Easy conditioning far beyond Gaussian

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2 Stability by conditioning

3 Methodology for Estimating Conditional Distributions

4 Application

5 Conclusion

A motivating example in medicine

- Cohort of 443 female patients from the University hospital of Bern, provided by Pr. Stute.

n	Age	BMI	TotalC	HDLC	BP
1	58	22.15	5.93	1.85	100
2	52	30.25	3.65	1.06	120
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- Apply risk calculators such as SCORE2 with imputed inputs.
- Data publicly available on Zenodo

Analytical conditioning approach

Goal: Sample from the conditional distribution $f_{\mathbf{X_1}|\mathbf{X_2}}$ of a random vector $\mathrm{X}_1 \in \mathbb{R}^l$ given an observation of x_2 of $\mathrm{X}_2 \in \mathbb{R}^m$, based on a sample of $\mathrm{X} = (x_{1i}, x_{2i})_{i=1}^n$ previously acquired.

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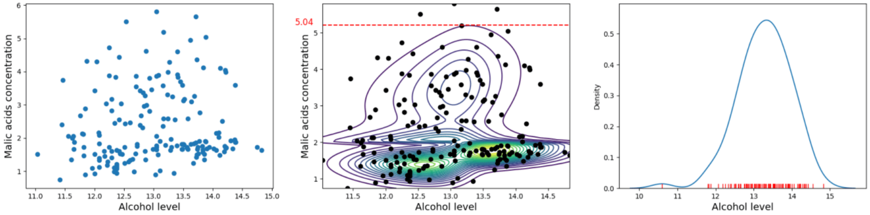
  2. to perform analytical conditioning to obtain $\hat{f}_{\mathbf{X_1}|\mathbf{X_2}}$ for a new observation x_2
- We will assume a **parametric form** for the joint distribution and use **analytical formulas for conditioning** instead of approximations such as MCMC methods.

Example

Chemical analysis of wines grown in the same region in Italy, 178 observations.



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The Gaussian case

- Let $\mathbf{X} \sim \mathcal{N}_d(\mu, \Sigma)$, $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2)^t$ with $\mathbf{X}_1 \in \mathbb{R}^l$, $\mathbf{X}_2 \in \mathbb{R}^m$ and $l + m = d$ and
$$\Sigma = \begin{pmatrix} \Sigma_{1,1} & \Sigma_{1,2} \\ \Sigma_{2,1} & \Sigma_{2,2} \end{pmatrix}$$
with Σ_{22} non-singular.

  Then
$$\mathbf{X}_2 \sim \mathcal{N}_m(\mu_2, \Sigma_{22})$$
and
$$\mathbf{X}_1 | \mathbf{X}_2 = \mathbf{x}_2 \sim \mathcal{N}_l(\mu_{1.2}, \Sigma_{11.2})$$

  with $\mu_{1.2} = \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(\mathbf{x}_2 - \mu_2)$ and $\Sigma_{11.2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$.

- Limitations: asymmetry, heavy-tail, tail dependence ...

  $\rightarrow$ Model the joint distribution with a broader class of multivariate distributions, while still enjoying stability by conditioning.

Multivariate Student t-distribution

Let $\mathbf{X} \sim t_d(\mu, \Sigma, \nu)$ and $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2)^t$ with $\mathbf{X}_1 \in \mathbb{R}^l$, $\mathbf{X}_2 \in \mathbb{R}^m$ and $l + m = d$.

Then by, Ding [2016] :

$$X_2 \sim t_q(\mu_2, \Sigma_{22}, \nu)$$

and

$$\mathbf{X}_1 | \mathbf{X}_2 = \mathbf{x}_2 \sim t_p(\mu_{1.2}, \frac{\nu + d_2}{\nu + q} \Sigma_{11.2}, \nu + q)$$

with $\mu_{1.2} = \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(\mathbf{x}_2 - \mu_2)$, $\Sigma_{11.2} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$ and $d_2 = (\mathbf{X}_2 - \mu)^t \Sigma_{22}^{-1}(\mathbf{X}_2 - \mu)$, and Σ_{22} non-singular.

Beyond

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- Remaining limitations: multi-modal distributions, different type of marginals.

Transdimensional families of distributions

Let $d \geq 1$ and a product of spaces $\prod_{k=1}^{d} \mathcal{X}_k$, where $\mathcal{X}_k$ are assumed to be measure spaces, typically $\mathbb{R}$ or its subspaces.

$\mathcal{F}^{(d)} = \{f^{(d)}(\cdot;\theta); \theta \in \Theta^{(d)}\}$ a parametric family of pdfs on $\prod_{k=1}^{d} \mathcal{X}_k$ with parameters belonging to a set $\Theta^{(d)}$.

We define trans-dimensional family of pdfs by $\mathcal{F} = \bigcup_{d=1}^{D} \mathcal{F}^{(d)}$ with $1 \leq D \leq +\infty$.

We will question the stability of such families by marginalization and conditioning with respect to some components, [Faul et al., 2024].

Stability by conditioning

For f a positive pdf on $\prod_{k=1}^{d} \mathcal{X}_k$, $(\mathrm{i},\mathrm{j}) \in I_{\ell,m}^{d}$ and $(x_{j_1},\dots,x_{j_m})$ observed:

$$f_{\mathrm{i}|\mathrm{j}}(\cdot|(x_{j_1},\dots,x_{j_m})) : (x_{i_1},\dots,x_{i_\ell}) \in \prod_{k=1}^{\ell} \mathcal{X}_{i_k} \to \frac{f_{[\mathrm{i},\mathrm{j}]}(x_{i_1},\dots,x_{i_\ell},x_{j_1},\dots,x_{j_m})}{f_{\mathrm{j}}(x_{j_1},\dots,x_{j_m})}$$

The conditioning operator is defined for $f^{(d)}(\cdot;\theta) \in \mathcal{F}^{(d)}$ as:

$$\mathrm{Cond}(f^{(d)}(\cdot,\theta)) = \left\{ f_{\mathrm{i}|\mathrm{j}}^{(d)}(\cdot|(x_{j_1},\dots,x_{j_m});\theta),\ (\mathrm{i},\mathrm{j}) \in I_{\ell,m}^{d},\ (x_{j_1},\dots,x_{j_m}) \in \prod_{k=1}^{m} \mathcal{X}_{i_k} \right\}$$

By applying it to the trans-dimensional family of pdf $\mathcal{F}$ we get:

$$\mathrm{Cond}(\mathcal{F}) = \bigcup_{d=1}^{D} \left\{ \mathrm{Cond}(f^{(d)}(\cdot;\theta)),\ \theta \in \Theta^{(d)} \right\}$$

A trans-dimensional family of probability distributions $\mathcal{F}$ is said to be stable by conditioning if $\mathrm{Cond}(\mathcal{F}) \subset \mathcal{F}$.

Extension to finite mixtures

For $\mathcal{F}^{(d)} = \{f^{(d)}(\cdot;\theta); \Theta \in \Theta^{(d)}\}$ define the mixing operator as:

$$\text{Mix}(\mathcal{F}^{(d)}) = \left\{ \sum_{k=1}^{K} \alpha_k f^{(d)}(\cdot;\theta_k), \quad K \geq 1, \quad \theta_1, \ldots, \theta_K \in \Theta^{(d)}, \right.$$
$$\left. , \ \alpha_1, \ldots, \alpha_K \geq 0 \quad \text{s.t.} \quad \sum_{k=1}^{K} \alpha_k = 1 \right\}$$

and for the transdimensional case:

$$\text{Mix}(\mathcal{F}) = \bigcup_{d=1}^{D} \text{Mix}(\mathcal{F}^{(d)})$$

Extension to finite mixtures

Theorem [Faul et al., 2024]

If a parametrized family of trans-dimensional probability distributions $\mathcal{F}$ is stable by conditioning (resp. marginalization) then $Mix(\mathcal{F})$ is also stable by conditioning (resp. marginalization).

Example of mixture of Gaussians:

$$f(\mathbf{x}_1|\mathbf{x}_2) = \sum_{i=1}^{K} \frac{\alpha_i \mathcal{N}_m(\mathbf{x}_2|\mu_{i,2}, \Sigma_{i,22})}{\sum_{j=1}^{K} \alpha_j \mathcal{N}_m(\mathbf{x}_2|\mu_{l,2}, \Sigma_{l,22})} \mathcal{N}_l(\mathbf{x}_1|\mu_{i,1.2}, \Sigma_{i,11.2})$$

The conditional distribution is a Gaussian mixture distribution with weights:

$$\tilde{\alpha}_i(\mathbf{x}_2) = \frac{\alpha_i \mathcal{N}_m(\mathbf{x}_2|\mu_{i,2}, \Sigma_{i,22})}{\sum_{j=1}^{K} \alpha_j \mathcal{N}_m(\mathbf{x}_2|\mu_{j,2}, \Sigma_{j,22})}$$

Furthermore, stability by conditioning is preserved by univariate transformations of the marginals.

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- Let remind that the density of a Gaussian mixture model (GMM) with K components is given by:

$$\psi(x_1, \dots, x_d, \Theta) = \sum_{k=1}^{K} \alpha_j \phi(x_1, \dots, x_d; \mu_k, \Sigma_k), \ \forall \mathrm{x} = (x_1, \dots, x_n) \in \mathbb{R}^d$$

with $\Theta = \{\alpha_i, \mu_i, \Sigma_i\}_{i=1}^{K}$.

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  with $\Theta = \{\alpha_i, \mu_i, \Sigma_i\}_{i=1}^{K}$.
- The density of a GMCM with parameters Θ is given by:

$$c_{gmc}(u_1, \ldots, u_d; \Theta) = \frac{\psi(\Psi_1^{-1}(u_1), \ldots, \Psi_d^{-1}(u_d))}{\prod_{i=1}^{d} \psi_i(\Psi_i^{-1}(u_i))}, \;\; 0 \leq u_1, \ldots, u_d \leq 1$$

  where ψ_j and Ψ_j^{-1} denote the marginal df and inverse cdf of the GMM along the j-th dimension .

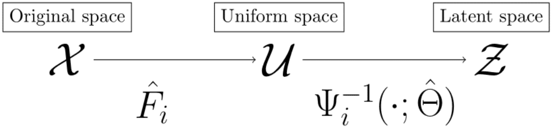
Estimate the joint multivariate distribution with copulas

From $\mathcal{D} = (x_{1i}, \ldots, x_{di})_{i=1}^{n}$ d-dimensional sample with i.i.d observations, estimate the joint distribution by:

- Estimate the marginal distribution by $\hat{F}_1, \ldots, \hat{F}_d$.
- By PIT, transform to approximately uniform pseudo-samples $\hat{u}_{ji} = \hat{F}_j(x_{ji}), \ \forall j \in \{1, \ldots, d\}$
- Fit a parametric copula by ML

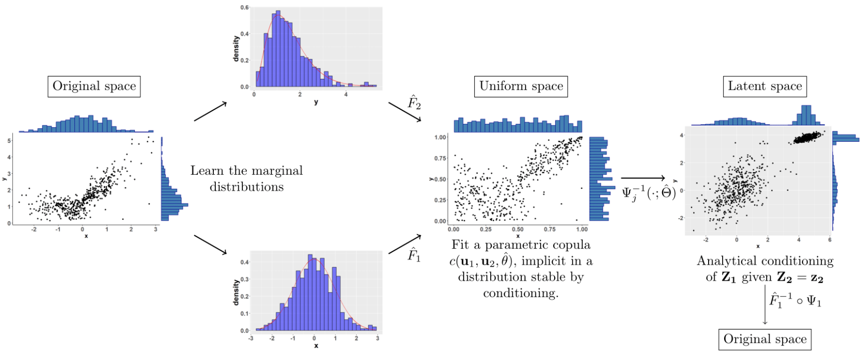
$$\hat{\theta} \in \underset{\theta \in \Theta}{\operatorname{argmin}} \prod_{i=1}^{n} c(\hat{u}_{1i}, \ldots, \hat{u}_{di}; \theta)$$

Conditioning in the latent space



- For a new point $x_2 \in \mathcal{X}$, transform to the a point in the latent space $z_2 \in \mathcal{Z}$.
- The joint distribution is approximately stable under conditioning, allowing us to perform conditioning effectively in the space $\mathcal{Z}$
- Transform back the samples to the original space by $x_1 = \hat{F}_1^{-1}(\Psi_1(z_1))$.

Algorithm Overview



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Analytical example: Meta Gaussian mixture model

2-dimensional meta-Gaussian mixture model i.e Gaussian mixture copula with different marginals.

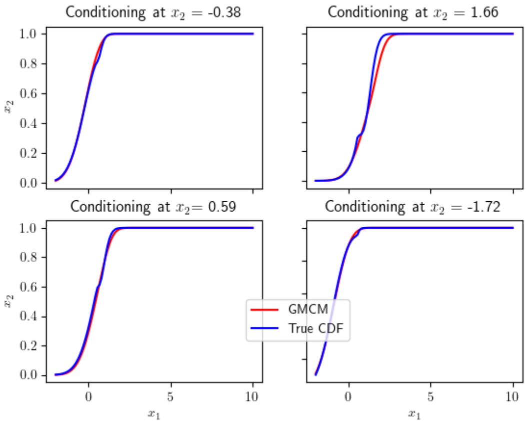

Figure 1: Comparison of true conditional cdf and estimated conditional cdf at various locations. The data follows a meta-Gaussian mixture model distribution.

Real Data: Wisconsin Cancer Data

569 patients on 30 features of the cell nuclei obtained from a digitized image of a fine needle aspirate (FNA) of a breast mass. For each patient the cancer was diagnosed as malignant or benign. We selected subset of 5 variables.

	ES	VS
GC	1.896	0.848
GMCM	**1.845**	**0.823**
TGMM	1.854	0.826
CKDE	2.007	1.979

Table 1: Comparison of various methods based on the mean of scoring rules over the test set for the Wisconsin dataset.

Application: Missing value imputation

Wisconsin Breast Cancer Dataset, adding 10% of missing values at random.

Metric	GMCM	MICE
Energy Score	**0.1908**	0.1989
Computational Time (s)	**112.3**	211.7

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- Design a versatile algorithm to estimate/sample from a conditional distribution.
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- Extend the algorithm to handle discrete variables and missing values.

Thank You

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ANY QUESTIONS ?

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