Tensor Graphical Lasso (TeraLasso)

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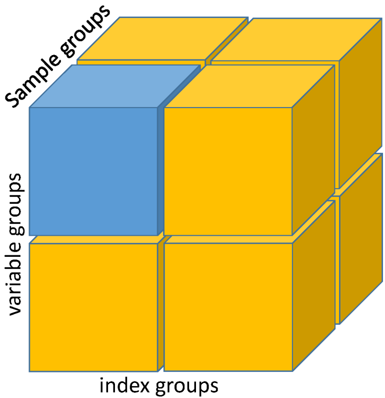
Multi-indexed data

- Sample groups
  $\Rightarrow$ Data from mixed populations[1]
- Variable groups
  $\Rightarrow$ Data from different modalities[2]
- Index groups
  $\Rightarrow$ Data indexed over diverse domains[3]



[1] G. McLachlan and D. Peel. Finite mixture models. John Wiley and Sons, 2004.

[2] Y. Yilmaz and A. Hero, Multimodal Event Detection in Twitter Hashtag Networks, Journ. of Signal Processing Systems, pp.1-16, 2016.

[3] K. Greenewald, S. Zhou, A.O. Hero, The Tensor Graphical Lasso (TeraLasso) arxiv1705.03983, 2017.

Data cube of heterogeneous data

Multi-indexed data array:

$$\mathbf{Z} = \{Z_{i_1,\ldots,i_K}\}_{i_1,\ldots,i_K}^{d_1,\ldots,d_K}, \qquad d = \prod_{i=1}^{K} d_k$$

Applications:

- predicting genome expression over time
- predicting weather from spatio-temporal climatological data
- human gait detection from low resolution video
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Common traits of these applications:

- the indices index over different types of domains
- the content of the arrays is complex and high dimensional
- the content is noisy and of high variability

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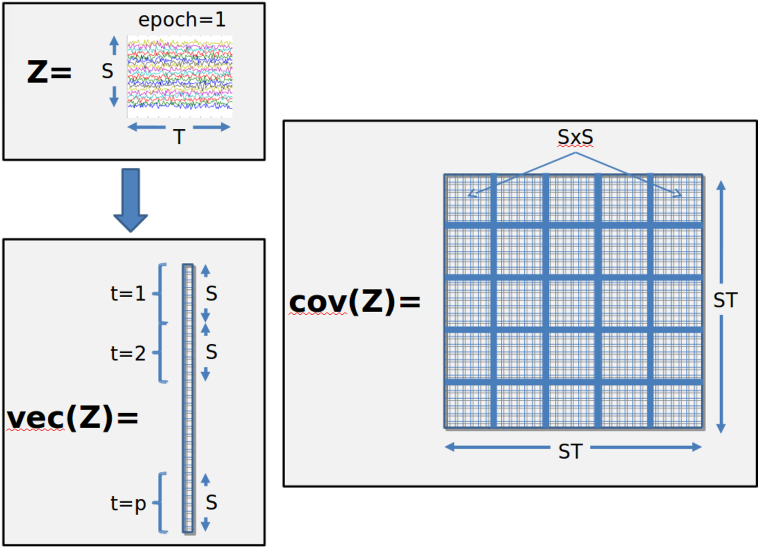
First order models not sufficient: much of the information lies in covariance

Covariance representation $d_1 = S, d_2 = T$

$\mathbf{\Sigma}$ =cov($\mathbf{Z}$) takes partitioned form



Measurement matrix and sample covariance

	Sample 1	Sample 2	...	Sample n
Variable 1	Z_{11}	Z_{12}	...	Z_{1n}
Variable 2	Z_{21}	Z_{22}	...	Z_{2n}
$\vdots$	$\vdots$	$\vdots$	...	$\vdots$
Variable d	Z_{d1}	Z_{n2}	...	Z_{dn}

$d \times n$ measurement matrix $\mathbb{Z}$ has i.i.d. columns $\mathbf{Z}_i$ with $\boldsymbol{\Sigma} = \mathrm{cov}(\mathbf{Z}_i)$

$$\mathbb{Z} = \begin{bmatrix} Z_{11} & \cdots & \cdots & Z_{1n} \\ \vdots & \ddots & \ddots & \vdots \\ Z_{d1} & \cdots & \cdots & Z_{dn} \end{bmatrix} = [\mathbf{Z}_1, \cdots, \mathbf{Z}_n]$$

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$d \times d$ *sample covariance matrix*:

$$\begin{aligned} \mathbf{S}_n &= (n-1)^{-1} \sum_{i=1}^{n} (\mathbf{Z}_i - \overline{\mathbf{Z}})(\mathbf{Z}_i - \overline{\mathbf{Z}})^T \\ &= (n-1)^{-1} \mathbb{Z}(\mathbf{I} - n^{-1}\mathbf{1}\mathbf{1}^T)\mathbb{Z}^T \end{aligned}$$

Empirical estimation of covariance under multivariate normal model

Multivariate normal model for $\mathbb{Z}$

$$\log f(\mathbb{Z}|\mathbf{\Sigma}) = \frac{n}{2}\log\det(\mathbf{\Sigma}^{-1}) - \frac{n-1}{2}\mathrm{tr}\left(\mathbf{S}_n\mathbf{\Sigma}^{-1}\right)$$

Maximum likelihood covariance estimator $\hat{\mathbf{\Sigma}} = \hat{\mathbf{\Omega}}^{-1}$ =soln to convex program[1]

$$\hat{\mathbf{\Omega}} = \mathrm{argmin}_{\mathbf{\Omega}}\mathrm{tr}(\mathbf{S}_n\mathbf{\Omega}) - c_n\log\det(\mathbf{\Omega})$$

Note that there are $p = d(d+1)/2 = O(d^2)$ unknown parameters in $\mathbf{\Sigma}$

Requirements:

1. $n \geq O(d)$ for MLE to be unique and have finite variance
2. $n \geq O(d^2)$ for estimator to be accurate (Bühlmann&VanDeGeer, 2011)

$$E[\|\hat{\mathbf{\Sigma}} - \mathbf{\Sigma}\|_F^2] = O\left(d^2/n\right)$$

[1] $c_n = \frac{n}{n-1}$

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If $\boldsymbol{\Omega}$ has structure can obtain $E[\|\hat{\boldsymbol{\Sigma}} - \boldsymbol{\Sigma}\|_F^2] = O\left(d/n\right)$, e.g. for sparse $\boldsymbol{\Omega}$

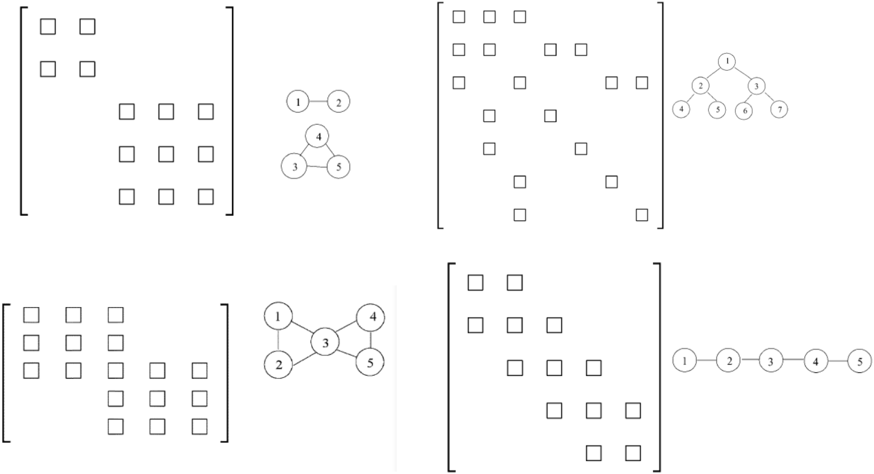
$$\hat{\boldsymbol{\Omega}} = \mathrm{argmin}_{\boldsymbol{\Omega}}\mathrm{tr}(\mathbf{S}_n\boldsymbol{\Omega}) - c_n\log\det(\boldsymbol{\Omega}) + \lambda\|\boldsymbol{\Omega}\|_1 \qquad (GLasso)$$

[1] $c_n = \frac{n}{n-1}$

Many types of covariance structure have been studied

- Sparse structured covariance
  - Banded covariance model: Bickel-Levina (2008)
  - Sparse eigendecomposition model: Johnstone-Lu (2007)
  - Stein shrinkage towards identity: Ledoit-Wolf (2005), Chen-Weisel-Eldar-H (2010)
- Sparse inverse covariance: Gaussian graphical models
  - Glasso: Freidman-Hastie,-Tibshirani(2007), Wiesel-Eldar-H (2010).
  - l_1-regularized logistic: Wainright, Ravikumar, Lafferty (2006)
  - Bayesian sparse cov estimation: Rajaratnam-Massam-Carvalho (2008)
  - Sparse Kronecker GGM (Matrix Normal):Allen-Tibshirani (2010), Tsiligkaridis-Zhou-H (2012), Greenewald-H (2014)
- Covariance sparsity testing
  - Sphericity test for multivariate Gaussian: Wilks (1935)
  - Maximal correlation test: Moran (1980), Eagleson (1983), Jiang (2004), Zhou (2007), Cai and Jiang (2011)
  - Independence screening (Fan 2007, Rajaratnam-H, 2011)
- Inverse covariance sparsity testing
  - Partial correlation hub screening (Rajaratnam-H 2012)
  - Sparse prediction and regression by correlation screening (SPARCS) (Firouzi-Rajaratnam-H 2017)

Graphical representations of $\mathbf{\Sigma}$ or $\mathbf{\Sigma}^{-1}$



Wiesel, Eldar and H IEEE TSP 2010

Sparsity in covariance vs sparsity in inverse covariance

Sparsity models

- Sparse correlation ($\mathbf{\Sigma}$) graphical models:
  - Most correlation are zero, few marginal dependencies
  - Examples: M-dependent processes, moving average (MA) processes
- Sparse inverse-correlation ($\mathbf{K} = \mathbf{\Sigma}^{-1}$) graphical models
  - Most inverse covariance entries are zero, few conditional dependencies
  - Examples: Markov random fields, autoregressive (AR) processes, global latent variables

- Sometimes correlation matrix and its inverse are both sparse
- Often only one of them is sparse

Refs: Meinshausen-Bühlmann (2006), Friedman (2007), Bannerjee (2008), Wiesel-Eldar-H (2010) .

Most physical processes are sparse in inverse covariance

Let $p^t(x, y)$ be a space-time process satisfying Poisson equation

$$\frac{\nabla^2 p^t}{\nabla x^2} + \frac{\nabla^2 p^t}{\nabla y^2} = W^t$$

where $W^t = W^t(x, y)$ is driving process.
For small Δ_x, Δ_y, p satisfies the difference equation:

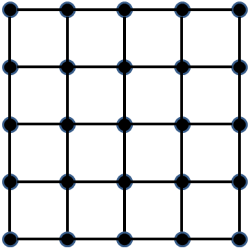
$$X^t_{i,j} = \frac{(X^t_{i+1,j} + X^t_{i-1,j})\Delta^2 y + (X^t_{i,j+1} + X^t_{i,j-1})\Delta^2 x - W^t_{i,j}\Delta^2 x \Delta^2 y}{2(\Delta^2 x + \Delta^2 y)}$$

In matrix form, as before: $[\mathbf{I} - \mathbf{A}]\mathbf{X}^t = \mathbf{W}^t$ and

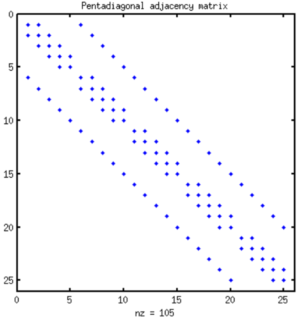
$$\mathbf{\Omega} = \mathrm{cov}^{-1}(\mathbf{X}^t) = \sigma^2_W [\mathbf{I} - \mathbf{A}][\mathbf{I} - \mathbf{A}]^T$$

$\mathbf{A}$ is sparse "pentadiagonal" matrix.

Example: 5×5 Poisson random field graphical model



Graph G_K on $\mathbb{R}^2$



corresp. **K** adjacency matrix

Gauss-Markov random field from Poisson equation on 90×90 grid

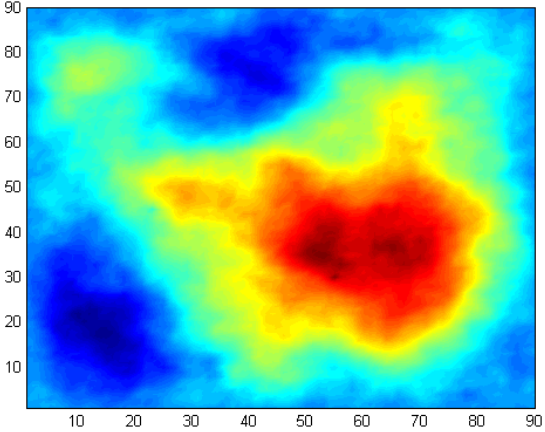
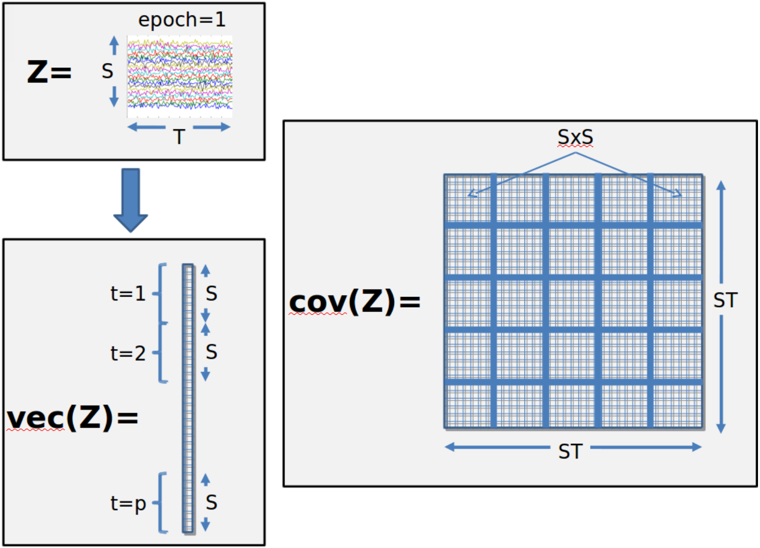


Figure: Poisson random field. $\mathbf{W}^t = \mathbf{N}_{iso} + sin(\omega_1 t)\mathbf{e}_1 + sin(\omega_2 t)\mathbf{e}_2$ ($\omega_1 = 0.025$, $\omega_2 = 0.02599$, SNR=0dB).

Kronecker product models: covariance representation

$\mathbf{\Sigma} = \text{cov}(\mathbf{Z})$ takes partitioned form



Kronecker product representation of covariance matrices

Let **A** be a $p \times p$ matrix and **B** be a $q \times q$ matrix. For $d = pq$ the Kronecker product of **A** and **B** is the $d \times d$ matrix

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & \cdots & a_{1p}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{p1}\mathbf{B} & \cdots & a_{pp}\mathbf{B} \end{bmatrix}$$

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Kronecker product properties (VanLoan-Pitsianis 1992)[a]:

- $\mathbf{A} \otimes \mathbf{B}$ is p.d. if $\mathbf{A}$ and $\mathbf{B}$ are p.d.
- $(\mathbf{A} \otimes \mathbf{B})^{-1} = \mathbf{A}^{-1} \otimes \mathbf{B}^{-1}$ if $\mathbf{A}$ and $\mathbf{B}$ are invertible.
- $\det(\mathbf{A} \otimes \mathbf{B}) = \det\mathbf{A} \det\mathbf{B}$
- For any $pq \times pq$ matrix $\mathbf{D}$

$$\|\mathbf{D} - \mathbf{A} \otimes \mathbf{B}\|_F^2 = \|\mathcal{R}(\mathbf{D}) - \mathrm{vec}(\mathbf{A})\mathrm{vec}(\mathbf{B})^T\|_F^2$$

Van Loan and Pitsianis (1993). "Approximation with Kronecker products." *Linear algebra for large scale and real-time applications*

Kronecker product model for inverse covariance

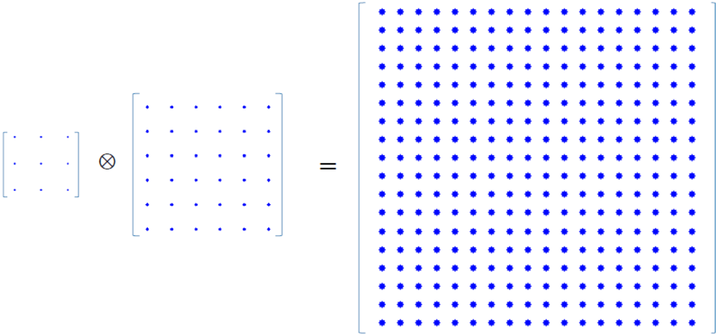


Figure: 18×18 covariance matrix has 18*17/2=153 unknown cross-correlation parameters. Kronecker product covariance model reduces this to $3 + 15 = 18$ parameters.

Leads to Kronecker MLE (matrix normal): Dawid (1981), Werner-Jansson-Stoica (2008), Tsiligkaridis-H-Zhou (2013)

Aka: matrix normal model, transposable covariance model, flip-flop covariance

Sparse Kronecker product model for inverse covariance

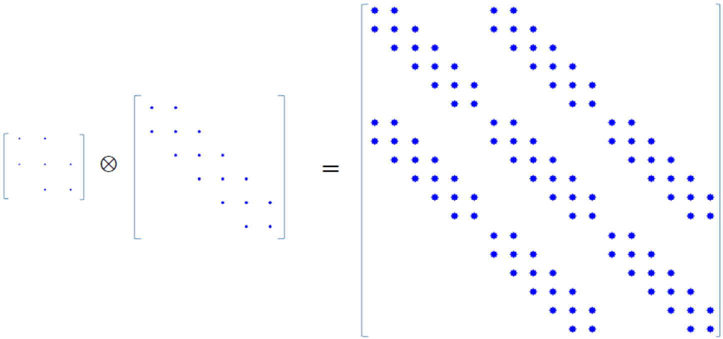


Figure: A sparse Kronecker product covariance model reduces number of parameters from 153 to 7 unknown correlation parameters.

Leads to KGlasso (sparse matrix normal): Allen-Tibshirani (2010), Yin-Li (2012), Tsiligkaridis-H-Zhou (2013)

Sparse matrix variate normal model: the KGlasso

Let $\mathbf{Z}$ ($p \times q$) follow the matrix normal normal distribution with inverse covariance matrix $\mathbf{\Omega} = \mathbf{X} \otimes \mathbf{Y}$. If

$$\|\mathbf{\Omega}\|_0 \leq O(pq)$$

then the matrix variate normal model is said to be sparse.

Maximize sparsity penalized likelihood function to estimate $\mathbf{\Omega}$

$$(\hat{\mathbf{X}}, \hat{\mathbf{Y}}) = \mathrm{argmin}_{\mathbf{X},\mathbf{Y}} J_\lambda(\mathbf{X}, \mathbf{Y})$$

where

$$J_\lambda(\mathbf{X}, \mathbf{Y}) = \mathrm{tr}\{\mathbf{S}_n(\mathbf{X} \otimes \mathbf{Y})\} - \log(|\mathbf{X}|\,|\mathbf{Y}|) + \lambda_X \|\mathbf{X}\|_1 + \lambda_Y \|\mathbf{Y}\|_1$$

Alternating minimization (flip-flop) algorithms

- Transposable regularized covariance algorithm (Allen-Tibshirani 2010)
- KGlasso algorithm (Tsiligkaridis-Zhou-H 2012)

Application: windspeed prediction (10×10 patch - Arctic to Norwegian sea)

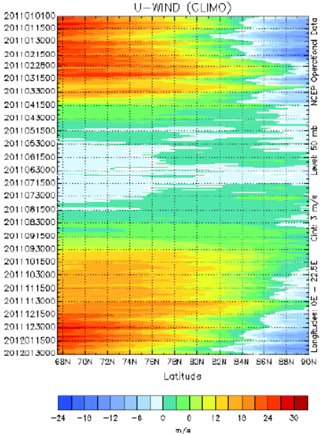
Region extending over latitudes 90-67.5 degrees N and longitudes 0-22.5 degrees E

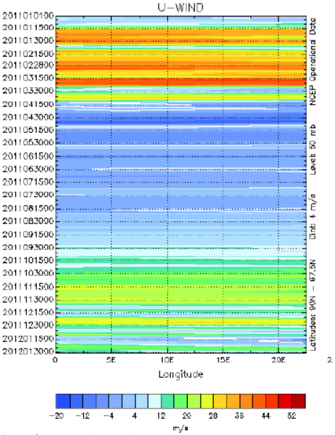
- $S = 100$ (10×10 spatial grid)
- $T = 8$ (2 day time window)
- $n = 224$ (over period 2003-2007)

Tsiligkaridis, H (2013). Covariance estimation in high D via kronecker product expansions. *IEEE Trans on Signal Processing*

Application: NCEP 10×10 patch over Arctic to Norwegian sea

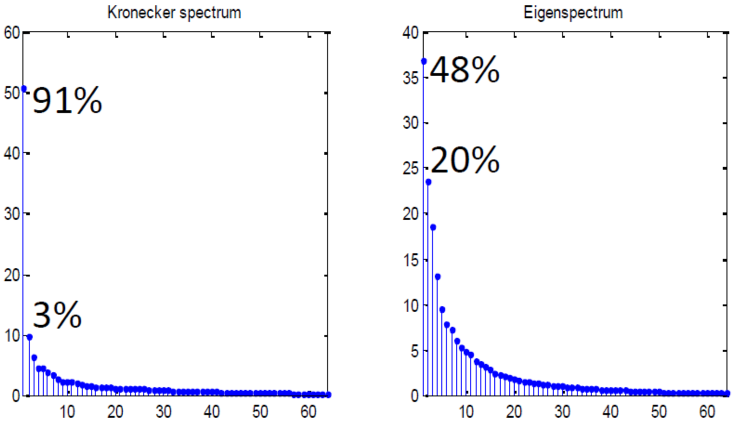
U component of windspeed





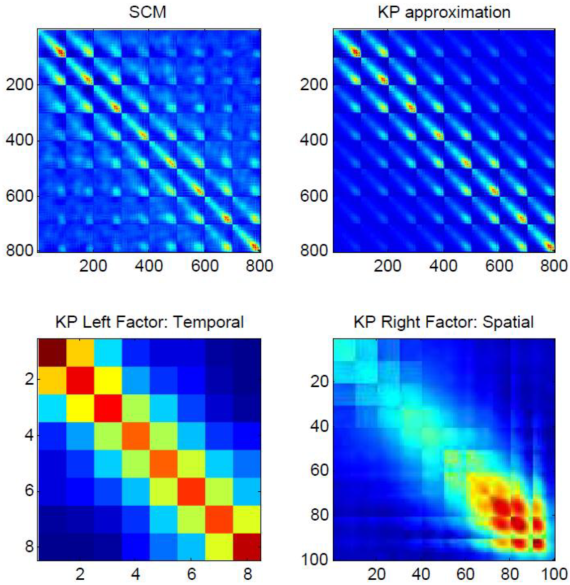
Lat (90-67.5) and long (0-22.5) is over 2.5 degree increments

Application: NCEP 10×10 over Arctic to Norwegian sea



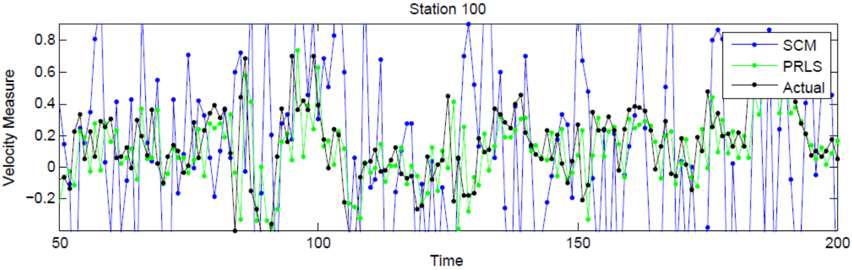
- Kronecker spectrum (left) significantly more concentrated than eigenspectrum (right)

Application: NCEP 10×10 patch over Arctic to Norwegian sea



Application: NCEP 10×10 patch over Arctic to Norwegian sea

When use PRLS for prediction get higher prediction accuracy



- Prediction by regularized sample covariance matrix (SCM):
  - Sample covariance $\hat{\mathbf{\Sigma}} = \hat{\mathbf{S}}_n$ is rank deficient
  - Min-norm (Moore-Penrose inverse) used on OLS predictor
- Prediction by Kronecker approximation to covariance
  - $\hat{\mathbf{\Sigma}} = \hat{\mathbf{\Sigma}}_X \otimes \hat{\mathbf{\Sigma}}_Y$ is full rank
  - Use $\hat{\mathbf{\Omega}}$ directly in OLSE predictor

Tsiligkaridis and Hero (2013). Covariance estimation in high D via kronecker product expansions. *IEEE Trans on Signal Processing*

TeraLasso: Kronecker sum covariance and inverse covariance model

Define Kronecker sum for two matrices $\mathbf{A} \in \mathbb{R}^{m \times m}$, $\mathbf{B} \in \mathbb{R}^{n \times n}$

$$\mathbf{A} \oplus \mathbf{B} \stackrel{\text{def}}{=} \mathbf{A} \otimes \mathbf{I}_n + \mathbf{I}_m \otimes \mathbf{B}$$

- Kronecker sum covariance model for $p = 2$ (Rudelson 2017)[a]

$$\mathbf{\Sigma} = \mathbf{A} \oplus \mathbf{B}$$

- Sparse Kronecker sum precision model for $p = 2$ (BiGlasso) (Kalaitzis 2013)[b]

$$\mathbf{\Sigma}^{-1} = \mathbf{A} \oplus \mathbf{B}$$

- Tensor-graphical Lasso (TeraLasso): (Greenewald 2017)[b]

$$\mathbf{\Sigma}^{-1} = \mathbf{\Psi}_1 \oplus \ldots \oplus \mathbf{\Psi}_p$$

[a] Rudelson and Zhou (2017). Errors-in-variables models with dependent measurements. *Elec Journ of Statistics*

[b] Kalaitzis, Lafferty, Lawrence, Zhou (2013). The bigraphical lasso. *Int. Conf. on Machine Learning, ICML*

[c] Greenewald, Zhou, and Hero (2017). Tensor Graphical Lasso (TeraLasso). arXiv:1705.03983.

Properties of Kronecker sum

Kronecker sum $\mathbf{A} \oplus \mathbf{B} \stackrel{\text{def}}{=} \mathbf{A} \otimes \mathbf{I}_n + \mathbf{I}_m \otimes \mathbf{B}$ satisfies[2]

- Associativity: $\mathbf{A}_1 \oplus (\mathbf{A}_2 \oplus \mathbf{A}_3) = (\mathbf{A}_1 \oplus \mathbf{A}_2) \oplus \mathbf{A}_3$

[2] A.J. Laub (2005), *Matrix analysis for scientists and engineers,"* *SIAM Press*

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- Linearity in $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$
- Distributivity:

$$\begin{aligned} & c_A(\mathbf{A}_1 \oplus \mathbf{A}_2 \oplus \mathbf{A}_3) + c_B(\mathbf{B}_1 \oplus \mathbf{B}_2 \oplus \mathbf{B}_3) \\ & \quad = (c_A\mathbf{A}_1 + \mathbf{c}_B\mathbf{B}_1) \oplus (c_A\mathbf{A}_2 + \mathbf{c}_B\mathbf{B}_2) \oplus (c_A\mathbf{A}_3 + \mathbf{c}_B\mathbf{B}_3) \end{aligned}$$

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- Eigendecomposition: if $\mathbf{A}_k = \mathbf{U}_k \boldsymbol{\Lambda}_k \mathbf{U}_k^T$ is SVD

$$\mathbf{A}_1 \oplus \cdots \oplus \mathbf{A}_K = (\mathbf{U}_1 \oplus \cdots \oplus \mathbf{U}_K)(\boldsymbol{\Lambda}_1 \oplus \cdots \oplus \boldsymbol{\Lambda}_K)(\mathbf{U}_1 \oplus \cdots \oplus \mathbf{U}_K)^T$$

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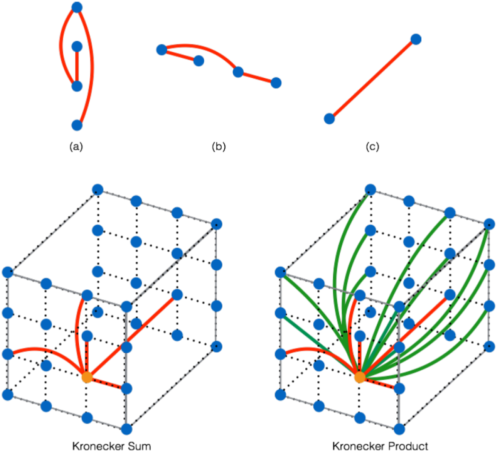
Kronecker sum vs Kronecker product

The Kronecker sum gives more flexible and sparser covariance representations



$\mathbf{A} \oplus \mathbf{B} \oplus \mathbf{C}$ $\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{C}$

64 total edges 184 total edges

TeraLasso: a sparse Kronecker sum precision matrix estimator

TeraLasso estimator of $\mathbf{\Omega} = \mathbf{\Sigma}^{-1} \in \kappa_p^\sharp$

$$\hat{\mathbf{\Omega}} = \arg\min_{\mathbf{\Omega} \in \kappa_p^\sharp} \left\{ -\log|\mathbf{\Omega}| + \mathrm{tr}(\hat{\mathbf{S}}\mathbf{\Omega}) + \sum_{k=1}^{K} \rho_k m_k |\mathbf{\Psi}_k|_{1,\mathrm{off}} \right\}$$

where $m_k = \prod_{i \neq k} d_i = p/d_k$ and

$$\hat{S} = \frac{1}{n} \sum_{i=1}^{n} \mathrm{vec}(\mathbf{Z}_i^T)\mathrm{vec}(\mathbf{Z}_i^T)^T$$

and

$$\kappa_{\mathrm{p}}^\sharp = \{\mathbf{A} \succ 0 : \exists B_k \in \mathbb{R}^{d_k \times d_k} \text{ s.}t.\ \mathbf{A} = \mathbf{B}_1 \oplus \ldots \oplus \mathbf{B}_K\}$$

Convergent convex optimization via gradient-based descent, e.g., first order FISTA[a]

[a] Greenewald, Zhou, and Hero (2017). Tensor Graphical Lasso (TeraLasso). arXiv:1705.03983

TeraLasso: statistical convergence rates

(**A1**) Sparsity assumption card$(\mathcal{S}_k) \leq s_k$, where $\mathcal{S}_k$ is support set of k-th Kronecker factor Ψ_k.

(**A2**) Eigenvalues of $\mathbf{\Omega}$ satisfy $0 < \lambda_i < \infty$

Theorem

*(**Frobenius Error Bound**)[a]. Suppose the assumptions (A1)-(A2) hold, and that $\hat{\mathbf{\Omega}}$ is a minimizer with $\rho_k = a\frac{1}{k}\sqrt{\frac{\log d}{nm_k}}$. Then with probability at least $1 - 2(K+1)exp(-c\log d)$*

$$\|\hat{\mathbf{\Omega}} - \mathbf{\Omega}_0\| \leq \frac{C\|\mathbf{\Sigma}_0\|_2}{\lambda_{\min}(\mathbf{\Sigma}_0)}\sqrt{(K+1)(s+d)\frac{\log d}{n \min_k m_k}}$$

Compare to Glasso (Rothman 2008)[b], (Zhou)[c]. If $\Omega \in \kappa_p^\sharp$ then

$\Rightarrow$ TeraLasso statistical convergence rate is faster by a factor of $\min_k m_k$.

[a] Greenewald, Zhou, and Hero (2017). Tensor Graphical Lasso (TeraLasso). arXiv:1705.03983.

[b] Rothman, Bickel, Levina, Zhu (2008). Sparse permutation invariance covariance estimation, *Elec. Journ. Statistics*.

[c] Zhou, Rütimann, Xi, Bülmann (2011). High dimensional covariance estiamtion based on GGMs. *NIPS*.

TeraLasso: runtime comparisons for random Erdös-Renyi

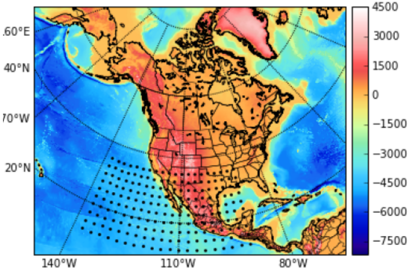
K	p	d_k	n	TeraLasso Runtime (s)	BiGLasso Runtime (s)
2	100	10	10	.0131	.84
2	625	25	10	.0147	6.81
2	2500	50	10	.0272	161
2	5625	75	10	.0401	1690
2	10^4	100	10	.0664	
2	2.5×10^5	500	10	1.62	
2	10^6	1000	10	23.2	
2	4×10^6	2000	10	427	
3	10^6	100	10	3.52	NA
3	8×10^6	200	10	11.2	NA
3	1.25×10^8	500	10	32.6	NA
3	1×10^9	1000	10	70.0	NA
4	10^4	10	10	.281	NA
4	1.6×10^5	20	10	.649	NA
4	6.25×10^6	50	10	10.8	NA
4	1.00×10^9	178	10	88.4	NA
5	1.16×10^9	65	10	124	NA

- TeraLasso speedup wrt BiGlasso by 2 to 4 orders of magnitude ($10^2 - 10^4$)
- Teralasso is scalable to many many variables

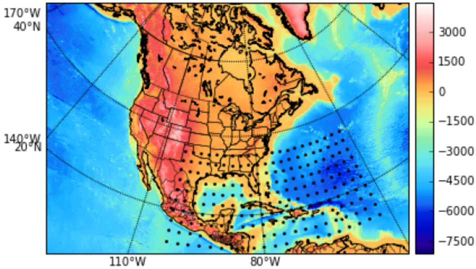
$$\text{Terralasso/iter} \Rightarrow O(\sum_{k=1}^{K} d_k^3) \qquad \text{Glasso/iter}^{a} \Rightarrow O(p^3) = O\left(\prod_{k=1}^{K} d_k^3\right)$$

[a] Guillot, Rajaratnam, Rolfs, Maleki, Wong (2012). Iterative thresholding algorithm for sparse inverse covariance estimation. *NIPS*.

Application to NCEP wind speed data

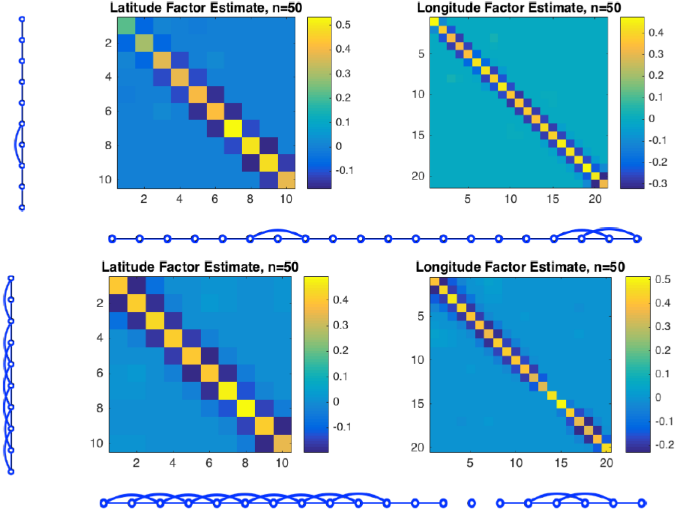


10 × 20 grid for western US



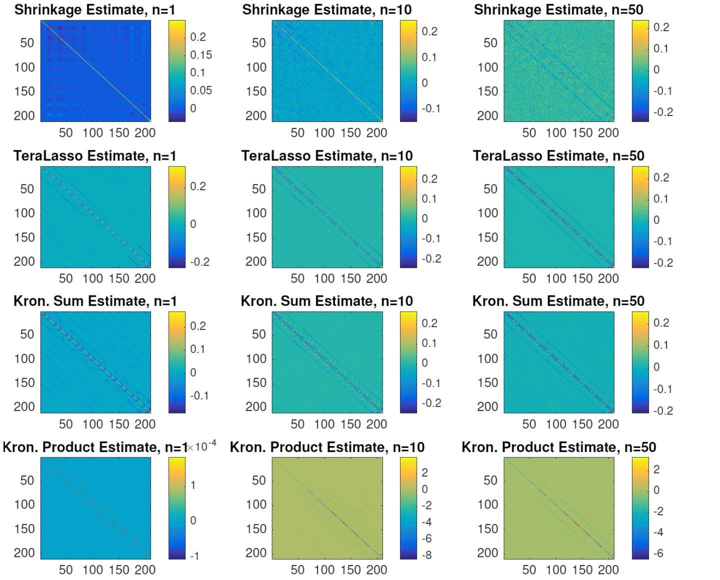
10 × 20 grid for eastern US

TeraLasso factors for spatial-only model ($K = 2$) (NCEP data)



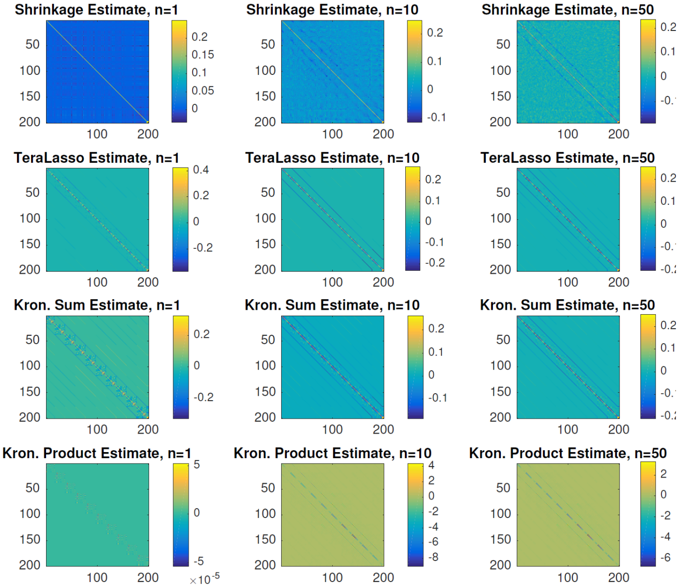
Top: Eastern grid. Bottom: Western grod. Kronecker sum factors for $d_1 = 10, d_2 = 20$

Comparisons for spatial-only model ($K = 2$) (NCEP data)



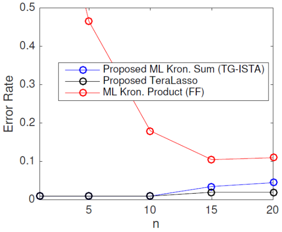
Eastern grid: inverse spatial covariance estimates for $d_1 = 10, d_2 = 20$

Comparisons for spatial-only model ($K = 2$) (NCEP data)

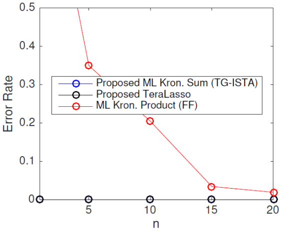


Western grid: inverse spatial covariance estimates for $d_1 = 10, d_2 = 20$

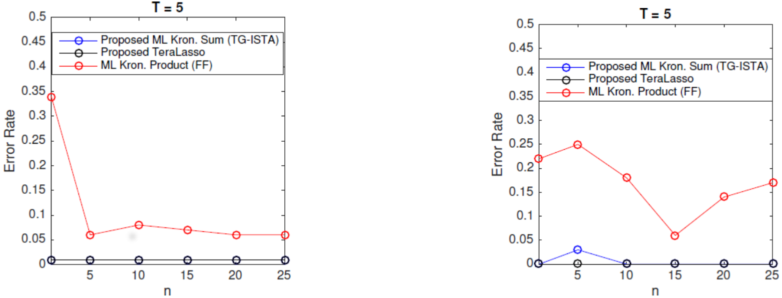
$K = 2$ vs $K = 3$ TeraLasso for season classification (NCEP data)



(a) Eastern grid



(b) Western grid

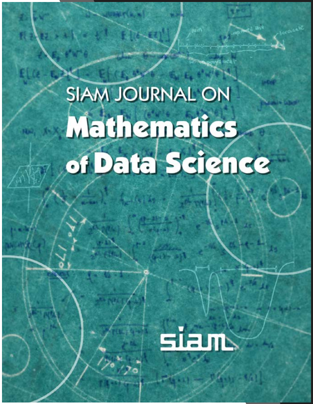


Top: $K = 2$. Bottom: $K = 3$ w/ $d_1 = 10, d_2 = 20, d_3 = 5$

Conclusions

- Value of Kronecker covariance representations for multi-indexed arrays
- Sparse Kronecker product model for matrix normal distributions (KLasso)
  - Reduces complexity of model from $O(p^2q^2)$ to $O(p+q)$
  - Bilinear non-convex objective function
- Sparse Kronecker sum model for matrix normal distributions (TeraLasso)
  - Reduces complexity of model even further than KLasso
  - Linear convex objective function

New journal



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