Copula Entropy

Theory and Applications

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October 24, 2020

Contents

Copula Theory

Definition (Copula)

[a] Given N random variables $\mathbf{X} = (X_1, \ldots, X_N) \in \mathcal{R}^N$. Let $\{u_i = F_i(x_i), i = 1, \ldots, N\}$ be the marginal distribution functions of $\mathbf{X}$. A N-dimensional copula $C : \mathcal{I}^N \rightarrow \mathcal{I}(\mathcal{I} = [0, 1])$ of $\mathbf{X}$ is a function with following properties:

1. C is grounded and N-increasing;
2. $C(1, \ldots, 1, u_i, 1, \ldots, 1) = u_i$.

[a] Roger B Nelsen. *An introduction to copulas.* Springer, 2007.

- The probabilistic theory on **representation** of statistical dependence

Copula Theory

Theorem (Sklar's Theorem)

[a] *Given a random vector* $\mathbf{X} = (X_1, \ldots, X_N)$*, its CDF* $\mathbf{F}(\mathbf{x})$ *can be represented as*

$$\mathbf{F}(\mathbf{x}) = C(u_1, \ldots, u_N), \tag{1}$$

where C *is a copula function,* $\{u_i\}$ *are marginal distribution functions of* $\mathbf{X}$*. If* $\{F_i\}$ *are continuous, then* C *is unique.*

[a] M. Sklar. "Fonctions de repartition an dimensions et leurs marges". In: *Publ. Inst. Statist. Univ. Paris* 8 (1959), pp. 229–231.

Corollary

The probabilistic density function (PDF) $p(x)$ *of* $\mathbf{X}$ *can be represented as*

$$p(\mathbf{x}) = c(\mathbf{u}) \prod_{i=1}^{N} p_i(x_i), \tag{2}$$

where $\{p_i, i = 1, \ldots, N\}$ *are marginal density functions of* $\mathbf{X}$*, and* c *is copula density.*

- the core of copula theory
- seperating dependence representation with properties of individual variables

Copula Entropy: Theory

Definition (Copula Entropy)

Let $\mathbf{X}$ be random variables with marginals $\mathbf{u}$ and copula density $c(\mathbf{u})$. Copula Entropy of $\mathbf{X}$ is defined as

$$H_c(\mathbf{x}) = -\int_{\mathbf{u}} c(\mathbf{u}) \log c(\mathbf{u}) d\mathbf{u}. \tag{3}$$

Theorem

Mutual Information of $\mathbf{X}$ is equavalent to its negative copula entropy.

$$I(\mathbf{x}) = -H_c(\mathbf{x}). \tag{4}$$

Corollary

$$H(\mathbf{x}) = \sum_i H_i(x_i) + H_c(\mathbf{x}). \tag{5}$$

- the theory of statistical independence measure
- the bridge between copula theory and information theory[1]

[1] Jian Ma and Zengqi Sun. "Mutual information is copula entropy". In: *Tsinghua Science & Technology* 16.1 (2011). See also arXiv preprint arXiv:0808.0845 (2008), pp. 51–54.

Copula Entropy: Theory

- Axiomatic Properties of Copula Entropy
  - multivariate
  - symmetric
  - non-negative, 0 iff independence
  - invariant to monotonic transformation
  - equivalent to correlation coefficient in Gaussian cases
- An ideal measure compared with others

Table: Comparison with other independence measures.

	Copula Entropy	Distance Correlation	HSIC
Definition	copula based	generalised corr	corr in RKHS
Multivariate	Yes	distance multivariance	dHSIC
Invariance	monotonic trans	No	No
Gaussanity	equivalent to cc	unclear	unclear
Computation	low	high	high

Copula Entropy: Estimation

- **Non-Parametric** Estimation Method[2]
  1. estimating empirical copula density with rank statistics
  2. estimating copula entropy with kNN entropy estimation method
- Advantages
  - distribution-free, non-parametric
  - tuning-free, insensitive to parameters
  - good convergence
  - easy to implement
  - low computation burden

[2] Jian Ma and Zengqi Sun. "Mutual information is copula entropy". In: *Tsinghua Science & Technology* 16.1 (2011). See also arXiv preprint arXiv:0808.0845 (2008), pp. 51–54.

Association Discovery[3]

[3] Jian Ma. "Discovering Association with Copula Entropy". In: *arXiv preprint arXiv:1907.12268* (2019).

Copula Entropy: Association Discovery

- Problem
  - To discover association relationship between random variables from data
- History
  - An old and fundamental problem since statistics birth
- Related Methods
  - Pearson Correlation Coefficient
  - Regression

Copula Entropy: Association Discovery

- Traditional association measures
  - Pearson Correlation Coefficient

$$r_{XY} = corr(X, Y) = \frac{cov(X, Y)}{\delta_X \delta_Y} \tag{6}$$

  - Spearman's ρ and Kendall's τ

$$\rho_{XY} = 12 \int_u \int_v C(u, v) dudv - 3 \tag{7}$$

$$\tau_{XY} = 4 \int_u \int_v C(u, v) dC(u, v) - 1 \tag{8}$$

- Why Copula Entropy?

Table: Theoretical comparison between CE and CC.

	CC	CE
linearity	linear	nonlinear
Order	2	≥ 2
Assumption	Gaussian	None
variate	bivariate	multivariate

Copula Entropy: Association Discovery

Experiments on the NHANES data

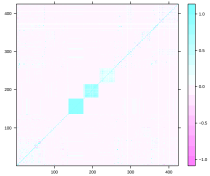
- Objectives of NHANES
  - to monitor trends and emerging issues of population health
  - to investigate its relationship with risk factors, nutritions and environmental exposures, etc.
- NHANES (2013-2014)
  - 14,332 persons from 30 different survey locations were selected;
  - Of those selected, 10,175 interviewed and 9,813 examined;
  - 5 groups of data: demographics, dietary, examination, laboratory, and questionnaire.
- Experimental data

  The laboratory data, which includes 423 variables from blood, urine, oral rinse and vaginal/Penile swabs.
- Missing values

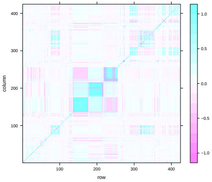
  The missing values were filled with the mean of their corresponding variables.

Copula Entropy: Association Discovery

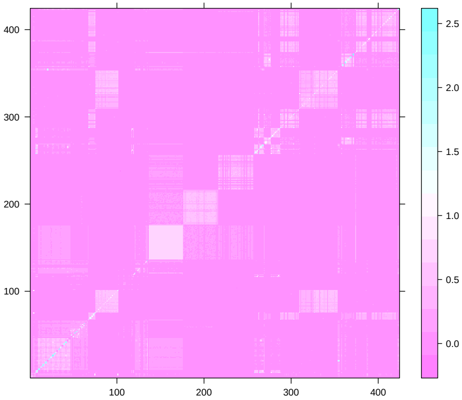
- Results - Correlation matrices



Pearson's r



Spearman's ρ



Copula Entropy

Copula Entropy: Association Discovery

- Results - Variable groups with meanings

Table: Variable groups with biomedical meanings discovered with CE.

Group	Index	Variables
1	288-302	Polycyclic Aromatic Hydrocarbones (PAH) - Urine
	68-75	Copper, Selenium & Zinc - Serum
	395-420	Urine Metals
2	358-373	Blood Lead, cadmium, total Mercury, Selenium, and Manganese
	269-276	Blood mercury: inorganic, ethyl and methyl
3	277-287	Oral Glucose Tolerance Test
	258-262	Insulin
	7-9	Cholesterol-LDL, Triglyceride&Apoliprotein(ApoB), WTSAF2YR-Fasting Subsample 2 Year MEC Weight, LBXAPB-Apolipoprotein (B) (mg/dL), LBDAPBSI-Apolipoprotein (B) (g/L)
4	10-46	Standard Biochemistry Profile
	137-176	Human Papillomavirus (HPV) - Oral Rinse
5	76-101	Personal Care and Consumer Product chemicals and Metabolites
	327-353	Phthalates and Plasticizers Metabolites - Urines

Structure Learning[4]

[4] Jian Ma and Zengqi Sun. "Dependence structure estimation via copula". In: *arXiv preprint arXiv:0804.4451* (2008).

Copula Entropy: Structure Learning

- Problem
  - To learn statistical structure among random variables from data
- Graph Representation
  - A probability density is represented with a directed or indirected graph, of which each node represents a random variable, and each edge represents a (conditional) dependence relation between two random variables
- Related Methods
  - Chow-Liu Algorithm

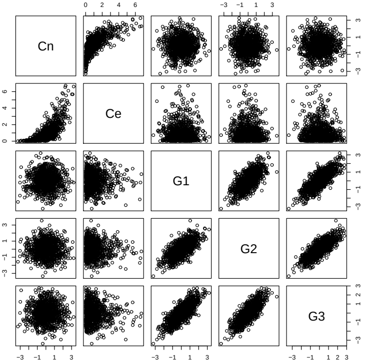
Copula Entropy: Structure Learning

- Our Algorithm
  1. computing dependence matrix $\mathbf{W}_x$ of data x with CE estimation
  2. constructing dependence structure T from $\mathbf{W}_x$ with MST algorithm
- Advantages
  - distribution-free, non-parametric
  - tuning-free, insensitive to parameters
  - easy to implement
  - low computation burden

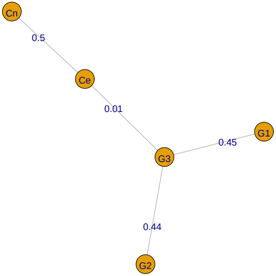
Copula Entropy: Structure Learning

- Simulated Experiment

  5 random variables: the first three are Gaussian and the others two are governed by Gaussian copula with margins as normal distribution and exponential distribution respectively



Simulated data

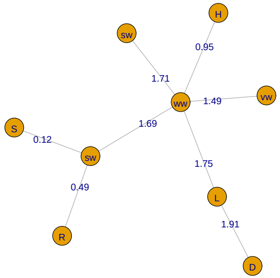


Learned graph

Copula Entropy: Structure Learning

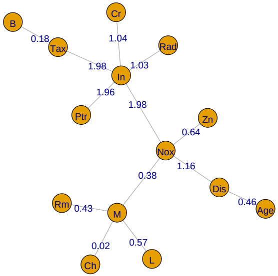
- Experiment on real data
  - Abalone data

    Predicting the age of abalone from physical measurements



  - Boston housing data

    Concerns housing values in suburbs of Boston



Variable Selection[5]

[5] Jian Ma. "Variable Selection with Copula Entropy". In: *Chinese Journal of Applied Probability and Statistics* (accepted). See also arXiv preprint arXiv:1910.12389 (2019).

Copula Entropy: Variable Selection

- Problem
  - To select a 'right' subset of variables from the whole group for building classification or regression models with good predictability and interpretability
- History
  - An old and basic problem in statistics and machine learning
- Related Problems
  - Feature Selection
  - Model Selection

Copula Entropy: Variable Selection

- Existing methods - Likelihood with penalty
  - Information Criteria
    with penalty on the number of parameters in the models

$$\mathbf{AIC} = -2L + 2p \tag{9}$$

$$\mathbf{BIC} = -2L + p \log N \tag{10}$$

  - Penalized GLMs
    with penalty on the nonzero coefficients in the GLMs
    - LASSO
    - Ridge Regression
    - Elastic Net

$$\min_{\beta}\{L(\beta; y, \mathbf{X}) + \lambda_1||\beta||_1 + \lambda_2||\beta||_2^2\} \tag{11}$$

    - Adaptive LASSO

$$\min_{\beta}\{L(\beta; y, \mathbf{X}) + \lambda\sum_{j=1}^{p} w_j|\beta_j|\} \tag{12}$$

Copula Entropy: Variable Selection

- Existing methods - Statistical independence measures
  - Distance Correlation

$$\mathbf{dCor}(X, Y) = \frac{\nu^2(X, Y)}{\sqrt{\nu^2(X)\nu^2(Y)}}, \tag{13}$$

    where $\nu^2(X, Y)$ be distance covariance.
  - Hilbert-Schmidt Independence Criterion (HSIC)

$$\mathbf{dHSIC}(P(\mathbf{X})) = ||\Pi(P(X_1)\otimes, \ldots, \otimes P(X_d)) - \Pi(P(\mathbf{X}))||, \tag{14}$$

    where Π be the mean embedding function associated with kernel functions.

Copula Entropy: Variable Selection

- CE based method
  To select variables based on ranks of their negative CE values with target
- Advantages
  - model-free, non-parametric
  - tunning-free, insensitive to parameters
  - interpretable with physical meanings
  - supported by rigorous math
  - science instead of art, compared with existing methods
  - easy to implement, low computation burden

Copula Entropy: Variable Selection

Experiments on the UCI heart disease data

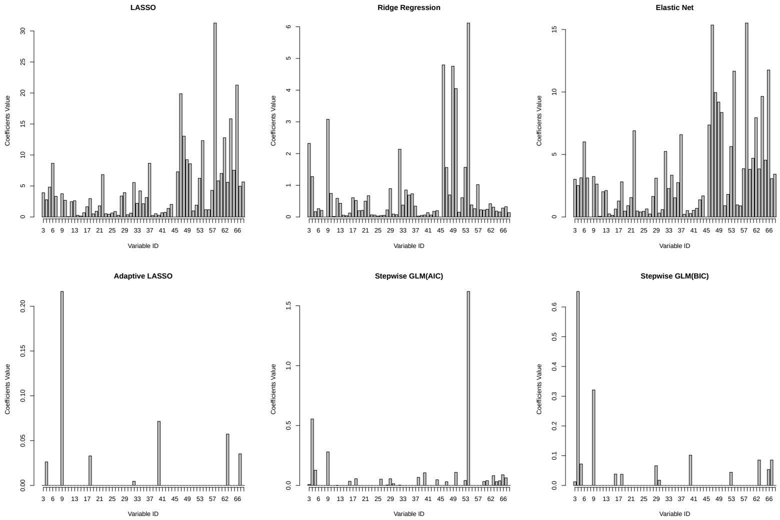
- Overview of the data
  The data set contains 4 databases (899 samples) concerning heart disease diagnosis. All attributes are numeric-valued. The data was collected from the four following locations:
  - Cleveland clinic foundation;
  - Hungarian Institute of Cardiology, Budapest;
  - V.A. medical center, long beach, CA;
  - University hospital, Zurich, Switzerland.
- Attributes
  The data has 76 attributes (#58 'num' for diagnosis). Of them, 13 attributes are recommended by professionals as clinical relevant.

Table: Recommended attributes.

ID	3	4	9	10	12	16	19
Name	age	sex	cp	trestbps	chol	fbs	restecg
ID	32	38	40	41	44	51	58
Name	thalach	exang	oldpeak	slope	ca	thal	num

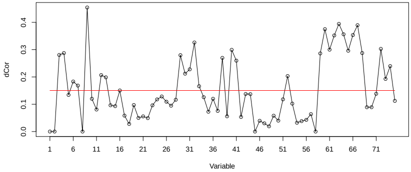
Copula Entropy: Variable Selection

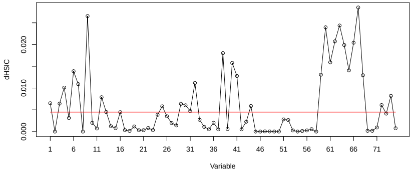
- Results - Coefficients of penalized likelihood based models

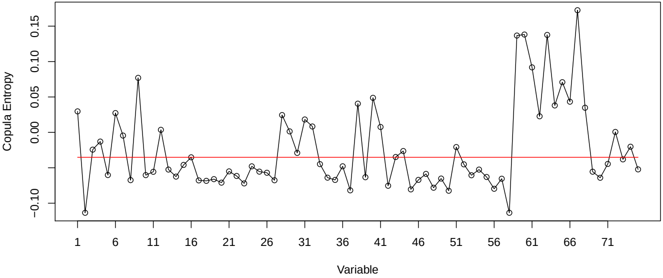


Copula Entropy: Variable Selection

- Results - with statistical dependence measures (dCor, dHSIC, CE)







Copula Entropy: Variable Selection

- Results - Prediction accuracy

  the selected variables present the best prediction accuracy.

Model	Accuracy(%)
SVM(Recommended variables)	84.20
SVM(CE)	**84.76**
SVM(dCor)	82.76
SVM(dHSIC)	84.54
Stepwise GLM(AIC)	51.8
Stepwise GLM(BIC)	49.1
LASSO	79.2
Ridge Regression	63.0
Elastic Net	75.9
Adaptive LASSO	35.7

Copula Entropy: Variable Selection

- Results - Selected variables

  Copula Entropy selects more 'right' variables than the other methods do.

Method	Selected Variables' ID	✓
Recommended variables	3,4,9,10,12,16,19,32,38,40,41,44,51	13
CE	3,4,6,7,9,12,16,28-32,38,40,41,44,51,59-68	**11**
dHSIC	3,4,6,7,9,12,13,16,25,29-32,38,40,41,44,59-68	10
dCor	3,4,6,7,9,12,13,16,28-33,38,40,41,52,59-68	9
Stepwise GLM(AIC)	3,4,5,9,12,16,18,20,26,29,30,32,40,44,47,50,53,54,60,61,63,65-67	8
Stepwise GLM(BIC)	3,4,5,9,16,18,29,30,40,53,63,66,67	5
Adaptive LASSO	4,6,9,18,32,40,63,67	4
LASSO		
Ridge Regression	all except 8,45	-
Elastic Net		

Copula Entropy: Application IV

Causal Discovery[6]

[6] Jian Ma. "Estimating Transfer Entropy via Copula Entropy". In: *arXiv preprint arXiv:1910.04375* (2019).

Copula Entropy: Causal Discovery

- Problem
  - To infer causality from time series data by *estimating Transfer Entropy*
- History & Significance
  - Causality is one of the oldest topics in philosophy.
  - Causal discovery is a central problem of all sciences.
- Correlation vs Causality
  - Correlation does not mean causation.
  - Correlation is only helpful for prediction while causality means intervention and control.

Copula Entropy: Causal Discovery

- Causality measures
  - Wiener's Principle
    Cause should improve the prediction of effect.
  - Granger Causality
    improvement measured by the variance of prediction error

$$\delta^2(Y_{t+1}|Y_t, X_t) < \delta^2(Y_{t+1}|Y_t) \tag{15}$$

  - Transfer Entropy
    improvement on the uncertainty of prediction measured by Shannon entropy

$$\begin{aligned} TE &= \sum p(Y_{t+1}, Y^t, X_t) \log \frac{p(Y_{t+1}|Y^t, X_t)}{p(Y_{t+1}|Y^t)} && (16) \\ &= H(Y_{t+1}|Y^t) - H(Y_{t+1}|Y^t, X_t) && (17) \\ &= I(Y_{t+1}, X_t|Y^t) && (18) \end{aligned}$$

- Issue on TE
  difficult to estimate, some think impossible without model assumptions

Copula Entropy: Causal Discovery

- TE via CE

Proposition

Transfer Entropy can be represented with only Copula Entropy.

Proof.

$$
\begin{aligned}
TE &= \sum p(Y_{t+1}, Y^t, X_t) \log \frac{p(Y_{t+1}|Y^t, X_t)}{p(Y_{t+1}|Y^t)} && (19)\\
&= \sum p(Y_{t+1}, Y^t, X_t) \log \frac{p(Y_{t+1}, Y^t, X_t)p(Y^t)}{p(Y_{t+1}, Y^t)p(Y^t, X_t)} && (20)\\
&= I(Y_{t+1}; Y^t; X_t) - I(Y_{t+1}; Y^t) - I(Y^t; X_t) && (21)\\
&= -H_c(Y_{t+1}; Y^t; X_t) + H_c(Y_{t+1}; Y^t) + H_c(Y^t; X_t) && (22)\\
&= -H_c(Y_{t+1}, Y^t, X_t) + H_c(Y_{t+1}, Y^t) + H_c(Y^t, X_t) - H_c(Y^t) && (23)
\end{aligned}
$$

□

- Non-parametric TE estimation method
  1. estimating three or four CE terms in (23);
  2. calculating TE for these estimated CEs.
- inheriting all the merits of non-parametric CE estimation

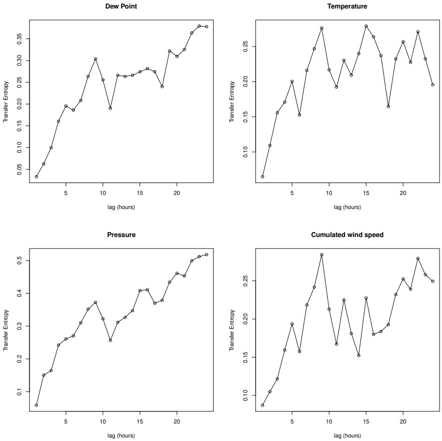
Copula Entropy: Causal Discovery

Experiments on the UCI Beijing PM2.5 data

- Overview of the data
  - Time
    hourly data from 2010-01-01 to 2014-12-31, which results in 43824 samples with missing values.
  - Observations
    - PM2.5 data of US Embassy in Beijing
    - Meteorological data from Beijing Capital International Airport
  - Meteorological factors
    dew point, temperature, pressure, cumulated wind speed, combined wind direction, cumulated hours of snow, cumulated hours of rain.
- Experimental data
  - the first four factors used in the experiments;
  - 1000 samples without missing values (2010-04-02$\sim$2010-05-14).

Copula Entropy: Causal Discovery

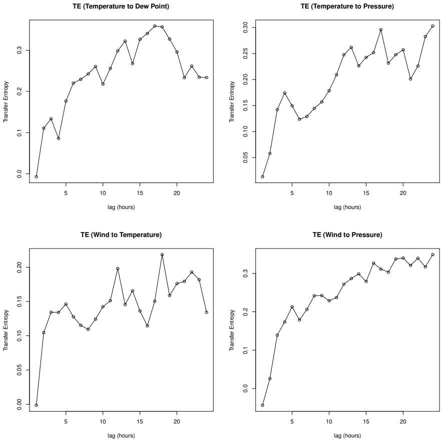
- Results - Effects of meteorological factors on PM2.5



- Two phrases
  - Sharp increase phrase: the first 9 hours time lag, and peak at about 9 hours lag;
  - Flat increase phrase: TE of Dew point and pressure increase with relatively flat rate while TE of temp. and cumulated wind speed does increase any more.
- Interpretation
  - The effects do not show immediately and are cumulating processes.

Copula Entropy: Causal Discovery

- Results - Effects between meteorological factors



- Temp. to Dew Point & Pressure
- Wind to Temp. & Pressure
  - Wind changes temperature in 3 hours later and
  - Wind changes pressure in 5 hours later.

Summary

- The theory of Copula Entropy was developed from copula theory, and a non-parametric method for estimating CE was proposed.
- CE was proposed to test statistical independence and conditional independence (transfer entropy).
- CE was applied to solve four fundamental statistical problems, including association discovery, structure learning, variable selection, and causal discovery.

References

1. Jian Ma and Zengqi Sun. "Mutual information is copula entropy". In: *Tsinghua Science & Technology* 16.1 (2011). See also arXiv preprint arXiv:0808.0845 (2008), pp. 51–54
2. Jian Ma. "Discovering Association with Copula Entropy". In: *arXiv preprint arXiv:1907.12268* (2019)
3. Jian Ma and Zengqi Sun. "Dependence structure estimation via copula". In: *arXiv preprint arXiv:0804.4451* (2008)
4. Jian Ma. "Variable Selection with Copula Entropy". In: *Chinese Journal of Applied Probability and Statistics* (accepted). See also arXiv preprint arXiv:1910.12389 (2019)
5. Jian Ma. "Estimating Transfer Entropy via Copula Entropy". In: *arXiv preprint arXiv:1910.04375* (2019)
6. Jian Ma. "copent: Estimating Copula Entropy in R". . In: *arXiv preprint arXiv:2005.14025* (2020)

http://arxiv.org/a/ma_j_3

Softwares

https://cran.r-project.org/package=copent

pip install copent

https://github.com/majianthu

The package **copent**[7] in R and Python for estimating copula entropy are available on CRAN and PyPI respectively. The source codes are provided on GitHub.

[7] Jian Ma. "copent: Estimating Copula Entropy in R". . In: *arXiv preprint arXiv:2005.14025* (2020).

Enjoy the Powerful Copula Entropy!