Imputing Missing Data with the Gaussian Copula

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Based on joint work with Yuxuan Zhao, Eric Landgrebe, and Eliot Shekhtman

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Data table

age	gender	state	income	education	$\cdots$
29	F	CT	\$53,000	college	$\cdots$
57	?	NY	\$19,000	high school	$\cdots$
?	M	CA	\$102,000	masters	$\cdots$
41	F	NV	\$23,000	?	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$		

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goals:

- impute missing entries?
- estimate confidence for imputations?
- quantify impact of imputation on downstream analyses?
- identify related features?

Data table

n examples (patients, respondents, assets)
p features (tests, questions, performance indicators)

$$\begin{bmatrix} & X & \end{bmatrix} = \begin{bmatrix} X_{11} & \cdots & X_{1p} \\ \vdots & \ddots & \vdots \\ X_{n1} & \cdots & X_{np} \end{bmatrix}$$

- x^i, ith row of X, is feature vector for ith example
- x_j, jth column of X, gives values for jth feature across all examples

Classic approach: low rank matrix completion

- (+) efficient algorithms
- (+) theoretical guarantees
- (+) works well when
  - true rank r is small compared to min(n,p)
  - or when true matrix is approximately low rank
- (-) works poorly for ordinal or mixed data
  - requires additional parameters (e.g., a loss function) to map from low rank parameter to ordinal observations
  - (-) fit with cross-validation $\implies$ slow!

Why low rank?

squareish data matrices $n \sim p$ for large n, p

- $(+)$ often approximately low rank
- $(+)$ Udell and Townsend 2019: approximate rank grows as $\log(n + p)$ under rather general assumptions

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skinny data matrices

- (-) are unlikely to be (very) low rank $\ll \min(n, p)$
- $(+)$ have lots of observations per column, so can estimate more complex model per column

Imputation challenge depends on the data

- size: skinny (small p) versus wide (large p)
- type: continuous, ordinal, binary, categorical, or mixed
- access: offline data vs streaming data

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Goals for imputation:

- high accuracy
- quantified uncertainty (e.g., confidence intervals)
- estimate impact on downstream analyses
- understand correlations between features

Outline

Gaussian copula model

Imputation

Approximate EM

Performance

Low-rank Gaussian copula

Gaussian copula model

We say $x \sim \mathrm{GC}(\Sigma, f) \in \mathbf{R}^p$ follows the *Gaussian copula model* with parameters Σ and $f : \mathbf{R}^p \to \mathbf{R}^p$ if

- *copula:* $z \sim \mathcal{N}(0, \Sigma)$
- *marginals:* $x = f(z)$ for $f = (f_1, \ldots, f_n)$ entrywise monotonic, i.e.,

$$x_j = f_j(z_j), \qquad j = 1, \ldots, p$$

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- models *nonlinear rulers*
- separates interations from marginals

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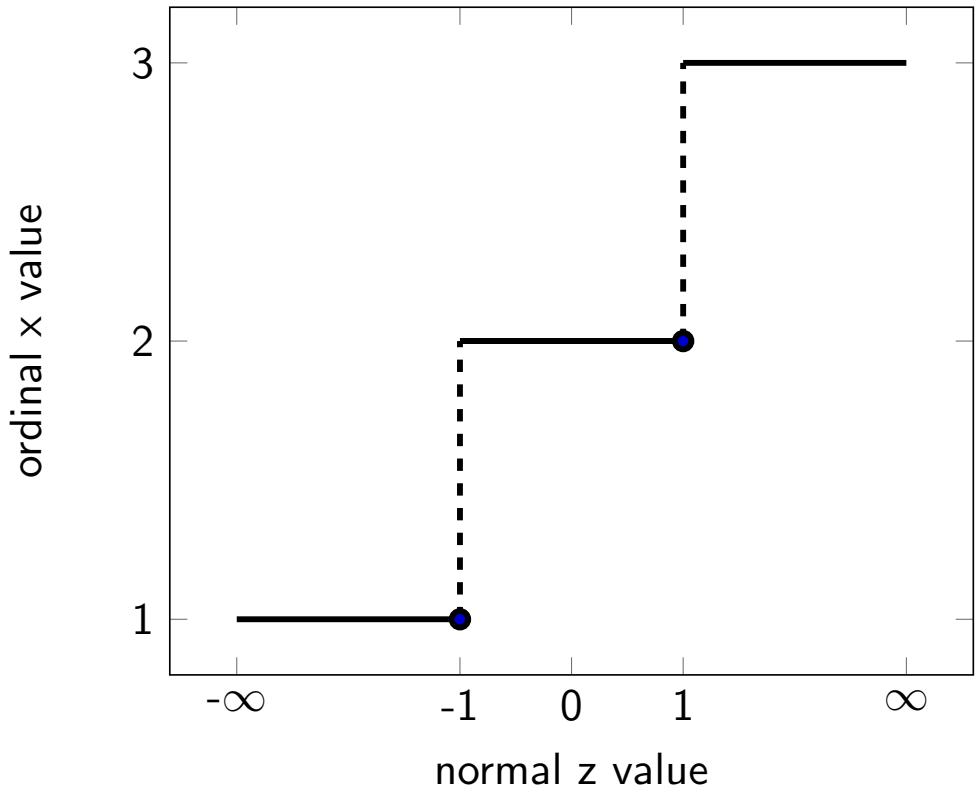
why use a copula?

- models *nonlinear rulers*
- separates interations from marginals
- Sklar's theorem: any multivariate joint distribution can be written in terms of univariate marginal distribution functions and a copula which describes the dependence structure

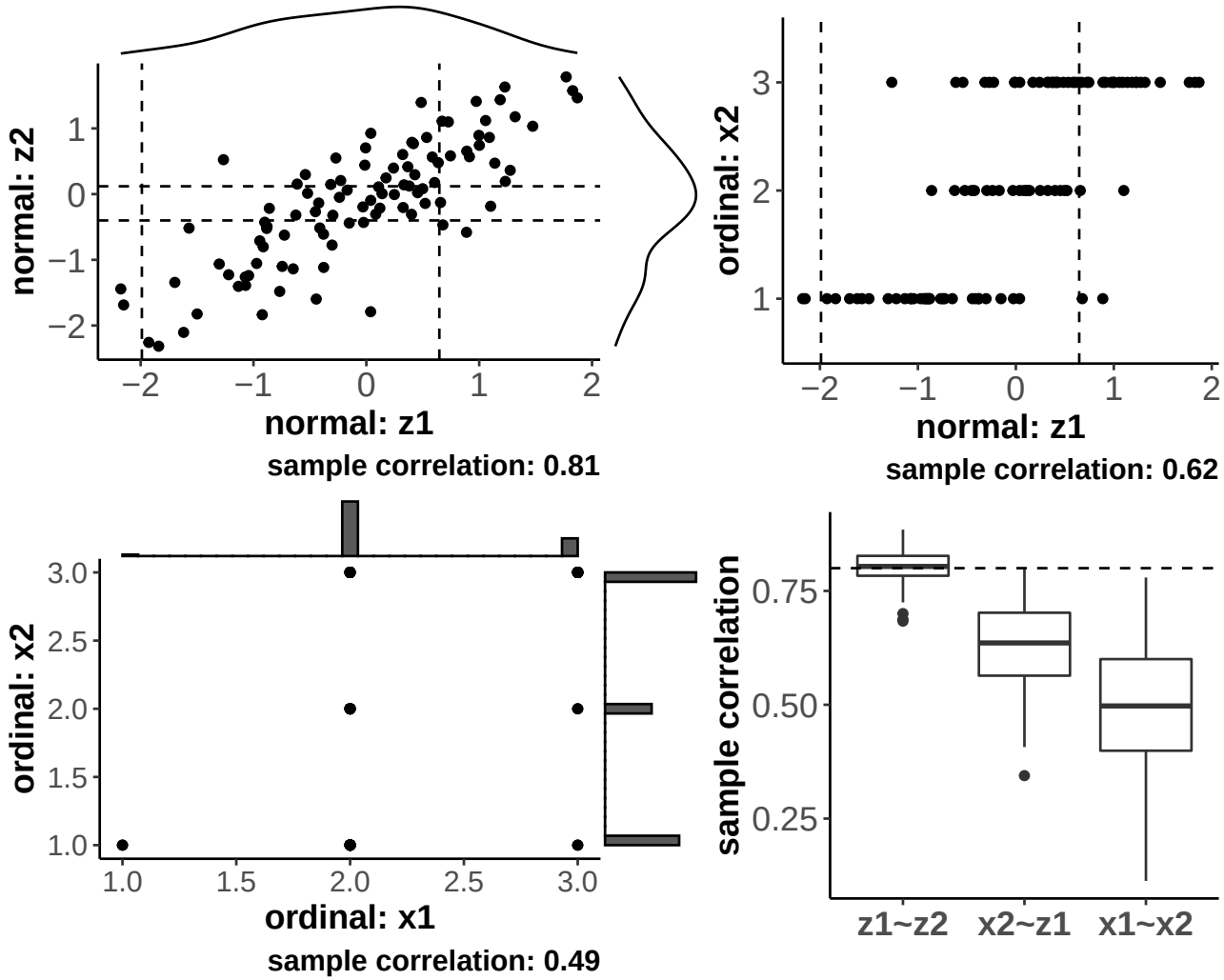
Example: cutoff function f generates ordinal data



- when x has a continuous distribution, f is invertible
- when x has a discrete distribution, f is not invertible
- we write f^{-1} for the set-valued mapping

$$z \in f^{-1}(x) \quad \Longleftrightarrow \quad x = f(z)$$

Marginals distort correlations



Related work

- Hoff et al. 2007: Gaussian copula for ordinal data, fit with MCMC
- Han and Liu 2014: Gaussian copula for real valued data
- Ganti et al. 2015: low rank model with nonlinear marginals, not probabilistic
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our method:

- handles real, boolean, ordinal, and missing data
- fully probabilistic ($\implies$ confidence intervals for estimates)
- no hyperparameters (rank, etc)
- fit with fast approximate EM

Outline

Given parameters, imputation is easy

- invertible marginals $f = (f_1, \ldots, f_p)$ (or estimates)
- copula Σ
- observed entries x_{obs} of new row $x \in \mathbf{R}^p$, obs $\subset \{1, \ldots, p\}$
- missing entries mis $= \{1, \ldots, p\} \setminus$ obs

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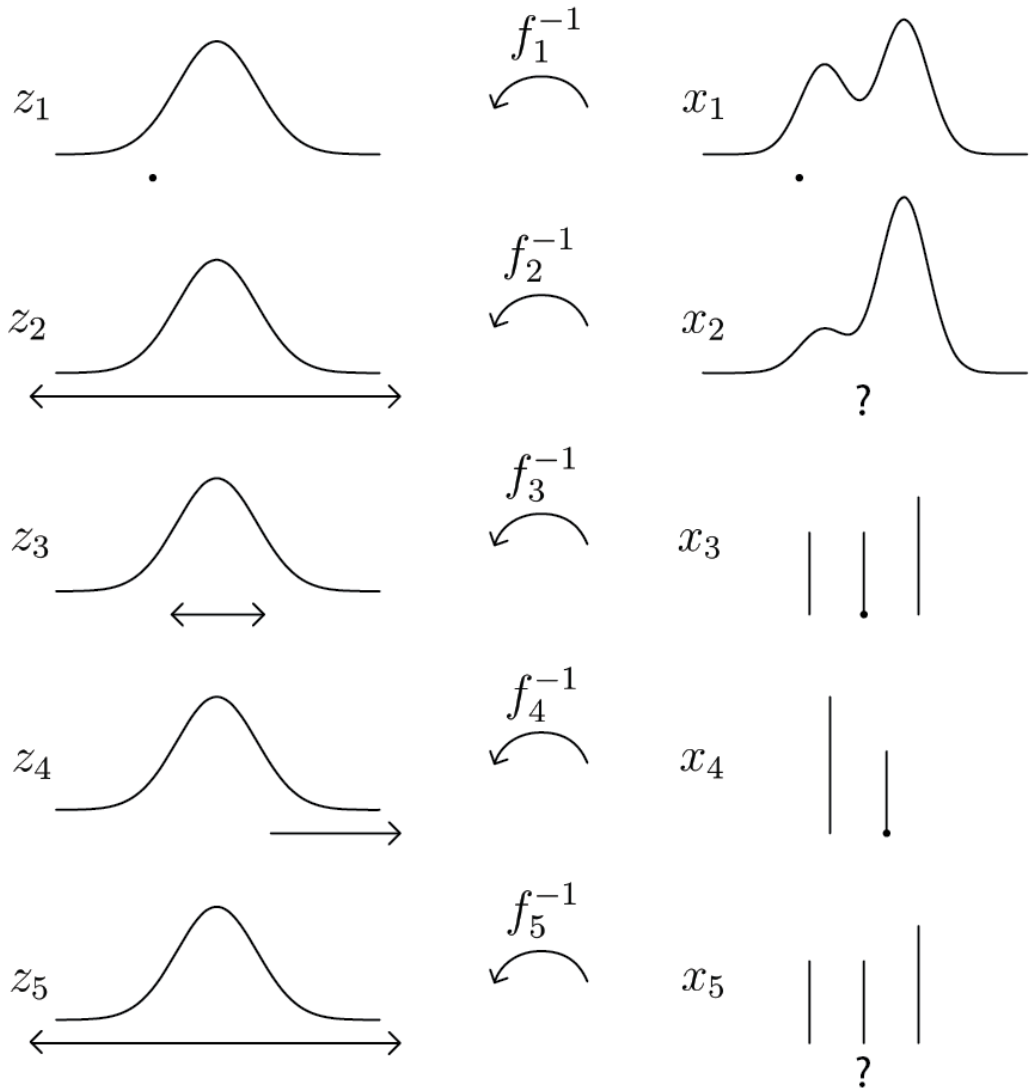
- map back to observed space using marginals $\hat{x}_{\text{mis}} = f(\hat{z}_{\text{mis}})$

Missing or mixed data: latent vector z not known



latent z is constrained to product of intervals

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$$\begin{aligned} \hat{z}_{\text{mis}} &= \mathbb{E}[z_{\text{mis}} \mid x_{\text{obs}}] = \mathbb{E}[\Sigma_{\text{mis,obs}} \Sigma_{\text{obs,obs}}^{-1} z_{\text{obs}} \mid x_{\text{obs}}] \\ &= \Sigma_{\text{mis,obs}} \Sigma_{\text{obs,obs}}^{-1} \mathbb{E}[z_{\text{obs}} \mid x_{\text{obs}}] \end{aligned}$$

- map back to observed space using marginals $\hat{x}_{\text{mis}} = f(\hat{z}_{\text{mis}})$

Outline

Estimating the model

Gaussian copula model

- $z \sim \mathcal{N}(0, \Sigma)$
- $x = f(z)$, $f = (f_1, \ldots, f_n)$ entrywise monotonic

two parameters to estimate

- *marginals:* monotone functions $f_1, \ldots, f_p$
- *copula:* correlation matrix $\Sigma \in \mathbf{R}^{p \times p}$

Estimating the marginals

- Gaussian matrix Z:
  - columns $\mathcal{N}(0, 1)$
- (partially) observed matrix X:
  - column j has observed empirical distribution with CDF F_j

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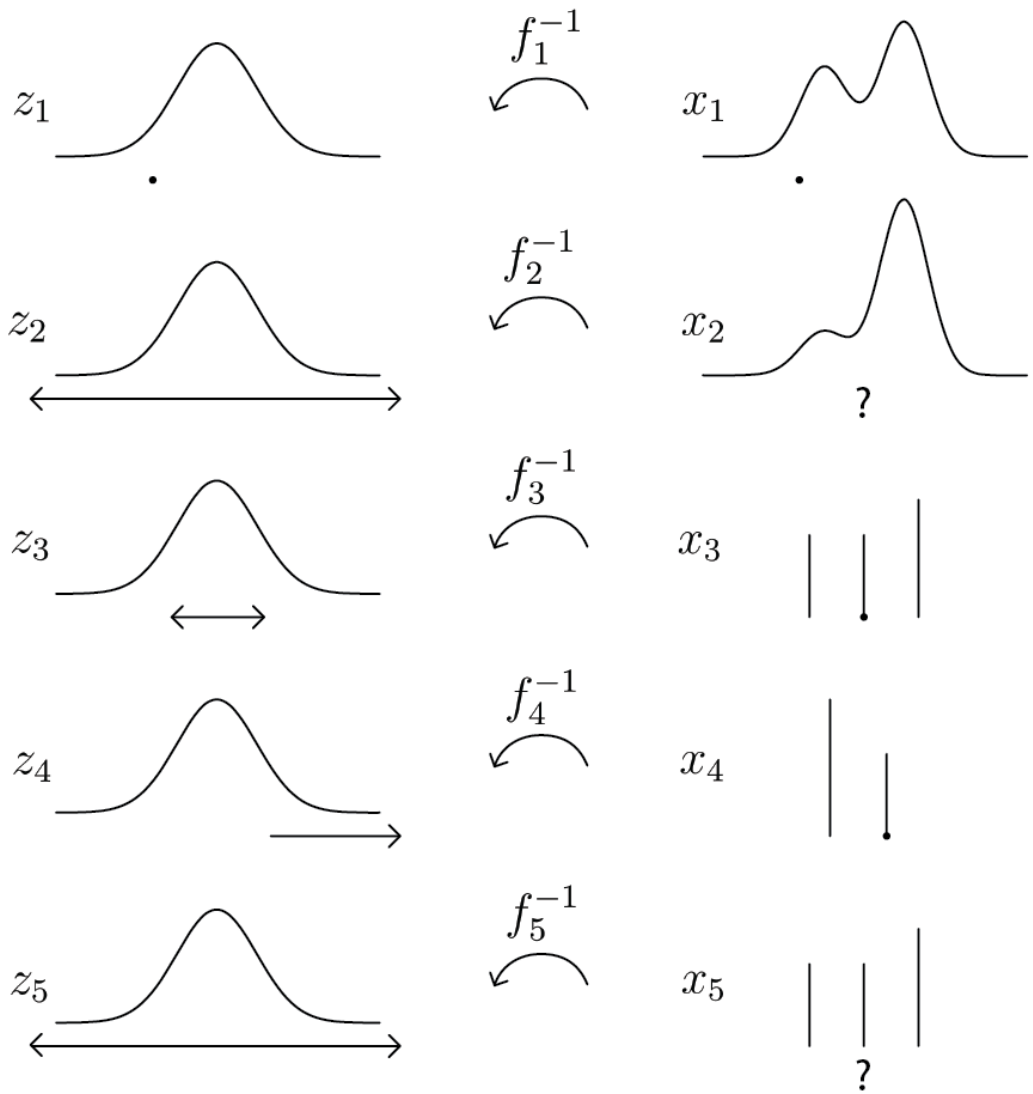
estimate f_j for each column $j = 1, \ldots, p$ by matching quantiles:

$$\hat{f}_j^{-1}(x_j^i) = \Phi^{-1}\left(\frac{n_j}{n_j + 1}\hat{F}_j(x_j^i)\right).$$

our convention: for discrete data, $\hat{F}_j$ is set-valued.

Matching quantiles



Warmup: estimate copula for complete cts data

given

- observed matrix $X \in \mathbf{R}^{n \times p}$
- invertible marginals $f = (f_1, \ldots, f_p)$ (or estimates)

estimate copula Σ using maximum likelihood estimation:

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- compute latent $z^i = f^{-1}(x^i)$ for each row x^i
- log likelihood is

$$\ell(\Sigma; X) = c - \frac{\log(|\Sigma|)}{2} - \frac{1}{2}\operatorname{Tr}(\Sigma^{-1} \sum_{i=1}^{n} \frac{1}{n} z^i (z^i)^\top),$$

maximized by the empirical covariance $G = \frac{1}{n}\sum_{i=1}^{n} z^i (z^i)^\top$

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  maximized by the empirical covariance $G = \frac{1}{n}\sum_{i=1}^{n} z^i (z^i)^\top$
- scale $\hat{\Sigma}$ to correlation matrix:
  set $D = \mathbf{diag}(G)$ and scale $\hat{\Sigma} \leftarrow D^{-1/2} G D^{-1/2}$

Estimating the copula: missing or discrete

given

- observed entries x^i_{obs} for each row $x^i \in \mathbf{R}^p$, $i = 1, \ldots, n$
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idea: estimate copula Σ using maximum likelihood estimation?

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$$\ell(\Sigma; \{x_{\mathcal{O}_i^i}\}_{i=1}^n) = \frac{1}{n} \sum_{i=1}^n \log \left(\int_{z^i \in f^{-1}(x^i)} \phi(z^i; 0, \Sigma) dz^i \right),$$

where $\phi(z; 0, \Sigma)$ is the pdf of a Gaussian with mean 0 and correlation Σ.

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- truncated Gaussian integral is hard to compute or optimize

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- truncated Gaussian integral is hard to compute or optimize
- instead: use EM

EM algorithm for Gaussian Copula

EM algorithm for Gaussian Copula:

- **Input:** observed entries X_{obs}, marginals f
- **Initialize:** $t = 0$, $\hat{\Sigma} = I$.
- For $t = 0, 1, 2, \ldots$
  1. E-step: $G = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}\left[zz^T | x_{\text{obs}}^i, \hat{\Sigma}, f \right]$.
  2. M-step: $D = \textbf{diag}(G)$; scale $\hat{\Sigma} \leftarrow D^{-1/2} G D^{-1/2}$.

  until convergence.
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properties:

- every step increases likelihood $\mathbb{P}(X_{\text{obs}}; \hat{\Sigma})$
- consistent estimate for Σ if data MAR
- E step is challenging; our approximate EM method uses a fast approximation based on 1D integrals.

Outline

Copula-EM imputes well and quickly

Synthetic data experiment:

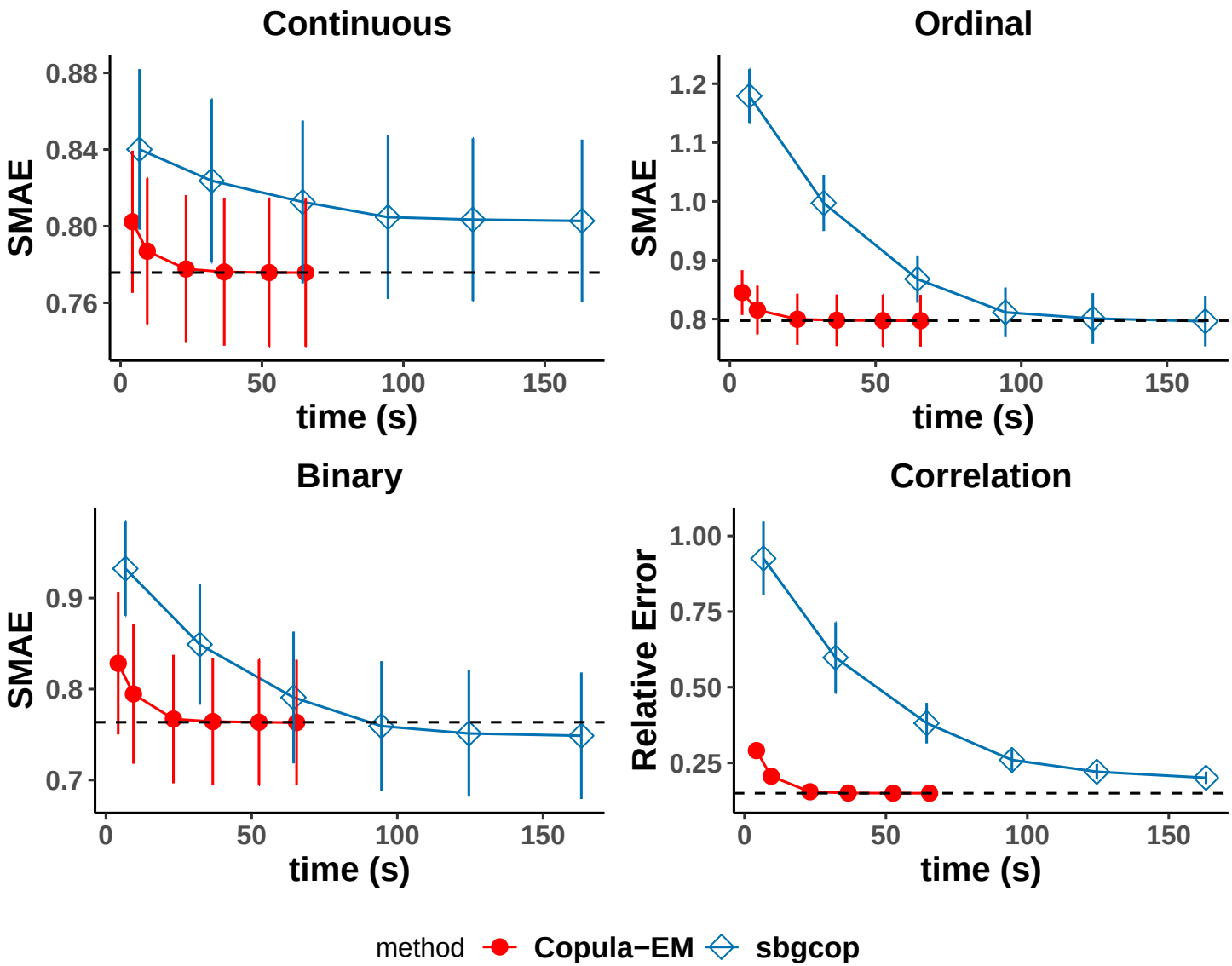
- $p = 15$, $n = 2000$. Correlation Σ is random. First five columns have exponential distributions, next five are binary, and last five are ordinal with five levels.

Define scaled mean absolute error

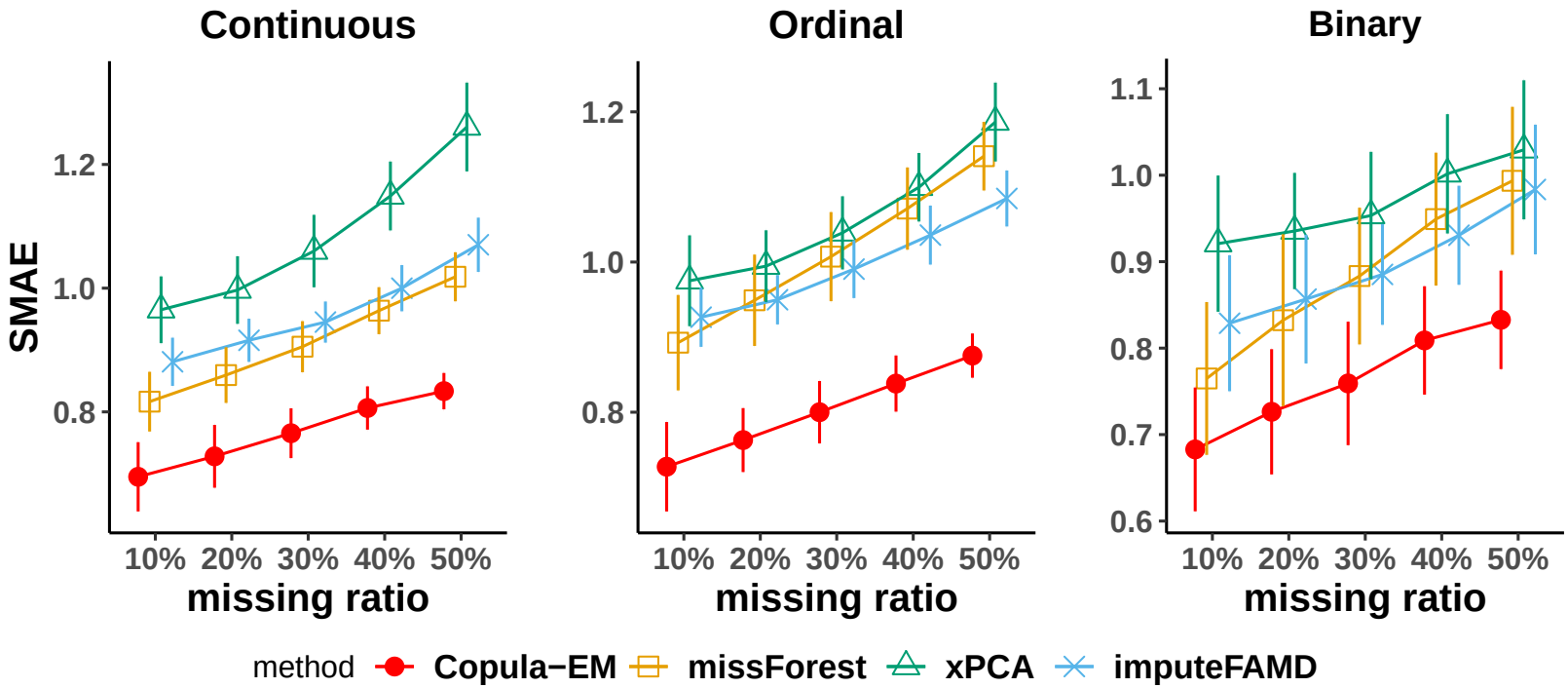
$$\text{SMAE}(\hat{x}, x, \text{obs}) := \frac{||\hat{x} - x||_1}{||\text{median}(x) - x||_1}$$

(Median imputation has SMAE $= 1$.)

Copula-EM imputes faster than MCMC



Gaussian copula has best accuracy



Gaussian copula for survey data

- General Social Survey data
- 1 continuous, 17 ordinal variables with 2–48 levels
- 25% of data missing
- mask additional 10% of data

Table: Imputation Error (SMAE) on Five GSS Variables

Variable	Copula-EM	sbgcop	missForest	xPCA	imputeFAMD
CLASS	**0.736(0.11)**	1.098(0.15)	0.782(0.09)	0.795(0.08)	0.797(0.10)
LIFE	**0.758(0.13)**	0.994(0.19)	0.828(0.17)	0.783(0.11)	0.821(0.11)
HEALTH	**0.886(0.08)**	1.257(0.17)	1.143(0.18)	0.908(0.10)	0.947(0.04)
HAPPY	**0.894(0.08)**	1.332(0.13)	1.079(0.15)	1.003(0.15)	1.001(0.10)
INCOME	**0.897(0.05)**	0.952(0.03)	0.944(0.18)	1.090(0.15)	0.996(0.01)

Gaussian copula yields insights

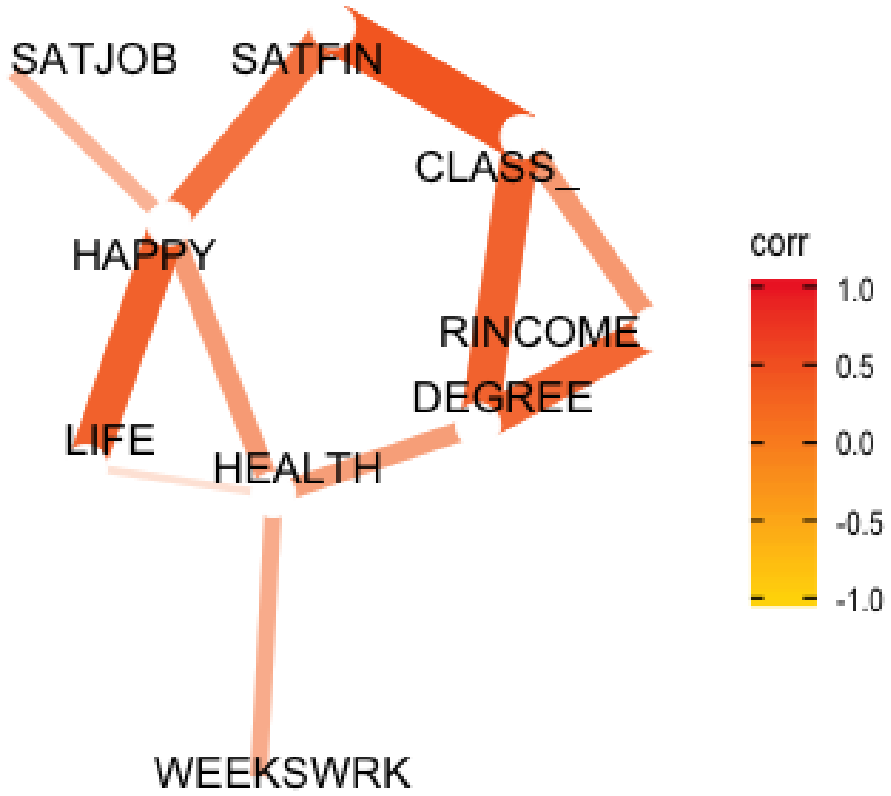


Figure: Large correlations ($|\cdot| > 0.3$) between a few interesting variables from GSS data.

Gaussian copula model outperforms on MovieLens

MovieLens data:

- 207 movies with $\geq$ 1000 ratings
- all users who rate at least one of those 207 movies
- 75% missing rate
- mask additional 10% of data

Table: Imputation Error on 207 Movies

Algorithm	MAE	RMSE
Column Median	0.702(0.004)	1.001(0.004)
Copula-EM	**0.579(0.004)**	**0.880(0.005)**
GLRM (BvSLoss)	0.595(0.004)	0.892(0.004)
softImpute	0.602(0.004)	0.883(0.004)
xPCA	0.613(0.004)	0.897(0.004)
imputeFAMD	0.646(0.005)	0.991(0.005)
missForest	0.669(0.004)	1.015(0.006)

True rank?

selecting the best rank using 5-fold cross validation,

- xPCA uses rank 6
- GLRM model uses rank 8
- softImpute model uses rank 99
- Copula EM model uses full rank covariance Σ

Outline

Low-rank Gaussian copula

Low-rank Gaussian copula model:

- $z \sim \mathcal{N}(0, WW^\top + \sigma I)$
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- low rank + diagonal covariance $\Sigma = WW^\top + \sigma I$
- latent z follows probabilistic PCA model

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- fewer parameters
  - covariance has $O(p)$ parameters for constant r
- faster to estimate
  - for dense data, $O(np)$ flops per EM iteration
  - for sparse data, flops per EM iteration $\sim$ #observations
- insensitive to the chosen rank (unlike low rank models)
  - doesn't overfit
  - generally, bigger is (very modestly) better

Simulation Setting

- Generate $X = f(Z)$ where $Z = TW^\top + \sigma E$.
- $T \in \mathbf{R}^{500 \times k}, W \in \mathbf{R}^{200 \times k}, E \in \mathbf{R}^{500 \times 200}$ with standard normal entries
- Continuous data: set $k = 10, \sigma^2 = 0.1$, missing ratio 40%.
  - Low rank: $X = f(Z) = Z$
  - High rank: $X = f(Z) = Z^3$ (entrywise)
- Ordinal (1-5) and binary data: set $k = 5$, missing ratio 60%.
  - High SNR: $\sigma^2 = 0.1$
  - Low SNR: $\sigma^2 = 0.5$

Simulation: accuracy

Continuous	LRGC	PPCA	softImpute	MMMF-ℓ_2	MMC
Low Rank	.347(.004), $r = 10$	**.338**(**.004**), $r = 10$	.371(.004), $r = 117$	.364(.003)	.633(.007), $r = 130$
High Rank	**.517**(**.011**), $r = 10$	.690(.010), $r = 10$	.703(.005), $r = 104$	.696(.006)	.824(.011), $r = 137$
1-5 ordinal	LRGC	PPCA	softImpute	MMMF-BvS	MMMF-ℓ_1
High SNR	**.358**(**.008**), $r = 5$	.501(.010), $r = 6$	.582(.011), $r = 83$	.407(.007)	.410(.007)
Low SNR	**.788**(**.013**), $r = 5$	.863(.013), $r = 5$	.951(.015), $r = 38$	.850(.011)	.863(.011)
Binary	LRGC	PPCA	MMMF-hinge	MMMF-logistic	MMMF-ℓ_1
High SNR	**.103**(**.003**), $r = 5$	.116(.002), $r = 6$	.140(.002)	.117(.002)	.224(.005)
Low SNR	**.205**(**.006**), $r = 5$	.208(.005), $r = 5$	.234(.006)	.217(.005)	.265(.009)

Table: Imputation error (NRMSE for continuous and MAE for ordinal) reported over 20 repetitions, with rank r for available methods. Maximum margin matrix completion (`MMMF`) are trained at rank 199, implemented using generalized low rank model (GLRM). Monotonic matrix completion (MMC) is aimed at high rank matrix completion.

Simulation: confidence intervals are calibrated

Low Rank Data	LRGC	PPCA	LRMC	MI-PCA
Empirical coverage rate	0.927(.002)	0.940(.001)	0.878(.006)	0.933(.002)
Interval length	1.273(.004)	1.264(.004)	1.129(.015)	1.267(.004)
Run time (in seconds)	6.9(.5)	3.4(.7)	2.7(.4)	189.8(15.4)
High Rank Data	**LRGC**	**PPCA**	**LRMC**	**MI-PCA**
Empirical coverage rate	0.927(.002)	0.943(.002)	0.925(.004)	0.948(.002)
Interval length	3.614(.068)	9.086(.248)	6.546(.191)	9.307(.249)
Run time (in seconds)	7.2(1.2)	0.4(.1)	3.1(.6)	220.0(30.2)

Table: 95% Confidence intervals on synthetic continuous data over 20 repetitions. LRMC stands for low rank matrix completion (Chen et al. 2019). MI-PCA stands for multiple imputation based on PCA (Josse et al. 2011).

Movielens 1M: identify entries with lowest error

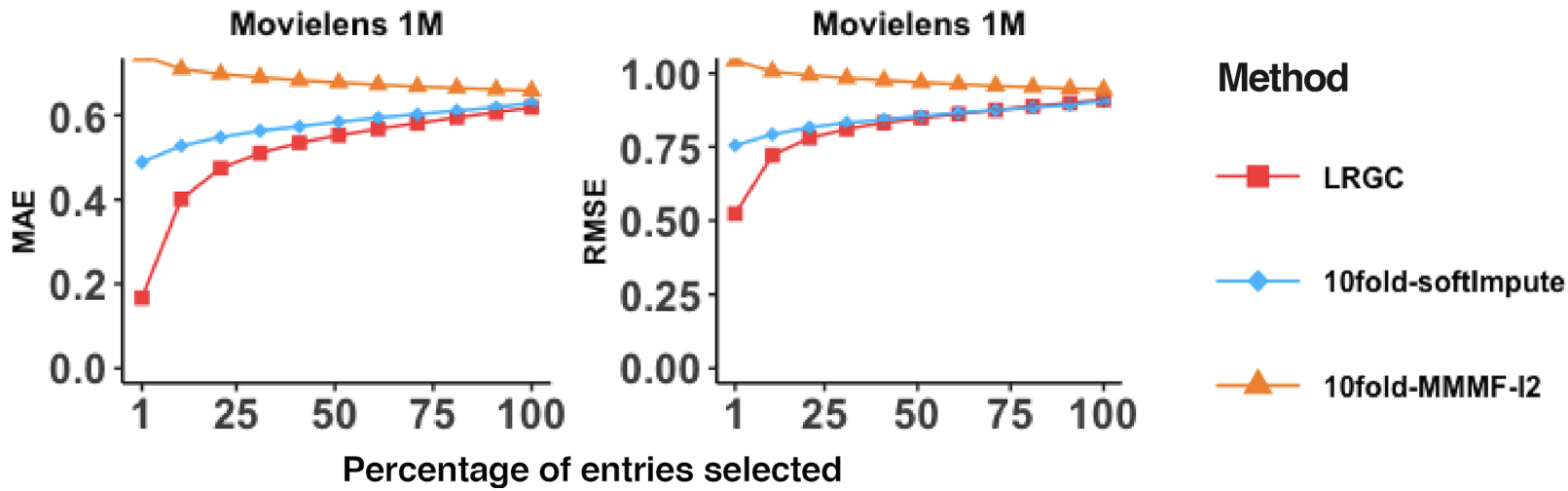

Figure: Movie rating dataset from 6040 users and 3952 movies with 4.19% observation. We select movies with at least 50 ratings, which yields size 6040×2514. The imputation error is plotted at the best tuning parameter over 5 repetitions.

Implementations

- Python: `https://github.com/udellgroup/online_mixed_gc_imp`
  - batch, minibatch, and online EM algorithm
- R: `https://github.com/udellgroup/mixedgcImp`
  - full-rank and low-rank EM algorithm

Conclusion

Gaussian copula model for data imputation:

- no hyperparameters
- outperforms fancier nonparametric methods
- yields confidence intervals for imputations
- fast and easy to estimate for moderate p or (with low rank covariance) large p

references:

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Outline

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