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ABSTRACT

The estimation of a precision matrix has an important role in several research fields. In high dimensional settings, one of the most prominent approaches to estimate the precision matrix is the Lasso norm penalized convex optimization. This framework guarantees the sparsity of the estimated precision matrix. However, it does not control the eigenspectrum of the obtained estimator. Moreover, Lasso penalization shrinks the largest eigenvalues of the estimated precision matrix. In this article, we focus on D-trace estimation methodology of a precision matrix. We propose imposing a negative trace penalization on the objective function of the D-trace approach, aimed to control the eigenvalues of the estimated precision matrix. Through extensive numerical analysis, using simulated and real datasets, we show the advantageous performance of our proposed methodology.

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Hannan-Quinn information criterion;
D-trace; gene expression;
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1. Introduction

The estimation of a high dimensional inverse covariance or precision matrix has attracted significant interest recently. It is an important problem in genetics (Stifanelli et al. 2013), medicine (Ryali et al. 2012), climate studies (Zerenner et al. 2014), finance (Goto and Xu 2015), etc. Moreover, it has a crucial role in various machine learning methodologies, such as classification and forecasting (McLachlan 2004).

Under the assumption of multivariate normality of data, the zero entry of the precision matrix at the position (i, j) indicates the conditional independence between the variables X^i and X^j , given all the other variables $X^{-(i,j)}$ (Dempster 1972). In other words, the precision matrix represents the statistical dependency among normally distributed variables. In high dimensional settings, the precision matrix is usually sparse, since some of the variables do not interact.

The sparse precision matrix is related to the Gaussian Graphical Models (GGM) (Lauritzen 1996). It is an undirected graph $G = (N, E)$, where the set of nodes, $N = \{1, \dots, p\}$, contains the indexes of the variables. The set of edges, $E \subseteq N \times N$, consists of the pair indexes (i, j) , that correspond to $\omega_{ij} \neq 0$, for $1 \leq i, j \leq p$. Thus, the GGM is a useful framework for illustrating the structure of dependencies among normally distributed variables.

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In this article, we focus on estimating a high dimensional precision matrix and the selection of corresponding GGM (known as covariance selection). Throughout the article we assume that observed sample data matrix, $\mathbf{X}_{n \times p}$, is mean centered, where each row $X_i = (X_{i1}, \dots, X_{ip})$ is a p -variate normal random vector, i.i.d. for $i = 1, \dots, n$, and has a covariance matrix Σ with corresponding precision matrix $\Omega = \Sigma^{-1}$.

A considerable research is devoted to the estimation of precision matrices in high dimensional settings, where the number of variables may potentially exceed the number of observations. The regularization framework has gained a substantial attention. The most popular approach is the Lasso or ℓ_1 norm regularization (Tibshirani 1996), which is convex and addresses the sparsity requirement of the estimated matrix. Banerjee et al. (2006) proposed the ℓ_1 norm penalized log-likelihood maximization approach, which is known in literature as Graphical Lasso or GLASSO estimator (see also Yuan and Lin 2007; Friedman, Hastie, and Tibshirani 2008; Rothman et al. 2008). On the other hand, Fan, Feng, and Wu (2009) proposed to employ adaptive ℓ_1 norm and SCAD (Smoothly Clipped Absolute Deviation) penalties to reduce the bias of the GLASSO estimator. van Wieringen and Peeters (2016) proposed the estimation of the precision matrix through ℓ_2 norm penalized log-likelihood maximization. Finally, Avagyan, Alonso, and Nogales (2017) proposed to improve the performance of the GLASSO estimator through k -root transformation of the sample covariance matrix.

Several authors studied non-likelihood based approaches for estimating either the precision matrix or the GGM. Meinshausen and Bühlmann (2006) introduced the Neighborhood Selection approach to estimate the GGM. Yuan (2010) proposed a similar approach to estimate each column of the precision matrix by using a Dantzig selector. Cai, Liu, and Luo (2011) proposed the constrained ℓ_1 norm minimization estimator known as CLIME. Zhang and Zou (2014) proposed a precision estimation method through ℓ_1 norm penalized D-trace loss minimization (hereafter, DT estimator) and Avagyan, Alonso, and Nogales (2016) proposed DT estimator using adaptive ℓ_1 norm penalization.

In this article, we focus on the DT estimator. As mentioned earlier, the ℓ_1 regularization induces sparsity in the estimated precision matrix. However, this framework does not control the eigenvalues of the estimated matrix. Moreover, as the penalty parameter increases (i.e., the matrix becomes sparser), the largest eigenvalues of the estimator decrease considerably and the smallest eigenvalues increase insignificantly. As a result, the eigenspectrum of the estimator shrinks. Therefore, it would be natural to expect that by controlling the eigenvalues of the estimated precision matrix through an additional constraint we may potentially improve the performance of the estimated matrix. Moreover, in practice, one may require the estimated precision matrix to have proper determinant, condition number or trace.

We propose an extension of DT estimator with an eigenvalue constraint. We employ an additional regularization of the objective function of the DT estimator through negative trace penalization. This penalty sustains the stability of the eigenvalues and diminishes the significant decrease of the largest eigenvalues. Thus, the estimator becomes sparse without having to shrink its eigenspectrum significantly. Through extensive simulation study, we show that the proposed methodology outperforms the DT in terms of several measures. Further, we propose a new penalty parameter selection procedure

based on Hannan-Quinn Information Criterion (HQIC). In the simulation study, we employ BIC and HQIC approaches to select the penalty parameters.

The rest of the manuscript is organized as follows. In Sec. 2, we describe the proposed methodology. In Sec. 3, we describe the penalty parameter selection process. In Sec. 4, we exhaustively evaluate the statistical loss and GGM prediction performance of the proposed methodology and compare them with that of DT and GLASSO methods. In Sec. 5, we apply the proposed methodology to an empirical application: prediction of breast cancer state using Linear Discriminant Analysis. Finally, we provide the conclusions in Sec. 6.

2. Proposed methodology

Before proceeding with the proposed methodology, we introduce the following notations. For any vector $\mathbf{a} = (a_1, \dots, a_p)^T \in \mathbb{R}^p$, we define the ℓ_2 norm by $\|\mathbf{a}\|_2 = \sqrt{\sum_{j=1}^p a_j^2}$. For any symmetric matrix $\mathbf{A} = [a_{ij}]_{1 \leq i,j \leq p}$, we denote the Frobenius norm by $\|\mathbf{A}\|_2 = \sqrt{\sum_{i=1}^p \sum_{j=1}^p a_{ij}^2}$, the ℓ_∞ norm by $\|\mathbf{A}\|_\infty = \max_{1 \leq i,j \leq p} |a_{ij}|$, the matrix ℓ_1 norm by $\|\mathbf{A}\|_{\ell_1} = \max_{1 \leq j \leq p} \sum_{i=1}^p |a_{ij}|$, the componentwise ℓ_1 norm by $\|\mathbf{A}\|_1 = \sum_{i=1}^p \sum_{j=1}^p |a_{ij}|$, and the spectral norm by $\|\mathbf{A}\|_{sp} = \sup_{\|\mathbf{x}\|_2 \leq 1} \|\mathbf{A}\mathbf{x}\|_2$. For any two symmetric $p \times p$ matrices A and B , we write $A \geq B$ if the matrix $A - B$ is positive semidefinite.

Zhang and Zou (2014) have proposed the D-trace loss function, defined as:

$$f_{DT}(\Omega, \Sigma) = \frac{1}{2} \text{trace}(\Omega^2 \Sigma) - \text{trace}(\Omega). \quad (1)$$

By regularizing the $f_{DT}(\Omega, \Sigma)$ function through a ℓ_1 norm of Ω , Zhang and Zou (2014) proposed the ℓ_1 penalized D-trace loss minimization estimator or DT. This estimator is defined as the solution of the following optimization problem:

$$\hat{\Omega}_{DT} = \arg \min_{\Omega \geq \epsilon I} \frac{1}{2} \text{trace}(\Omega^2 S) - \text{trace}(\Omega) + \tau \|\Omega\|_1, \quad (2)$$

where $S = (1/n) \sum_{i=1}^n X_i X_i^T$ is the sample covariance matrix, $\tau > 0$ is the associated penalty parameter and ϵ is a small positive value (we fix $\epsilon = 10^{-8}$). The constraint $\Omega \geq \epsilon I$ guarantees the positive definiteness of the matrix $\hat{\Omega}_{DT}$. In this article, we also penalize the diagonal entries of Ω . To solve the problem (2), Zhang and Zou (2014) developed an algorithm based on the Alternating Direction Method.

As discussed in Sec. 1, this article addresses the eigenvalue control of DT estimator. The ℓ_1 norm penalization guarantees the sparsity of the estimated precision matrix for a well-selected parameter τ . However, as τ increases (i.e., $\hat{\Omega}_{DT}$ becomes sparser), the eigenspectrum of the estimated matrix shrinks, i.e., the largest eigenvalues decrease significantly and the smallest eigenvalues increase insignificantly.

In order to illustrate the shrinkage of the eigenvalues, we consider a simple example. Assume that the true precision matrix has a known sparse structure given by *Model 2* described in Sec. 4.1. We set the values $p = 100$ and $n = 100$. Figure 1(a) shows the eigenvalues of DT estimator for different values of τ . Note that, as the parameter τ increases (i.e., the matrix becomes sparser), the largest eigenvalues of the DT estimator decrease significantly towards a constant. As a result, the trace of the matrix decreases significantly due to ℓ_1 norm penalization (see Figure 1(b)).

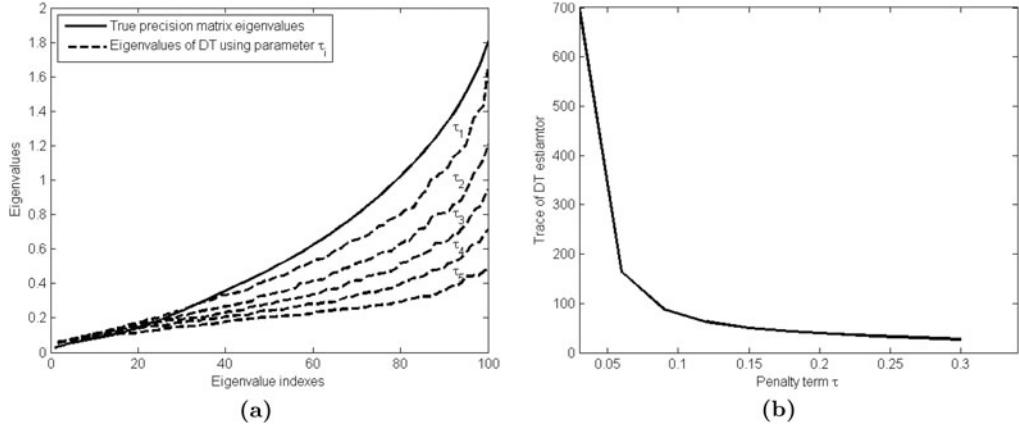


Figure 1. (a) Eigenvalues of DT estimator for different penalty parameters, where $\tau_1 < \dots < \tau_5$, (b) Trace of DT estimator for $\tau \in [0.03; 0.3]$.

In order to control the eigenspectrum of the estimator $\hat{\Omega}_{DT}$, an additional constraint is required (see Liu, Wang, and Zhao 2014, for covariance matrix estimation). We note that the decrement of the largest eigenvalues of the estimated matrix is associated with the decrease of its trace. We propose to impose an additional penalization in the problem (2) through a negative trace of Ω . In this way, we propose the DT estimator with Eigenvalue Control (or shortly, DTEC). Our proposed estimator is the solution of the following optimization problem.

$$\hat{\Omega}_{DTEC} = \arg \min_{\Omega \geq I} \frac{1}{2} \text{trace}(\Omega^2 S) - \text{trace}(\Omega) + \tau \|\Omega\|_1 - \gamma \text{trace}(\Omega), \quad (3)$$

where $\tau > 0$ and $\gamma > 0$ are penalty parameters. More specifically, the additional penalty term $-\gamma \text{trace}(\Omega)$ in problem (3) endorses the trace (and, therefore, the largest eigenvalues) of the estimated precision matrix not to decrease significantly. Thus, the eigenvalues (especially the largest ones) of the matrix $\hat{\Omega}_{DTEC}$ will be closer to the true ones, than those of the matrix $\hat{\Omega}_{DT}$. Even though in practice the true eigenvalues are unknown, the estimated precision matrix will have more proper eigenspectrum (or condition number, determinant, etc.) if we employ an additional constraint. This in turn will lead to better performance of the estimated precision matrix. Note that a similar approach (although with a different reasoning) has been considered to improve GLASSO estimator (Maurya 2014). In this context, the results indicated that the joint penalization provides better results than standard GLASSO estimator.

Furthermore, we can write our proposed estimator as the solution of the following optimization problem:

$$\hat{\Omega}_{DTEC} = \arg \min_{\Omega \geq I} \frac{1}{2} \text{trace}(\Omega^2 S) - (1 + \gamma) \text{trace}(\Omega) + \tau \|\Omega\|_1. \quad (4)$$

Note that we can solve the problem (4) using the same algorithm as for the problem (2), with minor modifications. We illustrate the performance of the proposed methodology on a particular example. Assume that the true precision matrix has the structure used above. In Figure 2, we present the eigenvalues of true matrix Ω and the eigenvalues of the estimators DT and DTEC. Figure 2(a) illustrates the eigenvalues of

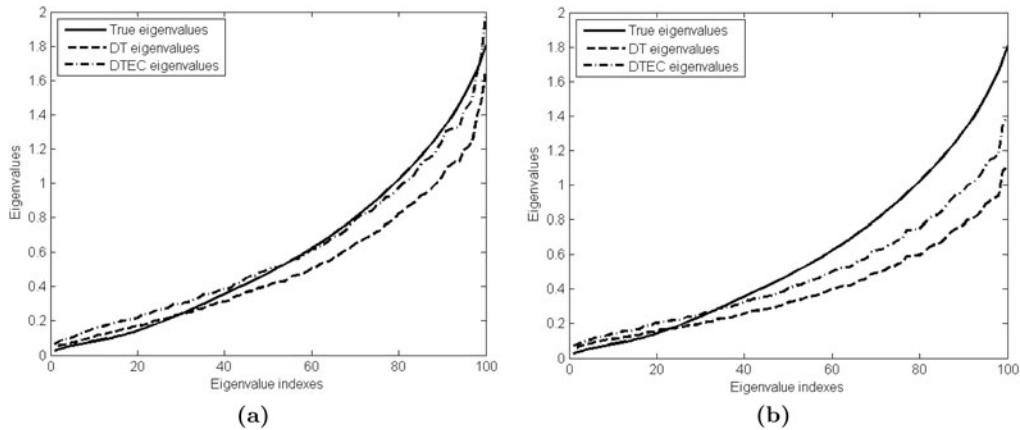


Figure 2. Eigenvalues of the true precision matrix and estimators DT, DTEC obtained through (a) optimal penalty parameters, (b) BIC selection approach.

the optimal (i.e., oracle) estimators in terms of the Frobenius norm loss (see Sec. 4.2 for a formal definition). In other words, DT and DTEC estimators are obtained using the penalty parameters that minimize the Frobenius norm loss assuming that Ω is known. Figure 2(b) shows the eigenvalues of DT and DTEC estimators obtained through BIC approach described in Sec. 3. From both figures we can see that the eigenvalues of DTEC estimator are larger than those of DT estimator. Moreover, the largest eigenvalues of DTEC estimator are much closer to the eigenvalues of Ω than those of DT. Therefore, the trace penalization diminishes the significant decrease of the largest eigenvalues of DT estimator.

In Sec. 4, through an exhaustive simulation study, we show that our proposed DTEC estimator outperforms the DT estimator in terms of several statistical performance measures including those for graphical models.

3. Penalty parameter selection

The performance of the estimated precision matrix greatly depends on the penalty parameter. Moreover, the penalty parameter controls the sparsity pattern of the estimated matrix. In this article, we suggest the use of a criterion based on the log-likelihood function of the Gaussian model. We define the score function as

$$SF(\tau) = -\log \det \hat{\Omega}(\tau) + \text{trace}\left(S\hat{\Omega}(\tau)\right) + k \times nz(\tau), \quad (5)$$

where $nz(\tau) = \text{card}\{(i,j) : 1 \leq i \leq j \leq p, [\hat{\Omega}(\tau)]_{ij} \neq 0\}$ and k is degrees of freedom. We select the parameter by $\hat{\tau} = \arg\min_{\tau} SF(\tau)$. The advantage of the suggested criterion is twofold. First, it is more effective than the techniques based on the cross-validation in terms of the computational time. Second, it accounts the sparsity characteristics of $\hat{\Omega}$. Further, we consider the following degrees of freedom:

$$k_{\text{BIC}} = \frac{\log n}{n}, \quad (6)$$

$$k_{HQIC} = \frac{2 \log \log n}{n}. \quad (7)$$

The choice k_{BIC} corresponds to the Bayesian Information Criterion (BIC) which is proposed by Yuan and Lin (2007) for precision matrix estimation methodologies. On the other hand, the choice k_{HQIC} corresponds to the Hannan-Quinn Information Criterion (HQIC) (Hannan and Quinn 1979), which is consistent and asymptotically well-behaved (van der Pas and Grünwald 2014). This is a novel criterion in this framework (to the best of our knowledge, it has not been employed for selecting the penalty terms of the precision matrix estimation methods) and a little attention has been paid to the HQIC, in general.

We note that our proposed methodology requires selection of two parameters, τ and γ . For this reason, we define the following multivariate score function to select these parameters simultaneously:

$$MSF(\tau, \gamma) = -\log \det \hat{\Omega}(\tau, \gamma) + \text{trace}\left(S\hat{\Omega}(\tau, \gamma)\right) + k \times nz(\tau), \quad (8)$$

where $\hat{\Omega}(\tau, \gamma)$ is the estimated precision matrix for given values τ and γ . We select the parameters $\hat{\tau}$ and $\hat{\gamma}$ by $(\hat{\tau}, \hat{\gamma}) = \operatorname{argmin}_{\tau, \gamma} MSF(\tau, \gamma)$.

4. Simulation study

In this section, we conduct a simulation analysis to evaluate the performance of our proposed methodology. In Sec. 4.1, we detail the considered models (i.e., patterns) for the true precision matrix Ω . In Sec. 4.2, we describe the performance evaluation. Finally, in subsection 4.3, we provide the discussion of the results.

4.1. Considered models

We perform a simulation study through six different patterns for the precision matrix with varying sizes. The considered models for the matrix Ω are the following:

- i. Deterministic patterns
- ii. *Model 1.* Tridiagonal design: $\omega_{ii} = 1$, $\omega_{i,i-1} = \omega_{i-1,i} = 0.45$ and others are 0.
- iii. *Model 2.* Tridiagonal design with varying entries: $\Omega = D^{1/2}\Omega_1D^{1/2}$, where D is a diagonal matrix with entries $D_{ii} = \frac{4i+p-5}{5(p-1)}$, $i = 1, \dots, p$ and Ω_1 is a matrix defined in the *Model 1*.
- iv. *Model 3.* Light-tailed (decaying) design: $\omega_{ij} = 0.6^{|i-j|}$.
- v. *Model 4.* A block-diagonal matrix, with four equally sized blocks along the diagonal, with a light-tailed model in each block.
- vi. Random patterns (generated using the MATLAB command *sprandsym*)
- vii. *Model 5.* A random p.d. matrix, with approximately 20% of non-zero entries.
- viii. *Model 6.* A random p.d. matrix, with approximately 50% of non-zero entries.

For each precision matrix model, we simulate multivariate normal random samples with zero mean. We set $n = 100$ and $p = 100, 200$ and 300 . The number of replications is 100.

4.2. Performance evaluation

To evaluate the performance of a precision matrix estimator, we use several losses and measures. In particular, we consider the Kullback–Leibler loss (KLL) and the Reverse Kullback–Leibler loss (RKLL), defined as

$$\text{KLL}(\hat{\Omega}, \Omega) = \text{trace}(\Omega^{-1}\hat{\Omega}) - \log \det(\Omega^{-1}\hat{\Omega}) - p, \quad (9)$$

$$\text{RKLL}(\hat{\Omega}, \Omega) = \text{trace}(\Omega\hat{\Omega}^{-1}) - \log \det(\Omega\hat{\Omega}^{-1}) - p, \quad (10)$$

respectively. We also consider matrix losses: the Frobenius norm, the spectral norm and the matrix ℓ_1 norm, defined respectively as

$$\ell_2(\hat{\Omega}, \Omega) = \|\hat{\Omega} - \Omega\|_2, \quad (11)$$

$$\ell_{\text{sp}}(\hat{\Omega}, \Omega) = \|\hat{\Omega} - \Omega\|_{\text{sp}}, \quad (12)$$

$$\ell_1(\hat{\Omega}, \Omega) = \|\hat{\Omega} - \Omega\|_{\ell_1}. \quad (13)$$

In order to evaluate the sparsity pattern of the precision matrix estimator (i.e., GGM selection performance), we compute Specificity, Sensitivity, Matthews Correlation Coefficient (Matthews 1975) and F_1 score (Powers 2011), defined as

$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}}, \quad (14)$$

$$\text{Sensitivity} = \frac{\text{TP}}{\text{TP} + \text{FN}}, \quad (15)$$

$$\text{MCC} = \frac{\text{TP} \times \text{TN} - \text{FP} \times \text{FN}}{\sqrt{(\text{TP} + \text{FP})(\text{TP} + \text{FN})(\text{TN} + \text{FP})(\text{TN} + \text{FN})}}, \quad (16)$$

$$F_1 = 2 \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}, \quad (17)$$

where TP, TN, FP and FN are the number of correctly estimated non-zero entries (true positives), the number of correctly estimated zero entries (true negatives), the number of incorrectly estimated non-zero entries (false positives) and the number of incorrectly estimated zero entries (false negatives), respectively. In (17), we define Precision = TP/(TP + FP) and Recall = TP/(TP + FN). The values of MCC are in [-1,1], and the closer the MCC to one is, the better the classification is. On the other hand, the values of F_1 score are in [0,1], and the closer the F_1 to one is, the better the classification is. It is worth to note that both MCC and F_1 are commonly used to evaluate the performance of binary classifiers (in our context, we consider these measures for the overall evaluation of the GGM selection). However, we put MCC above F_1 score, because MCC takes into account all four classification categories (thus, it is more informative), whereas F_1 score highly depends on the specification of positive categories (Chicco 2017).

We compare our proposed estimator with DT and GLASSO. We select the penalty parameters of these methods using univariate BIC and HQIC criteria. On the other hand, the parameters τ and γ of the proposed estimator DTEC are selected using multivariate BIC and HQIC criteria. Moreover, since the trace of the estimated matrix decreases when τ increases, we consider $\gamma = \tau$ in the proposed problem (3) as a naive case. We call the obtained estimator simplified DTEC or SDTEC, which is defined as

the solution of the following optimization problem:

$$\hat{\Omega}_{\text{SDTEC}} = \arg \min_{\Omega \geq I} \frac{1}{2} \text{trace}(\Omega^2 S) - (1 + \tau) \text{trace}(\Omega) + \tau \|\Omega\|_1. \quad (18)$$

In this way, we can calibrate only one parameter instead of two, which leads to saving the computational time.

4.3. Discussion of results

Tables 1–6 summarize the simulation results. Each table reports the averages over 100 replications and the standard deviations of the corresponding measures. We organize the discussion of our results as follows. First, we compare our proposed estimator DTEC with DT and GLASSO estimators when the penalty parameters are selected using the BIC approach. Next, we discuss the same comparison when the parameters are selected using the HQIC approach. Finally, we compare BIC and HQIC approaches through the corresponding measures.

First, we observe that when the parameters are selected through BIC approach, the estimator DTEC outperforms DT in terms of all statistical losses for almost all the models (except of model 3, in terms of KLL). The estimator DTEC outperforms DT for models 2, 4, 5, 6 in terms of MCC, for model 2 in terms of F_1 . On the other hand, DT outperforms DTEC for model 1 in terms of MCC, for models 1, 3, 4, 5, 6 in terms of F_1 . Furthermore, we observe that GLASSO provides high statistical losses and low GGM prediction measures.

Second, the results show that when the parameters are selected through HQIC approach, the estimator DTEC outperforms DT in terms of all statistical losses for almost all the models (except of model 2, in terms of KLL). On the other hand, DTEC outperforms DT for models 1, 2, 4, 5 in terms of MCC, for models 1, 2 in terms of F_1 . DT method outperforms DTEC for models 3, 4, 5 in terms of F_1 . Furthermore, we observe that GLASSO outperforms all the other estimators for model 6 in terms of F_1 . However, for the other models GLASSO provides poor results.

Finally, we conduct a comparison BIC and HQIC based on the corresponding losses and measures. We observe, that BIC provides higher statistical losses, whereas HQIC provides lower statistical losses for all considered approaches (including DT and GLASSO methods). Moreover, estimators obtained through BIC provide higher MCC than those for HQIC, and higher F_1 for models 1, 2. Estimators obtained through HQIC provide higher F_1 for models 3, 4, 5, 6 than those for BIC.

In sum, the proposed DTEC estimation method provides better performance than DT and GLASSO methods for most of the models in terms of several statistical losses and GGM prediction measures. Moreover, we observe that this conclusion holds if we consider the simplified SDTEC method (i.e., when $\gamma = \tau$), since it performs as good as DTEC estimator. This finding leads to saving significantly the computational time without sacrificing too much the performance.

Table 1. Average measures (with standard deviations) over 100 replications for Model 1.

p		BIC			HQIC			GLASSO
		DT	DTEC	SDTEC	DT	DTEC	SDTEC	
KL	100	10.68 (0.61)	10.82 (1.03)	10.67 (1.24)	18.95 (1.38)	8.94 (0.62)	9.43 (0.68)	14.14 (1.11)
	200	31.07 (1.15)	24.92 (1.22)	25.05 (1.19)	49.43 (1.90)	23.23 (0.88)	22.76 (1.05)	39.96 (3.29)
RKLL	100	46.62 (1.14)	38.66 (1.53)	38.12 (1.28)	81.80 (4.85)	35.41 (1.05)	35.66 (1.25)	68.39 (4.64)
	200	13.32 (0.87)	9.18 (0.69)	8.84 (1.23)	31.91 (2.92)	10.28 (0.88)	7.55 (0.48)	21.58 (2.30)
ℓ_1	100	43.52 (1.90)	20.54 (1.35)	21.09 (0.99)	90.22 (4.41)	29.11 (1.28)	17.49 (1.10)	67.97 (7.58)
	200	64.93 (2.07)	33.28 (2.89)	31.64 (1.02)	154.36 (12.41)	43.36 (1.43)	29.10 (1.68)	121.38 (11.46)
ℓ_2	100	4.77 (0.13)	3.64 (0.24)	3.51 (0.31)	6.76 (0.18)	4.19 (0.17)	3.22 (0.23)	5.90 (0.25)
	200	8.21 (0.13)	5.40 (0.28)	5.54 (0.15)	10.52 (0.14)	6.99 (0.13)	4.76 (0.29)	9.70 (0.33)
ℓ_{sp}	100	10.03 (0.11)	6.98 (0.42)	6.74 (0.13)	13.31 (0.27)	8.49 (0.12)	6.38 (0.32)	12.49 (0.31)
	200	1.18 (0.04)	1.03 (0.06)	1.02 (0.06)	1.40 (0.03)	1.15 (0.06)	0.99 (0.07)	1.39 (0.04)
Sens	100	1.30 (0.03)	1.08 (0.05)	1.09 (0.05)	1.46 (0.02)	1.24 (0.05)	1.04 (0.06)	1.07 (0.06)
	200	1.30 (0.03)	1.11 (0.05)	1.10 (0.04)	1.49 (0.02)	1.27 (0.04)	1.10 (0.05)	1.15 (0.03)
Spec	100	0.98 (0.03)	0.82 (0.05)	0.80 (0.05)	1.21 (0.02)	0.89 (0.04)	0.75 (0.05)	1.10 (0.03)
	200	1.13 (0.02)	0.87 (0.04)	0.88 (0.03)	1.30 (0.01)	1.02 (0.03)	0.81 (0.04)	1.23 (0.03)
F_1	100	1.13 (0.02)	0.91 (0.04)	0.89 (0.03)	1.34 (0.02)	1.03 (0.02)	0.87 (0.04)	0.86 (0.03)
	200	1 (0)	1 (0)	1 (0)	1 (0)	1 (0)	1 (0)	1 (0)
MCC	100	0.971 (0.002)	0.981 (0.005)	0.977 (0.009)	0.945 (0.009)	0.944 (0.006)	0.964 (0.006)	0.963 (0.002)
	200	0.995 (0.0005)	0.992 (0.001)	0.992 (0.0006)	0.978 (0.003)	0.981 (0.001)	0.984 (0.003)	0.987 (0.0006)
	300	0.995 (0.0003)	0.993 (0.001)	0.993 (0.0003)	0.987 (0.003)	0.982 (0.0007)	0.988 (0.001)	0.987 (0.0006)
	100	0.710 (0.016)	0.787 (0.047)	0.764 (0.080)	0.585 (0.035)	0.581 (0.031)	0.669 (0.033)	0.665 (0.015)
	200	0.871 (0.012)	0.795 (0.023)	0.818 (0.012)	0.640 (0.026)	0.667 (0.012)	0.697 (0.035)	0.734 (0.013)
	300	0.834 (0.009)	0.787 (0.030)	0.767 (0.009)	0.664 (0.042)	0.595 (0.008)	0.679 (0.025)	0.669 (0.008)
	100	0.683 (0.019)	0.772 (0.054)	0.745 (0.091)	0.532 (0.043)	0.527 (0.038)	0.634 (0.041)	0.629 (0.018)
	200	0.865 (0.013)	0.795 (0.027)	0.805 (0.014)	0.590 (0.033)	0.624 (0.014)	0.661 (0.043)	0.706 (0.015)
	300	0.823 (0.010)	0.767 (0.036)	0.745 (0.010)	0.617 (0.053)	0.530 (0.010)	0.636 (0.032)	0.623 (0.011)

Table 2. Average measures (with standard deviations) over 100 replications for Model 2.

	p	BIC			HQIC			GLASSO
		DT	DTEC	SDTEC	DT	DTEC	SDTEC	
KL	100	11.59 (0.56)	11.34 (0.82)	11.26 (0.72)	20.72 (1.58)	9.47 (0.87)	10.12 (0.80)	15.42 (1.22)
	200	30.95 (1.20)	27.00 (1.34)	27.62 (1.18)	56.26 (1.40)	23.57 (0.84)	23.80 (1.11)	43.11 (3.37)
RKLL	300	46.77 (1.07)	42.42 (1.44)	42.30 (1.42)	95.97 (2.85)	36.36 (2.39)	37.62 (2.10)	75.74 (4.01)
	100	14.80 (0.80)	9.46 (1.02)	9.36 (0.55)	37.27 (3.83)	10.77 (1.51)	8.06 (0.74)	24.48 (2.81)
ℓ_1	200	43.04 (2.09)	22.00 (1.69)	23.50 (1.13)	113.36 (3.82)	28.90 (1.21)	18.60 (1.09)	77.13 (9.03)
	300	64.52 (1.85)	35.95 (1.57)	35.61 (1.04)	204.31 (8.71)	43.31 (4.54)	31.38 (1.85)	143.87 (11.53)
ℓ_2	100	3.21 (0.09)	2.36 (0.21)	2.36 (0.10)	4.83 (0.12)	2.71 (0.19)	2.09 (0.17)	4.25 (0.16)
	200	5.24 (0.11)	3.57 (0.21)	3.76 (0.13)	7.53 (0.05)	4.43 (0.11)	3.18 (0.18)	3.26 (0.11)
ℓ_{sp}	300	6.41 (0.08)	4.65 (0.14)	4.62 (0.09)	9.56 (0.08)	5.36 (0.24)	4.28 (0.23)	8.85 (0.15)
	100	1.04 (0.06)	0.86 (0.08)	0.86 (0.07)	1.44 (0.03)	0.99 (0.08)	0.84 (0.09)	1.36 (0.04)
Sens	200	1.17 (0.05)	0.95 (0.07)	0.98 (0.06)	1.54 (0.01)	1.09 (0.08)	0.90 (0.09)	1.46 (0.03)
	300	1.18 (0.05)	0.99 (0.06)	0.99 (0.06)	1.57 (0.01)	1.12 (0.06)	0.97 (0.07)	1.51 (0.02)
Spec	100	0.88 (0.05)	0.70 (0.07)	0.70 (0.06)	1.32 (0.03)	0.78 (0.07)	0.64 (0.07)	1.20 (0.04)
	200	1.02 (0.05)	0.77 (0.06)	0.80 (0.05)	1.46 (0.01)	0.89 (0.06)	0.70 (0.07)	1.36 (0.03)
F_1	300	1.02 (0.04)	0.81 (0.04)	0.81 (0.04)	1.51 (0.01)	0.90 (0.05)	0.77 (0.06)	1.43 (0.02)
	100	1 (0)	1 (0)	1 (0)	0.996 (0.004)	1 (0)	1 (0)	0.999 (0.001)
MCC	200	1 (0)	1 (0)	1 (0)	0.990 (0.005)	1 (0)	1 (0)	0.998 (0.001)
	300	1 (0)	1 (0)	1 (0)	0.979 (0.007)	1 (0)	1 (0)	0.996 (0.003)

Table 3. Average measures (with standard deviations) over 100 replications for Model 3.

p	BIC			HQIC				
	DT	DTEC	SDTEC	GLASSO	DT	DTEC	SDTEC	GLASSO
KLL	15.75 (0.51)	15.36 (1.04)	15.38 (1.21)	22.98 (0.72)	13.74 (0.41)	14.19 (0.69)	14.17 (0.68)	20.78 (0.68)
	34.09 (0.73)	33.40 (1.06)	33.41 (0.99)	50.60 (1.09)	33.30 (2.05)	30.52 (1.14)	30.36 (1.13)	46.51 (1.63)
	51.30 (1.43)	51.72 (1.32)	50.76 (1.08)	81.73 (1.97)	51.13 (0.92)	50.57 (1.13)	50.20 (1.42)	75.77 (2.78)
RKLL	36.58 (1.75)	27.02 (1.87)	27.02 (3.49)	64.83 (3.02)	28.74 (1.23)	22.43 (2.12)	23.20 (2.28)	55.48 (2.78)
	82.40 (2.42)	60.70 (3.75)	61.39 (1.90)	150.16 (4.85)	78.86 (8.90)	52.59 (3.11)	49.66 (3.62)	131.92 (7.13)
	122.81 (5.61)	100.01 (6.10)	91.82 (2.17)	252.30 (9.36)	122.47 (3.12)	84.75 (4.95)	91.86 (2.36)	224.33 (2.05)
ℓ_2	10.34 (0.08)	9.63 (0.28)	9.65 (0.15)	11.41 (0.06)	9.84 (0.09)	9.20 (0.25)	9.29 (0.29)	11.14 (0.07)
	14.99 (0.07)	14.04 (0.20)	14.08 (0.08)	16.51 (0.06)	14.84 (0.38)	13.59 (0.21)	13.38 (0.22)	16.21 (0.11)
	18.35 (0.12)	17.57 (0.24)	17.24 (0.08)	20.53 (0.10)	18.34 (0.08)	16.89 (0.24)	17.24 (0.09)	20.23 (0.02)
ℓ_1	3.48 (0.04)	3.37 (0.05)	3.36 (0.05)	3.58 (0.02)	3.42 (0.04)	3.31 (0.05)	3.32 (0.05)	3.59 (0.03)
	200	3.54 (0.03)	3.43 (0.04)	3.44 (0.04)	3.64 (0.02)	3.53 (0.03)	3.41 (0.04)	3.40 (0.04)
	300	3.56 (0.03)	3.48 (0.03)	3.46 (0.03)	3.65 (0.01)	3.56 (0.03)	3.44 (0.03)	3.46 (0.03)
ℓ_{sp}	100	3.22 (0.02)	3.07 (0.04)	3.06 (0.06)	3.44 (0.01)	3.11 (0.02)	2.96 (0.06)	3.38 (0.01)
	200	3.29 (0.01)	3.14 (0.03)	3.15 (0.02)	3.49 (0.01)	3.26 (0.06)	3.07 (0.03)	3.45 (0.01)
	300	3.29 (0.02)	3.19 (0.03)	3.15 (0.02)	3.53 (0.01)	3.29 (0.01)	3.10 (0.02)	3.35 (0.03)
Sens	100	0.047 (0.001)	0.043 (0.005)	0.045 (0.008)	0.046 (0.003)	0.070 (0.002)	0.060 (0.012)	0.059 (0.015)
	200	0.025 (0.007)	0.021 (0.001)	0.021 (0.006)	0.022 (0.001)	0.029 (0.009)	0.032 (0.004)	0.035 (0.005)
	300	0.020 (0.001)	0.014 (0.001)	0.016 (0.004)	0.012 (0.001)	0.020 (0.005)	0.018 (0.002)	0.016 (0.004)
Spec	100	NA (NA)						
	200	NA (NA)						
	300	NA (NA)						
MCC	100	NA (NA)						
	200	NA (NA)						
	300	NA (NA)						
F_1	100	0.090 (0.003)	0.083 (0.009)	0.086 (0.015)	0.088 (0.006)	0.131 (0.004)	0.113 (0.021)	0.111 (0.026)
	200	0.049 (0.001)	0.042 (0.002)	0.041 (0.001)	0.043 (0.003)	0.056 (0.018)	0.062 (0.008)	0.069 (0.009)
	300	0.039 (0.002)	0.029 (0.002)	0.032 (0.007)	0.025 (0.002)	0.039 (0.001)	0.036 (0.003)	0.032 (0.008)

Spec and MCC are excluded for model 3, because these measurements are not defined for dense models.

Table 4. Average measures (with standard deviations) over 100 replications for Model 4.

p		BIC			HQIC			GLASSO	GLASSO
		D _T	DTEC	SDTEC	D _T	DTEC	SDTEC		
KL	100	16.30 (0.87)	14.95 (0.89)	15.04 (1.11)	22.60 (0.70)	13.34 (0.43)	13.76 (0.66)	13.81 (0.57)	20.30 (0.74)
	200	33.45 (0.70)	32.81 (0.81)	32.81 (0.77)	50.07 (0.33)	33.13 (1.58)	29.90 (1.00)	29.99 (1.28)	45.91 (1.17)
RKLL	300	50.87 (2.20)	50.87 (1.39)	49.88 (1.07)	80.98 (2.57)	50.40 (0.82)	49.56 (1.10)	49.77 (1.15)	75.33 (0.94)
	100	38.63 (3.35)	25.97 (1.98)	26.27 (3.16)	62.60 (2.81)	27.41 (1.23)	21.54 (1.86)	22.44 (1.77)	53.10 (2.97)
ℓ_1	200	79.96 (2.53)	59.01 (3.29)	59.50 (1.85)	147.07 (1.35)	78.35 (7.20)	51.97 (2.60)	48.86 (4.40)	128.79 (5.14)
	300	121.68 (8.59)	97.93 (5.57)	90.04 (2.26)	247.89 (1.87)	119.69 (2.68)	82.66 (4.39)	89.30 (3.37)	221.61 (4.06)
ℓ_2	100	10.24 (0.19)	9.37 (0.17)	9.38 (0.26)	11.15 (0.06)	9.55 (0.09)	8.93 (0.23)	9.04 (0.23)	10.86 (0.09)
	200	14.77 (0.08)	13.81 (0.18)	13.85 (0.09)	16.32 (0.01)	14.70 (0.33)	13.44 (0.19)	13.19 (0.27)	16.01 (0.08)
ℓ_{sp}	300	18.20 (0.19)	17.39 (0.22)	17.06 (0.09)	20.37 (0.13)	18.16 (0.08)	16.69 (0.22)	17.03 (0.17)	20.08 (0.05)
	100	3.47 (0.04)	3.33 (0.05)	3.33 (0.06)	3.56 (0.02)	3.39 (0.04)	3.27 (0.06)	3.29 (0.05)	3.56 (0.03)
Sens	200	3.53 (0.02)	3.43 (0.03)	3.43 (0.03)	3.62 (0.01)	3.53 (0.03)	3.41 (0.05)	3.39 (0.05)	3.63 (0.02)
	300	3.56 (0.03)	3.48 (0.03)	3.45 (0.04)	3.65 (0.01)	3.56 (0.03)	3.43 (0.04)	3.46 (0.04)	3.66 (0.02)
MCC	100	3.14 (0.04)	2.95 (0.04)	2.95 (0.06)	3.29 (0.01)	3.00 (0.03)	2.85 (0.06)	2.88 (0.06)	3.24 (0.02)
	200	3.25 (0.01)	3.11 (0.03)	3.11 (0.02)	3.45 (0.005)	3.24 (0.05)	3.05 (0.03)	3.01 (0.05)	3.41 (0.01)
Spec	300	3.28 (0.02)	3.18 (0.03)	3.13 (0.02)	3.51 (0.01)	3.27 (0.02)	3.08 (0.04)	3.13 (0.03)	3.48 (0.008)
	100	0.132 (0.009)	0.133 (0.009)	0.134 (0.012)	0.130 (0.005)	0.170 (0.006)	0.155 (0.014)	0.151 (0.015)	0.150 (0.009)
F ₁	200	0.070 (0.001)	0.066 (0.001)	0.066 (0.001)	0.064 (0.001)	0.073 (0.009)	0.079 (0.005)	0.083 (0.007)	0.075 (0.003)
	300	0.050 (0.002)	0.044 (0.001)	0.046 (0.007)	0.040 (0.001)	0.051 (0.001)	0.049 (0.002)	0.047 (0.003)	0.045 (0.005)
	100	0.988 (0.005)	0.987 (0.004)	0.987 (0.007)	0.982 (0.003)	0.962 (0.003)	0.973 (0.010)	0.976 (0.011)	0.960 (0.008)
	200	0.990 (0.0007)	0.993 (0.001)	0.993 (0.0006)	0.992 (0.001)	0.988 (0.008)	0.984 (0.003)	0.981 (0.005)	0.981 (0.003)
	300	0.990 (0.001)	0.995 (0.0009)	0.993 (0.0004)	0.996 (0.001)	0.990 (0.001)	0.992 (0.002)	0.993 (0.002)	0.991 (0.001)
	100	0.262 (0.011)	0.261 (0.012)	0.262 (0.012)	0.234 (0.011)	0.224 (0.011)	0.237 (0.016)	0.240 (0.015)	0.194 (0.016)
	200	0.168 (0.005)	0.178 (0.005)	0.179 (0.004)	0.167 (0.005)	0.164 (0.013)	0.155 (0.008)	0.150 (0.013)	0.140 (0.009)
	300	0.126 (0.007)	0.143 (0.005)	0.137 (0.003)	0.142 (0.006)	0.125 (0.004)	0.130 (0.006)	0.136 (0.005)	0.124 (0.004)
	100	0.227 (0.011)	0.229 (0.015)	0.228 (0.011)	0.220 (0.006)	0.265 (0.008)	0.251 (0.014)	0.246 (0.014)	0.237 (0.009)
	200	0.128 (0.002)	0.122 (0.002)	0.121 (0.002)	0.119 (0.002)	0.132 (0.012)	0.139 (0.007)	0.145 (0.010)	0.133 (0.005)
	300	0.093 (0.003)	0.084 (0.002)	0.087 (0.001)	0.077 (0.002)	0.094 (0.002)	0.091 (0.003)	0.088 (0.004)	0.085 (0.002)

Table 5. Average measures (with standard deviations) over 100 replications for Model 5.

p		BIC			HQIC			GLASSO
		DT	DTEC	SDTEC	DT	DTEC	SDTEC	
KL	100	13.31 (0.57)	12.24 (0.89)	12.31 (0.85)	23.60 (1.46)	10.85 (0.50)	10.74 (0.68)	18.88 (1.18)
	200	37.39 (2.16)	33.20 (1.48)	33.40 (1.63)	61.96 (2.50)	31.80 (1.57)	29.98 (0.91)	52.96 (2.65)
RKLL	300	60.49 (0.88)	55.62 (1.65)	55.45 (1.63)	98.60 (3.20)	52.01 (0.88)	51.28 (1.23)	88.28 (2.93)
	100	27.05 (1.96)	18.62 (2.24)	18.55 (2.18)	59.02 (5.66)	18.63 (1.36)	13.55 (1.25)	40.76 (4.44)
ℓ_1	200	84.32 (7.61)	52.24 (3.82)	52.55 (4.21)	175.09 (11.44)	64.22 (6.25)	41.93 (2.78)	135.28 (11.54)
	300	157.43 (4.16)	105.24 (6.54)	104.93 (5.40)	301.02 (15.68)	120.35 (3.04)	87.20 (5.30)	251.68 (13.73)
ℓ_2	100	1.83 (0.04)	1.58 (0.06)	1.58 (0.06)	2.65 (0.05)	1.63 (0.05)	1.44 (0.06)	2.44 (0.07)
	200	2.94 (0.08)	2.54 (0.06)	2.54 (0.07)	3.97 (0.04)	2.70 (0.09)	2.37 (0.07)	3.79 (0.07)
ℓ_{sp}	300	3.74 (0.04)	3.39 (0.07)	3.39 (0.07)	4.94 (0.04)	3.53 (0.13)	3.31 (0.15)	4.79 (0.05)
	100	1.25 (0.03)	1.21 (0.05)	1.21 (0.05)	1.47 (0.02)	1.20 (0.04)	1.15 (0.05)	1.42 (0.02)
Sens	200	1.63 (0.05)	1.56 (0.05)	1.56 (0.05)	1.74 (0.05)	1.57 (0.07)	1.50 (0.06)	1.72 (0.01)
	100	1.84 (0.08)	1.78 (0.14)	1.78 (0.14)	2.05 (0.01)	1.83 (0.46)	1.77 (0.39)	2.04 (0.01)
Spec	200	0.76 (0.02)	0.73 (0.03)	0.73 (0.03)	0.84 (0.01)	0.72 (0.03)	0.68 (0.03)	0.80 (0.01)
	100	0.90 (0.01)	0.87 (0.02)	0.87 (0.02)	0.92 (0.00)	0.87 (0.02)	0.84 (0.02)	0.90 (0.01)
MCC	200	0.85 (0.06)	0.83 (0.13)	0.83 (0.12)	0.89 (0.01)	0.87 (0.24)	0.86 (0.25)	0.88 (0.01)
	100	0.144 (0.006)	0.131 (0.01)	0.131 (0.01)	0.156 (0.015)	0.183 (0.01)	0.167 (0.014)	0.212 (0.020)
F ₁	200	0.068 (0.007)	0.062 (0.005)	0.062 (0.006)	0.065 (0.005)	0.088 (0.010)	0.082 (0.005)	0.091 (0.011)
	300	0.043 (0.001)	0.037 (0.002)	0.037 (0.002)	0.046 (0.003)	0.059 (0.002)	0.049 (0.003)	0.048 (0.002)
Spec	200	0.980 (0.002)	0.986 (0.005)	0.987 (0.005)	0.957 (0.009)	0.954 (0.007)	0.966 (0.008)	0.965 (0.007)
	100	0.991 (0.004)	0.994 (0.002)	0.994 (0.002)	0.982 (0.004)	0.979 (0.008)	0.983 (0.003)	0.962 (0.009)
MCC	200	0.992 (0.0005)	0.995 (0.0009)	0.995 (0.0008)	0.989 (0.002)	0.981 (0.001)	0.989 (0.002)	0.989 (0.004)
	100	0.240 (0.011)	0.249 (0.012)	0.249 (0.013)	0.184 (0.013)	0.210 (0.014)	0.222 (0.014)	0.156 (0.015)
F ₁	200	0.165 (0.008)	0.170 (0.006)	0.170 (0.007)	0.116 (0.009)	0.148 (0.011)	0.153 (0.008)	0.098 (0.009)
	300	0.114 (0.004)	0.121 (0.004)	0.120 (0.004)	0.105 (0.005)	0.099 (0.005)	0.109 (0.005)	0.095 (0.005)
Spec	200	0.235 (0.008)	0.221 (0.013)	0.220 (0.013)	0.234 (0.014)	0.267 (0.011)	0.254 (0.013)	0.268 (0.012)
	100	0.123 (0.010)	0.115 (0.008)	0.114 (0.009)	0.115 (0.011)	0.143 (0.008)	0.142 (0.006)	0.145 (0.012)
MCC	200	0.080 (0.002)	0.069 (0.004)	0.070 (0.004)	0.084 (0.005)	0.104 (0.003)	0.087 (0.003)	0.104 (0.008)
	300							

Table 6. Average measures (with standard deviations) over 100 replications for Model 6.

p		BIC			HQIC			
		DT	DTEC	SDTEC	GLASSO	DT	DTEC	SDTEC
KL	100	19.67 (1.86)	19.40 (1.11)	19.50 (1.01)	30.42 (1.69)	15.71 (1.31)	16.71 (0.96)	16.78 (0.95)
	200	46.30 (2.29)	45.63 (1.51)	45.37 (1.41)	70.47 (2.69)	39.99 (1.71)	41.51 (1.39)	41.70 (1.36)
RKLL	300	84.45 (3.63)	77.81 (2.66)	77.58 (3.08)	119.27 (3.64)	74.74 (1.45)	70.72 (1.62)	71.73 (1.12)
	100	44.73 (7.44)	32.36 (3.44)	32.99 (3.16)	88.30 (8.13)	28.10 (5.37)	23.06 (2.65)	23.25 (3.15)
ℓ_1	200	114.93 (10.88)	83.67 (5.63)	83.04 (4.78)	217.72 (13.82)	84.49 (7.47)	67.50 (4.59)	67.04 (6.11)
	300	234.17 (16.41)	147.95 (9.38)	148.14 (9.74)	383.36 (20.13)	189.14 (8.01)	123.71 (8.36)	126.28 (3.56)
ℓ_2	100	2.24 (0.10)	2.04 (0.07)	2.05 (0.07)	2.84 (0.04)	1.93 (0.12)	1.79 (0.08)	1.80 (0.09)
	200	3.19 (0.07)	2.95 (0.06)	2.95 (0.06)	4.08 (0.04)	2.95 (0.07)	2.80 (0.07)	2.79 (0.08)
ℓ_{sp}	300	4.19 (0.08)	3.72 (0.07)	3.72 (0.08)	5.11 (0.04)	3.96 (0.05)	3.53 (0.08)	3.55 (0.05)
	100	1.56 (0.05)	1.52 (0.05)	1.53 (0.04)	1.78 (0.01)	1.45 (0.06)	1.42 (0.05)	1.42 (0.05)
Sens	200	1.87 (0.02)	1.85 (0.02)	1.85 (0.02)	1.97 (0.01)	1.84 (0.02)	1.83 (0.04)	1.83 (0.03)
	300	2.09 (0.05)	2.01 (0.03)	2.01 (0.03)	2.29 (0.01)	2.06 (0.04)	1.99 (0.03)	1.99 (0.03)
Spec	100	0.71 (0.03)	0.67 (0.03)	0.68 (0.03)	0.88 (0.01)	0.63 (0.04)	0.61 (0.03)	0.61 (0.03)
	200	0.82 (0.01)	0.79 (0.03)	0.79 (0.03)	0.90 (0.006)	0.79 (0.02)	0.77 (0.05)	0.77 (0.04)
MCC	300	0.85 (0.01)	0.82 (0.03)	0.82 (0.03)	0.90 (0.004)	0.84 (0.01)	0.81 (0.03)	0.81 (0.01)
	100	0.094 (0.018)	0.079 (0.010)	0.078 (0.010)	0.097 (0.014)	0.155 (0.027)	0.128 (0.018)	0.128 (0.020)
F ₁	200	0.040 (0.004)	0.031 (0.003)	0.031 (0.003)	0.040 (0.005)	0.066 (0.007)	0.049 (0.007)	0.049 (0.009)
	300	0.022 (0.004)	0.021 (0.003)	0.021 (0.003)	0.025 (0.003)	0.033 (0.003)	0.035 (0.004)	0.031 (0.002)

5. Real data application

In this section, we conduct an empirical analysis through real-data example. In particular, we focus on the problem of predicting breast cancer patients (subjects) with pathological complete response (pCR) using Linear Discriminant Analysis (LDA). For this application we use a dataset which contains gene expression levels of subjects with different stages of breast cancer. The dataset consists of 22,283 gene expression levels of 271 subjects. There are 58 subjects with pCR and 213 subjects with residual disease (RD). The applied dataset is available in the website of the National Center for Biotechnology Information (<http://www.ncbi.nlm.nih.gov/>).

First, following the analysis by Cai, Liu, and Luo (2011), we divide the dataset into training and testing sets with sizes 227 and 44 (almost 5/6 and 1/6 of the observations), respectively. For the testing set, we randomly select 9 subjects with pCR and 35 subjects with RD (roughly 1/6 of the subjects in each group). The training set contains the remaining subjects. Second, based on the training set we perform two sample t-tests between two groups and select the most significant 200 genes with the smallest p-values. Third, using the training set, we estimate the precision matrix Ω with the DT, DTEC, SDTEC and GLASSO methods. Finally, we use the estimated precision matrix in the LDA score function, defined as $\delta_t(Y) = Y^T \hat{\Omega} \hat{\mu}_t - \frac{1}{2} \hat{\mu}_t^T \hat{\Omega} \hat{\mu}_t$, where $t = 1, 2$ ($t = 1$ for pCR and $t = 2$ for RD) and $\hat{\mu}_t$ is the within group average, calculated using the training data. We classify the subject Y through the classification rule $\hat{t} = \text{argmax} \delta_t(Y)$. To measure the prediction accuracy, we use Specificity, Sensitivity, MCC and F_1 . We consider TP and TN as the number of correctly predicted RD and pCR, respectively, and FP and FN as the number of erroneously predicted RD and pCR, respectively. We repeat this process 100 times. We report the average measurements in Table 7.

Our findings show that for both selection criteria the GLASSO method provides the highest Sensitivity, but it attains the lowest Specificity and MCC. On the other hand, the DTEC approach provides the highest Specificity and dominates all the other estimators in terms of MCC. We note that all methods provide very similar results in terms of the F_1 score. However, as mentioned earlier, we find MCC more informative than F_1 score. The results also show that SDTEC performs as good as the DTEC estimator. Furthermore, we observe that the obtained Specificity and MCC of the considered estimators are higher for BIC than the same for HQIC, whereas the Sensitivity and F_1 of the estimators are higher for HQIC than the same for BIC.

Table 7. Average pCR/RD classification measurements over 100 replications.

BIC				
Method	Specificity	Sensitivity	MCC	F_1
DT	0.692	0.749	0.378	0.818
DTEC	0.719	0.742	0.392	0.816
SDTEC	0.713	0.744	0.389	0.817
GLASSO	0.461	0.790	0.232	0.816
HQIC				
Method	Specificity	Sensitivity	MCC	F_1
DT	0.559	0.787	0.312	0.827
DTEC	0.606	0.778	0.341	0.827
SDTEC	0.606	0.777	0.340	0.826
GLASSO	0.443	0.802	0.231	0.823

In sum, for the considered application our proposed DTEC method (and its simplified version SDTEC) provides better classification performance than DT and GLASSO approaches. Therefore, employing additional penalization on the estimated precision matrix eigenvalues improves the estimate, even though the true precision matrix eigenvalues are unknown in this example.

6 Conclusions

In this article, we develop a new approach for estimating high dimensional precision matrices, using the ℓ_1 penalization framework. The proposed method imposes a negative trace penalization on the recently introduced DT estimator. The additional penalty term controls the eigenvalues of the precision matrix estimator and diminishes the reduction of its largest eigenvalues. We conduct an extensive simulation study where we use several statistical losses and measures for the estimation evaluation. The results show that our proposed methodology outperforms DT and GLASSO methods for most of the considered scenarios. In line with the popular BIC method we study the performance of another technique based on HQIC for selecting the penalty parameters. In contrast to its little use in practice, HQIC demonstrates lower statistical losses than BIC in the simulation study. Moreover, we illustrate the performance of our proposed approach through an empirical application aimed at predicting the patients with pCR using LDA. Furthermore, we propose a simplified version of our methodology, which leads to saving the computational time without having to sacrifice the performance.

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