Adaptive Bayesian Nonparametric Estimation of Mixed Discrete-Continuous Distributions under Smoothness and Sparsity

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Motivation and Questions

- Bayesian models based on mixtures:
 - convenient computationally
 - posterior contracts at optimal minimax rate (up to log) for smooth true densities (Shen, Tokdar, and Ghosal (2013), STG)
 - can be used for modeling discrete data through continuous latent variables
- ▶ Is it a good idea to use mixture models for discrete data?
- Will posterior contract at an optimal rate?
- Appropriate settings for asymptotics? Optimal rates?

Summary of Results

- Data Generating Process
 - ▶ support of discrete variables can become finer with *n* (sparse multinomials as in Hall and Titterington (1987))
 - probability mass function is "smooth"
- We establish lower bounds on estimation rates for multivariate discrete-continuous anisotropic distributions
- For mixture models, posterior contraction rates are equal to the derived lower bounds up to a log factor
- ▶ Excellent finite sample performance in simulations

DGP

- ▶ Continuous $x \in \mathbb{R}^{d_x}$
- ▶ Discrete $y = (y_1, ..., y_{d_y}), y_k \in \left\{\frac{1-1/2}{N_k}, \frac{2-1/2}{N_k}, ..., \frac{N_k-1/2}{N_k}\right\}.$
- ▶ A_y rectangle with center y and side lengths $(\frac{1}{N_1}, \dots, \frac{1}{N_{d_y}})$, $[0,1]^{d_y} = \bigcup_y A_y$
- DGP density-probability mass function

$$p_0(x,y) = \int_{A_y} f_0(x,\tilde{y}) d\tilde{y},$$

where f_0 is a density on $\mathbb{R}^{d_x} \times [0,1]^{d_y}$

So far, without loss of generality.

Anisotropic $(\beta_1, \ldots, \beta_d)$ -Holder Class $C^{L,\beta_1,\ldots,\beta_d}$

$$f \in C^{L,\beta_1,\ldots,\beta_d}$$
 if for any $k = (k_1,\ldots,k_d), \ \sum_{i=1}^d k_i/\beta_i < 1,$

$$|D^k f(z + \Delta z) - D^k f(z)| \leq L \sum_{j=1}^d |\Delta z_j|^{\beta_j (1 - \sum k_i/\beta_i)}$$

where $\Delta z_j = 0$ when $\sum_{i=1}^d k_i/\beta_i + 1/\beta_j < 1$.

- Is this definition standard?
- Ibragimov and Hasminskii (1984) did not restrict mixed derivatives
- ▶ When $\beta_j = \beta$, $\forall j$, $\beta_j (1 \sum k_i/\beta_i) = \beta \lfloor \beta \rfloor$, get standard definition for isotropic case.

Anisotropic $(\beta_1, \ldots, \beta_d)$ -Holder Class $C^{L,\beta_1,\ldots,\beta_d}$

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where $\Delta z_j = 0$ when $\sum_{i=1}^d k_i/\beta_i + 1/\beta_j < 1$.

- ► STG use $|\Delta z_i|^{\min(\beta_j k_j, 1)}$ instead of $|\Delta z_i|^{\beta_j (1 \sum k_i/\beta_i)}$
- It would not work in our proof of lower bounds
- Anisotropic Taylor expansion used in the proof of upper bounds can be obtained under our assumption

Theorem 1: Lower Bound on Estimation Rate

- lacksquare ${\cal A}$ collection of all subsets of $\{d_{\scriptscriptstyle X}+1,\ldots,d\}$, $d=d_{\scriptscriptstyle X}+d_{\scriptscriptstyle Y}$
- ▶ For $J \in A$, define $J^c = \{1, ..., d\} \setminus J$,

$$N_J = \prod_{k \in J} N_k, \qquad \beta_{J^c} = \left[\sum_{k \in J^c} \beta_k^{-1}\right]^{-1},$$

$$\beta_{\emptyset} = \infty$$
, and $N_{\emptyset} = 1$.

▶ Lower bound in TVD and Hellinger is

$$\min_{J \in \mathcal{A}} \left[\frac{N_J}{n} \right]^{\frac{\beta_J c}{2\beta_J c + 1}} = \left[\frac{N_{J_*}}{n} \right]^{\frac{\beta_J c}{2\beta_J c + 1}}$$

Special Case of Lower Bound: $d_x = 0$, $d_y = 1$

$$\min \left\{ \left[N_1/n \right]^{1/2}, n^{-\frac{\beta_1}{2\beta_1+1}} \right\}$$

- Parametric rate if N₁ is constant
- ▶ If N_1 is sufficiently fast then standard rate for estimation of β_1 -smooth functions
- Hall and Titterington (1987) obtained this lower bound for mean summed square error under slightly different smoothness definition

Special Case of Lower Bound: $d_x = 1$, $d_y = 1$

$$\min \left\{ [N_1/n]^{\frac{\beta_2}{2\beta_2+1}} \,, n^{-\frac{\beta_{1,2}}{2\beta_{1,2}+1}} \right\}$$

- ▶ Approximately, n/N_1 observations should be available for estimating β_2 -smooth conditional densities of x|y.
- ▶ If N_1 is sufficiently fast then we can exploit smoothness in y

Frequentist Literature on Smoothing Sparse Discrete Data

- ▶ N_k 's are constant: Aitchison and Aitken (1976), Hall, Racine, and Li (2004) (cross-validation)
- ▶ Burman (1987): lower bounds and discrete kernels for $d_y = 1$, $d_x = 0$, $\beta_1 = 2$.
- ▶ Hall and Titterington (1987): lower bounds and discrete kernels for $d_y = 1$, $d_x = 0$, general β_1 ; cross-validated bandwidth selection for $\beta_1 = 2$.
- ▶ Dong and Simonoff (1995): upper bounds for $d_x = 0$, $d_y \le 4$, $\beta_1 = \ldots = \beta_{d_y} = 4$, fast N_k 's
- Aerts et al. (1997): local polynomial smoothers for $d_x = 0$, general d_y , $\beta_1 = \ldots = \beta_{d_y}$, fast N_k 's.

Proof Sketch for Lower Bound

Th. 2.5 in Tsybakov (2008) (Ibragimov and Hasminskii (1977)):

$$\inf_{\hat{\rho}} \sup_{p_0 \in \mathcal{P}} P(d(\hat{\rho}, p_0) \geq \Gamma_n) \geq const > 0, \quad \text{if} \quad$$

- ▶ $\exists q_j, q_k \in \mathcal{P}$, $0 \leq j < k \leq M$
- ▶ $d(q_j, q_k) \ge 2\Gamma_n$,
- $ightharpoonup \sum_{j=1}^{M} KL(q_j, q_0)/M < \log(M)/8$

Proof Sketch for Lower Bound

$$q_j(x,y) = \int_{A_y} \left[1 + \Gamma_n \cdot \sum_i w_i^j \prod_{r=1}^d g(m_r(x_r - c_r^i)) \right] dx_{d_x + 1:d}$$

- $w_i^0 = 0, w_i^j \in \{0,1\}, i \in \{1,\ldots,\prod_{r=1}^d m_r\},$
- c_i center of rectangle with sides $(1/m_1,...,1/m_d)$
- g is infinitely smooth on [-1/2,1/2], 0 elsewhere, $\int g=0$
- $m_r = s^{-1/\beta_r^*}$
- ▶ $\beta_r^* = \beta_r$ for $r \notin J_*$ (x_r (treated as) continuous)
- ▶ $\beta_r^* = -\log(s)/\log N_r$ for $r \in J_*$ (smoothness at which we would be indifferent to treating x_r as continuous, $\beta_r^* \geq \beta_r$)
- ▶ The rest of the proof is similar to the continuous case.

Model

For $y \in \mathbb{R}^{d_y}$ and $x \in \mathbb{R}^{d_x}$,

$$p(x,y|\theta,m) = \int_{A_y} \sum_{i=1}^m \alpha_j \phi(x,\tilde{y};\mu_j,\sigma) d\tilde{y},$$

where $\theta = (\alpha_1, \mu_1, \dots, \alpha_m, \mu_m, \sigma)$, $\mu_j \in \mathbb{R}^d$, $\sigma^2 = (\sigma_1^2, \dots, \sigma_d^2)$ and ϕ - normal density with diagonal covariance.

- □ Π(θ|m)
- ► П(*m*)
- ► (Dirichlet process mixture should also work)

MCMC Estimation through Data Augmentation

- $X^n = (x_1, \ldots, x_n), Y^n = (y_1, \ldots, y_n)$
- Explicitly use latent variables $\tilde{y} = \{\tilde{y}_1, \dots, \tilde{y}_n\}$
- ▶ Introduce mixture allocation latent variables: $s = (s_1, ..., s_n)$,

$$x_i, \tilde{y}_i | s_i = j, \theta, m \sim N(\mu_j, \sigma)$$

- ▶ Gibbs sampler for $\theta, \tilde{y}, s | m, X^n, Y^n$
- $\blacktriangleright \theta | m, \tilde{y}, s, X^n, Y^n$, same as in simple Normal model.
- $ightharpoonup |\widetilde{y}_i| \ldots \sim N(\mu_{s_i}, \sigma) \cdot 1_{A_v}$
- $P(s_i = j | \ldots) \propto \alpha_j \phi(x_i, \tilde{y}_i; \mu_j, \sigma)$
- Reversible jump for m (or Dirichlet process mixture)

Assumptions on DGP for Upper Bound

For $J = \{d' + 1, \dots, d_y\}$, $y = (y_{J^c}, y_J)$, define marginal pmf

$$\pi_0(y_J) = \int \int_{A_{y_J}} f_0(x, \tilde{y}) d\tilde{y} dx$$

and conditional pdf

$$f_{0|J}(x,\tilde{y}_{J^c}|y_J) = \int_{A_{VJ}} f_0(x,\tilde{y}) d\tilde{y} / \pi_0(y_J)$$

Assume that for any y_J

- $\qquad \qquad \bullet \quad 0 < \frac{\pi}{N_J} \le \pi_0(y_J) \le \frac{\pi}{N_J} < \infty$

Upper Bound on Posterior Contraction Rate

 ϵ_n is an upper bound on the posterior contraction rate if

$$\Pi\left(p:\ d(p_0,p)>const\cdot\epsilon_n\bigg|Y^n,X^n
ight)\overset{Pr}{
ightarrow}0.$$

Theorem 2: under standard assumptions on priors and smoothness assumptions on f_0 from the previous slide

$$\epsilon_n = \left[\frac{N_J}{n}\right]^{\frac{\beta_J c}{2\beta_J c + 1}} \cdot (\log n)^t,$$

which coincides with the lower bound up to $(\log n)^t$ when $J = J_*$.

(x can have unbounded support but with sub-exponential tails and envelope function L that behaves like f_0 in the tails)

Previous Posterior Asymptotics Results for Constant N_k 's

- ► Norets and Pelenis (2012) weak consistency for mixtures with a variable number of components
- DeYoreo and Kottas (2017) weak consistency for Dirichlet process mixtures
- ▶ Canale and Dunson (2015) contraction rates for Dirichlet process mixtures (dimension in their rate is $d_y + d_x$, which is non-optimal for constant N_k 's)

Assumptions on Prior

- ▶ $\Pi(\alpha_1, ..., \alpha_m | m)$ is Dirichlet(a/m, ..., a/m), a > 0
- Prior density for locations μ_{ir}^{x} is bounded below by

$$\exp(-b_2\mu^{\tau_2})$$

and

$$1 - \Pi(\mu_i^x \in [-x, x]^{d_x}) \le \exp(-b_3 x^{\tau_3})$$

- Prior density for locations μ_j^y is bounded away from zero on $[0,1]^{d_y}$.
- ▶ Prior for σ_r is inverse Gamma (not a standard conditionally conjugate prior).

Proof: Sufficient Conditions

Ghosal, Ghosh, and Vaart (2000): posterior contracts at rate ϵ_n if

- $\triangleright Z_i \stackrel{iid}{\sim} p_0, Z^n = (Z_1, \ldots, Z_n)$
- $p_0 \in \mathcal{P}$ space of densities w.r.t. a σ -finite measure
- ▶ d Hellinger or total variation distance
- $ightharpoonup \mathcal{P}_n$ is a sieve satisfying

$$\log J(\epsilon_n, \mathcal{P}_n, d) \le c_1 n \epsilon_n^2 \quad (J - \text{metric entropy})$$

$$\Pi(\mathcal{P}_n^c) \le c_3 \exp\{-(c_2 + 4) n \epsilon_n^2\}$$

▶ Prior thickness condition for Kullback-Leibler neighborhoods

$$\mathcal{K}(p_0, \epsilon_n) = \left\{ p: \int p_0 \log(p_0/p) < \epsilon_n^2, \int p_0 [\log(p_0/p)]^2 < \epsilon_n^2 \right\}$$

$$\Pi(\mathcal{K}(p_0, \epsilon_n)) \ge c_4 \exp\{-c_2 n \epsilon_n^2\}$$

Proof: Approximation Idea

Approximation results are key, e.g., need to find (θ^*, m) s.t. $KL(p_0(x, y), p(x, y | \theta^*, m)) \le \epsilon_n^2$.

Consider first $J = \{d_x + 1, \dots, d\}$.

- $p_0(x,y) = \pi_0(y)p_0(x|y)$
- ▶ For $\sigma^y \to 0$, $\int_{A_y} \phi(\tilde{y}, y', \sigma^y) \approx 1$ when y = y', 0 otherwise.

$$\pi_0(y) pprox \int_{A_y} \sum_{y'} \pi_0(y') \phi(\tilde{y}, y', \sigma^y) d\tilde{y}$$

From STG: ∀y',

$$p_0(x|y') \approx \sum_{j=1}^{m_x} \alpha_{j|y'} \phi(x; \mu_{j|y'}, \sigma^x)$$

Proof: Approximation Idea

Combine the approximations from the previous slide into

$$p_0(x,y) \approx \int_{A_y} \sum_{y'} \sum_{j=1}^{m_x} \alpha_{j|y'} \pi_0(y') \phi(x; \mu_{j|y'}, \sigma^x) \phi(\tilde{y}, y', \sigma^y) d\tilde{y}$$
$$= p(x, y|\theta^*, m)$$

Next, need to find a neighborhood of θ^* , S_{θ^*} , for which approximation error is still below ϵ_n and its prior probability $\geq \exp\{-c_2n\epsilon_n^2\}$.

Proof: Prior Probability of KL neighborhoods

For example, consider m (isotropic case, $\beta_j = \beta$).

▶ If we need approximation error $\Gamma_n \cdot log(n)^t$ for the conditionals, where $\Gamma_n = [N_J/n]^{\frac{\beta}{2\beta+d_x}}$, from STG:

$$m_{x}=c_{1}\Gamma_{n}^{-d_{x}/\beta}(\log n)^{c_{2}}$$

- ▶ Total # of mixture components: $m = N_J \cdot c_1 \Gamma_n^{-d_x/\beta} (\log n)^{c_2}$

$$c_1 N_J \Gamma_n^{-d_x/\beta} (\log n)^{c_2} \le n [\Gamma_n \log(n)^t]^2 \quad \Leftrightarrow$$

$$c_1 N_J / n (\log n)^{c_2 - 2t} \le \Gamma_n^{2 + d_x/\beta} \quad \Leftrightarrow$$

$$t > c_2 / 2$$

Proof: $J \neq \{d_x + 1, \dots, d\}$

- Approximation argument above is easy to adapt
- (Hellinger, TVD, KL) distances and ratios for mixed discrete-continuous distributions are bounded by distances and ratios for the corresponding latent variable densities.
- ▶ Bounds on entropy for mixture of multivariate normals from previous literature also apply for the same reason (to $J = \{d_x + 1, ..., d\}$ case as well).

Evaluating Model Quality

Cross Validated Log Scoring Rule

$$\sum_{i=1}^n \log p(z_i|Z^{n/i}) \approx \sum_{i=1}^n \log \frac{1}{K} \sum_{k=1}^K p(z_i|Z^{n/i}, \theta^k)$$

▶ We use: Modified Cross Validated Log Scoring Rule: Randomly order sample observations and use the first n₁ observations for inference and the rest for evaluation. Repeat this process several times and compare means or medians.

$$\sum_{n_1+1}^{n} \log p(z_i|Z^{n_1})$$

Labor Market Participation

- Source: Norets and Pelenis (2012)
- ► Gerfin (1996) cross-section dataset. Compare probit, kernel (Hall et al. (2004)) and FMMN.
- ▶ Binary dependent variable Labor force participation dummy.
- Independent variables: Log of non-labor income, Age, Education, Number of young children, Number of old children, Foreign dummy.
- Number of observations: T=872. Split into two samples of $T_1=650$ and $T_2=222$ observations. Use T_1 as an estimation sample, and T_2 as a prediction sample for 50 different random splits.

Comparison of Different Models

Table: Modified cross-validated log scores and classification rates

Model	Log Score		% Correct pred-ns	
	Mean	Median	Mean	Median
Probit	-137.23	-136.69	66.08%	66.37%
Kernel	-138.21	-135.99	65.91%	65.77%
FMMN(m=1)	-137.27	-136.81	66.02%	65.77%
FMMN(m=2)	-132.30	-131.86	67.95%	68.02%
FMMN(m=3)	-133.32	-132.60	67.76%	67.57%
FMMN(m=4)	-133.13	-131.86	68.21%	68.02%

Future Work

- Check that results go though for Dirichlet process mixtures
- Simulations/applications for variable m or Dirichlet process mixtures
- Extend results from Norets and Pati (2017) for continuous conditional densities to mixed discrete-continuous case.
- Implement MCMC for direct estimation of conditional distributions (extend Norets (2017))

Power of log in the rate for continuous case

$$\epsilon_n = n^{-\beta/(2\beta+d)} (\log n)^t$$

$$t > \frac{d(1+1/\beta+1/\tau) + \max\{\tau_1, 1, \tau_2/\tau\}}{2+d/\beta} + \max\left\{0, \frac{1-\tau_1}{2}\right\}$$

- \triangleright β smoothness level
- \triangleright d dimension of (y,x)
- ▶ τ : $f_0(z) \le c \exp(-b||z||^{\tau})$
- $T_1: \Pi(m=i) \propto \exp(-b_1 i (\log i)^{\tau_1})$
- ▶ τ_2 : $\exp(-b_2\mu^{\tau_2}) \le \text{prior density for } \mu_{jk}^y$.

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