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# Penalising Model Component Complexity: A Principled, Practical Approach to Constructing Priors<sup>1</sup>

Daniel Simpson, Håvard Rue, Andrea Riebler, Thiago G. Martins and Sigrunn H. Sørbye

*Abstract.* In this paper, we introduce a new concept for constructing prior distributions. We exploit the natural nested structure inherent to many model components, which defines the model component to be a flexible extension of a base model. Proper priors are defined to penalise the complexity induced by deviating from the simpler base model and are formulated after the input of a user-defined *scaling* parameter for that model component, both in the univariate and the multivariate case. These priors are invariant to reparameterisations, have a natural connection to Jeffreys’ priors, are designed to support Occam’s razor and seem to have excellent robustness properties, all which are highly desirable and allow us to use this approach to define default prior distributions. Through examples and theoretical results, we demonstrate the appropriateness of this approach and how it can be applied in various situations.

*Key words and phrases:* Bayesian theory, interpretable prior distributions, hierarchical models, disease mapping, information geometry, prior on correlation matrices.

## 1. INTRODUCTION

The field of Bayesian statistics began life as a sub-branch of probability theory. From the 1950s onward, a number of pioneers built upon the Bayesian framework and applied it with great success to real world

problems. The true Bayesian “moment” began with the advent of Markov chain Monte Carlo (MCMC) methods. Coupled with user-friendly implementations of MCMC, such as OpenBUGS, JAGS, R-INLA, and Stan, the uptake of Bayesian models has exploded across fields of research from astronomy to anthropology, linguistics to zoology. Limited only by their data, their patience and their imaginations, applied researchers have constructed and applied increasingly complex Bayesian models. The spectacular flexibility of the Bayesian paradigm as an applied modelling toolbox has had a number of important consequences for modern science [see, e.g., the special issue of Statistical Science (Volume 29, Number 1, 2014) devoted to Bayesian success stories].

The challenge underlying the proliferation of Bayesian methods is that it is significantly easier to build, implement and use a complex model than it is to understand what it is doing. This is particularly true when the model is built to be potentially more complicated than the data in the sense that there are potentially many more parameters than there are observations. For these models, a balance between predictive power and

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parsimony is controlled by prior specification. Unfortunately, there has been very little work done on setting priors for these models outside of high-dimensional regression problems, for which the mathematics is tractable. In this paper, we propose a new technique for specifying priors that can be applied to a large number of applied Bayesian models.

The problem of constructing sensible priors on model parameters becomes especially pressing when developing general software for Bayesian computation. As developers of the R-INLA (see <http://www.r-inla.org/>) package, which performs approximate Bayesian inference for latent Gaussian models (Rue, Martino and Chopin, 2009, Lindgren, Rue and Lindström, 2011, Martins et al., 2013), we are left with two unpalatable choices. We could force the user of R-INLA to explicitly define a joint prior distribution for all parameters in the model. Arguably, this is the correct thing to do, however, the sea of confusion around how to properly prescribe priors makes this undesirable in practice. The second option is to provide default priors. These, as currently implemented, are chosen by the second author to be something he views as sensible. Default prior specification is also present implicitly in the OpenBUGS and Stan manuals, which contain a large number of fully-worked Bayesian analyses of real problems complete with prior specifications. In this case, we do not know precisely the thinking that underscores the choice of prior, but we do know that they have been hugely influential. This is not a satisfactory state of affairs.

This paper is our attempt to provide a broad, useful framework for building priors for a large class of hierarchical models. The priors we develop, which we call *Penalised Complexity* or PC priors, are informative priors. The information in these priors is specified in terms of four underlying principles. This has a twofold purpose. The first purpose is to communicate the exact information that is encoded in the prior in order to make the prior interpretable and easier to elicit. PC priors have a single parameter that the user must set, which controls the amount of flexibility allowed in the model. This parameter can be set using “weak” information that is frequently available (Gelman, 2006), or by appealing to some other subjective criterion such as “calibration” under some assumptions about future experiments (Draper, 2006).

Following in the footsteps of Lucien Le Cam (“Basic Principle 0. Do not trust any principle.” Le Cam, 1990) and (allegedly) Groucho Marx (“Those are my principles, and if you don’t like them. . . well, I have others.”),

the second purpose of building PC priors from a set of principles is to allow us to change these principles when needed. For example, in Sections 4.5 and 7 we modify single principles for, respectively, modelling and computational reasons. This gives the PC prior framework the advantage of flexibility without sacrificing its simple structure. We stress that the principles provided in this paper do not absolve modellers of the responsibility to check their suitability (see, e.g., Palacios and Steel, 2006, who argued that the principles underlying the reference prior approach are inappropriate for spatial data). This is in line with David Draper’s call for “transparent subjectivity” in Bayesian modelling (Draper, 2006).

We believe that PC priors are general enough to be used in realistically complex statistical models and are straightforward enough to be used by general practitioners. Using only weak information, PC priors represent a unified prior specification with a clear meaning and interpretation. The underlying principles are designed so that desirable properties follow automatically: invariance regarding reparameterisations, connection to Jeffreys’ prior, support of Occam’s razor principle and empirical robustness to the choice of the flexibility parameter. We do not claim that the priors we propose are optimal or unique, nor do we claim that the principles are universal. Instead, we make the more modest claim that these priors are useful, understandable, conservative and better than doing nothing at all.

### 1.1 The Models Considered in This Paper

While the goals of this paper are rather ambitious, we will necessarily restrict ourselves to a specific class of hierarchical model, namely additive models. The models we consider have a nontrivial unobserved latent structure. This latent structure is made up of a number of *model components*, the structure of which is controlled by a small number of *flexibility parameters*. We are interested in latent structures in which each model component is added for modelling purposes. We do not focus on the case where the hierarchical structure is added to increase the robustness of the model (See Chapter 10 of Robert, 2007, for a discussion of types of hierarchical structure). This *additive model* viewpoint is the key to understanding many of the choices we make, in particular the concept of the “base model,” which is covered in detail in Section 2.4.

An example of the type of model we are considering is the spatial survival model proposed by Henderson, Shimakura and Gorst (2002), where the log-hazard rate

is modelled according to a Cox proportional hazard model as

$$\log\left(\frac{\text{hazard}_j}{\text{baseline}}\right) = \beta_0 + \sum_{i=1}^p \beta_i x_{ij} + u_{r_j} + v_j,$$

where  $x_{ij}$  is the  $i$ th covariate for case  $j$ ,  $u_{r_j}$  is the value of the spatial structured random effect for the region  $r_j$  in which case  $j$  occurred, and  $v_j$  is the subject specific log-frailty. Let us focus on a *model component*  $\mathbf{u} \sim N(0, \tau^{-1}\mathbf{Q}^{-1})$ , where  $\mathbf{Q}$  is the structure matrix of the first-order intrinsic CAR model on the regions and  $\tau$  is an inverse scaling parameter (Rue and Held, 2005, Chapter 3). The model component  $\mathbf{u}$  has one flexibility parameter  $\tau$ , which controls the scaling of the structured random effect. The other model components are  $\mathbf{v}$  and  $\boldsymbol{\beta}$ , which have one and zero (assuming a uniform prior on  $\boldsymbol{\beta}$ ) flexibility parameters, respectively. We will consider this case in detail in Section 5.

We emphasise that we are not interested in the case where the number of flexibility parameters grows as we enter an asymptotic regime (here as the number of cases increases). The only time we consider models where the number of parameters grows in an “asymptotic” way is Section 4.5, where we consider sparse linear models. In that section, we discuss a (possibly necessary) modification to the prior specification given below (specifically Principle 3 in Section 3). We also do not consider models with discrete components.

## 1.2 Outline of the Paper

The plan of the paper is as follows. Section 2 contains an overview of common techniques for setting priors for hierarchical models. In Section 3, we will define our principled approach to design priors and discuss its connection to the Jeffreys’ prior. In Section 4, we will study properties of PC priors near the base model and its behaviour in a Bayesian hypothesis testing setting. Further, we provide explicit risk results in a simple hierarchical model and discuss the connection to sparsity priors. In Section 5, we discuss the BYM-model for disease mapping with a possible smooth effect of an ecological covariate, and we suggest a new parameterisation of the model in order to facilitate improved control and interpretation. Section 6 extends the method to multivariate parameters and we derive principled priors for correlation matrices in the context of the multivariate probit model. Section 7 contains a discussion of how to extend the framework of PC priors to hierarchical models by defining joint PC priors over model components that take the model structure into

account. This technique is demonstrated on an additive logistic regression model. We end with a discussion in Section 8. The Appendix host technical details and additional results.

## 2. A GUIDED TOUR OF NONSUBJECTIVE PRIORS FOR BAYESIAN HIERARCHICAL MODELS

The aim of this section is to review the existing methods for setting nonsubjective priors for parameters in Bayesian hierarchical models. We begin by discussing objective priors, which are frequently put forward as a “gold standard” of prior specification. The second class of priors that we survey are what we call “risk averse priors,” that is priors that come from the culture of a field rather than from specific principles. Finally, we survey the more recent concept of “weakly-informative” priors. We then consider a special class of priors that are important for hierarchical models, namely priors that encode some notion of a base model. Finally, we investigate the main concepts that we feel are most important for setting priors for parameters in hierarchical models, and we look at related ideas in the literature.

In order to control the size of this section, we have made two major decisions. The first is that we are focussing exclusively on methods of prior specification that could conceivably be used in all of the examples in this paper. The second is that we focus entirely on priors for prediction. It is commonly (although not exclusively Bernardo, 2011, Rousseau and Robert, 2011, Kamary et al., 2014) held that we need to use different priors for testing than those used for prediction. We return to this point in Section 4.3. A discussion of alternative priors for the specific examples in this paper is provided in the relevant section. We also do not consider data-dependent priors or empirical Bayes procedures.

### 2.1 Objective Priors

The concept of prior specification furthest from expert elicitation priors is that of “objective” priors (Bernardo, 1979, Berger, 2006, Berger, Bernardo and Sun, 2009, Ghosh, 2011, Kass and Wasserman, 1996). These aim to inject as little information as possible into the inference procedure. Objective priors are often strongly design-dependent and are not uniformly accepted amongst Bayesians on philosophical grounds; see, for example, discussion contributions to Berger (2006) and Goldstein (2006), but they are useful (and used) in practice. The most common constructs in this



family are Jeffreys' noninformative priors and their extension "reference priors" (Berger, Bernardo and Sun, 2009). If chosen carefully, the use of noninformative priors will lead to appropriate parameter estimates as demonstrated in several applications by Kamary and Robert (2014). It can be also shown theoretically that, for sufficiently nice models, the posterior resulting from a reference prior analysis matches the results of classical maximum likelihood estimation to second order (Reid, Mukerjee and Fraser, 2003).

While reference priors have been successfully used for classical models, they have a less triumphant history for hierarchical models. The practical reason for this is that reference priors are notoriously difficult to derive for complicated models. A second barrier to the routine use of reference priors for hierarchical models is that they depend on the ordering of the parameters. In some applications, there may be a natural ordering, however, in many situations, such as the ones encountered in this paper, any imposed ordering will be unnatural. Berger, Bernardo and Sun (2015) proposed some *ad hoc* solutions to this problem, however it is not clear how to apply these to even moderately complex hierarchical models (see the comment of Rousseau, 2015). In spite of these shortcomings, the reference prior framework is the only complete framework for specifying prior distributions.

## 2.2 Ad Hoc, Risk Averse and Computationally Convenient Prior Specification

The most common nonsubjective approach to prior specification for hierarchical models is to use a prior that has been previously used in the literature for a similar problem. This *ad hoc* approach is viewed as "good practice" in many applied communities. It may be viewed as a *risk averse* strategy, in which the choice of prior has been delegated to another researcher. The assumption is that the community of people using this prior are doing it for a good reason and continuing this practice is less risky than positing a different prior specification. In the best cases, the chosen prior was originally selected in a careful, problem independent manner for a similar problem to the one the statistician is solving (e.g., the priors in Gelman et al., 2013). More commonly, these priors have been carefully chosen for the problem they were designed to solve (such as the priors in Muff et al., 2015) and are inappropriate for the new application. The lack of a dedicated "expert" guiding these prior choices can lead to troubling inference. Worse still is the idea that, as the prior was

selected from the literature or is in common use, there is some sort of justification for it.

Other priors in the literature have been selected for purely computational reasons. The main example of these priors are conjugate priors for exponential families (Robert, 2007, Section 3.3), which facilitate easy implementation of a Gibbs sampler. While Gibbs samplers are an important part of the historical development of Bayesian statistics, we tend to favour modern sampling methods based on the joint distribution, such as those implemented in Stan, as they tend to perform better.

Some priors from the literature are not sensible. An extreme example of this is the enduring popularity of the  $\Gamma(\varepsilon, \varepsilon)$  prior, with a small  $\varepsilon$ , for inverse variance (precision) parameters, which has been the "default"<sup>2</sup> choice in the WinBUGS (Spiegelhalter et al., 1995) example manuals. However, this prior is well known to be a choice with severe problems; see the discussion in Fong, Rue and Wakefield (2010) and Hodges (2014). Another example of a bad "vague-but-proper" prior is a uniform prior on a fixed interval for the degrees of freedom parameter in a Student  $t$ -distribution. The results in the Supplementary Material (Simpson et al., 2016) show that these priors, which are also used in the WinBUGS manual, get increasingly informative as the upper bound increases.

One of the unintentional consequences of using risk averse priors is that they will usually lead to independent priors on each of the hyperparameters. For complicated models that are overparameterised or partially identifiable, we do not think this is necessarily a good idea, as we need some sort of shrinkage or sparsity to limit the flexibility of the model and avoid overfitting. The tendency towards overfitting is a property of the full model and independent priors on the components may not be enough to mitigate it (Pati, Pillai and Dunson, 2014, He, Hodges and Carlin, 2007, He and Hodges, 2008).

While the tone of this section has been quite negative, we do not wish to give the impression that all inference obtained using risk averse or computationally convenient priors will not be meaningful. We only want to point out that a lot of work needs to be put into checking the suitability of the prior for the particular application before it is used. Furthermore, the suitability (or not) of a specific joint prior specification will depend in subtle and complicated ways on the

<sup>2</sup>We note that this recommendation has been revised, however these priors are still widely used in the literature.

global model specification. An interesting, but computationally intensive, method for reasserting the role of an “expert” into a class of ad hoc priors is the method of *calibrated Bayes* (Rubin, 1984, Browne and Draper, 2006), where the hyper-parameters in the prior are chosen to ensure that, under correct model specification, the credible sets are also confidence regions.

### 2.3 Weakly Informative Priors

Between objective and expert priors lies the realm of “weakly informative” priors (Gelman, 2006, Gelman et al., 2008, Evans and Jang, 2011, Polson and Scott, 2012). These priors are constructed by recognising that while you usually do not have strong prior information about the value of a parameter, it is rare to be completely ignorant. For example, when estimating the height and weight of an adult, it is sensible to select a prior that gives mass neither to people who are five metres tall, nor to those who only weigh two kilograms. This use of weak prior knowledge is often sufficient to regularise the extreme inferences that can be obtained using maximum likelihood (Le Cam, 1990) or noninformative priors. To date, there has been no attempt to construct a general method for specifying weakly informative priors.

Some known weakly informative priors, like the half-Cauchy distribution on the standard deviation of a normal distribution, can lead to better predictive inference than reference priors (Polson and Scott, 2012). There are no general theoretical results that show how to build priors with good risk properties for the broader class of models we are interested in, but the intuition is that weakly informative priors can strike a balance between fidelity to a strong signal, and shrinkage of a weak signal. We interpret this as the prior on the flexibility parameter (the standard deviation) allowing extra model complexity, but not forcing it.

### 2.4 Priors Specified Using a Base Model

One of the key challenges when building a prior for a hierarchical model is finding a way to control against over-fitting. In this section, we consider a number of priors that have been proposed in the literature that are linked through the abstract concept of a “base model.” This can be seen as a specific type of “weak information” that is especially important for nested models.

**DEFINITION 1.** For a model component with density  $\pi(\mathbf{x}|\xi)$  controlled by a flexibility parameter  $\xi$ , the base model is the “simplest” model in the class. For notational clarity, we will take this to be the model corresponding to  $\xi = 0$ . It will be common for  $\xi$  to be

nonnegative. The flexibility parameter is often a scalar, or a number of independent scalars, but it can also be a vector-valued parameter.

This allows us to interpret  $\pi(\mathbf{x}|\xi)$  as a *flexible extension* of the base model, where increasing values of  $\xi$  imply increasing allowance of deviations from the base model. The idea of a base model is reminiscent of a “null hypothesis” and thinking of what a sensible hypothesis to test for  $\xi$  is a good way to specify a base model. We emphasise, however, that we are not using this model to do testing, but rather to control flexibility and reduce over-fitting thereby improving predictive performance.

A few simple examples will fix the idea.

*Gaussian random effects.* Let  $\mathbf{x}|\xi$  be a multivariate Gaussian with zero mean and precision matrix  $\tau\mathbf{I}$  where  $\tau = \xi^{-1}$ . Here, the base model puts all the mass at  $\xi = 0$ , which is appropriate for random effects where the natural reference is absence of these effects. In the multivariate case and conditional on  $\tau$ , we can allow for correlation among the model components where the uncorrelated case is the base model.

*Spline model.* Let  $\mathbf{x}|\xi$  represent a spline model with smoothing parameter  $\tau = 1/\xi$ . The base model is the infinite smoothed spline which can be a constant or a straight line, depending on the order of the spline or in general the null space of its penalty matrix. This interpretation is natural when the spline model is used as a flexible extension to a constant or in generalised additive models, which can be viewed as a flexible extension of a generalised linear model.

*Time dependence.* Let  $\mathbf{x}|\xi$  denote an auto-regressive model of order 1, unit variance and lag-one correlation  $\rho$ . Depending on the application, then either  $\xi = \rho$  and the base model is “no dependence in time” or  $\xi = 1 - \rho$  and the base model is no change in time.

The base model primarily finds a home in the idea of “spike-and-slab” priors (George and McCulloch, 1993, Ishwaran and Rao, 2005). These models specify a prior on  $\xi$  as a mixture of a point mass at the base model and a diffuse absolutely continuous prior over the remainder of the parameter space. These priors successfully control over-fitting and simultaneously perform prediction and model selection. The downside is that they are computationally unpleasant and specialised tools need to be built to do inference for these models. Furthermore, as the number of flexibility parameters increases, exploring the entire posterior quickly becomes infeasible.

In order to further consider what a nonatomic prior must look like to take advantage of the base model, we consider the following Informal Definition 1.

**INFORMAL DEFINITION 1.** A prior  $\pi(\xi)$  *forces overfitting* (or *overfits*) if the prior places insufficient mass at the base model.

A prior that overfits will drag the posterior towards the more flexible model and the base model will have almost no support in the posterior, even in the case where the base model is the true model. Hence, when using an overfitting prior, we are unable to distinguish between flexible models that are supported by the data and flexible models that are a consequence of the prior choice.

Informal Definition 1 is both uncontroversially true and completely useless because it relies on the vague notion of “insufficient mass.” This condition can be made very precise, at the cost of being impossible to verify for complex models (Ghosal, Ghosh and van der Vaart, 2000, Theorem 2.4).

The aim of this paper is to provide practical advice for setting priors, and so we commit the cardinal sin of mathematical sloppiness in an attempt to find a “rule of thumb” for ensuring there is sufficient prior mass around the base model. Hence, we say that *a prior overfits if its density in a sensible parameterisation is zero at the base model*. In Section 3, we argue that a “sensible parameterisation” is in terms of the square-root of a Kullback–Leibler divergence between the base model and a more flexible model. These terms are similar to the balls found in the asymptotic theory of Ghosal, Ghosh and van der Vaart (2000) with one important difference: because we set priors one component at a time (rather than all at once), this condition can be easily checked numerically and the remainder of the paper is devoted to using this condition to build a system for specifying priors. This practical version of Informal Definition 1 will rule out a number of suitable priors, but we believe it is a useful triage method for choosing priors that ensure we do not accidentally force our model to be more complex than necessary.

## 2.5 Desiderata for Setting Joint Priors on Flexibility Parameters in Hierarchical Models

We conclude this tour of prior specifications by detailing what we look for in a joint prior for parameters in a hierarchical model and pointing out priors that have been successful in fulfilling at least some of these. This list is quite personal, but we believe that it is broadly sensible. We wish to emphasise that the

desiderata listed below only make sense in the context of hierarchical models with *multiple model components* and it does not make sense to apply them to less complex models. The remainder of the paper can be seen as our attempt to construct a system for specifying priors that at least partially consistent with this list.

*D1: The prior should not be noninformative.* Even if it was possible to compute a noninformative prior for a specific hierarchical model, we are not convinced it would be a good idea. Our primary concern is the stability of inference. In particular, if a model is over-parameterised, that is, too flexible, these priors are likely to lead to badly over-fitted posteriors. Outside the realm of formally noninformative priors, emphasising “flatness” can lead to extremely prior-sensitive inferences (Gelman, 2006). This should not be interpreted as us calling for massively informative priors, but rather a recognition that for complex models, a certain amount of extra information needs to be injected to make useful inferences.

*D2: The prior should be aware of the model structure.* Roughly speaking, we want to ensure that if a subset of the parameters control a single aspect of the model, the prior on these parameters is set jointly. This also suggests using a parameterisation of the model that, as much as possible, has parameters that only control one aspect of the model. Specific examples of this can be found in Sections 5 and 7, as well as He, Hodges and Carlin (2007) and He and Hodges (2008).

*D3: When reusing the prior for a different analysis, changes in the problem should be reflected in the prior.* A prior specification should be explicit about what needs to be changed when applying it to a similar but different problem. An easy example is that the prior on the scaling parameter of a spline model needs to depend on the number of knots (Sørbye and Rue, 2014). Cui et al. (2010) suggested an approach for partitioning degrees of freedom to individual effects in a hierarchical model. By putting a prior on these, they induced a prior for the respective smoothing parameter. This approach has several attractive features, and one is that the range of the degrees of freedom for a spline model depends on the number of knots. Furthermore, it is invariant to a range of reparameterisations, however, its applicability is limited, but can be slightly improved using approximations proposed by Lu, Hodges and Carlin (2007) and Reich and Hodges (2008).

*D4: The prior should limit the flexibility of an over-parameterised model.* This desideratum is related to

the discussion in Section 2.4. It is unlikely that priors that do not have good shrinkage properties will lead to good inference for hierarchical models.

*D5: Restrictions of the prior to identifiable submanifolds of the parameter space should be sensible.* As more data appears, the posterior will contract to a submanifold of the parameter space. For an identifiable model, this submanifold will be a point. Unfortunately, a number of the more complex models that are formulated in real applications have parameters that cannot be identified. In these partially identifiable (Gustafson, 2005) or singular (Watanabe, 2009) models, the prior is still present in the limiting posterior. In these cases, it is vital to specify it carefully. A case where it is not desirable to have a noninformative prior on this submanifold is given in Fuglstad et al. (2015).

*D6: The prior should control what a parameter does, rather than its numerical value.* A sensible method for setting priors should be (at least locally) indifferent to the parameterisation used. It does not make sense, for example, for the posterior to depend on whether the modeller prefers working with the standard deviation, the variance, or the precision of a Gaussian random effect.

The idea of using the distance between two models as a reasonable scale to think about priors dates back to Jeffreys (1946) pioneering work to obtain priors that are invariant to reparameterisation. Bayarri and García-Donato (2008) build on the early ideas of Jeffreys (1961) to derive objective priors for computing Bayes factors for Bayesian hypothesis tests; see also Robert, Chopin and Rousseau (2009), Section 6.4. They use divergence measures between the competing models to derive the required proper priors, and call those derived priors divergence-based (DB) priors. Given the prior distribution on the parameter space of a full encompassing model, Consonni and Veronese (2008) used Kullback–Leibler projection, in the context of Bayesian model comparison, to derive suitable prior distributions for candidate submodels.

*D7: The prior should be computationally feasible.* If our aim is to perform applied inference, we need to ensure that inference can be performed within our computational budget. This will always lead to a very delicate trade-off between modelling and computation that needs to be evaluated for each problem.

*D8: The prior should perform well.* This is the most difficult desideratum to fulfill. Ideally, we would like to ensure that, for some appropriate quantities of interest, the estimators produced using these priors have appropriate theoretical guarantees. It could be that we desire good posterior contraction, asymptotic normality,

good predictive performance under mis-specification, robustness against outliers, admissibility in the Stein sense or any other “objective” property. At the present time, there is essentially no knowledge of any of these desirable features for the types of models that we are considering in this paper. As this gap in the literature closes, it may be necessary to update recommendations on how to set a prior for a hierarchical model to make them consistent with this new knowledge.

### 3. PENALISED COMPLEXITY PRIORS

In this section, we will outline our approach to constructing *penalised complexity priors* (PC priors) for a univariate parameter, postponing the extensions to the multivariate case to Section 6.1. These priors, which are fleshed out in further sections, satisfy most of the desiderata listed in Section 2.5. We demonstrate these principles by deriving the PC prior for the precision of a Gaussian random effect.

#### 3.1 A Principled Definition of the PC Prior

We will now state and discuss our principles for constructing a prior distribution for  $\xi$ .

*Principle 1: Occam’s razor.* We invoke the principle of parsimony, for which simpler model formulations should be preferred until there is enough support for a more complex model. Our simpler model is the base model, hence we want the prior to penalise deviations from it. From the prior alone, we should prefer the simpler model and the prior should be decaying as a function of a measure of the increased complexity between the more flexible model and the base model.

*Principle 2: Measure of complexity.* We base our measure of complexity on the Kullback–Leibler divergence (KLD) (Kullback and Leibler, 1951)

$$\begin{aligned} \text{KLD}(\pi(\mathbf{x}|\xi) \parallel \pi(\mathbf{x}|\xi = 0)) \\ = \int \pi(\mathbf{x}|\xi) \log\left(\frac{\pi(\mathbf{x}|\xi)}{\pi(\mathbf{x}|\xi = 0)}\right) d\mathbf{x}. \end{aligned}$$

The KLD is ubiquitous in the theory of Bayesian statistics and is once again appropriate for the task at hand as it measures the information lost when approximating a flexible model by the base model. Combining Principle 1 with a measure of complexity based on the KLD says that we want the prior to have high mass in areas where replacing the flexible model by the base model will not lead to much information loss. We note that the asymmetry of the KLD is not troubling in this context as we are interested in measuring how much more



complex a model is than the base model, which does not need to be reversible. A good analogy would be that, when walking between home and a destination, the appropriate measure “distance” is time, which is not necessarily symmetric in a hilly city, rather than physical distance, which is symmetric. In order to use the KLD with Principle 1, we need it to be interpretable as a “distance.” Using either asymptotic considerations (to relate to the Fisher-information metric) or Pinsker’s inequality (to relate it to the total-variation distance), it becomes clear that the natural way to use the KLD in to define the (unidirectional) distance between two models with densities  $f$  and  $g$  is  $d(f\|g) = \sqrt{2 \text{KLD}(f\|g)}$ . Hence, we consider  $d$  to be a measure of complexity of the model  $f$  when compared to model  $g$ .

*Principle 3: Constant rate penalisation.* Penalising the deviation from the base model parameterised with the distance  $d$ , we use a constant decay-rate  $r$ , so that the prior satisfies the memoryless property

$$\frac{\pi_d(d + \delta)}{\pi_d(d)} = r^\delta, \quad d, \delta \geq 0$$

for some constant  $0 < r < 1$ . This will ensure that the relative prior change by an extra  $\delta$  does not depend on  $d$ , which is a reasonable choice without extra knowledge (see the discussion on tail behaviour in Section 2.4). Deviating from the constant rate penalisation implies the assignment of different decay rates to different areas of the parameter space. However, this will require a concrete understanding of the distance scale for a particular problem; see Section 4.5. Further, the mode of the prior is at  $d = 0$ , that is, the base model. The constant rate penalisation assumption implies an exponential prior on the distance scale,  $\pi(d) = \lambda \exp(-\lambda d)$ , for  $r = \exp(-\lambda)$ . This corresponds to the following prior on the original space:

$$(3.1) \quad \pi(\xi) = \lambda e^{-\lambda d(\xi)} \left| \frac{\partial d(\xi)}{\partial \xi} \right|.$$

In some cases,  $d$  is upper bounded and we use a truncated exponential as the prior for  $d$ .

*Principle 4: User-defined scaling.* The final principle needed to completely define a PC prior is that the *user* has an idea of a sensible size for the parameter of interest or a property of the corresponding model component. This is similar to the principle behind weakly informative priors. In this context, we can select  $\lambda$  by controlling the prior mass in the tail. This condition is of the form

$$(3.2) \quad \text{Prob}(Q(\xi) > U) = \alpha,$$

where  $Q(\xi)$  is an interpretable transformation of the flexibility parameter,  $U$  is a “sensible,” user-defined upper bound that specifies what we think of as a “tail event” and  $\alpha$  is the weight we put on this event. This condition allows the user to prescribe how informative the resulting PC prior is.

The PC prior procedure is invariant to reparameterisation, since the prior is defined on the distance  $d$ , which is then transformed to the corresponding prior for  $\xi$ . This is a major advantage of PC priors, since we can construct the prior without taking the specific parameterisation into account.

The PC prior construction is consistent with the desiderata listed in Section 2.5. Limited flexibility (D4), controlling the effect rather than the value (D6), and informativeness (D1) follow from Principles 1, 2 and 4, respectively. Lacking more detailed theory for hierarchical models, Principle 3 is consistent with existing theory (D8). We argue that computational feasibility (D7) follows from restricting our search to absolutely continuous priors. Building “structurally aware” priors (D2) is discussed in Sections 5 and 7. The idea that a prior should change in an appropriate way when the model changes is discussed in Section 5. The desideratum that the prior is meaningful on identifiable submanifolds (D5) is discussed in the context of spatial statistics in Fuglstad et al. (2015).

### 3.2 Are the Tails of PC Priors Too Light?

While the careful specification of the prior near the base model is necessary to control against overfitting, it is also necessary to consider the tail behaviour in order to ensure that complexity is not being penalised too harshly. Adhering to Principle 3 leaves PC priors with exponential tails on a distance scale. Contrary to this, Gelman (2006), Gelman et al. (2008) argue that, when setting priors on the standard deviation of a normal distribution, heavy tails are necessary for robustness (O’Hagan and Pericchi, 2012). Unfortunately, this theory is only developed for inferring location-scale families or natural parameters in exponential families and it is unclear how to generalize these results to the types of models we are considering. Piironen and Vehtari (2015) suggest that the heavy tails induced by a half-Cauchy prior leads to poor numerical behaviour even in advanced MCMC implementations like Stan and recommend using a Student  $t$ -distribution with more than 2 degrees of freedom. Ghosh, Li and Mitra (2015) show that using priors with Cauchy-like tails on regression coefficients in logistic regression can lead to unusually large inferred coefficients. In our experiments,

we have found little difference between half-Cauchy and exponential tails, whereas we found huge differences between exponential and Gaussian tails, which performed badly when the data was generated from a moderately flexible model. Hence, we did not find compelling evidence that we needed to replace the exponential prior in Principle 3 with heavier tailed prior.

### 3.3 The PC Prior for the Precision of a Gaussian Random Effect

The classical notion of a random effect has proven to be a convenient way to introduce association and unobserved heterogeneity. We will now derive the PC prior for the precision parameter  $\tau$  for a Gaussian random effect  $\mathbf{x}$ , where  $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \tau^{-1}\mathbf{R}^{-1})$ , with  $\mathbf{R} \succeq 0$  known. In allowing  $\mathbf{R}$  to be indefinite, this derivation also includes popular intrinsic models such as CAR and thin-plate spline models (Rue and Held, 2005). The natural base model is the absence of random effects, which corresponds to  $\tau = \infty$ . In the rank deficient case, the natural base model is that the effect belongs to the nullspace of  $\mathbf{R}$ , which also corresponds to  $\tau = \infty$ . This base model leads to a useful negative result.

**THEOREM 1.** *Let  $\pi_\tau(\tau)$  be an absolutely continuous prior for  $\tau > 0$  where  $E(\tau) < \infty$ , then  $\pi_d(0) = 0$  and the prior overfits (in the sense of the practical version of Informal Definition 1).*

The proof is given in the Supplementary Material. Note that all commonly used  $\Gamma(a, b)$  priors with expected value  $a/b < \infty$  will overfit. Frühwirth-Schnatter and Wagner (2010, 2011) demonstrate overfitting due to Gamma priors and suggest using a (half) Gaussian prior for the standard deviation to overcome this problem, as suggested by Gelman (2006); See also Roos and Held (2011) and the discussion of Lunn et al. (2009).

The PC prior for  $\tau$  is, except for in the specification of  $\lambda$ , independent of  $\mathbf{R}$  and is derived in Appendix A.1 as a type-2 Gumbel distribution

$$(3.3) \quad \pi(\tau) = \frac{\lambda}{2} \tau^{-3/2} \exp(-\lambda \tau^{-1/2}), \quad \tau > 0, \lambda > 0.$$

The density is given in equation (3.3) and has no integer moments. This prior also corresponds to an exponential distribution with rate  $\lambda$  for the standard deviation. The parameter  $\lambda$  determines the magnitude of the penalty for deviating from the base model and higher values increase this penalty. As previously, we can determine  $\lambda$  by imposing a notion of *scale* on the random effects. This requires the user to specify  $(U, \alpha)$

so that  $\text{Prob}(1/\sqrt{\tau} > U) = \alpha$ . This implies that  $\lambda = -\ln(\alpha)/U$ . As a rule of thumb, the marginal standard deviation of  $\mathbf{x}$  with  $\mathbf{R} = \mathbf{I}$ , after the type-2 Gumbel distribution for  $\tau$  is integrated out, is about  $0.31U$  when  $\alpha = 0.01$ . This means that the choice  $(U = 0.968, \alpha = 0.01)$  gives  $\text{Stdev}(\mathbf{x}) \approx 0.3$ . The interpretation of the marginal standard deviation of a random effect is more direct and intuitive than choosing hyperparameters of a given prior.

The new prior is displayed in Figure 1 for  $(U = 0.968, \alpha = 0.01)$ , together with the popular  $\Gamma(1, b)$  prior, where the shape is 1 and rate is  $b$ . We selected  $b$  so that the marginal variance for the random effects are equal for the two priors. Panel (a) shows the two priors on the precision scale and panel (b) shows the two priors on the distance scale. The priors for low precisions are quite different, and so are the tail behaviours. For large  $\tau$ , the new prior behaves like  $\tau^{-3/2}$ , whereas the Gamma prior goes like  $\exp(-b\tau)$ . This is a direct consequence of the importance the new prior gives to the base model, that is, the absence of random effects. Panel (b) demonstrates that the Gamma prior has density zero at distance zero, and hence, does not prevent over-fitting.

We end with a cautionary note about scaling issues for these models and our third desideratum. If  $\mathbf{R}$  is full-rank, then it is usually scaled, or can be scaled, so that  $(\mathbf{R}^{-1})_{ii} = 1$  for all  $i$ , hence  $\tau$  represents the marginal precision. This leads to a simple interpretation of  $U$ . However, this is usually not the case if  $\mathbf{R}$  is singular like for spline and smoothing components; see Sørbye and Rue (2014) for a discussion of this issue. Let the columns of  $\mathbf{V}$  represent the null-space of  $\mathbf{R}$ , so that  $\mathbf{R}\mathbf{V} = \mathbf{0}$ . For smoothing spline models, the null-space is a low-dimensional polynomial and  $\mathbf{R}$  defines the penalty for deviating from the null space (Rue and Held, 2005, Section 3). In order to unify the interpretation of  $U$ , we can scale  $\mathbf{R}$  so that the geometric mean (or some typical value) of the marginal variances of  $\mathbf{x}|\mathbf{V}^T \mathbf{x} = \mathbf{0}$  is one. In this way,  $\tau$  represents the precision of the (marginal) deviation from the null space.

### 3.4 The Effect of $\lambda$

Our fourth principle asserts that the scale of the prior should be chosen by the user. This injects a very specific avenue of subjectivity into PC priors and it is worth investigating how important this choice is. In our experiences working with these priors, we have found that they are almost always insensitive to this parameter providing that it is not set to an extremely poor value. An easy example of this is found in Section 4.4,

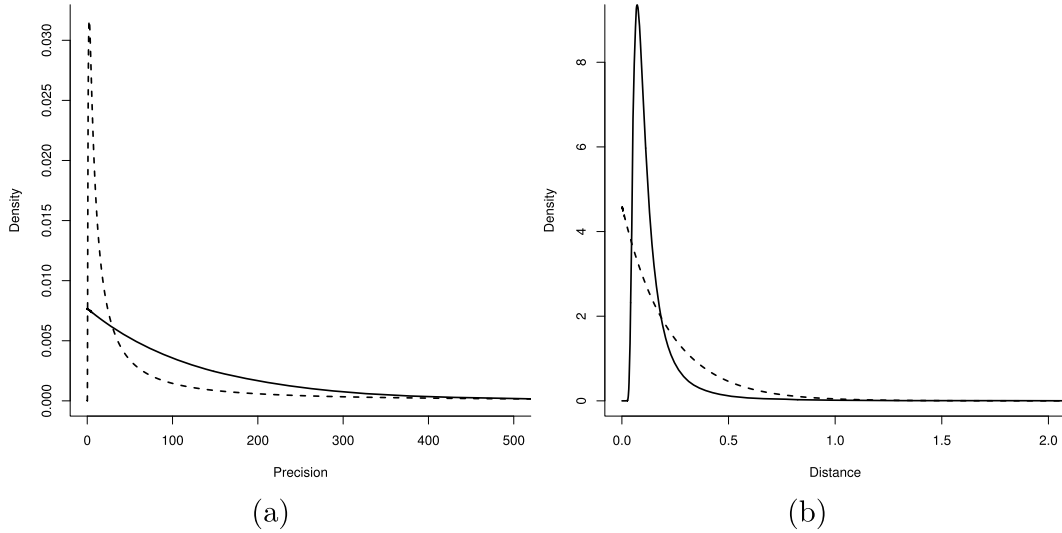


FIG. 1. Panel (a) displays the new prior (dashed) with parameters ( $U = 0.968, \alpha = 0.01$ ), and the  $\Gamma(\text{shape} = 1, \text{rate} = b)$  prior (solid). The value of  $a$  is computed so that the marginal variances for the random effects are equal for the two priors, which leads to  $b = 0.0076$ . Panel (b) shows the same two priors on the distance scale demonstrating that the density for the Gamma prior is zero at distance zero.

where a poor specification of  $\lambda$  leads to a very strong prior that is in conflict with the data.

A more interesting case when the posterior is sensitive to the choice of scaling was discussed by [Guo, Rue and Riebler \(2015\)](#). They considered prior specification in bivariate meta-analysis models, where they attempt to simultaneously combine information on sensitivity and specificity of a treatment. As meta-analyses typically only combine a small number of studies, the prior sensitivity that they found is not particularly surprising and that PC prior framework allows for a sensible way of constructing informative expert priors.

We conclude this discussion with a simulation study that shows that PC priors are fairly insensitive to the choice of  $\lambda$  when there is at least a moderate amount of information. In particular, we will consider the interesting problem of inferring the degrees of freedom parameter  $\nu$  in a Student  $t$ -distribution. This is a challenging problem for medium-sized datasets, as tail properties are hard to estimate without a lot of data.

To investigate the properties of the PC prior on  $\nu$  and compare it with the exponential prior on  $\nu$ , we performed a simulation experiment using the model  $y_i = \varepsilon_i$ ,  $i = 1, \dots, n$ , where  $\varepsilon$  is Student  $t$  distributed with unknown d.o.f. and fixed unit precision. Similar results are obtained for more involved models ([Martins and Rue, 2013](#)). We simulated data sets with  $n = 100, 1000, 10,000$ . For the d.o.f. we used  $\nu = 5, 10, 20, 100$ , to study the effect of the priors under different levels of the kurtosis. For each of the

12 scenarios, we simulated 1000 different data sets, for each of which we computed the posterior distribution of  $\nu$  using one-dimensional quadrature. Then we formed the equal-weight mixture over all the 1000 realisations to approximate the expected behaviour of the posterior distribution over different realisations of the data. Figure 2 shows the 0.025, 0.5 and 0.975-quantiles of this mixture of posterior distributions of  $\nu$  when using the PC prior with  $U = 10$  and  $\alpha = 0.2, 0.3, 0.4, 0.5, 0.6, 0.7$  and  $0.8$ , and the exponential prior, as recommended by [Geweke \(2006\)](#), with mean 5, 10, 20 and 100. Each row in Figure 2 corresponds to a different d.o.f. while each column corresponds to a different sample size  $n$ .

The full details of the simulation study, as well as more information about the Student  $t$  case, can be found in the Supplementary Material.

The first row in Figure 2 displays the results with  $\nu = 100$  in the simulation which is close to Gaussian observations. Using the PC priors results in wide credible intervals in the presence of few data points, but as more data are provided the model learns about the high d.o.f. Using an exponential prior for  $\nu$ , the posterior quantiles obtained depend strongly on the mean of the prior. This difference seems to remain even with  $n = 1000$  and  $n = 10,000$ , indicating that the prior still dominates the data. For all scenarios, the intervals obtained with the exponential prior for  $\nu$  look similar, with the exception of scenarios with low d.o.f. and high sample size, for which the information in the data

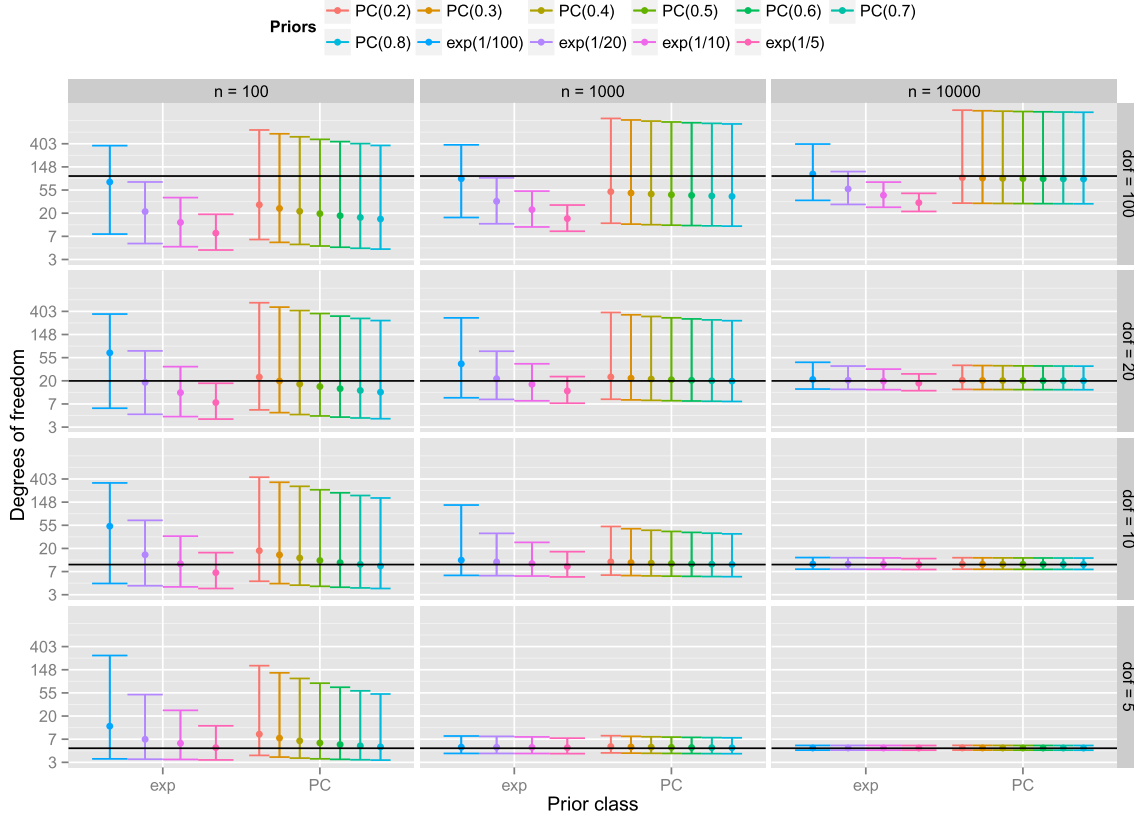


FIG. 2. The 0.025-, 0.5- and 0.975-quantile estimates obtained from an equal-weight mixture of posterior distributions of  $\nu$  when fitting a Student  $t$ -errors model with different priors for  $\nu$  over 1000 datasets, for each of the 12 scenarios with sample sizes  $n = 100, 1000, 10,000$  and d.o.f.  $\nu = 100, 20, 10, 5$ . The first four intervals in each scenario correspond to exponential priors with mean 100, 20, 10, 5, respectively. The last seven intervals in each scenario correspond to the PC prior with  $U = 10$  and  $\alpha = 0.2, 0.3, 0.4, 0.5, 0.6, 0.7$  and  $0.8$ .

is strong enough to dominate this highly informative prior.

If we study Figure 2 column-wise and top-down, we note that the performance of the PC priors are barely affected by the change in  $\alpha$ . They seem to be almost insensitive to the choice of  $\alpha$  and perform well for all sample sizes. For the exponential priors when  $n = 100$ , we basically see no difference in inference for  $\nu$  comparing the near Gaussian scenario ( $\nu = 100$ ) with the strongly heavy tailed one ( $\nu = 5$ ). The implication is that the results will be much more influenced by the choice of the mean in the exponential prior than by the d.o.f. in the data. Similarly, the exponential priors continue to be highly informative even for large sample sizes. This informative behaviour can be seen in particular in the first row ( $\nu = 100$ ).

We also inspected the coverage at a 95% level for all priors and simulation settings. The coverage probabilities for all PC priors were very similar and always at least 0.9, whereby they tended to be a bit too high compared to the nominal level. For the exponential priors,

the results are ambiguous, either the coverage probabilities are sensible while still being higher than the nominal level or they are far too low, in several settings even zero.

This example sheds light on the consistency issue discussed by Lid Hjort et al. (2010), Chapter 1. A prior distribution represents prior belief, learnt before data is observed, but it also fully specifies the Bayesian learning model. As more data arrives, it is expected that the learning model goes in the right direction. If it does not, then the learning model (prior) has not been set well, even though the prior might be appropriate as representing prior beliefs. In the Supplementary Material, we show that priors on  $\nu$  with finite mean do not respect the Occam's razor principle will invariably lead to bad learning models. Figure 2 illustrates this point for the case of exponential priors.

#### 4. SOME PROPERTIES OF PC PRIORS

In this section, we investigate some basic properties of PC priors for simple models. In particular, we will



investigate when the behaviour in the neighbourhood of the base model or the tail behaviour is important to obtain sensible results. For most moderate-dimensional models, we find that the behaviour at the base model is fundamentally important, while the tail behaviour is less important. In contrast, in very high-dimensional settings, we find that a heavier tail than that implied by the principle of constant rate penalisation is required for sound statistical inference.

For reasons of mathematical tractability, in this section we restrict ourselves to a much smaller set of models than in the rest of the paper. Sections 4.1–4.3 focus on *direct observations of a single component model*, while Sections 4.4–4.5 focus on estimating the mean of a normal distribution with known variance. None of these models fall within the family of realistically complicated models that are the focus of this paper. Unfortunately, there is very little theory for the types of hierarchical models we are considering, so we are forced to consider these simpler models in order to gain intuition for the more interesting cases.

#### 4.1 Behaviour Near the Base Model

To understand the PC prior construction better, we can study what happens near  $\xi = 0$  using the connection between KLD and the Fisher information metric. We will assume the model is sufficiently regular at  $\xi = 0$  to make the following formal asymptotic arguments work. Let  $I(\xi)$  be the Fisher information at  $\xi$ . Using the well-known asymptotic expansion (Watanabe, 2009, Remark 1.4),

$$\begin{aligned} \text{KLD}(\pi(\mathbf{x}|\xi) \parallel \pi(\mathbf{x}|\xi = 0)) \\ = \frac{1}{2} I(0) \xi^2 + \text{higher order terms}, \end{aligned}$$

a standard expansion reveals that our new prior behaves like

$$\pi(\xi) = I(\xi)^{1/2} \exp(-\lambda m(\xi)) + \text{higher order terms}$$

for  $\lambda\xi$  close to zero. Here,  $m(\xi)$  is the distance defined by the metric tensor  $I(\xi)$ ,  $m(\xi) = \int_0^\xi \sqrt{I(s)} ds$ , using tools from information geometry. Close to the base model, the PC prior is a tilted Jeffreys' prior for  $\pi(\mathbf{x}|\xi)$ , where the amount of tilting is determined by the distance on the Riemannian manifold to the base model scaled by the parameter  $\lambda$ . The user-defined parameter  $\lambda$  thus determines the degree of informativeness in the prior.

#### 4.2 Large Sample Behaviour Under the Base Model

A good check when specifying a new class of priors is to consider the asymptotic properties of the induced posterior. In particular, it is useful to ensure that, for large sample sizes, we achieve frequentist coverage. While the Bernstein–von Mises theorem ensures that, for sufficiently well-behaved models where the true parameter lies in the centre of the parameter space, asymptotic coverage is independent of (sensible) prior choice, the situation may be different when the true parameter lies on the boundary of the parameter space. In most examples in this paper, the base model defines the boundary of the parameter space and prior choice now plays an important role (Bochkina and Green, 2014).

When the true parameter lies at the boundary of the parameter space, there are two possible cases to be considered. In the regular case, where the derivative of the log-likelihood at this point is asymptotically zero, Bochkina and Green (2014) showed that the large-sample behaviour depends entirely on the behaviour of the prior near zero. Furthermore, if the prior density is finite at the base model, then the large sample behaviour is identical to that of the maximum likelihood estimator (Self and Liang, 1987). Hence Principle 1 ensures that PC priors induce the correct asymptotic behaviour. Furthermore, the invariance of our construction implies good asymptotic behaviour for any reparameterisation.

#### 4.3 PC Priors and Bayesian Hypothesis Testing

PC priors are not built to be hypothesis testing priors and we do not recommend their direct use as such. We will show, however, that they lead to consistent Bayes factors and suggest an invariant, weakly informative decision theory-based approach to the testing problem. With an eye towards invariance, in this section we will consider the re-parameterisation  $\zeta = d(\xi)$ .

In order to show the effects of using PC priors as hypothesis testing priors, let us consider the large-sample behaviour of the precise test  $\zeta = 0$  against  $\zeta > 0$ . We can use the results of Bochkina and Green (2014) to show the following in the regular case.

**THEOREM 2.** *Under the conditions of Bochkina and Green (2014), the Bayes factor for the test  $H_0 : \zeta = 0$  against  $H_1 : \zeta > 0$ , is consistent when the prior for  $\zeta$  does not overfit. That is,  $B_{01} \rightarrow \infty$  under  $H_0$  and  $B_{01} \rightarrow 0$  under  $H_1$ , where  $B_{01}$  denotes the Bayes factor for candidate model  $M_0$  against candidate model  $M_1$ .*

Johnson and Rossell (2010) point out for regular models, that the rates at which these Bayes factors go

to their respective limits under  $H_0$  and  $H_1$  are not symmetric. This suggests that the finite sample properties of these tests will be suboptimal. The asymmetry can be partly alleviated using the moment and inverse moment prior construction of [Johnson and Rossell \(2010\)](#), which can be extended to this parameter invariant formulation in a straightforward way (see [Rousseau and Robert, 2011](#)). The key idea of nonlocal priors is to modify the prior density so that it is approximately zero in the neighbourhood of  $H_0$ . This forces a separation between the null and alternative hypotheses that helps balance the asymptotic rates. Precise rates are given in the Supplementary Material.

The construction of nonlocal priors highlights the usual dichotomy between Bayesian testing and Bayesian predictive modelling: in the large sample limit, priors that lead to well-behaved Bayes factors have bad predictive properties and vice versa. In a far-reaching paper, [Bernardo \(2011\)](#) suggested that this dichotomy is the result of asking the question the wrong way. Rather than using Bayes factors as an “objective” alternative to a proper decision analysis, [Bernardo \(2011\)](#) suggests that reference priors combined with a well-constructed invariant loss function allows for predictive priors to be used in testing problems. This also suggests that PC priors can be used in place of reference priors to construct a consistent, coherent and invariant hypothesis testing framework based on decision theory.

#### 4.4 Risk Results for the Normal Means Model

A natural question to ask when presented with a new approach for constructing priors is *are the resulting estimators any good?* In this section, we investigate this question for the analytically tractable normal means model:

$$(4.1) \quad \begin{aligned} y_i | x_i, \sigma &\sim \mathcal{N}(x_i, 1), \quad x_i | \sigma \sim \mathcal{N}(0, \sigma^2), \\ \sigma &\sim \pi_d(\sigma), \quad i = 1, \dots, p. \end{aligned}$$

This model is the simplest one considered in this paper and gives us an opportunity to investigate whether constant rate penalisation, which was used to argue for an exponential prior on the distance scale, makes sense in this context. For the precision parameter of a Gaussian random effect, the distance parameter is the standard deviation,  $d = \sigma$ , which allows us to leverage our understanding of this parameter and consider alternatives to this principle.

Let  $\mathbf{x}_0 \equiv (x_1, \dots, x_p)$  denote the unknown vector of means. Then, for an estimator  $\delta(\cdot)$ , define the mean-square risk as  $R(\mathbf{x}_0, \delta) = E(\|\mathbf{x}_0 - \delta(\mathbf{y})\|^2)$ , where the

expectation is taken over data  $\mathbf{y} \sim N(\mathbf{x}_0, \mathbf{I})$ . The standard estimator  $\delta_0(\mathbf{y}) = \mathbf{y}$  is the best invariant estimator and obtains constant minimax risk  $R(\mathbf{x}_0, \delta_0) = p$ . Classical results of [James and Stein \(1961\)](#), [Stein \(1981\)](#) show that this estimator can be improved upon. We will consider the risk properties of the Bayes’ estimators, which in this case is the posterior mean.

By noting that  $E(x_i | \mathbf{y}, \sigma) = y_i(1 - E(\kappa | \mathbf{y}))$  for the shrinkage parameter  $\kappa = (1 + \sigma^2)^{-1}$ , [Polson and Scott \(2012\)](#) derived the general form of the mean-square risk. Using a half-Cauchy distribution on the standard deviation  $\sigma$ , as advocated by [Gelman \(2006\)](#), the resulting density for  $\kappa$  has a horseshoe shape with infinite peaks at zero and one. The estimators that come from this horseshoe prior have good frequentist properties as the shape of the density of  $\kappa$  allows the component to have any level of shrinkage. In general, the density for  $\kappa$  is related to  $\pi_d(\sigma)$  by

$$\pi_\kappa(\kappa) = \pi_d(\sqrt{\kappa^{-1} - 1}) \frac{1}{2\sqrt{\kappa^3 - \kappa^4}}.$$

Straightforward asymptotics shows how the limit behaviour of  $\pi_d(\sigma)$  transfers into properties of  $\pi_\kappa(\kappa)$ .

**THEOREM 3.** *If  $\pi_d(\sigma)$  has tails lighter than a Student  $t$ -distribution with 2 degrees of freedom, then  $\pi_\kappa(0) = 0$ . If  $\pi_d(d) \leq \mathcal{O}(d)$  as  $d \rightarrow 0$ , then  $\pi_\kappa(1) = 0$ .*

This result suggests that the PC prior will shrink strongly, putting relatively little prior mass near zero shrinkage, due to the relatively light tail of the exponential. The scaling parameter  $\lambda$  controls the decay of the exponential, and the effect of  $\lambda = -\log(\alpha)/U$ , with  $\alpha = 0.01$ , on the implied priors on  $\kappa$  is shown in Figure 3(a) for various choices of  $U$ . For moderate  $U$ , the PC prior still places a lot of prior mass near  $\kappa = 0$ , in spite of the density being zero at that point. This suggests that the effect of the light tail induced by the principle of constant penalisation rate, is less than Theorem 3 might suggest. For comparison, the horseshoe curve induced by the half-Cauchy prior is shown as the dotted line in Figure 3(a). This demonstrates that PC priors with sensible scaling parameter place more mass at intermediate shrinkage values than the half-Cauchy, which concentrates the probability mass near  $\kappa = 0$  and  $\kappa = 1$ . The overall interpretation of Figure 3(a) is that, for large enough  $U$ , the PC prior will lead to a slightly less efficient estimator than the half-Cauchy prior, while for small signals we expect them to behave similarly.

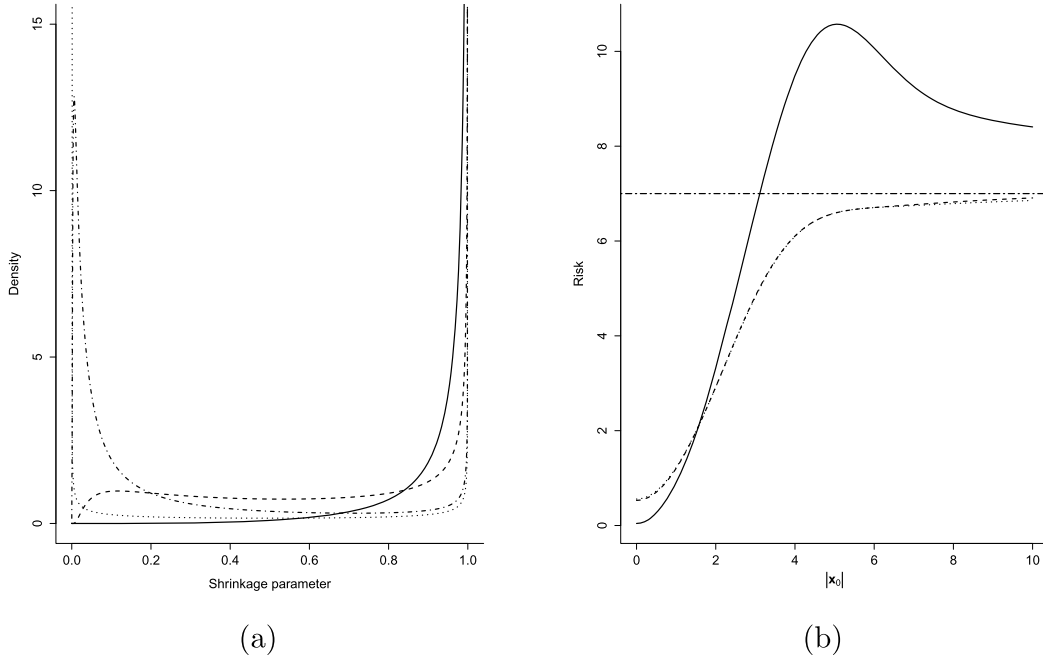


FIG. 3. Display (a) shows the implied prior on the shrinkage parameter  $\kappa$  for several different priors on the distance scale. These priors are the half-Cauchy (dotted) and PC priors with scaling parameter  $\lambda = -\log(0.01)/U$  for  $U = 1$  (solid),  $U = 5$  (dashed), and  $U = 20$  (dot-dashed). Display (b) shows the mean squared risk of the Bayes' estimators for the normal means model with  $p = 7$  corresponding to different priors on the distance parameter, against  $\|x_0\|$ . The dash-dashed horizontal line is the risk of the naïve minimax estimator  $\delta_0(\mathbf{x}) = \mathbf{x}$ . The solid line corresponds to the PC prior with  $U = 1$ . The dashed and dotted lines, which are essentially overlaid, correspond respectively to the PC prior with  $U = 5$  and the half-Cauchy distribution.

Figure 3(a) demonstrates also to which extent  $U$  controls the amount of information in the prior. The implied shrinkage prior for  $U = 1$  (dot-dash line), corresponds to the weakly informative statement that the effect is not larger than  $3\sigma \approx 0.93$ , has almost no prior mass on  $\kappa < 0.5$ . This is consistent with the information used to build the prior: if  $\|x_0\| < 1$ , the risk of the trivial estimator  $\delta(\mathbf{y}) = \mathbf{0}$  is significantly lower than the standard estimator.

Figure 3(b) shows the risk using PC priors with  $U = 1$  (solid line),  $U = 5$  (dashed line), the half-Cauchy prior (dot-dashed line), as a function of  $\|x_0\|$ . The mean-squared risk exceeds the minimax rate for large  $\|x_0\|$  when  $U = 1$  which is consistent with the prior/data mis-match inherent in badly mis-specifying  $U = 1$ . By increasing  $U$  to 5, we obtain almost identical results to the half-Cauchy prior, with a slight difference only for really large  $\|x_0\|$ . Increasing  $U$  decreases the difference.

The risk results obtained for the normal means model suggests that the PC priors give rise to estimators with good classical risk properties, and that the heavy tail of the half-Cauchy is less important than the finite prior density at the base model. It also demonstrates that

we can put strong information into a PC prior, which we conjecture would be useful when the data consists of Poisson or Binomial responses with link functions like the log and logit, as we have strong structural prior knowledge about the plausible range for the linear predictor in these cases (Polson and Scott, 2012, Section 5).

#### 4.5 Sparsity Priors

When solving high-dimensional problems, it is often expedient to assume that the underlying truth is sparse, meaning that only a small number of the model components have a nonzero effect. Good Bayesian models that can recover sparse signals are difficult to build. Castillo and van der Vaart (2012) consider spike-and-slab priors, that first select a subset of the components to be nonzero and then place a continuous prior on these. These priors have been shown to have excellent theoretical properties, but their practical implementation requires a difficult stochastic search component. A more pleasant computational option builds a prior on the scaling parameter of the individual model components. In the common case where the component has a normal distribution, the shrinkage properties of

these priors have received a lot of attention. Two examples of scale-mixtures of normal distributions are the horseshoe prior (Carvalho, Polson and Scott, 2010, van der Pas, Kleijn and van der Vaart, 2014) and the Dirichlet–Laplace prior (Pati, Pillai and Dunson, 2014) which both were shown to have comparable asymptotic behaviour to spike-and-slab priors when attempting to infer the sparse mean of a high dimensional normal distribution. On the other hand, Castillo, Schmidt-Hieber and van der Vaart (2014) showed that the Bayesian generalisation of the LASSO (Park and Casella, 2008), which can be represented as a scale mixture of normals, gives rise to a posterior that contracts much slower than the minimax rate. This stands in contrast to the frequentist situation, where the LASSO obtains almost optimal rates.

For concreteness, let us consider the problem

$$y_i \sim \pi(y|\beta), \quad \beta \sim \mathcal{N}(\mathbf{0}, \mathbf{D}), \quad D_{ii}^{-1} \stackrel{\text{i.i.d.}}{\sim} \pi(\tau),$$

where  $\pi(y|\beta)$  is some data-generating distribution,  $\beta$  is a  $p$ -dimensional vector of covariate weights,  $\pi(\tau)$  is the PC prior in (3.3) for the precisions  $\{D_{ii}^{-1}\}$  of the covariate weights. Let us assume that the observed data was generated from the above model with true parameter  $\beta_0$  that has only  $s_0$  nonzero entries. We will assume that  $s_0 = o(p)$ . Finally, in order to ensure a priori exchangeability, we set the scaling parameter  $\lambda$  in each PC prior to be the same.

This then raises the question: does an exponential prior on the standard deviation, which is the PC prior in this section, make a good variable selection prior? In this section, we will show that the answer is no. The problem with the basic PC prior for this problem is that the base model has been incorrectly specified. The base model that a  $p$ -dimensional vector is sparse is not the same as the base model that each of the  $p$  components is independently zero and hence the prior encodes the wrong information. A more correct application of the principles in Section 3.1 would lead to a PC prior that first selects the number of nonzero components and then puts i.i.d. PC priors on each of the selected components. If we measure complexity by the number of nonzero components, the principle of constant rate penalisation requires an exponential prior on the number of components, which matches with the theory of Castillo and van der Vaart (2012). Hence, the failure of  $p$  independent PC priors to capture sparsity is not unexpected.

To conclude this section, we show the reason for the failure of independent PC priors to capture sparsity. The problem is that the induced prior over  $\beta$  must have

mass on values with a few large and many small components. Theorem 4 shows that the values of  $\lambda$  that puts sufficient weight on approximately sparse models does not allow these models to have any large components. Fortunately, the principled approach allows us to fix the problem by simply replacing the principle of constant rate penalisation with something more appropriate (and consistent with D8). Specifically, in order for the prior to put appropriate mass around models with the true sparsity, the prior on the standard deviation needs to have a heavier tail than an exponential.

As  $\pi(\tau)$  is an absolutely continuous distribution, the naïve PC prior will never result in exactly sparse signals. This leads us to take up the framework of Pati, Pillai and Dunson (2014), who consider the  $\delta$ -support of a vector

$$\text{supp}_\delta(\beta) = \{i : |\beta_i| > \delta\},$$

and define a vector  $\beta$  to be  $\delta$ -sparse if  $|\text{supp}_\delta(\beta)| \ll p$ . Following Pati, Pillai and Dunson (2014), we take  $\delta = \mathcal{O}(p^{-1})$ . As  $s_0 = o(p)$ , this ensures that the nonzero entries are small enough not to have a large effect on  $\|\beta\|$ .

For fixed  $\delta$ , it follows that the  $\delta$ -support of  $\beta$  has a Binomial( $p, \alpha_p$ ) distribution, where  $\alpha_p = \text{Prob}(|\beta_i| > \delta_p)$ . If we had access to an oracle that told us the true sparsity  $s_0$ , it would follow that a good choice of  $\lambda$  would ensure  $\alpha_p = p^{-1}s_0$ .

**THEOREM 4.** *Let  $S = |\text{supp}_{p^{-1}}(\beta)|$ . If the true sparsity  $s_0 = o(p)$ , then the oracle value of  $\lambda$  that ensures that the a priori expectation  $\mathbb{E}(S) = s_0$  grows like  $\lambda \sim \mathcal{O}(\frac{p}{\log(p)})$ .*

Theorem 4 shows that  $\lambda$  is required to increase with  $p$ , which corresponds to a vanishing upper bound  $U = \mathcal{O}(p^{-1} \log(p))$ . Hence, it is impossible for the above PC prior to have mass on signals that are simultaneously sparse and moderately sized.

The failure of PC priors to provide useful variable selection priors is essentially down to the tails specified by the principle of constant rate penalisation. This principle was designed to avoid having to interpret a change of concavity on the distance scale for a general parameter. However, in this problem, the distance is the standard deviation, which is a well-understood statistical quantity. Hence, it makes sense to put a prior on the distance with a heavier tail in this case. In particular, if we use a half-Cauchy prior in place of an exponential, we recover the horseshoe prior on  $\beta$ , which has good shrinkage properties. In this case Theorem 6 in the Supplementary Material, which is a generalisation



of Theorem 4, shows that the inverse scaling parameter of the half-Cauchy must be at least  $\mathcal{O}(p/\log(p))$ , which corresponds up to a log factor with the optimal contraction results of van der Pas, Kleijn and van der Vaart (2014). We note that this is the only situation we have encountered in which the exponential tails of PC priors are problematic.

## 5. DISEASE MAPPING USING THE BYM MODEL

The application to disease mapping using the popular BYM-model (Besag, York and Mollié, 1991) is particularly interesting since we are required to reparameterise the model to see it as a flexible extension of two base models to which it will shrink towards unless otherwise indicated by the data.

Mapping disease incidence is a huge field within public health and epidemiology, and good introductions to the field exist (Lawson, 2006, 2009, Wakefield, Best and Waller, 2000, Waller and Carlin, 2010). The observed counts  $y_i$  in area  $i$  with  $i = 1, \dots, n$  are commonly assumed to be conditionally independent Poisson variables with mean  $E_i \exp(\eta_i)$ , where  $\{E_i\}$  are the expected number of cases. In the BYM-model, the log relative risk is given by  $\eta_i = \mu + \mathbf{z}_i^T \boldsymbol{\beta} + u_i + v_i$  where  $\mu$  is the overall intercept,  $\boldsymbol{\beta}$  measures the effect of possibly region specific covariates  $\mathbf{z}_i$ ,  $\mathbf{v}$  is a zero mean Gaussian with precision matrix  $\tau_v \mathbf{I}$  and represents an unstructured random effect. In contrast,  $\mathbf{u}$  is a spatial component saying that nearby regions are similar. A first-order intrinsic Gaussian Markov random field model (Rue and Held, 2005, Chapter 3) was introduced by Besag, York and Mollié (1991) as a model for  $\mathbf{u}$ . Let  $\mathcal{G}$  be the conditional independence graph of  $\mathbf{u}$ , where  $\partial i$  denotes the set of neighbours to node  $i$  and let  $n_{\partial i}$  be the corresponding number of neighbours. The conditional distribution of  $u_i$  is

$$u_i | \mathbf{u}_{-i}, \quad \tau_u \sim \mathcal{N}\left(\frac{1}{n_{\partial i}} \sum_{j \in \partial i} u_j, 1/(n_{\partial i} \tau_u)\right),$$

where  $\tau_u$  is the precision parameter; see Rue and Held (2005), Chapter 3, for details. This model is intrinsic and penalises local deviation from its null space, which is a constant level in the case of one connected component (Rue and Held, 2005, Section 3). If the map has islands, the definition of the null-space is more complex, see Hodges (2014), Section 5.2.1. To prevent confounding with the intercept, we impose the constraint that  $\mathbf{1}^T \mathbf{u} = 0$ .

To complete the model, we need the prior specification for the intercept and the fixed-effects  $\boldsymbol{\beta}$ , as well

as the prior for the two precision parameters  $\tau_u$  and  $\tau_v$ . There are two main issues with the BYM model and the choice of priors. The first, related to Desideratum D3, is that the spatial component is not *scaled* (see Section 3.3). The marginal variance after imposing the  $\mathbf{1}^T \mathbf{u} = 0$  constraint is not standardised, meaning that any recommended prior (like those suggested by Bernardinelli, Clayton and Montomoli, 1995) cannot be transferred from one graph to another, since the generalised variance depends on the graph; see Sørbye and Rue (2014). The second issue, related to Desideratum D2, is that the structured component  $\mathbf{u}$  cannot be seen independently from the unstructured component  $\mathbf{v}$ . This means that the priors for  $\tau_u$  and  $\tau_v$  should be (heavily) dependent, and not independent as it is usually assumed.

To resolve these issues, we assume a scaled spatially structured component  $\mathbf{u}^*$  where the generalised variance, computed as the geometric mean of the marginal variances is equal to one; see Section 3.3 and Sørbye and Rue (2014), Riebler et al. (2016). We then rewrite the log relative risk as

$$(5.1) \quad \eta_i = \mu + \mathbf{z}_i^T \boldsymbol{\beta} + \frac{1}{\sqrt{\tau}} (\sqrt{1-\phi} v_i + \sqrt{\phi} u_i^*),$$

where  $0 \leq \phi \leq 1$  is a mixing parameter. The marginal precision contribution from  $\mathbf{u}^*$  and  $\mathbf{v}$  is  $1/\tau$ , whereas the fraction of this variance explained by the spatial term  $\mathbf{u}^*$  and the random effects  $\mathbf{v}$ , are  $\phi$  and  $1-\phi$ , respectively. Note that the two hyperparameters  $(\tau, \phi)$  control very different parts of the prior and this naturally allows for independent prior specification. First, we notice that the type-2 Gumbel prior applies to the precision  $\tau$ , as the natural base model is no effect from  $\mathbf{u}^*$  and  $\mathbf{v}$ . For a fixed marginal precision, the base model is no spatial dependency, that is,  $\phi = 0$ . An increased value of  $\phi$  will blend in spatial dependency keeping the marginal precision constant, hence more of the variability will be explained by  $\mathbf{u}^*$  and the ratio is  $\phi$ . The PC prior for  $\phi$  is derived in Appendix A.2 and depends on the graph  $\mathcal{G}$ . Our notion of *scale* can be used to set  $(U, \alpha)$  so that  $\text{Prob}(\phi < U) = \alpha$  which determines the degree of penalisation. Similar re-parameterisations have been discussed by Dean, Ugarte and Militino (2001), who did not consider the scaling, and Wakefield (2007), who scaled the variance by the arithmetic rather than geometric mean. The difference between these two scalings is subtle: the arithmetic mean of the variances is a good way of finding a representative value of the variance,

whereas the geometric mean can be interpreted as finding the variance of a consensus Gaussian distribution by logarithmically pooling the information each of the marginal distributions (Genest, Weerahandi and Zidek, 1984). Hence, the geometric mean scaling is consistent with desideratum D6 as it averages the “meaning” of the individual variances in the context of their individual Gaussian distributions rather than the averaging the values. Neither Dean, Ugarte and Militino (2001) nor Wakefield (2007) considered the differences in the complexity of the two components when setting the prior on  $\phi$ .

Riebler et al. (2016) compared the new parameterisation and its (shrinkage) performance to alternative parameterisations in a simulation setting. Here, we reanalyse larynx cancer mortality for men, registered in 544 districts of Germany from 1986 to 1990 (Natário and Knorr-Held, 2003) to underline the learning abilities. The total number of deaths due to larynx cancer was 7283, which gives an average of 13.4 per region. An interesting part of modelling these data is the semi-parametric estimation of the covariate effect of lung cancer mortality rates in the same period. This covariate acts as an ecological covariate (Wakefield and Lyons, 2010) to account for smoking consumption, which is known to be the most important risk factor of the larynx cancer. As a smooth model for the ecological covariate  $\mathbf{z}$ , Natário and Knorr-Held (2003) used a second-order random walk model

$$\begin{aligned} \pi(\mathbf{z}|\tau_z) \\ (5.2) \quad &\propto (\tau_z \tau_z^*)^{(m-2)/2} \\ &\cdot \exp\left(-\frac{\tau_z \tau_z^*}{2} \sum_{i=3}^m (z_i - 2z_{i-1} + z_{i-2})^2\right), \end{aligned}$$

where  $m$  is the length of  $\mathbf{z}$ . This spline model penalises the estimated second-order differences and its null space is spanned by  $\mathbf{1}$  and  $(1, 2, \dots, m)$ . Similar to the spatial component in the BYM model, this model component is not standardised and  $\tau_z^*$  ensures that the generalised variance is one. The base model is here a straight line which reduces to a linear effect of the ecological covariate, and the type-2 Gumbel distribution is the resulting PC prior for  $\tau_z$ . The log relative risk results as  $\eta_i = \mu + z_i + \frac{1}{\sqrt{\tau}}(\sqrt{1-\phi}v_i + \sqrt{\phi}u_i^*)$ , where  $z_i$  follows the spline model in (5.2), and whereby the ecological covariate  $\mathbf{z}$  has been converted into the range  $1, 2, \dots, m$  for simplicity. See Rue and Held (2005), Chapter 3, for more details on this spline model, and Lindgren and Rue (2008) for an extension to irregular locations.

We use a constant prior for the intercept and parameters ( $U = 0.2/0.31, \alpha = 0.01$ ) for the precision  $\tau$ . For the prior for  $\phi$ , we use ( $U = 1/2, \alpha = 2/3$ ) which gives a  $2/3$  probability that the fraction of the marginal variance explained by the random effect  $\mathbf{v}$  is larger than  $1/2$ . For the precision in the spline model, we also used ( $U = 0.2/0.31, \alpha = 0.01$ ).

Figure 4(a) shows that the model learns from the data resulting in a posterior concentrated around 1. This implies that only the spatial component contributes to the marginal variance. The posterior for the precision  $\tau$  [panel (b)] is more concentrated than in earlier examples due to the relatively high average counts. The effect of the ecological covariate [panel (c)] seems to be shrunk towards the base model, that is, a straight line, and is much more linear than the various estimates by Natário and Knorr-Held (2003). We suppose that the reason lies in over-fitting due to their choice of priors.

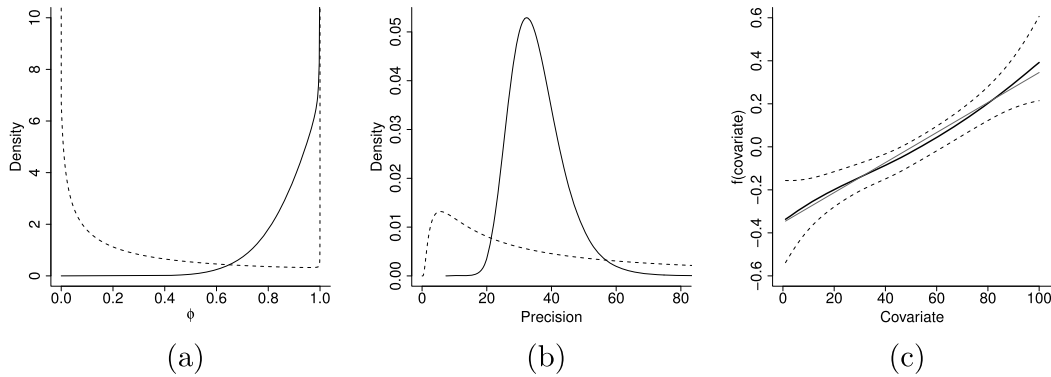


FIG. 4. The results for the larynx data in Germany using PC priors and the reparameterised BYM model. Panel (a) shows the prior density for the mixing parameter  $\phi$  (dashed) and the posterior density (solid). Panel (b) shows the prior density (dashed) and the posterior density (solid) for the precision  $\tau$ . Panel (c) shows the effect of the ecological covariate where the black solid line is the mean, the dashed lines are the upper and lower 0.025-quantiles and the gray solid line is the best linear fit to the mean.

The appropriateness of a linear effect of the ecological covariate, is also verified in [Sørbye and Rue \(2011\)](#).

## 6. MULTIVARIATE PROBIT MODELS

The examples considered thus far have been essentially univariate, with higher dimensional parameter spaces dealt with by assuming that independent priors are sensible when parameters are controlling different parts of the model. In this section, we will demonstrate that the PC prior methodology naturally extends to multivariate parameters and illustrate this by means of multivariate probit models.

Multivariate probit models have applications within sample surveys, longitudinal studies, group randomised clinical trials, analysis of consumer behaviour and panel data ([Talhouk, Doucet and Murphy, 2012](#)). They represent a natural extension of univariate probit models, where the probability for success at the  $i$ th subject is

$$(6.1) \quad \text{Prob}(y_i = 1 | \boldsymbol{\beta}) = \Phi(\mathbf{x}_i^T \boldsymbol{\beta}), \quad i = 1, \dots, n.$$

Here,  $\Phi(\cdot)$  is the cumulative distribution function for the standard Gaussian distribution,  $\mathbf{x}_i$  a set of fixed covariates with regression coefficients  $\boldsymbol{\beta}$ . The univariate probit model can be reformulated into a latent variable formulation which both improves the interpretation and eases computations. Let  $z_i = \mathbf{x}_i^T \boldsymbol{\beta} + \varepsilon_i$ , and define  $y_i = 1$  if  $z_i \geq 0$ , and  $y_i = 0$  if  $z_i < 0$ . When  $\{\varepsilon_i\}$  is standard multivariate Gaussian over all the  $n$  subjects, we obtain (6.1) after marginalising out  $\varepsilon_i$ . In the multivariate extension, we have  $m$  measurements of the  $i$ th subject,  $\{y_{ij} : j = 1, \dots, m\}$ . The latent vector for the  $i$ th subject is  $\mathbf{z}_i = \mathbf{X}_i^T \boldsymbol{\beta} + \boldsymbol{\varepsilon}_i$  where  $\boldsymbol{\varepsilon}_i \sim \mathcal{N}_m(\mathbf{0}, \mathbf{R})$ , and define  $y_{ij} = 1$  if  $z_{ij} \geq 0$ , and  $y_{ij} = 0$  if  $z_{ij} < 0$ . The dependence within each subject, is encoded through the matrix  $\mathbf{R}$ , which, in order to ensure identifiability, is restricted to be a correlation matrix.

A Bayesian analysis of a multivariate probit model requires a prior for the correlation matrix  $\mathbf{R}$ . For the saturated model for  $\mathbf{R}$ , [Barnard, McCulloch and Meng \(2000\)](#) demonstrate the joint uniform prior  $\pi(\mathbf{R}) \propto 1$  which gives highly informative marginals centred at zero; see [Talhouk, Doucet and Murphy \(2012\)](#) for applications of this prior within multivariate probit models. The joint Jeffreys' prior for  $\mathbf{R}$  was used by [Liu \(2001\)](#), which places most prior mass close to  $\pm 1$  in high dimension. [Chib and Greenberg \(1998\)](#) suggest using a multivariate Gaussian prior for  $\mathbf{R}$  restricted to the subset where  $\mathbf{R}$  is positive definite. Neither of these previously applied priors for  $\mathbf{R}$  is particularly convincing.

### 6.1 Extending the Univariate PC Prior Construction

The principles underlying the PC prior outlined in Section 3.1 can be extended to the multivariate setting  $\boldsymbol{\xi} \in \mathcal{M}$  with base model  $\boldsymbol{\xi} = \mathbf{0} \in \mathcal{M}$ . This multivariate extension has all the features of the univariate case. As many interesting multivariate parameters spaces are not  $\mathbb{R}^n$ , we will let  $\mathcal{M}$  be a subset of a smooth  $n$ -dimensional manifold. For example, when modelling covariance matrices  $\mathcal{M}$  will be the manifold of symmetric positive definite matrices, while the set of correlation matrices is a convex subset of that space. A nice introduction to models on manifolds can be found in [Byrne and Girolami \(2013\)](#), where the problem of constructing useful MCMC schemes is also considered.

Assume that  $d(\boldsymbol{\xi})$  has a nonvanishing Jacobian. For each  $r \geq 0$ , the level sets  $\boldsymbol{\theta} \in S_r = \{\boldsymbol{\xi} \in \mathcal{M} : d(\boldsymbol{\xi}) = r\}$  are a system of disjoint embedded submanifolds of  $\mathcal{M}$ , which we will assume to be compact ([Lee, 2003](#), Chapter 8). In the parlance of differential geometry, the submanifolds  $S_r$  are the leaves of a foliation and the decomposition  $\mathcal{M} = \mathbb{R}_+ \times (\bigsqcup_{r \geq 0} S_r)$  gives rise to a natural coordinate system on  $\mathcal{M}$ . Hence, the natural lifting of the PC prior concept onto  $\mathcal{M}$  is the prior that is exponentially distributed in  $d(\boldsymbol{\xi})$  and uniformly distributed on the leaves  $S_{d(\boldsymbol{\xi})}$ .

In some sense, this above definition is enough to be useful. A simple MCMC or optimisation scheme would proceed in a ‘‘coordinate ascent’’ manner, moving first in the distance direction and then along the leaf  $S_r$ . More efficient schemes, however, may be derived from a more explicit density. To this end, we can locally find a mapping  $\varphi(\cdot)$  such that  $(d(\boldsymbol{\xi}), \varphi(\boldsymbol{\xi})) = \mathbf{g}(\boldsymbol{\xi})$ . With this mapping, we get a local representation for the multivariate PC prior as

$$(6.2) \quad \pi(\boldsymbol{\xi}) = \frac{\lambda}{|S_{d(\boldsymbol{\xi})}|} \exp(-\lambda d(\boldsymbol{\xi})) |\det(\mathbf{J}(\boldsymbol{\xi}))|,$$

where  $J_{ij} = \frac{\partial g_i}{\partial \xi_j}$  is the Jacobian of  $\mathbf{g}$ . While the definition of multivariate PC priors is significantly more involved than in the univariate case, it is still useful. In general, computational geometry can be used to evaluate (6.2) approximately in low dimension. In the case where the level sets are simplexes or spheres, exact expressions for the PC prior can be found. These situations occur when  $d(\boldsymbol{\xi})$  can be expressed as

$$(6.3) \quad d(\boldsymbol{\xi}) = h(\mathbf{b}^T \boldsymbol{\xi}), \quad \mathbf{b} > \mathbf{0}, \boldsymbol{\xi} \in \mathbb{R}_+^n$$

or

$$(6.4) \quad d(\boldsymbol{\xi}) = h\left(\frac{1}{2} \boldsymbol{\xi}^T \mathbf{H} \boldsymbol{\xi}\right), \quad \mathbf{H} > \mathbf{0}, \boldsymbol{\xi} \in \mathbb{R}^n,$$

for some function  $h(\cdot)$  satisfying  $h(0) = 0$ , typically  $h(a) = \sqrt{2a}$ . The linear case will prove useful for deriving the PC prior for general correlation matrices in Section 6.2. The quadratic case will be fundamental to derive approximate multivariate PC priors for hierarchical models; see Section 7.

It is trivial to simulate from the PC prior when (6.3) or (6.4) holds. First, we sample  $d$  from the exponential distribution with rate  $\lambda$ . In the linear case (6.3), sample  $\mathbf{s}$  uniformly on an  $(n-1)$ -simplex [by sampling  $z_1, \dots, z_n$  independent from  $\text{Exp}(1)$  and set  $\mathbf{s} = \mathbf{z}/\mathbf{1}^T \mathbf{z}$ ] and compute  $\boldsymbol{\xi} = h^{-1}(d)\mathbf{s}/\mathbf{b}$ . In the quadratic case (6.4), sample  $\mathbf{s}$  uniformly on a unit sphere (by sampling independent standard Gaussians  $z_1, \dots, z_n$  and then set  $\mathbf{s} = \mathbf{z}/\sqrt{\mathbf{z}^T \mathbf{z}}$ ) and compute  $\boldsymbol{\xi} = \sqrt{2h^{-1}(d)}\mathbf{H}^{-1/2}\mathbf{s}$ . Using these direct simulation algorithms, it is a simple change of variables exercise to derive the densities for the PC priors. In the linear case with  $\mathbf{b} = \mathbf{1}$ , the PC prior is

$$\begin{aligned} \pi(\boldsymbol{\xi}) &= \lambda \exp(-\lambda d(\boldsymbol{\xi})) \times \frac{(n-1)!}{r(\boldsymbol{\xi})^{n-1}} \times |h'(r(\boldsymbol{\xi}))|, \\ (6.5) \quad r(\boldsymbol{\xi}) &= h^{-1}(d(\boldsymbol{\xi})), \end{aligned}$$

in the quadratic case with  $\mathbf{H} = \mathbf{I}$ , the PC prior is

$$\begin{aligned} \pi(\boldsymbol{\xi}) &= \lambda \exp(-\lambda d(\boldsymbol{\xi})) \frac{\Gamma(\frac{n}{2} + 1)}{n\pi^{\frac{n}{2}} r(\boldsymbol{\xi})^{n-2}} \left| h'\left(\frac{1}{2}r(\boldsymbol{\xi})^2\right) \right|, \\ (6.6) \quad r(\boldsymbol{\xi}) &= \sqrt{2h^{-1}(d(\boldsymbol{\xi}))}. \end{aligned}$$

The results for the general case,  $\mathbf{b} > \mathbf{0}$  and  $\mathbf{H} > \mathbf{0}$ , follows directly after a linear transformation of  $\boldsymbol{\xi}$ .

## 6.2 A Prior for General Correlation Matrices

Consider the model component  $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{R})$  where  $\mathbf{R}$  is a  $q \times q$  correlation matrix. The distance function to the base model, which corresponds to using the identity matrix as correlation matrix, is given by  $d(\mathbf{R}) = \sqrt{-\log(\det(\mathbf{R}))}$ . This distance function can be greatly simplified by considering a different parameterisation of the set of correlation matrices. Rapisarda, Brigo and Mercurio (2007) show that every correlation matrix can be written as  $\mathbf{R} = \mathbf{B}\mathbf{B}^T$ , where  $\mathbf{B}$  is a lower triangular matrix with first row given by a 1 on the diagonal (first position) and zeros in every other position

and, for rows  $i \geq 2$ , entries are given by

$$B_{ij} = \begin{cases} \cos(\theta_{ij}), & j = 1; \\ \cos(\theta_{ij}) \prod_{k=1}^{j-1} \sin(\theta_{ik}), & 2 \leq j \leq i-1; \\ \prod_{k=1}^{i-1} \sin(\theta_{ik}), & j = i; \\ 0, & i+1 \leq j \leq q, \end{cases}$$

where  $\theta_{ij} \in [0, \pi]$ . The advantage of this parameterisation is that the distance function is now given by

$$d(\mathbf{R}) = \sqrt{2 \sum_{i=2}^q \sum_{j=1}^{i-1} \gamma_{ij}},$$

where  $\gamma_{ij} = -\log(\sin(\theta_{ij})) \in [0, \infty)$  are the  $p = q(q-1)/2$  parameters. Using the  $\boldsymbol{\gamma}$ -parameterisation, we are in the linear case (6.3) and the PC prior is given by (6.5) with  $\boldsymbol{\xi} = \boldsymbol{\gamma}$ ,  $h(a) = \sqrt{2a}$  and  $n = p$ . The PC prior for  $\boldsymbol{\theta}$  follows directly after a change of variables exercise, and is simplified by noting that the two branches of the mapping  $\theta_{ij} = \theta_{ij}(\gamma_{ij})$  have the same Jacobian.

The scaling parameter  $\lambda$  controls the degree of compression of the parallelotope with vertices given by the column vectors of  $\mathbf{R}$ . For large values of  $\lambda$ , most of the mass will be concentrated near parallelotopes with unit volume, while for small  $\lambda$ , the volume could be significantly less than one. This parameter may be difficult to visualise in practice, and we suggest calibrating the prior by drawing samples from the model component and selecting a value of  $\lambda$  for which this component behaves appropriately. Figure 5(a) shows the PC prior marginal for one of these correlations for an exchangeable PC prior on a  $3 \times 3$  correlation matrix, using  $\lambda = 10, 5$  and  $2$ . Decreasing  $\lambda$  makes the marginal less tightened up around zero.

There is a complication when interpreting the PC prior for  $\boldsymbol{\theta}$ , namely that it is not exchangeable due to the dependence of the Cholesky decomposition on the ordering of the random effects. This can be rectified by summing over all orderings, however, we have observed that this makes little difference in practice. While we do not necessarily recommend summing over the permutations in practice, for the figures in this section, we have computed the exchangeable PC prior.

## 6.3 The Six Cities Study and Exchangeable Random Effects

We will now illustrate the use of PC priors for  $\mathbf{R}$  and reanalyse a subset of the data from the Six Cities



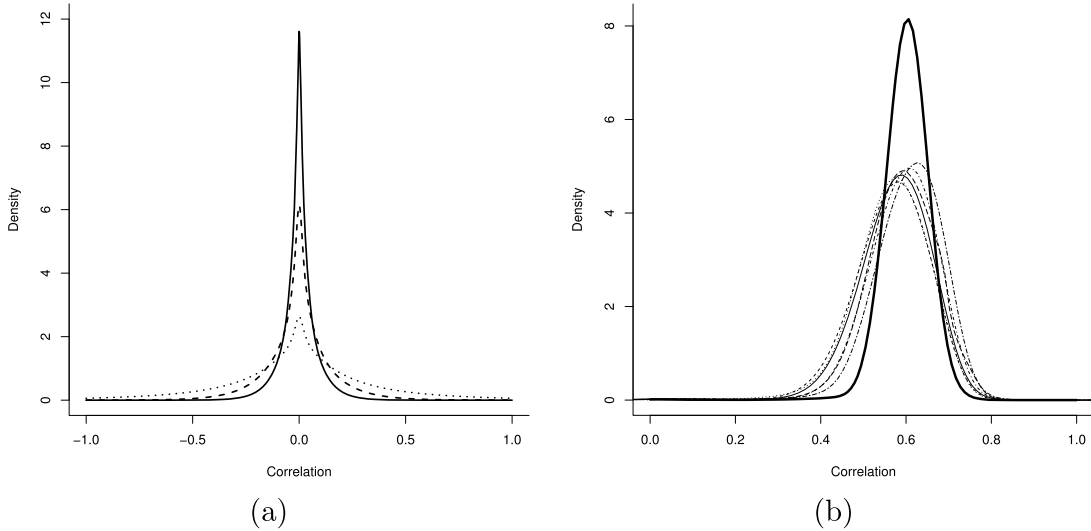


FIG. 5. Panel (a) shows the symmetric marginal prior density for the correlation computed from the PC prior for a  $3 \times 3$  correlation matrix with  $\lambda = 10$  (solid), 5 (dashed) and 2 (dotted). Panel (b) shows the posterior marginals for the correlations in the general model for the Six Cities study with  $\lambda = 0.1$ . The solid thick line is for the exchangeable model. The marginal densities in the general model are approximately identical.

study discussed by Chib and Greenberg (1998), Section 5.2, using the data as tabulated in their Table 3. The Six Cities study investigates the health effects of air pollution; refer to Chib and Greenberg (1998) for background. The response is the wheezing status from  $n = 537$  children in Ohio at ages 7, 8, 9 and 10 years, and the aim is to study the effect of the smoking habit of the mother to the response. The model is

$$\begin{aligned} \text{Prob}(y_{ij} = 1 | \boldsymbol{\beta}, \mathbf{R}) \\ = \Phi(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3}), \\ j = 1, \dots, m = 4, \end{aligned}$$

where covariates are  $\mathbf{x}_1$  representing age (centred at 9),  $\mathbf{x}_2$  for smoking (1 = yes, 0 = no), and their interaction  $\mathbf{x}_3$ , respectively. Chib and Greenberg (1998) used two models for  $\mathbf{R}$ , the saturated or general case with  $m(m-1)/2$  parameters, and the exchangeable case where all off-diagonal terms in  $\mathbf{R}$  are the same. Our analysis is made more comparable to Chib and Greenberg (1998) by adapting their  $\mathcal{N}_4(\mathbf{0}, 10^{-1}\mathbf{I})$  prior for  $\boldsymbol{\beta}$ .

We chose the decay-rate  $\lambda$  by sampling from the PC prior for various values of  $\lambda$ . We then estimated  $\text{Prob}(|\rho_{ij}| > 1/2)$  and found the values of  $\lambda$  where this probability was approximately 0.8 and 0.2. These two choices gave  $\lambda = 0.1$  and 1.0. We then ran two long MCMC chains to obtain posterior samples after disregarding the burn-in phase. The estimated posterior marginals for  $\beta_2$  (effect of smoking) are shown in Figure 6(a) (solid and dashed lines). The choice of  $\lambda$  seems

to have only a minor effect on the posterior marginal for the effect of smoking  $\beta_2$ .

Since all the estimated correlations in  $\mathbf{R}$  are somewhat similar in the general model for  $\mathbf{R}$  [Figure 5(b)], it is natural to investigate a simplified model with an exchangeable correlation matrix where all correlations are the same,  $\rho$ . For positive definiteness, we require  $-1/(m-1) < \rho < 1$ . The fact that positive and negative correlations are apparently very different, makes the selection of the prior for  $\rho$  challenging. Due to the invariance property of the PC priors, this asymmetry is automatically accounted for and the potential problem goes away. We can easily compute the PC prior for  $\rho$  for any fixed base value  $\rho_0$ . For  $\rho_0 = 0$ , which is the same base model as the correlation matrix PC prior, the distance function to the base model is

$$d(\rho) = \sqrt{-\log((1 + (m-1)\rho)(1 - \rho)^{m-1})}$$

and the prior follows directly after noting that in this case we must also allow for  $\xi < 0$ . The PC prior is shown in Figure 6(b) for  $\lambda = 0.1$  (solid) and 1.0 (dashed). The PC prior automatically adjusts the prior density for  $\rho < 0$  and  $\rho > 0$  due to the constraint  $\rho > -1/(m-1)$ .

A second potential issue is the following: as we are changing the model for  $\mathbf{R}$ , we should, in order to get comparable results, use a comparable prior. By reusing the values  $\lambda = 0.1$  and 1.0 from the general case, we define the prior for  $\rho$  to penalise the distance from the

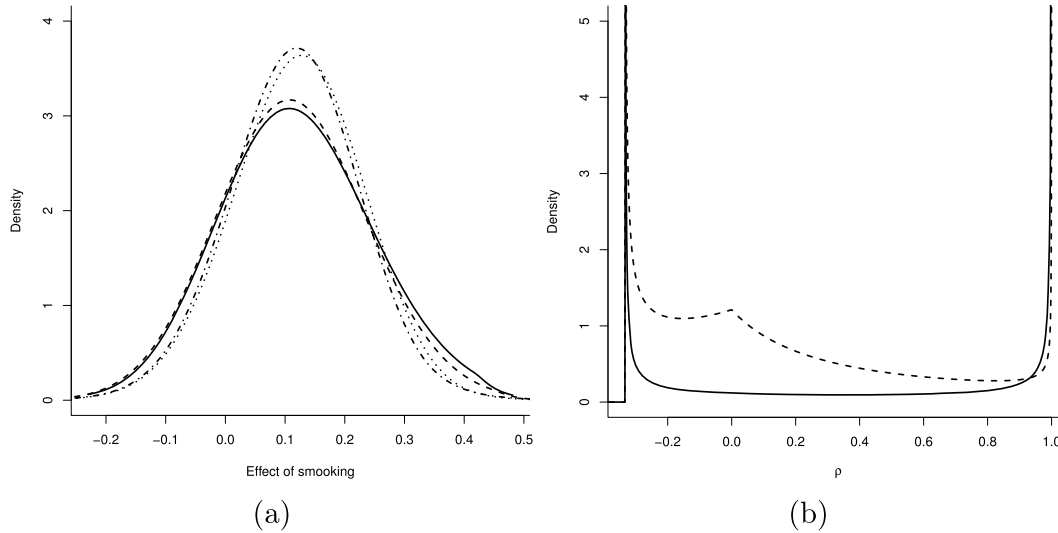


FIG. 6. Panel (a) shows the estimated posterior marginal for  $\beta_2$  (the effect of smoking) for both the general model for  $\mathbf{R}$  [ $\lambda = 0.1$  (solid) and  $\lambda = 1.0$  (dashed)] and the exchangeable model [ $\lambda = 0.1$  (dotted) and  $\lambda = 1.0$  (dashed-dotted)]. Panel (b) shows the PC prior for the exchangeable case with base-model  $\rho = 0$ , for  $\lambda = 0.1$  (solid) and 1.0 (dashed).

base model the same way in both parameterisations of  $\mathbf{R}$ . In this sense, the prior is the same for both models. We can then conclude that the reduced variability of about 10% for  $\beta_2$  as shown in Figure 6(a) for  $\lambda = 0.1$  (dotted) and  $\lambda = 1.0$  (dashed-dotted), is due to the more restrictive exchangeable model for  $\mathbf{R}$  and not an unwanted effect from the prior distributions for  $\mathbf{R}$ .

The results obtained with the PC priors are in this example in overall agreement with those reported in Chib and Greenberg (1998).

## 7. DISTRIBUTING THE VARIANCE: HIERARCHICAL MODELS, AND ALTERNATIVE DISTANCES

For complex models, it is unlikely that practitioners will be able to provide information about the relative effect of each component in an hierarchical model. Hence, we can no longer build informative independent priors on each component but need to consider the global model structure. Looking back to the example in Section 5, we were not able to control jointly the variance contribution from the spline and the combined spatial/random effect term. It could be argued that in these simple situations, this is less of a problem as priors could easily be tuned to account for this effect and this strategy is well within current statistical practice. In this section, we argue and demonstrate that it is possible to control overall variance automatically using the PC prior framework. This requires, in concordance with Desideratum D2, that the priors on the individual scaling parameters for each component change

as the global model changes. We will demonstrate this by considering a logistic regression model with several linear and nonlinear effects, and show how we can take the global structure into account to control the overall variance of the linear predictor, and controlling how each term contributes to it. To achieve this, we will use a multivariate PC prior on the fractions of how much each component contributes to the variance of the linear predictor.

The broader message of this section is that the PC prior framework can be used to build priors that respect the global graphical structure of the underlying model. Additionally, it is possible to build these priors automatically for new models and data-sets (which can be integrated into software like R-INLA or Stan). The priors depend on the graphical structure and the model design (or covariate values), but do not, of course, depend on the observations. Following this path into the future, we happily give up global invariance of reparameterisation, as we are adding another source of information to our prior construction. Additional to knowledge of the base model and the strength of the penalisation, we also require expert information about the structure of the model. As with the previous two information sources, this is not particularly onerous to elicit.

Our practical approach to handle multivariate PC priors in this setting is to use a Taylor expansion around the base model, and approximate it using a first- or second-order expansion. When the base model is an

interior point in the parameter space, then the second-order approximation equation (6.4) gives the PC prior in equation (6.6), while the linear approximation equation (6.3) is appropriate if the base model is at the border of the parameter space leading to the PC prior in equation (6.5). For the quadratic approximation, it is well known that

$$(7.1) \quad \text{KLD} = \frac{1}{2}(\xi - \xi_0)^T I(\xi_0)(\xi - \xi_0) + \text{higher order terms},$$

where  $\xi_0$  is the base model and  $I(\xi_0)$  is the Fisher information at the base model. This approximation has resemblance to the generalisation by Kass and Wasserman (1995), Section 3 of early ideas by Jeffreys (1961) for the purpose of hypothesis testing in the multivariate case. Equation (7.1) is not unsound as measure of complexity by itself, and adopting this as our second principle for practical/computational reasons, then equation (6.6) will be the corresponding PC prior, but will not longer be invariant for reparameterisation. Hence, care needs to be taken in order to choose a parameterisation for the second-order expansion to be sensible. This parameterisation is typically motivated by a variance-stabilising transformation.

To fix ideas, we will discuss a dataset from Hastie and Tibshirani (1987) about a retrospective sample of males in a heart-disease high-risk region of the Western Cape, South Africa. These data are available as heart in the R-package catdata, and we will use the model suggested by Wood and Kohn (1998), Section 6.4, changing the link to logit. A total of 462 subjects are classified of have had ( $y_i = 1$ ) a heart attack or not ( $y_i = 0$ ), and the measured risk factors are age at onset (Age), systolic blood pressure (BP) and low density lipoprotein cholesterol (CR). We use standardised covariates in this analysis. The linear predictor is

$$\eta = \mu \mathbf{1} + \tau^{-1/2} \times g(\text{Age}, \text{BP}, \text{CR}),$$

where  $g(\cdot)$  is some smooth function of the covariates. At this top-level, we can use the structural information provided by the model to elicit the amount of variability we expect from covariates. This information can be incorporated in the prior for the precision parameter  $\tau$ . We assume here that the effect of covariates  $g(\cdot)$  have zero mean and “unit variance.” We use the phrase “unit variance” for  $\beta_x \mathbf{x}$  to describe a standardised covariate  $\mathbf{x}$  and a covariate weight  $\beta_x$  with unit variance. The predicted probabilities from the regression model might mostly be in the range [0.05, 0.95] leading to an interval [−2.94, 2.94] on the linear predictor scale. We

take the marginal standard deviation of the effect of the covariates to be 2.94/1.96, which gives parameters  $U = 4.84$  and  $\alpha = 1\%$  in the PC prior for the precision in a Gaussian random effect (3.3). This prior will shrink the effect of the covariates towards the intercept, which is the first base model.

At the next level in the model, we use an additive model for the covariates and distribute the unit variance among the covariates,

$$g(\text{Age}, \text{BP}, \text{CR}) = \sqrt{w_1}g_1(\text{Age}) + \sqrt{w_2}g_2(\text{BP}) + \sqrt{w_3}g_3(\text{CR}),$$

where the weights live on a 2-simplex, that is,  $w_1 + w_2 + w_3 = 1$  and  $w_i \geq 0$ , and  $\{g_i(\cdot)\}$  are smooth functions (with unit variance). The variance contribution from covariate Age, say, is then  $w_1$ . Without additional knowledge, it is reasonable to treat them equally, meaning that the base model for the weights is  $w_1 = w_2 = w_3 = 1/3$ . This reflects an a priori assumption of (conditional) exchangeability between these model components.

Further, one level down, we continue to distribute the variance, but now for each  $g_i(\cdot)$  function and between a linear and (purely) nonlinear effect. For covariate Age, this becomes

$$g_1(\text{Age}) = \sqrt{1 - \phi_1}\beta_1\text{Age} + \sqrt{\phi_1}f_1(\text{Age}), \quad \phi_1 \geq 0.$$

Here, both  $\beta_1$  and  $f_1(\cdot)$  have unit variance, and  $f_1(\cdot)$  is a smooth (purely) nonlinear function. The natural base model is  $\phi_1 = 0$  meaning that the variance in  $g_1(\text{Age})$  is only explained by the linear effect, as we do not want to involve deviations from the linear effect without support from data.

Figure 7(a) displays the graphical structure of the recursive decomposition of the variance of  $g(\text{Age}, \text{BP}, \text{CR})$ . By following the path from the top node to the relevant node, we can determine the fraction of the variance explained by that node. For example, the relative contribution to the variance from the linear effect of covariate Age, is  $w_1(1 - \phi_1)$ , and the relative contribution to the variance from  $g_3(\text{CR})$  is  $w_3$ .

In order to proceed with the analysis and computation of the PC prior, we need to make some specific choices for the linear effects  $\{\beta_i\}$  and the (purely) nonlinear effects  $\{f_i(\cdot)\}$ . For  $\beta_i$ , we use independent zero mean Gaussians with unit variance, and for the nonlinear effect, we use the second-order random walk (5.2) which corresponds to the integrated Wiener process used by Wood and Kohn (1998); see Lindgren and Rue (2008). Figure 7(b) displays the histogram of samples

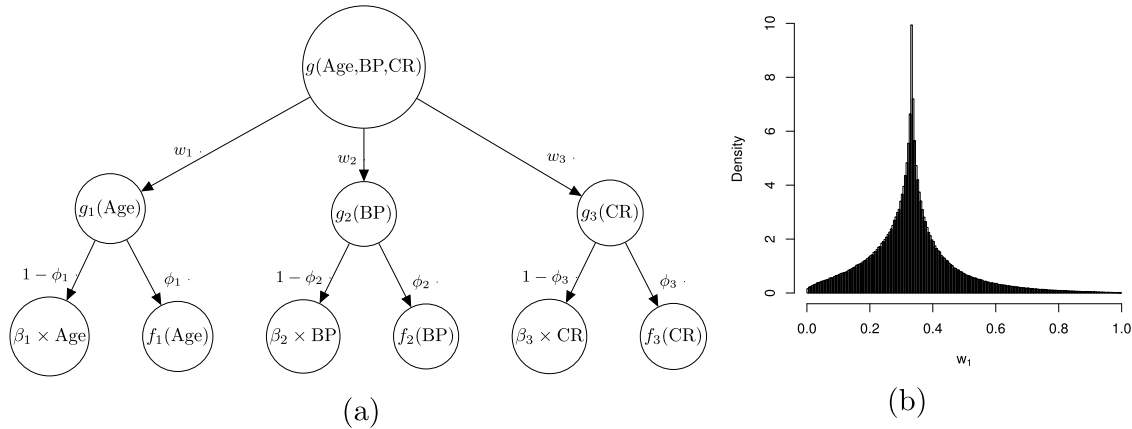


FIG. 7. Panel (a) displays the recursive structure of how the additive effect of the covariates are built up, to control the variance contributed from each of the model terms to the linear predictor. Panel (b) shows the histogram of  $w_1$  from a typical joint PC prior for  $\mathbf{w}$  using  $\lambda = 0.3$ .

for the first weight component  $w_1$  sampled from a typical PC prior for the weights  $\mathbf{w}$  using  $\lambda = 0.3$ . The histogram is centred at the base model  $w_1 = 1/3$ , but still supports weights close to 0 meaning that the covariate Age does not contribute to the linear predictor, and close to 1 meaning that *only* Age contributes to the linear predictor.

The PC prior in this example is computed as follows. The priors for  $\phi$  follows the computations described in Appendix A.2. The joint prior for  $\mathbf{w}$ , depends on the values for  $\phi$  (but not too much in this example) and, therefore, has to be recomputed when there is any change in  $\phi$ . We use here (6.6) as an approximation to the multivariate PC prior which only requires a numerical estimate of the Hessian matrix at the base model. More details are available in Appendix A.3. The results were obtained using R-INLA. The covariate estimates (given in the Supplementary Material) are comparable to those in Wood and Kohn (1998) obtained using MCMC based on independent diffuse and flat priors.

## 8. DISCUSSION

Priors are the Bayesian's greatest tool, but they are also the greatest point for criticism: the arbitrariness of prior selection procedures and the lack of realistic sensitivity analysis (which is addressed in Roos and Held, 2011 and Roos et al., 2014) are serious arguments that current Bayesian practice need to be significantly improved. In this paper, we have provided a principled, widely applicable method for specifying priors on parameters that are difficult to directly elicit from expert knowledge. These PC priors can be vague, weakly informative, or strongly informative depending

on the way the user tunes an intuitive scaling parameter. The key feature of these priors is that they explicitly lay out the assumptions underlying them and, as such, these assumptions and principles can be directly critiqued and accordingly modified.

PC priors are defined on individual components. This distinguishes PC priors, from reference priors, in which the priors depend on the global model structure. This global dependence is required to ensure a proper posterior. However, the modern applied Bayesian is far more likely to approach their modelling using a component-wise and often additive approach. The directed acyclic graph—approach pioneered by the WinBUGS inference engine, is now a standard tool for specification of general Bayesian models. The additive approach pioneered by Hastie and Tibshirani (1990) is now a standard approach within generalised regression based models. Hence, the ability to specify priors in a component-wise manner is a useful feature. It is worth noting that none of the examples in this paper have known reference priors. We believe that PC priors are a valuable addition to the literature on prior choice. They are not designed as, and should not be interpreted as, a replacement for reference priors, but rather a method to solve a different set of problems.

This is not the whole story of PC priors. We still have to work them out on a case by case basis, construct better guidance for choosing the scaling using knowledge of the global model (like the link-function and the likelihood family), and make them the default choice in packages like R-INLA. We aware that this is an ambitious goal. First, R-INLA is a rather general purpose software which allows the user to specify arbitrary models given that they fit into the modelling language. The example of how the definition of



the PC prior changes under a sparsity assumption illustrates this challenge. Second, not all cases are straight forward to work out. The over-dispersion parameter in the negative binomial distribution, considered as an extension of the Poisson distribution, cannot be separated from the mean in the commonly known parameterisation. Hence, we cannot compute the PC prior without knowing a typical value for the mean. Re-thinking the negative binomial model and using a different parameterisation, such as one using the parameters mean and variance-to-mean-ratio, may however help here. We also need to get more experience deriving joint priors for two or more parameters, such as a joint prior for the skewness and kurtosis deviation from a Gaussian (Jones and Pewsey, 2009). We also have not considered PC priors on discrete parameters. To do this, we need to find a sensible, computationally tractable notion of distance for these problems. In this paper, we have focused on generic specification, however Fuglstad et al. (2015) show that, in the case of hyperparameters for Gaussian random fields, if the distance knows about the structure of the model component, the resulting priors perform very well. Hence, there is more work to be done on tailoring distance measures to specific problem classes.

Several of the examples in this paper have used the notion that model components can be regarded as a flexible extension of a base model. This idea has natural links to Bayesian nonparametrics. In particular, we consider many of the examples, such as the logistic GAM model in Section 7, as a nonparametric model that has been firmly rooted in a simpler parametric model. We believe that this decomposition of the model into favoured parametric and extra nonparametric components improves the interpretability of these models in many applications. This is related to the ideas of Kennedy and O’Hagan (2001), where the nonparametric component can be used to “calibrate” the covariate effect. An alternative interpretation of this decomposition is that the nonparametric part adds “robustness” to the linear model and the flexibility parameter gives an indication of how far from the simple, interpretable, base model the data requires you to depart.

There is a great deal of scope for further theoretical work on this problem. First, it would be useful to understand better the effect of the prior tail on the inference. The results in this paper suggest that an exponential tail is sufficiently heavy in low-dimensional problems, and the heavy tailed half-Cauchy distribution only gives different results in the high dimensional sparse setting. However, it is not clear that this is truly

a problem with the tail, as an examination of the base model suggests that it is not shrinking towards sparse models. Hence, the question is “are heavy tails necessary in high dimensions, or are they just more forgiving of our poor prior specification?” Staying in the realm of sparse models, it would be interesting to see if the models in Section 7 could be extended to high dimensional sparse models. It may be possible to take inspiration in this case from the Dirichlet–Laplace construction of Bhattacharya et al. (2012). More generally, there are open questions relating to the large sample properties of hierarchical models with PC priors, hypothesis testing for flexible models, Stein-type risk properties for PC priors and robustness against mis-specification.

The current practice of prior specification is not in a good shape. While there has been a strong growth of Bayesian analysis in science, the research field of “practical prior specification” has been left behind. There are few widely applicable guidelines for how this could or should be done in practice. We hope that with this new principled approach to prior construction, we can reduce the number of “cut and paste” prior choices from other similar research articles, and instead use the derived tools in this paper to specify weakly informative or informative priors with a well defined shrinkage. As always, if the user knows of a better prior for their case, then they should use it. However, having a better default proposal for how to construct priors is a significant advantage. The PC prior framework was constructed because of our work with scientists on applied problems and came out of a desire to derive and explain the prior information that we were putting into hierarchical models. As such, we believe that these priors are “fit for purpose” as tool for real-world applied statistics.

These new PC prior have made a difference to how we do and see Bayesian analysis. We feel much more confident that the priors we are using do not force over-fitting, and the notion of *scale*, which determines the magnitude of the effects, really simplifies the interpretation of the results. The fact that the prior specification reduces to a notion of *scale*, makes them very easy to interpret and communicate. We feel that PC priors lay out a new route forward towards more sound Bayesian analysis. Jimmie Savage (Lindley, 1983) suggested that we “build our models as big as elephants,” while J. Bertrand (Le Cam, 1990) told us to “give [him] four parameters and [he] shall describe an elephant; with five, it will wave its trunk.” The modern practice of Bayesian statistics can be seen as a battle between these two elephants, and with PC priors we hope to make it a fair fight.

## APPENDIX: DERIVATION OF PC PRIORS

### A.1 The PC Prior for the Precision in a Multivariate Normal Distribution

Let  $\mathcal{N}^{(p)}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  denote a multivariate normal distribution with dimension  $p$ . The Kullback–Leibler divergence from  $\mathcal{N}_1^{(p)}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$  to  $\mathcal{N}_0^{(p)}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$  is

$$\begin{aligned} \text{KLD}(\mathcal{N}_1^{(p)} \parallel \mathcal{N}_0^{(p)}) \\ \text{(A.1)} = \frac{1}{2} \left\{ \text{tr}(\boldsymbol{\Sigma}_0^{-1} \boldsymbol{\Sigma}_1) + (\boldsymbol{\mu}_0 - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}_0^{-1} (\boldsymbol{\mu}_0 - \boldsymbol{\mu}_1) \right. \\ \left. - p - \ln \left( \frac{|\boldsymbol{\Sigma}_1|}{|\boldsymbol{\Sigma}_0|} \right) \right\}. \end{aligned}$$

In our setting,  $\mathcal{N}_1^{(p)}$  denotes the flexible model and  $\mathcal{N}_0^{(p)}$  the base model.

To derive the PC prior for  $\tau$  where  $\boldsymbol{\Sigma}_1 = \mathbf{R}/\tau$ ,  $\mathbf{R}$  is a fixed matrix and  $\boldsymbol{\Sigma}_0 = \mathbf{0}$ , we will study the limiting behaviour when  $\boldsymbol{\Sigma}_0 = \mathbf{R}/\tau_0$  for a high fixed value of  $\tau_0$ . In the end, we will look at the limit  $\tau_0 \rightarrow \infty$ . For simplicity, assume  $\mathbf{R}$  has full rank. We then get  $\text{KLD} = \frac{p}{2} \frac{\tau_0}{\tau} (1 + \frac{\tau}{\tau_0} \ln(\frac{\tau}{\tau_0}) - \frac{\tau}{\tau_0}) \rightarrow \frac{p}{2} \frac{\tau_0}{\tau}$ , when  $\tau \ll \tau_0$ , and hence  $d(\tau) = \sqrt{p\tau_0/\tau}$ . We assign an exponential prior with rate  $\tilde{\lambda}$  to  $d$  and derive the prior for  $\tau$  using the ordinary change of variable transformation where we set  $\lambda = \tilde{\lambda} \sqrt{p\tau_0}$ . This leads to the type-2 Gumbel distribution with parameter  $\lambda$  see equation (3.3).

### A.2 The PC Prior for the Mixing Parameter in the BYM-Model

We will now derive the PC prior for the mixing parameter  $\phi$  in the new parameterisation for the BYM model. Let  $\mathbf{u}$  be a  $n$ -dimensional standardised Gaussian model with zero mean and precision matrix  $\mathbf{R} > 0$ ,  $\mathbf{v}$  be an independent zero mean random effects with unit variance  $\mathcal{N}(\mathbf{0}, \mathbf{I})$ , and where the mixing parameter  $\phi$  satisfies  $0 \leq \phi \leq 1$ . The more flexible model is  $\sqrt{1-\phi}\mathbf{v} + \sqrt{\phi}\mathbf{u}$ , and the base model is  $\mathbf{v}$  (i.e., the model flexible model when  $\phi = 0$ ). Let  $\boldsymbol{\Sigma}_0 = \mathbf{I}$  and  $\boldsymbol{\Sigma}_1(\phi) = (1-\phi)\mathbf{I} + \phi\mathbf{R}^{-1}$ , then

$$\begin{aligned} 2 \text{KLD}(\phi) &= \text{tr}(\boldsymbol{\Sigma}_1(\phi)) - n - \ln |\boldsymbol{\Sigma}_1(\phi)| \\ &= n\phi \left( \frac{1}{n} \text{tr}(\mathbf{R}^{-1}) - 1 \right) \\ &\quad - \ln |(1-\phi)\mathbf{I} + \phi\mathbf{R}^{-1}| \end{aligned}$$

and  $d(\phi) = \sqrt{2 \text{KLD}(\phi)}$ . The interesting case is when  $\mathbf{R}$  is sparse, for which  $\text{tr}(\mathbf{R}^{-1})$  is quick to compute (Erisman and Tinney, 1975, Rue and Martino, 2007). For the determinant term, we can massage

the expression to facilitate the speedup of computing with sparse matrices. Using the matrix identity  $(\mathbf{I} + \mathbf{A}^{-1})^{-1} = \mathbf{A}(\mathbf{A} + \mathbf{I})^{-1}$ , we get  $|(1-\phi)\mathbf{I} + \phi\mathbf{R}^{-1}| = |\phi^{-1}\mathbf{R}|^{-1} |\frac{1-\phi}{\phi}\mathbf{R} + \mathbf{I}|$ . An alternative approach, is to compute the eigenvalues  $\{\gamma_i\}$  of  $\mathbf{R}$ , which we need to do only once. Let  $\tilde{\gamma}_i = 1/\gamma_i$ , and we get  $|(1-\phi)\mathbf{I} + \phi\mathbf{R}^{-1}| = \prod_{i=1}^n (1 - \phi + \phi\tilde{\gamma}_i)$ .

In the case where  $\mathbf{R}$  is singular, we introduce linear constraint(s) to ensure that any realisation of  $\mathbf{u}$  is in its null-space. It is now easier to use the latter computational strategy, but redefine  $\tilde{\gamma}_i$  as  $1/\gamma_i$  if  $\gamma_i > 0$  and  $\tilde{\gamma}_i = 0$  if  $\gamma_i = 0$ .

The PC prior for the mixing parameter in the hierarchical models in Section 7 generalise the BYM-model as the base model is more general. Let  $\boldsymbol{\Sigma}_1(\phi) = (1-\phi)\mathbf{S}_1 + \phi\mathbf{S}_2$ , and where the base model is  $\boldsymbol{\Sigma}_0 = \boldsymbol{\Sigma}_1(1/2)$ . The costly task is to compute  $\det(\boldsymbol{\Sigma}_1(\phi))$  for a sequence of  $\phi$ 's. Using the Matrix determinant lemma:  $\det(\mathbf{A} + \mathbf{U}\mathbf{V}^T) = \det(\mathbf{I} + \mathbf{V}^T\mathbf{A}^{-1}\mathbf{U}) \det(\mathbf{A})$  for compatible matrices  $\mathbf{A}$  (invertible),  $\mathbf{V}$  and  $\mathbf{U}$ , we can reduce the computational cost to essential one evaluation of  $\det(\boldsymbol{\Sigma}_1(\phi))$ .

### A.3 The PC Prior for the Variance Weights in Additive Models

The joint PC prior of the weights  $\mathbf{w}$  in Section 7 is computed as follows. Let  $\boldsymbol{\eta}^*$  be the standardised linear predictor and  $\mathbf{x}_i$  the  $i$ th vector of standardised covariates, then the model considered in Section 7 can be written as  $\boldsymbol{\eta}^* = \sum_i \sqrt{w_i}(\sqrt{1-\phi_i}\beta_i\mathbf{x}_i + \sqrt{\phi_i}\mathbf{A}_i\mathbf{f}_i)$ , where  $\mathbf{A}_i$  is a sparse matrix extracting the required elements (or linear combinations thereof) of the Gaussian vector  $\mathbf{f}_i$  representing the scaled second-order random walk model. The covariance for the linear predictor is then  $\text{Cov}(\boldsymbol{\eta}^*) = \sum_i w_i((1-\phi_i)\mathbf{x}_i\mathbf{x}_i^T + \phi_i\mathbf{A}_i\text{Cov}(\mathbf{f}_i)\mathbf{A}_i^T)$ . In order to improve the second-order approximation equation (6.6), we reparameterise the weights following the ideas in compositional data analysis (Aitchison, 2003), using new parameters  $\tilde{w}_i = \log(w_i/w_n)$ , for  $i = 1, \dots, n-1$  for  $n$  components. This makes  $\text{Cov}(\boldsymbol{\eta}^*)$  a function of  $\tilde{\mathbf{w}}$  with base model at  $\tilde{\mathbf{w}} = \mathbf{0}$ . The KLD can then be computed from equation (A.1), and the PC prior follows from a numerical approximation to the Hessian matrix of the KLD and equation (6.6).

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## SUPPLEMENTARY MATERIAL

**Supplement to “Penalising Model Component Complexity: A Principled, Practical Approach to Constructing Priors”** (DOI: [10.1214/16-STS576SUPP](https://doi.org/10.1214/16-STS576SUPP); .pdf). The supplementary material contains the proofs of all theorems contained in the paper. It also contains a detailed description of the Student  $t$ -simulation study used in Section 3.4. The R-code for analysing all examples and generating the corresponding figures in this report, is available at [www.r-inla.org/examples/case-studies/](http://www.r-inla.org/examples/case-studies/).

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