Supplementary material for: Multiresolution dictionary learning for conditional distributions

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1 Full conditionals

Introduce the latent variable $S_i \in \{1,\ldots,k\}$, for $i=1,\ldots,n$, denoting the multiscale level used by the ith subject. Assuming data are normalized prior to analysis, we let $\mu \sim \mathcal{N}(0,I)$ and $\sigma = \mathcal{IG}(a,b)$ for the means and variances of the dictionary densities. Let n_{B_j} be the number of observations allocated to node B_j . Each Gibbs sampler iteration can be summarized in the following steps.

1. Update S_i by sampling from the multinomial full conditional with

$$\Pr(S_i = j \mid -) = \frac{\pi_{B_j(x_i)} f_{B_j(x_i)}(y_i)}{\sum_{h=1}^k \pi_{B_h(x_i)} f_{B_h(x_i)}(y_i)}$$

- 2. Update stick-breaking random variable $V_{B_j(x_i)}$, for $j=1,\ldots,k$ and $i=1,\ldots,n$, from $\mathrm{Beta}(\beta_p,\alpha_p)$ with $\beta_p=1+n_{B_j}$ and $\alpha_p=\alpha+\sum_{B_h(x_i)\in de\{B_j(x_i)\}}n_{B_h(x_i)}$.
- 3. Update $(\mu_{B_j(x_i)}, \sigma_{B_j(x_i)})$ by sampling from

$$\mu_{B_j} \sim \mathcal{N}\left(\bar{y}_{B_j} n_{B_j} / \sigma_{B_j}, (1 + n_{B_j} / \sigma_{B_j})^{-1}\right)$$

$$\sigma_{B_j} \sim \mathcal{IG}\left(a_{\sigma}, b + 0.5 \sum_{\{i: S_i = j, x_i \in B_j\}} \left(y_i - \mu_{B_j}\right)^2\right)$$

with $a_{\sigma} = a + n_{B_i}/2$, \bar{y}_{B_i} being the average of the observation $\{y_i\}$ allocated to node B_i .

2 Predictions

Consider the case we want to predict the response y_{n+1} for a future subject based on the predictors x_{n+1} and (y_1, \ldots, y_n) . For each tree level, the new vector of predictors x_n is allocated to subsets having closer centers with respect some metric. We will consider the euclidean metric. Then, for a new observation the predictive density is defined as

$$p(y_{n+1}|x_{n+1}, y_1, \dots, y_n) = \int f(y_{n+1}|x_{n+1}, \Omega) dp(\Omega|y_1, \dots, y_n)$$
 (1)

with $f\left(y_{n+1}|x_{n+1},\Omega\right)$ defined as in (1) and Ω being the set of all parameters involved, i.e. weights, location and scale parameters. In order to make inference on the predictive density of y_{n+1} , at the sth Gibbs sampler iteration, we will first sample parameters involved in $\ref{eq:total_scale}$ from its posterior, i.e. $\Omega^{(s)} \sim p\left(\Omega|y_1,\ldots,y_n\right)$ and then we will sample $y_{n+1}^{(s)}$ from $p\left(y_{n+1}|x_{n+1},\Omega^{(s)}\right)$. Let us assume the number of iterations is S an a burn-in of b is considered. Then, given the sequence $\left(y_{n+1}^{(b+1)},\ldots,y_{n+1}^{(S)}\right)$, summaries of the predictive density such as mean, variance and quantiles can be computed.

3 Partition Tree Schematic

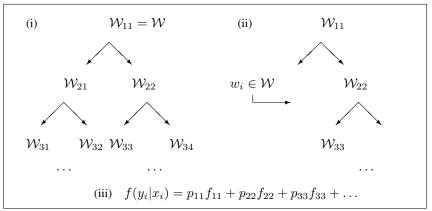


Figure 1: (i) Multiscale partition of the data. (ii) Path through the tree for $x_i \in \mathbb{R}^p$. (iii) Conditional density of y_i given x_i defined as a convex combination of densities along the path.

4 Synthetic examples

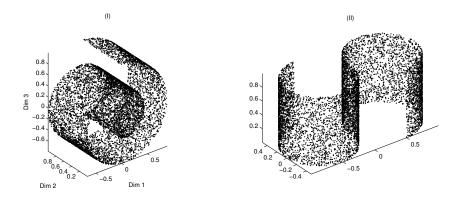


Figure 2: Non-linear manifolds: Swissroll (I) and S-Manifold (II) embedded in \mathcal{R}^3

Table 1: Linear manifold example 1: Mean and standard deviations of squared errors under multiscale stick-breaking (MSB), CART and Lasso for sample size 50 and 100 for different simulation scenarios.

| | | | | r = 5 | | r = 10 | | | |
|---------|-----|--------------------|---------------------|----------------------|---------------------|---------------------|----------------------|---------------------|--|
| p | n | | MSB | CART | LASSO | MSB | CART | LASSO | |
| 1e + 04 | 50 | MSE STD TIME | 0.18 0.32 3 | 0.31 0.30 2 | 0.25 0.42 1 | 0.22 0.24 3 | 0.58 0.54 3 | 0.22 0.30 1 | |
| 1e + 04 | 100 | MSE STD TIME | 0.18 0.26 5 | 0.27 0.42 5 | 0.26 0.46 2 | 0.20 0.23 5 | 0.41 0.46 5 | 0.52 0.78 1 | |
| 1e + 05 | 50 | MSE STD TIME | $0.35 \\ 0.53 \\ 3$ | $0.45 \\ 0.77 \\ 25$ | $0.89 \\ 1.04 \\ 2$ | $0.16 \\ 0.21 \\ 3$ | $0.33 \\ 0.46 \\ 27$ | $0.20 \\ 0.31 \\ 2$ | |
| 1e + 05 | 100 | MSE STD TIME | $0.43 \\ 0.59 \\ 7$ | 0.88 1.29 50 | $0.52 \\ 0.70 \\ 5$ | $0.17 \\ 0.24 \\ 7$ | 0.50 0.75 51 | $0.31 \\ 0.49 \\ 5$ | |
| 5e + 05 | 50 | MSE STD TIME | 0.11 0.15 5 | 0.16 0.24 90 | 0.15 0.19 11 | 0.83 1.01 5 | 2.26 2.60 121 | 0.92 3.69 10 | |
| 5e + 05 | 100 | MSE STD TIME | 0.003 0.16 10 | 0.17 0.23 214 | 0.08 0.13 43 | 0.13 1.12 8 | 1.37 1.81 227 | 1.06 1.50 42 | |
| 7e + 05 | 50 | MSE STD TIME | 1.70 2.18 6 | 1.48 2.47 121 | 1.47 1.63 12 | 0.66 0.87 7 | 1.65 1.49 151 | 1.07 0.95 13 | |
| 5e + 05 | 100 | MSE STD TIME | 0.69 0.94 13 | 1.36 1.47 321 | 0.82 1.28 41 | 0.78 1.03 12 | 1.52 1.34 325 | 1.43 2.11 44 | |

Table 2: Linear manifold example 2: Mean and standard deviations of squared errors under multiscale stick-breaking (MSB), CART and Lasso for different sample sizes

| | | | | r=2 | | | r = 5 | |
|----------|-----|------------|--------------|--------------|--------------|--------------|--------------|--------------|
| p | n | | MSB | CART | LASSO | MSB | CART | LASSO |
| 10e + 03 | 100 | MSE STD | 1.54 1.70 | 1.78 1.72 | 2.37 0.89 | 0.84 1.38 | 1.25 1.35 | 1.62 1.47 |
| 50e + 03 | 100 | MSE STD | 0.76 1.04 | 0.97 1.21 | 1.77 3.13 | 0.88 1.00 | 1.53 1.59 | 1.43 2.73 |
| 10e + 04 | 100 | MSE STD | 0.77 0.94 | 1.01 1.13 | 1.61 1.85 | 0.67 0.82 | 0.46 0.61 | 0.97 1.16 |
| 20e + 04 | 100 | MSE STD | 0.86 1.30 | 0.90 1.35 | 1.41 1.41 | 0.74 0.95 | 1.09 1.98 | 0.78 0.95 |

Table 3: Non-linear manifold - MFA: Mean and standard deviations of squared errors under multiscale stick-breaking (MSB), CART and Lasso for different sample sizes for different simulations sampled from a mixture of factor analyzers

| | | | | N = 10 | <u> </u> | | N = 5 | |
|----------|-----|--------------------|----------------------|---------------------|--------------------|--------------------|---------------------|--------------------|
| p | n | SIM | MSB | CART | LASSO | MSB | CART | LASSO |
| 50e + 03 | 100 | MSE STD TIME | 0.23 0.34 5 | 0.42 0.59 24 | 0.36 0.43 3 | 0.17 0.18 7 | 0.43 0.69 27 | 0.22 0.23 3 |
| 50e + 03 | 200 | MSE STD TIME | 0.23 0.33 10 | 0.42 0.56 51 | 0.27 0.23 8 | 0.17 0.19 12 | 0.22 0.38 56 | 0.20 0.25 7 |
| 10e + 04 | 100 | MSE STD TIME | 0.67 1.04 9 | 1.35 2.26 47 | 1.32 1.36 6 | 0.15 0.23 6 | 0.17 0.19 44 | 0.22 0.23 5 |
| 10e + 04 | 200 | MSE STD TIME | 0.64 0.95 15 | 1.37 1.77 99 | 0.85 1.29 15 | 0.15 0.24 11 | 0.26 0.42 89 | 0.15 0.24 15 |
| 30e + 04 | 100 | MSE STD TIME | 0.26 0.39 9.28 | 0.39 0.51 125 | 0.31 0.52 18 | 0.63 0.80 9 | 1.40 1.24 145 | 1.01 1.46 17 |
| 30e + 04 | 200 | MSE STD TIME | 0.25 0.36 15 | 0.47 0.88 262 | 0.26 0.43 40 | 0.63 0.80 13 | 1.17 2.11 283 | 0.92 1.04 43 |
| 30e + 04 | 300 | MSE STD TIME | 0.25 0.36 15 | 0.30 0.41 463 | 0.30 0.48 73 | 0.62 0.89 16 | 1.42 1.85 465 | 0.70 0.94 89 |

Table 4: Non-linear manifold - Swissroll and S-Manifold: Mean and standard deviations of squared errors under multiscale stick-breaking (MSB), CART and Lasso for different sample sizes for different simulation scenarios.

| | | | SWISSROLL | | | S-Manifold | | |
|----------|-----|------|-----------|------|-------|------------|------|-------|
| p | n | | MSB | CART | LASSO | MSB | CART | LASSO |
| | | MSE | 0.25 | 0.46 | 0.38 | 0.67 | 0.70 | 0.77 |
| 10e + 03 | 100 | STD | 0.24 | 0.53 | 0.40 | 0.76 | 0.80 | 0.85 |
| | | TIME | 5 | 5 | 1 | 4 | 5 | 1 |
| | | MSE | 0.24 | 0.44 | 0.25 | 0.38 | 0.38 | 0.84 |
| 10e + 04 | 50 | STD | 0.24 | 0.42 | 0.29 | 0.40 | 0.35 | 0.80 |
| | | TIME | 3 | 22 | 2 | 5 | 7 | 1 |
| | | MSE | 0.24 | 0.43 | 0.17 | 0.25 | 0.30 | 0.70 |
| 10e + 04 | 100 | STD | 0.26 | 0.55 | 0.22 | 0.22 | 0.25 | 0.50 |
| | | TIME | 6 | 48 | 7 | 7 | 50 | 7 |
| | | MSE | 0.24 | 0.67 | 0.29 | 0.35 | 0.40 | 0.73 |
| 20e + 04 | 50 | STD | 0.23 | 0.50 | 0.29 | 0.22 | 0.30 | 0.40 |
| | | TIME | 4 | 38 | 5 | 3 | 40 | 5 |
| | | MSE | 0.25 | 0.78 | 0.33 | 0.37 | 0.37 | 0.70 |
| 20e + 04 | 100 | STD | 0.26 | 0.74 | 0.36 | 0.25 | 0.27 | 0.55 |
| | | TIME | 6 | 96 | 13 | 6 | 98 | 14 |
| | | MSE | 0.17 | 0.47 | 0.23 | 0.16 | 0.20 | 0.35 |
| 50e + 04 | 50 | STD | 0.23 | 0.43 | 0.22 | 0.20 | 0.19 | 0.40 |
| · | | TIME | 5 | 126 | 10 | 5 | 130 | 15 |
| | | MSE | 0.17 | 0.33 | 0.19 | 0.11 | 0.25 | 0.56 |
| 50e + 04 | 100 | STD | 0.21 | 0.46 | 0.23 | 0.14 | 0.20 | 0.61 |
| | | TIME | 11 | 230 | 25 | 10 | 254 | 27 |