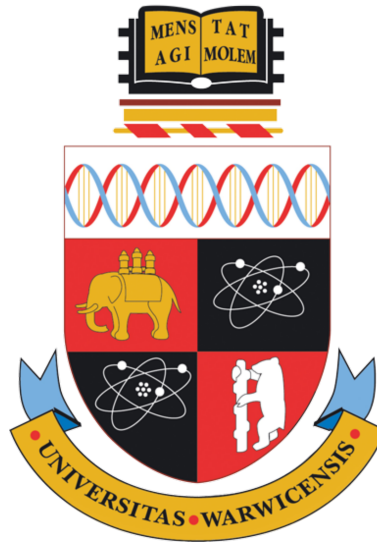# University of Warwick

Markov Melding

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Contents

Abstract

Markov melding is a Bayesian generic approach to combining evidence from multiple sources. Each evidence source is modelled by separate submodels, which are then joined by a process called melding. This process, its motivations and inference on the resulting melded model are the primary topics of study in this dissertation. We discuss one simple example of melding, as well as one more involved example involving the use of computational techniques to perform inference.

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This dissertation was typeset using `bookdown` (Xie 2016), plots produced using `ggplot2` (Wickham 2016) and written in `R` (R Core Team 2018). The associated code can be found at the GitHub repo `github.com/athowes/meld`.

Chapter 1

Introduction

It is rare that societally relevant questions can be addressed entirely by a single study (Royal Society, Academy of Medical Sciences 2018). Well-founded policy and informed public discourse therefore depend upon taking into account all available evidence evenhandedly. More and more, this evidence is in terms of data; with vast amounts now becoming available in all sectors of society. The sources of this data are varied and diverse, making it challenging to analyse simultaneously. As a result, there is a need for statistical methodology able to synthesise disparate evidence across multiple sources.

Using all available data has a range of benefits. From a statistical point of view evidence synthesis is typically associated with more precise estimates, just as with an increase in sample size. Any single given study or model typically harbors biases. Integrating multiple models may help to mitigate the effect of bias in any particular model. Furthermore, taking into account multiple sources of evidence gives a fuller and more realistic unstanding of the uncertainty involved.

Evidence synthesis is particularly relevant when the required quantity is difficult to measure directly, or otherwise a challenge to obtain complete, reliable, unbiased information about. There are many situations in which it is impossible to carry out a randomised controlled trial or other highly informative study and only partial data sources are available. For instance in the monitoring of pandemics, only fragmented, biased surveillance data is available (Presanis et al. 2014). Effective public health response depends on up-to-date severity information. Evidence synthesis provides a feasible solution using only the available data.

Meta-analysis, also known as systematic review, is one quantitative approach to combining

evidence from multiple studies. Classically, it has been frequentist in nature and typically focused on combining sources of evidence which are in some sense alike, such as multiple studies of the same kind.

Multiparameter Evidence Synthesis (MPES) (Welton et al. 2012) provides a more general approach, set within a Bayesian framework. The only requirement of MPES is that each study is informative about a shared parameter. Bayesian statistics provides a flexible and systematic approach to combining prior knowledge with data from multiple, potentially disparate, sources. The Bayesian paradigm also allows uncertainty to be quantified and propagated through the models such that information is shared between models.

Computational tools such as Markov chain Monte Carlo (MCMC) (Gilks, Richardson, and Spiegelhalter 1995) facilitate fitting complex Bayesian models. Using MCMC, Ades and Cliffe (2002) demonstrate the application of MPES to HIV data in the context of prenatal screening policy. MPES is now the key method (Hickman et al. 2013) used by the UK government to estimate HIV prevalence; accomplished using "a collection of census, surveillance and survey-type prevalence data" (Public Health England 2008).

Markov melding (Goudie et al. 2019) is a recent approach to MPES which introduces a generic framework for combining modular evidence sources. In Chapter 2 we explain the route taken by Goudie et al. (2019) to constructing a joint model over all of the considered sources of evidence. In Chapter 3 we discuss computational methods for conducting inference on this model. Finally, we conclude in Chapter 4.

Chapter 2

Model specification

Markov melding is a Bayesian procedure based on the construction and integration of a collection of graphical models; one for each of the separate evidence components. we begin this chapter by introducing Bayesian statistics in Section 2.1 and outlining how models might be constructed using a Bayesian networks, a type of graphical model, in Section 2.2.

2.1 Bayesian statistics

Consider observable data $Y \in \mathcal{Y}$. Statistical models simplify reality by using parameters $\theta \in \Theta$ to explain the processes governing Y. In Bayesian statistics, the unknown quantities such as Y and θ are treated as random variables. A statistical model $\mathcal{M}$ is then defined entirely by the joint probability distribution $p(\theta, Y)$, encompassing all beliefs about the parameters, data and their interdependence.

This distribution $p(\theta, Y)$ can be decomposed into a product of the likelihood $p(Y \mid \theta)$ and the prior $p(\theta)$ distributions. Having observed the data $Y = y$, the likelihood function $\mathcal{L}(\theta \mid y) = p(y \mid \theta)$ expresses how probable the generation of data y is under parameter setting θ. The prior distribution $p(\theta)$ can be interpreted as embodying subjective judgments about the plausibility of the different parameter settings in advance of seeing the data. Alternatively, from an objective Bayesian point of view, a prior which is in some sense non-informative about the parameters should be chosen. In either setting there is significant freedom in prior-specification which is left to the practitioner.

Statistical inference is the process of learning about the underlying parameters once the data $Y = y$ has been observed. In Bayesian statistics, this is achieved using probability theory via the eponymous Bayes' rule

$$p(\theta \,|\, y) = \frac{p(y \,|\, \theta)p(\theta)}{p(y)}. \tag{2.1}$$

The posterior distribution $p(\theta \,|\, y)$ represents updated beliefs about the parameters conditional on the observed data. The marginal likelihood $p(y)$ is a constant which normalises the product $p(y \,|\, \theta)p(\theta)$ to a valid probability distribution which integrates to one. Calculating the marginal likelihood is often difficult, preventing exact Bayesian inference from being tractable. However, during this chapter we will concentrate on statistical modelling, mostly ignoring potential computational difficulties for the time being.

Bayes' rule (2.1) can also be written in the form

$$p(\theta \,|\, y) \propto p(y \,|\, \theta)p(\theta) = p(y, \theta), \tag{2.2}$$

omitting the dependence on the marginal likelihood. Indeed, in practice Equation (2.2) is the form of Bayes' rule most widely useful. To demonstrate the application of Bayesian inference to a statistical model we present the following example.

Example 2.1: Poisson likelihood and conjugate Gamma prior

Consider the Poisson-Gamma statistical model $p(\lambda, Y_1, \ldots, Y_n)$ defined as

$$(Prior) \qquad \lambda \sim \text{Gamma}(a, b), \tag{2.3}$$

$$(Likelihood) \qquad Y_i \sim \text{Pois}(\lambda), \quad i = 1, \ldots, n. \tag{2.4}$$

The parameter of interest is the rate $\lambda > 0$, the data $Y = (Y_1, \ldots, Y_n)$ and $a, b > 0$ are fixed hyperparameters (parameters of the prior distribution). Having observed data $y_1, \ldots, y_n$, in terms of probability density functions the prior and likelihood are

$$(Prior) \qquad p(\lambda) = \frac{b^a}{\Gamma(a)} \lambda^{a-1} e^{-b\lambda} \propto \lambda^{a-1} e^{-b\lambda}. \tag{2.5}$$

$$(Likelihood) \qquad \mathcal{L}(\lambda) = \prod_{i=1}^{n} p(y_i \mid \lambda) = \prod_{i=1}^{n} \frac{\lambda^{y_i} e^{-\lambda}}{\lambda!} \propto \lambda^{\sum_{i=1}^{n} y_i} e^{-n\lambda}, \tag{2.6}$$

This particular prior has been chosen as it has functional form matching that of Equation (2.6), making it relatively simple to calculate the posterior distribution using Equation (2.2), as follows

$$p(\lambda \mid y_1, \dots, y_n) \propto \mathcal{L}(\lambda) p(\lambda) \propto \lambda^{\sum_{i=1}^{n} y_i} e^{-n\lambda} \cdot \lambda^{a-1} e^{-b\lambda}$$

$$= \lambda^{a-1+\sum_{i=1}^{n} y_i} e^{-(b+n)\lambda} \propto \mathrm{Gamma}\left(a + \sum_{i=1}^{n} y_i, b + n\right). \tag{2.7}$$

After updating conditional on the observed data, the posterior distribution (2.7) is of the same family, a Gamma distribution, as the prior distribution (2.5). This property is called conjugacy and allows exact Bayesian inference to be performed in some situations.

Having observed the data $\{1, 1, 2, 4, 1, 4\}$, Figure (2.1) shows the posterior distribution contracting as beliefs about the rate parameter become stronger. $\qquad \square$

2.2   Graphical models

The particular features of the joint distribution $p(\theta, Y)$ can be constructed in many ways. Note that typically both θ and Y are multivariate, so specifying $p(\theta, Y)$ may be no small task. Probabilistic graphical models (PGMs) (Bishop 2006) are one popular and useful tool for this purpose.

A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is defined by a set of vertices $\mathcal{V}$ together with a set of edges $\mathcal{E}$, where each edge connects a pair of vertices. In a PGM, the vertices represent random variables and the edges represent probabilistic relationships between the random variables. Bayesian networks are a particular type of PGM in which conditional dependencies (defined below) are the probabilistic relationships represented by the edges (Bishop 2006).

Consider random variables $Z_k \in \mathcal{Z}_k$, $k = 1, \dots, K$ with joint distribution $p(Z_1, \dots, Z_K)$. Z_k is conditionally independent from Z_l given Z_m, written $Z_k \perp Z_l \mid Z_m$, if and only if
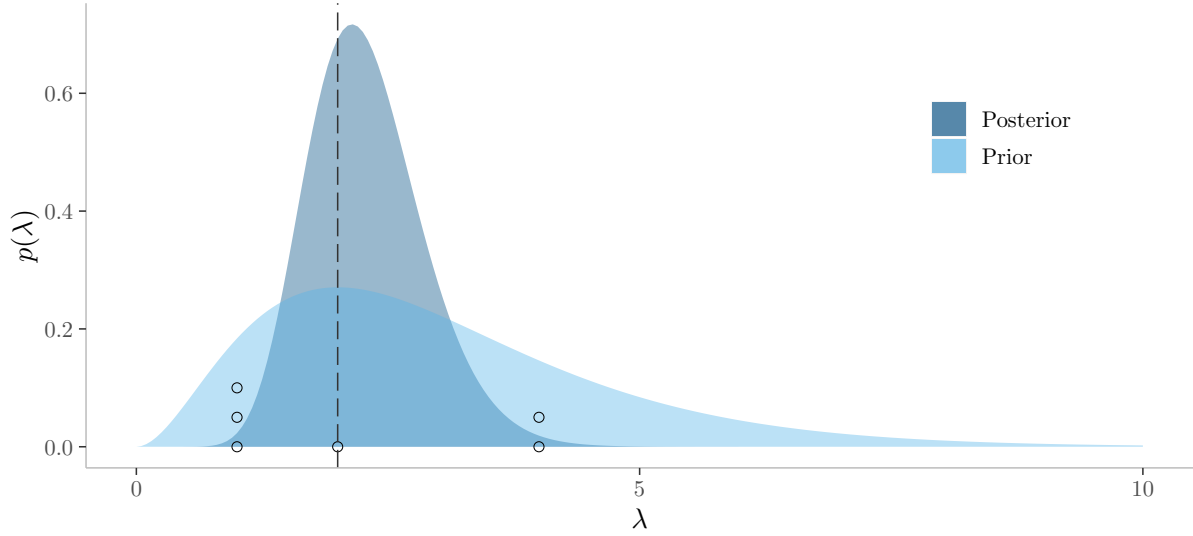
Figure 2.1: Particular example of Bayesian inference for the Poisson-Gamma model. The prior hyperparameters are $a = 3$ and $b = 1$. Data, plotted as open circles, is simulated from a Poisson distribution with $\lambda = 2$ shown as the dashed line.
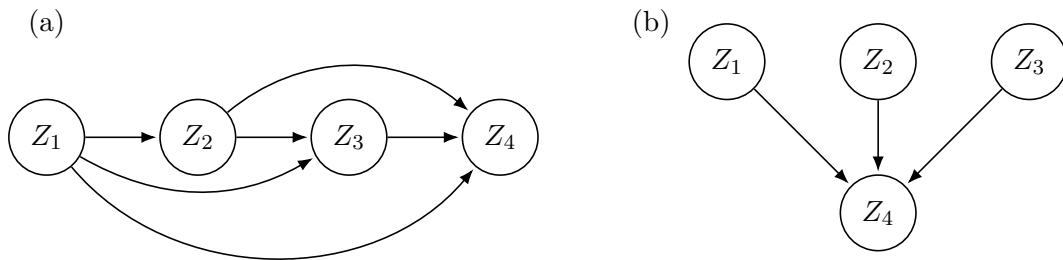

Figure 2.2: Directed acyclic graphs for the four variables $Z_1, \ldots, Z_4$.

$$p(Z_k, Z_l \,|\, Z_k) = p(Z_k \,|\, Z_k)p(Z_l \,|\, Z_k) \tag{2.8}$$

By repeated conditioning, it is always true that the joint distribution $p(Z_1, \ldots, Z_K)$ can be decomposed according to

$$p(Z_1, \ldots, Z_K) = p(Z_1)p(Z_2, \ldots, Z_K \,|\, Z_1) = p(Z_1)p(Z_2 \,|\, Z_1)p(Z_3, \ldots, Z_K \,|\, Z_1, Z_2)$$
$$= \cdots = p(Z_1)p(Z_2 \,|\, Z_1) \cdots p(Z_K \,|\, Z_1, \ldots, Z_{K-1}). \tag{2.9}$$

This factorisation can be represented by a particular kind of graph where the edges are directional, shown using arrows, and there are no directed cycles between the nodes. Graphs like this are called directed acyclic graphs (DAGs). A Bayesian network is a DAG where there is a directed edge from variable Z_k to Z_l if the conditional distribution of Z_l depends on Z_k. For example, the DAG corresponding to Equation (2.9) with $K = 4$ is shown in part (a) of Figure 2.2.

If Equation (2.8) holds then conditional densities of the form $p(Z_k \,|\, Z_l, Z_k)$ can be rewritten to remove the dependence on Z_l as follows

$$p(Z_k \,|\, Z_l, Z_k) = \frac{p(Z_k, Z_l \,|\, Z_k)}{p(Z_l \,|\, Z_k)} = \frac{p(Z_k \,|\, Z_k)p(Z_l \,|\, Z_k)}{p(Z_l \,|\, Z_k)} = p(Z_k \,|\, Z_k). \tag{2.10}$$

Equation (2.10) shows that conditional independence statements allow some of the dependencies, and hence directed edges in DAGs, to be removed. Suppose that $K = 4$ as before and each Z_1, Z_2 and Z_3 are conditionally independent from each other given Z_4. Then, Equation (2.9) may be rewritten as

$$p(Z_1, \ldots, Z_K) = p(Z_1)p(Z_2)p(Z_3)p(Z_4 \,|\, Z_1, Z_2, Z_3), \tag{2.11}$$

and the corresponding DAG redrawn taking into account this structure (part (b) of Figure 2.2).

It is visually clear that conditional independence statements result in sparser graphs, thereby reducing model complexity. More generally, given a set of conditional independence statements, joint probability distributions may be rewritten as

$$p(Z_1, \ldots, Z_K) = \prod_{k=1}^{K} p(Z_k \,|\, \mathrm{pa}(Z_k)), \qquad\qquad (2.12)$$

where Z_k is only conditionally dependent only on its parents $\mathrm{pa}(Z_k)$. In the corresponding DAG, there is a directed edge from each $Z_l \in \mathrm{pa}(Z_k)$ to Z_k. For example, in Figure 2.2, $\mathrm{pa}(Z_4) = \{Z_1, Z_2, Z_3\}$.

Bayesian networks allow complex models $p(Z_1, \ldots, Z_k)$ to be built up from the simpler building blocks of $p(Z_k \,|\, \mathrm{pa}(Z_k))$. In the context of Bayesian statistics, supposing the prior parameter is multivariate $\theta = (\theta_1, \ldots, \theta_K)$ then the prior distribution may be decomposed according to $\prod_{k=1}^{K} p(\theta_k \,|\, \mathrm{pa}(\theta_k))$. The statistical model $p(\theta, Y)$ may then be written as a product of the prior with the likelihood $p(Y \,|\, \mathrm{pa}(Y))$. Bayesian models which are built up in stages this way are known as hierarchical models.

These models possess the flexibility required to model the varied data sources necessary for evidence synthesis. Furthermore, domain experts can often efficaciously express their beliefs via Bayesian networks due to their ease of interpretability.

2.3   Modular models

Having introduced the necessary prerequisites, we may now discuss how they might be used to synthesise evidence.

Consider multiple sources of observable data $Y_m \in \mathcal{Y}_m$ with $m = 1, \ldots M$. Each Y_m is, at least to some extent, directly informative about a shared parameter ϕ which is common to all of the models. Therefore, for each evidence source, define a statistical model $p_m(\phi, \psi_m, Y_m)$, which will be henceforth called a submodel. For each submodel the parameters are (ϕ, ψ_m): the link parameter $\phi \in \Phi$ together with model specific parameters $\psi_m \in \Psi_m$ unique to each submodel.

It is essential that each of the submodels agree conceptually on what the link parameter ϕ represents: conversations in which the participants do not agree on the basic tenants are rarely productive. It is worth mentioning this fact because in some models the interpretation of parameters can be subtle. For example, in a regression the regression coefficient of a covariate implicitly takes into account the inclusion and exclusion of all other potential covariates; thereby

making it a different parameter in different models and rarely an appropriate link parameter. It is therefore safest if ϕ has a clear interpretation linked to the real world.

Given the collection of submodels $p_m(\phi, \psi_m, Y_m)$, the aim of the joining operation in Markov melding (Goudie et al. 2019) is to produce a joint distribution $p(\phi, \psi_1, \ldots, \psi_M, Y_1, \ldots, Y_M)$ over all parameters and observable data. Synthesising a joint distribution is attractive as it facilitates the propagation of uncertainty between the submodels. Additionally, the joint distribution defines a statistical model to which general methodological tools can be applied. Higher quality inference about ϕ is typically the primary aim of evidence synthesis, although due to the sharing of information between the submodels it may be that inference for ψ_m $m = 1, \ldots, M$ is also improved.

The joining of submodels is best suited to situations where the model specific observed quantities Y_m are relatively distinct. The more unique information there is dispersed across the different submodels, the greater the potential benefits of evidence synthesis. On the other extreme, the observed data $Y_m = Y$ may be identical for each of the M submodels (with different likelihood components say). This is in some sense unappealing as each of the submodels then offers a competing explanation for the data generating mechanism. Such a collection of beliefs cannot be reasonably held confidently by a single individual simultaneously. Rather, the individual may have to assign prior probabilities to each of the models being true. Then, if the link parameter plays different roles in the different submodels, although Markov melding may be possible it might not be advisable. In machine learning, multiple models may be trained on the same data and aggregated for the purposes of prediction (Bishop 2006). However, in this setting the focus is not on model building, interpretation or uncertainty quantification.

Markov melding extends and unifies previous work, particularly Markov combination (Dawid and Lauritzen 1993) and Bayesian melding (Poole and Raftery 2000) which we review here. In particular, Markov combination considers joining submodels where an added simplifying assumption is made; whilst Bayesian melding provides the methodological inspiration for overcoming this assumption.

2.4 Markov combination

As above consider the collection of submodels $p_m(\phi, \psi_m, Y_m)$, $m = 1, \ldots, M$. Each submodel features a prior distribution on the link parameter ϕ which in the simplest case is specified

directly with $p_m(\phi, \psi_m, Y_m) = p_m(\psi_m, Y_m \mid \phi)p_m(\phi)$ such that $\mathrm{pa}(\phi) = \emptyset$. Alternatively, the prior can be accessed by marginalising out both ψ_m and Y_m as follows

$$p_m(\phi) = \iint p_m(\phi, \psi_m, Y_m)d\psi_m dY_m. \tag{2.13}$$

An important property of the prior distributions is consistency; where the marginals $p_m(\phi)$ of the link parameter ϕ are called consistent if

$$\forall m \; p_m(\phi) = p(\phi). \tag{2.14}$$

If the prior marginals are consistent then the submodels each have the same beliefs about ϕ in advance of seeing the data. As a result, all of the submodels and their associated beliefs could theoretically reasonably be held by a single individual without any self-contradiction. (That being said, in practice a single practitioner may justifiably place different priors on the same parameter depending on the particular likelihood component. This might be the case if there exists a conjugate prior, as in Example 2.1, for example.)

Supposing that assumption (2.14) holds, Dawid and Lauritzen (1993) define a joint model $p_{\mathrm{comb}}(\phi, \psi_1, \ldots, \psi_M, Y_1, \ldots, Y_M)$ called the Markov combination of the submodels $p_1, \ldots, p_M$. In advance of justification, this joint model p_{comb} is

$$p_{\mathrm{comb}}(\phi, \psi_1, \ldots, \psi_M, Y_1, \ldots, Y_M) = \frac{\prod_{m=1}^{M} p_m(\phi, \psi_m, Y_m)}{p(\phi)^{M-1}}. \tag{2.15}$$

The construction of p_{comb} is based on prior consistency together with an additional assumption. This assumption is that, conditional on the link parameter, the models are independent. To be exact

$$\forall m \neq \ell \; (\psi_m, Y_m) \perp (\psi_\ell, Y_\ell) \mid \phi, \tag{2.16}$$

where conditional independence is defined as in Equation (2.8). Figure (2.3) illustrates this assumption using a DAG for $M = 2$ submodels.

In some sense, the truth of this assumption justifies the use of seperate submodels, rather than a single monolithic model which is specified at the outset. Just as with DAGs, conditional

independence statements simplify the process of modelling: it is easier to specify a collection of submodels than it is to additionally consider their interactions. This is particularly pertinent if the observable data Y_m are from different background areas. Here, the modelling process naturally decomposes such that different domain experts are consultated for each data source, resuling in submodel specifications. In this situation, the conditional independence assumption also seems, in general, quite reasonable.
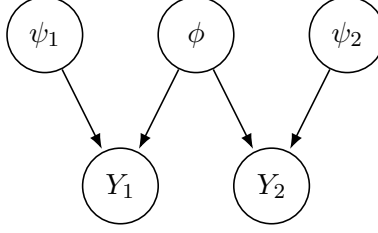

Figure 2.3: Directed acyclic graph corresponding to Equation (2.16) for $M = 2$.

The structure of Equation (2.15) is then explained by applying these two assumptions to a hypothetical joint model

$$
\begin{aligned}
p(\phi, \psi_1, \ldots, \psi_M, Y_1, \ldots, Y_M) &= p(\phi)\, p(\psi_1, \ldots, \psi_M, Y_1, \ldots, Y_M \mid \phi) \\
&\overset{(2.16)}{=} p(\phi) \prod_{m=1}^{M} p_m(\psi_m, Y_m \mid \phi) \\
&= p(\phi) \prod_{m=1}^{M} \frac{p_m(\phi, \psi_m, Y_m)}{p_m(\phi)} \qquad (2.17) \\
&\overset{(2.14)}{=} \frac{\prod_{m=1}^{M} p_m(\phi, \psi_m, Y_m)}{p(\phi)^{M-1}}, \qquad (2.18)
\end{aligned}
$$

where the result is exactly that of Equation (2.15).

Markov combination has the attractive property that submodel marginals and submodel-specific conditional distributions are preserved, that is $p_{\text{comb}}(\phi, \psi_m, Y_m) = p_m(\phi, \psi_m, Y_m)$ and $p_{\text{comb}}(\psi_m, Y_m \mid \phi) = p_m(\psi_m, Y_m \mid \phi)$ for all m (Goudie et al. 2019). This can be shown via

$$p_{\text{comb}}(\phi, \psi_m, Y_m) = \int p_{\text{comb}}(\phi, \psi_1, \dots, \psi_M, Y_1, \dots, Y_M) d\psi_{-m} dY_{-m}$$

$$= \int p(\phi) \prod_{m=1}^{M} p_m(\psi_m, Y_m \mid \phi) d\psi_{-m} dY_{-m}$$

$$= p(\phi) p_m(\psi_m, Y_m \mid \phi) = p_m(\phi, \psi_m, Y_m), \tag{2.19}$$

where the notation $d\psi_{-m} dY_{-m}$ refers to integration with respect to each of the model specific parameters and observed quantites except from ψ_m and Y_m. Similarly

$$p_{\text{comb}}(\psi_m, Y_m \mid \phi) = \frac{p_{\text{comb}}(\phi, \psi_m, Y_m)}{p(\phi)} = \frac{p(\phi, \psi_m, Y_m)}{p(\phi)} = p_m(\psi_m, Y_m \mid \phi). \tag{2.20}$$

In its form, the Markov melded joint model is similar to that of Markov combination. This is because both methods assume the conditional independence assumption, given by Equation (2.16). The primary difference is that Markov melding does not assume that the prior marginals of the link parameter are consistent. Instead, these marginals are "melded" by a process similar to that developed in Bayesian melding, which we will now detail.

2.5 Bayesian melding

The presence of multiple priors on a given quantity also arises in the study of simulation models. Bayesian melding (Poole and Raftery 2000) is motivated by this challenge and aims to perform inference on deterministic simulation models $M : \theta \to \phi$. The outputs $\phi \in \Phi \subseteq \mathbb{R}^p$ are a function of the inputs $\theta \in \Theta \subseteq \mathbb{R}^n$ only, such that $\phi = M(\theta)$. There may exist data relating to one or both of θ and ϕ which we denote by Y_θ and Y_ϕ respectively. Irrespective of the simulation model M, a statistical model $p(\theta, \phi, Y_\theta, Y_\phi)$ can be specified which Poole and Raftery (2000) additionally assume can be decomposed into a product of independent prior and likelihood components

$$p(\theta, \phi, Y_\theta, Y_\phi) = p(Y_\theta \mid \theta) p(\theta) p(Y_\phi \mid \phi) p(\phi). \tag{2.21}$$

We call this distribution the joint premodel prior distribution. It may be marginalised to find the premodel prior distributions $p(\theta)$ and $p(\phi)$ respectively.

Bayesian melding builds upon a previous approach called Bayesian synthesis (Raftery, Givens, and Zeh 1995). In this approach, the model M is incorporated into the joint premodel distribution to create a joint postmodel distribution $\pi(\theta, \phi, Y_\theta, Y_\phi)$. Poole and Raftery (2000) describe that this is done by restricting $p(\theta, \phi, Y_\theta, Y_\phi)$ to the submanifold $\{(\theta, \phi, Y_\theta, Y_\phi) : \phi = M(\theta)\}$, such that

$$\pi(\theta, \phi, Y_\theta, Y_\phi) \propto \begin{cases} p(\theta, M(\theta), Y_\theta, Y_\phi), & \text{if } \phi = M(\theta) \\ 0, & \text{otherwise.} \end{cases} \tag{2.22}$$

The marginal postmodel prior distribution for θ is then

$$\pi(\theta) = p(\theta \,|\, \phi = M(\theta)) \tag{2.23}$$

However, in a discussion of the paper, Wolpert (1995) call attention to the fact that conditional distributions of the form (2.23) are ill-defined and therefore subject to what is known as the Borel-Kolmogorov paradox. A key repercussion of this fact is that the postmodel distribution depends on how M is parametrised. Furthermore, Schweder and Hjort (1996) show that any postmodel distribution can be obtained by arbitrary parametrisation of M. These observations place serious concern on the usefulness of Bayesian synthesis, motivating the development of Bayesian melding.

The problem that Wolpert (1995) find arises because in Bayesian synthesis, as well as the premodel marginal prior distribution $p(\phi)$, there is an additional prior on the output ϕ. In particular, applying the deterministic model M to the premodel marginal prior distribution on inputs $p(\theta)$ results in a model-induced prior on outputs ϕ denoted by $p^\star(\phi)$. If M^{-1} exists then this prior is given by

$$p^\star(\phi) = p(M^{-1}(\phi))|J(\phi)|, \tag{2.24}$$

where $J(\phi)$ is the Jacobian of the transformation. The two priors are typically inconsistent as they are based on different information.

A simple approach to rectifying this problem would be not to attempt to place a separate prior on outputs ϕ, instead relying on the prior induced by applying M to $p(\theta)$ However, in hopes of combining both information from the premodel prior and that of the model induced prior, Bayesian melding instead replaces $p(\phi)$ and $p^\star(\phi)$ by a single melded output prior $\tilde{p}(\phi)$. For their

particular motivating application, relating to a population dynamics model for bowhead whales, Poole and Raftery (2000) do this by taking the (normalised) geometric mean of the two priors as follows

$$\tilde{p}(\phi) \propto p(\phi)^{0.5} p^{\star}(\phi)^{0.5} \tag{2.25}$$

Equation (2.25) is an example of a broader class of pooling operations which mathematically combine probability distributions. More examples will be discussed further in the next section.

Poole and Raftery (2000) propose then inverting the prior $\tilde{p}(\phi)$ to the input space to define a melded input prior $\tilde{p}(\theta)$ as (omitting some details)

$$\begin{aligned}
\tilde{p}(\theta) &= \tilde{p}(M(\theta)) \left(\frac{p(\theta)}{p^{\star}(M(\theta))} \right) \\
&\propto p(\theta) \left(\frac{p(M(\theta))}{p^{\star}(M(\theta))} \right)^{1-\alpha}.
\end{aligned} \tag{2.26}$$

Equation (2.26) corresponds to the original input prior $p(\theta)$ weighted, according to α, by a ratio of the output prior and the model induced prior evaluated at $\phi = M(\theta)$ for given value of $\theta \in \Theta$.

To conclude discussion of Bayesian melding, having observed $Y_\theta = y_\theta$ and $Y_\phi = y_\phi$ a standard Bayesian posterior for θ can be then defined as follows

$$\pi(\theta \,|\, y_\phi, y_\theta) \propto p(y_\theta \,|\, \theta) p(y_\phi \,|\, M(\theta)) \tilde{p}(\theta), \tag{2.27}$$

allowing inference to proceed as usual.

2.6   Combining expert opinion

The prior pooling step, for which Equation (2.25) is one instance, in Bayesian melding has methodological similarities with previous work on combining the opinions of multiple experts (O'Hagan et al. 2006). Most relevant from this literature is mathematical aggregation, where distributions are elicited independently from each expert individually and then combined by some mathematical rule. The primary alternative to mathematical aggregation is behavioural

aggregation, where the group of experts interact and a single distribution is elicited from the group after discussion. In the case of Markov melding, in general the practitioners who originally developed each of the submodels may not be willing and able to justify their choices as would be required in behavioural aggregation.

Just as it is important that the submodels in Markov melding have a shared concept of the link parameter, Clemen and Winkler (1999) caution that "the mathematical and behavioural approaches ... assume that the experts have ironed out differences in definitions and that they agree on exactly what is to be forecast or assessed"; also noting that "practising risk analysts know these are strong assumptions".

In order to outline some of the proposed (O'Hagan et al. 2006) approaches, suppose each of a group of n experts are independently asked their beliefs about an unknown quantity θ, resulting in elicited distributions $f_i(\theta), i = 1, \ldots, n$. The simplest and most widely used technique within mathematical aggregation is opinion pooling, where a consensus distribution $f(\theta)$ is obtained as some function of the individual distributions $\{f_1(\theta), \ldots, f_n(\theta)\}$. Two of the most common examples are the linear opinion pool (2.28) and logarithmic opinion pool (2.29) defined respectively as

$$f(\theta) \propto \sum_{i=1}^{n} w_i f_i(\theta), \tag{2.28}$$

$$f(\theta) \propto \prod_{i=1}^{n} f_i(\theta)^{w_i}, \tag{2.29}$$

where $f(\theta)$ is normalised to a probability density function. The weights w_i can be chosen freely, either giving more weight to some experts than others or choosing to weight all of the experts equally.

Dictatorial pooling, in which one experts opinion is chosen as the consensus distribution, is special case of linear opinion pooling. To see this, set $w_j = 0$ for all $j \neq i$ in Equation (2.28) such that $f(\theta) = f_i(\theta)$. In Section 2.5, the suggestion to set $\tilde{p}(\phi) = p^\star(\phi)$ is an example of dictatorial pooling. The method used by Poole and Raftery (2000), geometric pooling given by Equation (2.25), is an example of logarithmic pooling with $w_i = 1/M$. Another special case of logarithmic opinion pooling is the product of experts pooling (Hinton 2002) which sets $w_i = 1$ for all i such that

$$f(\theta) \propto \prod_{i=1}^{n} f_i(\theta). \tag{2.30}$$

Figure (2.4) shows the Product of Experts, logarithmic and linear opinion pooling applied to various Gaussian distributions. Note that in the Product of Experts pooling, there are no weights. Or, another way of looking at it, the weights are fixed to be $w_1 = w_2 = 1$.

The Product of Experts is named as such because it gives each expert the benefit of the doubt in assuming that their beliefs are correct. The result, as most clearly illustrated by row (g, h, i) of Figure (2.4), is that the regions where the experts overlap has to be the truth. Logarithmic pooling is slightly more doubtful of the experts but still produces relatively contracted pooled beliefs in comparison to the more cautious linear pooling. O'Hagan et al. (2006) find that "while the linear opinion pool has been quite widely used in practice, the logarithmic opinion pool has been largely ignored, perhaps because it is perceived to lead to unrealistically strong aggregated beliefs".

Row (a, b, c) of Figure (2.4) prompt another consideration: to what extend should expert agreement lead to higher confidence. To use an analogy, suppose you and a group of friends want to decide whether or not to eat at a certain restaurant. If each friend expresses a positive opinion about the restaurant then may seem reasonable to be more confident than any given friend about the restaurant. However, if each friend bases their opinion solely on a positive review of the restaurant in that week's paper then this effectively would be double counting; in reality there is only one "expert" - the journalist.

2.7   Markov melding

If the marginals are inconsistent, that is condition (2.14) fails to hold, then the approach of Markov combination requires some modification. Just as pooling is used to reconcile disagreement between the premodel prior and induced prior in Bayesian melding, the inconsistent prior marginals $p_m(\phi)$ can be also pooled to allow Bayesian inference to proceed. The resulting pooled prior $p_{\text{pool}}(\phi)$ is such that

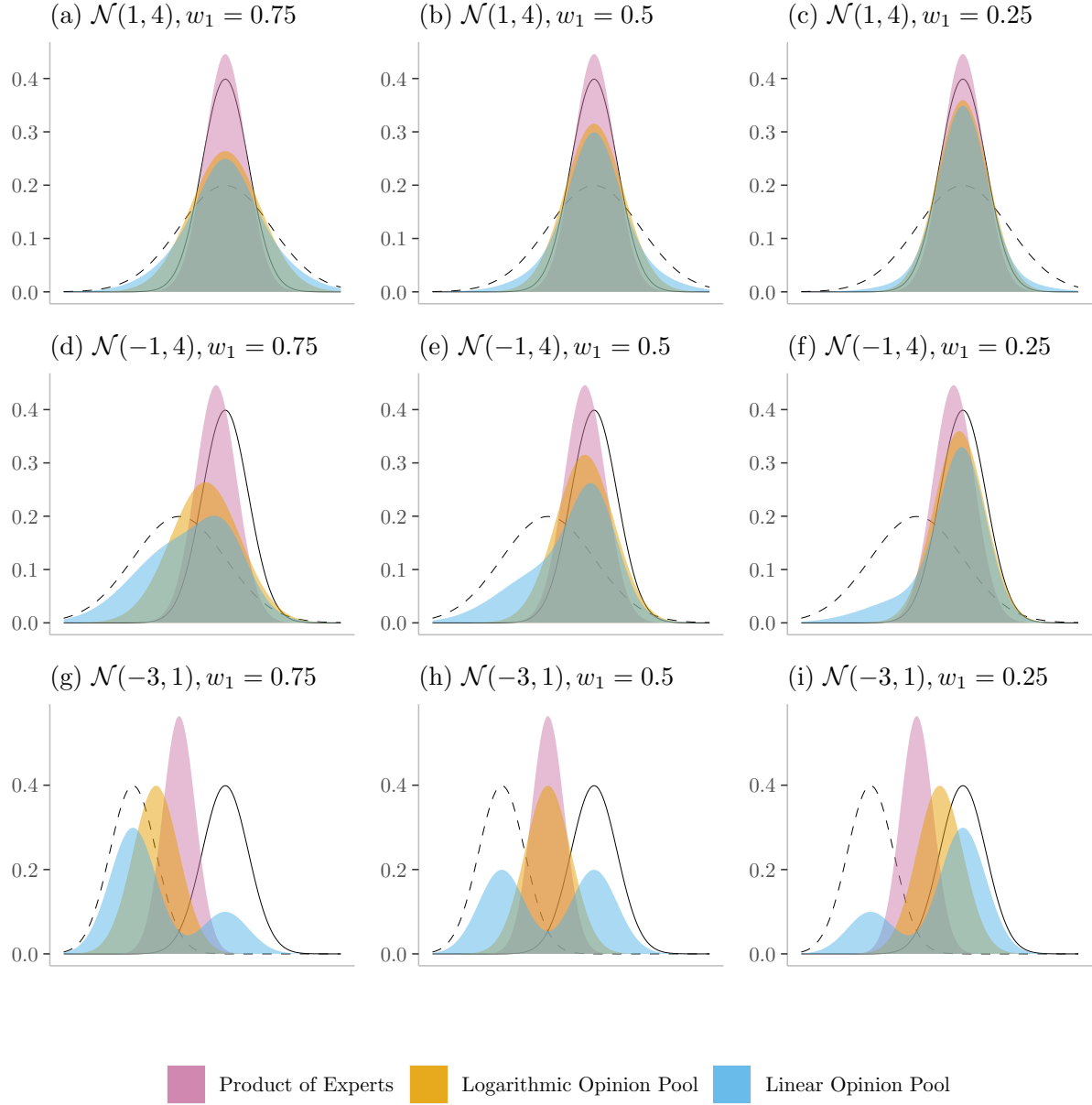$$p_{\text{pool}}(\phi) = g(p_1(\phi), \ldots, p_M(\phi)), \tag{2.31}$$

Figure 2.4: Opinion pooling of solid line $\mathcal{N}(1,1)$ with dashed line Gaussians, specified by plot text. Dashed line Gaussians are weighted w_1 with $w_2 = 1 - w_1$. Reproduced with alternations from Goudie et al. (2019).

for some choice of pooling function g. As discussed in Section 2.6, many possible pooling functions are possible and could be reasonably justified depending on the situation. That being said, some choices of pooling function may be more computational efficient and so attractive from a practical point of view.

The Markov melded joint model p_meld can be achieved by replacing $p(\theta)$ in Equation (2.17) with the pooled prior (2.31) such that

$$p_\text{meld}(\phi, \psi_1, \ldots, \psi_M, Y_1, \ldots, Y_M) = p_\text{pool}(\phi) \prod_{m=1}^{M} \frac{p_m(\phi, \psi_m, Y_m)}{p_m(\phi)} \tag{2.32}$$

This construction is equivalent to altering each of the submodels by a procedure Goudie et al. (2019) call marginal replacement and then applying Markov combination. In particular, the marginal $p_m(\phi)$ of the original submodel is replaced by $p_\text{pool}(\phi)$ resulting in the replacement submodel

$$p_\text{repl,m}(\phi, \psi_m, Y_m) = p_m(\psi_m, Y_m \mid \phi) p_\text{pool}(\phi). \tag{2.33}$$

After marginal replacement has occurred it is possible to apply Markov combination to the collection of replacement submodels $\{p_\text{repl,m}\}_{m=1,\ldots,M}$ since they have consistent marginals, such that

$$
\begin{aligned}
p_\text{comb}(\phi, \psi_1, \ldots, \psi_M, Y_1, \ldots, Y_M) &= \frac{\prod_{m=1}^{M} p_\text{repl,m}(\phi, \psi_m, Y_m)}{p_\text{pool}(\phi)^{M-1}} \\
&= \frac{\prod_{m=1}^{M} p_m(\psi_m, Y_m \mid \phi) p_\text{pool}(\phi)}{p_\text{pool}(\phi)^{M-1}} \\
&= p_\text{pool}(\phi) \prod_{m=1}^{M} p_m(\psi_m, Y_m \mid \phi) \\
&= p_\text{pool}(\phi) \prod_{m=1}^{M} \frac{p_m(\psi_m, Y_m, \phi)}{p_m(\phi)}.
\end{aligned}
\tag{2.34}
$$

The result is equal to that of the Markov melded joint model, Equation (2.32).

Since a joint model has been obtained, Bayesian inference can proceed as usual. Given observed data $Y_m = y_m$ for $m = 1, \ldots, M$, under the Markov melded model (2.32) the joint posterior distribution is
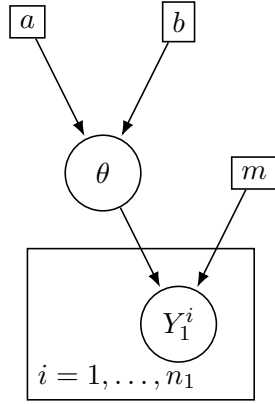
$$p_{\text{meld}}(\phi, \psi_1, \ldots, \psi_M \mid y_1, \ldots, y_M) \propto p_{\text{pool}}(\phi) \prod_{m=1}^{M} \frac{p_m(\phi, \psi_m, y_m)}{p_m(\phi)}, \tag{2.35}$$

which is called the Markov melded posterior.

We present the following pedagogical example of Markov melding with $M = 2$ submodels which, as with Example 3.1, uses conjugacy to enable exact Bayesian computation.

Example 2.2: Binomial and Geometric submodels with conjugate Beta priors

(a) Submodel 1: $p_1(\theta, Y_1)$ (b) Submodel 2: $p_2(\theta, Y_2)$
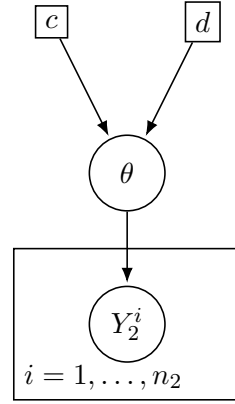

Figure 2.5: Further to the notation introduced in Section 2.2, constants may be included in DAGs with square boxes, whereas random variables have circular boxes. Rectangular boxes (sometimes called plates) are drawn around sections of the diagram which are repeated across the indices indicated.

Consider the following two submodels, illustrated as DAGs in Figure 2.5.

Submodel 1 Define the first submodel $p_1(\theta, Y_1)$ as

$$\theta \sim \text{Beta}(a, b), \tag{2.36}$$

$$Y_1^i \sim \text{Bin}(m, \theta), \quad i = 1, \ldots, n_1, \tag{2.37}$$

where $a = 2$, $b = 3$ and $m = 10$ are known and $Y_1 = (Y_1^1, \ldots, Y_1^{n_1})$.

Suppose the true value of $\theta = 0.4$. We simulate observed data $Y_1 = y_1$ and of size $n_1 = 3$ from this submodel, resulting in $y_1 = \{3, 5, 4\}$. Conditioning on the observed data, inference can be done exactly as the prior is conjugate. The posterior distribution is given by

$$p_1(\theta \mid y_1) \propto p_1(y_1 \mid \theta)p_1(\theta) = \prod_{i=1}^{n_1} \binom{m}{y_1^i} \theta^{y_1^i}(1-\theta)^{m-y_1^i} \cdot \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}\theta^{a-1}(1-\theta)^{b-1}$$

$$\propto \theta^{\tau_1+a-1}(1-\theta)^{n_1 m-\tau_1+b-1} \propto \text{Beta}(\tau_1+a, n_1 m-\tau_1+b), \tag{2.38}$$

where $\sum_{i=1}^{n_1} y_1^i = \tau_1$.

Submodel 2 The second submodel $p_2(\theta, Y_2)$ is such that

$$\theta \sim \text{Beta}(c, d) \tag{2.39}$$

$$Y_2 \sim \text{Geo}(\theta), \quad i = 1, \ldots, n_2, \tag{2.40}$$

where $c = 5$ and $d = 4$ are known and $Y_1 = (Y_2^1, \ldots, Y_2^{n_2})$.

We again simulate observed data $Y_2 = y_2$ this time of size $n_2 = 6$, resulting in $y_2 = \{2, 0, 1, 0, 0, 1\}$. This submodel, like the one before, is conjugate and the posterior distribution is simply

$$p_2(\theta \mid y_2) \propto p_2(y_2 \mid \theta)p_2(\theta) = \prod_{i=1}^{n_2}(1-\theta)^{y_2^i}\theta \cdot \frac{\Gamma(c)\Gamma(d)}{\Gamma(c+d)}\theta^{c-1}(1-\theta)^{d-1}$$

$$\propto \theta^{n_2+c-1}(1-\theta)^{\tau_2+d-1} \propto \text{Beta}(n_2+c, \tau_2+d), \tag{2.41}$$

where $\sum_{i=1}^{n_2} y_2^i = \tau_2$.

Melded model This is a simple situation: the link parameter is $\phi = \theta$, and there are no model specific parameters $\psi_1 = \psi_2 = \emptyset$. Notice with this hyperparameter setting, there is not consistency between the two Beta priors, given by Equations (2.36) and (2.39), on the link parameter. For this reason, Markov melding is an appropriate methodological choice to perform inference.

To facilitate Markov melding, we pool the inconsistent prior distributions $p_1(\theta)$ and $p_2(\theta)$. Using the Product of Experts pooling (2.30) gives the pooled prior to be
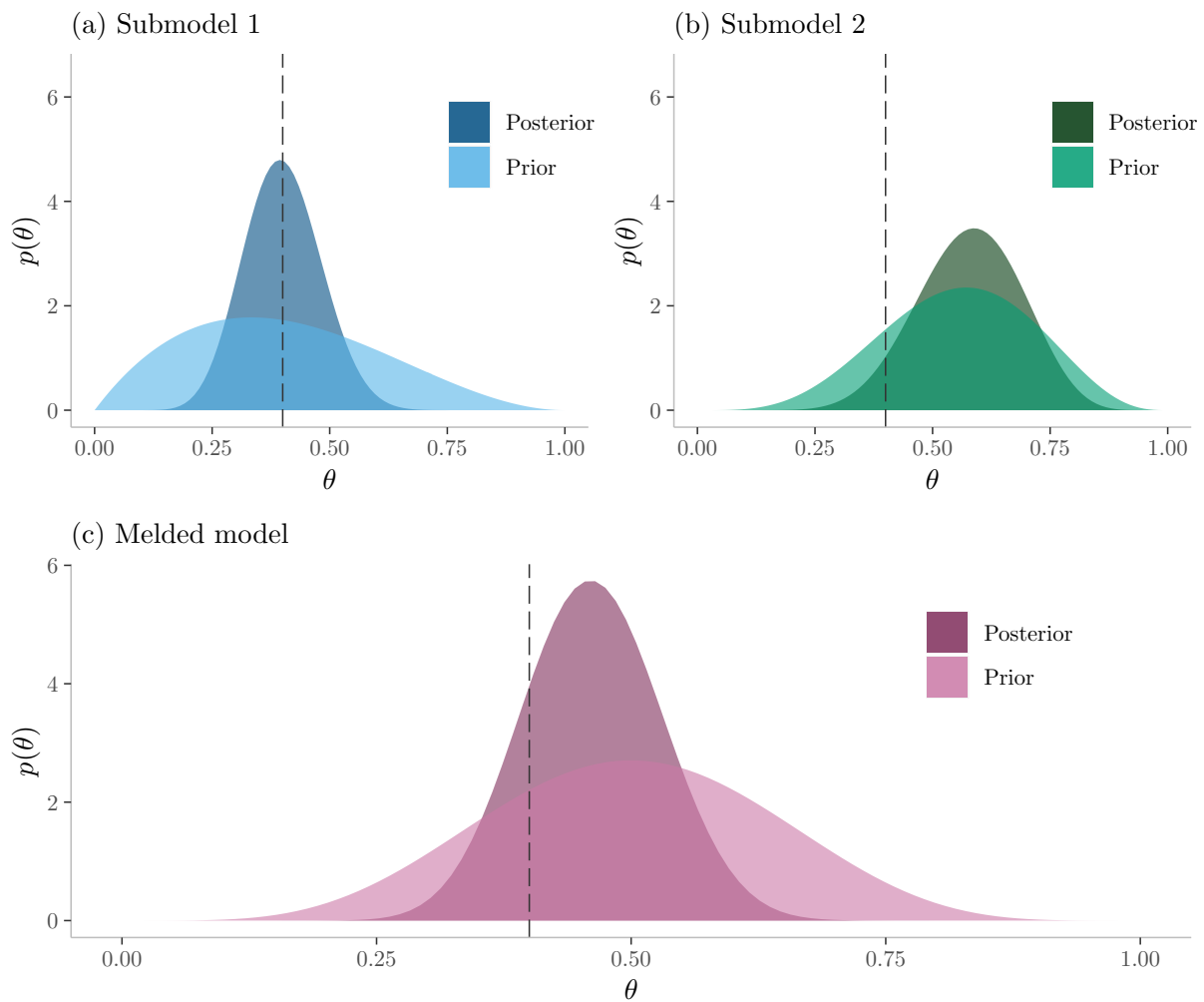
Figure 2.6: Parts (a) and (b) show the standard Bayesian updating of the prior for submodels one and two respectively. Part (c) shows the PoE pooled prior and Markov melded posterior.

$$p_{\text{pool}}(\theta) \propto \text{Beta}(a, b) \cdot \text{Beta}(c, d) \propto \theta^{a-1}(1-\theta)^{b-1} \cdot \theta^{c-1}(1-\theta)^{d-1}$$
$$= \theta^{a+c-2}(1-\theta)^{b+d-2} \propto \text{Beta}(a+c-1, b+d-1). \qquad (2.42)$$

By Equation (2.35), the relevant Markov melded posterior is

$$p_{\text{meld}}(\theta \,|\, y_1, y_2) \propto p_{\text{pool}}(\theta) \prod_{m=1}^{2} \frac{p_m(\theta \,|\, y_m)}{p_m(\theta)} \propto p_1(\theta)p_2(\theta) \prod_{m=1}^{2} \frac{p_m(\theta \,|\, y_m)}{p_m(\theta)}$$
$$\propto p_1(\theta \,|\, y_1)p_2(\theta \,|\, y_2)$$
$$\propto \text{Beta}(\tau_1 + a + n_2 + c - 1, n_1 m - \tau_1 + b + \tau_2 + d - 1). \qquad (2.43)$$

In fact, in general under Product of Experts pooling, the melded posterior is proportional to the product of the submodel posteriors

$$p_{\text{meld}}(\phi, \psi_1, \ldots, \psi_M \,|\, y_1, \cdots, y_M) \propto p_{\text{pool}}(\phi) \prod_{m=1}^{M} \frac{p_m(\phi, \psi_m, y_m)}{p_m(\phi)}$$
$$= \prod_{m=1}^{M} p_m(\phi, \psi_m, y_m)$$
$$\propto \prod_{m=1}^{M} p_m(\phi, \psi_m \,|\, y_m). \qquad (2.44)$$

Figure 2.6 shows that both the melded prior (2.42) and Markov melded posterior (2.43) occupy a centrist position between the two submodels.

Suppose rather than Product of Experts pooling we use logarithmic pooling with weights w_m for submodel m such that $w_1 + w_2 = 1$. The pooled prior is then

$$p_{\text{pool}}(\theta) \propto \text{Beta}(a, b)^{w_1} \cdot \text{Beta}(c, d)^{w_2} \propto \theta^{w_1(a-1)}(1-\theta)^{w_1(b-1)} \cdot \theta^{w_2(c-1)}(1-\theta)^{w_2(d-1)}$$
$$\propto \text{Beta}(w_1 a + w_2 c - w_1 - w_2 + 1, w_1 b + w_2 d - w_1 - w_2 + 1) \propto \text{Beta}(e, f), \qquad (2.45)$$

where $e = w_1 a + w_2 c - w_1 - w_2 + 1$ and $f = w_1 b + w_2 d - w_1 - w_2 + 1$. Using this pooled prior, the Markov melded posterior is given by

$$p_{\text{meld}}(\theta \mid y_1, y_2) \propto p_{\text{pool}}(\theta) \prod_{m=1}^{2} \frac{p_m(\theta \mid y_m)}{p_m(\theta)}$$

$$\propto \text{Beta}(e, f) \frac{\text{Beta}(\tau_1 + a, n_1 m - \tau_1 + b)}{\text{Beta}(a, b)} \frac{\text{Beta}(n_2 + c, \tau_2 + d)}{\text{Beta}(c, d)}$$

$$\propto \theta^{e + \tau_1 + n_2 - 1}(1 - \theta)^{f + n_1 m - \tau_1 + \tau_2 - 1}$$

$$\propto \text{Beta}(e + \tau_1 + n_2, f + n_1 m - \tau_1 + \tau_2) \tag{2.46}$$

Note that setting $w_1 = w_2 = 1$ gives, as in Equation (2.43), a $\text{Beta}(a + c + \tau_1 + n_2 - 1, b + d + n_1 m - \tau_1 + \tau_2 - 1)$ distribution. Figure 2.7 shows the results of Markov melding for three weight settings. In parts (a) and (c) the weighting amounts to dictatorial pooling to submodels one and two respectively. Part (b), in contrast, is a geometric mean between the two submodels. Under these circumstances of the particular pooling is of little consequence to the Markov melded posterior. $\qquad\square$
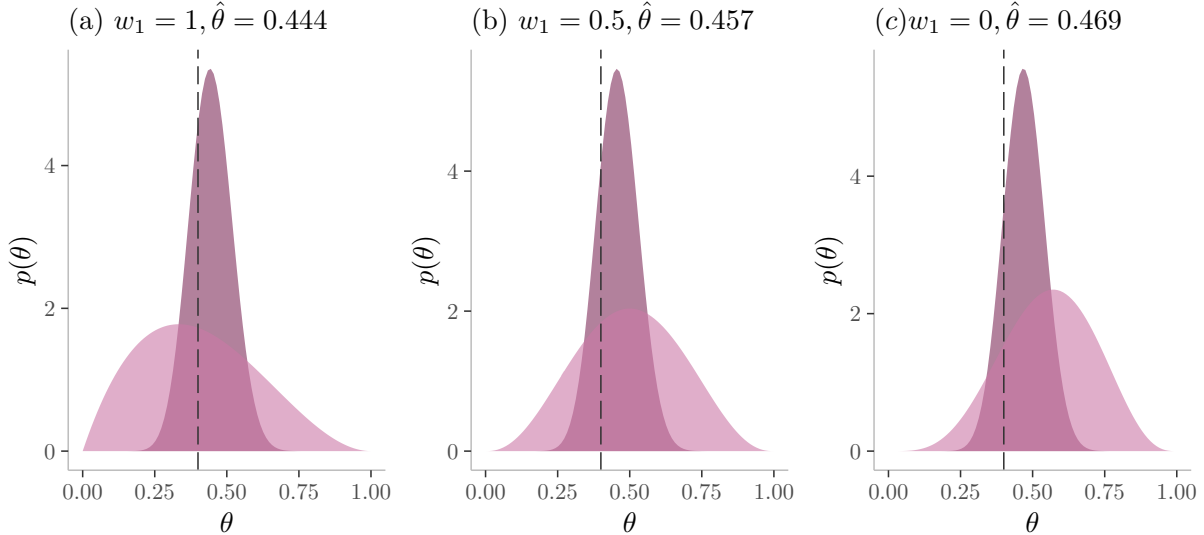

Figure 2.7: Markov melding using logarithmically pooled priors with various weights. The weighting w_1, with $w_2 = 1 - w_1$, as well as the posterior mean $\hat{\theta} = \mathbb{E}[\theta \mid y_1, y_2]$ is given above each plot.

Example 2.2 shows that, for a simple tractable case, Markov melding behaves as one would hope.

Chapter 3

Computation

The primary goal in Bayesian computation is to find expectations of functions with respect to the posterior distribution, or in our case the Markov melded posterior given by Equation (2.35). Many relevant quantities, such as probabilities or risks, can be cast as integrals as the following example demonstrates.

Example 3.1: Bayesian decision theory

In assessing developments in evidence-based medicine, Ashby and Smith (2000) argue that a Bayesian approach is the natural framework for decision making under uncertainty. Suppose $\mathcal{A}$ is the space of possible decisions with elements $a \in \mathcal{A}$ and there exists a utility function $U : \mathcal{A} \to \mathbb{R}^+$ weighing up the drawbacks and benefits of each decision. Then, it is clear to see that the optimal decision is to select the decision $a^\star$ which maximises this utility. Leaving aside the problem of specifying U, most (if not all) of the time the utility also depends on additional variables which we are uncertain about. If these additional variables are (leadingly) denoted by $\theta \in \Theta$ then our definition of U may be expanded so that $U : \mathcal{A} \times \Theta \to \mathbb{R}^+$. Now, in order to make well-informed decisions, we must take into account our uncertainty about θ. Having observed data $y \in \mathcal{Y}$ informative about θ, the distribution which represents this uncertainty is the posterior $p(\theta \mid y)$. Rather than computing utilities, we now must calculate expected utilities. This is done by integrating out our uncertainty about θ as follows

$$\mathbb{E}_{p(\theta \mid y)}[U(a, \theta)] = \int U(a, \theta) p(\theta \mid y) d\theta. \tag{3.1}$$

The optimal decision now is to select the action maximising this expected utility. The upshot is that Equation (3.1) amounts to computing expectations with respect to the posterior. □

3.1   Monte Carlo methods

Monte Carlo, a general class of simulation-based methods, are a prevailing technique for scalable computation of integrals like that of Equation (3.1). For ease of notation rather than the posterior, we consider a general probability density function $\pi(x)$ where $x \in \mathcal{X}$. The relevant integral is then

$$\mathbb{E}_\pi[\varphi(x)] = \int \varphi(x)\pi(x)dx \tag{3.2}$$

where $\varphi : \mathcal{X} \to \mathbb{R}$ is an arbitrary test function.

By sampling points independently from the probability density function $X_i \sim \pi(x)$ for $i = 1, \ldots, N$, $\pi(x)$ may be approximated by the empirical distribution

$$\widehat{\pi}(x) = \frac{1}{N}\sum_{i=1}^N \delta_{X_i}(x). \tag{3.3}$$

This facilitates the approximation of expectations by using $\widehat{\pi}(x)$ in place of $\pi(x)$ such that

$$\mathbb{E}_\pi[\varphi(x)] = \int \varphi(x)\pi(x)dx \approx \int \varphi(x)\widehat{\pi}(x)dx = \frac{1}{N}\sum_{i=1}^N \varphi(X_i) := \bar{\varphi}_N. \tag{3.4}$$

By the strong law of large numbers, granted the expectation exists, then the Monte Carlo estimator will converge

$$\lim_{N\to\infty} \bar{\varphi}_N = \mathbb{E}_\pi[\varphi(x)] \tag{3.5}$$

almost surely. In addition, the rate of convergence can be monitored by estimating the variance of the Monte Carlo estimator $\bar{\varphi}_N$ as

$$\sigma_N^2 = \frac{1}{N^2}\sum_{i=1}^N \left(\varphi(x_i) - \bar{\varphi}_N\right)^2, \tag{3.6}$$

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and then applying the central limit theorem such that

$$\frac{\bar{\varphi}_N - \mathbb{E}_\pi[\varphi(x)]}{\sigma_N} \sim \mathcal{N}(0,1). \tag{3.7}$$

These principles, both the approximation of the empirical distribution via Equation (3.3) and the convergence of the Monte Carlo estimator, are illustrated in Figure (3.1) for a simple exponential distribution with rate parameter $\lambda = 1$.

3.2 Markov chain Monte Carlo

It is typically not possible to generate independent samples from the relevant distribution directly. This is especially true for complex models and in high dimensions, as with Markov melding.

Markov chain Monte Carlo (MCMC) is a flexible and broad class of algorithms for sampling from probability distributions unable to be sampled from directly. In MCMC, rather than drawing independent samples, the sample at iteration i depends on that of the previous iteration $i-1$; the result being a a Markov chain of samples. By careful specification, the stationary distribution of this Markov chain can be set to correspond to the distribution π. As a result, if the Markov chain is run until it reaches convergence then it can more-or-less be used in place of direct samples from π. There are many diagnostic tools which can be used to check if the chain appears to have converged, the simplest being heuristic examinination of trace-plots which show the positions of the chain over time. However, convergence is not something which is possible to prove so disgression must be taken.

Due to dependence on the previous value, samples from a Markov chain are typically positively correlated, thereby reducing the amount of information each sample contains about π. This autocorrelation should be taken into account when calculating the standard error of Monte carlo estimates, see for example Gelman, Rubin, and others (1992). One popular metric of this sort is the effective sample size (ESS) (Robert and Casella 2013) which can be interpreted as the number of independent samples the correlated samples would be equivalent to.
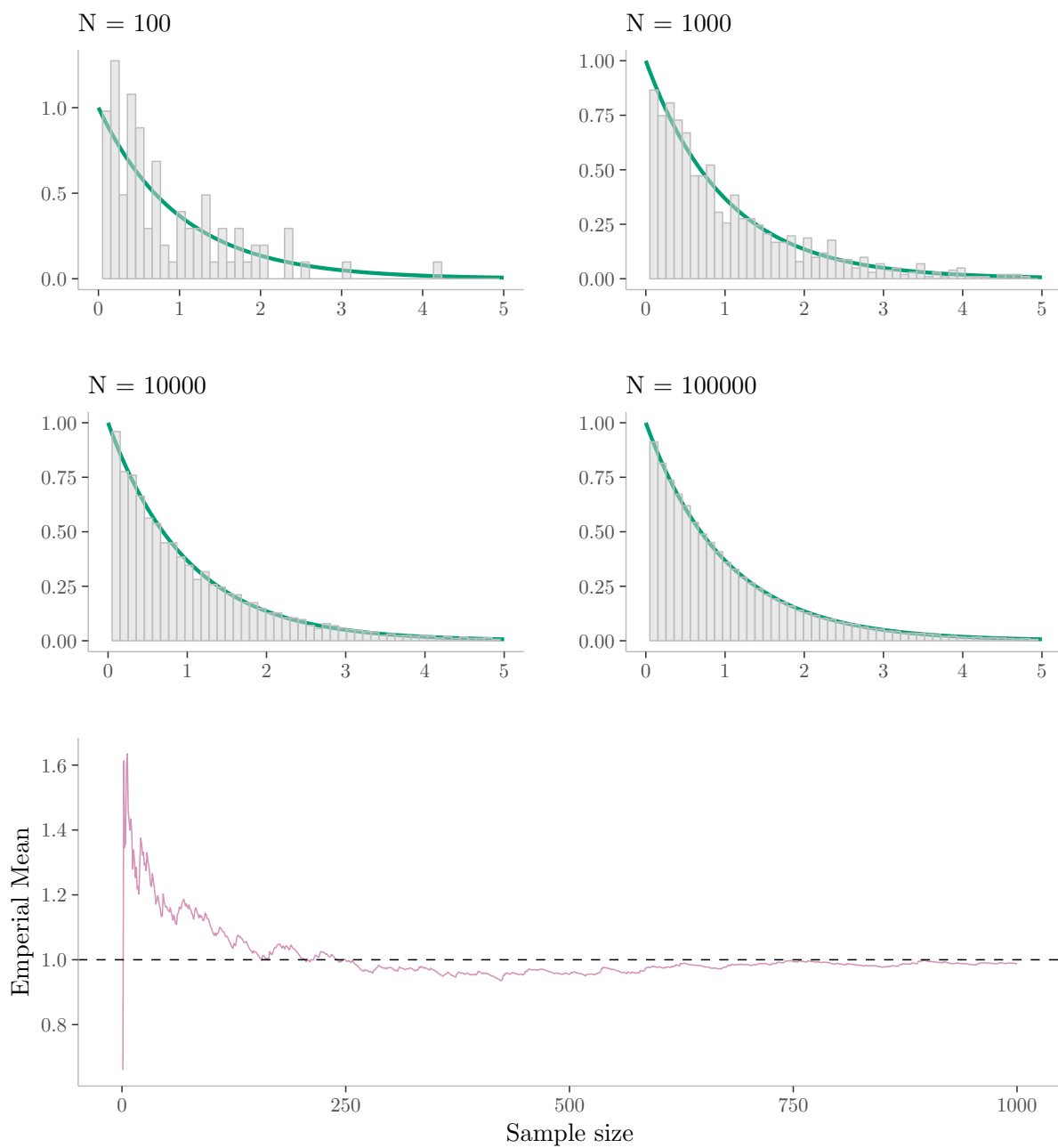
Figure 3.1: Above: Emperical distributions generated by samples $X_i \sim \text{Exp}(1)$ for $i = 1, \ldots, N$ for N of varying order of magnitude with exact $\text{Exp}(1)$ distribution plotted in green. Below: Convergence of the empirical mean, in pink, to the true mean plotted as dashed grey line.

3.2.1 Metropolis-Hastings

Algorithm 1: Metropolis-Hastings sampler

Target density π, initialise $x^{(0)}$;

for $i = 1, 2, \ldots, N$ **do**

    Set current value $x = x^{(i-1)}$;

    Draw candidate value $x^\star \sim q(\cdot \,|\, x)$;

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

    Let $\alpha = \min(1, r)$, where $r = \frac{\pi(x^\star)/q(x^\star \,|\, x)}{\pi(x)/q(x \,|\, x^\star)}$;

    if $\alpha > u$ **then**

        $x^{(i)} = x^\star$;

    else

        $x^{(i)} = x$;

end for

The Metropolis-Hastings (MH) algorithm dates back to foundational work of Metropolis et al. (1953) and Hastings (1970). At each iteration i, the next step $x^\star$ is suggested according to a user-specified proposal distribution $q(\cdot \,|\, x)$ conditional on the current location $x = x^{(i-1)}$. Candidate values $x^\star$ are accepted with probability α, else the Markov chain remains at the current location x. The value of the acceptance probability α is calculated by

$$\alpha = \mathbb{P}[x^\star \text{ accepted}] = \min(1, r)$$

$$= \min\left(1, \frac{R(x^\star, x)}{R(x, x^\star)}\right) = \min\left(1, \frac{\pi(x^\star)/q(x^\star \,|\, x)}{\pi(x)/q(x \,|\, x^\star)}\right), \tag{3.8}$$

where r is the ratio of target-to-proposal density ratios R at the candidate $x^\star$ and current x values.

In Bayesian statistics typically the target distribution π is such that

$$\pi(x) = \frac{\gamma(x)}{Z}, \tag{3.9}$$

where the normalising constant $Z = \int \gamma(x) dx$ is computationally intractable. To be specific,

π is the product of the likelihood and prior and Z is the marginal likelihood. Therefore, it is crucial that Equation (3.8) only requires the point-wise evaluation of γ and not π since $\pi(x)/\pi(z) = \gamma(x)/\gamma(z)$.

The efficiency of MH depends greatly on the user's choice of proposal distribution $q(\cdot \,|\, x)$. A common option is to consider proposal distributions which are symmetric about the current value x, thereby simplifying the acceptance probability $\alpha = \min\{1, \pi(x^\star)/\pi(x)\}$ since $q(x \,|\, x^\star) = q(x^\star \,|\, x)$. This algorithm is called random walk Metropolis (RWM). Roberts, Gelman, and Gilks (1997) show that, under certain conditions, the acceptance rate for RWM which minimises autocorrelation is 0.44 for one-dimensional proposals tending asymptotically to 0.234 as the dimension increases.

By setting $\pi(x) = p_{\text{meld}}(\phi, \psi_1, \ldots, \psi_M \,|\, y_1, \ldots, y_M)$ the general MH algorithm can be applied to target the Markov melded posterior. The proposal distribution is then of the form $q(\phi^\star, \psi_1^\star, \ldots, \psi_M^\star \,|\, \phi, \psi_1, \ldots, \psi_M)$, where $(\phi^\star, \psi_1^\star, \ldots, \psi_M^\star)$ are the candidate values and $(\phi, \psi_1, \ldots, \psi_M)$ are the current values of the chain.

The acceptance probability $\alpha = \min(1, r)$ for moves $(\phi, \psi_1, \ldots, \psi_M) \to (\phi^\star, \psi_1^\star, \ldots, \psi_M^\star)$ can be calculated via

$$r = \frac{R(\phi^\star, \psi_1^\star, \ldots, \psi_M^\star, \phi, \psi_1, \ldots, \psi_M)}{R(\phi, \psi_1, \ldots, \psi_M, \phi^\star, \psi_1^\star, \ldots, \psi_M^\star)}, \tag{3.10}$$

where $R(\phi^\star, \psi_1^\star, \ldots, \psi_M^\star, \phi, \psi_1, \ldots, \psi_M)$ is the target-to-proposal density ratio

$$R(\phi^\star, \psi_1^\star, \ldots, \psi_M^\star, \phi, \psi_1, \ldots, \psi_M) = \frac{p_{\text{pool}}(\phi^\star) \prod_{m=1}^{M} \frac{p_m(\phi^\star, \psi_m^\star, y_m)}{p_m(\phi^\star)}}{q(\phi^\star, \psi_1^\star, \ldots, \psi_M^\star \,|\, \phi, \psi_1, \ldots, \psi_M)} \tag{3.11}$$

For Markov melding, due to the possible quantity of parameters $(\phi, \psi_1, \ldots, \psi_M)$, it is likely difficult to find a suitable choice of proposal distribution $q(\phi^\star, \psi_1^\star, \ldots, \psi_M^\star \,|\, \phi, \psi_1, \ldots, \psi_M)$ such that moves are accepted with reasonable probability.

3.2.2   Metropolis-within-Gibbs

The general MH algorithm ignores the modular structure of the submodels. As a result both of this structure and the difficulty of full parameter moves, it may be more appealing to update submodel components separately.

Gibbs sampling (S. Geman and Geman 1987) is an MCMC algorithm which updates component-wise. In fact, Gibbs sampling is a special case of MH where the acceptance rate can be calculated to be identically one. Returning to the more general notation, suppose that x can be written as a p-dimensional vector such that $x = (x_1, \ldots, x_p)$. In Gibbs sampling at each iteration i only one of the components x_j where $j \in 1, \ldots p$ is updated. In particular, x_j is sampled from its full conditional distribution, defined as

$$\pi_{X_j \mid X_{-j}}(x_j | x_{-j}) = \frac{\pi(x)}{\int \pi(x) dx_j}, \tag{3.12}$$

where the notation x_{-j} refers to the subvector of x excluding the jth element. There are multiple ways of choosing the component j to update at each iteration: it can be chosen uniformly using random-scan Gibbs sampling, or iterated over deterministically using systematic-scan Gibbs sampling. Having selected a component to update x_j, informally speaking Gibbs sampling moves perpendicular to the directions spanned by each of the other components x_{-j}. If components x_j and x_k are say positively correlated then increases in x_j are typically accompanied by increases in $x_k, k \neq j$. In this situation, Gibbs sampling may not be efficient as it struggles to find the relevant region using perpendicular moves.

From a computational point of view, requiring that the full conditionals of π are available and can be sampled from is often restrictive. For Markov melding, the full conditionals of p_{meld} may not be available and as a result generic Gibbs sampling is not generally applicable. Instead, Goudie et al. (2019) propose the use of the Metropolis-within-Gibbs (Muller 1991) (MWG) algorithm.

Algorithm 2: (Random-scan) Metropolis-within-Gibbs sampler

Target density π, initialise $x^{(0)} := (x_1^{(0)}, \ldots, x_p^{(0)})$;

for $i = 1, 2, \ldots, N$ **do**

$\quad$ Set current value $x = x^{(i-1)}$;

$\quad$ Draw $j \sim \mathcal{U}\{1, \ldots, p\}$;

$\quad$ Draw $x_j^\star \sim q_j(\cdot \,|\, x)$;

$\quad$ Set $x^\star = (x_1, \ldots, x_j^\star, \ldots, x_p)$;

$\quad$ Draw $u \sim \mathcal{U}(0, 1)$;

$\quad$ Let $\alpha = \min(1, r)$, where $r = \frac{\gamma(x^\star)/q(x^\star \,|\, x)}{\gamma(x)/q(x \,|\, x^\star)}$;

$\quad$ **if** $\alpha > u$ **then**

$\quad\quad$ $x^{(i)} = x^\star$;

$\quad$ **else**

$\quad\quad$ $x^{(i)} = x$;

end for

MWG unifies MH and Gibbs sampling by utilising componentwise MH proposals rather than sampling from the full conditionals exactly. As such, MWG does not require access to the full conditionals and as a result is more generally applicable. Of course, if for some index j the full conditional is available then it is a valid MH update and can be used.

As with MH, the user must specify the proposal distributions, in this case $q_j(\cdot \,|\, x_j^{(i-1)})$ for each of the p components. For random walk type proposals the resulting algorithm known as random walk Metropolis-within-Gibbs (RWM-within-Gibbs). This algorithm is studied in the context of optimal scaling by Neal and Roberts (2006) who show that, as with RWM, the optimal acceptance rate is 0.44 for one-dimensional proposals again tending to 0.234 for higher dimension as with Roberts, Gelman, and Gilks (1997).

Now, to target Equation (2.35) using MWG, define the components of $(\phi, \psi_1, \ldots, \psi_M)$ be the link parameter ϕ and each of the model specific parameters ψ_m, $m = 1, \ldots, M$ respectively as would be expected. Suppose the initial values $(\phi^{(0)}, \psi_1^{(0)}, \ldots, \psi_M^{(0)})$ are given.

Model specific parameter updates In Markov melding, it is assumed (2.16) that the ψ_m are conditionally independent given ϕ. Supposing this assumption is reasonable, it would therefore be expected that Gibbs and MWG sampling would be relatively efficient for model specific

parameters. For each of ψ_m for $m = 1, \ldots, M$ define a proposal distribution $q_m(\cdot \,|\, \psi_m)$. The target-to-proposal density ratio is then

$$R(\phi, \psi_1, \ldots, \psi_m^\star, \ldots, \psi_M, \phi, \psi_1, \ldots, \psi_m, \ldots, \psi_M)$$

$$= p_{\text{pool}}(\phi) \prod_{j=1}^M \frac{p_j(\phi, \psi_j, y_j)}{p_j(\phi)} \frac{1}{q_m(\psi_m^\star \,|\, \psi_m)}$$

$$= p_{\text{pool}}(\phi) \prod_{j \neq m} \frac{p_j(\phi, \psi_j, y_j)}{p_j(\phi)} \cdot \frac{p_m(\phi, \psi_m^\star, y_m)}{p_m(\phi)} \frac{1}{q_m(\psi_m^\star \,|\, \psi_m)}. \tag{3.13}$$

In calculating r via (3.10) factors not dependent on submodel m, as well as the pooled prior, cancel leaving

$$r = \frac{p_m(\phi, \psi_m^\star, y_m) \cdot \frac{1}{q_m(\psi_m^\star \,|\, \psi_m)}}{p_m(\phi, \psi_m, y_m) \cdot \frac{1}{q_m(\psi_m \,|\, \psi_m^\star)}}. \tag{3.14}$$

Equation (3.14) precisely corresponds to updating ψ_m conditional on the link parameter ϕ for inference performed on the mth alone. With each submodel having been specified as it is, it's reasonable to expect that inference for each submodel individually is tractable via MH. As such, it is possible to calculate the ratio in Equation (3.14) for each $m = 1, \ldots, M$.

Link parameter updates In contrast to the above, one would expect the link parameter ϕ to have covariance structure with each of the model specific parameters: potentially making link parameter updates relatively inefficient. For the link parameter ϕ define a proposal distribution $q(\cdot \,|\, \phi)$. The target-to-proposal density ratio is

$$R(\phi, \psi_1, \ldots, \psi_M, \phi^\star, \psi_1, \ldots, \psi_M) = p_{\text{pool}}(\phi^\star) \prod_{m=1}^M \frac{p_m(\phi^\star, \psi_m, y_m)}{p_m(\phi^\star)} \cdot \frac{1}{q(\phi^\star \,|\, \phi)}. \tag{3.15}$$

If Product of Experts pooling is used then the marginal distributions of the link parameter cancel, leaving

$$R(\phi, \psi_1, \ldots, \psi_M, \phi^\star, \psi_1, \ldots, \psi_M) \propto \prod_{m=1}^M p_m(\phi^\star) \prod_{m=1}^M \frac{p_m(\phi^\star, \psi_m, y_m)}{p_m(\phi^\star)} \cdot \frac{1}{q(\phi^\star \,|\, \phi)}$$

$$= \prod_{m=1}^M p_m(\phi^\star, \psi_m, y_m) \cdot \frac{1}{q(\phi^\star \,|\, \phi)}. \tag{3.16}$$

However, in general, in order to calculate Equation (3.15) the prior marginal distributions $p_m(\phi)$ and the closely related p_{pool} must be evaluated. If $p_m(\phi)$ is not tractable, Goudie et al. (2019) suggest using an approximation $\hat{p}_m(\phi)$ found using kernel density estimation with samples drawn from the prior marginal given by Equation (2.13). Samples can be drawn by forward Monte Carlo: simulating the statistical relationships (which typically are standard distributions) top-down in the DAG representation of the submodel until the node corresponding to ϕ is reached.

In the following example, we demonstrate the use of MCMC for Markov melding two different types of meta-analysis.

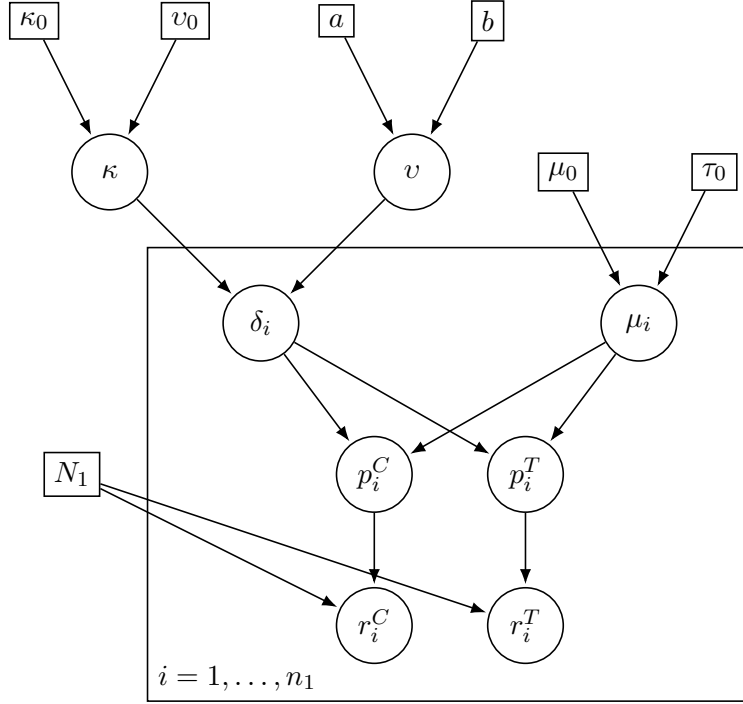*Example 3.2: Metropolis-within-Gibbs for Markov melding*

Figure 3.2: DAG representing Submodel 1

Submodel 1 Standard meta-analysis usually assumes that either effects are common across studies (fixed-effects) or drawn from a probability distribution (random-effects). T. Smith, Spiegelhalter, and Thomas (1995) present a fully Bayesian approach to random-effects meta-analysis. They use this model to study the effectiveness of a treatment (selective decontamination of the digestive tract) which aims to prevent patients acquiring infections whilst in intensive care units (ICUs). We present an adapted version of the model as follows.

Consider $n_1 = 5$ trials $i = 1, \ldots, n_1$ each with both a control (C) and treatment (T) group of size $N_1 = 10$. In trial i, individuals within group $j \in \{C, T\}$ are assumed to have independent probability p_i^j of developing an infection. The numbers of infections in the control and treatment groups for trial i are r_i^C and r_i^T respectively. Assume that μ_i is the average infection rate for the ith trial and δ_i is the true treatment effect, both on the log-odds scale. Following T. Smith, Spiegelhalter, and Thomas (1995), we place an uninformative Gaussian prior on each μ_i, with fixed prior mean $\mu_0 = 0$ and precision $\tau_0 = 0.25$ hyperparameters. The prior on each δ_i is also Gaussian mean κ and precision τ. Uninformative hyperpriors (3.17) and (3.18) are placed on both κ and τ with $\kappa_0 = 0$, $\tau = 0.1$, $a = 3$, $b = 1$. Clinical trials aim to assess treatment effectiveness and therefore the mean (log-odds scale) treatment effect κ is the parameter of interest. The full model $p_1(\kappa, \upsilon, \delta, \mu, p^C, p^T, r^C, r^T)$ is then

$$\kappa \sim \mathcal{N}(\kappa_0, \upsilon_0^{-1}), \tag{3.17}$$

$$\upsilon \sim \text{Gamma}(a, b), \tag{3.18}$$

$$\delta_i \sim \mathcal{N}(\kappa, \upsilon^{-1}), \tag{3.19}$$

$$\mu_i \sim \mathcal{N}(\mu_0, \tau_0^{-1}), \tag{3.20}$$

$$p_i^C = \frac{e^{\mu_i - \delta_i/2}}{1 + e^{\mu_i - \delta_i/2}}, \ p_i^T = \frac{e^{\mu_i + \delta_i/2}}{1 + e^{\mu_i + \delta_i/2}}, \tag{3.21}$$

$$r_i^C \sim \text{Bin}(N_1, p_i^C), \ r_i^T \sim \text{Bin}(N_1, p_i^T), \quad i = 1, \ldots, n_1, \tag{3.22}$$

where the vectors $\delta, \mu, p^C, p^T, r^C, r^T$ are each of length n_1, e.g. $\delta = (\delta_1, \ldots, \delta_{n_1})$. Observed data for Submodel 1 is $Y_1 = (r^C, r^T)$. For this example, we forward simulate the observed data $Y_1 = y_1$ (with $N_1 = 10$ and $n_1 = 5$) from $\delta_i \sim \mathcal{N}(-0.25, 4^{-1})$, $\mu_i \sim \mathcal{N}(-1, 2^{-1})$, resulting in $r^C = \{8, 8, 11, 6, 5\}$, $r^T = \{2, 2, 5, 11, 4\}$.

The probabilities $p = (p_i^C, p_i^T)$ are an (invertible) deterministic transformation of (μ_i, δ_i). Therefore, each probability has an induced distribution via Equation (2.24). Had a prior been specified on p then the situation would have been identical to that of Poole and Raftery (2000) where there exist multiple priors on parameters in a deterministic simulation model. To resolve issues of this sort Goudie et al. (2019) propose using Bayesian melding (introduced in Section 2.5) however in this instance we choose not to place a prior on p; implicitly accepting the distribution induced by μ_i and δ_i. In particular, for p_i^C (a similar statement is true for p_i^T) we have the inverse transformation

$$\mu_i - \delta_i/2 = \mathrm{logit}(p_i^C) = \log \frac{p_i^C}{1 - p_i^C}, \qquad (3.23)$$

with corresponding Jacobian

$$\left| \frac{\delta(\mu_i - \delta_i/2)}{\delta p_i} \right| = \frac{1}{p_i^C(1 - p_i^C)}. \qquad (3.24)$$

As linear transformations of Gaussian distributions, $\mu_i \pm \delta_i/2$ are Gaussian with mean and variance given by

$$\mathbb{E}[\mu_i - \delta_i/2 | \mu_0, \tau_0, \kappa, \upsilon] = \mu_0 - \kappa/2, \qquad (3.25)$$

$$\mathbb{E}[\mu_i + \delta_i/2 | \mu_0, \tau_0, \kappa, \upsilon] = \mu_0 + \kappa/2, \qquad (3.26)$$

$$\mathbb{V}[\mu_i \pm \delta_i/2 | \mu_0, \tau_0, \kappa, \upsilon] = \tau_0^{-1} + \upsilon^{-1}/4. \qquad (3.27)$$

Therefore, defining $(\tau_0^{-1} + \upsilon^{-1}/4)^{-1} = \omega$, the distributions of p_i^C and p_i^T are given by

$$p(p_i^C \,|\, \mu_0, \tau_0, \kappa, \upsilon) = \frac{\omega}{\sqrt{2\pi}} \exp\left(-\frac{\omega}{2} \left(\log \frac{p_i^C}{1 - p_i^C} - (\mu_0 - \kappa/2) \right)^2 \right) \frac{1}{p_i^C(1 - p_i^C)}, \qquad (3.28)$$

$$p(p_i^T \,|\, \mu_0, \tau_0, \kappa, \upsilon) = \frac{\omega}{\sqrt{2\pi}} \exp\left(-\frac{\omega}{2} \left(\log \frac{p_i^T}{1 - p_i^T} - (\mu_0 + \kappa/2) \right)^2 \right) \frac{1}{p_i^T(1 - p_i^T)}. \qquad (3.29)$$

Having calculated distributions (3.28) and (3.29) dependence on (μ, δ) can be omitted. Given (r^C, r^T) (and additionally omitting dependence on fixed hyperparameters) the posterior distribution is then

$$p_1(\kappa, \upsilon, p^C, p^T \mid r^C, r^T)$$

$$\propto \prod_{i=1}^{n_1} \binom{N_1}{r_i^C} p_i^{Cr_i^C} (1-p_i^C)^{N_1-r_i^C} \frac{\omega}{\sqrt{2\pi}} \exp\left(-\frac{\omega}{2}\left(\log\frac{p_i^C}{1-p_i^C} - (\mu_0 - \kappa/2)\right)^2\right) \frac{1}{p_i^C(1-p_i^C)}$$

$$\cdot \prod_{i=1}^{n_1} \binom{N_1}{r_i^T} p_i^{Tr_i^T} (1-p_i^T)^{N_1-r_i^T} \frac{\omega}{\sqrt{2\pi}} \exp\left(-\frac{\omega}{2}\left(\log\frac{p_i^T}{1-p_i^T} - (\mu_0 + \kappa/2)\right)^2\right) \frac{1}{p_i^T(1-p_i^T)}$$

$$\cdot \frac{\tau_0}{\sqrt{2\pi}} \exp\left(-\frac{\tau_0}{2}(\mu-\mu_0)^2\right) \cdot \frac{b^a}{\Gamma(a)} \tau^{a-1} \exp(-b\tau)$$

$$\propto \prod_{i=1}^{n_1} \{p_i^{Cr_i^C-1}(1-p_i^C)^{N_1-r_i^C-1}\} \omega^{n_1} \exp\left(-\frac{\omega}{2}\sum_{i=1}^{n_1}\left(\log\frac{p_i^C}{1-p_i^C} - (\mu_0 - \kappa/2)\right)^2\right)$$

$$\cdot \prod_{i=1}^{n_1} \{p_i^{Tr_i^T-1}(1-p_i^T)^{N_1-r_i^T-1}\} \omega^{n_1} \exp\left(-\frac{\omega}{2}\sum_{i=1}^{n_1}\left(\log\frac{p_i^T}{1-p_i^T} - (\mu_0 + \kappa/2)\right)^2\right)$$

$$\cdot \exp\left(-\frac{\upsilon_0}{2}(\kappa-\kappa_0)^2\right) \upsilon^{a-1} \exp(-b\upsilon) \tag{3.30}$$

Often it is more computationally convenient to work in terms of logarithms as this allows products to be replaced with sums. The log-posterior is

$$\log p(\kappa, \upsilon, p^C, p^T \mid r^C, r^T)$$

$$\propto \sum_{i=1}^{n_1} \{(r_i^C - 1)\log p_i^C + (N_1 - r_i^C - 1)\log(1-p_i^C)$$

$$+ (r_i^T - 1)\log p_i^T + (N_1 - r_i^T - 1)\log(1-p_i^T)$$

$$- \frac{\omega}{2}\left(\log\frac{p_i^C}{1-p_i^C} - (\mu_0 - \kappa/2)\right)^2 - \frac{\omega}{2}\left(\log\frac{p_i^T}{1-p_i^T} - (\mu_0 + \kappa/2)\right)^2\}$$

$$+ 2n_1\omega - \frac{\upsilon_0}{2}(\kappa-\kappa_0)^2 + (a-1)\log\upsilon - b\upsilon := \ell_1 \tag{3.31}$$

To target the posterior (3.30) we use RWM-within-Gibbs. The initialisation values are chosen to be 0.5 for each of the probabilities and otherwise chosen according to the prior means $(\kappa^{(0)}, \upsilon^{(0)}) = (\kappa_0, a/b) = (0, 1/3)$. The proposal distribution for each component is Gaussian with indivual componentwise standard deviation parameters tuned to achieve close to the optimal one-dimensional acceptance rate 0.44 (Roberts, Gelman, and Gilks (1997) note that there is "little value" in finely tuning algorithms to exact values).

Table 3.1: Scaling and resultant acceptance rates for each component.

	κ	υ	p_1^C	p_2^C	p_3^C	p_4^C	p_5^C	p_1^T	p_2^T	p_3^T	p_4^T	p_5^T
σ	3.000	3.500	0.300	0.250	0.300	0.250	0.200	0.150	0.150	0.250	0.300	0.200
Acceptance	0.427	0.452	0.384	0.407	0.398	0.381	0.411	0.438	0.437	0.406	0.397	0.447

To determine an appropriate number of Markov chain samples for the problem at hand one method is to consider the ESS. To this end, Vats, Flegal, and Jones (2015) calculate a lower bound on the number of effective samples required to estimate a vector of length p with $100(1 - \alpha)\%$ confidence and a relative tolerance of ϵ. Additionally, they define a multivariate ESS which takes into account cross-correlation across the Markov chain components. Both these methods are implemented in the `R` package `mcmcse` (J. M. Flegal et al. 2017).

In order to estimate the mean, of length $p = 12$, with 97.5% confidence and a tolerance of $\epsilon = 0.025$ the required number of effective samples is approximately 40000. Based on a short trial chain, the number of simulations required to achieve this ESS is 2800000 (although this may seem high, at every iteration only one component is proposed and therefore the chain is highly auto-correlated). That being said, the algorithm is not prohibitively computationally intensive, so we choose to run 5000000 iterations.

Table 3.2: Posterior mean (PM), true value and posterior standard deviation (PSD) for each component.

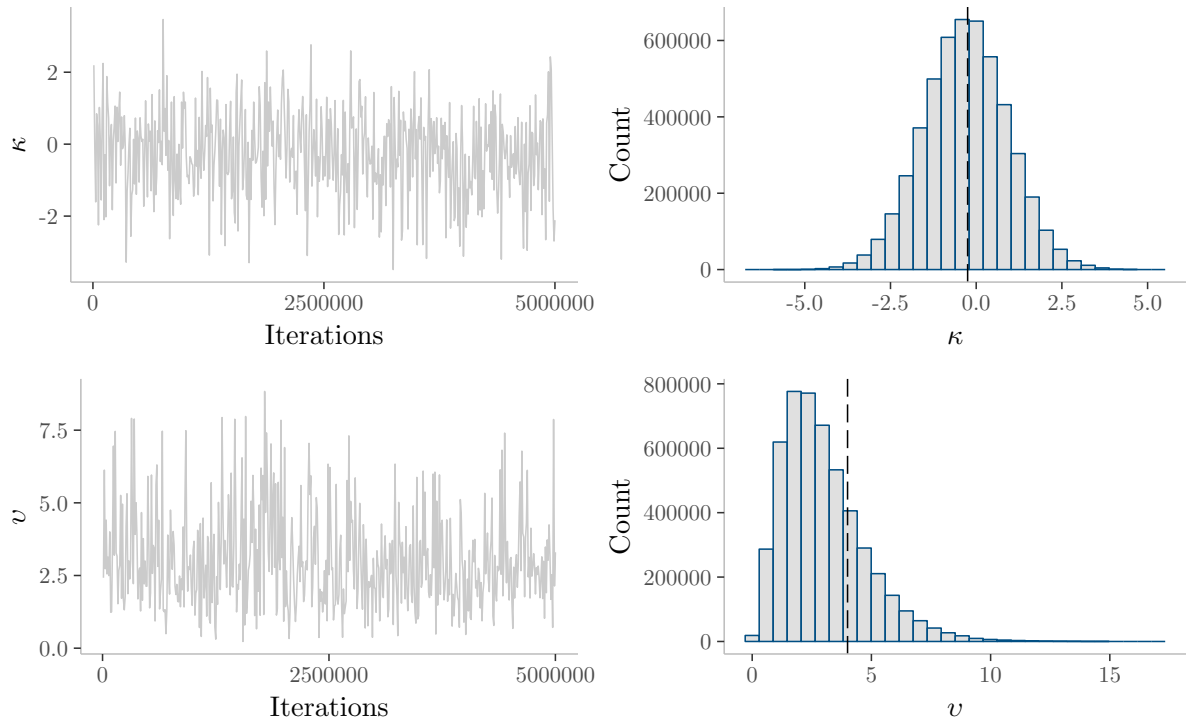|	κ	υ	p_1^C	p_2^C	p_3^C	p_4^C	p_5^C	p_1^T	p_2^T	p_3^T	p_4^T	p_5^T
PM	-0.314	2.991	0.359	0.265	0.502	0.219	0.172	0.124	0.124	0.262	0.546	0.215
Truth	-0.250	4.000	0.214	0.360	0.464	0.296	0.236	0.134	0.324	0.308	0.421	0.221
PSD	1.229	1.731	0.102	0.093	0.106	0.088	0.079	0.068	0.069	0.093	0.107	0.087

Figure 3.3: Submodel 1 posterior traceplots and histograms for the parameters κ and υ, with truth shown on the histogram as a dashed black line. Similar plots for the ten other probability parameters are presented in Appendix A. Note that for this, and all subsequent, traceplots the chains have first been thinned for graphical display reasons.
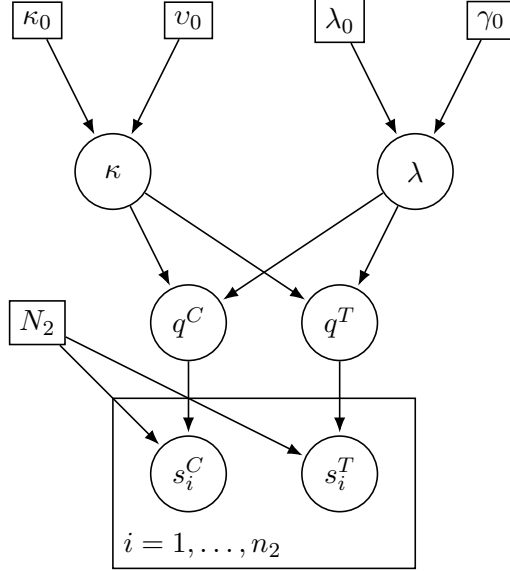
Figure 3.4: DAG representing Submodel 2

Submodel 2 For the second submodel we consider a fixed-effects meta-analysis. The full model $p_2(\kappa, \lambda, q^C, q^T, r^C, r^T)$ is given by

$$\kappa \sim \mathcal{N}(\kappa_0, \upsilon_0^{-1}), \tag{3.32}$$

$$\lambda \sim \mathcal{N}(\lambda_0, \gamma_0^{-1}), \tag{3.33}$$

$$q^C = \frac{e^{\lambda - \kappa/2}}{1 + e^{\lambda - \kappa/2}}, \ q^T = \frac{e^{\lambda + \kappa/2}}{1 + e^{\lambda + \kappa/2}}, \tag{3.34}$$

$$s_i^C \sim \text{Bin}(N_2, q^C), \ s_i^T \sim \text{Bin}(N_2, q^T), \quad i = 1, \ldots, n_2. \tag{3.35}$$

To facilitate Markov melding, inference about the underlying parameters κ and λ is conducted rather than the probabilities q^C and q^T - which typically would seem to be the more natural option. Indeed for a fixed effects meta-analysis more generally it would likely be preferable to directly place priors on the probabilities (for example a Beta prior would be conjugate to the Binomial likelihood). Setting this fact aside, the posterior distribution given (s^C, s^T) is

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$$p_2(\kappa, \lambda \mid s^C, s^T)$$

$$\propto \prod_{i=1}^{n_2} \binom{N_2}{s_i^C} \left(\frac{e^{\lambda - \kappa/2}}{1 + e^{\lambda - \kappa/2}} \right)^{s_i^C} \left(\frac{1}{1 + e^{\lambda - \kappa/2}} \right)^{N_2 - s_i^C} \left(\frac{1}{1 + e^{\lambda - \kappa/2}} \right)^2$$

$$\cdot \prod_{i=1}^{n_2} \binom{N_2}{s_i^T} \left(\frac{e^{\lambda + \kappa/2}}{1 + e^{\lambda + \kappa/2}} \right)^{s_i^T} \left(\frac{1}{1 + e^{\lambda + \kappa/2}} \right)^{N_2 - s_i^T} \left(\frac{1}{1 + e^{\lambda + \kappa/2}} \right)^2$$

$$\cdot \frac{\upsilon_0}{\sqrt{2\pi}} \exp\left(-\frac{\upsilon_0}{2} (\kappa - \kappa_0)^2 \right) \cdot \frac{\gamma_0}{\sqrt{2\pi}} \exp\left(-\frac{\gamma_0}{2} (\lambda - \lambda_0)^2 \right)$$

$$\propto \left(\frac{e^{\lambda - \kappa/2}}{1 + e^{\lambda - \kappa/2}} \right)^{\sum_{i=1}^{n_2} s_i^C} \left(\frac{1}{1 + e^{\lambda - \kappa/2}} \right)^{2 + n_2 N_2 - \sum_{i=1}^{n_2} s_i^C}$$

$$\cdot \left(\frac{e^{\lambda + \kappa/2}}{1 + e^{\lambda + \kappa/2}} \right)^{\sum_{i=1}^{n_2} s_i^T} \left(\frac{1}{1 + e^{\lambda + \kappa/2}} \right)^{2 + n_2 N_2 - \sum_{i=1}^{n_2} s_i^T}$$

$$\cdot \exp\left(-\frac{\upsilon_0}{2} (\kappa - \kappa_0)^2 \right) \cdot \exp\left(-\frac{\gamma_0}{2} (\lambda - \lambda_0)^2 \right), \tag{3.36}$$

again using a transformation of variables (with Jacobians $(1 + e^{\lambda - \kappa/2})^{-2}$). The log posterior is

$$= \log p(\kappa, \lambda \mid s^C, s^T)$$

$$\propto \sum_{i=1}^{n_2} s_i^C \log\left(\frac{e^{\lambda - \kappa/2}}{1 + e^{\lambda - \kappa/2}} \right) + (2 + n_2 N_2 - \sum_{i=1}^{n_2} s_i^C) \log\left(\frac{1}{1 + e^{\lambda - \kappa/2}} \right)$$

$$+ \sum_{i=1}^{n_2} s_i^T \log\left(\frac{e^{\lambda + \kappa/2}}{1 + e^{\lambda + \kappa/2}} \right) + (2 + n_2 N_2 - \sum_{i=1}^{n_2} s_i^T) \log\left(\frac{1}{1 + e^{\lambda + \kappa/2}} \right)$$

$$- \frac{\upsilon_0}{2} (\kappa - \kappa_0)^2 - \frac{\gamma_0}{2} (\lambda - \lambda_0)^2 := \ell_2 \tag{3.37}$$

Table 3.3: Scaling and acceptance rate for κ and λ.

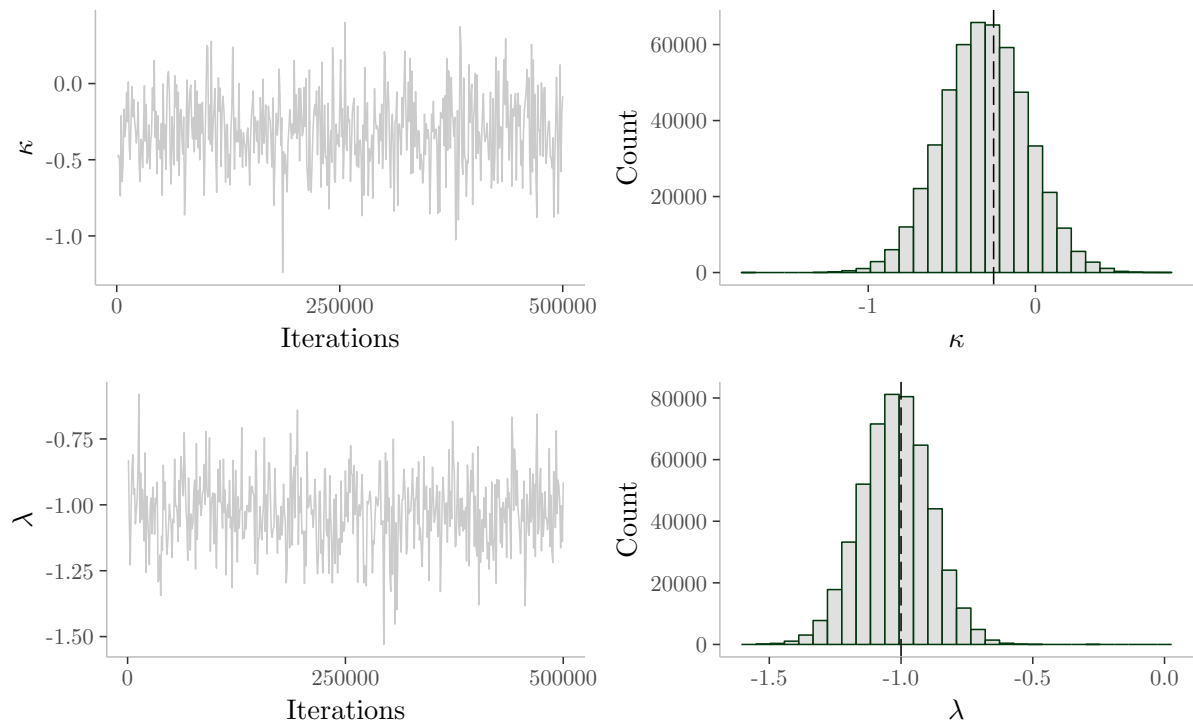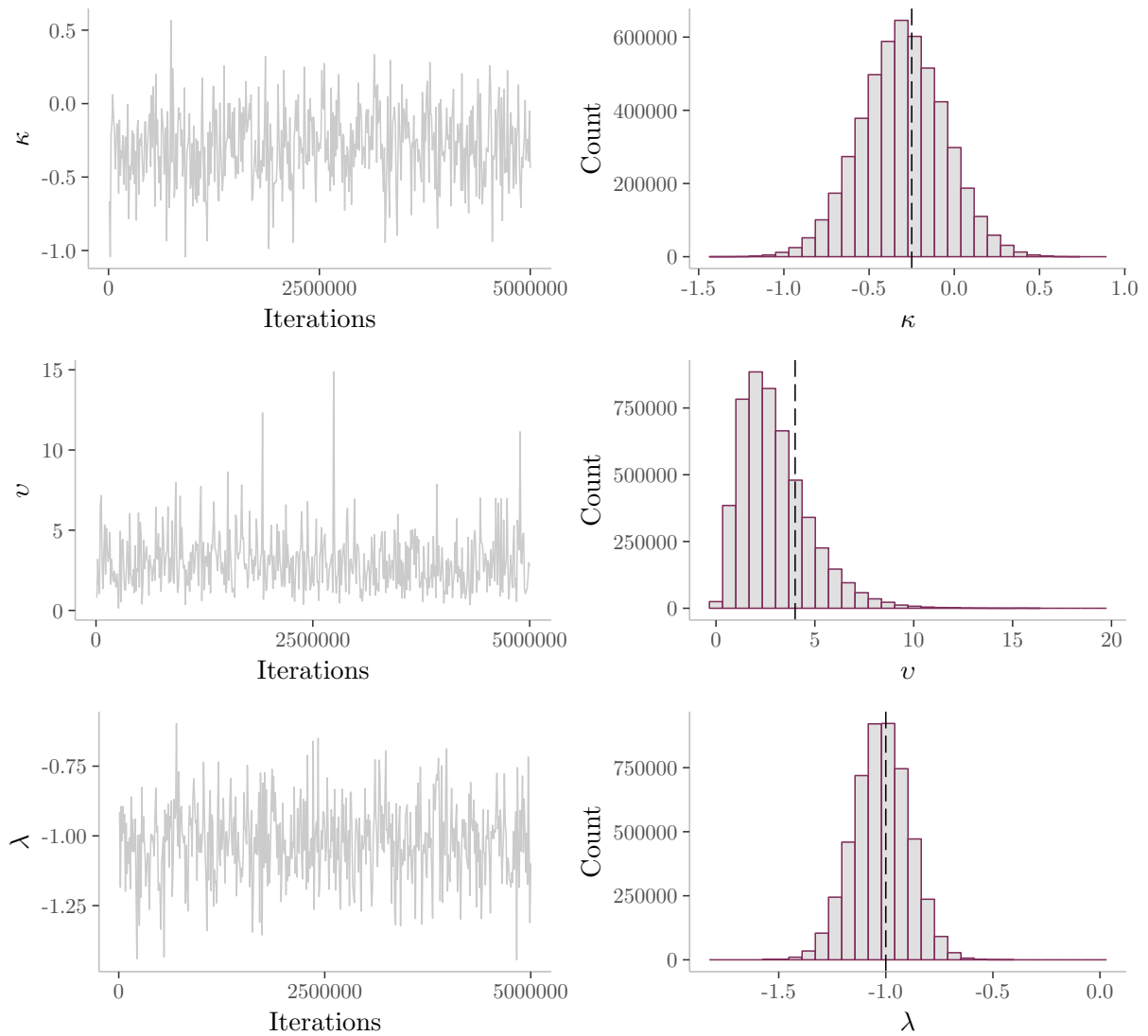|	κ	λ
σ	0.550	0.300
Acceptance	0.472	0.452

Figure 3.5: Submodel 2 posterior traceplots and histograms for the parameters κ and λ, with truth shown on the histogram as a dashed black line.

Table 3.4: Posterior mean (PM), true value and posterior standard deviation (PSD) for κ and λ.

	κ	λ
PM	-0.303	-1.021
Truth	-0.250	-1.000
PSD	0.253	0.131

Melded model

$$p_{\text{meld}}(\kappa, \upsilon, p^C, p^T, \lambda \,|\, r^C, r^T, s^C, s^T)$$
$$\propto p_{\text{pool}}(\kappa)\frac{p_1(\kappa, \upsilon, p^C, p^T \,|\, r^C, r^T)}{p_1(\kappa)}\frac{p_1(\kappa, \upsilon, p^C, p^T \,|\, r^C, r^T)}{p_2(\kappa)} \tag{3.38}$$

$$p_{\text{meld}}(\kappa, \upsilon, p^C, p^T, \lambda \,|\, r^C, r^T, s^C, s^T) \propto p_1(\kappa, \upsilon, p^C, p^T \,|\, r^C, r^T)p_1(\kappa, \upsilon, p^C, p^T \,|\, r^C, r^T) \tag{3.39}$$

$$\log p_{\text{meld}}(\kappa, \upsilon, p^C, p^T, \lambda \,|\, r^C, r^T, s^C, s^T)$$
$$\propto \log p_1(\kappa, \upsilon, p^C, p^T \,|\, r^C, r^T) + \log p_2(\kappa, \upsilon, p^C, p^T \,|\, r^C, r^T)$$
$$\propto \ell_1 + \ell_2 \tag{3.40}$$

```
## Warning in rbind(vscale, accept): number of columns of result is not a
## multiple of vector length (arg 1)
```

Table 3.5: Scaling and acceptance rate for κ and λ.

	κ	λ	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	N
σ	0.550	0.300	0.550	0.300	0.550	0.300	0.550	0.300	0.550	0.300	0.550	0.300	0.55
Acceptance	0.291	0.452	0.384	0.408	0.398	0.381	0.411	0.438	0.439	0.407	0.396	0.448	0.16

Figure 3.6: Melded model posterior traceplots and histograms for the parameters κ, υ and λ, with truth shown on the histogram as a dashed black line.

3.3 Sequential Monte Carlo

In some situations, where the submodels are complex, it may be challenging to directly sample from the full Markov melded posterior using Metropolis-within-Gibbs. Goudie et al. (2019) therefore propose a sequential approach, in which information from the submodels is added step-by-step. At a high-level, it is an example of Sequential Monte Carlo (SMC) which we outline the connection to here.

Consider a probability density function $\pi(x)$ as before defined on the state space $\mathcal{X}$. Following Lindsten et al. (2017), if $\mathcal{X}$ is a product space it may be decomposed into a Cartesian product of subspaces according to

$$\mathcal{X} := \mathcal{X}_T = \widetilde{\mathcal{X}}_1 \times \widetilde{\mathcal{X}}_2 \times \cdots \times \widetilde{\mathcal{X}}_T. \tag{3.41}$$

Elements $x \in \mathcal{X}$ in the product space may be written as $x := x_T = (\widetilde{x}_1, \ldots, \widetilde{x}_T)$. Both the elements of the subspaces and the subspaces themselves are denoted with tildes, so that $\widetilde{x}_t \in \widetilde{\mathcal{X}}_t$, for $1 \leq t \leq T$. A sequence of auxiliary probability distributions $\pi_1, \ldots \pi_T$ can be defined on the spaces $\mathcal{X}_t$ of lower dimension $1 \leq t \leq T$ than $\mathcal{X}_T$. $\pi_t(x_t) := \pi_t(\widetilde{x}_1, \cdots, \widetilde{x}_t)$ for $t = 1, \ldots, T$. The final auxiliary distribution is chosen to coincide with the target distribution, such that

$$\pi = \pi_T. \tag{3.42}$$

Collections of auxiliary distributions with the two properties, (3.41) and (3.42), are called a sequential decomposition of the target distribution π.

Sequential Monte Carlo (SMC) methods are a general class of Monte Carlo algorithms designed for situations where sequential decompositions are applicable. The distributions $\pi_1, \pi_2, \cdots, \pi_T = \pi$ are approximated sequentially, allowing information from previous iterations to inform the sampling strategy as it proceeds.

3.3.1 Multi-stage Metropolis-within-Gibbs

Define $(\phi, \psi_1, \ldots, \psi_M) = \theta_M = \theta \in \Theta$, then the full parameter space Θ may be decomposed such that $\Theta = \Phi \times \Psi_1 \times \cdots \times \Psi_M$. Define the sequence of subspaces $\Theta_\ell = \Phi \times \Psi_1 \times \cdots \times \Psi_m$

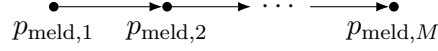$p_{\mathrm{meld},1}$ $p_{\mathrm{meld},2}$ $\cdots$ $p_{\mathrm{meld},M}$

Figure 3.7: Computational flow of the multi-stage Metropolis-within-Gibbs sampler for Markov melding. Stages labeled with target auxiliary distribution. Adapted to Markov melding context from Lindsten et al. (2017)

with respective elements $\theta_\ell = (\phi, \psi_1, \ldots, \psi_\ell)$ for $\ell = 1, \ldots, M$. The subspaces are of increasing dimension such that $\Theta_1 \subseteq \cdots \subseteq \Theta_\ell \subseteq \cdots \subseteq \Theta_M$ with the final subspace $\Theta_M = \Theta$.

It remains to construct a sequence of auxiliary probability distributions $p_{\mathrm{meld},l}$ defined on the subspaces Θ_ℓ such that the Mth distribution coincides with the posterior

$$p_{\mathrm{meld},M}(\theta_M) = p_{\mathrm{meld},M}(\phi, \psi_1, \ldots, \psi_M) = p_{\mathrm{meld}}(\phi, \psi_1, \ldots, \psi_M \mid y_1, \ldots, y_M) \tag{3.43}$$

The posterior (2.35) includes a product of the submodel posteriors $p_m(\phi, \psi_m \mid y_m)$ and conditional on ϕ, the mth submodel is the only source of information about ψ_m. It therefore seems reasonable that when $\Psi_m \subseteq \Theta_\ell$ this information $p_m(\phi, \psi_m \mid y_m)$ about ψ_m is included in the auxiliary probability distribution.

On the other hand, informally speaking, information about the link parameter is ϕ is dispersed across the M submodels. For this reason there is flexibility about how the auxiliary distributions should be defined to take this into account. This flexibility can be encapsulated by the possible factorisations of the pooled prior

$$p_{\mathrm{pool}}(\phi) = \prod_{m=1}^{M} p_{\mathrm{pool},m}(\phi). \tag{3.44}$$

Two example factorisations are $p_{\mathrm{pool},m}(\phi) = p_{\mathrm{pool}}(\phi)^{1/M}$ and $p_{\mathrm{pool},m}(\phi) = p_m(\phi)$.

Therefore, the ℓth stage posterior over the parameters $\theta_\ell \in \Theta_\ell$ is defined to be

$$p_{\mathrm{meld},l}(\theta_\ell \mid y_1, \ldots, y_\ell) \propto \prod_{m=1}^{\ell} \left(\frac{p_m(\phi, \psi_m, y_m)}{p_m(\phi)} p_{\mathrm{pool},m}(\phi) \right) \tag{3.45}$$

where indeed Equation (3.43) holds.

To sample from this sequence of auxiliary distributions, Goudie et al. (2019) generalise a previous two-stage computational approach of Lunn et al. (2013). With the introduction of each additional parameter, the relevant Markov chains may be initialised as before at the corresponding elements of $(\phi^{(0)}, \psi_1^{(0)}, \ldots, \psi_M^{(0)})$.

Stage 1. For the first stage, the auxiliary target distribution is the 1st stage posterior $p_{\text{meld},1}(\phi, \psi_1 \,|\, y_1)$. Samples $(\phi^{(h,1)}, \psi_1^{(h,1)})$ for $h = 1, \ldots, H_1$ from this distribution can typically be drawn using standard MCMC methods such as MWG. If $p_{\text{pool},1}(\phi) = p_1(\phi)$ then the first stage posterior corresponds to the standard posterior $p_m(\phi, \psi_m \,|\, y_m)$. This may present computational advantages as often a given submodel may have been fit and samples will be already available. This factor may motivate setting the first submodel to be the most computational intensive submodel for which samples are available.

Stage ℓ. Following stage $\ell - 1$, samples $(\theta^{(h,\ell-1)})$ for $h = 1, \ldots, H_{\ell-1}$ from the $(\ell-1)^{\text{th}}$ stage posterior $p_{\text{meld},\ell-1}(\theta_{\ell-1} \,|\, y_1, \ldots, y_{\ell-1})$ are available. In stage ℓ a Metropolis-within-Gibbs sampler targeting $p_{\text{meld},l}(\theta_{\ell-1}, \psi_\ell \,|\, y_1, \ldots, y_\ell)$ on the space $\Theta_\ell = \Theta_{\ell-1} \times \Psi_\ell$ is constructed.

Keeping $\theta_{\ell-1}$ fixed, the parameter ψ_m is updated as usual using a Metropolis-Hastings step. This chain can be initialsed at $\psi_m^{(0)}$. The target-to-proposal density ratio is equivalent, with respect to the calculation of r as in Equation (3.14), to

$$R(\theta_{\ell-1}, \psi_\ell^\star, \theta_{\ell-1}, \psi_\ell) = p_\ell(\phi, \psi_\ell^\star, y_\ell) \cdot \frac{1}{q(\psi_\ell^\star \,|\, \psi_\ell)} \tag{3.46}$$

Now, to update the parameters $\theta_{\ell-1}$ the empirical distribution generated by the draws $(\theta^{(h,\ell-1)})$ for $h = 1, \ldots, H_{\ell-1}$ is used as proposal. This is equivalent to drawing an index $d \sim \mathcal{U}(\{1, \ldots, H_{\ell-1}\})$ and setting $\theta_{\ell-1}^\star = \theta_{\ell-1}^{(d,\ell-1)}$, a process commonly known as resampling. The resulting target-to-proposal density ratio simplifies as a result

$$
\begin{aligned}
&R(\theta_{\ell-1}^\star, \psi_\ell, \theta_{\ell-1}, \psi_\ell) \\
&= \frac{p_\ell(\phi^\star, \psi_\ell, y_\ell)}{p_\ell(\phi^\star)} p_{\text{pool},\ell}(\phi^\star) \prod_{m=1}^{\ell-1} \left(\frac{p_m(\phi^\star, \psi_m^\star, y_m)}{p_m(\phi^\star)} p_{\text{pool},m}(\phi^\star) \right) \cdot \frac{1}{q(\theta_{\ell-1}^\star \,|\, \theta_{\ell-1})} \\
&= \frac{p_\ell(\phi^\star, \psi_\ell, y_\ell)}{p_\ell(\phi^\star)} p_{\text{pool},\ell}(\phi^\star) \frac{p_{\text{meld},\ell-1}(\phi^\star, \theta_{\ell-1}^\star \,|\, y_1, \ldots, y_{\ell-1})}{p_{\text{meld},\ell-1}(\phi^\star, \theta_{\ell-1}^\star \,|\, y_1, \ldots, y_{\ell-1})} \\
&= \frac{p_\ell(\phi^\star, \psi_\ell, y_\ell)}{p_\ell(\phi^\star)} p_{\text{pool},\ell}(\phi^\star),
\end{aligned}
\tag{3.47}
$$

facilitating fast computation.

Chapter 4

Conclusion

- **Study selection** Throughout this dissertation, as well as Goudie et al. (2019), it is assumed that the set of studies to be synthesised is prespecified. In reality this is often not the case. The order of inclusion is important

- **Model misspecification**

- **Scalability** Multi-stage Metropolis-within-Gibbs operates sequentially: each stage ℓ can only be completed after the previous stage $\ell - 1$ has been. To put it another way, the computational flow is indexed by the chain $\{1, \ldots, M\}$ as in Figure 3.7. An alternative, proposed by Lindsten et al. (2017) in a broader SMC context, is to instead utilise divide-and-conquer by operating on a tree $\mathcal{T}$. Particularly for joining many submodels, this may result in significant computational gains as the resulting algorithm would be more easily parallelisable.

Appendix A

Appendix

A.1 Submodel 1
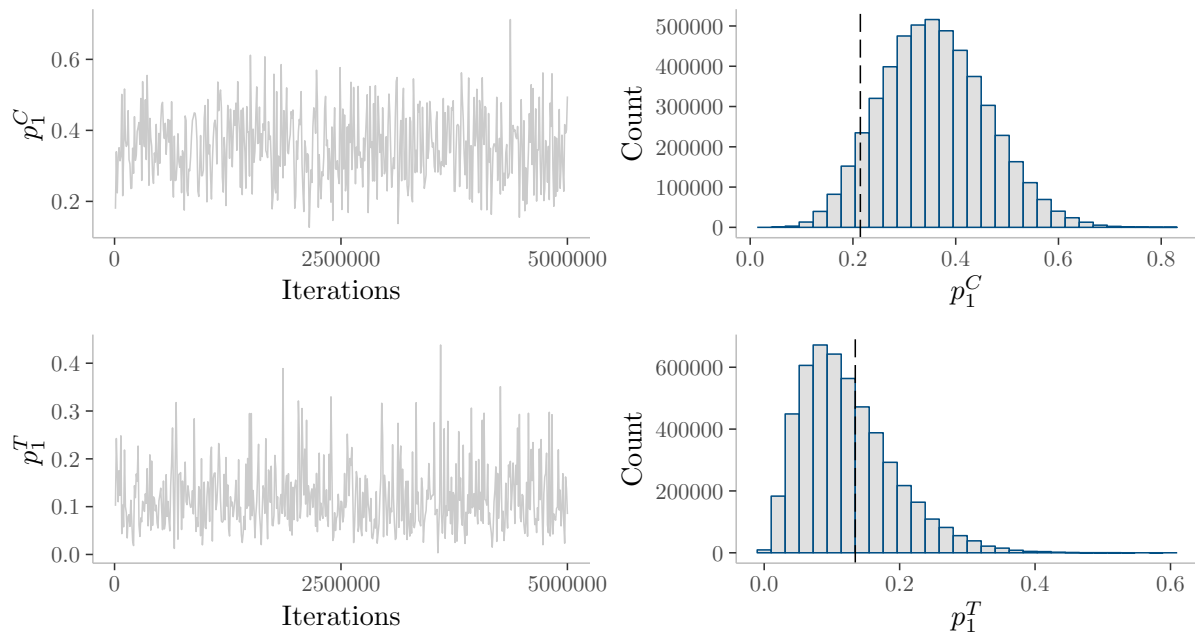
Figure A.1: Submodel 1 posterior traceplots and histograms for p_1^C and p_1^T
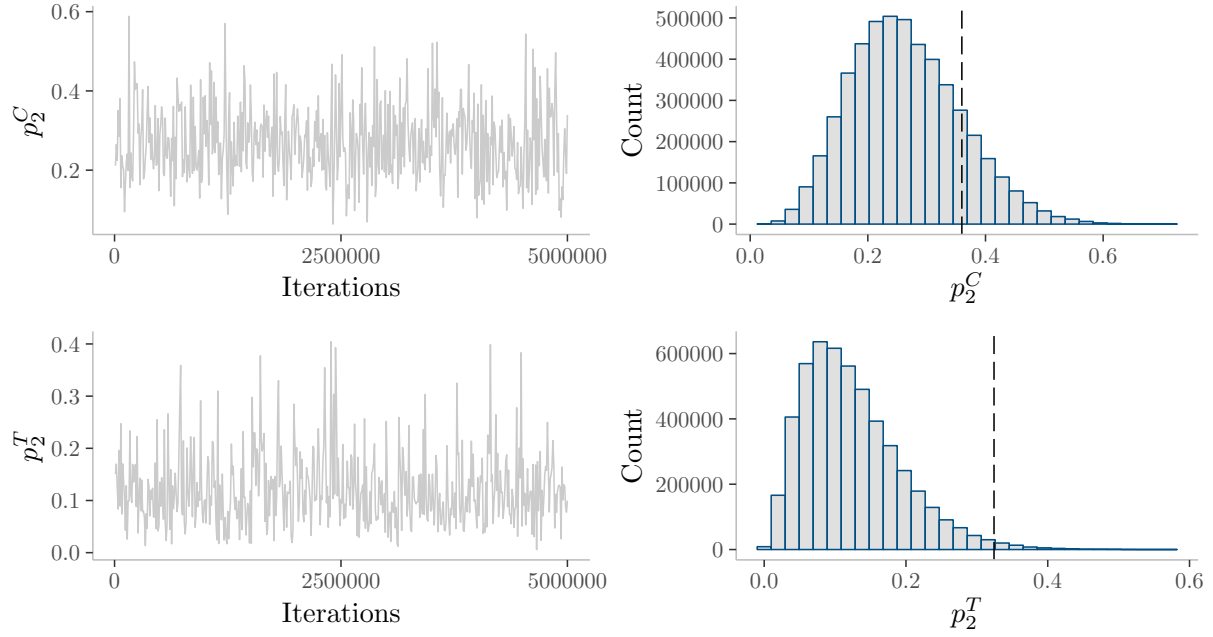
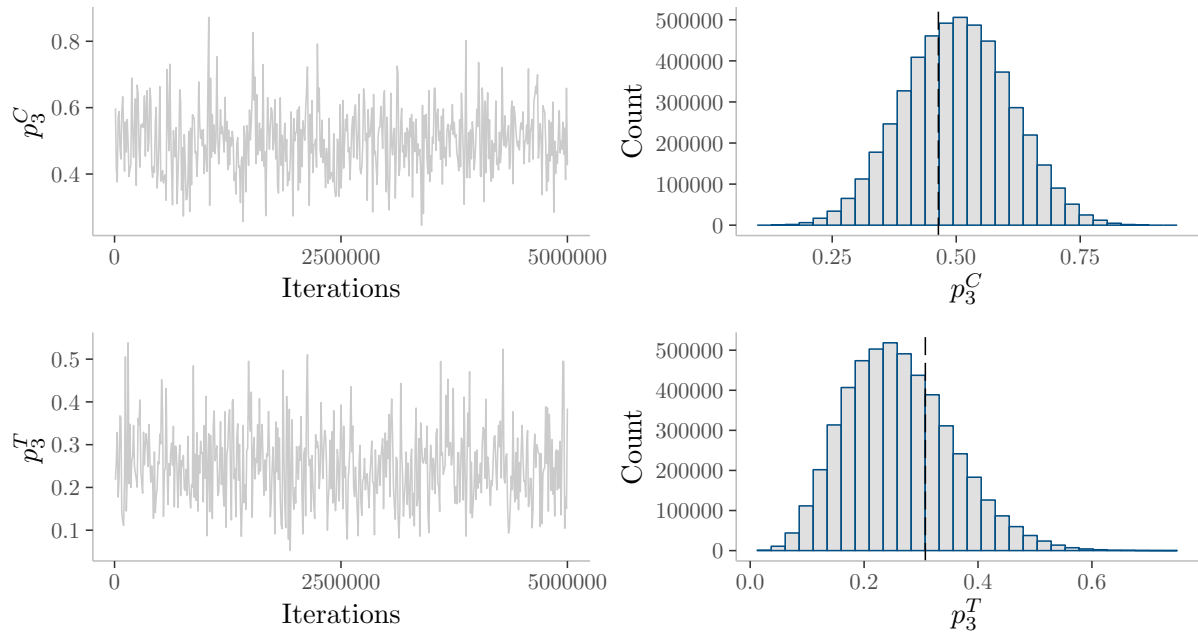Figure A.2: Submodel 1 posterior traceplots and histograms for p_2^C and p_2^T

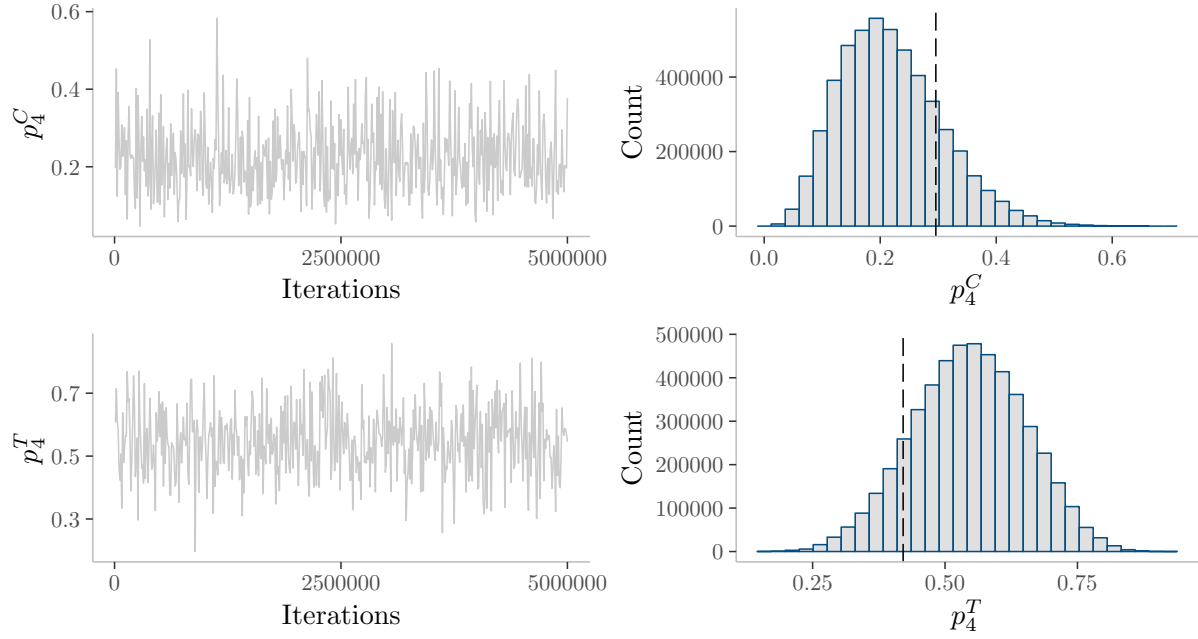Figure A.3: Submodel 1 posterior traceplots and histograms for p_3^C and p_3^T

Figure A.4: Submodel 1 posterior traceplots and histograms for p_4^C and p_4^T
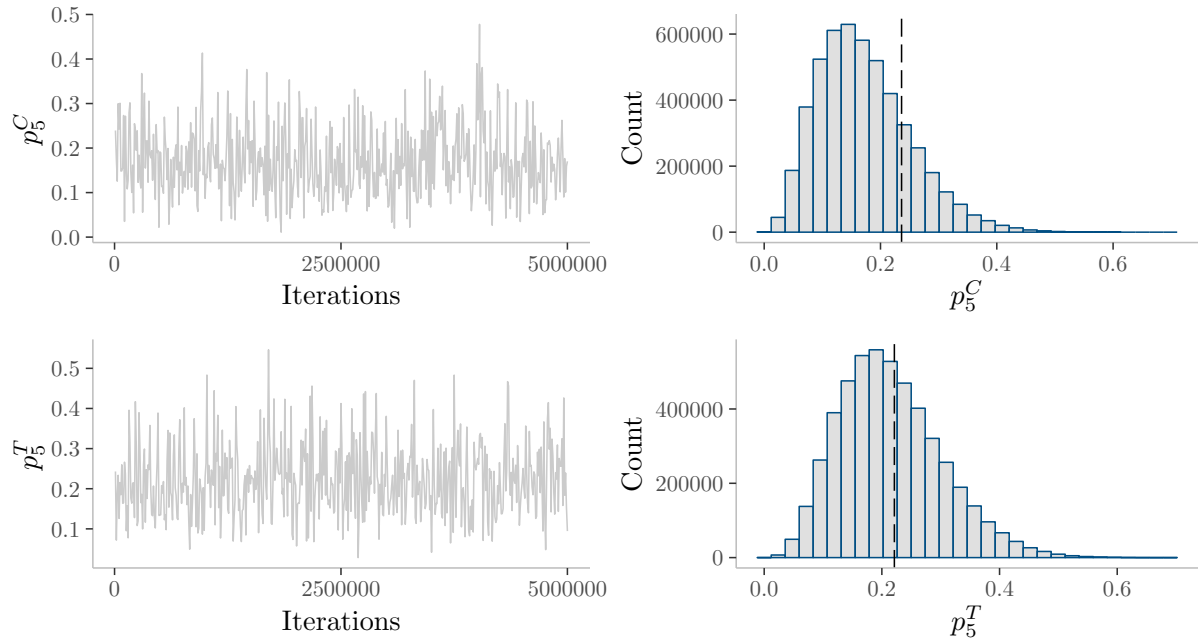

Figure A.5: Submodel 1 posterior traceplots and histograms for p_5^C and p_5^T
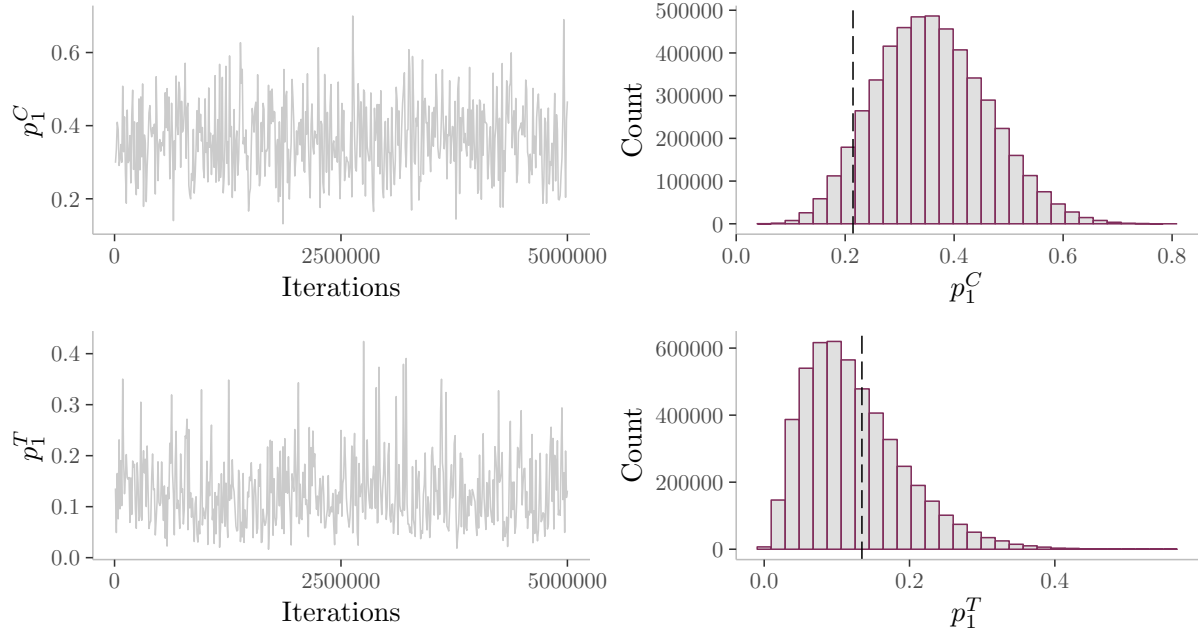
A.2 Melded model

Figure A.6: Melded model posterior traceplots and histograms for p_1^C and p_1^T
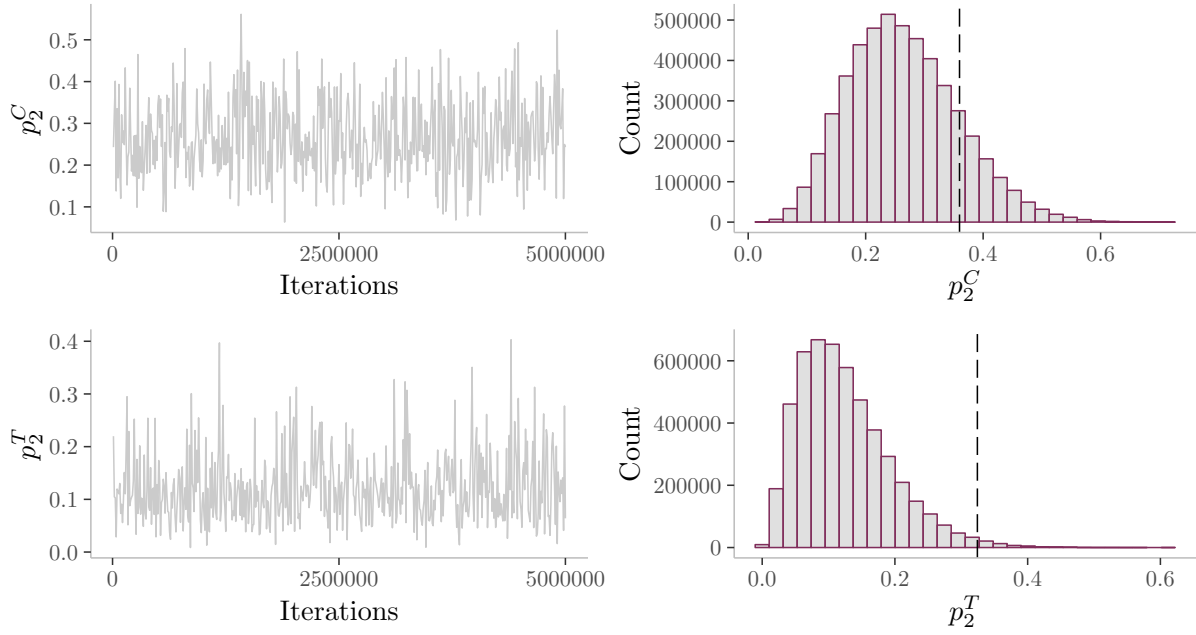
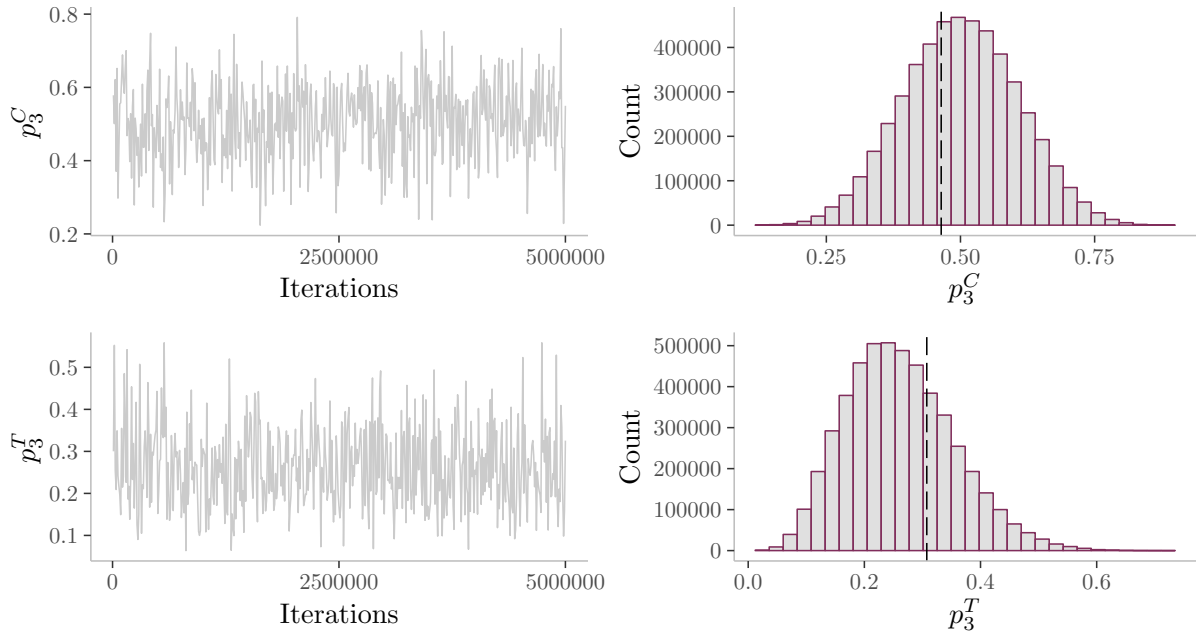Figure A.7: Melded model posterior traceplots and histograms for p_2^C and p_2^T

Figure A.8: Melded model posterior traceplots and histograms for p_3^C and p_3^T
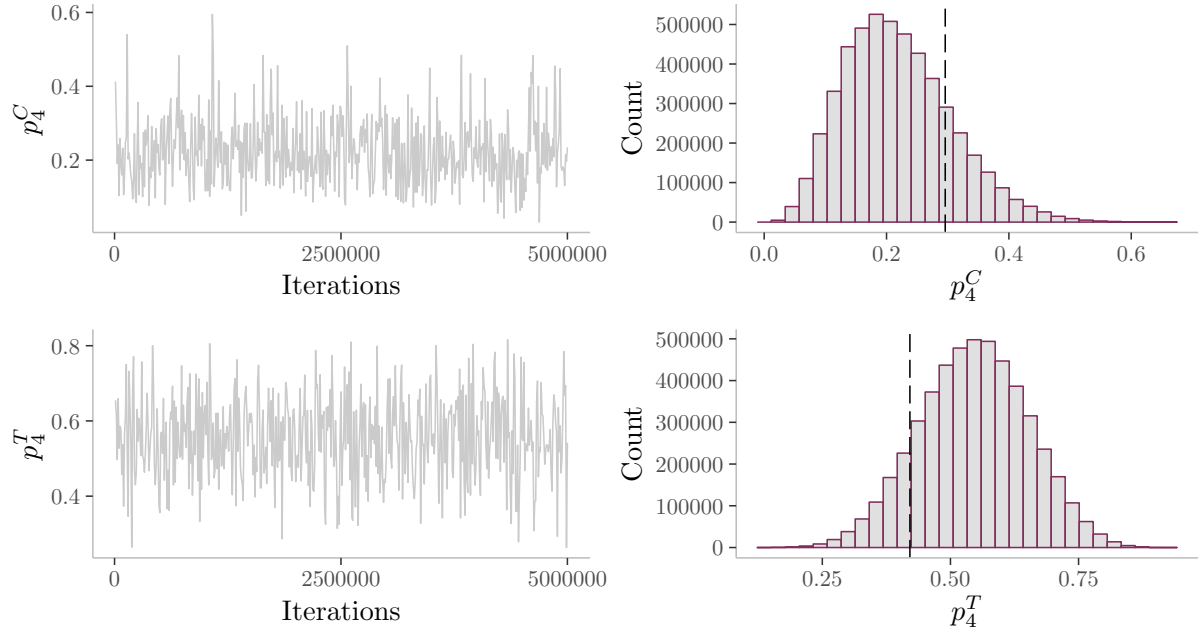
Figure A.9: Melded model posterior traceplots and histograms for p_4^C and p_4^T
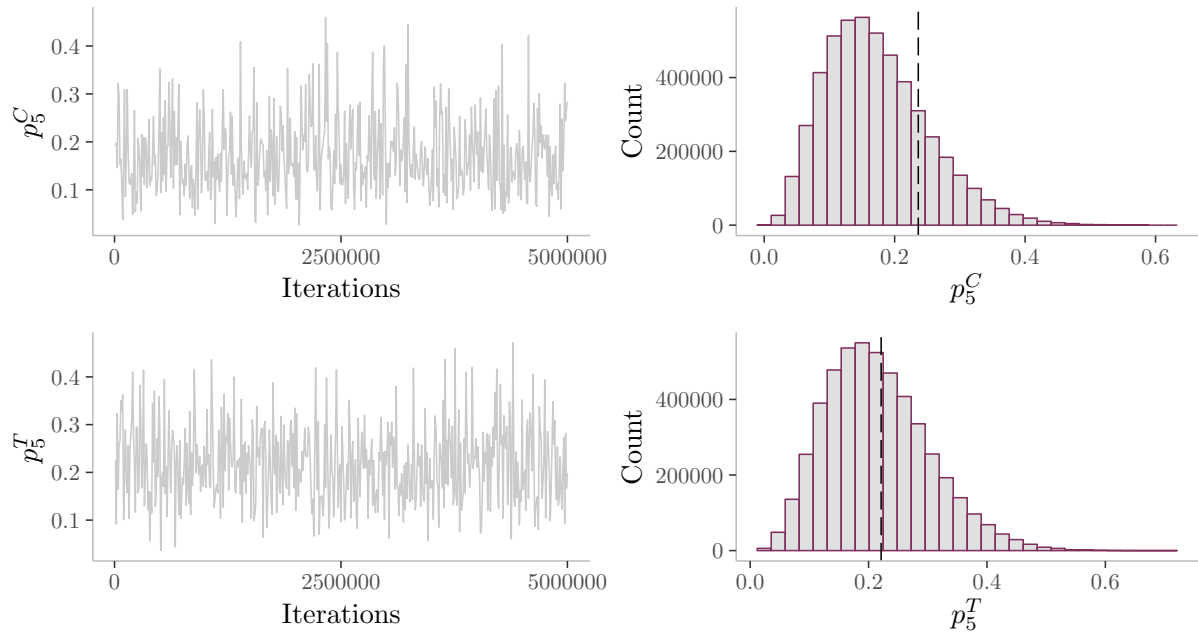

Figure A.10: Melded model posterior traceplots and histograms for p_5^C and p_5^T

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