Fast Computing via Recursive Dyadic Partitioning for Statistical Dependency

Workshop on Frame Theory and Sparse Representation for Complex Data
June 1, 2017

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Agenda

I. Statistical Dependence
II. Distance Correlation
III. Fast Algorithm
IV. Simulations
V. An Application

I. Statistical Dependence

- Correlation
- Shortcoming of Pearson's linear correlation
- Related works

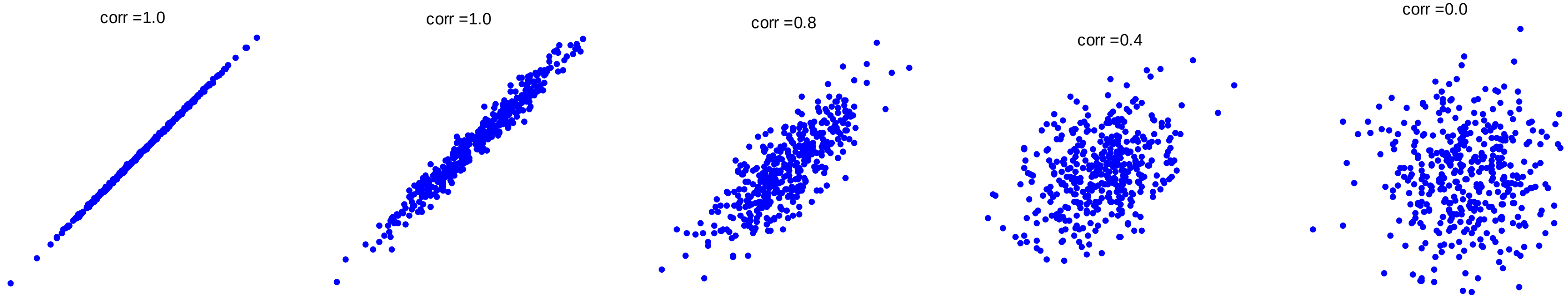
Linear Dependency (Pearson's)

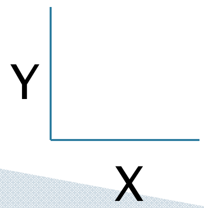
- Pearson's linear correlation coefficient:

$$\mathrm{Corr}(X,Y) = \frac{Cov(X,Y)}{\sqrt{Var(X)Var(Y)}}$$

- Karl Pearson (1895)

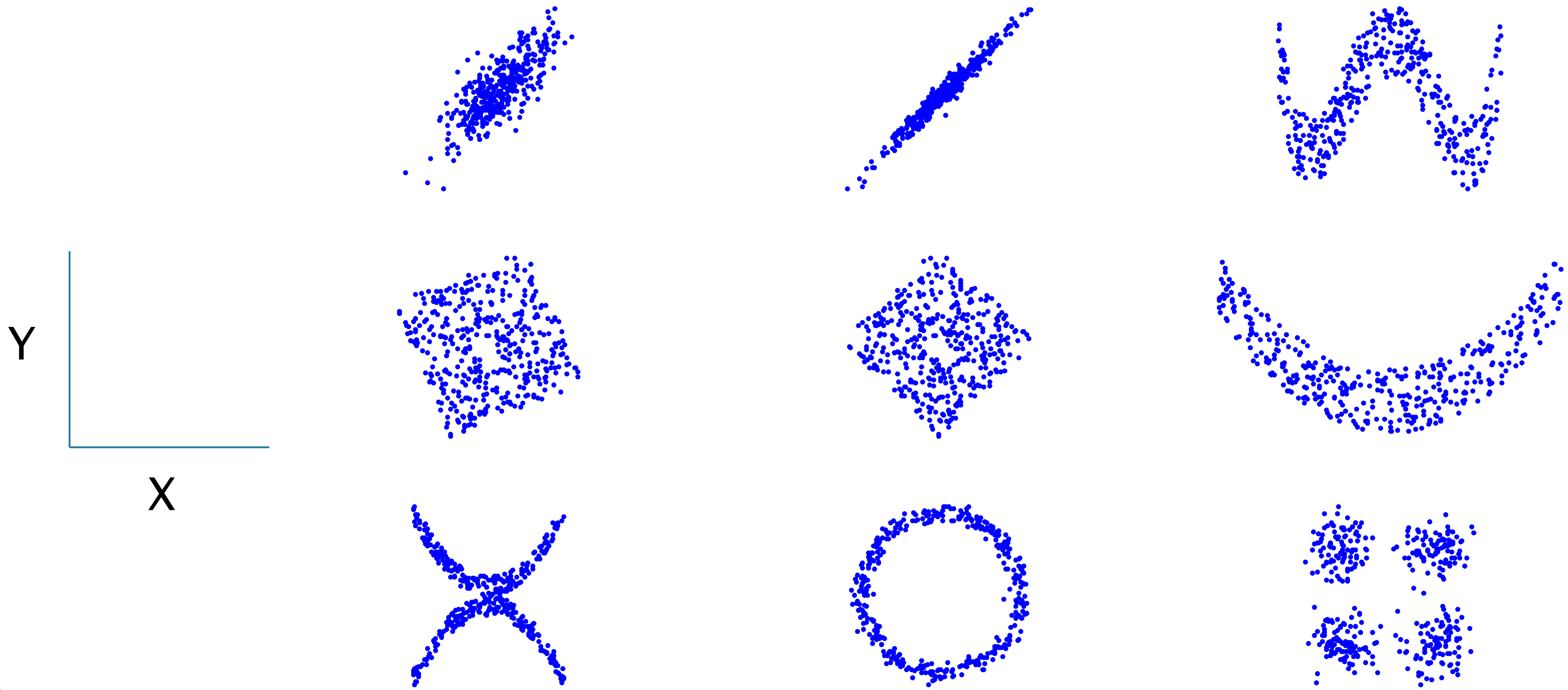
Corr=1.0 Corr=1.0 Corr=0.8 Corr=0.4 Corr=0.0



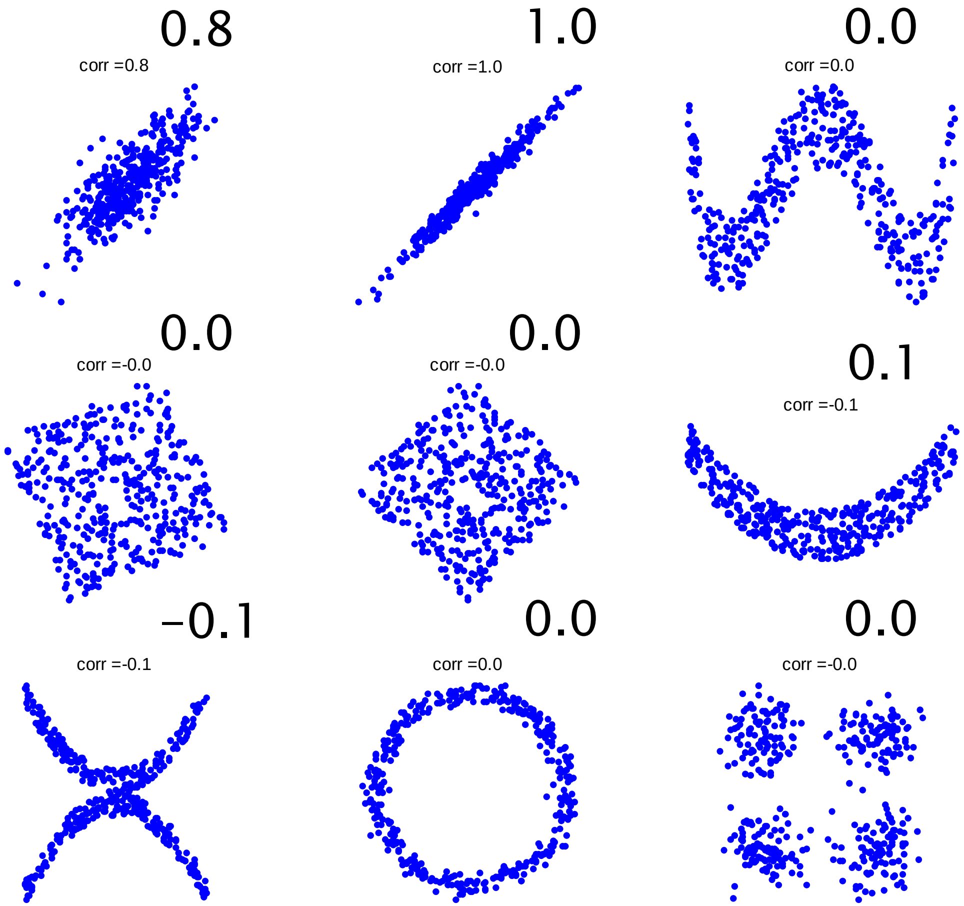


Nonlinearity

- Dependency could be complicated



Pearson's corr. not effective

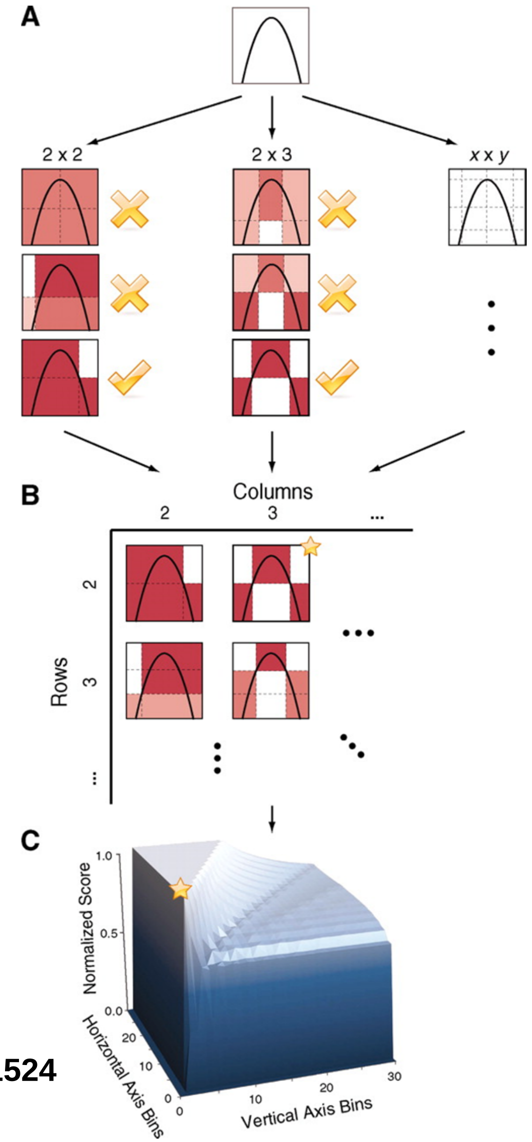


Related work

- Alternating Conditional Expectations or backfitting algorithm (ACE). Breiman and Friedman. JASA 1985.
- Kernel Canonical Correlation Analysis (KCCA). Bach and Jordan. JMLR 2002.
- (Copula) Maximum Mean Discrepancy (MMD, CMMD). Gretton, Borgwardt, Rasch, Scholkopf, and Smola. JMLR 2012. Poczos, Ghahramani, and Schneider. ICML, 2012.
- Maximal Information Coefficient (MIC). Reshef et al. Science, 2011.
- Randomized Dependence Coefficient (RDC). Lopez-Paz, Hennig, and Scholkopf. NIPS 2013.

Maximal Information Coefficient (MIC)

- Science, 2011
- "A Correlation for the 21st Century" – Terry Speed



Computing MIC For each pair (X, Y), the MIC algorithm finds the x-by-y grid with the highest induced mutual information.

D N Reshef et al. Science 2011;334:1518-1524

Kendall's τ

- 1938
- Let, $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ be a set of observations of the joint random variables X and Y respectively
- Kendall τ coefficient

$$\tau = \frac{1}{\binom{n}{2}} \sum_{1 \le i < j \le n} \operatorname{sign}[(x_i - x_j)(y_i - y_j)]$$

- $-1 \le \tau \le 1$

Comparison

- Comparison between dependence measures

Name of Coeff.	Comp. cost
Pearson's ρ	n
Spearman's ρ	$n \log n$
Kendall's τ	$n \log n$
CCA	n
KCCA	n^3
ACE	n
MIC	2^n
MMD	n^2
CMMD	n^2
RDC	$n \log n$
dCor	$n^2 \rightarrow n \ \log n$

II. Distance Correlation

1. Distance correlation
2. Sample dCor
3. An example

How to measure statistical dependence?

- Independence: f(x,y)=f(x)f(y)
  - Joint density is the multiplication of two marginal densities
- Hope:
  - X and Y independent if and only if corr(X,Y)=0
  - If X=c_1·Y+c_2, then corr(X,Y)=1
- Pearson's correlation coefficient not effective

Distance covariance

- Gabor J. Szekely, 2005, 2007 (AoS), 2009 (AoAS), 2012 (SPL), 2014 (AoS)
- Distance covariance: (population version)

$$\mathcal{V}^2(X,Y) = \left\|\phi_{X,Y}(t,s) - \phi_X(t)\phi_Y(s)\right\|_w^2$$

$$:= \int_{R^{p+q}} \left|\phi_{X,Y}(t,s) - \phi_X(t)\phi_Y(s)\right|^2 w(t,s)dt\, ds$$

where $\phi_{X,Y}$, ϕ_X, and ϕ_Y are characteristic func.

- Weight $w(t,s) = (|t|_p^{1+p}|s|_q^{1+q})^{-1}$ to ensure the above integral is well defined…

Distance correlation

- Correlation:

$$dCor = \frac{\mathcal{V}\,(X,Y)}{\sqrt{\mathcal{V}(X,X)\cdot\mathcal{V}(Y,Y)}}$$

A Fact

- An equation:

$$2\pi \int_{-\infty}^{\infty} (F(x) - G(x))^2 = \underbrace{\int_{-\infty}^{\infty} \frac{\left|\hat{f}(t) - \hat{g}(t)\right|^2}{t^2} dt}_{\text{Distance correlation}}$$

- Distance correlation ~ difference between cumulative distribution functions.

Sample Distance Covariance

- Pairwise distances: $a_{ij} = \|X_i - X_j\|, 1 \le i, j \le n$
- Similarly, $b_{ij} = \|Y_i - Y_j\|$
- Centered matrix:

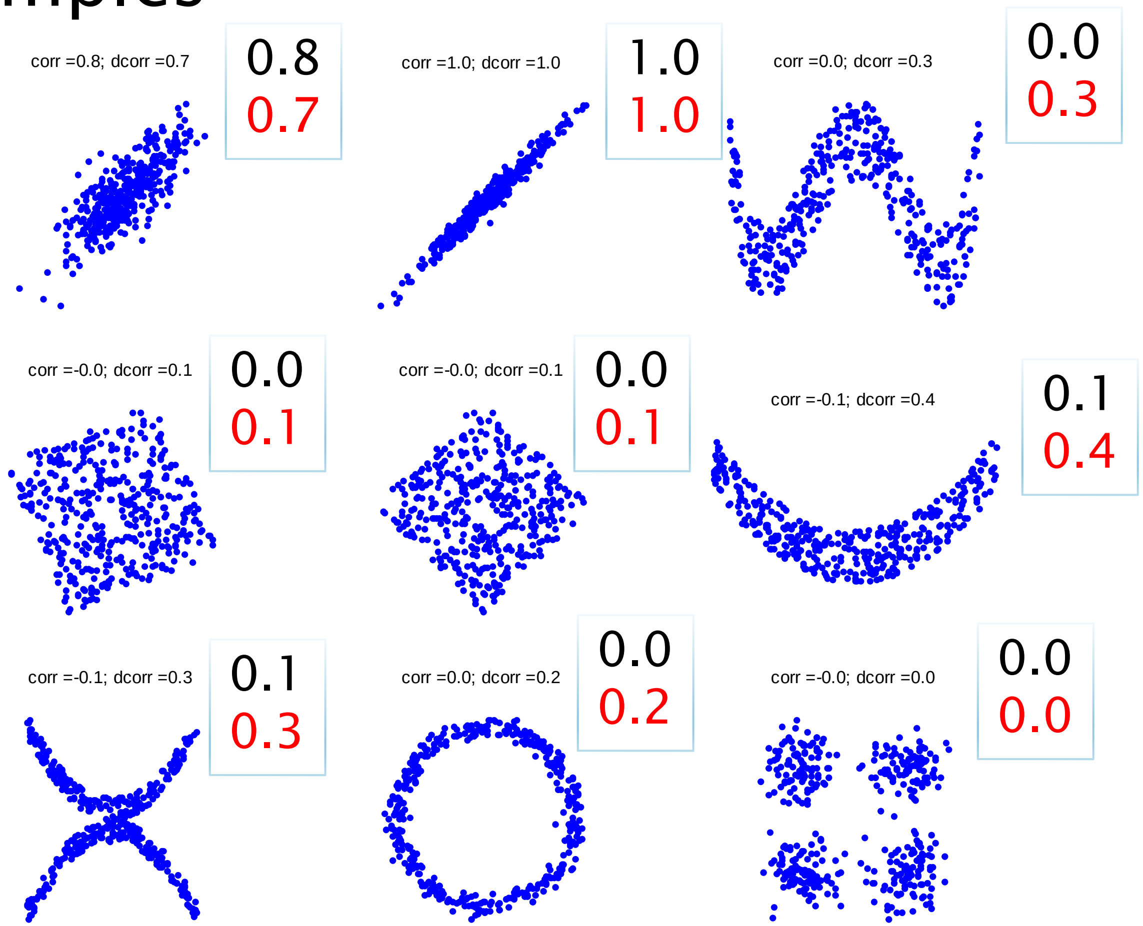
$$A_{ij} = \begin{cases} a_{ij} - \frac{\sum_{\ell=1}^{n} a_{i\ell}}{n-2} - \frac{\sum_{k=1}^{n} a_{kj}}{n-2} + \frac{\sum_{k,\ell=1}^{n} a_{k\ell}}{(n-1)(n-2)}, & i \neq j; \\ 0, & i = j \end{cases}$$

- Similarly, B_{ij}.
- An unbiased estimator of $\mathcal{V}^2(X,Y)$:

$$(A \cdot B) = \frac{\sum_{i \neq j} A_{ij} B_{ij}}{n(n-3)}$$

Compare with Dist. Corr.

- Same examples



III. Fast Algorithm

- Reformulation
- Partials sums
- 2-D dyadic partitioning and updating

Reformulation

- Requiring pairwise distances undesirable (n^2)
- Denote $a_{i\cdot} = \sum_{\ell=1}^{n} a_{i\ell}$, $1 \le i \le n$; similarly for $b_{i\cdot}$
- Denote $a_{\cdot\cdot} = \sum_{i,\ell=1}^{n} a_{i\ell}$; similarly for $b_{\cdot\cdot}$
- We have

$$(A \cdot B) = \frac{\sum_{i\neq j} a_{ij} b_{ij}}{n(n-3)} - \frac{2\sum_{i=1}^{n} a_{i\cdot} b_{i\cdot}}{n(n-2)(n-3)} + \frac{a_{\cdot\cdot} b_{\cdot\cdot}}{n(n-1)(n-2)(n-3)}$$

Main ideas towards an O(n log n) algorithm

- $a_{i\cdot}$ and $b_{i\cdot}$ can be related to partial sums – O(n) algorithm
- We designed a ***dyadic updating*** scheme to compute for

$$\sum_{i \neq j} a_{ij} b_{ij} = \sum_{i \neq j} |x_i - x_j| \cdot |y_i - y_j|$$

- An O(n log n) algorithm

Fast method for ALL $a_{i\cdot}$ ($b_{i\cdot}$)

- Recall $a_{i\cdot} = \sum_{l=1}^{n} a_{il} = \sum_{l=1}^{n} |x_i - x_l|$
- Sorting $x_1, x_2, \ldots, x_n$ takes (on average) $O(n \log n)$
- Computes ALL $\alpha_i = \sum_{l:\, x_l < x_i} 1$ takes $O(n)$
- Computes ALL $\beta_i = \sum_{l:\, x_l < x_i} x_l$ takes $O(n)$
- Note

$$a_{i\cdot} = \sum_{i=1}^{n} x_i + (2\alpha_i - n)x_i - 2\beta_i$$

- Overall, computing for ALL $a_{i\cdot}$'s takes $O(n \log n)$

Fast Method for cross terms

- Recall we want to compute for

$$\sum_{i \neq j} a_{ij} b_{ij} = \sum_{i \neq j} |x_i - x_j| \cdot |y_i - y_j|$$

- Define $S_{ij} = \text{sign}\big[(x_i - x_j)(y_i - y_j)\big]$
- We have

$$\begin{aligned}
\sum_{i \neq j} a_{ij} b_{ij} &= \sum_{i \neq j} |x_i - x_j| \cdot |y_i - y_j| \\
&= \sum_{i=1}^{n} \sum_{j:j \neq i} (x_i y_i + x_j y_j - x_i y_j - x_j y_i) S_{ij} \\
&= \sum_{i=1}^{n} \left[x_i y_i \sum_{j:j \neq i} S_{ij} + \sum_{j:j \neq i} x_j y_j S_{ij} - x_i \sum_{j:j \neq i} y_j S_{ij} - y_i \sum_{j:j \neq i} x_j S_{ij} \right]
\end{aligned}$$

Fast Method (2)

- We need to compute for all $1 \leq i \leq n$,

$$\sum_{j:j\neq i} c_j S_{ij}$$

- For an i, we have

Partial sum

$$\sum_{j:j\neq i} c_j S_{ij}$$

$$= \sum_{j} c_j - c_i \boxed{- 2 \sum_{j:j<i}} c_j \boxed{- 2 \sum_{j:\, y_j<y_i}} c_j$$

$$\boxed{+ 4 \sum_{j:j<i, y_j<y_i}} c_j$$

Need some efforts!

Relation to Fast Kendall's τ

Recall Kendall τ coefficient

$$\tau = \frac{1}{\binom{n}{2}} \sum_{1 \le i < j \le n} \operatorname{sign}[(x_i - x_j)(y_i - y_j)] = \frac{1}{\binom{n}{2}} \sum_{1 \le i < j \le n} S_{ij}$$

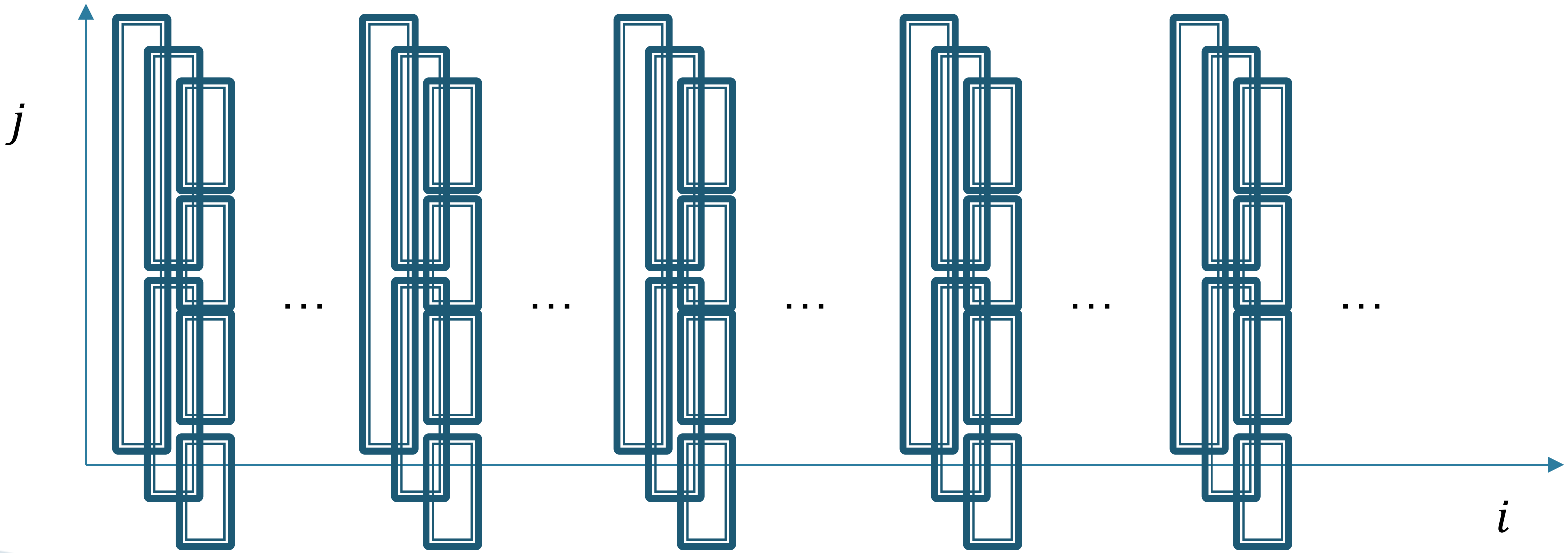
- Equivalent to $c_j \equiv 1$
- Knight (JASA 1966) and Christensen (2005)
- AVL tree structure (Adelson-Velskii and Landis 1962)

Fast Method (3)

- For an i, need to compute for

$$\sum_{j:j<i,y_j<y_i} c_j$$

- An *dyadic partitioning/updating* scheme:

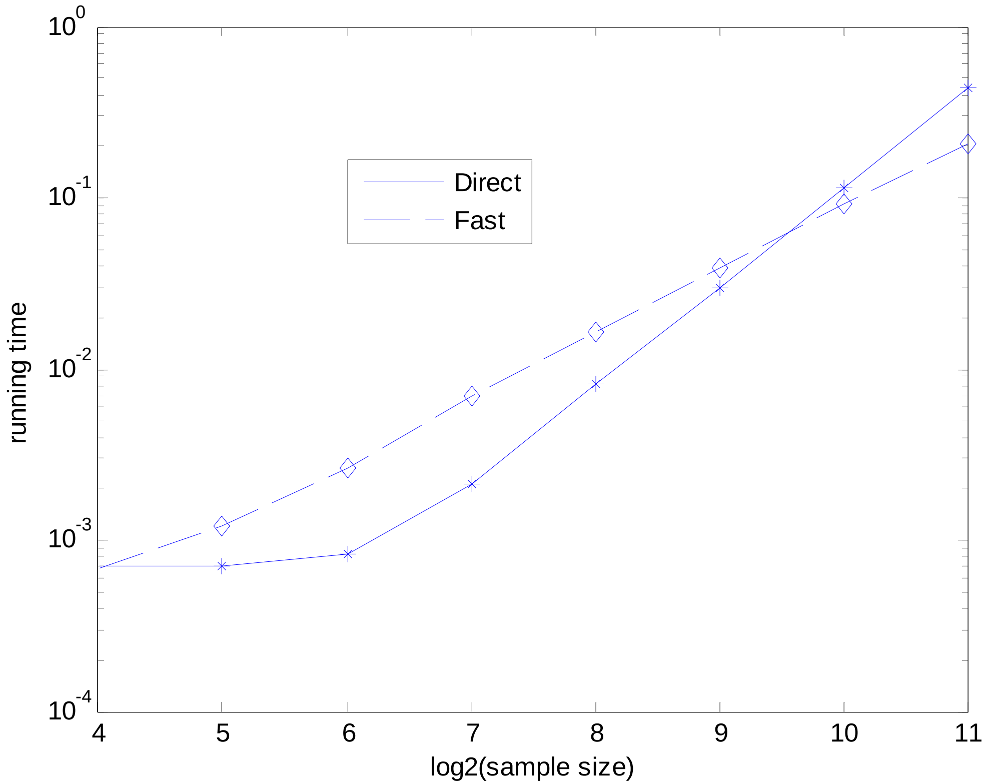


IV. Numerical Experiments

- Implementation
- Effects of large sample simulation
- Convergence

MATLAB implementation

- Compare with direct implementation

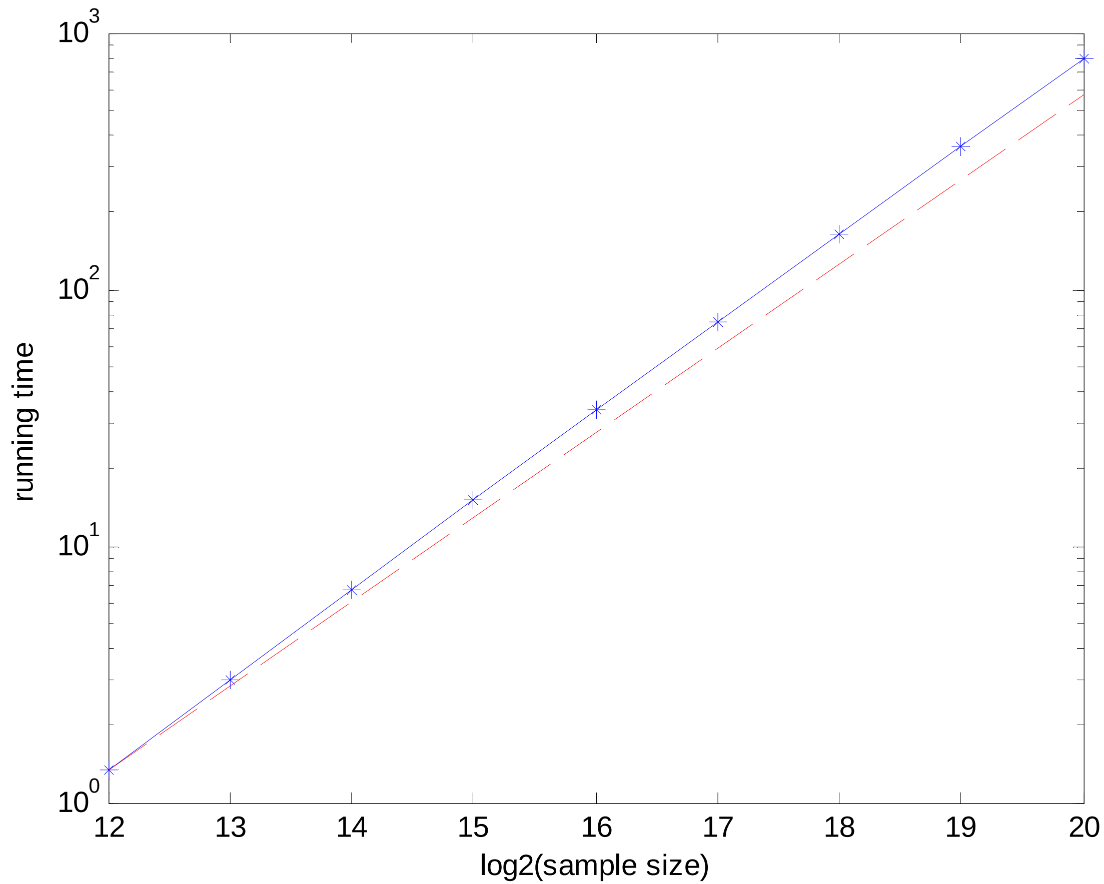


- When sample size > 2000, MATLAB is out of memory

MATLAB implementation (2)

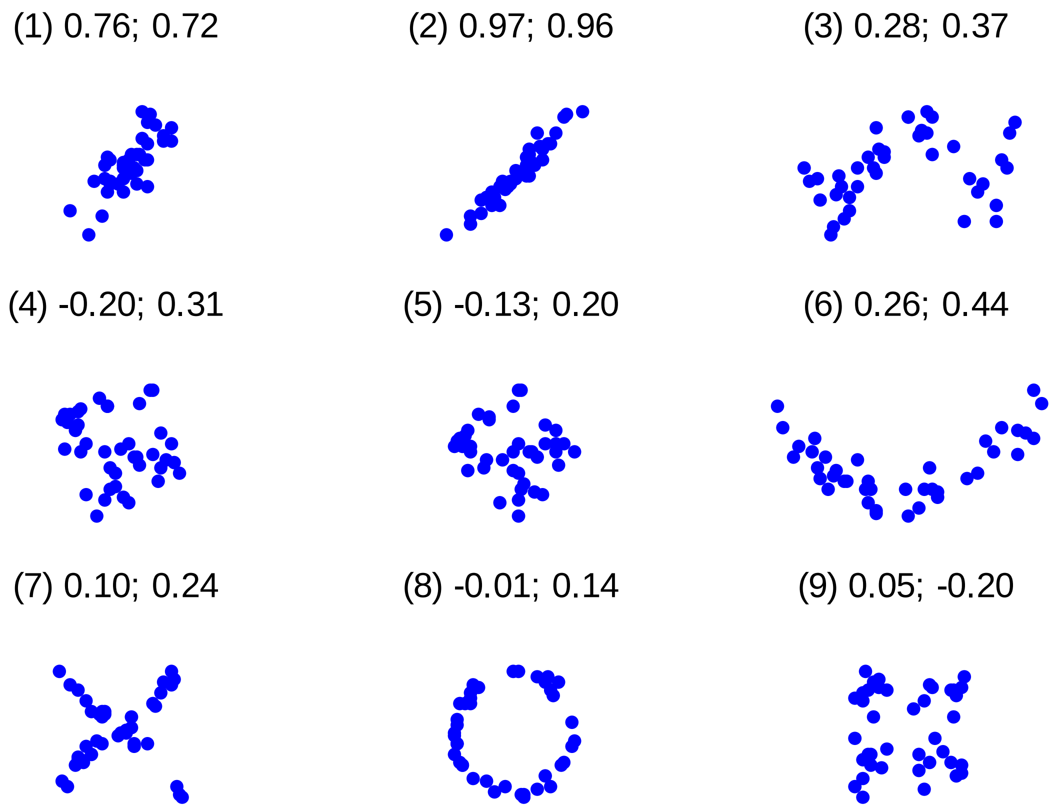
- Running time vs sample size (n)
- For n=1M, about 3min. on a laptop
- Dash line:

  O(n log n) complexity



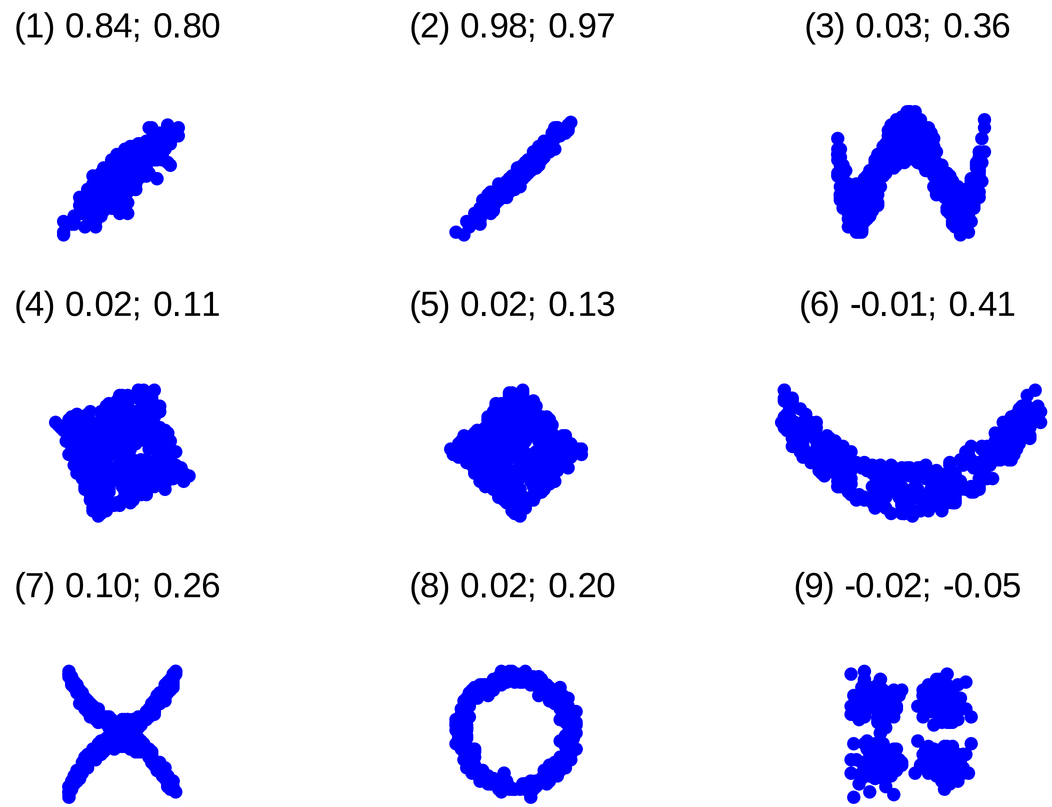
Effect of Large Sample Simulations

- Small sample (n=40)



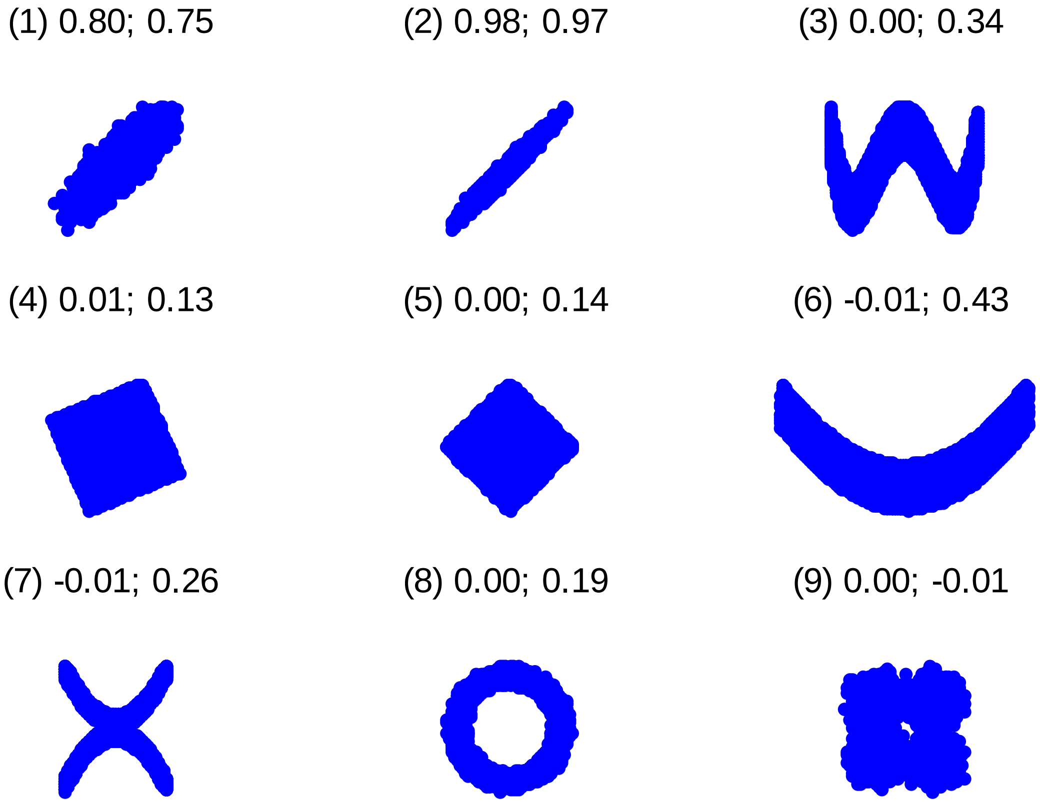
Effect of Large Sample Simulations

- Small sample (n=400)



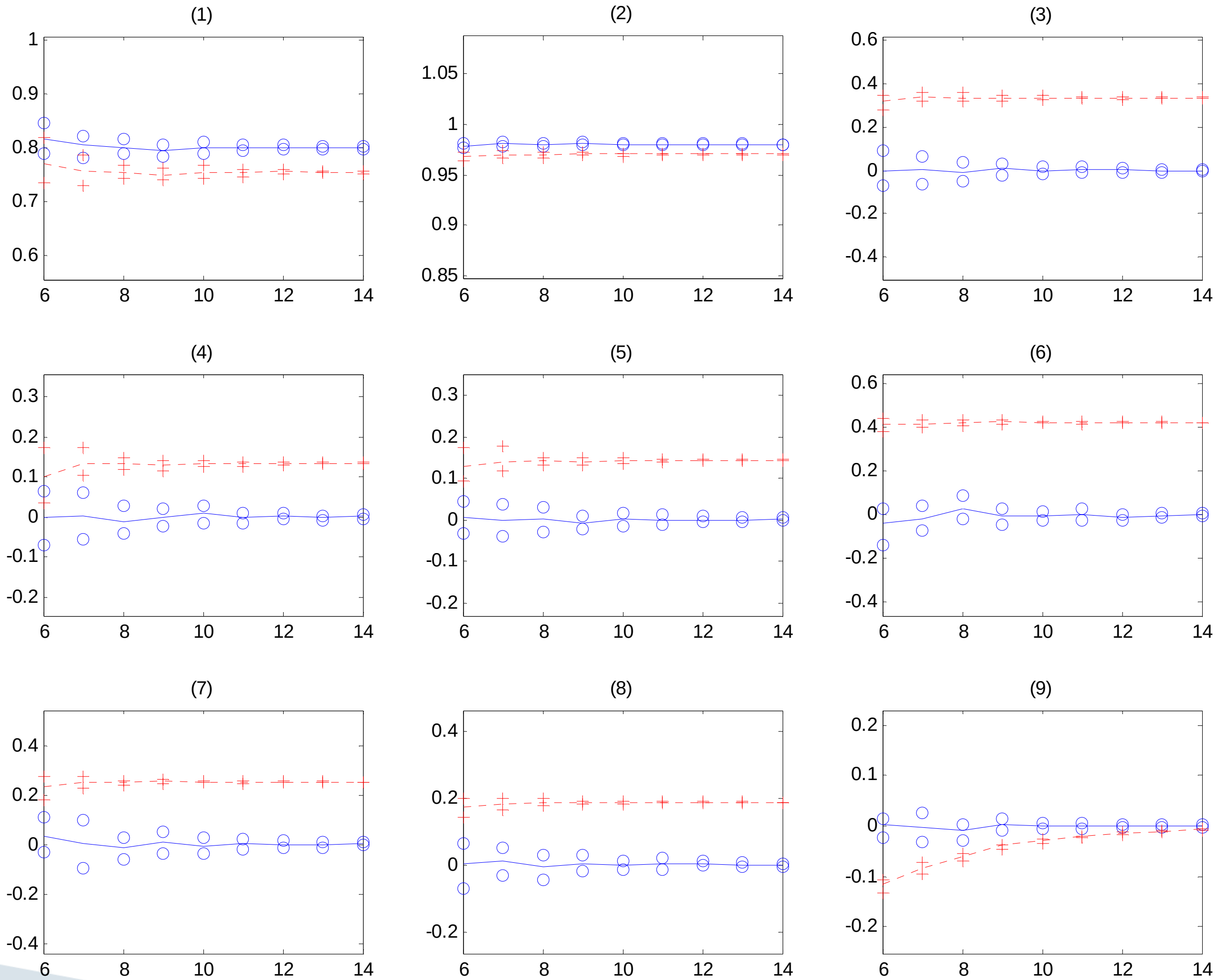
Effect of Large Sample (2)

- Large sample (n=10,000)



Convergence Study

- Convergence of sample correlations



V. Apply in Variable Screening

- Sure independence screening
- DC-SIS
- Improvement

dCor in Sure Screening

- Sure screening
- Li. et al JASA 2012, propose dCor in SURE screening
- More extensive simulation studies with sample size from n=200 to n=20,000…

SURE Variable Screening

- Setting

$$y \sim X_1, X_2, \ldots, X_p$$

- p is large; # of observation, small
- sure independence screening (SIS), Fan and Lv (JRSS-B 2008):
  - Compute marginal utility function
  - Retain the largest few
  - Asymptotic theory: “sure screening property”
  - marginal utility function: the Pearson's correlation

DC-SIS

- sure independence screening procedure based on the distance correlation
- marginal utility function: distance correlation
- Li. et al (JASA 2012)

Improvements via distCorr

- Experiment setting

$$(1.a):\ Y = c_1\beta_1 X_1 + c_2\beta_2 X_2 + c_3\beta_3 1(X_{12} < 0) + c_4\beta_4 X_{22} + \varepsilon,$$

$$(1.b):\ Y = c_1\beta_1 X_1 X_2 + c_3\beta_2 1(X_{12} < 0) + c_4\beta_3 X_{22} + \varepsilon,$$

$$(1.c):\ Y = c_1\beta_1 X_1 X_2 + c_3\beta_2 1(X_{12} < 0) X_{22} + \varepsilon,$$

$$(1.d):\ Y = c_1\beta_1 X_1 + c_2\beta_2 X_2 + c_3\beta_3 1(X_{12} < 0) + \exp(c_4|X_{22}|)\varepsilon,$$

- $p = 2000, 5000.$ $n = 200 \rightarrow 20{,}000.$

Improvements via distCorr (2)

- When $n = 200$

Table 1. The 5%, 25%, 50%, 75%, and 95% quantiles of the minimum model size $\mathcal{S}$ out of 500 replications in Example 1

$\mathcal{S}$	SIS					SIRS					DC-SIS				
Model	5%	25%	50%	75%	95%	5%	25%	50%	75%	95%	5%	25%	50%	75%	95%
Case 1: $p = 2000$ and $\sigma_{ij} = 0.5^{\lvert i-j \rvert}$															
(1.a)	4.0	4.0	5.0	7.0	21.2	4.0	4.0	5.0	7.0	45.1	4.0	4.0	4.0	6.0	18.0
(1.b)	68.0	578.5	1180.5	1634.5	1938.0	232.9	871.5	1386.0	1725.2	1942.4	5.0	9.0	24.5	73.0	345.1
(1.c)	395.9	1037.2	1438.0	1745.0	1945.1	238.5	805.0	1320.0	1697.0	1946.0	6.0	10.0	22.0	59.0	324.1
(1.d)	130.5	611.2	1166.0	1637.0	1936.5	42.0	304.2	797.0	1432.2	1846.1	4.0	5.0	9.0	41.0	336.2

- When $n = 20{,}000$

$\mathcal{S}$	SIS					SIRS					DC-SIS				
Model	5%	25%	50%	75%	95%	5%	25%	50%	75%	95%	5%	25%	50%	75%	95%
Case 1: $p = 2000$ and $\sigma_{ij} = 0.5^{\lvert i-j \rvert}$															
(1.a)	4	4	6	10	22	4	5	6	10	20	4	5	6	9	20
(1.b)	76	551	1180	1592	1918	237	814	1269	1789	1959	4	6	8	11	14
(1.c)	591	922	1364	1781	1941	342	827	1354	1637	1930	6	6	6	8	11
(1.d)	8	237	726	1310	1827	58	273	919	1444	1878	4	4	6	8	1001

Conclusion

- A fast algorithm to measure dependence: fast dCor
- Nearly linear complexity: O(n log n)
- Reference: "Fast Computing for Distance Covariance", Technometrics 2016

Name of Coeff.	Comp. cost
Pearson's ρ	n
Spearman's ρ	$n \log n$
Kendall's τ	$n \log n$
CCA	n
KCCA	n^3
ACE	n
MIC	2^n
MMD	n^2
CMMD	n^2
RDC	$n \log n$
dCor	$n^2 \rightarrow n \log n$