = \frac{k \cdot \exp\left\{ -\frac{(v'_{removed} - v_{removed})^2}{2\theta_3'^2} \right\}}{\Delta z \theta_3^2 \sqrt{2\pi}} \tag{38}$$

2.4.2 Prior ratio (depth part): $\frac{p(\mathbf{c}'|k)}{p(\mathbf{c}|k)}$

$$\frac{p(\mathbf{c}' \mid k-1)}{p(\mathbf{c} \mid k)} = \frac{\Gamma(\sum_{i=1}^{k-1} \alpha'_i)\Gamma(\alpha_{removed})\Delta z}{\Gamma(\sum_{i=1}^{k} \alpha_i) h_{removed}^{\alpha_{removed}-1}} \prod_{\substack{i \\ h_i \neq h'_i}} \frac{h_i^{\alpha_i - 1}}{h_i'^{\alpha'_i - 1}} \tag{39}$$

For the case when $\alpha = 1$,

$$\frac{p(\mathbf{c}' \mid k)}{p(\mathbf{c} \mid k)} = \frac{\Delta z}{k+1} \tag{40}$$

2.4.3 Prior ratio (parameter part): $\frac{p(\mathbf{v}'|k)}{p(\mathbf{v}|k)}$

1. **Single uniform parameter**.

$$\frac{p(\mathbf{v}' \mid k-1)}{p(\mathbf{v} \mid k)} = \Delta v_{removed} \tag{41}$$

2. **Single Gaussian parameter**.

$$\frac{p(\mathbf{v}' \mid k-1)}{p(\mathbf{v} \mid k)} = (\sigma_{removed}\sqrt{2\pi} \exp\left\{ \frac{(v_{removed} - \mu_{removed})^2}{2\sigma_{removed}} \right\}) \tag{42}$$

3. **Multiple uniform and Gaussian parameters**.

$$\frac{p(\mathbf{v}' \mid k-1)}{p(\mathbf{v} \mid k)} = TODO \tag{43}$$

References

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