Abstract

In a variety of disciplines such as social sciences, psychology, medicine and economics, the recorded data are considered to be noisy measurements of latent variables connected by some causal structure. This corresponds to a family of graphical models known as the structural equation model with latent variables. While linear non-Gaussian variants have been well-studied, inference in nonparametric structural equation models is still underdeveloped. We introduce a sparse Gaussian process parameterization that defines a non-linear structure connecting latent variables, unlike common formulations of Gaussian process latent variable models. The sparse parameterization is given a full Bayesian treatment without compromising Markov chain Monte Carlo efficiency. We compare the stability of the sampling procedure and the predictive ability of the model against the current practice.

1 CONTRIBUTION

A cornerstone principle of many disciplines is that observations are noisy measurements of hidden variables of interest. This is particularly prominent in fields such as social sciences, psychology, marketing and medicine. For instance, data can come in the form of social and economical indicators, answers to questionnaires in a medical exam or marketing survey, and instrument readings such as fMRI scans. Such indicators are treated as measures of latent factors such as the latent ability levels of a subject in a psychological study, or the abstract level of democratization of a country. The literature on structural equation models (SEMs) (Bartholomew et al., 2008; Bollen, 1989) approaches such problems with directed graphical models, where each node in the graph is a noisy function of its parents. The goals of the analysis include typical applications of latent variable models, such as projecting points in a latent space (with confidence regions) for ranking, clustering and visualization; density estimation; missing data imputation; and causal inference (Pearl, 2000; Spirtes et al., 2000).

This paper introduces a nonparametric formulation of SEMs with hidden nodes, where functions connecting latent variables are given a Gaussian process prior. An efficient but flexible sparse formulation is adopted. To the best of our knowledge, our contribution is the first full Gaussian process treatment of SEMs with latent variables.

We assume that the model graphical structure is given. Structural model selection with latent variables is a complex topic which we will not pursue here; a detailed discussion of model selection is left as future work. Asparouhov and Muthén (2009) and Silva et al. (2006) discuss relevant issues. Our goal is to be able to generate posterior distributions over parameters and latent variables with scalable sampling procedures with good mixing properties, while being competitive against non-sparse Gaussian process models.

In Section 2 we specify the likelihood function for our structural equation models and its implications. In Section 3 we elaborate on priors, Bayesian learning, and a sparse variation of the basic model which is able to handle larger datasets. Section 4 describes a Markov chain Monte Carlo (MCMC) procedure. Section 5 evaluates the usefulness of the model and the stability of the sampler in a set of real-world SEM applications with comparisons to modern alternatives. Finally, in Section 6 we discuss related work.

2 THE MODEL: LIKELIHOOD

Let $G$ be a given directed acyclic graph (DAG). For simplicity, in this paper we assume that no observed variable is a parent in $G$ of any latent variable. Many SEM applications are of this type (Bollen, 1989; Silva et al., 2006), and this will simplify our presentation. Likewise, we will treat models for continuous variables only. Although cyclic SEMs are also well-defined for the linear case (Bollen, 1989; Silva et al., 2006),
non-linear cyclic models are not trivial to define and as such we will exclude them from this paper.

Let $\mathcal{X}$ be our set of latent variables and $X_i \in \mathcal{X}$ be a particular latent variable. Let $X_{P_i}$ be the set of parents of $X_i$ in $G$. The latent structure in our SEM is given by the following generative model: if the parent set of $X_i$ is not empty, $X_i = f_i(X_{P_i}) + \zeta_i$, where $\zeta_i \sim \mathcal{N}(0, \nu_\zeta)$ \hspace{1cm} (1)

$\mathcal{N}(m, v)$ is the Gaussian distribution with mean $m$ and variance $v$. If $X_i$ has no parents (i.e., it is an exogenous latent variable, in SEM terminology), it is given a mixture of Gaussians marginal\(1\).

The measurement model, i.e., the model that describes the distribution of observations $Y$ given latent variables $\mathcal{X}$, is as follows. For each $Y_j \in Y$ with parent set $X_{P_j}$, we have

$Y_j = \lambda_{j0} + X_{P_j}^T \Lambda_j + \epsilon_j$, where $\epsilon_j \sim \mathcal{N}(0, \nu_\epsilon)$ \hspace{1cm} (2)

Error terms $\{\epsilon_j\}$ are assumed to be mutually independent and independent of all latent variables in $\mathcal{X}$. Moreover, $\Lambda_j$ is a vector of linear coefficients $\Lambda_j = [\lambda_{j1} \ldots \lambda_{j|X_{P_j}|}]^T$. Following SEM terminology, we say that $Y_j$ is an indicator of the latent variables in $X_{P_j}$.

An example is shown in Figure 1(a). Following the notation of Bollen (1989), squares represent observed variables and circles, latent variables. SEMs are graphical models with an emphasis on sparse models where: 1. latent variables are dependent according to a directed graph model; 2. observed variables measure (i.e., are children of) very few latent variables. Although sparse latent variable models have been the object of study in machine learning and statistics (e.g., Wood et al. (2006); Zou et al. (2006)), not much has been done on exploring nonparametric models with dependent latent structure (a loosely related exception being dynamic systems, where filtering is the typical application). Figure 1(b) illustrates how modeling can be affected by discarding the structure among latent variables.

2.1 Identifiability Conditions

Latent variable models might be unidentifiable. In the context of Bayesian inference, this is less of a theoretical issue than a computational one: unidentifiable models might lead to poor mixing in MCMC, as discussed in Section 5. Moreover, in many applications, the latent embedding of the data points is of interest itself, or the latent regression functions are relevant for causal inference purposes. In such applications, an unidentifiable model is of limited interest. In this Section, we show how to derive sufficient conditions for identifiability.

Consider the case where a latent variable $X_i$ has at least three unique indicators $Y_i \equiv \{Y_{i\alpha}, Y_{i\beta}, Y_{i\gamma}\}$, in the sense that no element in $Y_i$ has any other parent in $G$ but $X_i$. It is known that in this case (Bollen 1989) the parameters of the structural equations for each element of $Y_i$ are identifiable (i.e., the linear coefficients and the error term variance) up to a scale and sign of the latent variable. This can be resolved by setting the linear structural equation of (say) $Y_{i\alpha}$ to $Y_{i\alpha} = X_i + \epsilon_{i\alpha}$. The distribution of the error terms is then identifiable. The distribution of $X_i$ follows from a

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\(1\)For simplicity of presentation, in this paper we adopt a finite mixture of Gaussians marginal for the exogenous variables. However, introducing a Dirichlet process mixture of Gaussians marginal is conceptually straightforward.

\(2\)Another consequence of modeling latent dependencies is reducing the number of parameters of the model: a SEM with a linear measurement model can be seen as a type of module network (Segal et al. 2005) where the observed children of a particular latent $X_i$ share the same nonlinearities propagated from $X_i$: in the context of Figure 1 each indicator $Y_i \in \{Y_1, \ldots, Y_7\}$ has a conditional expected value of $\lambda_{i0} + \lambda_{i1} f_2(X_2)$ for a given $X_1$; function $f_2(\cdot)$ is shared among the indicators of $X_2$. 

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deconvolution between the observed distribution of an element of \( Y \), and the identified distribution of the error term.

Identifiability of the joint of \( \mathcal{X} \) can be resolved by multivariate deconvolution under extra assumptions. For instance,\(^{\text{[3]}}\) describes the problem in the context of kernel density estimation (with known joint distribution of error terms, but unknown joint of \( Y \)).

Assumptions for the identifiability of functions \( f_i(\cdot) \), given the identifiability of the joint of \( \mathcal{X} \), have been discussed in the literature of error-in-variables regression (Fan and Truong,\(^{\text{[1]}}\), Carroll et al.,\(^{\text{[2]}}\)). Error-in-variables regression is a special case of our problem, where \( X_i \) is observed but \( X_{P_i} \) is not. However, since we have \( Y_{ia} = X_i + \epsilon_i \), this is equivalent to an error-in-variables regression \( Y_{ia} = f_i(X_{P_i}) + \epsilon_{ia} + \zeta_i \), where the compound error term \( \epsilon_{ia} + \zeta_i \) is still independent of \( X_{P_i} \).

It can be shown that such identifiability conditions can be exploited in order to identify causal directionality among latent variables under additional assumptions, as discussed by\(^{\text{[4]}}\) for the fully observed case.\(^{\text{[5]}}\) A brief discussion is presented in the Appendix. In our context, we focus on the implications of identifiability on MCMC (Section 5).

### 3 THE MODEL: PRIORS

Each \( f_i(\cdot) \) can be given a Gaussian process prior (Rasmussen and Williams,\(^{\text{[6]}}\)). In this case, we call this class of models the GPSEM-LV family, standing for Gaussian Process Structural Equation Model with Latent Variables. Models without latent variables and measurement models have been discussed by Friedman and Nachman\(^{\text{[7]}}\).

#### 3.1 Gaussian Process Prior and Notation

Let \( X_i \) be an arbitrary latent variable in the graph, with latent parents \( X_{P_i} \). We will use \( X^{(d)} \) to represent the \( d \)-th \( X \) sampled from the distribution of random vector \( X \), and \( X^{(d)} \) indexes its \( i \)-th component. For instance, \( X^{(d)} \) is the \( d \)-th sample of the parents of \( X_i \). A training set of size \( N \) is represented as \( \{Z^{(1)}, \ldots, Z^{(N)}\} \), where \( Z \) is the set of all variables. Lower case \( x \) represents fixed values of latent variables, and \( x^{1:N} \) represents a whole set \( \{x^{(1)}, \ldots, x^{(N)}\} \).

For each \( x_{P_i} \), the corresponding Gaussian process prior for function values \( f_i^{1:N} \equiv \{f_i^{(1)}, \ldots, f_i^{(N)}\} \) is

\[
f_i^{1:N} \mid x_i^{1:N} \sim \mathcal{N}(0, K_i)
\]

where \( K_i \) is an \( N \times N \) kernel matrix (Rasmussen and Williams,\(^{\text{[6]}}\)), as determined by \( x_i^{1:N} \). Each corresponding \( x_i^{(d)} \) is given by \( f_i^{(d)} + \xi_i^{(d)} \), as in Equation (1).

MCMC can be used to sample from the posterior distribution over latent variables and functions. However, each sampling step in this model costs \( O(N^3) \), making sampling very slow when \( N \) is at the order of hundreds, and essentially undoable when \( N \) is in the thousands. As an alternative, we introduce a multilayered representation adapted from the pseudo-inputs model of Snelson and Ghahramani\(^{\text{[8]}}\). The goal is to reduce the sampling cost down to \( O(M^2N) \), \( M < N \). \( M \) can be chosen according to the available computational resources.

#### 3.2 Pseudo-inputs Review

We briefly review the pseudo-inputs model (Snelson and Ghahramani,\(^{\text{[8]}}\)) in our notation. As before, let \( X^{(d)} \) represent the \( d \)-th data point for some \( X \). For a set \( X_i^{1:N} \equiv \{X_i^{(1)}, \ldots, X_i^{(N)}\} \) with corresponding parent set \( X_{P_i}^{1:N} \equiv \{X_{P_i}^{(1)}, \ldots, X_{P_i}^{(N)}\} \) and corresponding latent function values \( f_i^{1:N} \), we define a pseudo-input set \( X_i^{1:M} \equiv \{X_i^{(1)}, \ldots, X_i^{(M)}\} \) such that

\[
f_i^{1:N} \mid x_{P_i}^{1:N}, \tilde{f}_i, \bar{X}_i^{1:M} \sim \mathcal{N}(K_{i;N,M}K_{i;M}^{-1} \tilde{f}_i, \tilde{V}_i)
\]

\[
\tilde{f}_i \mid \bar{X}_i^{1:M} \sim \mathcal{N}(0, K_{i;E,M})
\]

where \( K_{i;N,M} \) is a \( N \times M \) matrix with each \( (j,k) \) element given by the kernel function \( k_i(X_i^{(j)}, \bar{X}_i^{(k)}) \). Similarly, \( K_{i;E,M} \) is a \( M \times M \) matrix where element \( (j,k) \) is \( k_i(X_i^{(j)}, \bar{X}_i^{(k)}) \). It is important to notice that each pseudo-input \( X_i^{(d)} \), \( d = 1, \ldots, M \), has the same dimensionality as \( X_{P_i} \). The motivation for this is that \( \bar{X}_i \) works as an alternative training set, with the original prior predictive means and variances being recovered if \( M = N \) and \( \bar{X}_i = X_{P_i} \).

Let \( k_{i;E,M} \) be the \( d \)-th row of \( K_{i;N,M} \). Matrix \( \tilde{V}_i \) is a diagonal matrix with entry \( \tilde{v}_{i;dd} \) given by \( \tilde{v}_{i;dd} = k_i(X_{P_i}^{(d)}, X_{P_i}^{(d)}) - k_{i;E,M}^{-1} k_{i;E,M} \). This implies that all latent function values \( \{f_i^{(1)}, \ldots, f_i^{(N)}\} \) are conditionally independent.
fitting, since pseudo-inputs are in fact free parameters, and the model. This is practical but sometimes prone to over-placement for the pseudo-inputs can be learned, since sampling procedure. By conditioning on the data, a good stead we put a prior on the pseudo-inputs and extend the optimization techniques to choose pseudo-input values. In- stead we optimize the pseudo-inputs model is best seen as a variation of the Gaussian process prior rather than an approximation to it (Titsias, 2009).

In our setup, there is limited motivation to optimize the pseudo-inputs since the inputs themselves are random vari- ables. For instance, we show in the next section that the cost of sampling pseudo-inputs is no greater than the cost of sampling latent variables, while avoiding cumbersome optimization techniques to choose pseudo-input values. Instead we put a prior on the pseudo-inputs and extend the sampling procedure. By conditioning on the data, a good placement for the pseudo-inputs can be learned, since $\bar{X}_p$ and $\bar{X}(d)$ are dependent in the posterior. This is illustrated by Figure 2. Moreover, it naturally provides a protection against overfitting.

A simple choice of priors for pseudo-inputs is as follows: each pseudo-input $X^{(d)}_i$, $d = 1, \ldots, M$, is given a $N(\mu_i^d, \Sigma_i^d)$ prior, independent of all other random variables. A partially informative (empirical) prior can be easily defined in the case where, for each $X_k$, we have the freedom of choosing a particular indicator $Y_q$ with fixed structural equation $Y_q = X_k + \epsilon_q$ (see Section 2.1), implying $E[X_k] = E[Y_q]$. This means if $X_q$ is a parent $X_i$, we set the respective entry in $\mu_i^d$ (recall $\mu_i^d$ is a vector with an entry for every parent of $X_i$) to the empirical mean of $Y_q$. Each prior covariance matrix $\Sigma_i^d$ is set to be diagonal with a common variance.

Alternatively, we would like to spread the pseudo-inputs a priori: other things being equal, pseudo-inputs that are too close to each can be wasteful given their limited number. One prior, inspired by space-filling designs from the experimental design literature [Santner et al., 2003], is

$$p(x_i^{1:M}) \propto \det(D_i)$$

the determinant of a kernel matrix $D_i$. We use a squared exponential covariance function with characteristic length scale of 0.1 (Rasmussen and Williams, 2006), and a “nugget” constant that adds $10^{-4}$ to each diagonal term. This prior has support over a $[−L, L]^{|X_p|}$ hypercube. We set $L$ to be three times the largest standard deviation of observed variables in the training data. This is the pseudo-input prior we adopt in our experiments, where we center all observed variables at their empirical means.

### 3.4 Other Priors

We adopt standard priors for the parametric components of this model: independent Gaussians for each coefficient $\lambda_{ij}$, inverse gamma priors for the variances of the error terms and a Dirichlet prior for the distribution of the mixture indicators of the exogenous variables.

## 4 INFEERENCE

We use a Metropolis-Hastings scheme to sample from our space of latent variables and parameters. Similarly to Gibbs sampling, we sample blocks of random variables while conditioning on the remaining variables. When the corresponding conditional distributions are canonical, we sample directly from them. Otherwise, we use mostly standard random walk proposals.

Conditioned on the latent variables, sampling the parameters of the measurement model is identical to the case of classical Bayesian linear regression. The same can be said of the sampling scheme for the posterior variances of each $\zeta_i$. Sampling the mixture distribution parameters for the exogenous variables is also identical to the standard Bayesian
case of Gaussian mixture models. Details are described in the Appendix.

We describe the central stages of the sampler for the sparse model. The sampler for the model with full Gaussian process priors is simpler and analogous, and also described in the Appendix.

4.1 Sampling Latent Functions

In principle, one can analytically marginalize the pseudo-functions $f_i^{1:M}$. However, keeping an explicit sample of the pseudo-functions is advantageous when sampling latent variables $X_i^{(d)}$, $d = 1, \ldots, N$: for each child $X_i$ of $X$, only the corresponding factor for the conditional density of $f_i^{(d)}$ needs to be computed (at a $O(M)$ cost), since function values are independent given latent parents and pseudo-functions. This issue does not arise in the fully-observed case of [Snelson and Ghahramani (2006)], who do marginalize the pseudo-functions.

Pseudo-functions and functions $\{f_i^{1:M}, f_i^{1:N}\}$ are jointly Gaussian given all other random variables and data. The conditional distribution of $f_i^{1:M}$ given everything, except itself and $\{f_j^{1}, \ldots, f_j^{N}\}$, is Gaussian with covariance matrix

$$\Sigma_i = (K_{i:M}^{-1} + K_{i:M}^T V_i^{-1} + I/v_{i:C}) K_{i:M} K_{i:M}^{-1}$$

where $V_i$ is defined in Section 3.2 and $I$ is a $M \times M$ identity matrix. The total cost of computing this matrix is $O(NM^2 + M^3) = O(NM^2)$. The corresponding mean is

$$\tilde{\Sigma}_i \propto K_{i:M} V_i^{-1} + I/v_{i:C} X_i^{1:N}$$

where $x_i^{1:N}$ is a column vector of length $N$.

Given that $f_i^{1:M}$ is sampled according to this multivariate Gaussian, we can now sample $\{f_j^{1}, \ldots, f_j^{N}\}$ in parallel, since this becomes a mutually independent set with univariate Gaussian marginals. The conditional variance of $f_j^{(d)}$ is $v_j^{(d)} = 1/(1/v_{i:C} + 1/v_i)$, where $v_{i:C}$ is defined in Section 3.2.

The corresponding mean is $\tilde{\Sigma}_i x_i^{1:N} / v_{i:C}$. The conditional density $\pi_i(x_i^{(d)} | f_i^{1:M})$ of the kernel function used by $K_i$ and $K_iN$ is a Gaussian with covariance $\Sigma_i$. Fast submatrix updates of $K_i$ and $K_iN$ are required in order to calculate $l_i(x_i^{(d)})$ at a $O(NM^2)$ cost, which can be done by standard Cholesky updates [Seeger (2004)]. The total cost is therefore $O(NM^2)$ for a full sweep over all pseudo-inputs.

The conditional density $p(x_i^{(d)} | f_i^{1:M}, x_i)$ is known to be sharply peaked for moderate sizes of $M$ (at the order of hundreds) [Titsias et al. (2009)], which may cause mixing problems for the Markov chain. One way to mitigate this effect is to also propose a value $\bar{x}_i^{(d)}$ jointly with $x_i^{(d)}$, which is possible at no additional cost. We propose the pseudo-function using the conditional $p(f_i^{(d)} | \bar{x}_i^{(d)}, x_i$).

The Metropolis-Hastings acceptance probability for this variation is then simplified to $\min\left\{1, p(x_i^{(d)} | \bar{x}_i^{(d)}) / l_i(x_i^{(d)})\right\}$, where

$$\tilde{l}_i(x_i^{(d)}) = \tilde{\pi}_i(x_i^{(d)}) \times \prod_{d=1}^N v_{i:C}^{-1/2} e^{-\frac{(f_i^{(d)} - x_i^{(d)} - k_{i,d} \bar{x}_i^{(d)})^2}{2v_{i:C}}}$$

Finally, consider the proposal for latent variables $X_i^{(d)}$. For each latent variable $X_i$, the set of latent variable instantiations $\{X_i^{(1)}, X_i^{(2)}, \ldots, X_i^{(N)}\}$ is mutually independent given the remaining variables. We propose each new latent variable value $x_i^{(d)}$ in parallel, and accept or reject it based on a Gaussian random walk proposal centered at the current value $x_i^{(d)}$. We accept the move with probability $\min\left\{1, h_{X_i}(x_i^{(d)}) / h_{X_i}(x_i^{(d)})\right\}$ where, if $X_i$ is not an exogenous variable in the graph,

$$h_{X_i}(x_i^{(d)}) = e^{-\frac{(x_i^{(d)} - f_i^{(d)})^2}{2v_{i:C}}} \times \prod_{C_i \in X_{C_i}} p(f_{C_i}^{(d)} | \tilde{x}_C, x_i^{(d)}) \times \prod_{C_i \in X_{C_i}} p(y_{C_i}^{(d)} | \tilde{x}_C)$$

where $X_{C_i}$ is the set of latent children of $X_i$ in the graph, and $Y_{C_i}$ is the corresponding set of observed children.
The conditional \( p(\nu_i^{(d)} | \bar{\nu}_i, \bar{x}_i, x_i^{(d)}) \), which follows from \(^3\), is a non-linear function of \( x_i^{(d)} \), but crucially does not depend on any \( x_i \) variable except point \( d \). The evaluation of this factor costs \( O(M^2) \). As such, sampling all latent values for \( X_i \) takes \( O(NM^2) \).

The case where \( X_i \) is an exogenous variable is analogous, given that we also sample the mixture component indicators of such variables.

5 EXPERIMENTS

In this evaluation Section \(^4\), we briefly illustrate the algorithm in a synthetic study, followed by an empirical evaluation on how identifiability matters in order to obtain an interpretable distribution of latent variables. We end this section with a study comparing the performance of our model in predictive tasks against common alternatives.

5.1 An Illustrative Synthetic Study

We generated data from a model of two latent variables \( (X_1, X_2) \) where \( X_2 = 4X_1^2 + \epsilon_2, \epsilon_1 = X_1 + \epsilon_i \) for \( i = 1, 2, 3 \) and \( Y_i = X_2 + \epsilon_i \), for \( i = 4, 5, 6 \). \( X_1 \) and all error terms follow standard Gaussians. Given a sample of 150 points from this model, we set the structural equations for \( Y_1 \) and \( Y_2 \) to have a zero intercept and unit slope for identifiability purposes. Observed data for \( Y_1 \) against \( Y_2 \) is shown in Figure \(^3\)(a), which suggests a noisy quadratic relationship (plotted in \(^3\)(b), but unknown to the model).

We run a GPSEM-LV model with 50 pseudo-inputs. The expected posterior value of each latent pair \( \{X_1^{(d)}, X_2^{(d)}\} \) for \( d = 1, \ldots, 150 \) is plotted in Figure \(^3\)(c). It is clear that we were able to reproduce the original non-linear functional relationship given noisy data using a pseudo-inputs model.

For comparison, the output of the Gaussian process latent variable model (GPLVM, \(^5\)Lawrence 2005) with two hidden variables is shown in Figure \(^3\)(d). GPLVM here assumes that the marginal distribution of each latent variable is a standard Gaussian, but the measurement model is non-parametric. In theory, GPLVM is as flexible as GPSEM-LV in terms of representing observed joints. However, it does not learn functional relationships among latent variables, which is often of central interest in SEM applications (Bollen 1989). Moreover, since no marginal dependence among latent variables is allowed, the model adapts itself to find (unidentifiable) functional relationships between the exogenous latent variables of the true model and the observables, analogous to the case illustrated by Figure \(^1\)(b).

As a result, despite GPLVM being able to depict, as expected, some quadratic relationship (up to a rotation), it is noisier than the one given by GPSEM-LV.

5.2 MCMC and Identifiability

We now explore the effect of enforcing identifiability constraints on the MCMC procedure. We consider the dataset Consumer, a study \(^6\) with 333 university students in Greece (Bartholomew et al. 2008). The aim of the study was to identify the factors that affect willingness to pay more to consume environmentally friendly products. We selected 16 indicators of environmental beliefs and attitudes, measuring a total of 4 hidden variables. For simplicity, we will call these variables \( X_1, \ldots, X_4 \). The structure among latents is \( X_1 \rightarrow X_2, X_1 \rightarrow X_3, X_2 \rightarrow X_3, X_2 \rightarrow X_4 \). Full details are given by Bartholomew et al. (2008). All observed variables have a single latent parent in the corresponding DAG. As discussed in Section \(^1\), the corresponding measurement model is identifiable by fixing the structural equation for one indicator of each variable to have a zero intercept and unit slope (Bartholomew et al. 2008). If the assumptions described in the references of Section \(^1\) hold, then the latent functions are also identifiable. We normalized the dataset before running the MCMC inference algorithm.

An evaluation of the MCMC procedure is done by running and comparing 5 independent chains, each starting from a different point. Following Lee (2007), we evaluate convergence using the EPSR statistic (Gelman and Rubin 1992), which compares the variability of a given marginal posterior within each chain and between chains. We calculate this statistic for all latent variables \( \{X_1, X_2, X_3, X_4\} \) across all 333 data points.

A comparison is done against a variant of the model where the measurement model is not sparse: instead, each observed variable has all latent variables as parents, and no

\(^{3}\)MATLAB code to run all of our experiments is available at http://www.homepages.ucl.ac.uk/~ucgtrbd/code/gpsem.zip

\(^{4}\)Some implementation details: we used the squared exponential kernel function \( k(x_p, x_q) = a \exp(-\frac{1}{2b}||x_p - x_q||^2) + 10^{-4} \delta_{pq} \), where \( \delta_{pq} = 1 \) if \( p = q \) and 0 otherwise. The hyperprior for \( a \) is a mixture of a gamma (1, 20) and a gamma (10, 10) with equal probability each. The same (independent) prior is given to \( b \). Variance parameters were given inverse gamma (2, 1) priors, and the linear coefficients were given Gaussian priors with a common large variance of 5. Exogenous latent variables were modeled as a mixture of five Gaussians where the mixture distribution is given a Dirichlet prior with parameter 10. Finally, for each latent \( X_i \) variable we choose one of its indicators \( Y_j \) and fix the corresponding edge coefficient to 1 and intercept to 0 to make the model identifiable. We perform 20,000 MCMC iterations with a burn-in period of 2000 (only 6000 iterations with 1000 of burn-in for the non-sparse GPSEM-LV due to its high computational cost). Small variations in the priors for coefficients (using a variance of 10) and variance parameters (using an inverse gamma (2, 2)), and a mixture of 3 Gaussians instead of 5, were attempted with no significant differences between models.

\(^{5}\)There was one latent variable marginally independent of everything else. We eliminated it and its two indicators, as well as the REC latent variable that had only 1 indicator.
coefficient are fixed. The differences are noticeable and illustrated in Figure 4. Box-plots of EPSR for the 4 latent variables are shown in Figure 5. It is difficult to interpret or trust an embedding that is strongly dependent on the initialization procedure, as it is the case for the unidentifiable model. As discussed by Palomo et al. (2007), identifiability might not be a fundamental issue for Bayesian inference, but it is an important practical issue in SEMs.

5.3 Predictive Verification of the Sparse Model

We evaluate how well the sparse GPSEM-LV model performs compared against two parametric SEMs and GPLVM. The linear structural equation model is the SEM, where each latent variable is given by a linear combination of its parents with additive Gaussian noise. Latent variables without parents are given the same mixture of Gaussians model as our GPSEM-LV implementation. The quadratic model includes all quadratic and linear terms, plus first-order interactions, among the parents of any given latent variable. This is perhaps the most common non-linear SEM used in practice (Bollen and Paxton, 1998; Lee, 2007). GPLVM is fit with 50 active points and the rbf kernel with automatic relevance determination (Lawrence, 2005). Each sparse GPSEM model uses 50 pseudo-points.

We performed a 5-fold cross-validation study where the average predictive log-likelihood on the respective test sets is reported. Three datasets are used. The first is the Consumer dataset, described in the previous section.

The second is the Abalone data (Asuncion and Newman, 2007), where we postulate two latent variables, “Size” and “Weight.” Size has as indicators the length, diameter and height of each abalone specimen, while Weight has as indicators the four weight variables. We direct the relationship among latent variables as Size → Weight.

The third is the Housing dataset (Asuncion and Newman, 2007; Harrison and Rubinfeld, 1978), which includes indicators about features of suburbs in Boston that are relevant for the housing market. Following the original study (Harrison and Rubinfeld, 1978, Table IV), we postulate three latent variables: “Structural,” corresponding to the structure of each residence; “Neighborhood,” corresponding to an index of neighborhood attractiveness; and “Accessibility,” corresponding to an index of accessibility within Boston. The corresponding 11 non-binary ob-

The analysis by (Harrison and Rubinfeld, 1978, Table IV)
In order to get more stable results, we use a subset of the indicators of accessibility (Friedman and Nachman, 2000). For the non-sparse GPSEM, we subsampled all of the points in each cross-validation fold, compared to the sparse alternative. Notice that while the quadratic polynomial model shows some overfitting, the Abalone study is known for having clear functional relationships among variables, as also discussed by Friedman and Nachman (2000). In this case, there is a substantial difference between the non-linear models and the linear one, although GPLVM seems suboptimal in this scenario where observed variables can be easily clustered into groups. Finally, functional relationships among variables in Housing are not as clear (Friedman and Nachman, 2000), with multimodal residuals. GPSEM still shows an advantage, but all SEMs are suboptimal compared to GPLVM. One explanation is that the DAG on which the models rely is not adequate. Structure learning might be necessary to make the most out of nonparametric SEMs.

Although results suggest that the sparse model behaved better than the non-sparse one (which was true of some cases found by Snelson and Ghahramani, 2006, due to heteroscedasticity effects), such results should be interpreted with care. Abalone had to be subsampled in the non-sparse case. Mixing is harder in the non-sparse model since all the data are dependent. While we believe that with larger sample sizes and denser latent structures the non-sparse model should be the best, large sample sizes are too expensive to process and, in many SEM applications, latent variables have very few parents.

It is also important to emphasize that the wallclock sampling time for the non-sparse model was an order of magnitude larger than the sparse case with $M = 50$ — even considering that 3000 training points were used by the sparse model in the Abalone experiment, against 300 points by the non-sparse alternative.
Table 1: Average predictive log-likelihood in a 5-fold cross-validation setup. The five methods are the GPSEM-LV model with 50 pseudo-inputs (GPS), GPSEM-LV with standard Gaussian process priors (GP), the linear and quadratic structural equation models (LIN and QDR) and the Gaussian process latent variable model (GPL) of Lawrence (2005), a nonparametric factor analysis model. For Abalone, GP uses a subsample of the training data. The p-values given by a paired Wilcoxon signed-rank test, measuring the significance of positive differences between sparse GPSEM-LV and the quadratic model, are 0.03 (for Consumer), 0.34 (Abalone) and 0.09 (Housing).

6 RELATED WORK

Non-linear factor analysis has been studied for decades in the psychometrics literature. A review is provided by Yalcin and Amemiya (2001). However, most of the classic work is based on simple parametric models. A modern approach based on Gaussian processes is the Gaussian process latent variable model of Lawrence (2005). By construction, factor analysis cannot be used in applications where one is interested in learning functions relating latent variables, such as in causal inference. For embedding, factor analysis is easier to use and more robust to model misspecification than SEM analysis. Conversely, it does not benefit from well-specified structures and might be harder to interpret. Bollen (1989) discusses the interplay between factor analysis and SEM. Practical non-linear structural equation models are discussed by Lee (2007), but none of such approaches rely on nonparametric methods. Gaussian processes latent structures appear mostly in the context of dynamical systems (e.g., Ko and Fox (2009)). However, the connection is typically among data points only, not among variables within a data point, where online filtering is the target application.

7 CONCLUSION

The goal of graphical modeling is to exploit the structure of real-world problems, but the latent structure is often ignored. We introduced a new nonparametric approach for SEMs by extending a sparse Gaussian process prior as a fully Bayesian procedure. Although a standard MCMC algorithm worked reasonably well, it is possible as future work to study ways of improving mixing times. This can be particularly relevant in extensions to ordinal variables, where the sampling of thresholds will likely make mixing more difficult. Since the bottleneck of the procedure is the sampling of the pseudo-inputs, one might consider a hybrid approach where a subset of the pseudo-inputs is fixed and determined prior to sampling using a cheap heuristic. New ways of deciding pseudo-input locations based on a given measurement model will be required. Evaluation with larger datasets (at least a few hundred variables) remains an open problem. Finally, finding ways of determining the graphical structure is also a promising area of research.

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We use a MCMC sampler to draw all variables of interest from the posterior distribution of a GPSEM model. Let $M$ denote the number of pseudo-inputs per latent function $f_i(\cdot)$, $N$ be the sample size, $V$ the number of latent variables and $K$ the common number of Gaussian mixture components for each exogenous latent variable.

The sampler is a standard Metropolis-Hastings procedure with block sampling: random variables are divided into blocks, where we sample each block conditioning on the current values of the remaining blocks.

We consider both the non-sparse and sparse variations of GPSEM. The blocks are as follows for the non-sparse GPSEM:

- the linear coefficients for the structural equation of each observed variable $Y_j$: $\{\lambda_0\} \cup \Lambda_j$
- the conditional variance for the structural equation of each observed variable $Y_j$: $\nu_{w_j}$
- the $d$-th instantiation of each latent variable $X_i, x_i^{(d)}$
- the set of latent function values $\{f_i^{(1)}, \ldots, f_i^{(N)}\}$ for each particular endogenous latent variable $X_i$
- the conditional variance for the structural equation of each latent variable $X_i$: $\nu_{z_i}$
- the set of latent mixture component indicators $\{z_i^{(1)}, \ldots, z_i^{(N)}\}$ for each particular exogenous latent variable $X_i$
- the set of means $\{\mu_i^{(1)}, \ldots, \mu_i^{(K)}\}$ for the mixture components of each particular exogenous latent variable $X_i$
- the set of variances $\{\upsilon_{i1}, \ldots, \upsilon_{iK}\}$ for the mixture components of each particular exogenous latent variable $X_i$
- mixture distribution $\pi_i$ corresponding to the probability over mixture components for exogenous latent variable $X_i$

The blocks for the sparse model are similar, except that

- all instantiations of a given latent variable $x_i^{(d)}$, for $d = 1, 2, \ldots, N$, are mutually independent conditioned on the functions, pseudo-inputs and pseudo-functions. As such, they can be treated as a single block of size $N$, where all elements are sampled in parallel;
- the $d$-th instantiation of each pseudo-input $x_i^{(d)}$ for $d = 1, 2, \ldots, M$
- all instantiations of latent functions and pseudo-latents functions $\{f_i^{(1)}, \ldots, f_i^{(N)}, f_i^{(1)}, \ldots, f_i^{(M)}\}$ for any particular $X_i$ are conditionally multivariate Gaussian and can be sampled together.

We adopt the convention that, for any particular step described in the following procedure, any random variable that is not explicitly mentioned should be considered fixed at the current sampled value. Moreover, any density function that depends on such implicit variables uses the respective implicit values.

Our implementation uses code for submatrix Cholesky updates from the library provided by Seeger (2004).

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**APPENDIX A: FURTHER MCMC DETAILS**

We use a MCMC sampler to draw all variables of interest from the posterior distribution of a GPSEM model. Let $M$ denote the number of pseudo-inputs per latent function $f_i(\cdot)$, $N$ be the sample size, $V$ the number of latent variables and $K$ the common number of Gaussian mixture components for each exogenous latent variable.
The measurement model

The measurement model can be integrated out in principle, if we adopt a conjugate normal-inverse gamma prior for the linear regression of observed variables $Y$ on $X$. However, we opted for a non-conjugate prior in order to evaluate the convergence of the sampler when this marginalization cannot be done (as in alternative models with non-Gaussian error terms).

Given the latent variables, the corresponding conditional distributions for the measurement model parameters boil down to standard Bayesian linear regression posteriors. In our Metropolis-Hastings scheme, our proposals correspond to such conditionals, as in Gibbs sampling (and therefore have an acceptance probability of 1).

Let $X_{P_j}$ be the parents of observed variable $Y_j$ in the graph and let the $d$-th instantiation of the corresponding regression input be $x^{(d)}_{P_j} \equiv [x^{(d)}_{P_1}, \ldots, x^{(d)}_{P_J}]$. Let each coefficient $\lambda_j$ have an independent Gaussian prior with mean zero and variance $\upsilon$. Conditioned on the error variance $\upsilon_{ci}$, the posterior distribution of the vector $[\lambda_j, \ldots, \lambda_J|x_{P_j}, \upsilon] \equiv \mathcal{N}(0, \upsilon_{ci}^{-1})$ is multivariate Gaussian with covariance $\mathbf{S_j} \equiv (\sum_{d=1}^N x^{(d)}_{P_j} x^{(d)}_{P_j}^T + \upsilon_{ci}^{-1})^{-1}$ and mean $\mathbf{S_j} \sum_{d=1}^N x^{(d)}_{P_j} y^{(d)}_{j}$, where $I$ is a $(|X_{P_j}| + 1) \times (|X_{P_j}| + 1)$ identity matrix.

The derivative for the case where some coefficients $\lambda_k$ are fixed to constants is analogous.

For a fixed set of linear coefficients $\{\lambda_{j0}\} \cup \Lambda_j$, we now sample the conditional variance $\upsilon_{ci}$. Let this variance have a inverse gamma prior $(\alpha, \beta)$. Its conditional distribution is an inverse gamma $(\alpha', \beta')$, where $\alpha' = \alpha + N/2$, $\beta' = \beta + \sum_{d=1}^N (y^{(d)}_j)^2/2$, and $\hat{\upsilon}_{ci} \equiv \upsilon_{ci} - \lambda_{j0} - \Lambda_j x^{(d)}_{P_j}$.

The structural model: non-sparse GPSEM

For all $i = 1, 2, \ldots, V$ and $d = 1, 2, \ldots, N$, we propose each new latent variable $x^{(d)}_i$ individually, and accept or reject it based on a Gaussian random walk proposal centered at the current value $x^{(d)}_i$. We accept the move with probability

$$
\min \left\{ 1, \frac{g_{X_i}(x^{(d)}_i)}{g_{X_i}(x^{(d)}_i)} \right\}
$$

where, if $X_i$ is not an exogenous variable in the graph,

$$
g_{X_i}(x^{(d)}_i) = e^{-\frac{(y^{(d)}_i - f^{(d)}_i(x^{(d)}_i))^2}{2\upsilon_{ci}}} \times \prod_{X_{ci}} p(f^{(d)}_i | f^{(d)}_i) \times \prod_{Y_i} p(y^{(d)}_i | X^{(d)}_{P_i})
$$

Recall that $f^{(d)}_i$ is a function of the parents $X_{P_i}$ of $X_i$ in the graph. The $d$-th instantiation of such parents assume the value $x^{(d)}_{P_i}$. We use $f^{(d)}_i$ as a shorthand notation for $f_i(x^{(d)}_i)$. Moreover, let $X_{ci}$ denote the latent children of $X_i$ in the graph. The symbol $f^{(d)}_i$ refers to the respective function values taken by $f_i$ in data points $\{1, 2, \ldots, d-1, d+1, \ldots, N\}$. Function $p(f^{(d)}_i | f^{(d)}_i)$ is the conditional density of $f^{(d)}_i$ given $f^{(d)}_i$, according to the Gaussian process prior. The evaluation of this factor costs $O(N^2)$ using standard submatrix Cholesky updates (Smyth, 2004). As such, sampling all latent values for $X_i$ takes $O(N^3)$.

Finally, $Y_i$ denotes the observed children of $X_i$, and function $p(y^{(d)}_i | X^{(d)}_{P_i})$ is the corresponding density of observed child $Y_i$ evaluated at $y^{(d)}_i$, given its parents (which includes $X^{(d)}_{P_i}$) and (implicit) measurement model parameters. This factor can be dropped if $y^{(d)}_i$ is missing.

If variable $X_i$ is an exogenous variable, then the factor $e^{-\frac{(y^{(d)}_i - f^{(d)}_i)^2}{2\upsilon_{ci}}}$ gets substituted by

$$
e^{-\frac{1}{2}(z^{(d)}_i - \mu^{(d)}_i)^2}/\upsilon_{ci}^{(d)}
$$

where $z^{(d)}_i$ is the latent mixture indicator for the marginal mixture of Gaussians model for $X_i$, with means $\{\mu_1, \ldots, \mu_K\}$ and variances $\{\upsilon_{11}, \ldots, \upsilon_{KK}\}$.

Given all latent variables, latent function values $\{f^{(1)}_i, \ldots, f^{(N)}_i\}$ are multivariate Gaussian with covariance matrix

$$
\mathbf{S}_{f_i} \equiv (\mathbf{K}_i^{-1} + 1/\upsilon_{ci})^{-1}
$$

where $\mathbf{K}_i$ is the corresponding kernel matrix and $I$ is a $N \times N$ identity matrix.

We sample from this conditional as in a standard Gibbs update. Sampling each latent conditional variance $\upsilon_{ci}$ can also be done by sampling from its conditional. Let $\upsilon_{ci}$ have an inverse gamma prior $(\alpha_c, \beta_c)$. The conditional distribution for this variance given all other random variables is inverse gamma $(\alpha'_c, \beta'_c)$, where $\alpha'_c = \alpha_c + N/2$ and $\beta'_c = \beta_c + \sum_{d=1}^N (y^{(d)}_i)^2/2$.

We are left with sampling the mixture model parameters that correspond to the marginal distributions of the exogenous latent variables. Once we condition on the latent variables, this is completely standard. If each mixture mean parameter $\mu_{ij}$ is given an independent Gaussian prior with mean zero and variance $\upsilon_{ij}$, its conditional distribution is also Gaussian with mean $\upsilon_{ij}^{-1}/\upsilon_{ij} + 1/\upsilon_{ij}$ and variance $1/\upsilon_{ij}$. If $\upsilon_{ij}^{-1}/\upsilon_{ij} + 1/\upsilon_{ij}$ is fixed, then the remaining variables is also Gaussian with variance $\upsilon_{ij}^{-1}=1/(1/\upsilon_{ij} + 1/\upsilon_{ij})$, where $Z_i$ is the subset of $1, 2, \ldots, N$ such that $d \in Z_i$ if and only if $z^{(d)}_i = j$. The corresponding mean is given by $\upsilon_{ij}^{-1}/\upsilon_{ij} + \sum_{d=1}^N (x^{(d)}_i - \mu_{ij})^2/2$.

The conditional probability $P(\zeta^{(d)}_i = j \mid \text{everything else})$ is proportional to $\sum_{d=1}^N \upsilon_{ij}^{-1}/\upsilon_{ij} + 1/\upsilon_{ij} + 1/\upsilon_{ij}$ and $\upsilon_{ij}^{-1} = \upsilon_{ij}^{-1}/\upsilon_{ij} + \sum_{d=1}^N (x^{(d)}_i - \mu_{ij})^2/2$. Finally, given a Dirichlet prior distribution $(\alpha_1, \ldots, \alpha_K)$ for each $\pi_1$, its conditional is also Dirichlet with parameter vector $(\alpha_1 + |Z_1|, \ldots, \alpha_K + |Z_K|)$.

APPENDIX B: A NOTE ON DIRECTIONALITY DETECTION

The assumption of linearity of the measurement model is not only a matter of convenience. In SEM applications, observed variables are carefully chosen to represent different aspects of latent concepts of interest and often have a single latent parent. As such, it is plausible that children of a particular latent variable are different noisy linear transformations of the target latent variable. This differs from other applications of latent variable Gaussian process models such as those introduced by Lawrence (2005), where measurements are not designed to explicitly account for target latent variables of interest. Moreover, this linearity condition has important implications on distinguishing among candidate models.
Implications for Model Selection

We assumed that the DAG $G$ is given. A detailed discussion of model selection is left as future work. Instead, we discuss some theoretical aspects of a very particular but important structural feature that will serve as a building block to more general model selection procedures, in the spirit of [Hoyer et al. (2008a)]. Determining sufficient conditions for the subproblem of detecting edge directionality from the data. Given a measurement model for two latent variables $X_1$ and $X_2$, we need to establish conditions in which we can test whether the only correct latent structure is $X_1 \rightarrow X_2$, $X_2 \rightarrow X_1$, the disconnected structure, or either directionality. The results of [Hoyer et al. (2008a)] can be extended to the latent variable case by exploiting the conditions of identifiability discussed in Section 2.1 as follows.

Our sufficient conditions are a weaker set of assumptions than that of [Silva et al. (2006)]. We assume that $X_1$ has at least two observable children which are not children of $X_2$ and vice-versa. Call these sets $\{Y_1, Y_1'\}$ and $\{Y_2, Y_2'\}$, respectively. Assume all error terms $\{\epsilon_i\} \cup \{\zeta_i\}$ are non-Gaussian\footnote{Variations where $\epsilon_i$ and latent error terms are allowed to be Gaussian, as in our original model description are also possible and will be treated in the future.} The variance of all error terms is assumed to be nonzero. As in [Hoyer et al. (2008a)], we also assume $X_1$ and $X_2$ are unconfounded.

To test whether the model where $X_1$ and $X_2$ are independent becomes easy in this case: the independence model entails that (say) $Y_1$ and $Y_2$ are marginally independent. This can be tested using the nonparametric marginal independence test of [Gretton et al. (2007)].

For the nontrivial case where latent variables are dependent, the results of Section 2.1 imply that the measurement model of $\{X_1 \rightarrow Y_1, X_1 \rightarrow Y_1'\}$ is identifiable up to the scale and sign of the latent variables, including the marginal distributions of $\epsilon_1$ and $\epsilon_1'$. An analogous result applies to $\{X_2, Y_2, Y_2'\}$.

Since the measurement model $\{Y_1, Y_1', Y_2, Y_2'\}$ of $\{X_1, X_2\}$ is identifiable, assume without loss of generality that the linear coefficients corresponding to $X_1 \rightarrow Y_1$ and $X_2 \rightarrow Y_2$ are fixed to 1, i.e., $Y_1 = X_1 + \epsilon_1$ and $Y_2 = X_2 + \epsilon_2$. Also from Section 2.1, it follows that the distribution of $\{X_1, X_2\}$ can be identified under very general conditions. The main result of [Hoyer et al. (2008a)] can then be directly applied. That is, data generated by a model $X_2 = f(X_1) + \eta_2$, with $\eta_2$ being non-Gaussian and independent of $X_1$, cannot be represented by an analogous generative model $X_1 = g(X_2) + \eta_1$ except in some particular cases that are ruled out as implausible.

Practical Testing

The test for comparing $X_1 \rightarrow X_2$ against $X_2 \rightarrow X_1$ in [Hoyer et al. (2008a)] can be modified to our context as follows: we cannot regress $X_2$ on $X_1$ and estimate the residuals $\zeta_2$ since $X_1$ and $X_2$ are latent. However, we can do a error-in-variables regression of $Y_2$ on $Y_1$ using $Y_1'$ and $Y_2'$ as instrumental variables [Carroll et al. (2004)]; this means we find a function $h(\cdot)$ such that $Y_2 = h(X) + r$ and $Y_1 = X + w$, for non-Gaussian latent variables $r, w$ and $X$. We then calculate the estimated residuals $r$ of this regression, and test whether such residuals are independent of $Y_1$ [Gretton et al. (2007)]. If this is true, then we have no evidence to discard the hypothesis $X_1 \rightarrow X_2$.

The justification for this process is that, if the true model is indeed $X_2 = f(X_1) + \eta_2$, then $h(\cdot) = f(\cdot)$ and $r = \epsilon_2 + \eta_2$ in the limit of infinite data, since the error-in-variables regression model is identifiable in our case [Carroll et al. (2004)], with $X = X_1$ being a consequence of deconvolving $Y_1$ and $\epsilon_1$. By this result, $r$ will be independent of $Y_1$. However, if the opposite holds ($X_1 \leftarrow X_2$) then, as in [Hoyer et al. (2008a)], the residual is not in general independent of $Y_1$: given $X_1 (= X)$, there is a d-connecting path $Y_2 \leftarrow X_2 \rightarrow X_1 \leftarrow \eta_1$ [Pearl, 2000], and $r$ will be a function of $\eta_1$, which is dependent on $Y_1$. This is analogous to [Hoyer et al. (2008a)], but using a different family of regression techniques.

Error-in-variables regression is a special case of the Gaussian process SEM. The main practical difficulty on using GPSEM with the pseudo-inputs approximation in this case is that such pseudo-inputs formulation implies a heteroscedastic regression model [Snelson and Ghahramani, 2006]. One has either to use the GPSEM formulation without pseudo-inputs, or a model linear in the parameters but with an explicit, finite, basis dictionary on the input space.