

CrossCat: A Fully Bayesian Nonparametric Method for Analyzing Heterogeneous, High Dimensional Data

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Editor: David Blei

Abstract

There is a widespread need for statistical methods that can analyze high-dimensional datasets without imposing restrictive or opaque modeling assumptions. This paper describes a domain-general data analysis method called CrossCat. CrossCat infers multiple non-overlapping views of the data, each consisting of a subset of the variables, and uses a separate nonparametric mixture to model each view. CrossCat is based on approximately Bayesian inference in a hierarchical, nonparametric model for data tables. This model consists of a Dirichlet process mixture over the columns of a data table in which each mixture component is itself an independent Dirichlet process mixture over the rows; the inner mixture components are simple parametric models whose form depends on the types of data in the table. CrossCat combines strengths of mixture modeling and Bayesian network structure learning. Like mixture modeling, CrossCat can model a broad class of distributions by positing latent variables, and produces representations that can be efficiently conditioned and sampled from for prediction. Like Bayesian networks, CrossCat represents the dependencies and independencies between variables, and thus remains accurate when there are multiple statistical signals. Inference is done via a scalable Gibbs sampling scheme; this paper shows that it works well in practice. This paper also includes empirical results on heterogeneous tabular data of up to 10 million cells, such as hospital cost and quality measures, voting records, unemployment rates, gene expression measurements, and images of handwritten digits. CrossCat infers structure that is consistent with accepted findings and common-sense knowledge in multiple domains and yields predictive accuracy competitive with generative, discriminative, and model-free alternatives.

Keywords: Bayesian nonparametrics, Dirichlet processes, Markov chain Monte Carlo, multivariate analysis, structure learning, unsupervised learning, semi-supervised learning

Acknowledgments: The authors thank Kevin Murphy, Ryan Rifkin, Cameron Freer, Daniel Roy, Bill Lazarus, David Jensen, Beau Cronin, Rax Dillon, and the anonymous reviewers and editor for valuable suggestions. This work was supported in part by gifts from Google, NTT Communication Sciences Laboratory, and Eli Lilly & Co; by the Army Research Office under agreement number W911NF-13-1-0212; and by DARPA via the XDATA and PPAML programs. Any opinions, findings, and conclusions or recommendations expressed in this work are those of the authors and do not necessarily reflect the views of any of the above sponsors.

1. Introduction

High-dimensional datasets containing data of multiple types have become commonplace. These datasets are often represented as tables, where rows correspond to data vectors, columns correspond to observable variables or features, and the whole table is treated as a random subsample from a statistical population (Hastie, Tibshirani, Friedman, and Franklin, 2005). This setting brings new opportunities as well as new statistical challenges (NRC Committee on the Analysis of Massive Data, 2013; Wasserman, 2011). In principle, the dimensionality and coverage of some of these datasets is sufficient to rigorously answer to fine-grained questions about small sub-populations. This size and richness also enables the detection of subtle predictive relationships, including those that depend on aggregating individually weak signals from large numbers of variables. Challenges include integrating data of heterogeneous types (NRC Committee on the Analysis of Massive Data, 2013), suppressing spurious patterns (Benjamini and Hochberg, 1995; Attia, Ioannidis, et al., 2009), selecting features (Wasserman, 2011; Weston, Mukherjee, et al., 2001), and the prevalence of non-ignorable missing data.

This paper describes CrossCat, a general-purpose Bayesian method for analyzing high-dimensional mixed-type datasets that aims to mitigate these challenges. CrossCat is based on approximate inference in a hierarchical, nonparametric Bayesian model. This model is comprised of an “outer” Dirichlet process mixture over the columns of a table, with components that are themselves independent “inner” Dirichlet process mixture models over the rows. CrossCat is parameterized on a per-table basis by data type specific component models — for example, Beta-Bernoulli models for binary values and Normal-Gamma models for numerical values. Each “inner” mixture is solely responsible for modeling a subset of the variables. Each hypothesis assumes a specific set of marginal dependencies and independencies. This formulation supports scalable algorithms for learning and prediction, specifically a collapsed MCMC scheme that marginalizes out all but the latent discrete state and hyper parameters.

The name “CrossCat” is derived from the combinatorial skeleton of this probabilistic model. Each approximate posterior sample represents a *cross-categorization* of the input data table. In a cross-categorization, the variables are partitioned into a set of *views*, with a separate partition of the entities into *categories* with respect to the variables in each *view*. Each (*category*, *variable*) pair contains the sufficient statistics or latent state needed by its associated component model. See Figure 1 for an illustration of this structure. From the standpoint of structure learning, CrossCat finds multiple, cross-cutting categorizations or clusterings of the data table. Each non-overlapping system of categories is context-sensitive in that it explains a different subset of the variables. Conditional densities are straightforward to calculate and to sample from. Doing so first requires dividing the conditioning and target variables into views, then sampling a category for each view. The distribution on categories must reflect the values of the conditioning variables. After choosing a category it is straightforward to sample predictions or evaluate predictive densities for each target variable by using the appropriate component model.

Standard approaches for inferring representations for joint distributions from data, such as Bayesian networks, mixture models, and sparse multivariate Gaussians, each exhibit complementary strengths and limitations. Each method exhibits distinct strengths and weaknesses:

1. Bayesian networks and structure learning.

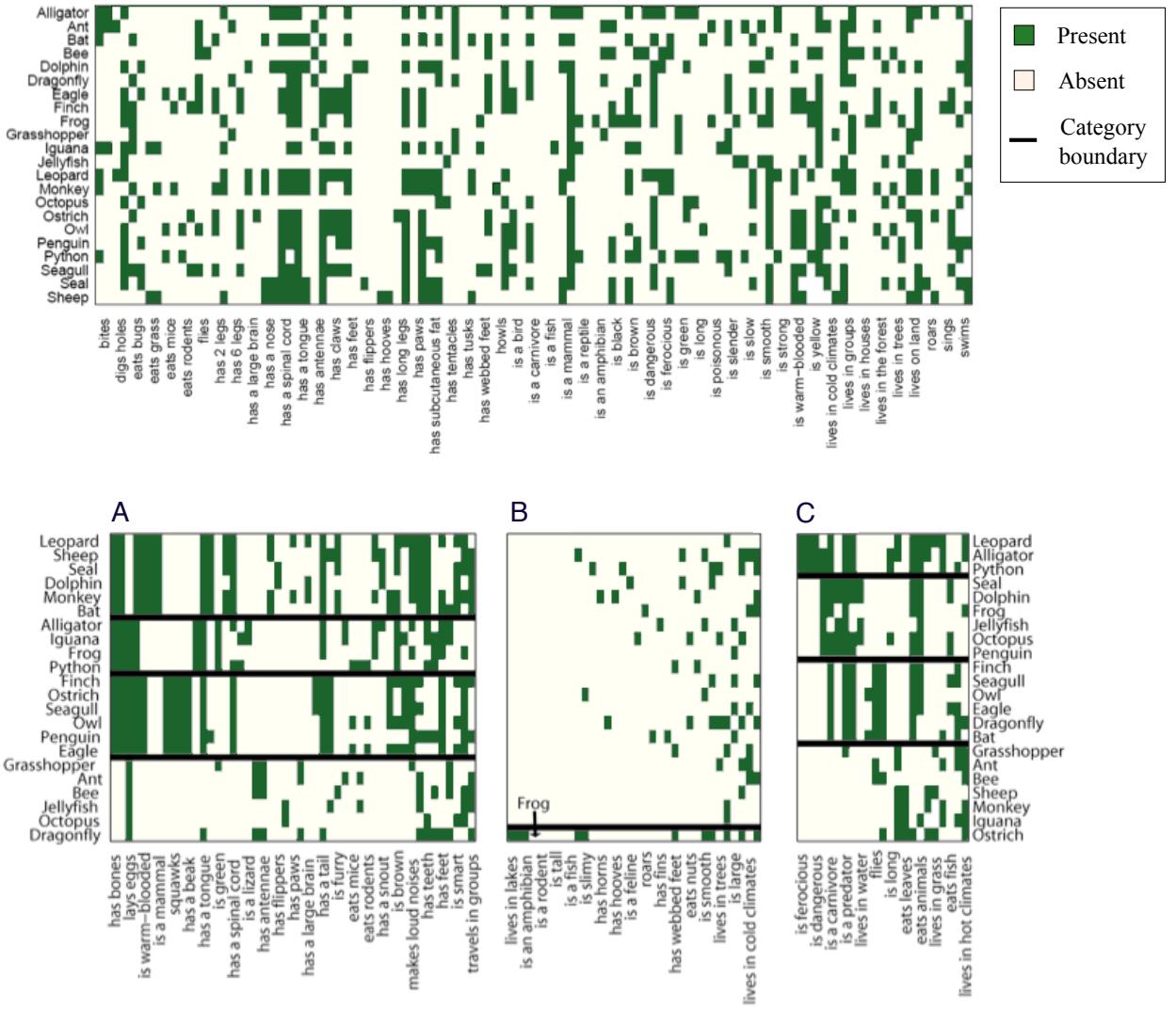


Figure 1: An illustration of the latent structure posited by cross-categorization on a dataset of common-sense judgments about animals. The figure shows the raw input data and one posterior sample from a dataset containing animals and their properties. CrossCat finds three independent signals, or *views*. A taxonomic clustering (left, A) comprises groups of mammals, amphibians and reptiles, birds, and invertebrates, and explains primarily anatomical and physiological variables. An ecological clustering (right, C) cross-cuts the taxonomic groups and specifies groups of carnivorous land predators, sea animals, flying animals, and other land animals, and explains primarily habitat and behavior variables. Finally all animals (except frogs) are lumped together into a cluster of miscellaneous features (center, B) that accounts for a set of idiosyncratic or sparse “noise” variables.

The main advantage offered by Bayesian networks in this setting is that they can use a separate network to model each group of variables. From a statistical perspective, Bayes nets may be effective for sufficiently large, purely discrete datasets where all variables are observed and no hidden variables are needed to accurately model the true data generator. The core modeling difficulty is that many relevant joint distributions are either impossible to represent using a Bayesian network or require prohibitively complex parameterizations. For example, without hidden variables, Bayes nets must emulate the effect of any hidden variables by implicitly marginalizing them out, yielding a dense set of connections. These artificial edges can reduce statistical efficiency: each new parent for a given node can multiplicatively increase the number of parameters to estimate (Elidan, Lotner, Friedman, and Koller, 2001; Elidan and Friedman, 2005). There are also computational difficulties. First, there are no known scalable techniques for fully Bayesian learning of Bayesian networks, so posterior uncertainty about the dependence structure is lost. Second, even when the training data is fully observed, i.e. all variables are observed, search through the space of networks is computationally demanding. Third, if the data is incomplete (or hidden variables are posited), a complex inference subproblem needs to be solved in the inner loop of structure search.

2. Parametric and semi-parametric mixture modeling.

Mixtures of simple parametric models have several appealing properties in this setting. First, they can accurately emulate the joint distribution within each group of variables by introducing a sufficiently large number of mixture components. Second, heterogeneous data types are naturally handled using independent parametric models for each variable chosen based on the type of data it contains. Third, learning and prediction can both be done via MCMC techniques that are linear time per iteration, with constant factors and iteration counts that are often acceptable in practice. Unfortunately, mixture models assume that all variables are (marginally) coupled through the latent mixture component assignments. As a result, posterior samples will often contain good categorizations for one group of variables, but these same categories treat all other groups of mutually dependent variables as noise. This can lead to dramatic under-fitting in high dimensions or when missing values are frequent; this paper includes experiments illustrating this failure mode. Thus if the total number of variables is small enough, and the natural cluster structure of all groups of variables is sufficiently similar, and there is enough data, mixture models may perform well.

3. Multivariate Gaussians with sparse inverse covariances.

High-dimensional continuous distributions are often modeled as multivariate Gaussians with sparse conditional dependencies (Meinshausen and Bühlmann, 2006). Several parameter estimation techniques are available; see e.g. (Friedman, Hastie, and Tibshirani, 2008). The pairwise dependencies produced by these methods form an undirected graph. The underlying assumptions are most appropriate when the number of variables and observations are sufficiently large, the data is naturally continuous and fully observed, and the joint distribution is approximately unimodal. A key advantage of these methods is the availability of fast algorithms for parameter estimation (though extensions for handling missing values require solving challenging non-convex optimization problems (Städler and Bühlmann, 2012)). These

methods also have two main limitations. First, the assumption of joint Gaussianity is unrealistic in many situations (Wasserman, 2011). Second, discrete values must be transformed into numerical values; this invalidates estimates of predictive uncertainty, and can generate other surprising behaviors.

CrossCat combines key computational and statistical strengths of each of these methods. As with nonparametric mixture modeling, CrossCat admits a scalable MCMC algorithm for posterior sampling, handles incomplete data, and does not impose restrictions on data types. CrossCat also preserves the asymptotic consistency of density estimation via Dirichlet process mixture modeling (Dunson and Xing, 2009), and can emulate a broad class of generative processes and joint distributions given enough data. However, unlike mixture modeling but like Bayesian network structure learning, CrossCat can also detect independencies between variables. The “outer” Dirichlet process mixture partitions variables into groups that are independent of one another. As with estimation of sparse multivariate Gaussians (but unlike Bayesian network modeling), CrossCat can handle complex continuous distributions and report pairwise measures of association between variables. However, in CrossCat, the couplings between variables can be nonlinear and heteroscedastic, and induce complex, multi-modal distributions. These statistical properties are illustrated using synthetic tests designed to strain the CrossCat modeling assumptions and inference algorithm.

This paper illustrates the flexibility of CrossCat by applying it to several exploratory analysis and predictive modeling tasks. Results on several real-world datasets of up to 10 million cells are described. Examples include measures of hospital cost and quality, voting records, US state-level unemployment time series, and handwritten digit images. These experiments show that CrossCat can extract latent structures that are consistent with accepted findings and common-sense knowledge in multiple domains. They also show that CrossCat can yield favorable predictive accuracy as compared to generative, discriminative, and model-free baselines.

The remainder of this paper is organized as follows. This section concludes with a discussion of related work. Section 2 focuses on generative model and approximate inference scheme behind CrossCat. Section 3 describes empirical results, and section 4 contains a broad discussion and summary of contributions.

1.1 Related Work

The observation that multiple alternative clusterings can often explain data better than a single clustering is not new to this paper. Methods for finding multiple clusterings have been developed in several fields, including by the authors of this paper (see e.g. Niu, Dy, and Jordan, 2010; Cui, Fern, and Dy, 2007; Guan, Dy, Niu, and Ghahramani, 2010; Li and Shafto, 2011; Rodriguez and Ghosh, 2009; Shafto, Kemp, Mansinghka, Gordon, and Tenenbaum, 2006; Shafto, Kemp, Mansinghka, and Tenenbaum, 2011; Ross and Zemel, 2006). For example, Ross and Zemel (2006) used an EM approach to fit a parametric mixture of mixtures and applied it to image modeling. As nonparametric mixtures and model selection over finite mixtures can behave similarly, it might seem that a nonparametric formulation is a small modification. In fact, nonparametric formulation presented here is based on a super-exponentially larger space of model complexities that includes all possible numbers and sizes of views, and for each view, all possible numbers and sizes of categories. This expressiveness is necessary for the broad applicability of CrossCat. Cross-validation over this set is intractable, motivating the nonparametric formulation and sampling scheme used in this paper.

It is instructive to compare and contrast CrossCat with related hierarchical Bayesian models that link multiple Dirichlet process mixture models, such as the nested Dirichlet process (Rodriguez, Dunson, and Gelfand, 2008) and the hierarchical Dirichlet process (Teh, Jordan, Beal, and Blei, 2006). See Jordan (2010) for a thorough review. This section contains a brief discussion of the most important similarities and differences. The hierarchical Dirichlet process applies independent Dirichlet processes to each dataset, whose atoms are themselves drawn from a single shared Dirichlet process. It thus enables a single pool of clusters to be shared and sparsely expressed in otherwise independent clusterings of several datasets. The differences are substantial. For example, with the hierarchical Dirichlet process, the number of Dirichlet processes is fixed in advance. In CrossCat, each atom on one Dirichlet process is associated with its own Dirichlet process, and inference is used to determine the number that will be expressed in a given finite dataset.

The nested Dirichlet process shares this combinatorial structure with CrossCat, but has been used to build very different statistical models. (Rodriguez et al., 2008) introduces it as a model for multiple related datasets. The model consists of a Dirichlet process mixture over datasets where each component is another Dirichlet process mixture models over the items in that dataset. From a statistical perspective, it can be helpful to think of this construction as follows. First, a top-level Dirichlet process is used to cluster datasets. Second, all datasets in the same cluster are pooled and their contents are modeled via a single clustering, provided by the lower-level Dirichlet process mixture model associated with that dataset cluster.

The differences between CrossCat and the nested Dirichlet process are clearest in terms of the nested Chinese restaurant process representation of the nested DP (Blei, Griffiths, Jordan, and Tenenbaum, 2004; Blei, Griffiths, and Jordan, 2010). In a 2-layer nested Chinese restaurant process, there is one customer per data vector. Each customer starts at the top level, sits a table at their current level according to a CRP, and descends to the CRP at the level below that the chosen table contains. In CrossCat, the top level CRP partitions the variables into views, and the lower level CRPs partition the data vectors into categories for each view. If there are K tables in top CRP, i.e. the dataset is divided into K views, then adding one datapoint leads to the seating of K new customers at level 2. Each of these customers is deterministically assigned to a distinct table. Also, whenever a new customer is created at the top restaurant, in addition to creating a new CRP at the level below, R customers are immediately seated below it (one per row in the dataset).

Close relatives of CrossCat have been introduced by the authors of this paper in the cognitive science literature, and also by other authors in machine learning and statistics. This paper goes beyond this previous work in several ways. Guan et al. (2010) uses a variational algorithm for inference, while Rodriguez and Ghosh (2009) uses a sampler for the stick breaking representation for a Pitman-Yor (as opposed to Dirichlet Process) variant of the model. CrossCat is instead based on samplers that (i) operate over the combinatorial (i.e. Chinese restaurant) representation of the model, not the stick-breaking representation, and (ii) perform fully Bayesian inference over all hyper-parameters. This formulation leads to CrossCat’s scalability and robustness. This paper includes results on tables with millions of cells, without any parameter tuning, in contrast to the 148x500 gene expression subsample analyzed in Rodriguez and Ghosh (2009). These other papers include empirical results comparable in size to the authors’ experiments from Shafto et al. (2006) and Mansinghka, Jonas, Petschulat, Cronin, Shafto, and Tenenbaum (2009); these are 10-100x smaller than some of the examples from this paper. Additionally, all the previous work on variants of the CrossCat model focused on clustering, and did not articulate its use as a general model for

high-dimensional data generators. For example, Guan et al. (2010) does not include predictions, although Rodriguez and Ghosh (2009) does discuss an example of imputation on a 51x26 table.

To the best of our knowledge, this paper is the first to introduce a fully Bayesian, domain-general, semi-parametric method for estimating the joint distributions of high-dimensional data. This method appears to be the only joint density estimation technique that simultaneously supports heterogeneous data types, detects independencies, and produces representations that support efficient prediction. This paper is also the first to empirically demonstrate the effectiveness of the underlying probabilistic model and inference algorithm on multiple real-world datasets with mixed types, and the first to compare predictions and latent structures from this kind of model against multiple generative, discriminative and model-free baselines.

2. The CrossCat Model and Inference Algorithm

CrossCat is based on inference in a column-wise Dirichlet process mixture of Dirichlet process mixture models (Escobar and West, 1995; Rasmussen, 2000) over the rows. The “outer” or “column-wise” Dirichlet process mixture determines which dimensions/variables should be modeled together at all, and which should be modeled independently. The “inner” or “row-wise” mixtures are used to summarize the joint distribution of each group of dimensions/variables that are stochastically assigned to the same modeling subproblem.

This paper presents the Dirichlet processes in CrossCat via the convenient Chinese restaurant process representation (Pitman, 1996). Recall that the Dirichlet process is a stochastic process that maps an arbitrary underlying base measure into a measure over discrete atoms, where each atom is associated with a single draw from the base measure. In a set of repeated draws from this discrete measure, some atoms are likely to occur multiple times. In nonparametric Bayesian mixture modeling, each atom corresponds to a set of parameters for some mixture component; “popular” atoms correspond to mixture components with high weight. The Chinese restaurant process is a stochastic process that corresponds to the discrete residue of the Dirichlet process. It is sequential, easy to describe, easy to simulate, and exchangeable. It is often used to represent nonparametric mixture models as follows. Each data item is viewed as a customer at a restaurant with an infinite number of tables. Each table corresponds to a mixture component; the customers at each table thus comprise the groups of data that are modeled by the same mixture component. The choice probabilities follow a simple “rich-gets-richer” scheme. Let m_j be the number of customers (data items) seated at a given table j , and z_i be the table assignment of customer i (with the first table $z_0 = 0$), then the conditional probability distribution governing the Chinese restaurant process with concentration parameter α is:

$$Pr(z_i = j) \propto \begin{cases} \alpha & \text{if } j = \max(\vec{z}) + 1 \\ m_j & \text{o.w.} \end{cases}$$

This sequence of conditional probabilities induces a distribution over the partitions of the data that is equivalent to the marginal distribution on equivalence classes of atom assignments under the Dirichlet process. The Chinese restaurant process provides a simple but flexible modeling tool: the number of components in a mixture can be determined by the data, with support over all logically possible clusterings. In CrossCat, the *number* of Chinese restaurant processes (over the rows) is determined by the number of tables in a Chinese restaurant process over the columns. The data

itself is modeled by datatype-specific component models for each dimension (column) of the target table.

2.1 The Generative Process

The generative process behind CrossCat unfolds in three steps:

1. **Generating hyper-parameters and latent structure.** First, the hyper-parameters $\vec{\lambda}_d$ for the component models for each dimension are chosen from a vague hyper-prior V_d that is appropriate¹ for the type of data in d . Second, the concentration parameter α for the outer Chinese restaurant process is sampled from a vague gamma hyper-prior. Third, a partition of the variables into views, \vec{z} , is sampled from this outer Chinese restaurant process. Fourth, for each view, $v \in \vec{z}$, a concentration parameter α_v is sampled from a vague hyper-prior. Fifth, for each view v , a partition of the rows \vec{y}^v is drawn using the appropriate inner Chinese restaurant process with concentration α_v .
2. **Generating category parameters for uncollapsed variables.** This paper uses u_d as an indicator of whether a given variable/dimension d is uncollapsed ($u_d = 1$) or collapsed ($u_d = 0$). For each uncollapsed variable, parameters $\vec{\theta}_c^d$ must be generated for each category c from a datatype-compatible prior model M_d .
3. **Generating the observed data given hyper-parameters, latent structure, and parameters.** The dataset $\mathbf{X} = \{x_{(r,d)}\}$ is generated separately for each variable d and for each category $c \in \vec{y}^v$ in the view $v = z_d$ for that variable. For uncollapsed dimensions, this is done by repeatedly simulating from a likelihood model L_d . For collapsed dimensions, we use an exchangeably coupled model ML_d to generate all the data in each category at once.

The details of the CrossCat generative process are as follows:

1. Generate α_D , the concentration hyper-parameter for the Chinese Restaurant Process over dimensions, from a generic Gamma hyper-prior: $\alpha_D \sim \text{Gamma}(k = 1, \theta = 1)$.
2. For each dimension $d \in D$:

- (a) Generate hyper-parameters $\vec{\lambda}_d$ from a data type appropriate hyper-prior with density $p(\vec{\lambda}_d) = V_d(\vec{\lambda}_d)$, as described above. Binary data is handled by an asymmetric Beta-Bernoulli model with pseudocounts $\vec{\lambda}_d = [\alpha_d, \beta_d]$. Discrete data is handled by a symmetric Dirichlet-Discrete model with concentration parameter λ_d . Continuous data is handled by a Normal-Gamma model with $\vec{\lambda}_d = (\mu_d, \kappa_d, \nu_d, \tau_d)$, where μ_d is the mean,

1. The hyper-prior must only assign positive density to valid hyper-parameter values and be sufficiently broad for the marginal distribution for a single data cell has comparable spread to the actual data being analyzed. We have explored multiple hyper-priors that satisfy these constraints on analyses similar to those from this paper; there was little apparent variation. Examples for strictly positive, real-valued hyper-parameters include vague $\text{Gamma}(k = 1, \theta = 1)$ hyper-prior, uniform priors over a broad range, and both linear and logarithmic discretizations. Our reference implementation uses a set of simple data-dependent heuristics to determine sufficiently broad ranges. Chinese restaurant process concentration parameters are given 100-bin log-scale grid discrete priors; concentration parameters for the finite-dimensional Dirichlet distributions used to generate component parameters for discrete data have the same form. For Normal-Gamma models, $\min(\vec{x}_{(.,d)}) \leq \mu_d \leq \max(\vec{x}_{(.,d)})$.

κ_d is the effective number of observations, v_d is the degrees of freedom, and τ_d is the sum of squares.

- (b) Assign dimension d to a view z_d from a Chinese Restaurant Process with concentration hyper-parameter α_D , conditional on all previous draws: $z_d \sim \text{CRP}(\{z_0, \dots, z_{d-1}\}; \alpha_D)$

3. For each view v in the dimension partition \vec{z} :

- (a) Generate α_v , the concentration hyper-parameter for the Chinese Restaurant Process over categories in view v , from a generic hyper-prior: $\alpha_v \sim \text{Gamma}(k = 1, \theta = 1)$.
- (b) For each observed data point (i.e. row of the table) $r \in R$, generate a category assignment y_r^v from a Chinese Restaurant Process with concentration parameter α_v , conditional on all previous draws: $y_r^v \sim \text{CRP}(\{y_0^v, \dots, y_{r-1}^v\}; \alpha_v)$
- (c) For each category c in the row partition for this view \vec{y}^v :
 - i. For each dimension d such that $u_d = 1$ (i.e. its component models are uncollapsed), generate component model parameters $\vec{\theta}_c^d$ from the appropriate prior with density $M_d(\cdot; \vec{\lambda}_d)$ using hyper-parameters $\vec{\lambda}_d$, as follows:
 - A. For binary data, we have a scalar θ_c^d equal to the probability that dimension d is equal to 1 for rows from category c , drawn from a Beta distribution: $\theta_c^d \sim \text{Beta}(\alpha_d, \beta_d)$, where values from the hyper-parameter vector $\vec{\lambda}_d = [\alpha_d, \beta_d]$.
 - B. For categorical data, we have a vector-valued $\vec{\theta}_c^d$ of probabilities, drawn from a symmetric Dirichlet distribution with concentration parameter λ_d : $\vec{\theta}_c^d \sim \text{Dirichlet}(\lambda_d)$.
 - C. For continuous data, we have $\vec{\theta}_c^d = (\mu_c^d, \sigma_c^d)$, the mean and variance of the data in the component, drawn from a Normal-Gamma distribution $(\mu_c^d, \sigma_c^d) \sim \text{NormalGamma}(\vec{\lambda}_d)$.
 - ii. Let $\vec{x}_{(.,d)}^c$ contain all $x_{(r,d)}$ in this component, i.e. for r such that $y_r^z = c$. Generate the data in this component, as follows:
 - A. If $u_d = 1$, i.e. d is uncollapsed, then generate each $x_{(r,d)}$ from the appropriate likelihood model $L_d(\cdot; \vec{\theta}_c^d)$. For binary data, we have $x_{(r,d)} \sim \text{Bernoulli}(\theta_c^d)$; for categorical data, we have $x_{(r,d)} \sim \text{Multinomial}(\vec{\theta}_c^d)$; for continuous data, we have $x_{(r,d)} \sim \text{Normal}(\mu_c^d, \sigma_c^d)$.
 - B. If $u_d = 0$, so d is collapsed, generate the entire contents of $\vec{x}_{(.,d)}^c$ by directly simulating from the marginalized component model that with density $ML_d(\vec{x}_{(.,d)}; \vec{\lambda}_d)$. One approach is to sample from the sequence of predictive distributions $P(x_{(r_i,d)} | \vec{x}_{(.,d)}^{r_i}, \vec{\lambda}_d)$, induced by M_d and L_d , indexing over rows r_i in c .

The key steps in this process can be concisely described:

$$\begin{aligned}
\alpha_D &\sim \text{Gamma}(k=1, \theta=1) \\
\vec{\lambda}_d &\sim V_d(\cdot) && \text{foreach } d \in \{1, \dots, D\} \\
z_d &\sim \text{CRP}(\{z_i \mid i \neq d\}; \alpha_D) && \text{foreach } d \in \{1, \dots, D\} \\
\alpha_v &\sim \text{Gamma}(k=1, \theta=1) && \text{foreach } v \in \vec{z} \\
y_r^v &\sim \text{CRP}(\{y_i^v \mid i \neq r\}; \alpha_v) && \text{foreach } v \in \vec{z} \text{ and } r \in \{1, \dots, R\} \\
\vec{\theta}_c^d &\sim M_d(\cdot; \vec{\lambda}_d) && \text{foreach } v \in \vec{z}, c \in \vec{y}^v, \text{ and } d \text{ such that } z_d = v \text{ and } u_d = 1 \\
\vec{x}_{(\cdot, d)}^c &= \{x_{(r, d)} \mid y_r^v = c\} \sim \begin{cases} \prod_r L_d(\vec{\theta}_c^d) & \text{if } u_d = 1 \\ ML_d(\vec{\lambda}_d) & \text{if } u_d = 0 \end{cases} && \text{foreach } v \in \vec{z} \text{ and each } c \in \vec{y}^v
\end{aligned}$$

2.2 The joint probability density

Recall that the following dataset-specific information is needed to fully specify the CrossCat model:

1. $V_d(\cdot)$, a generic hyper-prior of the appropriate type for variable/dimension d .
2. $\{u_d\}$, the indicators for which variables are uncollapsed.
3. $M_d(\cdot)$ and $L_d(\cdot) \forall d$ s.t. $u_d = 1$, a datatype-appropriate parameter prior (e.g. a Beta prior for binary data, Normal-Gamma for continuous data, or Dirichlet for discrete data) and likelihood model (e.g. Bernoulli, Normal or Multinomial).
4. $ML_d(\cdot) \forall d$ s.t. $u_d = 0$, a datatype-appropriate marginal likelihood model, e.g. the collapsed version of the conjugate pair formed by some M_d and L_d .
5. $T_d(\{x\})$, the sufficient statistics for the component model for some collapsed dimension d from a subset of the data $\{x\}$. Arbitrary non-conjugate component models can be numerically collapsed by choosing $T_d(\{x\}) = \{x\}$.

This paper will use **CC** to denote the information necessary to capture the dependence of CrossCat on the data \mathbf{X} . This includes the view concentration parameter α_D , the variable-specific hyper-parameters $\{\vec{\lambda}_d\}$, the view partition \vec{z} , the view-specific concentration parameters $\{\alpha_v\}$ and row partition $\{\vec{y}^v\}$, and the category-specific parameters $\{\vec{\theta}_c^d\}$ or sufficient statistics $T_d(\vec{x}_{(\cdot, d)})$. This paper will also overload ML_d, M_d, V_d, L_d , and CRP to each represent both probability density functions and stochastic simulators; the distinction should be clear based on context. Given this notation, we have:

$$\begin{aligned}
P(\mathbf{CC}, \mathbf{X}) &= P(\mathbf{X}, \{\vec{\theta}_c^d\}, \{\vec{y}^v, \alpha_v\}, \{\vec{\lambda}_d\}, \vec{z}, \alpha_D) \\
&= e^{-\alpha_D} \left(\prod_{d \in D} V_d(\vec{\lambda}_d) \right) \text{CRP}(\vec{z}; \alpha_D) \left(\prod_{v \in \vec{z}} e^{-\alpha_v} \text{CRP}(\vec{y}^v; \alpha_v) \right) \\
&\times \prod_{v \in \vec{z}} \prod_{c \in \vec{y}^v} \prod_{d \in \{i \text{ s.t. } z_i=v\}} \left(\begin{cases} ML_d(T_d(\vec{x}_{(\cdot, d)}^c); \vec{\lambda}_d) & \text{if } u_d = 1 \\ M_d(\vec{\theta}_c^d; \vec{\lambda}_d) \prod_{r \in c} L_d(x_{(r, d)}; \vec{\theta}_c^d) & \text{if } u_d = 0 \end{cases} \right)
\end{aligned}$$

2.3 Hypothesis space and modeling capacity

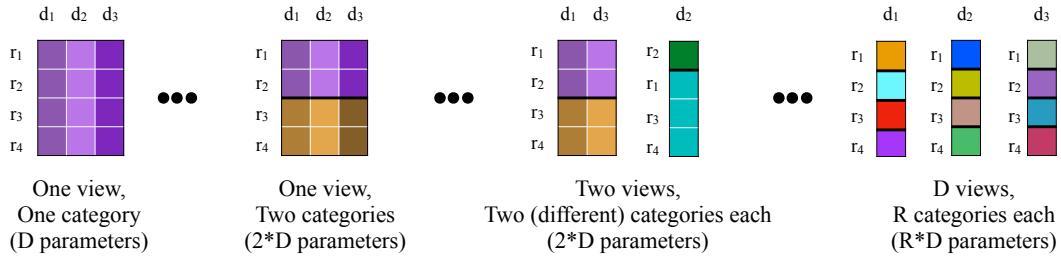


Figure 2: Model structures drawn from the space of all logically possible cross-categorizations of a 4 row, 3 column dataset. In each structure, all data values (cells) that are governed by the same parametric model are shown in the same color. If two cells have different colors, they are modeled as conditionally independent given the model structure and hyper-parameters. In general, the space of all cross-categorizations contains a broad class of simple and complex data generators. See the main text for details.

The modeling assumptions encoded in CrossCat are designed to enable it to emulate a broad class of data generators. One way to assess this class is to study the full hypothesis space of CrossCat, that is, all logically possible cross-categorizations. Figure 2 illustrates the version of this space that is induced by a 4 row, 3 column dataset. Each cross-categorization corresponds to a model structure — a set of dependence and independence assumptions — that is appropriate for some set of statistical situations. For example, conditioned on the hyper-parameters, the dependencies between variables and data values can be either dense or sparse. A group of dependencies will exhibit a unimodal joint distribution if they are modeled using only a single cluster. Strongly bimodal or multi-modal distributions as well as nearly unimodal distributions with some outliers are recovered by varying the number of clusters and their size. The prior favors stochastic relationships between groups of variables, but also supports (nearly) deterministic models; these correspond to structures with a large number of clusters that share low-entropy component models.

The CrossCat generative process favors hypotheses with multiple views and multiple categories per view. A useful rule of thumb is to expect $O(\log(D))$ views with $O(\log(R))$ categories each a priori. Asserting that a dataset has several views and several categories per view corresponds to asserting that the underlying data generator exhibits several important statistical properties. The first is that the dataset contains variables that arise from several distinct causal processes, not just a single one. The second is that these processes cannot be summarized by a single parametric model, and thus induce non-Gaussian or multi-modal dependencies between the variables.

2.4 Posterior Inference Algorithm

Posterior inference is carried out by simulating an ergodic Markov chain that converges to the posterior (Gilks, 1999; Neal, 1998). The state of the Markov chain is a data structure storing the cross-categorization, sufficient statistics, and all uncollapsed parameters and hyper-parameters. Figure

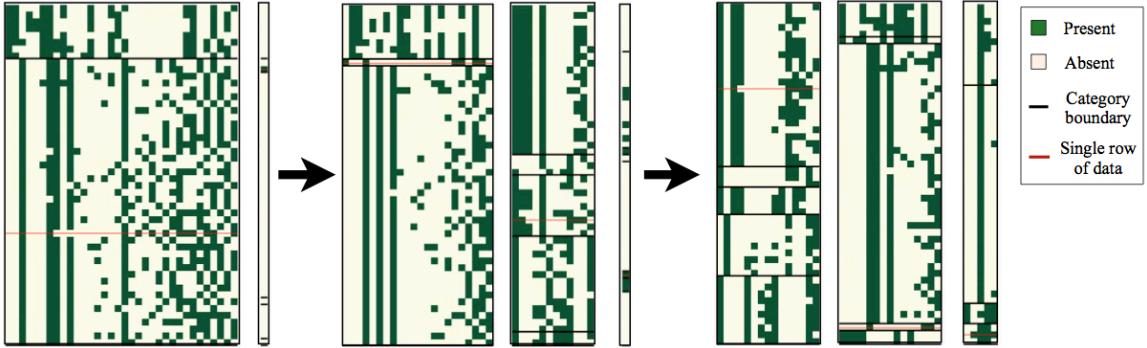


Figure 3: Snapshots of the Markov chain for cross-categorization on a dataset of human object-feature judgments. Each of the three states shows a particular cross-categorization that arose during a single Markov chain run, automatically rendered using the latent structure from cross-categorization to inform the layout. Black horizontal lines separate categories within a view. The red horizontal line follows one row of the dataset. Taken from left to right, the three states span a typical run of roughly 100 iterations; the first is while the chain appears to be converging to a high probability region, while the last two illustrate variability within that region.

3 shows several sampled states from a typical run of the inference scheme on the dataset from Figure 1.

The CrossCat inference Markov chain initializes a candidate state by sampling it from the prior². The transition operator that it iterates consists of an outer cycle of several kernels, each performing cycle sweeps that apply other transition operators to each segment of the latent state. The first is a cycle kernel for inference over the outer CRP concentration parameter α and a cycle of kernels over the inner CRP concentration parameters $\{\alpha_v\}$ for each view. The second is a cycle of kernels for inference over the hyper-parameters $\vec{\lambda}_d$ for each dimension. The third is a kernel for inference over any uncollapsed parameters $\vec{\theta}_c^d$. The fourth is a cycle over dimensions of an inter-view auxiliary variable Gibbs kernel that shuffles dimensions between views. The fifth is itself a cycle over views of cycles that sweep a single-site Gibbs sampler over all the rows in the given view. This chain corresponds to the default auxiliary variable Gibbs sampler that the Venture probabilistic programming platform (Mansinghka, Selsam, and Perov, 2014) produces when given the CrossCat model written as a probabilistic program.

More formally, the Markov chain used for inference is a cycle over the following kernels:

1. **Concentration hyper-parameter inference: updating α_D and each element of $\{\alpha_v\}$.** Sample α_D and all the α_v s for each view via a discretized Gibbs approximation to the posterior, $\alpha_D \sim P(\alpha_D | \vec{z})$ and $\alpha_v \sim P(\alpha_v | \vec{y}^v)$. For each α , this involves scoring the CRP marginal likelihood at a fixed number of grid points — typically ~ 100 — and then re-normalizing and sampling from the resulting discrete approximation.
2. Anecdotally, this initialization appears to yield the best inference performance overall. One explanation can be found by considering a representative subproblem of inference in CrossCat: performing inference in one of the inner CRP mixture models. A maximally dispersed initialization, with each of the N rows in its own category, requires $O(N^2)$ time for its first Gibbs sweep. An initialization that places all rows in a single category requires $O(1)$ time for its first sweep but can spend many iterations stuck in or near the “low resolution” model encoded by this initial configuration.

2. **Component model hyper-parameter inference: updating the elements of $\{\vec{\lambda}_d\}$.** For each dimension, for each hyper-parameter, discretize the support of the hyper-prior and numerically sample from an approximate hyper-posterior distribution. That is, implement an appropriately-binned discrete approximation to a Gibbs sampler for $\vec{\lambda}_d \sim P(\vec{\lambda}_d | \vec{x}_d, \vec{y}_{-d})$ (i.e. we condition on the vertical slice of the input table described by the hyper-parameters, and the associated latent variables). For conjugate component models, the probabilities depend only on the sufficient statistics needed to evaluate this posterior. Each hyper-parameter adjustment requires an operation linear in the number of categories, since the scores for each category (i.e. the marginal probabilities) must be recalculated, after each category's statistics are updated. Thus each application of this kernel takes time proportional to the number of dimensions times the maximum number of categories in any view.
3. **Category inference: updating the elements of $\{\vec{y}^v\}$ via Gibbs with auxiliary variables.** For each entity in each view, this transition operator samples a new category assignment from its conditional posterior. A variant of Algorithm 8 from (Neal, 1998) (with $m=1$) is used to handle uncollapsed dimensions.

The category inference transition operator will sample y_r^v , the categorization for row r in view v , according to its conditioned distribution given the other category assignments \vec{y}_{-r}^v , parameters $\{\vec{\theta}_c^d\}$ and auxiliary parameters. If $u_d = 0 \forall d$ s.t. $z_d = v$, i.e. there are no uncollapsed dimensions in this view, then this reduces to the usual collapsed Gibbs sampler applied to the subset of data within the view. Otherwise, let $\{\vec{\phi}^d\}$ denote auxiliary parameters for each uncollapsed dimension d (where $u_d = 1$) of the same form as $\vec{\theta}_c^d$. Before each transition, these parameters are chosen as follows:

$$\vec{\phi}^d \sim \begin{cases} \delta_{\vec{\theta}_c^d} & \text{if } y_r^v = y_j^v \iff r = j \\ M_d(\vec{\lambda}_d) & \text{o.w. } (y_r^v \in \vec{y}_{-r}^v) \end{cases}$$

In this section, c^+ will denote the category associated with the auxiliary variable. If $y_r^v \in \vec{y}_{-r}^v$, then $c^+ = \max(\vec{y}_{-r}^v) + 1$, i.e. a wholly new category will be created, and by sampling $\vec{\phi}^d$ this category will have newly sampled parameters. Otherwise, $c^+ = y_r^v$, i.e. row r was a singleton, so its previous category assignment and parameters will be reused.

Given the auxiliary variables, we can derive the target density of the transition operator by expanding the joint probability density:

$$\begin{aligned} y_r^v &\sim P(y_r^v | \vec{y}_{-r}^v, \{\vec{\lambda}_d, \{x_{(\cdot, d)}\} | d \text{ s.t. } z_d = v\}, \{\{\vec{\theta}_c^d | c \in \vec{y}_{-r}^v\} | d \text{ s.t. } z_d = v \text{ and } u_d = 1\}, \{\vec{\phi}^d\}) \\ &\propto \text{CRP}(y_r^v; \vec{y}_{-r}^v, \alpha_v) \prod_{d \in \{i \text{ s.t. } z_i=v\}} \left(\begin{cases} ML_d(T_d(\vec{x}_{(\cdot, d)}^c), \vec{\lambda}_d) & \text{if } u_d = 0 \\ M_d(\vec{\theta}_c^d; \vec{\lambda}_d) \prod_{r \in c} L_d(x_{(r, d)}; \vec{\theta}_c^d) & \text{if } u_d = 1 \text{ and } y_r^v \in \vec{y}_{-r}^v \\ M_d(\vec{\phi}_c^d; \vec{\lambda}_d) \prod_{r \in c} L_d(x_{(r, d)}; \vec{\phi}_c^d) & \text{if } u_d = 1 \text{ and } y_r^v = c^+ \notin \vec{y}_{-r}^v \end{cases} \right) \end{aligned}$$

The probabilities this transition operator needs can be obtained by iterating over possible values for y_r^v , calculating their joint densities, and re-normalizing numerically. These operations can be implemented efficiently by maintaining and incrementally modifying a representation of **CC**, updating sufficient statistics and a joint probability accumulator after each change

(Mansinghka, 2007). The complexity of resampling y_r^v for all rows r and views v is $O(VRCD)$, where V is the number of views, R the number of rows, C the maximum number of categories in any view, and D is the number of dimensions.

4. **Inter-view inference: updating the elements of \vec{z} via Gibbs with auxiliary variables.** For each dimension d , this transition operator samples a new view assignment z_d from its conditional posterior. As with the category inference kernel, this can be viewed as a variant of Algorithm 8 from (Neal, 1998) (with $m = 1$), applied to the “outer” Dirichlet process mixture model in CrossCat. This mixture has uncollapsed, non-conjugate component models that are themselves Dirichlet process mixtures.

Let v^+ be the index of the new view. The auxiliary variables are $\alpha_{v^+}, \vec{y}^{v^+}$ and $\{\theta_c^d \mid c \in \vec{y}^{v^+}\}$ (if $u_d = 1$). If $z_d \in \vec{z}^{-d}$, then $v^+ = \max(\vec{z}) + 1$, and the auxiliary variables are sampled from their priors. Otherwise, $v^+ = z_d$, and the auxiliary variables are deterministically set to the values associated with z_d . Given values for these variables, the conditional distribution for z_d can be derived as follows:

$$\begin{aligned} z_d &\sim P(z_d \mid \alpha_D, \vec{\lambda}_d, \vec{z}^{-d}, \alpha_{v^+}, \{\vec{y}^v\}, \{\{\theta_c^d \mid c \in \vec{y}^{z_j}\} \mid j \in D\}, \mathbf{X}) \\ &\propto \text{CRP}(z_d; \vec{z}^{-d}, \alpha_D) \prod_{c \in \vec{y}^d} \left(\begin{cases} M\mathcal{L}_d(T_d(\vec{x}_{(.,d)}^c), \vec{\lambda}_d) & \text{if } u_d = 1 \\ M_d(\vec{\theta}_c^d; \vec{\lambda}_d) \prod_{r \in c} L_d(x_{(r,d)}; \vec{\theta}_c^d) & \text{if } u_d = 0 \end{cases} \right) \end{aligned}$$

This transition operator shuffles individual columns between views, weighing their compatibility with each view by multiplying likelihoods for each category. A full sweep thus has time complexity $O(DVCR)$. Note that if a given variable is a poor fit for its current view, its hyper-parameters and parameters will be driven to reduce the dependence of the likelihood for that variable on its clustering. This makes it more likely for row categorizations proposed from the prior to be accepted.

Inference over the elements of \vec{z} can also be done via a mixture of a Metropolis-Hastings birth-death kernel to create new views with a standard Gibbs kernel to reassign dimensions among pre-existing views. In our experience, both transition operators yield comparable results on real-world data; the Gibbs auxiliary variable kernel is presented here for simplicity.

5. **Component model parameter inference: updating $\{\vec{\theta}_c^d \mid u_d = 1\}$.** Each dimension or variable whose component models are uncollapsed must be equipped with a suitable ergodic transition operator T that converges to the local parameter posterior $P(\vec{\theta}_c^d \mid \vec{x}_{(.,d)}^c, \vec{\lambda}_d)$. Exact Gibbs sampling is often possible when L_d and M_d are conjugate.

CrossCat’s scalability can be assessed by multiplying an estimate of how long each transition takes with an estimate of how many transitions are needed to get good results. The experiments in this paper use $\sim 10\text{-}100$ independent samples. Each sample was based on runs of the inference Markov chain with $\sim 100\text{-}1,000$ transitions. Taking these numbers as rough constants, scalability is governed by the asymptotic orders of growth. Let R be the number of rows, D the number of dimensions, V the maximum number of views and C the maximum number of categories. The memory needed to store the latent state is the sum of the memory needed to store the D hyper-parameters

and view assignments, the VC parameters/sufficient statistics, and the VR category assignments, or $O(D + VC + VR)$. Assuming a fully dense data matrix, the loops in the transition operator described above scale as $O(DC + RDVC + RDVC + DC) = O(RDVC)$, with the RD terms scaling down following the data density.

This paper shows results from both open-source and commercial implementations on datasets of up to ~ 10 million cells³. Because this algorithm is asymptotically linear in runtime with low memory requirements, a number of performance engineering and distributed techniques can be applied to reach larger scales at low latencies. Performance engineering details are beyond the scope of this paper.

2.5 Exploration and Prediction Using Posterior Samples

Each approximate posterior sample provides an estimate of the full joint distribution of the data. It also contains a candidate latent structure that characterizes the dependencies between variables and provides an independent clustering of the rows with respect to each group of dependent variables. This section gives examples of exploratory and predictive analysis problems that can be solved by using these samples. Prediction is based on calculating or sampling from the conditional densities implied by each sample and then either averaging or resampling from the results. Exploratory queries typically involve Monte Carlo estimation of posterior probabilities that assess structural properties of the latent variables posited by CrossCat and the dependencies they imply. Examples include obtaining a global map of the pairwise dependencies between variables, selecting those variables that are probably predictive of some target, and identifying rows that are similar in light of some variables of interest.

2.5.1 PREDICTION

Recall that **CC** represents a model for the joint distribution over the variables along with sufficient statistics, parameters, a partition of variables into views, and categorizations of the rows in the data \mathbf{X} . Variables representing the latent structure associated with a particular posterior sample \hat{CC}_s will all be indexed by s , e.g. z_d^s . Also let Y_v^+ represent the category assignment of a new row in view v , and let $\{t_i\}$ and $\{g_j\}$ be the sets of target variables and given variables in a given predictive query.

To generate predictions by sampling from the conditional density on targets given the data, we must simulate

$$\{\hat{x}_{t_i}\} \sim p(\{X_{t_i}\} | \{X_{g_i} = x_{g_i}\}, \mathbf{X})$$

Given a set of models, this can be done in two steps. First, from each model, sample a categorization from each view conditioned on the values of the given variables. Second, sample values for each target variable by simulating from the target variable's component model for the sampled category:

3. A variation on CrossCat was the basis of Veritable, a general-purpose machine learning system built by Navia Systems/Prior Knowledge Inc. This implementation became a part of Salesforce.com's predictive analytics infrastructure. At Navia, CrossCat was applied to proprietary datasets from domains such as operations management for retail, clinical virology, and quantitative finance.

$$\begin{aligned}
\hat{C}C_s &\sim p(\mathbf{CC}|\mathbf{X}) \\
c_v^s &\sim p(Y_v^+ | \{X_{g_j} = x_{g_j}\}, z_{g_j}^s = v) \\
\hat{x}_{t_i}^s &\sim p(X_{t_i} | c_{z_{t_i}}^s) = \int L(x_{t_i}; \vec{\theta}_{c_v^s}^{t_i}) M(\vec{\theta}_{c_v^s}^{t_i}; \vec{\lambda}_{t_i}) d\vec{\theta}
\end{aligned}$$

The category kernel from the MCMC inference algorithm can be re-used to sample from c_v^s . Also, sampling from $\hat{x}_{t_i}^s$ can be done directly given the sufficient statistics for data types whose likelihood models and parameter priors are conjugate. In other cases, either $\vec{\theta}$ will be represented as part of $\hat{C}C_s$ or sampled on demand.

The same latent variables are also useful for evaluating the conditional density for a desired set of predictions:

$$\begin{aligned}
p(\{X_{t_i} = x_{t_i}\} | \{X_{g_j} = x_{g_j}\}, \mathbf{X}) &\approx \frac{1}{N} \sum_s p(\{X_{t_i} = x_{t_i}\} | \{X_{g_j} = x_{g_j}\}, \mathbf{CC} = \hat{C}C_s) \\
&= \frac{1}{N} \sum_s \prod_{v \in \mathcal{Z}^s} p(\{X_{t_i} = x_{t_i} | z_{g_j}^s = v\} | Y_v^+ = c) p(Y_v^+ = c | \{X_{g_j} = x_{g_j} | z_{g_j}^s = v\})
\end{aligned}$$

Many problems of prediction can be reduced to sampling from and/or calculating conditional densities. Examples include classification, regression and imputation. Each can be implemented by forming estimates $\{X_{t_i}^*\}$ of the target variables. By default, the implementation from this paper implementation uses the mean of the predictive to impute continuous values. This is equivalent to choosing the value that minimizes the expected square loss under the empirical distribution induced by a set of predictive samples. For discrete values, the implementation uses the most probable value, equivalent to minimizing 0-1 loss, and calculates it by directly evaluating the conditional density of each possible value. This approach to prediction can also handle nonlinear and/or stochastic relationships within the set of target variables $\{X_{t_i}\}$ and between the given variables $\{X_{g_i}\}$ and the targets. It is easy to implement in terms of the same sampling and probability calculation kernels that are necessary for inference.

This formulation of prediction scales linearly in the number of variables, categories, and view. It is also sub-linear in the number of variables when dependencies are sparse, and parallelizable over the views, the posterior samples, and the generated samples from the conditional density. Future work will explore the space of tradeoffs between accuracy, latency and throughput that can be achieved using this basic design.

2.5.2 DETECTING DEPENDENCIES BETWEEN VARIABLES

To detect dependencies between groups of variables, it is natural to use a Monte Carlo estimate of the marginal posterior probability that a set of variables $\{q_i\}$ share the same posterior view. Using s as a superscript to select values from a specific sample, we have:

$$\begin{aligned}
Pr[z_{q_0} = z_{q_1} = \dots = z_{q_k} | \mathbf{X}] &\approx \frac{1}{N} \sum_s Pr[z_{q_0}^s = z_{q_1}^s = \dots = z_{q_k}^s | \hat{C}C_s] \\
&= \frac{\#(\{s | z_{q_0}^s = z_{q_1}^s = \dots = z_{q_k}^s\})}{N}
\end{aligned}$$

These probabilities also characterize the marginal dependencies and independencies that are explicitly represented by CrossCat. For example, pairwise co-assignment in \vec{z} determines⁴ pairwise marginal independence under the generative model:

$$X_{q_i} \perp\!\!\!\perp X_{q_j} \iff z_{q_i} \neq z_{q_j}$$

The results in this paper often include the “z-matrix” of marginal dependence probabilities $\mathbf{Z} = [Z_{(i,j)}]$, where $Z_{(i,j)} = 1 - Pr[X_i \perp\!\!\!\perp X_j | \mathbf{X}]$. This measure is used primarily for simplicity; other measures of the presence or strength of predictive relationships are possible.

2.5.3 ESTIMATING SIMILARITY BETWEEN ROWS

Exploratory analyses often make use of “similarity” functions defined over pairs of rows. One useful measure of similarity is given by the probability that two pieces of data were generated from the same statistical model (Tenenbaum and Griffiths, 2001; Ghahramani and Heller, 2006). CrossCat naturally induces a context-sensitive similarity measure between rows that has this form: the probability that two items come from the same category in some context. Here, contexts are defined by target variables, and comprise the set of views in which that variable participates (weighted by their probability). This probability is straightforward to estimate given a collection of samples:

$$1 - Pr[x_{(r,c)} \perp\!\!\!\perp x_{(r',c)} | \mathbf{X}, \vec{\lambda}_c] \approx \frac{\#(\{s | y_{(s,r)}^{z_c^s} = y_{(s,r')}^{z_c^s}\})}{N}$$

This measure relies on CrossCat’s detection of marginal dependencies to determine which variables are relevant in any given context. The component models largely determine how differences in each variable in that view will be weighted when calculating similarity.

2.6 Assessing Inference Quality

A central concern is that the single-site Gibbs sampler used for inference might not produce high-quality models or stable posterior estimates within practical running times. For example, the CrossCat inference algorithm might rapidly converge to a local minimum in which all proposals to create new views are rejected. In this case, even though the Gibbs sampler will appear to have converged, the models it produces could yield poor inference quality.

This section reports four experiments that illustrate key algorithmic and statistical properties of CrossCat. The first experiment gives a rough sense of inference efficiency by comparing the energies of ground truth states to the energies of states sampled from CrossCat on data generated by the model. The second experiment assesses the convergence rate and the reliability of estimates of posterior expectations on a real-world dataset. The third experiment explores CrossCat’s resistance to under-fitting and over-fitting by running inference on datasets of Gaussian noise. The fourth experiment assesses CrossCat’s predictive accuracy in a setting with a large number of distractors and a small number of signal variables. It shows that CrossCat yields favorable accuracy compared to several baseline methods.

4. This paper defines independence in terms of the generative process and latent variables. Two variables in different views are explicitly independent, but two variables in the same view are coupled through the latent cluster assignment. This is clear if there are multiple clusters. Even if there is just one cluster, if α_v remains nonzero as N goes to infinity, then eventually there will be more than one cluster. A predictive definition of independence in terms of nonzero mutual information will differ in some cases; a comparison between these candidate measures is beyond the scope of this paper..

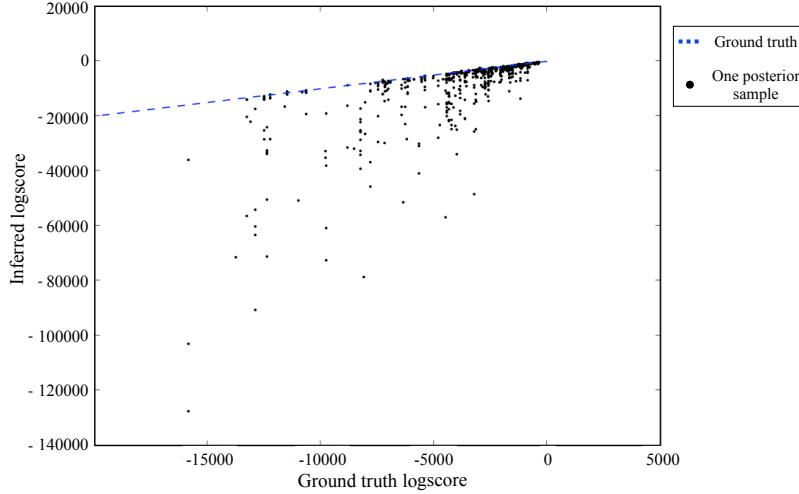


Figure 4: The joint density of the latent cross-categorization and training data for $\sim 1,000$ samples from CrossCat’s inference algorithm, compared to ground truth. Each point corresponds to a sample drawn from an approximation of the CrossCat posterior distribution after 200 iterations on data from a randomly chosen CrossCat model. Table sizes range from 10x10 to 512x512. Points on the blue line correspond to samples with the same joint density as the ground truth state. Points lying above the line correspond to models that most likely underestimate the entropy of the underlying generator, i.e. they have over-fit the data. CrossCat rarely produces such samples. Some points lie significantly below the line, overestimating the entropy of the generator. These do not necessarily correspond to “under-fit” models, as the true posterior will be broad (and may also induce broad predictions) when data is scarce.

The next experiment assesses the stability and efficiency of CrossCat inference on real-world data. Figure 5a shows the evolution of Monte Carlo dependence probability estimates as a function of the number of Markov chain iterations. Figure 5b shows traces of the number of views for each chain in the same set of runs. ~ 100 iterations appears sufficient for initializations to be forgotten, regardless of the number of views sampled from the CrossCat prior. At this point, Monte Carlo estimates appear to stabilize, and the majority of states (~ 40 of 50 total) appear to have 4, 5 or 6 views. This stability is not simply due to a local minimum: after 700 iterations, transitions that create or destroy views are still being accepted. However, the frequency of these transitions does decrease. It thus seems likely that the standard MCMC approach of averaging over a single long chain run might require significantly more computation than parallel chains. This behavior is typical for applications to real-world data. We typically use 10-100 chains, each run for 100-1,000 iterations, and have consistently obtained stable estimates.

The convergence measures from (Geweke, 1992) are also included for comparison, specifically the numerical standard error (NSE) and relative numerical efficiency (RNE) for the view CRP parameter α to assess autocorrelations (LeSage, 1999). NSE values near 0 and RNE values near 1 indicate approximately independent draws. These values were computed using a 0%, 4%, 8%, and 15% autocorrelation taper. NSE values were near zero and did not differ markedly: .023, .021, .018, and .018. Similarly, RSE values were near 1 and did not differ markedly: 1, 1.23, 1.66, and

1.54. These results suggest that there is acceptably low autocorrelation in the sampled values of the hyper-parameters.

The reliability of CrossCat reflects simple but important differences between the way single-site Gibbs sampling is used here and standard MCMC practice in machine learning. First, CrossCat uses independent samples from parallel chains, each initialized with an independent sample from the CrossCat prior. In contrast, typical MCMC schemes from nonparametric Bayesian statistics use dependent samples obtained by thinning a single long chain that was deterministically initialized. For example, Gibbs samplers for Dirichlet process mixtures are often initialized to a state with a single cluster; this corresponds to a single-view single-category state for CrossCat. Second, CrossCat performs inference over hyper-parameters that control the expected predictability of each dimension, as well as the concentration parameters of all Dirichlet processes. Many machine learning applications of nonparametric Bayes do not include inference over these hyper-parameters; instead, they are set via cross-validation or other heuristics.

There are mechanisms by which these differences could potentially explain the surprising reliability and speed of CrossCat inference as compared to typical Gibbs samplers. Recall that the regeneration time of a Markov chain started at its equilibrium distribution is the (random) amount of time it needs to “forget” its current state and arrive at an independent sample. For CrossCat, this regeneration time appears to be substantially longer than convergence time from the prior. States from the prior are unlikely to have high energy or be near high energy regions, unlike states drawn from the posterior. Second, hyper-parameter inference — especially those controlling the expected noise in the component models, not just the Dirichlet process concentrations — provides a simple mechanism that helps the sampler exit local minima. Consider a dimension that is poorly explained by the categorization in its current view. Conditioned on such a categorization, the posterior on the hyper-parameter will favor increasing the expected noisiness of the clusters, to better accommodate the data. Once the hyper-parameter enters this regime, the model becomes less sensitive to the specific clustering used to explain this dimension. This therefore also increases the probability that the dimension will be reassigned to any other pre-existing view. It also increases the acceptance probability for proposals that create a new view with a random categorization. Once a satisfactory categorization is found, however, the Bayesian Occam’s Razor favors reducing the expected entropy of the clusters. Similar dynamics were described in (Mansinghka, Kulkarni, Perov, and Tenenbaum, 2013); a detailed study is beyond the scope of this paper.

The third simulation, shown in Figure 7, illustrates CrossCat’s behavior on datasets with low-dimensional signals amidst high-dimensional random noise. In each case, CrossCat rapidly and confidently detects the independence between the “distractor” dimensions, i.e. it does not over-fit. Also, when the signal is strong or there are few distractors, CrossCat confidently detects the true predictive relationships. As the signals become weaker, CrossCat’s confidence decreases, and variation increases. These examples qualitatively support the use of CrossCat’s estimates of dependence probabilities as indicators of the presence or absence of predictive relationships. A quantitative characterization of CrossCat’s sensitivity and specificity, as a function of both sample size and strength of dependence, is beyond the scope of this paper.

Many data analysis problems require sifting through a large pool of candidate variables in settings where only a small fraction are relevant for any given prediction. The fourth experiment, shown in Figure 7, illustrates CrossCat’s behavior in this setting. The test datasets contain 10 “signal” dimensions generated from a 5-component mixture model, plus 10-1,000 “distractor” dimensions generated by an independent 3-component mixture that clusters the data differently. As the

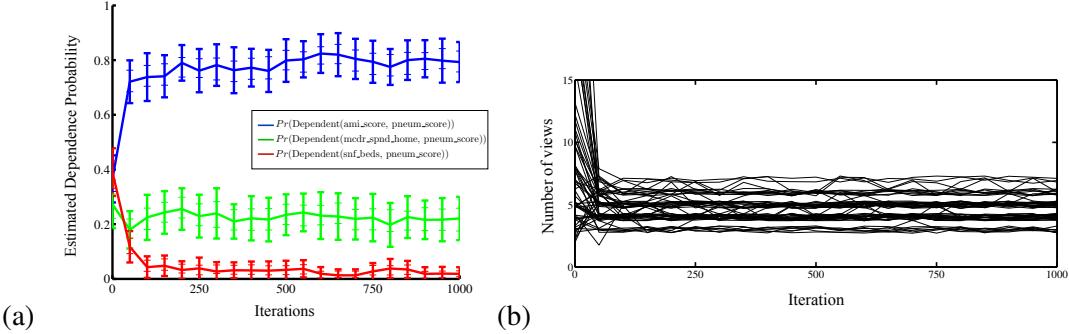


Figure 5: A quantitative assessment of the convergence rate of CrossCat inference and the stability of posterior estimates on a real-world health economics dataset. (a) shows the evolution of simple Monte Carlo estimates of the probability of dependence of three pairs of variables, made from independent chains initialized from the prior, as a function of the number of iterations of inference. Thick error bars show the standard deviation of estimates across 50 repetitions, each with 20 samples; thin lines show the standard deviation of estimates from 40 samples. Estimates stabilize after ~ 100 iterations. (b) shows the number of views for 50 of the same Markov chain runs. After ~ 100 iterations, states with 4, 5 or 6 views dominate the sample, and chains still can switch into and out of this region after 700 iterations.

number of distractors increases, the likelihood becomes dominated by the distractors. The experiment compares imputation accuracy for several methods — CrossCat; mixture modeling; column-wise averaging; imputation by randomly chosen values; and a popular model-free imputation technique (Hastie, Tibshirani, Sherlock, Eisen, Brown, and Botstein, 1999) — on problems with varying numbers of distractors. CrossCat remains accurate when the number of distractors is 100x larger than the number of signal variables. As expected, mixtures are effective in low dimensions, but inaccurate in high dimensions. When the number of distractors equals the number of signal variables, the mixture posterior grows bimodal, including one mode that treats the signal variables as noise. This mode dominates when the number of distractors increases further.

$1.0 - \Pr[X_i \perp\!\!\!\perp X_k | \mathbf{X}]$
for strong signal,
many distractors
($\rho = 0.7, D = 20$)

Moderate signal,
few distractors
($\rho = 0.5, D = 8$)

Moderate signal,
many distractors
($\rho = 0.5, D = 20$)

Weak signal,
few distractors
($\rho = 0.25, D = 8$)

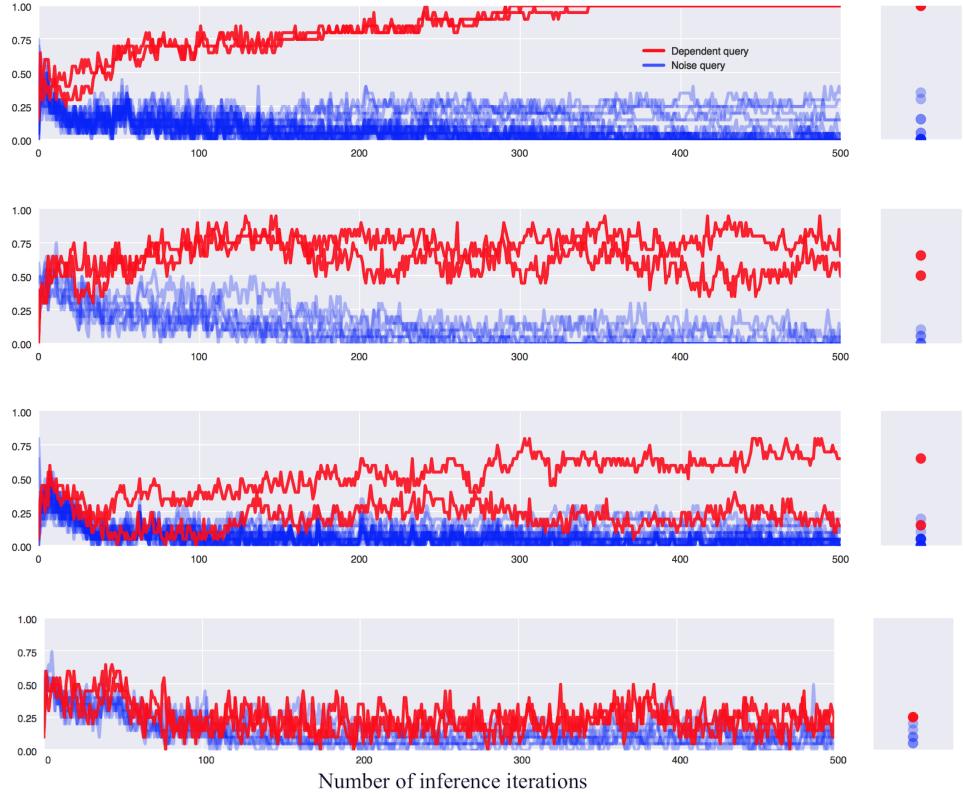


Figure 6: Detected dependencies given two correlated signal variables and multiple independent distractors. This experiment illustrates CrossCat’s sensitivity and specificity to pairwise relationships on multivariate Gaussian datasets with 100 rows. In each dataset, two pairs of variables have nonzero correlation ρ . The remaining $D - 4$ dimensions are uncorrelated distractors. Each row shows the inferred dependencies between 20 randomly sampled pairs of distractors (blue) and the two pairs of signal variables (red). See main text for further discussion.

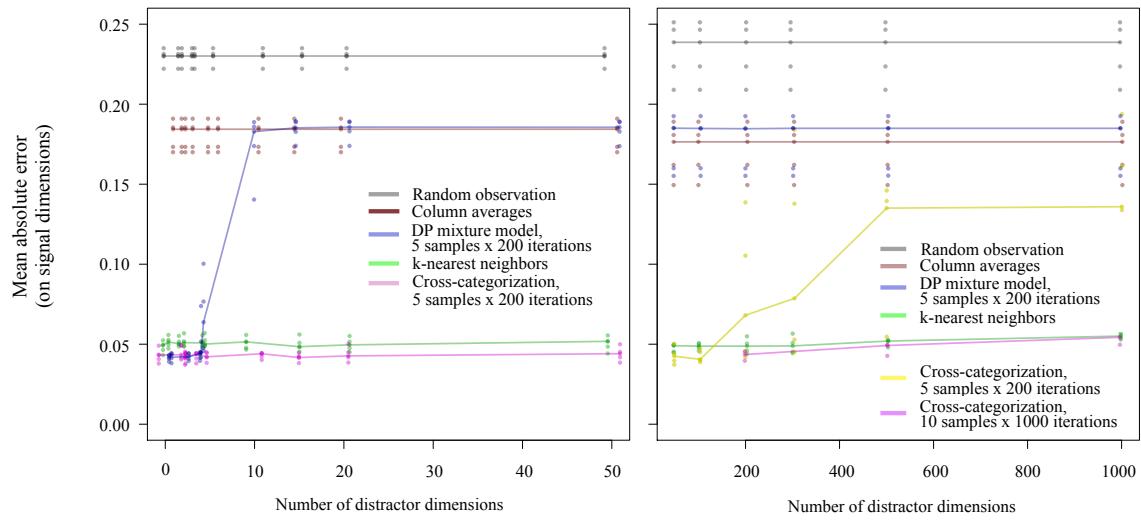


Figure 7: Predictive accuracy for low-dimensional signals embedded in high-dimensional noise. The data generator contains 10 “signal” dimensions described by a 5-cluster model to which distractor dimensions described by an independent 3-cluster model have been appended. The left plot shows imputation accuracies for up to 50 distractor dimensions; the right shows accuracies for 50-1,000 distractors. CrossCat is compared to mixture models as well as multiple non-probabilistic baselines (column-wise averaging, imputing via a random value, and a state-of-the-art extension to k-nearest-neighbors). The accuracy of mixture modeling drops when the number of distractors D becomes comparable to the number of signal variables S, i.e. when $D \approx S$. When $D > S$, the distractors get modeled instead of the signal. In contrast, CrossCat remains accurate when the number of distractors is 100 times larger than the number of signal variables. See main text for additional discussion.

3. Empirical Results on Real-World Datasets

This section describes the results from CrossCat-based analyses of several datasets. Examples are drawn from multiple fields, including health economics, pattern recognition, political science, and econometrics. These examples involve both exploratory analysis and predictive modeling. The primary aim is to illustrate CrossCat and assess its efficacy on real-world problems. A secondary aim is to verify that CrossCat produces useful results on data generating processes with diverse statistical characteristics. A third aim is to compare CrossCat with standard generative, discriminative, and model-free methods.

3.1 Dartmouth Atlas of Health Care

The Dartmouth Atlas of Health Care (Fisher, Goodman, Wennberg, and Bronner, 2011) is one output from a long-running effort to understand the efficiency and effectiveness of the US health care system. The overall dataset covers ~ 4300 hospitals that can be aggregated into ~ 300 hospital reporting regions. The extract analyzed here contains 74 variables that collectively describe a hospital's capacity, quality of care, and cost structure. These variables contain information about multiple functional units of a hospital, such as the intensive care unit (ICU), its surgery department, and any hospice services it offers. For several of these units, the amount each hospital bills to a federal program called Medicare is also available. The continuous variables in this dataset range over multiple orders of magnitude. Specific examples include counts of patients, counts of beds, dollar amounts, percentages that are ratios of counts in the dataset, and numerical aggregates from survey instruments that assess quality of care.

Due to its broad coverage of hospitals and their key characteristics, this dataset illustrates some of the opportunities and challenges described by the NRC Committee on the Analysis of Massive Data (2013). For example, given the range of cost variables and quality surveys it contains, this data could be used to study the relationship between cost and quality of care. The credibility of any resulting inferences would rest partly on the comprehensiveness of the dataset in both rows (hospitals) and columns (variables). However, it can be difficult to establish the absence of meaningful predictive relationships in high-dimensional data on purely empirical grounds. Many possible sets of predictors and forms of relationships need to be considered and rejected, without sacrificing either sensitivity or specificity. If the dataset had fewer variables, a negative finding would be easier to establish, both statistically and computationally, as there are fewer possibilities to consider. However, such a negative finding would be less convincing.

The dependencies detected by CrossCat reflect accepted findings about health care that may be surprising. The inferred pairwise dependence probabilities, shown in Figure 8, depict strong evidence for a dissociation between cost and quality. Specifically, the variables in block A are aggregated quality scores, for congestive heart failure (CHF_SCORE), pneumonia (PNEUM_SCORE), acute myocardial infarction (AMI_SCORE), and an overall quality metric (QUAL_SCORE). The probability that they depend on any other variable in the dataset is low. This finding has been reported consistently across multiple studies and distinct patient populations (Fisher, Goodman, Skinner, and Bronner, 2009). Partly due to its coverage in the popular press (Gawande, 2009), it also informed the design of performance-based funding provisions in the 2009 Affordable Care Act.

CrossCat identifies several other clear, coherent blocks of variables whose dependencies are broadly consistent with common sense. For example, Section B of Figure 8 shows that CrossCat has inferred probable dependencies between three variables that all measure hospice usage. The

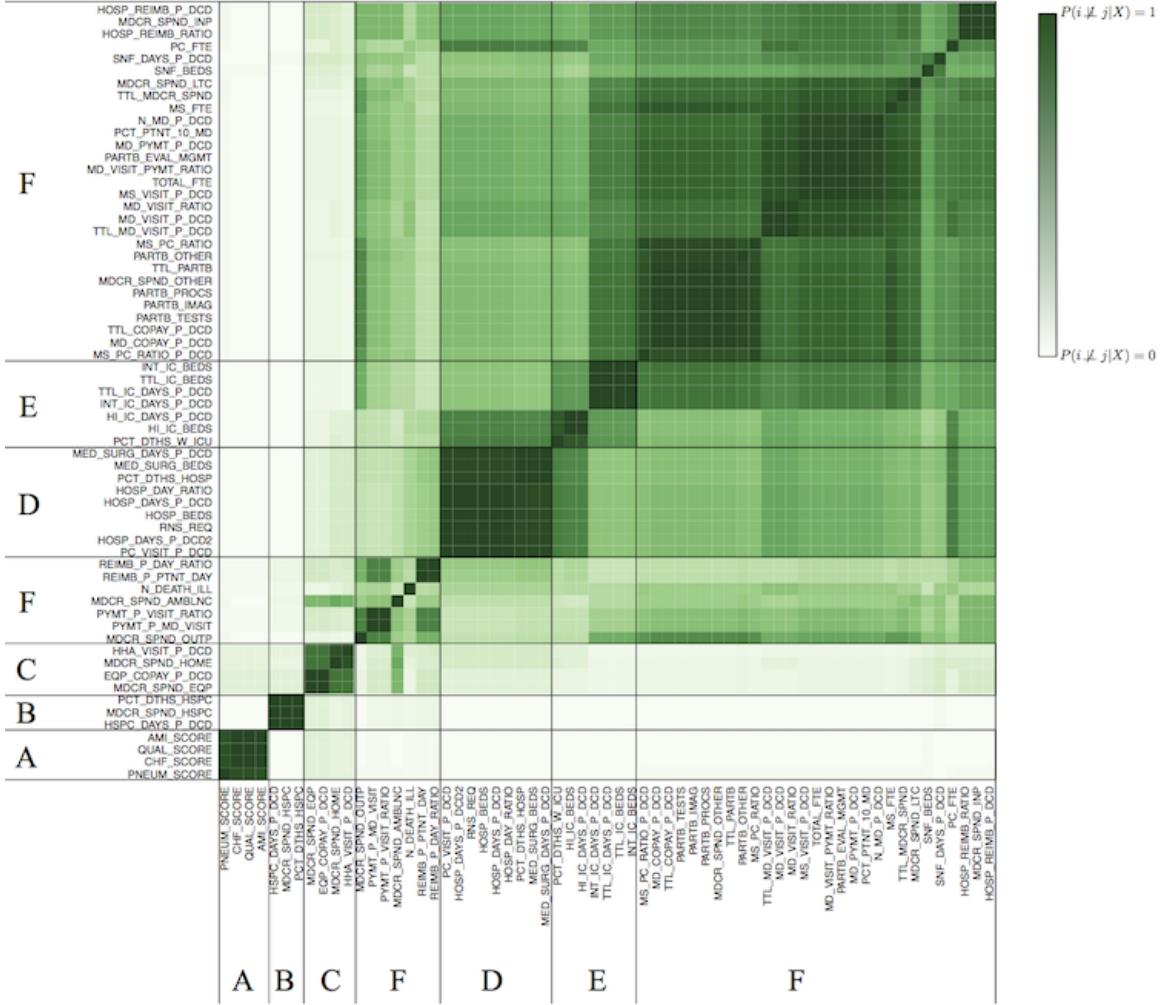


Figure 8: Dependencies between variables the Dartmouth Atlas data aggregated by hospital referral region. This figure shows the z-matrix $Z = [Z(i,j)]$ of pairwise dependence probabilities, where darker green represents higher probability. Rows and columns are sorted by hierarchical clustering and several portions of the matrix have been labeled. The isolation of [A] indicates that the quality score variables are almost certainly mutually dependent but independent of the variables describing capacity and cost structure. [B] contains three distinct but dependent measures of hospice cost and capacity: the percent of deaths in hospice, the number of hospice days per decedent, and the total Medicare spending on hospice usage. [C] contains spending on home health aides, equipment, and ambulance care. [D] shows dependencies between hospital stays, surgeries and in-hospital deaths. [E] contains variables characterizing intensive care, including some that probably interact with surgery, and others that interact with general spending metrics [F], such as usage of doctors' time and total full time equivalency (FTE) head count.

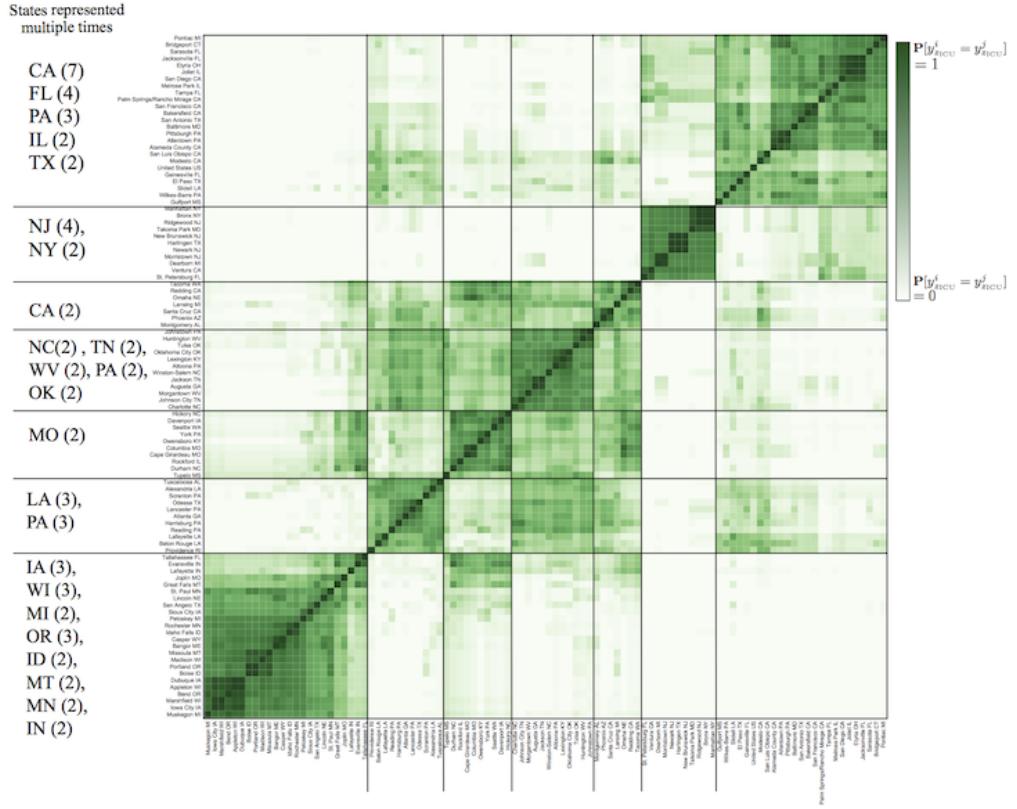


Figure 9: The pairwise similarity measure inferred by CrossCat in the context of ICU utilization. Each cell contains an estimate of the marginal probability that the hospital reporting regions corresponding to the row and column come from the same category in the view. The block structure in this matrix reflects regional variation in ICU utilization and in other variables that are probably predictive of it; examples include measures of hospital and intensive care capacity and usage.

dependencies within Section C reflect the proposition that the presence of home health aides — often consisting of expensive equipment — and overall equipment spending are probably dependent. The dark green bar for `MDCR_SPND_AMBLNC` with the variables in section C is also intuitive: home health care easily leads to ambulance transport during emergencies. Section D shows probable dependencies between the length of hospital stays, hospital bed usage, and surgery. This section and section E, which contains measures of ICU usage, are probably predictive of the general spending metrics in section F, such as total Medicare reimbursement, use of doctors' time, and total full time equivalent (FTE) head count. Long hospital stays, surgery, and time in the intensive care unit (ICU) are key drivers of costs, but not quality of care.

It has been proposed that regional differences explain variation in cost and capacity, but not quality of care (Gawande, 2009). This proposal can be explored using CrossCat by examining individual samples as well as the context-sensitive pairwise co-categorization probabilities (similarities) for hospitals. Figure 9 shows these probabilities in the context of time spent in the ICU. These prob-

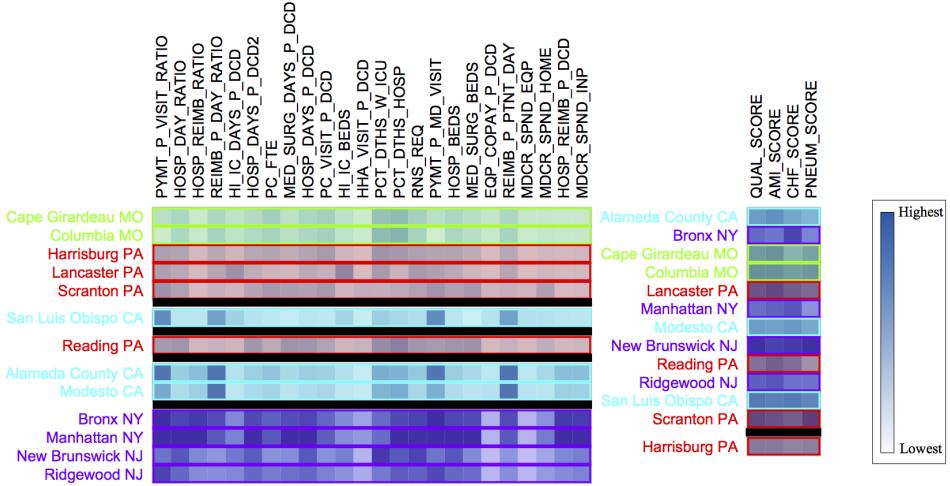


Figure 10: **Subset of a single posterior sample for the Dartmouth Health Atlas.** These entities have been color-coded according to geography. Variables related to quality are independent of geography (left), but variables related to usage of services are related to geography (right). This is in accord with a key finding from Gawande (2009).

abilities yield hospital groups that often contain adjacent regions, consistent with the idea that local variation in training or technique diffusion may contribute significantly to costs. Figure 10 shows results for regions from four states, coloring regions from the same state with the same color, with white space separating categories in a given view. Variables probably dependent on usage lead to geographically consistent partitions, while variables that are probably dependent on quality do not.

The models inferred by CrossCat can also be used to compare each value in the dataset with the values that are probable given the rest of the data. Figure 11 shows the predictive distribution on the number of physician visits for ICU patients for 10 hospital reporting regions. The true values are relatively probable for most of these regions. However, for McAllen, Texas, the observed value is highly improbable. McAllen is known for having exceptionally high costs and an unusually large dependence on expensive, equipment-based treatment rather than physician care. In fact, Gawande (2009) used McAllen to illustrate how significant the variation can be.

The imputation accuracy of CrossCat on this dataset is also favorable relative to multiple baselines. Figure 12 shows the results on versions of the Dartmouth Atlas of Health care where 5%-20% of the cells are censored at random. CrossCat performs favorably across this range, outperforming both simple model-free schemes and nonparametric Bayesian mixture modeling.

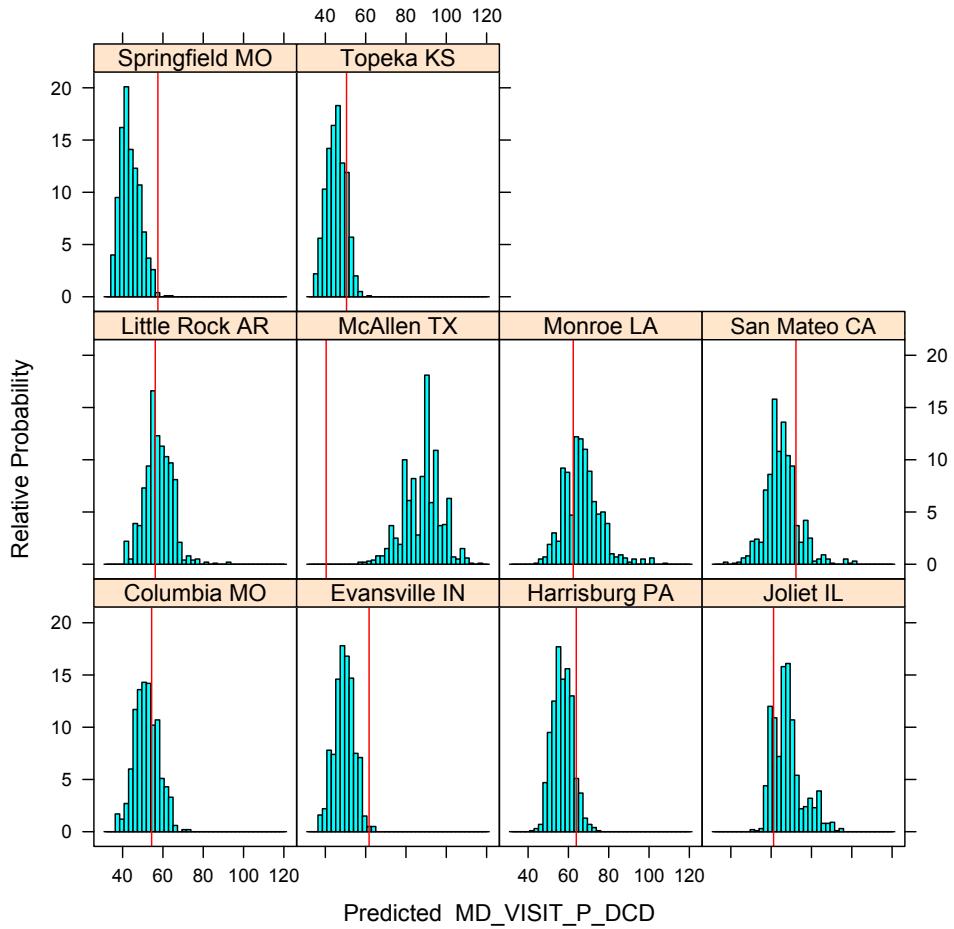


Figure 11: A comparison between the observed utilization of physicians their inferred predictive distributions, for 10 hospital reporting regions. McAllen, TX appears to under-utilize physicians relative to CrossCat's predictions based on the overall dataset. This is consistent with analyses of McAllen's equipment and procedure-intensive approach to care. Note that some predictive distributions are multi-modal, e.g. Joliet, IL.

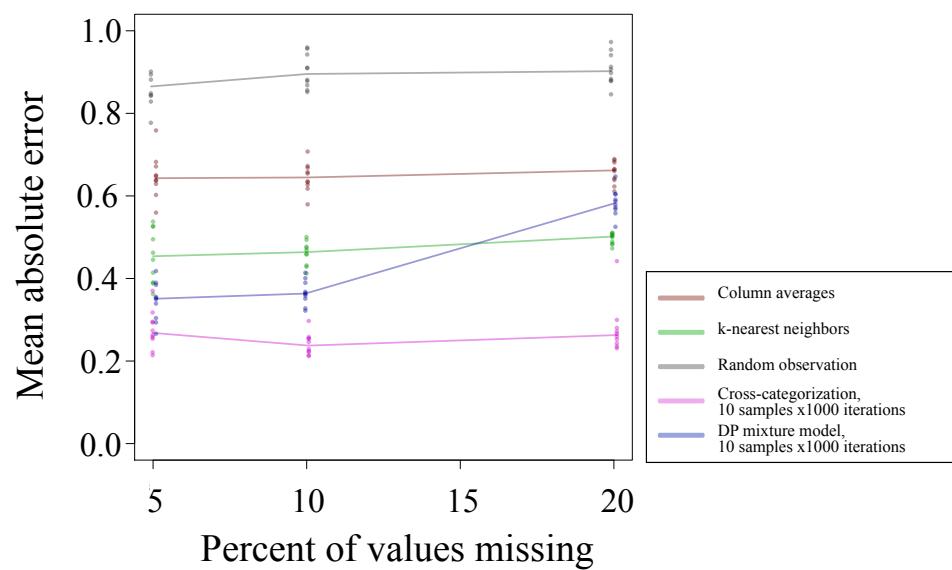


Figure 12: **A comparison of imputation accuracy under random censoring.** The error (y axis) as a function of the fraction of missing values (x axis) is measured on a scale that has been normalized by column-wise variance, so that high-variance variables do not dominate the comparison. CrossCat is more accurate than baselines such as column-wise averaging, imputation using a randomly chosen observation, a state-of-the-art variant of k-nearest-neighbors, and Dirichlet process mixtures of Gaussians. Also note the collapse of mixture modeling to column-wise averaging when the fraction of missing values grows sufficiently large.

3.2 Classifying Images of Handwritten Digits

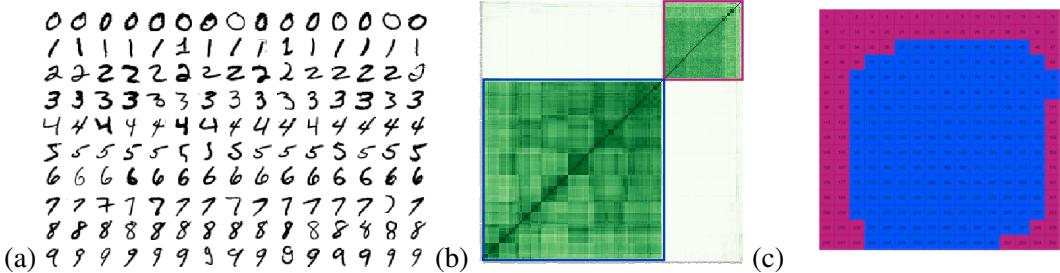


Figure 13: MNIST handwritten digits, feature z-matrix, and color-coded image pixel locations. (a) Fifteen visually rendered examples of handwritten digits for each number in the MNIST data set. Each image was converted to a binary feature vector for predictive modeling. CrossCat additionally treated the digit label as an additional feature; this value was observed for training examples and treated as missing for testing. (b) The dependence probabilities between pixel values distinguish two blocks of pixels, one containing the digit label. (c) Coloring the pixels from each block reveals the spatial structure in pixel dependencies. Blue pixels — pixels from the block with a blue border from figure (b) — pick out the foreground, i.e. pixels whose values depend on what digit the image contains. Magenta pixels pick out the common background, i.e. pixels whose values are independent of what digit is drawn.

The MNIST collection of handwritten digit images (LeCun and Cortes, 2011) can be used to explore CrossCat’s applicability to high-dimensional prediction problems from pattern recognition. Figure 13a shows example digits. For all experiments, each image was downsampled to 16x16 pixels and represented as a 256-dimensional binary vector. The digit label was treated as an additional categorical variable, observed for training examples and treated as missing for testing. Figure 13b shows the inferred dependence probabilities among pixels and between the digit label and the pixels. The pixels that are identified as independent of the digit class label lie on the boundary of the image, as shown in Figure 13c.

A set of approximate posterior samples from CrossCat can be used to complete partially observed images by sampling predictions for arbitrary subsets of pixels. Figure 14 illustrates this: each panel shows the data, marginal predictive images, and predicted image completions, for 10 images from the dataset, one per digit. With no data, all 10 predictive distributions are equivalent, but as additional pixels are observed, the predictions for most images concentrate on representations of the correct digit. Some digits remain ambiguous when $\sim 30\%$ of the pixels have been observed. The predictive distributions begin as highly multi-modal distributions when there is little to no data, but concentrate on roughly unimodal distributions given sufficiently many features.

The predictive distribution can also be used to infer the most probable digit, i.e. solve the standard MNIST multi-class classification problem. Figure 15 shows ROC curves for CrossCat on this problem. Each panel shows the tradeoff between true and false positives for each digit, aggregated from the overall performance on the underlying multi-class problem. The figure also includes ROC curves for Support Vector Machines with linear and Gaussian kernels. For these methods, the standard one-vs-all approach was used to reduce the multi-class problem into a set of binary classification problems. The regularization and kernel bandwidth parameters for the SVMs were set via cross-validation using 10% of the training data. 10 posterior samples from CrossCat

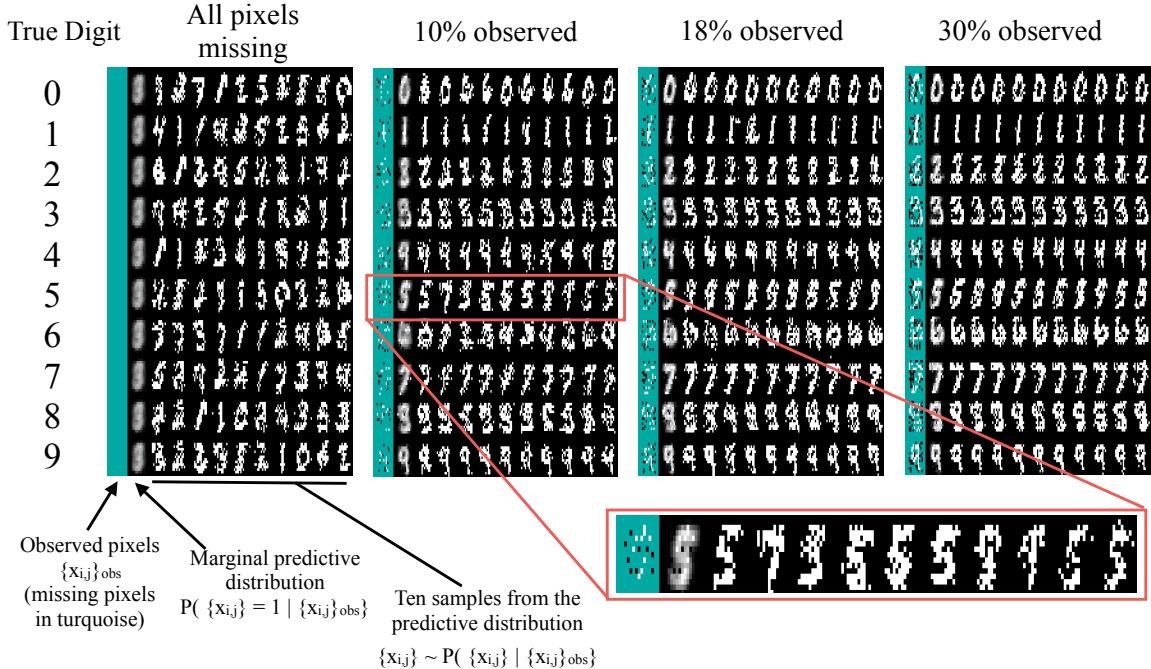


Figure 14: **Predicted images of handwritten digits given sparse observations.** CrossCat can be used to fill in missing pixels by sampling from their conditional density given the observed pixels. Each panel shows completion results for one image per digit; across panels, the fraction of observed pixels grows from 0 to 30%. The leftmost column shows the observed pixels in black and white, with missing pixels in turquoise. The second column from the left shows the marginal probabilities for each pixel. The 10 remaining columns show independent sampled predictions. In the leftmost panel, with no data, all 10 predictive distributions are equivalent. The predictive distribution collapses onto single digit classes (except for 8 and 6) after 18% of the digits have been observed. The marginal images for 1, 7, and 9 become resolvable to a single prototypical example after 10% of the 256 pixels have been observed. Others, such as 8, remain ambiguous.

were used, each obtained after 1,000 iterations of inference from a random initialization. CrossCat was more accurate than the linear discriminative technique; this is expected, as CrossCat induces a nonlinear decision boundary even if classifying based on a single posterior sample. Overall, the 10-sample model used here made less accurate predictions than the Gaussian SVM baseline. Also, in anecdotal runs that were scored by overall 0-1 loss rather than per-digit accuracy, performance was similarly mixed, and less favorable for CrossCat. However, the size of the kernel matrix for the Gaussian SVM scales quadratically, while CrossCat scales linearly. As a classifier, CrossCat thus offers different tradeoffs between accuracy, amount of training data, test-time parallelism (via the number of independent samples), and latency than standard techniques.

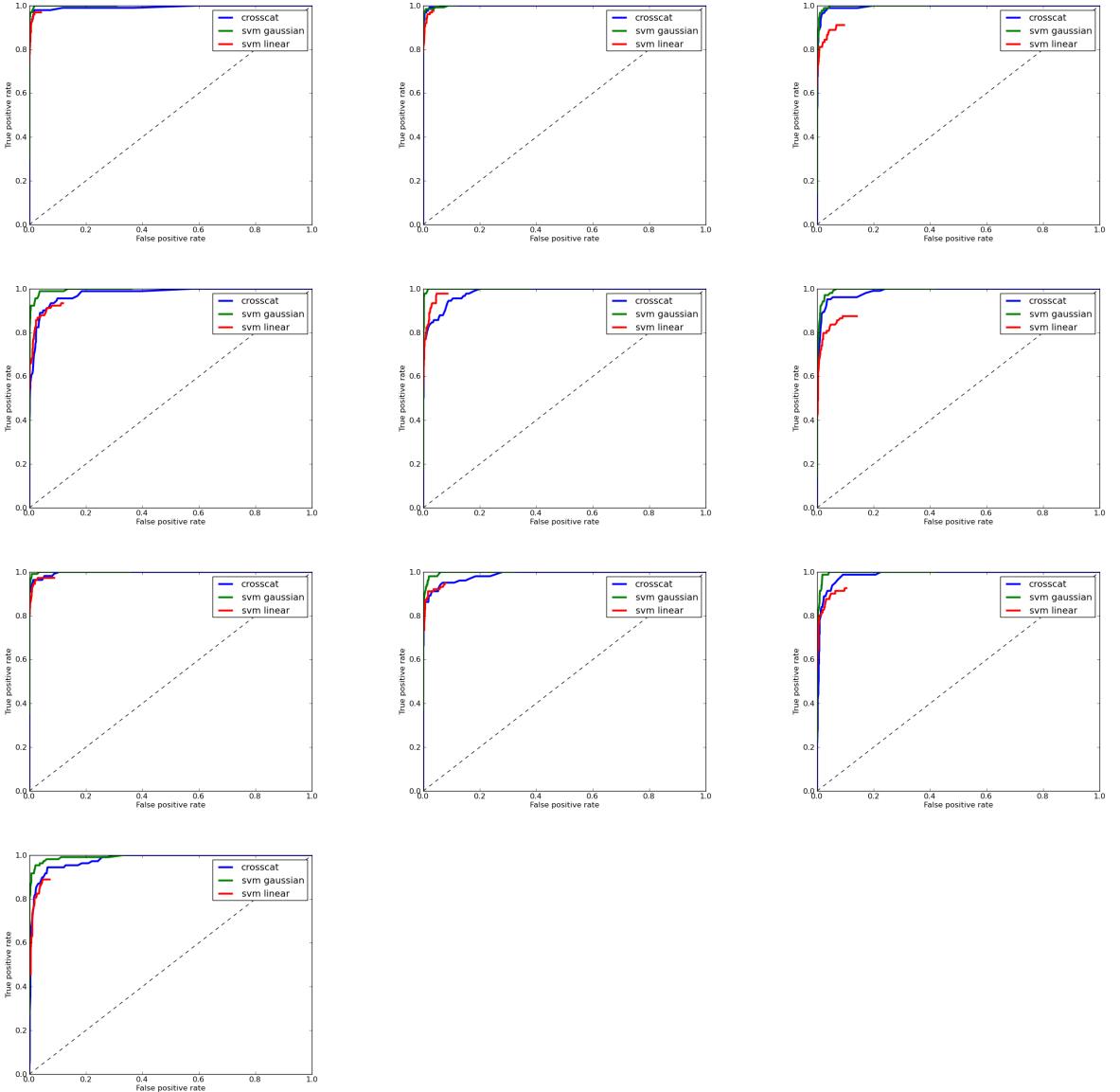


Figure 15: Classification accuracy on handwritten digits from MNIST. Each panel shows the true positive/false positive tradeoff curves for classifying each digit from 0 through 9. Digit images were represented as binary vectors, with one dimension per pixel. As with the image completion example from Figure 14, CrossCat was applied directly to this data, with the digit label appended as a categorical variable; no weighting or tuning for the supervised setting was done. Support vector machines (SVMs) with both linear and Gaussian kernels are provided as baselines. Regularization and kernel bandwidth parameters were chosen via cross-validation on 10% of the training data, with multiple classes treaded via a one-versus-all reduction. See the main text for further discussion.

3.3 Voting records for the 111th Senate

Voters are often members of multiple issue-dependent coalitions. For example, US senators sometimes vote according to party lines, and at other times vote according to regional interests. Because this common-sense structure is typical for the CrossCat prior, voting records are an important test case.

This set of experiments describes the results of a CrossCat analysis of the 397 votes held by the 111th Senate during the 2009-2010 session. In this dataset, each column is a vote or bill, and each row is a senator. Figure 16 shows the raw voting data, with several votes and senators highlighted. There are 106 senators; this is senators is larger than the size of the senate by 6, due to deaths, replacement appointments, party switches, and special elections. When a senator did not vote on a given issue, that datum is treated as missing. Figure 16 also includes two posterior samples, one that reflects partisan alignment and another that posits a higher-resolution model for the votes.

This kind of structure is also apparent in estimates that aggregate across samples. Dependence probabilities between votes are shown in Figure 17. The visible independencies between blocks are compatible with a common-sense understanding of US politics. The two votes in orange are partisan issues. The two votes in green have broad bipartisan support. The vote in yellow aimed at removing an energy subsidy for rural areas, an issue that cross-cuts party lines. The vote in purple stipulates that the Department of Homeland Security must spend its funding through competitive processes, with an exception for small businesses and women or minority-owned businesses. This issue subdivides the republican party, isolating many of the most fiscally conservative. Similarity matrices for the senators with respect to S. 160 (orange) and an amendment to H.R. 2997 (yellow) are shown in Figure 18, with the senators whose similarity values changed the most between these two bills highlighted in grey.

It is instructive to compare the latent structure and predictions inferred by CrossCat with structures and predictions from other learning techniques. As an individual voting record can be described by 397 binary variables and the missing values are negligible, Bayesian network structure learning is a suitable benchmark. Figure 19a shows the best Bayesian network structure found by structure learning using the search-and-score method implemented in the Bayes Net Toolbox for MATLAB (Murphy, 2001). This search is based on local moves similar to the transition operators from Giudici and Green (1999). The highest scoring graphs after 500 iterations contained between 143 and 193 links. Figure 19b shows the marginal dependencies between votes induced by this Bayesian network; these are sparser than those from CrossCat. Figure 19c shows the mean absolute errors for this Bayes net and for CrossCat on a predictive test where 25% of the votes were held out and predicted for senators in the test set. Bayes net CPT's were estimated using a symmetric Beta-Bernoulli model with hyper-parameter $\alpha = 1$. CrossCat predictions were based on four samples, each obtained after 250 iterations of inference. Compared to Bayesian network structure learning, CrossCat makes more accurate predictions and also finds more intuitive latent structures.

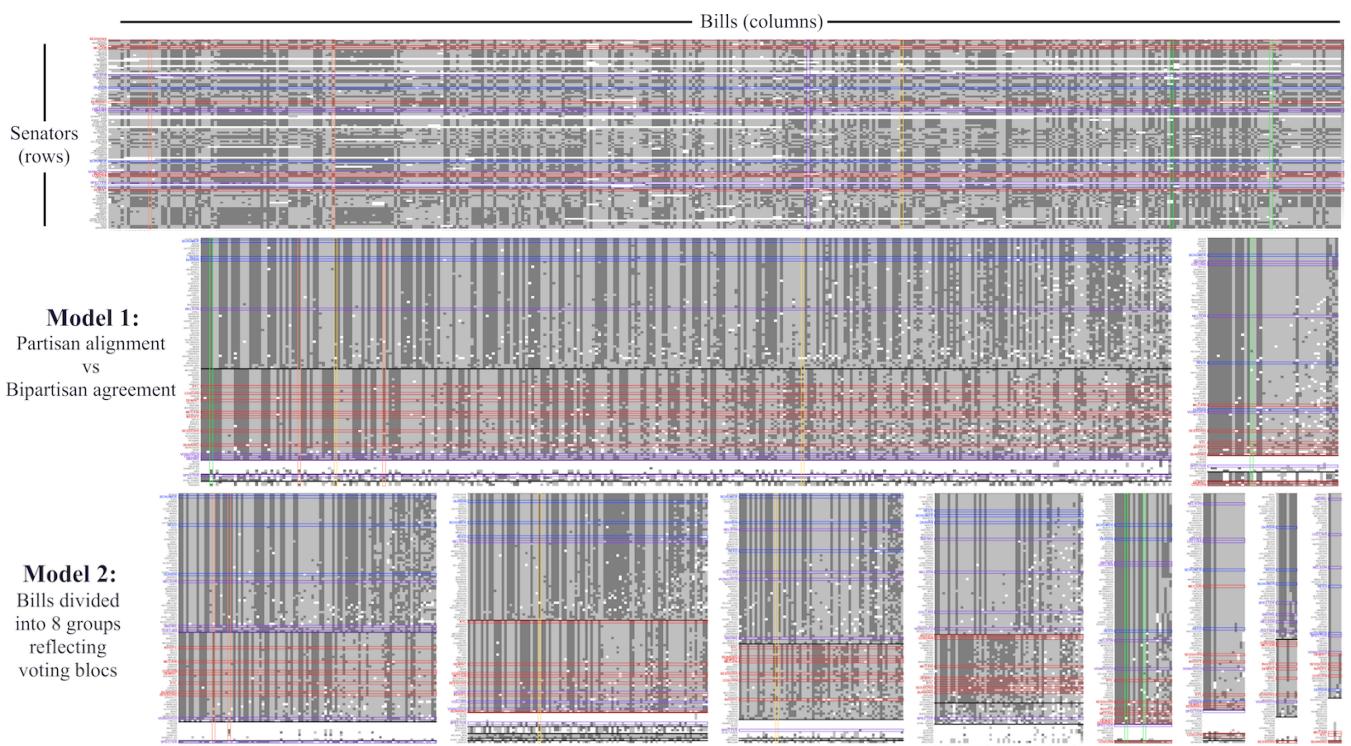


Figure 16: Voting records for the 111th US Senate (2009). (top) This includes 397 votes (yea in light grey, nay in dark grey) for 106 senators, including separate records for senators who changed parties or assumed other offices mid-term. Some senators are highlighted in colors based on their generally accepted identification as democrats (blue), moderates (purple), or republicans (red). See main text for an explanation of the colored bills. (middle) This row shows a simple or low resolution posterior sample that divides bills into those that exhibit partisan alignment and those with bipartisan agreement. Clusters of senators, generated automatically, are separated by thick black horizontal lines. (bottom) This row shows a sample that includes additional views and clusters, positing a finer-grained predictive model for votes that are treated as random in the middle row.

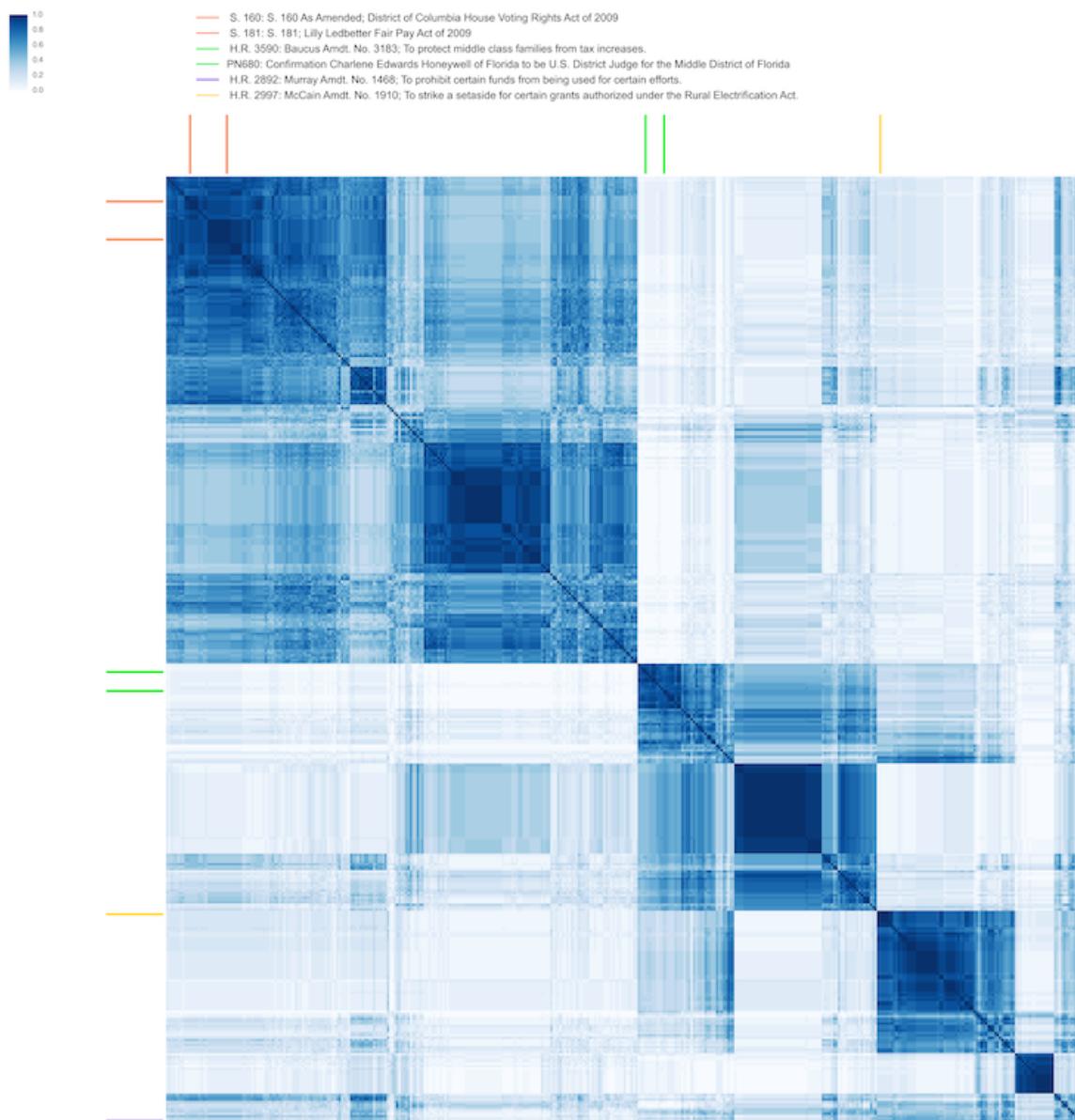


Figure 17: Pairwise dependence probabilities between bills. Blocks of bills with high probability of dependence include predominantly partisan issues (orange), issues with broad bipartisan support (green), and bills that divide senators along ideological or regional lines.

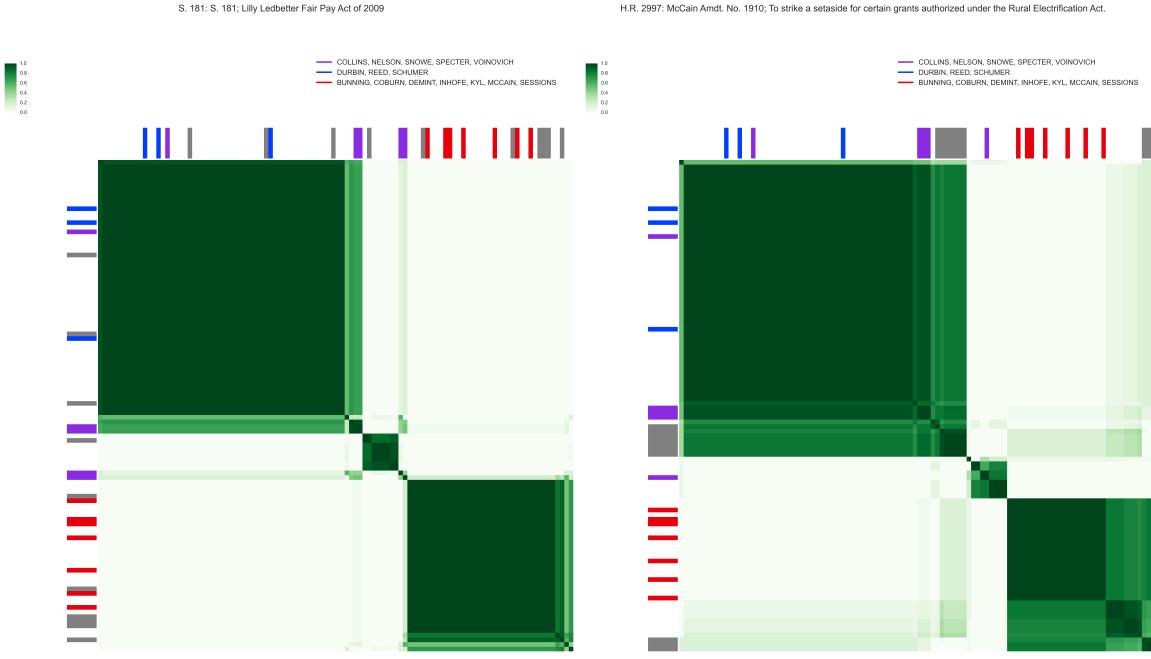


Figure 18: Context-sensitive similarity measures for senators with respect to partisan and special-interest issues. The left matrix shows senator similarity for S. 181, the Lilly Ledbetter Fair Pay Act of 2009, a bill whose senator clusters tend to respect party lines. The right matrix is for H.R. 2997, a bill designed to remove a subsidy for energy generation systems in rural areas. The grey senators are those whose similarities changed the most between these two bills.

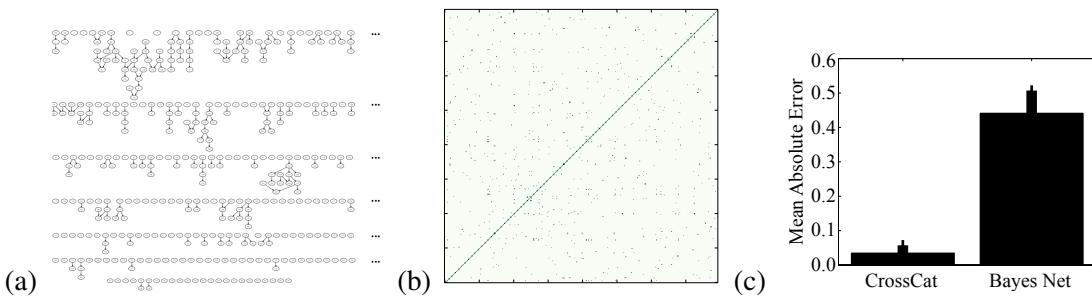


Figure 19: Comparison of latent structures and predictive accuracy for CrossCat and Bayesian network structure learning. (a) The Bayesian network structure found by structure learning; each node is a vote, and edge indicates a conditional dependence. (b) The sparse marginal dependencies induced by this Bayes net. (c) A comparison of the predictive accuracy of CrossCat and Bayesian networks. See main text for details and discussion.

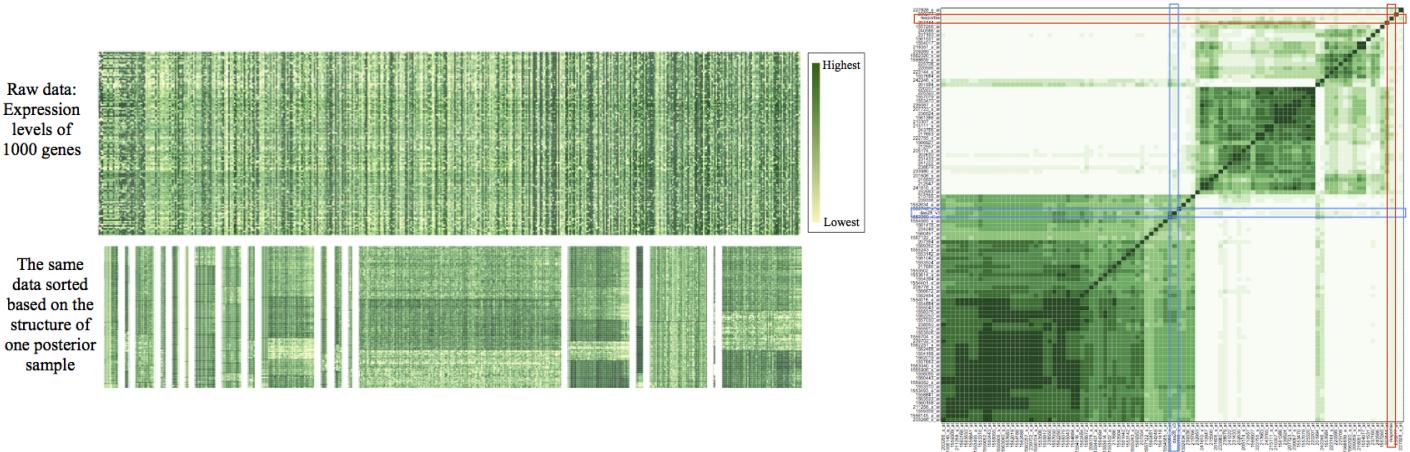


Figure 20: CrossCat inference results on gene expression data. (left) Expression levels for the top 1,000 highest-variance genes from Raponi et al. (2009) in original form and in the order induced by a single CrossCat sample. CrossCat was applied to a subset with roughly 1 million cells ($\sim 10,000$ probes by ~ 100 tissue samples). (right) Pairwise dependence probabilities between probe values and treatment response inferred from the GSE15258 dataset. The 100 probes most probably dependent on a 3-class treatment response variable, based on analysis of a subset with 1,000 probes, are shown outlined in red. The low inferred dependence probability suggests that the data does not support the existence of any prognostic biomarker. A standard disease activity score is shown outlined in blue; this measure is naturally dependent on many of the probes.

3.4 High-dimensional Gene Expression Data

High-throughput measurement techniques in modern biology generate datasets of unusually high dimension. The number of variables typically is far greater than the sample size. For example, microarrays can be used to assess the expression levels of 10,000 to 100,000 probe sequences, but due to the cost of clinical data acquisition, typical datasets may have just tens or hundreds of tissue samples. Exploration and analysis of this data can be both statistically and computationally challenging.

Individual samples from CrossCat can aid exploration of this kind of data. Figure 20 shows one typical sample obtained from the data in Raponi et al. (2009). The dataset had ~ 1 million cells, with 10,000 probes (columns) and 100 tissue samples (rows). This sample has multiple visually coherent views with ~ 50 genes, each reflecting a particular low-dimensional pattern. Some of these views divide the rows into clusters with “low”, “medium” or “high” expression levels; others reflect more complex patterns. The co-assignment of many probes to a single view could indicate the existence of a latent co-regulating mechanism. The structure in a single sample could thus potentially inform pathway searches and help generate testable hypotheses.

Posterior estimates from CrossCat can also facilitate exploration. CrossCat was applied to estimate dependence probabilities for a subset of the arthritis dataset from (Bienkowska, Dal-

gin, Batliwalla, Allaire, Roubenoff, Gregersen, and Carulli, 2009) (NCBI GEO accession number GSE15258). This dataset contains expression levels for $\sim 55,000$ probes, each measured for 87 patients. It also contains standard measures of initial and final disease levels and a categorical “response” variable with 3 classes. CrossCat was applied to subsets with 1,000 and 5,000 columns.

Figure 20 shows the 100 variables most probably predictive of a 3-class treatment response variable. The dependence probabilities with response (outlined in red) are all low, i.e. according to CrossCat, there is little evidence in favor of the existence of any prognostic biomarker. At first glance this may seem to contradict (Bienkowska et al., 2009), which reports 8-gene and 24-gene biomarkers with prognostic accuracies of 83%-91%. However, the test set from (Bienkowska et al., 2009) has 11 out-of-sample patients, 9 of whom are responders. Predicting according to class marginal probabilities would yield compatible accuracy. The final disease activation level, outlined in blue, does appear within the selected set of variables. CrossCat infers that it probably depends on many other gene expression levels; these genes could potentially reflect the progression of arthritis in physiologically or clinically useful ways.

3.5 Longitudinal Unemployment Data by State

This experiment explores CrossCat’s behavior on data where variables are tracked over time. The data are monthly state-level unemployment rates from 1976 to 2011, without seasonal adjustment, obtained from the US Bureau of Labor Statistics. The data also includes annual unemployment rates for every state. Figure 21 shows time series for 5 states, along with national unemployment rate and real Gross Domestic Product (GDP). Typical analyses of raw macroeconomic time series are built on assumptions about temporal dependence and incorporate multiple model-based smoothing techniques; see e.g. (Bureau of Labor Statistics, 2014). Cyclical macroeconomic dynamics, such as the business cycle, are demarcated using additional formal and informal techniques for assessing agreement across multiple indicators (National Bureau of Economic Research, 2010). For this analysis, the input data was organized as a table, where each row r represents a state, each column c represents a month, and each cell $x_{r,c}$ represents the unemployment rate for state r in month c . This representation removes all temporal cues.

CrossCat posits short-range, common-sense temporal structure in state-level employment rates. The top panel of Figure 21 shows the largest and smallest month in each of the views in a single posterior sample as vertical dashes. Figure 22a shows the frequency of years in each view; each view contains one or two temporally contiguous blocks. Figure 22b shows the raw unemployment rates sorted according to the cross-categorization from this sample. Different groups of states are affected by each phase of the business cycle in different ways, inducing different natural clusterings of unemployment rates.

CrossCat also detects long-range temporal structure that is largely in agreement with the officially designated phases of the business cycle. Figure 23 shows the dependence probabilities for all months, in temporal order, with business cycle peaks in black and troughs in red. The beginning of the 1980 recession aligns closely with a sharp drop in dependence probability; this indicates that during 1980 the states naturally cluster differently than they do in 1979. Three major US recessions — 1980, 1990, and late 2001 — align with these breakpoints. The beginning of the 2008 recession and the end of the 1980s recession (in 1984) both fall near sub-block boundaries; these are best seen at high resolution. Correspondence is not perfect, but this is expected: CrossCat is not analyzing

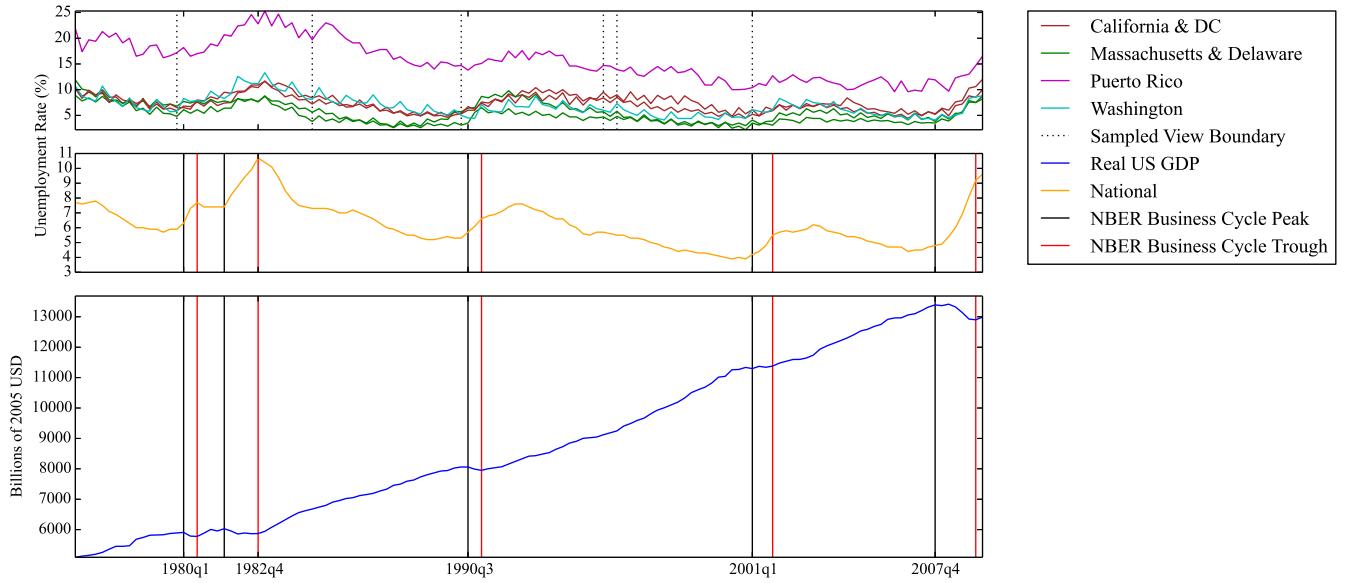


Figure 21: US state-level unemployment data aligned with official business cycle peaks and troughs.
 (top) Unemployment rates for five states from 1976 to 2009, colored according to one posterior sample.
 (middle) The national unemployment rate and business cycle peaks and troughs during the same period. Business cycle peaks and troughs are identified using multiple macroeconomic signals; see main text for details. Unemployment grows during recessions (intervals bounded on the left by black and on the right by red) and shrinks during periods of growth (intervals bounded on the left by red and on the right by black).
 (bottom) Real US gross domestic product (GDP) similarly decreases or stays constant during recessions and increases during periods of growth. View boundaries from the CrossCat sample pick out the business cycle turning points around 1980, 1990 and 2001.

the same data used to determine business cycle peaks and troughs, nor is it explicitly assuming any temporal dynamics.

Time series analysis techniques commonly assume temporal smoothness and sometimes also incorporate the possibility of abrupt changes (Ahn and Thompson, 1988; Wang and Zivot, 2000). CrossCat provides an alternative approach that makes weaker dynamical assumptions: temporal smoothness is not assumed at the outset but must be inferred from the data. This cross-sectional approach to the analysis of natively longitudinal data may open up new possibilities in econometrics. For example, it could be fruitful to apply CrossCat to a longitudinal dataset with multiple macroeconomic variables for each state, or to use CrossCat to combine temporal information at different timescales.

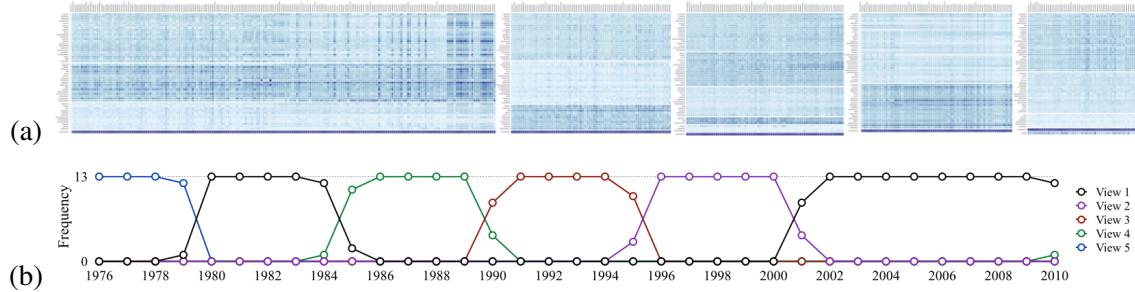


Figure 22: The temporal structure in a single posterior sample. (a) The complete state-level monthly employment rate dataset, sorted according to one posterior sample. This sample divides the months into 5 time periods, each inducing a different clustering of the states. (b) The frequency of years and quarters for each view shows that each view reflects temporal contiguity: each view either corresponds to a single, temporally contiguous interval or to the union of two such intervals. This temporal structure is not given to CrossCat, but rather inferred from patterns of unemployment across clusters of states.

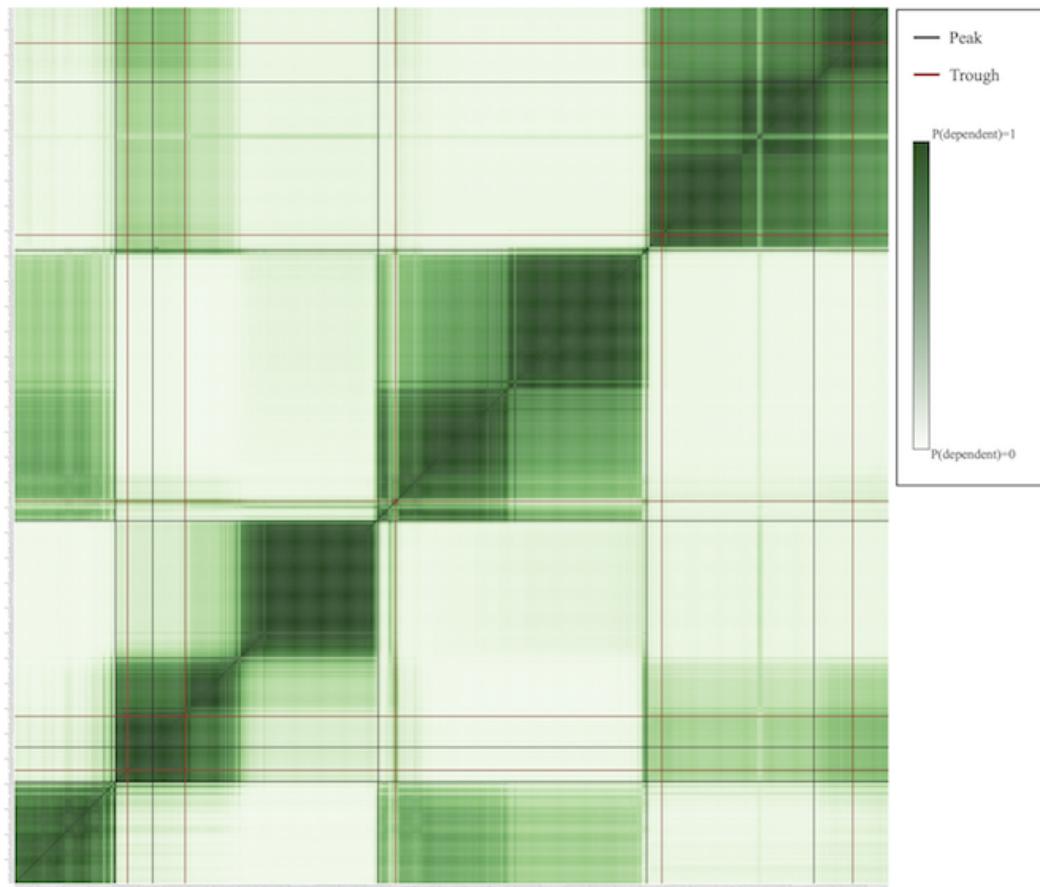


Figure 23: **Dependence probabilities between monthly unemployment rates.** Unemployment rates are sorted by date, beginning with 1976 in the bottom left corner, with business cycle peaks and troughs identified by the NBER in black and red. The beginnings of three major recessions — in the early 1980s, 1990s, and late 2001 — are identified by breaks in dependence probability: unemployment rates are dependent with high probability within these periods, and independent of rates from the previous period. See main text for more discussion.

4. Discussion

This paper contains two contributions. First, it describes CrossCat, a model and inference algorithm that together comprise a domain-general method for characterizing the full joint distribution of the variables in a high-dimensional dataset. CrossCat makes it possible to draw a broad class of Bayesian inferences and to solve prediction problems without domain-specific modeling. Second, it describes applications to real-world datasets and analysis problems from multiple fields. CrossCat finds latent structures that are consistent with accepted findings as well as common-sense knowledge and that can yield favorable predictive accuracy compared to generative and discriminative baselines.

CrossCat is expressive enough to recover several standard statistical methods by fixing its hyper-parameters or adding other deterministic constraints:

1. **Semi-supervised naive Bayes:** $\alpha = 0 \implies \#\text{(unique}(\vec{z})) = 1$ and $\alpha_0 = \epsilon$ with $\lambda_{\text{class}} = 0$

Assume that the dimension in the dataset labeled *class* contains categorical class labels, with a multinomial component model and symmetric Dirichlet prior, with concentration parameter λ_{class} . Because the outer CRP concentration parameter is 0, all features as well as the class label will be assigned to a single view. Because $\lambda_{\text{class}} = 0$, each category in this view will have a component model for the class label dimension that constrains the category to only contain data items whose class labels all agree:

$$y_0^i = y_0^j \iff x_{(i,\text{class})} = x_{(j,\text{class})}$$

This yields a model that is appropriate for semi-supervised classification, and related to previously proposed techniques based on EM for mixture models (Nigam, McCallum, Thrun, and Mitchell, 1999). Data from each class will be modeled by a separate set of clusters, with feature hyper-parameters (e.g. overall scales for continuous values, or levels of noise for discrete values) shared across classes. Data items whose class labels are missing will be stochastically assigned to classes based on how compatible their features are with the features for other data items in the same class, marginalizing out parameter uncertainty. Forcing the concentration parameter α_0 for the sole inner CRP to have a sufficiently small value ϵ ensures that there will only be a single cluster per class (with arbitrarily high probability depending on N and ϵ). These restrictions thus recover a version of the naive Bayesian classifier (for discrete data) and linear discriminant analysis (for continuous data), adding hyper-parameter inference.

2. **Nonparametric mixture modeling:** $\alpha = 0 \implies \#\text{(unique}(\vec{z})) = 1$

If the constraints on categorizations are relaxed, but the outer CRP is still constrained to generate a single view, then CrossCat recovers a standard nonparametric Bayesian mixture model. The current formulation of CrossCat additionally enforces independence between features. This assumption is standard for mixtures over high-dimensional discrete data. Mixtures of high-dimensional continuous distributions sometimes support dependence between variables within each component, rather than model all dependence using the latent component assignments. It would be easy and natural to relax CrossCat to support these component models and to revise the calculations of marginal dependence accordingly.

3. **Independent univariate mixtures:** $\alpha = \infty \implies \#\text{(unique}(\vec{z})) = D$

The outer CRP can be forced to assign each variable to a separate view by setting its concentration parameter α to ∞ . With this setting, each customer (variable) will choose a new table (view) with probability 1. In this configuration, CrossCat reduces to a set of independent Dirichlet process mixture models, one per variable. A complex dataset with absolutely no dependencies between variables can induce a CrossCat posterior that concentrates near this subspace.

4. **Clustering with unsupervised feature selection:** $\#\text{(unique}(\vec{z})) = 2$, with $\alpha_0 > 0$ but $\alpha_1 = 0$

A standard mixture must model noisy or independent variables using the same cluster assignments as the variables that support the clustering. It can therefore be useful to integrate mixture modeling with feature selection, by permitting inference to select variables that should be modeled independently. The “irrelevant” features can be modeled in multiple ways; one natural approach is to use a single parametric model that can independently adjust the entropy of its model for each dimension. CrossCat contains this extension to mixtures as a subspace.

The empirical results suggest that CrossCat’s flexibility in principle manifests in practice. The experiments show that can effectively emulate many qualitatively different data generating processes, including processes with varying degrees of determinism and diverse dependence structures. However, it will still be important to quantitatively characterize CrossCat’s accuracy as a density estimator.

Accuracy assessments will be difficult for two main reasons. First, it is not clear how to define a space of data generators that spans a sufficiently broad class of applied statistics problems. CrossCat itself could be used as a starting point, but key statistical properties such as the marginal and conditional entropies of groups of variables are only implicitly controllable. Second, it is not clear how to measure the quality of an emulator for the full joint distribution. Metrics from collaborative filtering and imputation, such as the mean squared error on randomly censored cells, do not account for predictive uncertainty. Also, the accuracy of estimates of joint distributions and conditional distributions can diverge. Thus the natural metric choice of KL divergence between the emulated and true joint distributions may be misleading in applications where CrossCat is used to respond to a stream of queries of different structures. Because there are exponentially many possible query structures, random sampling will most likely be needed. Modeling the likely query sequences or weighting queries based on their importance seems ultimately necessary but difficult.

In addition to these questions, CrossCat has several known limitations that could be addressed by additional research:

1. **Real-world datasets may contain types and/or shapes of data that CrossCat can only handle by transformation.**

First, several common data types are poorly modeled by the set of component models that CrossCat currently supports. Examples include timestamps, geographical locations, currency values, and categorical variables drawn from open sets. Additional parametric component models — or nonparametric models, e.g. for open sets of discrete values — could be integrated.

Second, it is unclear how to best handle time series data or panel/longitudinal settings. In the analysis of state-level monthly unemployment data, each state was represented as a row, and

each time point was a separate and a priori independent column. The authors were surprised that CrossCat inferred the temporal structure rather than under-fit by ignoring it. In retrospect, this is to be expected in circumstances where the temporal signal is sufficiently strong, such that it can be recovered by inference over the views. However, computational and statistical limitations seem likely to lead to under-fitting on panel data with sufficiently many time points and variables per time point.

One pragmatic approach to resolving this issue is to transform panel data into cross-sectional data by replacing the time series for each member of the population with the parameters of a time-series model. Separately fitting the time-series model could be done as a pre-processing step, or alternated with CrossCat inference to yield a joint Gibbs sampler. Another approach would be to develop a sequential extension to CrossCat. For example, the inner Dirichlet process mixtures could be replaced with nonparametric state machines (Beal, Ghahramani, and Rasmussen, 2001). Each view would share a common state machine, with common states, transition models, and observation models. Each group of dependent variables would thus induce a division of the data into subpopulations, each with a distinct hidden state sequence.

2. Discriminative learning can be more accurate than CrossCat on standard classification and regression problems.

Discriminative techniques can deliver higher predictive accuracy than CrossCat when input features are fully observed during both training and testing and when there is enough labeled training data. One possible remedy is to integrate CrossCat with discriminative techniques, e.g. by allowing “discriminative target” variables to be modeled by generic regressions (e.g. GLMs or Gaussian processes). These regressions would be conditioned on the non-discriminative variables that would still be modeled by CrossCat.

An alternative approach is to distinguish prediction targets within the CrossCat model. At present, the CrossCat likelihood penalizes prediction errors in all features equally. This could be fixed by e.g. deterministically constraining the Dirichlet concentration hyper-parameters for class-label columns to be equal to 0. This forces CrossCat to assign 0 probability density to states that put items from different classes into the same category in the view containing the class label. These purity constraints can be met by using categories that either exactly correspond to the finest-grained classes in the dataset or subdivide these classes. Conditioned on the hyper-parameters, this modification reduces joint density estimation to independent nonparametric Bayesian estimation of class-conditional densities (Mansinghka, Roy, Rifkin, and Tenenbaum, 2007).

3. Natural variations are challenging to test due to the cost and difficulty of developing fast implementations.

The authors found it surprising that a reliable and scalable implementation was possible. Several authors were involved in the engineering of multiple high-performance commercial implementations. One of these can be applied to multiple real-world, million-row datasets with typical runtimes ranging from minutes to hours (Obermeyer, Glidden, and Jonas, 2014). No fundamental changes to the Gibbs sampling algorithm were necessary to make it possible do to inference on these scales. Instead, the gains were due to standard software performance engineering techniques. Examples include custom numerical libraries, careful data structure design, and adopting a streaming architecture and compact latent state representation that

reduce the time spent waiting for memory retrieval. The simplicity of the Gibbs sampling algorithm thus turned out to be an asset for achieving high performance. Unfortunately, this implementation took man-years of software engineering, and is harder to extend and modify than slower, research-oriented implementations.

Probabilistic programming technology could potentially simplify the process of prototyping variations on CrossCat and incrementally optimizing them. For example, Venture (Mansinghka et al., 2014) can express the CrossCat model and inference algorithm from this paper in \sim 40 lines of probabilistic code. At the time of writing, the primary open-source implementation of CrossCat is \sim 4,000 lines of C++. New datatypes, model variations, and perhaps even more sophisticated inference strategies could potentially be tested this way. However, the performance engineering will still be difficult. As an alternative to careful performance engineering, the authors experimented with more sophisticated algorithms and initializations. Transition operators such as the split-merge algorithm from (Jain and Neal, 2000) and initialization schemes based on high-quality approximations to Dirichlet process posteriors (Li and Shafto, 2011) did not appear to help significantly. These complex approaches are also more difficult to debug and optimize than single-site Gibbs. This may be a general feature: reductions in the total number of iterations can easily be offset by increases in the computation time required for each transition.

There is a widespread need for statistical methods that are effective in high dimensions but do not rely on restrictive or opaque assumptions (NRC Committee on the Analysis of Massive Data, 2013; Wasserman, 2011). CrossCat attempts to address these requirements via a divide-and-conquer strategy. Each high-dimensional modeling problem is decomposed into multiple independent subproblems, each of lower dimension. Each of these subproblems is itself decomposed by splitting the data into discrete categories that are separately modeled using parametric Bayesian techniques. The hypothesis space induced by these stochastic decompositions contains proxies for a broad class of data generators, including some generators that are simple and others that are complex. The transparency of simple parametric models is largely preserved, without sacrificing modeling flexibility. It may be possible to design other statistical models around this algorithmic motif.

CrossCat formulates a broad class of supervised, semi-supervised, and unsupervised learning problems in terms of a single set of models and a single pair of algorithms for learning and prediction. The set of models and queries that can be implemented may be large enough to sustain a dedicated probabilistic programming language. Probabilistic programs in such a language could contain modeling constraints, translated into hyper-parameter settings, but leave the remaining modeling details to be filled in via approximate Bayesian inference. Data exploration using CrossCat samples can be cumbersome, and would be simplified by a query language where each query could reference previous results.

This flexibility comes with costs, especially in applications where only a single repeated prediction problem is important. In these cases, it can be more effective to use a statistical procedure that is optimized for this task, such as a discriminative learning algorithm. It seems unlikely that even a highly optimized CrossCat implementation will be able to match the performance of best-in-class supervised learning algorithms when data is plentiful and all features are fully observed.

However, just as with software, sophisticated optimizations also come with costs, and can be premature. For example, some researchers have suggested that there is an “illusion of progress” in classifier technology (Hand, 2006) in which algorithmic and statistical improvements documented

in classification research papers frequently do not hold up in practice. Instead, classic methods seem to give the best and most robust performance. One interpretation is that this is the result of prematurely optimizing based on particular notions of expected statistical accuracy. The choice to formalize a problem as supervised classification may similarly be premature. It is not uncommon for the desired prediction targets to change after deployment, or for the typical patterns of missing values to shift. In both these cases, a collection of CrossCat samples can be used unmodified, while supervised methods need to be retrained.

It is unclear how far this direct Bayesian approach to data analysis can be taken, or how broad is the class of data generating processes that CrossCat can emulate in practice. Some statistical inference problems may be difficult to pose in terms of approximately Bayesian reasoning over a space of proxy generators. Under-fitting may be difficult to avoid, especially for problems with complex couplings between variables that exceed the statistical capacity of fully factored models. Despite these challenges, our experiences with CrossCat have been encouraging. It is fortunate that, paraphrasing Box (1979), the statistical models that CrossCat produces can be simplistic yet still flexible and useful. We thus hope that CrossCat proves to be an effective tool for the analysis of high-dimensional data. We also hope that the results in this paper will encourage the design of other fully Bayesian, general-purpose statistical methods.

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