



Multivariate Gaussian and Student-*t* process regression for multi-output prediction

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Abstract

Gaussian process model for vector-valued function has been shown to be useful for multi-output prediction. The existing method for this model is to reformulate the matrix-variate Gaussian distribution as a multivariate normal distribution. Although it is effective in many cases, reformulation is not always workable and is difficult to apply to other distributions because not all matrix-variate distributions can be transformed to respective multivariate distributions, such as the case for matrix-variate Student-*t* distribution. In this paper, we propose a unified framework which is used not only to introduce a novel multivariate Student-*t* process regression model (MV-TPR) for multi-output prediction, but also to reformulate the multivariate Gaussian process regression (MV-GPR) that overcomes some limitations of the existing methods. Both MV-GPR and MV-TPR have closed-form expressions for the marginal likelihoods and predictive distributions under this unified framework and thus can adopt the same optimization approaches as used in the conventional GPR. The usefulness of the proposed methods is illustrated through several simulated and real-data examples. In particular, we verify empirically that MV-TPR has superiority for the datasets considered, including air quality prediction and bike rent prediction. At last, the proposed methods are shown to produce profitable investment strategies in the stock markets.

Keywords Multivariate Gaussian process · Multivariate Student-*t* process · Gaussian process regression · Student-*t* process regression · Multi-output prediction · Stock investment strategy · Industrial sector · Time series prediction

1 Introduction

Over the last few decades, Gaussian processes regression (GPR) has been proven to be a powerful and effective method for nonlinear regression problems due to many favorable properties, such as simple structure of obtaining and expressing uncertainty in predictions, the capability of capturing a wide variety of behavior by parameters and a natural Bayesian interpretation [5, 21]. In 1996, Neal [20] revealed that many Bayesian regression models based on neural network converge to Gaussian processes (GP) in the limit of an infinite number of hidden units [26]. GP has

been suggested as a replacement for supervised neural networks in nonlinear regression [17, 28] and classification [17]. Furthermore, GP has excellent capability of forecasting time series [6, 7].

Despite the popularity of GPR in various modeling tasks, there still exists a conspicuous imperfection, that is, the majority of GPR models are implemented for single response variables or considered independently for multiple responses variables without consideration of their correlation [5, 25]. In order to resolve the multi-output prediction problem, Gaussian process regression for vector-valued function is proposed and regarded as a pragmatic and straightforward method. The core of this method is to vectorize the multi-response variables and construct a “big” covariance, which describes the correlations between the inputs as well as between the outputs [2, 5, 8, 25]. This modeling strategy is feasible due to the fact that the matrix-variate Gaussian distributions can be reformulated as multivariate Gaussian distributions [8, 15]. Intrinsically, Gaussian process regression for vector-valued

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function is still a conventional Gaussian process regression model since it merely vectorizes multi-response variables, which are assumed to follow a developed case of GP with a reproduced kernel. As an extension, it is natural to consider more general elliptical processes models for multi-output prediction. However, the vectorization method cannot be used to extend multi-output GPR because the equivalence between vectorized matrix-variate and multivariate distributions only exists in Gaussian cases [15].

To overcome this drawback, in this paper we propose a unified framework which: (1) is used to introduce a novel multivariate Student-*t* process regression model (MV-TPR) for multi-output prediction, (2) is used to reformulate the multivariate Gaussian process regression (MV-GPR) that overcomes some limitations of the existing methods and (3) can be used to derive regression models of general elliptical processes. Both MV-GPR and MV-TPR have closed-form expressions for the marginal likelihoods and predictive distributions under this unified framework and thus can adopt the same optimization approaches as used in the conventional GPR. The usefulness of the proposed methods is illustrated through several simulated examples. Furthermore, we also verify empirically that MV-TPR has superiority in the prediction based on some widely used datasets, including air quality prediction and bike rent prediction. The proposed methods are then applied to stock market modeling which shows that the profitable stock investment strategies can be obtained.

The rest of the paper is organized as follows. Section 2 introduces some preliminaries of matrix-variate Gaussian and Student-*t* distributions with their useful properties. Section 3 presents the unified framework to reformulate the multivariate Gaussian process regression and to derive the new multivariate Student-*t* process regression models. Some numerical experiments by the simulated data and real data and the applications to stock market investment are presented in Sect. 4. Conclusion and discussion are given in Sect. 5.

2 Backgrounds and notations

Matrix-variate Gaussian and Student-*t* distributions have many useful properties, as discussed in the studies [10, 15, 31]. For completeness and easy referencing, below we list some of them which will be used in this paper.

2.1 Matrix-variate Gaussian distribution

Definition 1 The random matrix $X \in \mathbb{R}^{n \times d}$ is said to have a matrix-variate Gaussian distribution with mean matrix

$M \in \mathbb{R}^{n \times d}$ and covariance matrix $\Sigma \in \mathbb{R}^{n \times n}, \Omega \in \mathbb{R}^{d \times d}$ if and only if its probability density function is given by

$$p(X|M, \Sigma, \Omega) = (2\pi)^{-\frac{nd}{2}} \det(\Sigma)^{-\frac{d}{2}} \det(\Omega)^{-\frac{n}{2}} \times \text{etr}\left(-\frac{1}{2}\Omega^{-1}(X - M)^T \Sigma^{-1}(X - M)\right), \tag{1}$$

where $\text{etr}(\cdot)$ is exponential of matrix trace and Ω and Σ are positive semi-definite. It is denoted $X \sim \mathcal{MN}_{n,d}(M, \Sigma, \Omega)$. Without loss of clarity, it is denoted $X \sim \mathcal{MN}(M, \Sigma, \Omega)$.

Like multivariate Gaussian distribution, matrix-variate Gaussian distribution also possesses several important properties as follows.

Theorem 1 (Transposable) *If $X \sim \mathcal{MN}_{n,d}(M, \Sigma, \Omega)$, then $X^T \sim \mathcal{MN}_{d,n}(M^T, \Omega, \Sigma)$.*

The matrix-variate Gaussian is related to the multivariate Gaussian in the following way.

Theorem 2 (Vectorizable) *$X \sim \mathcal{MN}_{n,d}(M, \Sigma, \Omega)$ if and only if*

$$\text{vec}(X^T) \sim \mathcal{N}_{nd}(\text{vec}(M^T), \Sigma \otimes \Omega),$$

where $\text{vec}(\cdot)$ is the vector operator and \otimes is the Kronecker product (or called tensor product).

Furthermore, the matrix-variate Gaussian distribution is consistent under the marginalization and conditional distribution.

Theorem 3 (Marginalization and conditional distribution) *Let $X \sim \mathcal{MN}_{n,d}(M, \Sigma, \Omega)$ and partition X, M, Σ and Ω as*

$$X = \begin{bmatrix} X_{1r} \\ X_{2r} \end{bmatrix} \begin{matrix} n_1 \\ n_2 \end{matrix} = \begin{bmatrix} X_{1c} & X_{2c} \\ d_1 & d_2 \end{bmatrix}, \quad M = \begin{bmatrix} M_{1r} \\ M_{2r} \end{bmatrix} \begin{matrix} n_1 \\ n_2 \end{matrix} = \begin{bmatrix} M_{1c} & M_{2c} \\ d_1 & d_2 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \begin{matrix} n_1 & n_2 \end{matrix} \quad \text{and} \quad \Omega = \begin{bmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{bmatrix} \begin{matrix} d_1 \\ d_2 \end{matrix},$$

where n_1, n_2, d_1, d_2 is the column or row length of the corresponding vector or matrix. Then,

1. $X_{1r} \sim \mathcal{MN}_{n_1,d}(M_{1r}, \Sigma_{11}, \Omega)$,
 $X_{2r}|X_{1r} \sim \mathcal{MN}_{n_2,d}$
 $\left(M_{2r} + \Sigma_{21}\Sigma_{11}^{-1}(X_{1r} - M_{1r}), \Sigma_{22 \cdot 1}, \Omega\right);$
2. $X_{1c} \sim \mathcal{MN}_{n,d_1}(M_{1c}, \Sigma, \Omega_{11})$,
 $X_{2c}|X_{1c} \sim \mathcal{MN}_{n,d_2}$
 $\left(M_{2c} + (X_{1c} - M_{1c})\Omega_{11}^{-1}\Omega_{12}, \Sigma, \Omega_{22 \cdot 1}\right),$

where $\Sigma_{22 \cdot 1}$ and $\Omega_{22 \cdot 1}$ are the Schur complement [30] of Σ_{11} and Ω_{11} , respectively,

$$\Sigma_{22.1} = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}, \quad \Omega_{22.1} = \Omega_{22} - \Omega_{21}\Omega_{11}^{-1}\Omega_{12}.$$

2.2 Matrix-variate Student-t distribution

Definition 2 The random matrix $X \in \mathbb{R}^{n \times d}$ is said to have a matrix-variate Student- t distribution with the mean matrix $M \in \mathbb{R}^{n \times d}$ and covariance matrix $\Sigma \in \mathbb{R}^{n \times n}, \Omega \in \mathbb{R}^{d \times d}$ and the degree of freedom ν if and only if the probability density function is given by

$$p(X|\nu, M, \Sigma, \Omega) = \frac{\Gamma_n\left[\frac{1}{2}(\nu + d + n - 1)\right]}{\pi^{\frac{1}{2}dn}\Gamma_n\left[\frac{1}{2}(\nu + n - 1)\right]} \times \det(\Sigma)^{-\frac{d}{2}} \det(\Omega)^{-\frac{n}{2}} \times \det(\mathbf{I}_n + \Sigma^{-1}(X - M)\Omega^{-1}(X - M)^T)^{-\frac{1}{2}(\nu + d + n - 1)}, \tag{2}$$

where Ω and Σ are positive semi-definite, and

$$\Gamma_n(\lambda) = \pi^{n(n-1)/4} \prod_{i=1}^n \Gamma\left(\lambda + \frac{1}{2} - \frac{i}{2}\right).$$

We denote this by $X \sim \mathcal{MT}_{n,d}(\nu, M, \Sigma, \Omega)$. Without loss of clarity, it is denoted $X \sim \mathcal{MT}(\nu, M, \Sigma, \Omega)$.

Theorem 4 (Expectation and covariance) *Let $X \sim \mathcal{MT}(\nu, M, \Sigma, \Omega)$, then*

$$\mathbb{E}(X) = M, \quad \text{cov}(\text{vec}(X^T)) = \frac{1}{\nu - 2} \Sigma \otimes \Omega, \nu > 2.$$

Theorem 5 (Transposable) *If $X \sim \mathcal{MT}_{n,d}(\nu, M, \Sigma, \Omega)$, then $X^T \sim \mathcal{MT}_{d,n}(\nu, M^T, \Omega, \Sigma)$.*

Theorem 6 (Asymptotics) *Let $X \sim \mathcal{MT}_{n,d}(\nu, M, \Sigma, \Omega)$, then $X \xrightarrow{d} \mathcal{MN}_{n,d}(M, \Sigma, \Omega)$ as $\nu \rightarrow \infty$, where “ \xrightarrow{d} ” denotes the convergence in distribution.*

Theorem 7 (Marginalization and conditional distribution) *Let $X \sim \mathcal{MT}_{n,d}(\nu, M, \Sigma, \Omega)$ and partition X, M, Σ and Ω as*

$$X = \begin{bmatrix} X_{1r} \\ X_{2r} \end{bmatrix} \begin{matrix} n_1 \\ n_2 \end{matrix} = \begin{bmatrix} X_{1c} & X_{2c} \end{bmatrix} \begin{matrix} d_1 \\ d_2 \end{matrix}, \quad M = \begin{bmatrix} M_{1r} \\ M_{2r} \end{bmatrix} \begin{matrix} n_1 \\ n_2 \end{matrix} = \begin{bmatrix} M_{1c} & M_{2c} \end{bmatrix} \begin{matrix} d_1 \\ d_2 \end{matrix}$$

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \begin{matrix} n_1 \\ n_2 \end{matrix} \quad \text{and} \quad \Omega = \begin{bmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{bmatrix} \begin{matrix} d_1 \\ d_2 \end{matrix},$$

where n_1, n_2, d_1, d_2 is the column or row length of the corresponding vector or matrix. Then,

- $X_{1r} \sim \mathcal{MT}_{n_1,d}(\nu, M_{1r}, \Sigma_{11}, \Omega),$

$$X_{2r}|X_{1r} \sim \mathcal{MT}_{n_2,d}\left(\nu + n_1, M_{2r} + \Sigma_{21}\Sigma_{11}^{-1}(X_{1r} - M_{1r}), \Sigma_{22.1}, \Omega + (X_{1r} - M_{1r})^T \Sigma_{11}^{-1}(X_{1r} - M_{1r})\right);$$

- $X_{1c} \sim \mathcal{MT}_{n,d_1}(\nu, M_{1c}, \Sigma, \Omega_{11}),$

$$X_{2c}|X_{1c} \sim \mathcal{MT}_{n,d_2}\left(\nu + d_1, M_{2c} + (X_{1c} - M_{1c})\Omega_{11}^{-1}\Omega_{12}, \Sigma + (X_{1c} - M_{1c})\Omega_{11}^{-1}(X_{1c} - M_{1c})^T, \Omega_{22.1}\right),$$

where $\Sigma_{22.1}$ and $\Omega_{22.1}$ are the Schur complement of Σ_{11} and Ω_{11} , respectively,

$$\Sigma_{22.1} = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}, \quad \Omega_{22.1} = \Omega_{22} - \Omega_{21}\Omega_{11}^{-1}\Omega_{12}.$$

Remark 1 It can be seen that matrix-variate Student- t distribution has many properties similar to matrix-variate Gaussian distribution, and it converges to matrix-variate Gaussian distribution if its degree of freedom tends to infinity. However, matrix-variate Student- t distribution lacks the property of vectorizability (Theorem 2) [15]. As a consequence, Student- t process regression for multiple outputs cannot be derived by vectorizing the multi-response variables. In the next section, we propose a new framework to introduce multivariate Student- t process regression model.

3 Multivariate Gaussian and Student-t process regression models

3.1 Multivariate Gaussian process regression (MV-GPR)

If f is a multivariate Gaussian process on \mathcal{X} with vector-valued mean function $\mathbf{u} : \mathcal{X} \mapsto \mathbb{R}^d$, covariance function (also called kernel) $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ and positive semi-definite parameter matrix $\Omega \in \mathbb{R}^{d \times d}$, then any finite collection of vector-valued variables have a joint matrix-variate Gaussian distribution:

$$[\mathbf{f}(x_1)^T, \dots, \mathbf{f}(x_n)^T]^T \sim \mathcal{MN}(M, \Sigma, \Omega), n \in \mathbb{N},$$

where $\mathbf{f}, \mathbf{u} \in \mathbb{R}^d$ are row vectors whose components are the functions $\{f_i\}_{i=1}^d$ and $\{\mu_i\}_{i=1}^d$, respectively. Furthermore, $M \in \mathbb{R}^{n \times d}$ with $M_{ij} = \mu_j(x_i)$, and $\Sigma \in \mathbb{R}^{n \times n}$ with $\Sigma_{ij} = k(x_i, x_j)$. Sometimes Σ is called column covariance matrix, while Ω is row covariance matrix. We denote $f \sim \mathcal{MG}\mathcal{P}(\mathbf{u}, k, \Omega)$.

In conventional GPR methods, the noisy model $y = f(x) + \varepsilon$ is usually considered. However, for Student- t process regression such a model is analytically intractable [24]. Therefore, we adopt the method used in [24] and consider the noise-free regression model where the noise term is incorporated into the kernel function.

Given n pairs of observations $\{(x_i, y_i)\}_{i=1}^n, x_i \in \mathbb{R}^p, y_i \in \mathbb{R}^{1 \times d}$, we assume the following model:

$$f \sim \mathcal{MGP}(u, k', \Omega),$$

$$y_i = f(x_i), \text{ for } i = 1, \dots, n,$$

where

$$k' = k(x_i, x_j) + \delta_{ij}\sigma_n^2, \tag{3}$$

and $\delta_{ij} = 1$ if $i = j$, otherwise $\delta_{ij} = 0$. Note that the second term in (3) represents the random noises.

We assume $u = \theta$ as commonly done in GPR. By the definition of multivariate Gaussian process, it yields that the collection of functions $[f(x_1), \dots, f(x_n)]$ follow a matrix-variate Gaussian distribution:

$$[f(x_1)^T, \dots, f(x_n)^T]^T \sim \mathcal{MN}(\theta, K', \Omega),$$

where K' is the $n \times n$ covariance matrix of which the (i, j) -th element $[K']_{ij} = k'(x_i, x_j)$.

To predict a new variable $f_* = [f_{*1}, \dots, f_{*m}]^T$ at the test locations $X_* = [x_{n+1}, \dots, x_{n+m}]^T$, the joint distribution of the training observations $Y = [y_1^T, \dots, y_n^T]^T$ and the predictive targets f_* are given by

$$\begin{bmatrix} Y \\ f_* \end{bmatrix} \sim \mathcal{MN}\left(\theta, \begin{bmatrix} K'(X, X) & K'(X_*, X)^T \\ K'(X_*, X) & K'(X_*, X_*) \end{bmatrix}, \Omega\right), \tag{4}$$

where $K'(X, X)$ is an $n \times n$ matrix of which the (i, j) -th element $[K'(X, X)]_{ij} = k'(x_i, x_j)$, $K'(X_*, X)$ is an $m \times n$ matrix of which the (i, j) -th element $[K'(X_*, X)]_{ij} = k'(x_{n+i}, x_j)$, and $K'(X_*, X_*)$ is an $m \times m$ matrix with the (i, j) -th element $[K'(X_*, X_*)]_{ij} = k'(x_{n+i}, x_{n+j})$. Thus, taking advantage of conditional distribution of multivariate Gaussian process, the predictive distribution is

$$p(f_* | X, Y, X_*) = \mathcal{MN}(\hat{M}, \hat{\Sigma}, \hat{\Omega}), \tag{5}$$

where

$$\hat{M} = K'(X_*, X)^T K'(X, X)^{-1} Y, \tag{6}$$

$$\hat{\Sigma} = K'(X_*, X_*) - K'(X_*, X)^T K'(X, X)^{-1} K'(X_*, X), \tag{7}$$

$$\hat{\Omega} = \Omega. \tag{8}$$

Additionally, the expectation and the covariance are obtained:

$$E[f_*] = \hat{M} = K'(X_*, X)^T K'(X, X)^{-1} Y, \tag{9}$$

$$\begin{aligned} \text{cov}(\text{vec}(f_*^T)) &= \hat{\Sigma} \otimes \hat{\Omega} = [K'(X_*, X_*) \\ &- K'(X_*, X)^T K'(X, X)^{-1} K'(X_*, X)] \otimes \Omega. \end{aligned} \tag{10}$$

3.1.1 Kernel

Although there are two covariance matrices in the above regression model: the column covariance and the row covariance, only the column covariance depends on inputs and is considered as kernel since it contains our presumptions about the function we wish to learn and define the closeness and similarity between data points [22]. As in conventional GPR, the choice of kernels has a profound impact on the performance of multivariate Gaussian process regression (as well as multivariate Student- t process regression introduced later). A wide range of useful kernels have been proposed in the literature, such as linear, rational quadratic and Matérn [22]. But the squared exponential (SE) kernel is the most commonly used due to its simple form and many desirable properties such as smoothness and integrability with other functions, although it could oversmooth the data, especially financial data.

The squared exponential (SE) kernel is defined as:

$$k_{SE}(x, x') = s_f^2 \exp\left(-\frac{\|x - x'\|^2}{2\ell^2}\right),$$

where s_f^2 is the signal variance and can also be considered as an output-scale amplitude and the parameter ℓ is the input (length or time) scale [23]. The kernel can also be defined by automatic relevance determination (ARD):

$$k_{SEard}(x, x') = s_f^2 \exp\left(-\frac{(x - x')^T \Theta^{-1} (x - x')}{2}\right),$$

where Θ is a diagonal matrix with the element components $\{\ell_i^2\}_{i=1}^p$, which represents the length scales for each corresponding input dimension.

For convenience and the purpose of demonstration, SE kernel is used in all our experiments where there is only one input variable, while SEard is used in those with multiple input variables. It should be noted that there is no technical difficulty to use other kernels in our models.

3.1.2 Parameter estimation

The hyperparameters involved in the kernel and the row covariance matrix of MV-GPR need to be estimated from the training data. Many approaches used in the conventional GP models [27], such as maximum likelihood estimation (MLE), maximum a posteriori (MAP) and Markov chain Monte Carlo (MCMC), can be used for our proposed models. Although Monte Carlo methods can perform GPR without the need of estimating hyperparameters

[6, 18, 19, 28], the common approach is to estimate them by means of MLE due to the high computational cost of Monte Carlo methods. Therefore, as an example we consider parameter estimation using MLE. Compared to the conventional GPR model, Ω is an extra parameter; hence, the unknown parameters include the hyperparameters in the kernel, the noise variance σ_n^2 and the row covariance parameter matrix Ω .

Because Ω is positive semi-definite, it can be denoted as $\Omega = \Phi\Phi^T$, where

$$\Phi = \begin{bmatrix} \phi_{11} & 0 & \cdots & 0 \\ \phi_{21} & \phi_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{d1} & \phi_{d2} & \cdots & \phi_{dd} \end{bmatrix}.$$

To guarantee the uniqueness of Φ , the diagonal elements are restricted to be positive and denote $\phi_{ii} = \ln(\phi_{ii})$ for $i = 1, 2, \dots, d$.

In MV-GPR model, the observations follow a matrix-variate Gaussian distribution $Y \sim \mathcal{MN}_{n,d}(\boldsymbol{\theta}, K', \Omega)$ where K' is the noisy column covariance matrix with element $[K']_{ij} = k'(x_i, x_j)$ so that $K' = K + \sigma_n^2 \mathbf{I}$ where K is noise-free column covariance matrix with element $[K]_{ij} = k(x_i, x_j)$. As we know, there are hyperparameters in the kernel k so that we can denote $K = K_\theta$. The hyperparameter set denotes $\Theta = \{\theta_1, \theta_2, \dots\}$, thus

$$\frac{\partial K'}{\partial \sigma_n^2} = \mathbf{I}_n, \quad \frac{\partial K'}{\partial \theta_i} = \frac{\partial K_\theta}{\partial \theta_i}$$

According to the matrix-variate distribution, the negative log marginal likelihood of observations is

$$\begin{aligned} \mathcal{L} = & \frac{nd}{2} \ln(2\pi) + \frac{d}{2} \ln \det(K') + \frac{n}{2} \ln \det(\Omega) \\ & + \frac{1}{2} \text{tr}((K')^{-1} Y \Omega^{-1} Y^T). \end{aligned} \tag{11}$$

The derivatives of the negative log marginal likelihood with respect to parameter σ_n^2 , θ_i , ϕ_{ij} and ϕ_{ii} are as follows:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \sigma_n^2} &= \frac{d}{2} \text{tr}((K')^{-1}) - \frac{1}{2} \text{tr}(\alpha_{K'} \Omega^{-1} \alpha_{K'}^T), \\ \frac{\partial \mathcal{L}}{\partial \theta_i} &= \frac{d}{2} \text{tr}\left((K')^{-1} \frac{\partial K_\theta}{\partial \theta_i}\right) - \frac{1}{2} \text{tr}\left(\alpha_{K'} \Omega^{-1} \alpha_{K'}^T \frac{\partial K_\theta}{\partial \theta_i}\right), \\ \frac{\partial \mathcal{L}}{\partial \phi_{ij}} &= \frac{n}{2} \text{tr}[\Omega^{-1} (\mathbf{E}_{ij} \Phi^T + \Phi \mathbf{E}_{ji})] \\ &\quad - \frac{1}{2} \text{tr}[\alpha_\Omega (K')^{-1} \alpha_\Omega^T (\mathbf{E}_{ij} \Phi^T + \Phi \mathbf{E}_{ji})], \\ \frac{\partial \mathcal{L}}{\partial \phi_{ii}} &= \frac{n}{2} \text{tr}[\Omega^{-1} (\mathbf{J}_{ii} \Phi^T + \Phi \mathbf{J}_{ii})] \\ &\quad - \frac{1}{2} \text{tr}[\alpha_\Omega (K')^{-1} \alpha_\Omega^T (\mathbf{J}_{ii} \Phi^T + \Phi \mathbf{J}_{ii})], \end{aligned}$$

where $\alpha_{K'} = (K')^{-1} Y$, $\alpha_\Omega = \Omega^{-1} Y^T$, \mathbf{E}_{ij} is the $d \times d$ elementary matrix having unity in the (i, j) th element and zeros elsewhere, and \mathbf{J}_{ii} is the same as \mathbf{E}_{ij} but with the unity being replaced by $e^{\phi_{ii}}$. The details are provided in “Multivariate Gaussian process regression” in Appendix.

Hence, standard gradient-based numerical optimization techniques, such as conjugate gradient method, can be used to minimize the negative log marginal likelihood function to obtain the estimates of the parameters. Note that since the random noise is incorporated into the kernel function, the noise variance is estimated alongside the other hyperparameters.

3.1.3 Comparison with the existing methods

Compared with the existing multi-output GPR methods [2, 5, 25], our proposed method possesses several advantages.

Firstly, the existing methods have to vectorize the multi-output matrix in order to utilize the GPR models. It is complicated and not always workable if the numbers of outputs and observations are large. In contrast, our proposed MV-GPR has more straightforward form where the model settings, derivations and computations are all directly performed in matrix form. In particular, we use column covariance (kernel) and row covariance to capture all the correlations together in the multivariate outputs, rather than assuming a separate kernel for each output and constructing a “big” covariance matrix by Kronecker product as done in [5].

Secondly, the existing methods rely on the equivalence between vectorized matrix-variate Gaussian distribution and multivariate Gaussian distribution. However, this equivalence does not exist for other elliptical distributions such as matrix-variate Student- t distribution [15]. Therefore, the existing methods for multi-output Gaussian process regression cannot be applied to Student- t process regression. On the other hand, our proposed MV-GPR is based on matrix forms directly and does not require vectorization, so it can naturally be extended to MV-TPR as we will do in the next subsection.

Therefore, our proposed MV-GPR provides not only a new derivation of the multi-output Gaussian process regression model, but also a unified framework to derive more general elliptical processes models.

3.2 Multivariate Student- t process regression (MV-TPR)

In this subsection, we propose a new nonlinear regression model for multivariate response, namely multivariate Student- t process regression model (MV-TPR), using the

framework discussed in the previous subsections. MV-TPR is an extension to multi-output GPR, as well as an extension to the univariate Student-*t* process regression proposed in [24].

By definition, if \mathbf{f} is a multivariate Student-*t* process on \mathcal{X} with parameter $\nu > 2$, vector-valued mean function $\mathbf{u} : \mathcal{X} \mapsto \mathbb{R}^d$, covariance function (also called kernel) $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ and positive semi-definite parameter matrix $\Omega \in \mathbb{R}^{d \times d}$, then any finite collection of vector-valued variables have a joint matrix-variate Student-*t* distribution:

$$[\mathbf{f}(x_1)^T, \dots, \mathbf{f}(x_n)^T]^T \sim \mathcal{MT}(\nu, \mathbf{M}, \Sigma, \Omega), n \in \mathbb{N},$$

where $\mathbf{f}, \mathbf{u} \in \mathbb{R}^d$ are row vectors whose components are the functions $\{f_i\}_{i=1}^d$ and $\{\mu_i\}_{i=1}^d$, respectively. Furthermore, $\mathbf{M} \in \mathbb{R}^{n \times d}$ with $M_{ij} = \mu_j(x_i)$, and $\Sigma \in \mathbb{R}^{n \times n}$ with $\Sigma_{ij} = k(x_i, x_j)$. We denote $\mathbf{f} \sim \mathcal{MTP}(\nu, \mathbf{u}, k, \Omega)$.

Therefore, MV-TPR model can be formulated along the same line as MV-GPR based on the definition of multivariate Student-*t* process. We present the model briefly below.

Given n pairs of observations $\{(x_i, \mathbf{y}_i)\}_{i=1}^n, x_i \in \mathbb{R}^p, \mathbf{y}_i \in \mathbb{R}^{1 \times d}$, we assume

$$\begin{aligned} \mathbf{f} &\sim \mathcal{MTP}(\nu, \mathbf{u}, k', \Omega), \nu > 2, \\ \mathbf{y}_i &= \mathbf{f}(x_i), \text{ for } i = 1, \dots, n, \end{aligned}$$

where ν is the degree of freedom of Student-*t* process and the remaining parameters have the same meaning of MV-GPR model. Consequently, the predictive distribution is obtained as:

$$p(\mathbf{f}_* | X, Y, X_*) = \mathcal{MT}(\hat{\nu}, \hat{\mathbf{M}}, \hat{\Sigma}, \hat{\Omega}), \tag{12}$$

where

$$\hat{\nu} = \nu + n, \tag{13}$$

$$\hat{\mathbf{M}} = K'(X_*, X)^T K'(X, X)^{-1} Y, \tag{14}$$

$$\hat{\Sigma} = K'(X_*, X_*) - K'(X_*, X)^T K'(X, X)^{-1} K'(X, X_*), \tag{15}$$

$$\hat{\Omega} = \Omega + Y^T K'(X, X)^{-1} Y. \tag{16}$$

According to the expectation and the covariance of matrix-variate Student-*t* distribution, the predictive mean and covariance are given by

$$\mathbb{E}[\mathbf{f}_*] = \hat{\mathbf{M}} = K'(X_*, X)^T K'(X, X)^{-1} Y, \tag{17}$$

$$\begin{aligned} \text{cov}(\text{vec}(\mathbf{f}_*^T)) &= \frac{1}{\nu + n - 2} \hat{\Sigma} \otimes \hat{\Omega} \\ &= \frac{1}{\nu + n - 2} [K'(X_*, X_*) \\ &\quad - K'(X_*, X)^T K'(X, X)^{-1} K'(X, X_*)] \\ &\quad \otimes (\Omega + Y^T K'(X, X)^{-1} Y). \end{aligned} \tag{18}$$

In the MV-TPR model, the observations are followed by a matrix-variate Student-*t* distribution $Y \sim \mathcal{MT}_{n,d}(\nu, \boldsymbol{\theta}, K', \Omega)$. The negative log marginal likelihood is

$$\begin{aligned} \mathcal{L} &= \frac{1}{2}(\nu + d + n - 1) \ln \det(\mathbf{I}_n + (K')^{-1} Y \Omega^{-1} Y^T) \\ &\quad + \frac{d}{2} \ln \det(K') + \frac{n}{2} \ln \det(\Omega) \\ &\quad + \ln \Gamma_n\left(\frac{1}{2}(\nu + n - 1)\right) - \ln \Gamma_n\left(\frac{1}{2}(\nu + d + n - 1)\right) \\ &\quad + \frac{1}{2} dn \ln \pi \\ &= \frac{1}{2}(\nu + d + n - 1) \ln \det(K' + Y \Omega^{-1} Y^T) \\ &\quad - \frac{\nu + n - 1}{2} \ln \det(K') \\ &\quad + \ln \Gamma_n\left(\frac{1}{2}(\nu + n - 1)\right) - \ln \Gamma_n\left(\frac{1}{2}(\nu + d + n - 1)\right) \\ &\quad + \frac{n}{2} \ln \det(\Omega) + \frac{1}{2} dn \ln \pi. \end{aligned}$$

Therefore, the parameters of MV-TPR contain all the parameters in MV-GPR and one more parameter: the degree of freedom ν . The derivatives of the negative log marginal likelihood with respect to parameter $\nu, \sigma_n^2, \theta_i, \phi_{ij}$ and φ_{ii} are as follows:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \nu} &= \frac{1}{2} \ln \det(U) - \frac{1}{2} \ln \det(K') + \frac{1}{2} \psi_n\left(\frac{1}{2} \tau\right) \\ &\quad - \frac{1}{2} \psi_n\left(\frac{1}{2}(\tau + d)\right), \\ \frac{\partial \mathcal{L}}{\partial \sigma_n^2} &= \frac{(\tau + d)}{2} \text{tr}(U^{-1}) - \frac{\tau}{2} \text{tr}((K')^{-1}), \\ \frac{\partial \mathcal{L}}{\partial \theta_i} &= \frac{(\tau + d)}{2} \text{tr}\left(U^{-1} \frac{\partial K_\theta}{\partial \theta_i}\right) - \frac{\tau}{2} \text{tr}\left(\Sigma^{-1} \frac{\partial K_\theta}{\partial \theta_i}\right), \\ \frac{\partial \mathcal{L}}{\partial \phi_{ij}} &= -\frac{(\tau + d)}{2} \text{tr}[U^{-1} \alpha_\Omega^T (\mathbf{E}_{ij} \Phi^T + \Phi \mathbf{E}_{ji}) \alpha_\Omega] \\ &\quad + \frac{n}{2} \text{tr}[\Omega^{-1} (\mathbf{E}_{ij} \Phi^T + \Phi \mathbf{E}_{ji})], \\ \frac{\partial \mathcal{L}}{\partial \varphi_{ii}} &= -\frac{(\tau + d)}{2} \text{tr}[U^{-1} \alpha_\Omega^T (\mathbf{J}_{ii} \Phi^T + \Phi \mathbf{J}_{ii}) \alpha_\Omega] \\ &\quad + \frac{n}{2} \text{tr}[\Omega^{-1} (\mathbf{J}_{ii} \Phi^T + \Phi \mathbf{J}_{ii})], \end{aligned}$$

where $U = K' + Y \Omega^{-1} Y^T$, $\tau = \nu + n - 1$ and $\psi_n(\cdot)$ is the derivative of the function $\ln \Gamma_n(\cdot)$ with respect to ν . The details are provided in “Multivariate Student-*t* process regression” in Appendix.

Remark 2 It is known that the marginal likelihood function in GPR models is not usually convex with respect to the hyperparameters; therefore, the optimization algorithm may converge to a local optimum, whereas the global one provides better result [12]. As a result, the optimized

hyperparameters obtained by maximum likelihood estimation and the performance of GPR models may depend on the initial values of the optimization algorithm [6, 18, 28, 29]. A common strategy adopted by most GPR practitioners is a heuristic method. That is, the optimization is repeated using several initial values generated randomly from a prior distribution based on their expert opinions and experiences, for example, using ten initial values randomly selected from a uniform distribution. The final estimates of the hyperparameters are the ones with the largest likelihood values after convergence [6, 28, 29]. Further discussion on how to select suitable initial hyperparameters can be found in [9, 29]. In our numerical experiments, the same heuristic method is used for both MV-GPR and MV-TPR.

Remark 3 Another issue related to the Gaussian process and Student-*t* process models is the existence of the maximum likelihood estimators. To guarantee the existence of the MLE, one needs to show that there exists a solution to the system of equations that the derivatives of the marginal likelihood equal 0 and to prove that the Hessians at the solution are negative definite. However, due to the complex structure of these models and non-concavity of their likelihood functions, this issue has not been theoretically studied to the best of our knowledge, even for the conventional univariate Gaussian process regression models, although the numerical examples and applications in the literature have shown that the likelihood functions in the GPR models often have many local optima and the heuristic method discussed in Remark 2 need to be used in order to find an estimate as optimal as possible. For the MV-GPR and MV-TPR models, in practice we can impose a reasonable range for the parameters based on the data so that (local) optima of the marginal likelihoods always exist. In fact, our numerical examples demonstrate that the likelihood functions are not concave and there often exist multiple local optima; hence, several random initial values are used in order to find optimal estimates of the parameters. Of course, this procedure is not guaranteed to find the global optimum, but our experiments have provided much empirical evidence that for the proposed MV-GPR and MV-TPR (local) optima can be found and the models with these local optima as the estimates of the hyperparameters perform better than many existing models. As the focus of this paper is to propose multi-output prediction methods using Gaussian process and Student-*t* process and to demonstrate its usefulness through numerical examples and the maximum likelihood method is just an example for the model parameter estimation, the issue of the existence of MLE is not further studied here and will be investigated in our future work.

4 Experiments

In this section, we demonstrate the usefulness of MV-GPR and our proposed MV-TPR using some numerical examples, including simulated data and real data.

4.1 Simulated example

We first use simulation examples to evaluate the quality of the parameter estimation and the prediction performance of the proposed models.

4.1.1 Evaluation of parameter estimation

We generate random samples from a bivariate Gaussian process $y \sim \mathcal{MG}\mathcal{P}(0, k', \Omega)$, where k' is defined as in (3) with the kernel k_{SE} . The hyperparameters in k_{SE} are set as $[\ell, s_f^2] = [0.5, 2.5]$ and $\Omega = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$. The variance of the random noise in k' takes values $\sigma_n^2 = 0.1, 0.05$ and 0.01 . As explained in Sect. 3.1, in our models the random noises are included in the kernel; therefore, no additional random errors can be added when the random samples are generated; otherwise, two random error terms will result in identifiability issues in the parameter estimation. The covariate x has 100 equally spaced values in $[0, 1]$. We utilize the heuristic method discussed in Remark 2 to estimate the parameters. The experiment is repeated 50 times, and we use the parameter median relative error (pMRE) as a measure of the quality of the estimates [4]:

$$\text{pMRE} = \text{median} \left\{ \frac{|\hat{\theta}_i - \theta|}{\theta}, i = 1, 2, \dots, 50 \right\},$$

where $|\cdot|$ is the absolute value, $\hat{\theta}_i$ is the parameter estimates in repetition i and θ is the true parameter. The results are shown in Table 1.

The similar experiment is also conducted for MV-TPR, where the samples are generated from a bivariate Student-*t*

Table 1 The pMREs of MV-GP samples with different noise levels estimated by MV-GPR

Noise level σ_n^2	0.1	0.05	0.01
$\hat{\sigma}_n^2$	0.041	0.041	0.041
\hat{s}_f^2	0.235	0.235	0.238
$\hat{\ell}^2$	0.080	0.079	0.078
$\hat{\phi}_{11}$	0.284	0.280	0.271
$\hat{\phi}_{22}$	0.282	0.279	0.276
$\hat{\phi}_{12}$	0.645	0.645	0.632

Table 2 The pMREs of MV-TP samples with different noise levels estimated by MV-TPR

Noise level σ_n^2	0.1	0.05	0.01
$\hat{\sigma}_n^2$	0.053	0.058	0.061
\hat{s}_f^2	0.181	0.178	0.163
$\hat{\ell}^2$	0.083	0.075	0.071
$\hat{\varphi}_{11}$	0.015	0.015	0.014
$\hat{\varphi}_{22}$	0.013	0.013	0.013
$\hat{\varphi}_{12}$	0.007	0.007	0.007
$\hat{\nu}$	0.193	0.190	0.179

process $\mathbf{y} \sim \mathcal{MTP}(\nu, 0, k', \Omega)$ with the same true parameters as above and $\nu = 3$. The results are reported in Table 2.

It can be seen that most of the parameters are well estimated in both cases, except the parameters in the row covariance matrix (φ_{11} , φ_{22} and φ_{12}) in MV-GPR which are not as good but reasonable. This may be because the conjugate gradient optimization algorithm does not manage to reach the global maxima of the likelihood function. Better results may be achieved using optimal design for parameter estimation as discussed in [4]. In general, the estimates of the parameters are closer to the true values as the noise level decreases, but the improvement in terms of estimation accuracy is not significant.

4.2 Evaluation of prediction accuracy

Now, we consider a simulated data from two specific functions. The true model used to generate data is given by

$$\mathbf{y} = [f_1(x), f_2(x)] + [\varepsilon^{(1)}, \varepsilon^{(2)}],$$

$$f_1(x) = 2x \cos(x), \quad f_2(x) = 1.5x \cos(x + \pi/5),$$

where the random noise $[\varepsilon^{(1)}, \varepsilon^{(2)}] \sim \mathcal{MGP}(0, k_{SE}, \Omega)$. We select k_{SE} with parameter $[\ell, s_f^2] = [1.001, 5]$ and $\Omega = \begin{pmatrix} 1 & 0.25 \\ 0.25 & 1 \end{pmatrix}$. The covariate x has 100 equally spaced values in $[-10, 10]$ so that a sample of 100 observations for y_1 and y_2 are obtained.

For model training, we use fewer points with one part missing so that the z th training data points with $z =$

$\{3r + 1\}_{r=0}^{14} \cup \{3r + 2\}_{r=21}^{32}$ are selected for both y_1 and y_2 . The prediction is then performed for the remaining covariate values in the interval $[-10, 10]$. The RMSEs between the predicted values and the true ones from $f_1(x)$ and $f_2(x)$ are calculated. For comparison, the conventional GPR and TPR models are also applied to the two outputs independently. The above experiment is repeated 1000 times, and the ARMSE (average root mean square error), defined by

$$\text{ARMSE} = \frac{1}{N_r} \sum_{i=1}^{N_r} \left(\frac{1}{N_s} \sum_{j=1}^{N_s} (\hat{y}_l^{(ij)} - f_l^{(ij)})^2 \right)^{\frac{1}{2}}, \quad l = 1, 2,$$

is calculated. Here, N_r is the number of repeats, N_s is the number of data points, $f_l^{(ij)}$ is the j th true function value of f_l in the i th repetition and $\hat{y}_l^{(ij)}$ is the corresponding predicted value. The ARMSEs for both training and test points in $[-10, 10]$ are reported in Table 3, and an example of prediction is demonstrated in Fig. 1.

The similar experiment is also conducted for the case where the random noise follows a multivariate Student- t process $[\varepsilon^{(1)}, \varepsilon^{(2)}] \sim \mathcal{MTP}(3, 0, k_{SE}, \Omega)$. We select k_{SE} with parameter $[\ell, s_f^2] = [1.001, 5]$ and $\Omega = \begin{pmatrix} 1 & 0.25 \\ 0.25 & 1 \end{pmatrix}$. The resulted ARMSEs are presented in Table 4, and an example of prediction is demonstrated in Fig. 2.

From the tables and figures above, it can be seen that the multivariate process regression models are able to discover a more desired pattern in the gap compared with the conventional GPR and TPR models used independently. It also reveals that taking the correlations between the two outputs into consideration improves the accuracy of prediction compared with the methods of modeling each output independently. In particular, MV-TPR performs better than MV-GPR in the predictions for both types of noisy data while the performances by TPR and GPR are similar.

It is not surprising that in general MV-TPR works better than MV-GPR when the outputs have dependencies, because the former has more modeling flexibility with one more parameter which captures the degree of freedom. Theoretically, MV-TP converges to MV-GP if the degree of freedom tends to infinity, and to some extent, MV-GPR is a special case of MV-TPR. In the above experiment

Table 3 The ARMSE by the different models (multivariate Gaussian noisy data)

	Output 1 (y_1)				Output 2 (y_2)			
	MV-GPR	MV-TPR	GPR	TPR	MV-GPR	MV-TPR	GPR	TPR
Training	0.877	0.884	0.880	0.875	0.862	0.849	0.864	0.862
Test	1.453	1.309	1.869	1.869	1.282	1.145	1.478	1.480

Fig. 1 Predictions for MV-GP noise data using different models. From panels **a–d** predictions for y_1 by MV-GPR, MV-TPR, GPR and TPR. From panels **e–h** predictions for y_2 by MV-GPR, MV-TPR, GPR and TPR. The solid blue lines are predictions, the solid red lines are the true functions and the circles are the observations. The dash lines represent the 95% confidence intervals (colour figure online)

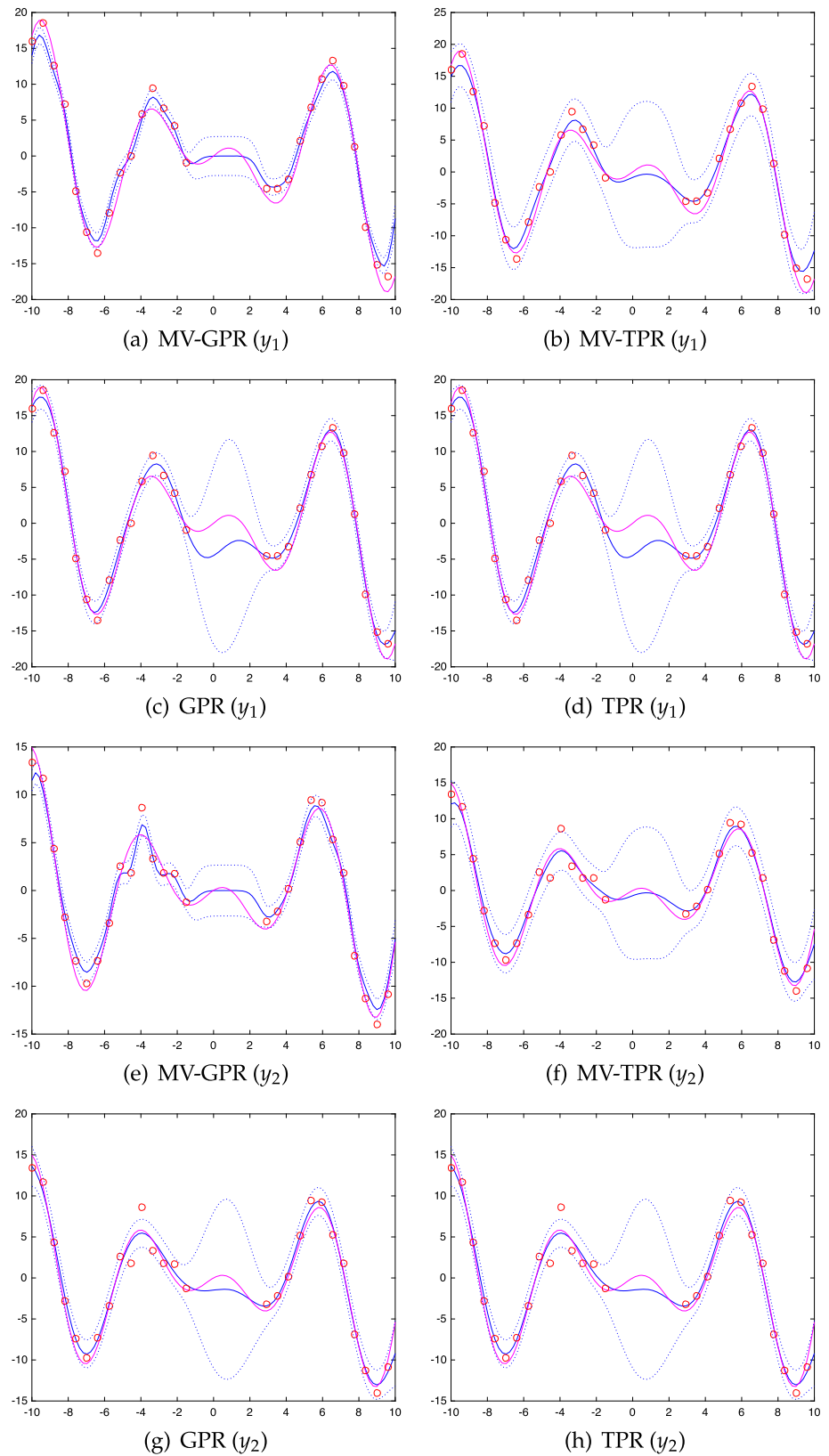


Table 4 The ARMSE by the different models (multivariate Student-*t* noisy data)

	Output 1 (y_1)				Output 2 (y_2)			
	MV-GPR	MV-TPR	GPR	TPR	MV-GPR	MV-TPR	GPR	TPR
Training	0.927	0.919	0.892	0.890	0.871	0.850	0.852	0.850
Test	1.496	1.332	1.870	1.867	1.315	1.156	1.520	1.521

because the observations, even generated from MV-GP, may contain outliers and the sample size (23 training points) is small, MV-TPR with a large degree of freedom may fit the data better than MV-GPR and hence provides a better prediction. These findings coincide with those in [24] in the context of univariate Student-*t* process regressions. On the other hand, while a training sample of size 23 may be too small for two-dimensional processes such that MV-TPR performs better than MV-GPR, it may be large enough for one-dimensional processes, leading to similar performances by TPR and GPR.

4.3 Real-data examples

We further test our proposed methods on two real datasets.¹ The selected mean function is zero offset, and the selected kernel is SEard. Before the experiments are conducted, all the data have been normalized by

$$\tilde{y}_i = \frac{y_i - \mu}{\sigma},$$

where μ and σ are the sample mean and standard deviation of the data $\{y_i\}_{i=1}^n$, respectively.

4.3.1 Bike rent prediction

This dataset contains the hourly and daily count of rental bikes between years 2011 and 2012 in Capital Bikeshare System with the corresponding weather and seasonal information [13]. There are 16 attributes. We test our proposed methods for multi-output prediction based on daily count dataset. After deleting all the points with missing attributes, we use the first 168 data points in the season autumn because the data are observed on a daily basis (1 week = 7 days) and the whole dataset is divided into eight subsets. (Each subset has 3-weeks' data points.) In the experiment, the input comprises eight attributes, including normalized temperature, normalized feeling temperature, normalized humidity, normalized wind speed, whether the day is holiday or not, day of the week, working day or not and weathersit. The output consists of two attributes, including the count of casual users (Casual) and the count of registered users (Registered).

¹ These datasets are from the UC Irvine Machine Learning Repository (<https://archive.ics.uci.edu/ml/index.php>).

The cross-validation method is taken as *k*-fold, where *k* = 8. Each subset is considered as a test set, and the remaining subsets are considered as a training set. Four models, including MV-GPR, MV-TPR, GPR (to predict each output independently) and TPR (to predict each output independently), are applied to the data, and predictions are made based on the divided training and test sets. The process is repeated for eight times, and for each subset's prediction, the MSE (mean square error) and the MAE (mean absolute error) are calculated. The medians of the eight MSEs and MAEs are then used to evaluate the performance for each output. Finally, the maximum median of all the outputs (MMO) is used to evaluate the overall performance of the multi-dimensional prediction. The results are shown in Table 5. It can be seen that MV-TPR significantly outperforms all the other models in terms of MSE and MAE, and MV-GPR performs the second best, while TPR is slightly better than GPR.

4.3.2 Air quality prediction

The dataset contains 9,358 instances of hourly averaged responses from an array of five metal oxide chemical sensors embedded in an Air Quality Chemical Multisensor Device with 15 attributes [11]. We delete all the points with missing attributes (887 points remaining). The first 864 points are considered in our experiment because the data are hourly observed (1 day = 24 h) and the whole dataset is divided into nine subsets. (Each subset has 4-days' data points, totally 864 data points.) In the experiment, the input comprises nine attributes, including time, true hourly averaged concentration CO in mg/m³ (COGT), true hourly averaged overall non-metanic hydrocarbons concentration in microg/m³ (NMHCGT), true hourly averaged benzene concentration in microg/m³ (C6H6GT), true hourly averaged NO_x concentration in ppb (NO_x), true hourly averaged NO₂ concentration in microg/m³ (NO₂), absolute humidity (AH), temperature (T) and relative humidity (RH). The output consists of five attributes, including PT08.S1 (tin oxide) hourly averaged sensor response, PT08.S2 (titania) hourly averaged sensor response, PT08.S3 (tungsten oxide) hourly averaged sensor response, PT08.S4 (tungsten oxide) hourly averaged sensor response and PT08.S5 (indium oxide) hourly averaged sensor response.

Fig. 2 Predictions for MV-TP noise data using different models. From panels **a–d** predictions for y_1 by MV-GPR, MV-TPR, GPR and TPR. From panels **e–h** predictions for y_2 by MV-GPR, MV-TPR, GPR and TPR. The solid blue lines are predictions, the solid red lines are the true functions and the circles are the observations. The dash lines represent the 95% confidence intervals (colour figure online)

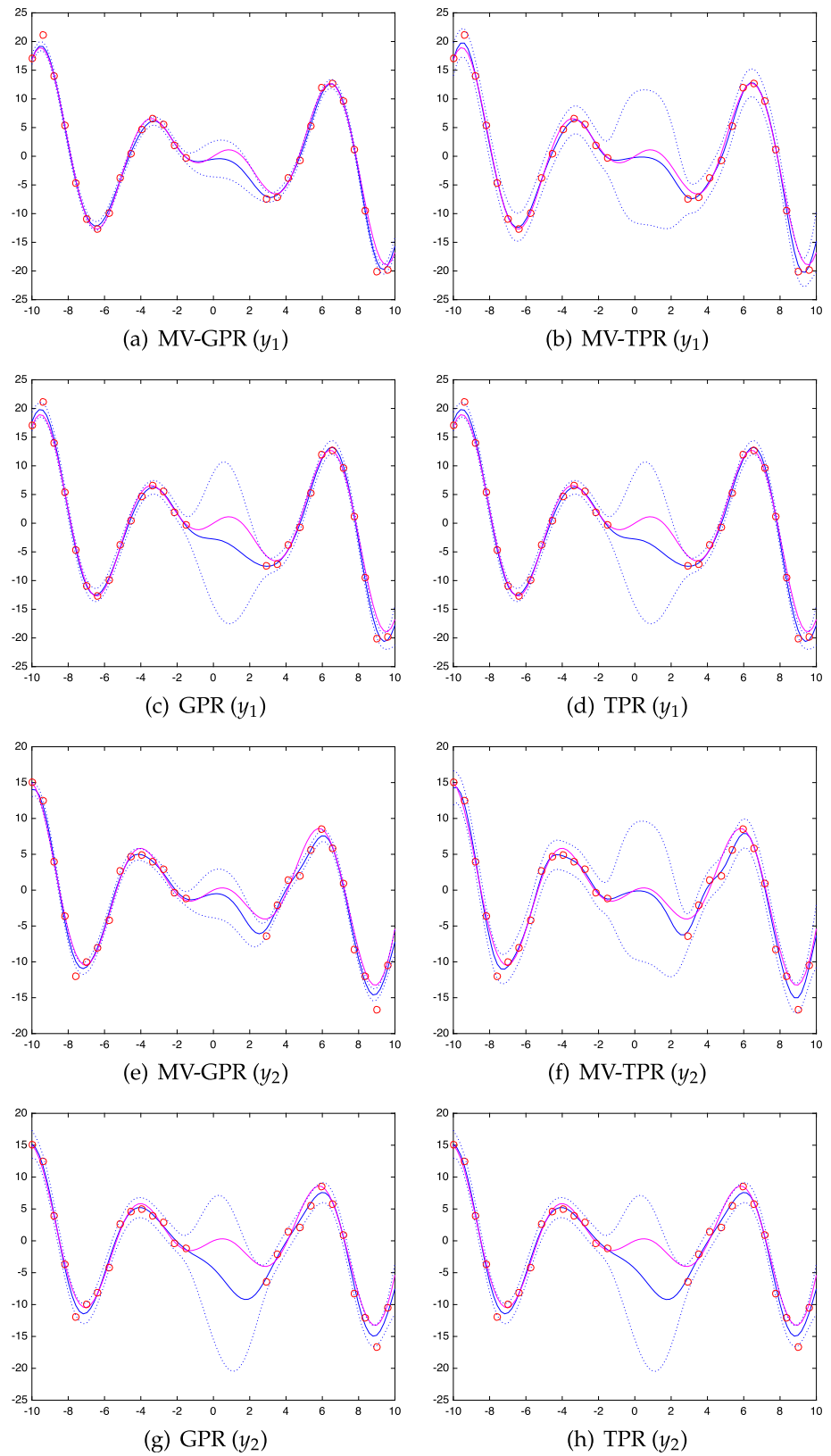


Table 5 Bike rent prediction results based on MSEs and MAEs

	MV-GPR	MV-TPR	GPR	TPR
(a) MSE				
Casual	0.411	0.334	0.424	0.397
Registered	0.982	0.903	1.134	1.111
MMO	0.982	0.903	1.134	1.111
(b) MAE				
Casual	0.558	0.488	0.540	0.546
Registered	0.897	0.855	0.916	0.907
MMO	0.897	0.855	0.916	0.907

The cross-validation method is taken as k -fold, where $k = 9$. The remaining modeling procedure is the same as in the bike rent prediction experiment, except that k is 9 so that the process is repeated nine times. The results are shown in Table 6. It can be observed that MV-TPR consistently outperforms MV-GPR, and in overall terms, MV-GPR does not perform as well as independent GPR. These results can likely be explained as follows. In fact, in our proposed framework, all the outputs are considered as a whole and the same kernel (and hyperparameters) is used for all the outputs, which may not be appropriate if different outputs have very different patterns (which is the case in this example). On the other hand, in the independent modeling different GPR models are used for different outputs and they can have different hyperparameters even though the kernel is the same, which may result in better prediction accuracy. It is noted that in this example, MV-

TPR still works better than MV-GPR because the former offers more modeling flexibility and is thus more robust to model misspecification. This finding is consistent with that by [24] for the univariate Student- t process.

4.4 Application to stock market investment

In the previous subsections, the examples show the usefulness of our proposed methods in terms of more accurate prediction. Furthermore, our proposed methods can be applied to produce trading strategies in the stock market investment.

It is known that the accurate prediction of future for an equity market is almost impossible. Admittedly, the more realistic idea is to make a strategy based on the Buy&Sell signal in the different prediction models [1]. In this paper, we consider a developed Dollar 100 (dD100) as a criterion of the prediction models. The dD100 criterion is able to reflect the theoretical future value of \$100 invested at the beginning, and traded according to the signals constructed by predicted value and the reality. The details of dD100 criterion are described in Sect. 4.4.2.

Furthermore, the equity index is an important measurement of the value of a stock market and is used by many investors making trades and scholars studying stock markets. The index is computed from the weighted average of the selected stocks' prices, so it is able to describe how the whole stock market in the consideration performs in a period, and thus many trading strategies of a stock or a portfolio have to take the information of the index into account. As a result, our experimental predictions for specific stocks are based on the indices as well.

Table 6 Air quality prediction results based on MSEs and MAEs

	MV-GPR	MV-TPR	GPR	TPR
(a) MSE				
PT08S1CO	0.091	0.065	0.079	0.074
PT08S2NMHC	8.16×10^{-5}	3.42×10^{-5}	1.91×10^{-7}	7.32×10^{-8}
PT08S3NOx	0.036	0.027	0.022	0.025
PT08S4NO2	0.015	0.014	0.010	0.009
PT08S5O3	0.092	0.073	0.060	0.067
MMO	0.092	0.073	0.079	0.074
(b) MAE				
PT08S1CO	0.240	0.204	0.212	0.223
PT08S2NMHC	6.39×10^{-3}	1.15×10^{-2}	1.80×10^{-4}	9.26×10^{-5}
PT08S3NOx	0.141	0.122	0.115	0.120
PT08S4NO2	0.095	0.089	0.079	0.073
PT08S5O3	0.231	0.210	0.199	0.205
MMO	0.240	0.210	0.212	0.223

4.4.1 Data preparation

We obtain daily price data, containing opening, closing and adjusted closing for the stocks (the details are shown in Sects. 4.4.3 and 4.4.4) and three main indices in the USA, Dow Jones Industrial Average (INDU), S&P500 (SPX) and NASDAQ (NDX) from Yahoo Finance in the period of 2013–2014. The log returns of the adjusted closing price and inter-day log returns are obtained by defining

$$\text{Log return: } LR_i = \ln \frac{ACP_i}{ACP_{i-1}},$$

$$\text{Inter-day log return: } ILR_i = \ln \frac{CP_i}{OP_i},$$

where ACP_i is the adjusted closing price of the i th day ($i > 1$), CP_i is the closing price of the i th day, and OP_i is the opening price of the i th day. Therefore, there are totally 503 daily log returns and log inter-day returns for all the stocks and indices from 2013 to 2014.

4.4.2 Prediction model and strategy

The sliding windows method is used for our prediction models, including GPR, TPR, MV-GPR and MV-TPR, based on the indices, INDU, SPX and NDX. The training sample is set as 303, which is used to forecast for the next 10 days, and the training set is updated by dropping off the earliest 10 days and adding on the latest 10 days when the window is moved. The sliding-forward process was run 20 times, resulting in a total of 200 prediction days, in groups of 10. The updated training set allows all the models and parameters to adapt the dynamic structure of the equity market [1]. Specifically, the inputs consist of the log returns of three indices, the targets are multiple stocks' log returns and standard exponential with automatic relevance determination (SEard) is used as the kernel for all of these prediction models.

It is noteworthy that the predicted log returns of stocks are used to produce a buy or sell signal for trading rather than to discover an exact pattern of the future. The signal BS produced by the predicted log returns of the stocks is defined by

$$BS_i = \hat{LR}_i - LR_i + ILR_i, i = 1, \dots, 200,$$

where $\{\hat{LR}_i\}_{i=1}^{200}$ are the predicted log returns of a specific stock and $\{LR_i\}_{i=1}^{200}$ are the true log returns, while $\{ILR_i\}_{i=1}^{200}$ are the inter-day log returns. The Buy&Sell strategy relying on the signal BS is described in Table 7.

It is noted that the stocks in our experiment are counted in Dollar rather than the number of shares, which means in theory we can precisely buy or sell a specific Dollar-valued stock. For example, if the stock price is \$37 when we only

Table 7 Buy&Sell strategy of dD100 investment

Decision	Condition
Buy	$\hat{LR}_i > 0$, and $BS_i > 0$ and we have the position of cash
Sell	$\hat{LR}_i < 0$, and $BS_i < 0$ and we have the position of share
Keep	No action is taken for the rest of the option

have \$20, we can still buy \$20-valued stock rather than borrowing \$17 and then buy 1 share. Furthermore, it is also necessary to explain why we choose the signal BS . By the definition, we rewrite it as:

$$\begin{aligned} BS_i &= \ln \left(\frac{\hat{ACP}_i}{ACP_{i-1}} \right) - \ln \left(\frac{ACP_i}{ACP_{i-1}} \right) + \ln \left(\frac{CP_i}{OP_i} \right) \\ &= \ln \left(\frac{\hat{ACP}_i}{ACP_{i-1}} \right) - \ln \left(\frac{ACP_i}{ACP_{i-1}} \right) + \ln \left(\frac{ACP_i}{AOP_i} \right) \\ &= \ln \left(\frac{\hat{ACP}_i}{AOP_i} \right), \end{aligned}$$

where $\{ACP_i\}_{i=0}^{200}$ are the last 201 adjusted closing prices for a stock, $\{CP\}_{i=1}^{200}$ are the last 200 closing prices, and $\{AOP\}_{i=1}^{200}$ are the adjusted opening prices. If $BS_i > 0$, the predicted closing price should be higher than the adjusted opening price, which means we can obtain the inter-day profit by buying the shares at the opening price² as long as the signal based on our predictions is accurate. Meanwhile, the opposite manipulation based on BS strategy means that we can avoid the inter-day loss by selling decisively at the opening price. Furthermore, the reasonable transaction fee 0.025% is considered in the experiment since the strategy might trade frequently.³ As a result, this is a reasonable strategy since we can definitely obtain a profit by buying the shares and cut the loss by selling the shares in time only if our prediction has no serious problem. It is also an executable strategy because the decision is made based on the next day's reality and our prediction models.

At last, BS signal varies in different prediction models so that we denote these Buy&Sell strategies based on MV-GPR, MV-TPR, GPR and TPR model as MV-GPR strategy, MV-TPR strategy, GPR strategy and TPR strategy, respectively.

² Actually, the value has to be considered as adjusted opening price since all the shares are counted in Dollar. The adjusted opening price is also easy to compute based on the real opening price and the dividend information.

³ The figure 0.025% is comprehensive consideration referred to NASDAQ website:<http://nasdaq.cchwallstreet.com/>.

Table 8 Three biggest “Chinese concept” stocks

Ticker	Exchange	Company
BIDU	NASDAQ	Baidu, Inc.
CTRP	NASDAQ	Ctrip.com International, Ltd.
NTES	NASDAQ	NetEase, Inc.

4.4.3 Chinese companies in NASDAQ

In recent years, the “Chinese concepts stock” has received an extensive attention among international investors owing to the fast development of Chinese economy and an increasing number of Chinese firms have been traded in the international stock markets [16]. The “Chinese concepts stock” refers to the stock issued by firms whose asset or earning have essential activities in Mainland China. Undoubtedly, all these “Chinese concept stocks” are heavily influenced by the political and economic environment of China together. For this reason, all these stocks have the

potential and unneglectable correlation theoretically, which is probably reflected in the movement of stock prices. The performance of multiple targets prediction, which takes the potential relationship into consideration, should be better. Therefore, the first real-data example is based on three biggest Chinese companies described in Table 8.

We apply MV-GPR, MV-TPR, GPR and TPR strategies, and the results are demonstrated in Fig. 3. Furthermore, Tables 12, 13 and 14 in “Appendix 2: Three Chinese stocks investment details” in Appendix summarize the results by period for each stock, respectively. In particular, the Buy&Sell signal examples for each stock are shown in Tables 15, 16 and 17 in “Appendix 2: Three Chinese stocks investment details” in Appendix, respectively, along with other relevant details.

From the view of Fig. 3, there is no doubt that a \$100 investment for each stock has sharply increased over 200 days period using Buy&Sell strategies no matter whether the stock went up or down during this period. In particular, the stock prices of BIDU and NTES rose up gradually while CTRP hit the peak and then decreased in a large

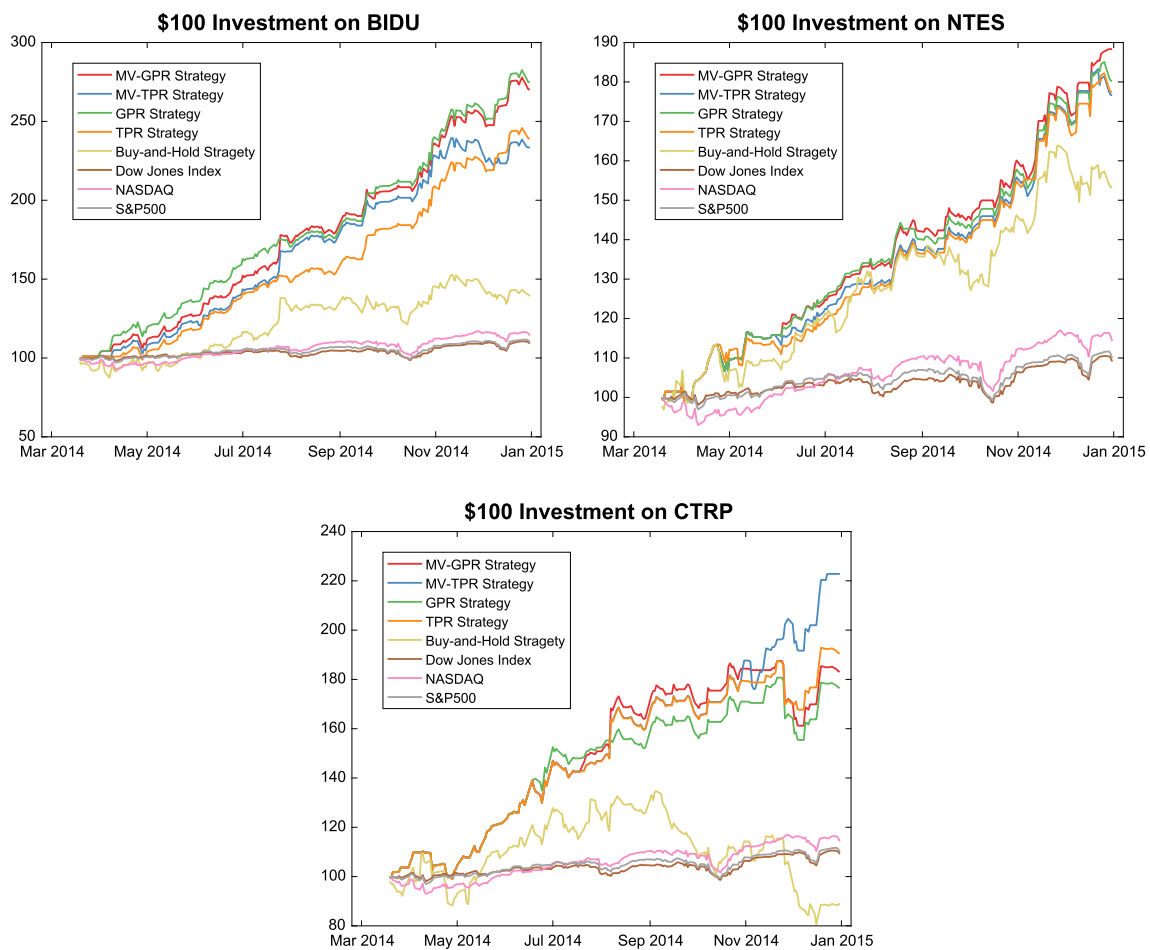


Fig. 3 The movement of invested \$100 in 200 days for three Chinese stocks in the US market. The top four lines in legend are Buy&Sell strategies based on four prediction models: MV-GPR, MV-TPR, GPR

and TPR, respectively. The last four lines are Buy&Hold strategies for the stock and for the three indices: INDU, NASDAQ and NDX, respectively

Table 9 Stock components of Dow 30

Ticker	Company	Exchange	Industry	Industry ⁴ (ICB)
DD	DuPont	NYSE	Chemical industry	Basic Materials
KO	Coca-Cola	NYSE	Beverages	Consumer Goods
PG	Procter and Gamble	NYSE	Consumer goods	Consumer Goods
MCD	McDonald's	NYSE	Fast food	Consumer Goods
NKE	Nike	NYSE	Apparel	Consumer Services
DIS	Walt Disney	NYSE	Broadcasting and entertainment	Consumer Services
HD	The Home Depot	NYSE	Home improvement retailer	Consumer Services
WMT	Wal-Mart	NYSE	Retail	Consumer Services
JPM	JPMorgan Chase	NYSE	Banking	Financials
GS	Goldman Sachs	NYSE	Banking, financial services	Financials
V	Visa	NYSE	Consumer banking	Financials
AXP	American Express	NYSE	Consumer finance	Financials
TRV	Travelers	NYSE	Insurance	Financials
UNH	UnitedHealth Group	NYSE	Managed health care	Health Care
JNJ	Johnson & Johnson	NYSE	Pharmaceuticals	Health Care
MRK	Merck	NYSE	Pharmaceuticals	Health Care
PFE	Pfizer	NYSE	Pharmaceuticals	Health Care
BA	Boeing	NYSE	Aerospace and defense	Industrials
MMM	3M	NYSE	Conglomerate	Industrials
GE	General Electric	NYSE	Conglomerate	Industrials
UTX	United Technologies	NYSE	Conglomerate	Industrials
CAT	Caterpillar	NYSE	Construction and mining equipment	Industrials
CVX	Chevron	NYSE	Oil and gas	Oil and Gas
XOM	ExxonMobil	NYSE	Oil and gas	Oil and Gas
CSCO	Cisco Systems	NASDAQ	Computer networking	Technology
IBM	IBM	NYSE	Computers and technology	Technology
AAPL	Apple	NASDAQ	Consumer electronics	Technology
INTC	Intel	NASDAQ	Semiconductors	Technology
MSFT	Microsoft	NASDAQ	Software	Technology
VZ	Verizon	NYSE	Telecommunication	Telecommunications

Note that the terms “industry” and “sector” are reversed from the Global Industry Classification Standard (GICS) taxonomy

scale. Anyway, the Buy&Sell strategies based on different prediction models have still achieved considerable profits compared with Buy&Hold strategies for the corresponding investments. However, the different prediction models have diverse performances for each stock. For BIDU, GPR-based models, including MV-GPR and GPR, outperform TPR-based models, including MV-TPR and TPR. For NTES, all the models for Buy&Sell strategy have a similar performance. Admittedly, TPR-based models, especially MV-TPR, have an outstanding performance for stock CTRP.

4.4.4 Diverse sectors in Dow 30

Owing to the globalization of capital, there has been a significant shift in the relative importance of national and economic influences in the world's largest equity markets

and the impact of industrial sector effects is now gradually replacing that of country effects in these markets [3]. Therefore, a further example is carried out under the diverse industrial sectors in Dow 30 from New York Stock Exchange (NYSE) and NASDAQ.

Initially, the classification of stocks based on diverse industrial sectors in Dow 30 has to be done. There are two main industry classification taxonomies, including Industry Classification Benchmark (ICB) and Global Industry Classification Standard (GICS). In our research, ICB is used to segregate markets into sectors within the macroeconomy. The stocks in Dow 30 are classified in Table 9.

Due to the multivariate process models considering at least two related stocks in one group, the first (Basic Materials) and the last industrial sector (Telecommunications), each consisting of only one stock, are excluded. As a result, our experiments are performed seven times for the

Table 10 Stock investment performance ranking under different strategies

Ticker	Industry	Buy&Sell strategy				Buy&Hold strategy			
		MV-GPR	MV-TPR	GPR	TPR	Stock	INDU	NDX	SPX
CVX	Oil and Gas	3rd	4th	2nd	<i>1st</i>	8th	7th	5th	6th
XOM	Oil and Gas	4th	2nd	3rd	<i>1st</i>	8th	7th	5th	6th
MMM	Industrials	2nd	3rd	<i>1st</i>	4th	5th	8th	6th	7th
BA	Industrials	<i>1st</i>	2nd	3rd	4th	8th	7th	5th	6th
CAT	Industrials	3rd	4th	2nd	<i>1st</i>	8th	7th	5th	6th
GE	Industrials	2nd	4th	3rd	<i>1st</i>	8th	7th	5th	6th
UTX	Industrials	2nd	4th	3rd	<i>1st</i>	8th	7th	5th	6th
KO	Consumer Goods	2nd	<i>1st</i>	3rd	4th	6th	8th	5th	7th
MCD	Consumer Goods	2nd	4th	<i>1st</i>	3rd	8th	7th	5th	6th
PG	Consumer Goods	3rd	4th	<i>1st</i>	2nd	5th	8th	6th	7th
JNJ	Health Care	3rd	2nd	<i>1st</i>	4th	6th	8th	5th	7th
MRK	Health Care	3rd	2nd	4th	<i>1st</i>	8th	7th	5th	6th
PFE	Health Care	4th	<i>1st</i>	3rd	2nd	8th	7th	5th	6th
UNH	Health Care	2nd	3rd	<i>1st</i>	4th	5th	8th	6th	7th
HD	Consumer Services	<i>1st</i>	4th	3rd	2nd	5th	8th	6th	7th
NKE	Consumer Services	2nd	3rd	4th	<i>1st</i>	5th	8th	6th	7th
WMT	Consumer Services	<i>1st</i>	4th	3rd	2nd	5th	8th	6th	7th
DIS	Consumer Services	3rd	2nd	<i>1st</i>	4th	5th	8th	6th	7th
AXP	Financials	2nd	4th	<i>1st</i>	3rd	8th	7th	5th	6th
GS	Financials	2nd	<i>1st</i>	3rd	4th	5th	8th	6th	7th
JPM	Financials	2nd	4th	<i>1st</i>	3rd	6th	8th	5th	7th
TRV	Financials	2nd	3rd	<i>1st</i>	4th	5th	8th	6th	7th
V	Financials	<i>1st</i>	4th	3rd	2nd	5th	8th	6th	7th
AAPL	Technology	4th	2nd	3rd	<i>1st</i>	5th	8th	6th	7th
CSCO	Technology	2nd	<i>1st</i>	3rd	4th	5th	8th	6th	7th
IBM	Technology	4th	<i>1st</i>	2nd	3rd	8th	7th	5th	6th
INTC	Technology	3rd	4th	2nd	<i>1st</i>	5th	8th	6th	7th
MSFT	Technology	2nd	4th	<i>1st</i>	3rd	5th	8th	6th	7th

seven grouped industrial sector stocks, including Oil & Gas, Industrial, Consumer Goods, Health Care, Consumer Services, Financials and Technology, respectively.

Secondly, the four models, MV-GPR, MV-TPR, GPR and TPR, are applied in the same way as in Sect. 4.4.3 and the ranking of stock investment performance is listed in Table 10. (The details are summarized in Table 18 in “Appendix 3: Final investment details of stocks in Dow 30” in Appendix.) On the whole, for each stock, there is no doubt that using Buy&Sell strategy is much better than using Buy&Hold strategy regardless of the industrial sector. Specifically, MV-GPR makes a satisfactory performance overall in the sectors, Industrials, Consumer Services and Financials, while MV-TPR has a higher ranking in Health Care in general.

Further analysis is considered using industrial sector portfolios, which consists of these grouped stocks by the same weight investment on each stock. For example, the Oil & Gas portfolio investment is \$100 with \$50 shares CVX and \$50 shares XOM, while the Technology portfolio investment is \$100 with the same \$20 investment on each stock in the

industrial sector Technology. The diverse industry portfolio investment performance ranking is listed in Table 11. (The details are described in Table 19 in “Appendix 3: Final investment details of stocks in Dow 30” in Appendix.) Apparently, the Buy&Sell strategies performed better than the Buy&Hold strategies. MV-GPR suits better in three industries, including Consumer Goods, Consumer Services and Financials, followed by TPR which performed best in Oil & Gas and Industrials. The optimal investment strategy in Health Care is MV-TPR, while in Technology industry, using GPR seems to be the most profitable.

5 Conclusion and discussion

In this paper, we have proposed a unified framework for multi-output regression and prediction. Using this framework, we introduced a novel multivariate Student-*t* process regression model (MV-TPR) and also reformulated the multivariate Gaussian process regression (MV-GPR) which overcomes

Table 11 Industry portfolio investment performance ranking under different strategies

Industry Portfolio	Buy&Sell strategy				Buy&Hold strategy			
	MV-GPR	MV-TPR	GPR	TPR	Stock	INDU	NDX	SPX
Oil and Gas	4th	3rd	2nd	<i>1st</i>	8th	7th	5th	6th
Industrials	2nd	4th	3rd	<i>1st</i>	8th	7th	5th	6th
Consumer Goods	<i>1st</i>	4th	2nd	3rd	7th	8th	5th	6th
Health Care	4th	<i>1st</i>	3rd	2nd	6th	8th	5th	7th
Consumer Services	<i>1st</i>	4th	3rd	2nd	5th	8th	6th	7th
Financials	<i>1st</i>	4th	2nd	3rd	5th	8th	6th	7th
Technology	4th	3rd	<i>1st</i>	2nd	5th	8th	6th	7th

some limitations of the existing methods. It could also be used to derive regression models of general elliptical processes. Under this framework, the model settings, derivations and computations for both MV-GPR and MV-TPR are all directly performed in matrix form. MV-GPR is a more straightforward method compared to the existing vectorization method and can be implemented in the same way as the conventional GPR. Similar to the existing Gaussian process regression for vector-valued function, our models are also able to learn the correlations between inputs and outputs, but with more convenient and flexible formulations. The proposed MV-TPR also possesses closed-form expressions for the marginal likelihood and the predictive distributions under this unified framework. Thus, the same optimization approaches as used in the conventional GPR can be adopted. The usefulness of the proposed methods is illustrated through several numerical examples. It is empirically demonstrated that MV-TPR has superiority in prediction in these examples, including the simulated examples, air quality prediction and bike rent prediction.

The proposed methods are also applied to stock market modeling and are shown to have the ability to make a profitable stock investment. For the three “Chinese concept stocks,” the Buy&Sell strategies based on the proposed models have more satisfactory performances, compared with the Buy&Hold strategies for the corresponding stocks and three main indices in the USA; in particular, the strategy based on MV-TPR has outstanding returns for NetEase among three stocks. When applied to the industrial sectors in Dow 30, the results indicate that the strategies based on MV-GPR have generally considerable performances in Industrials, Consumer Goods, Consumer Services and Financials sectors, while those based on MV-TPR can make maximum profit in Health Care sector.

It is noted that we used the squared exponential kernel for demonstration in all our experiments. However, it can be expected that other kernels or more complicated kernels may lead to better results, especially in the financial data examples, as the SE kernel may oversmooth data; see [22] for more details on the choice of kernels. In this paper, we assume that different outputs are observed at the same covariate values. In practice, different responses may be observed at different

locations. These cases are, however, difficult for the proposed framework since all the outputs have to be considered as a matrix in our models, rather than as a vector with adjustable length. Another issue worth noting is that, as discussed in Sect. 4.3.2, in our proposed framework all the outputs are considered as a whole and the same kernel (and hyperparameters) is used for all the outputs, which may not be appropriate if different outputs have very different patterns such as in the air quality example. Moreover, it is also important to further study how to improve the quality of the parameter estimates, for example using optimal design methods for parameter estimation as discussed in [4]. All of these problems are worth further investigation and exploration and will be our future works.

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Compliance with ethical standards

Conflict of interest The authors declare no conflict of interest.

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Appendix 1: Negative log marginal likelihood and gradient evaluation

Matrix derivatives

According to the chain rule of derivatives of matrix, there exists [14]: Letting $U = f(X)$, the derivatives of the function $g(U)$ with respect to X are

$$\frac{\partial g(U)}{\partial X_{ij}} = \text{tr} \left[\left(\frac{\partial g(U)}{\partial U} \right)^T \frac{\partial U}{\partial X_{ij}} \right],$$

where X is an $n \times m$ matrix. Additionally, there are another two useful formulas of derivative with respect to X :

$$\frac{\partial \ln \det(X)}{\partial X} = X^{-T}, \quad \frac{\partial}{\partial X} \text{tr}(AX^{-1}B) = -(X^{-1}BAX^{-1})^T,$$

where X is an $n \times n$ matrix, A is a constant $m \times n$ matrix and B is a constant $n \times m$ matrix.

Multivariate Gaussian process regression

For a matrix-variate observations $Y \sim \mathcal{MN}_{n,d}(M, \Sigma, \Omega)$ where $M \in \mathbb{R}^{n \times d}$, $\Sigma \in \mathbb{R}^{n \times n}$, $\Omega \in \mathbb{R}^{d \times d}$, the negative log likelihood is

$$\begin{aligned} \mathcal{L} = & \frac{nd}{2} \ln(2\pi) + \frac{d}{2} \ln \det(\Sigma) + \frac{n}{2} \ln \det(\Omega) \\ & + \frac{1}{2} \text{tr}(\Sigma^{-1}(Y - M)\Omega^{-1}(Y - M)^T), \end{aligned} \tag{19}$$

where actually $\Sigma = K + \sigma_n^2 \mathbf{I}$. As we know, there are several parameters in the kernel k so that we can denote $K = K_\theta$. The parameter set denotes $\Theta = \{\theta_1, \theta_2, \dots\}$. Besides, we denote the parameter matrix $\Omega = \Phi\Phi^T$ since Ω is positive semi-definite, where

$$\Phi = \begin{bmatrix} \phi_{11} & 0 & \cdots & 0 \\ \phi_{21} & \phi_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{d1} & \phi_{d2} & \cdots & \phi_{dd} \end{bmatrix}.$$

To guarantee the uniqueness of Φ , the diagonal elements are restricted to be positive and denote $\varphi_{ii} = \ln(\phi_{ii})$ for $i = 1, 2, \dots, d$. Therefore,

$$\frac{\partial \Sigma}{\partial \sigma_n^2} = \mathbf{I}_n, \quad \frac{\partial \Sigma}{\partial \theta_i} = \frac{\partial K_\theta}{\partial \theta_i}, \quad \frac{\partial \Omega}{\partial \phi_{ij}} = \mathbf{E}_{ij}\Phi^T + \Phi\mathbf{E}_{ji},$$

$$\frac{\partial \Omega}{\partial \varphi_{ii}} = \mathbf{J}_{ii}\Phi^T + \Phi\mathbf{J}_{ii},$$

where \mathbf{E}_{ij} is the $d \times d$ elementary matrix having unity in the (i,j)-th element and zeros elsewhere, and \mathbf{J}_{ii} is the same as \mathbf{E}_{ij} but with the unity being replaced by $e^{\varphi_{ii}}$.

The derivatives of the negative log likelihood with respect to σ_n^2 , θ_i , ϕ_{ij} and φ_{ii} are as follows. The derivative with respect to θ_i is

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \theta_i} = & \frac{d}{2} \frac{\partial \ln \det(\Sigma)}{\partial \theta_i} + \frac{1}{2} \frac{\partial}{\partial \theta_i} \text{tr}(\Sigma^{-1}(Y - M)\Omega^{-1}(Y - M)^T) \\ = & \frac{d}{2} \text{tr} \left[\left(\frac{\partial \ln \det(\Sigma)}{\partial \Sigma} \right)^T \frac{\partial \Sigma}{\partial \theta_i} \right] \\ & + \frac{1}{2} \text{tr} \left[\left(\frac{\partial \text{tr}(\Sigma^{-1}G)}{\partial \Sigma} \right)^T \frac{\partial \Sigma}{\partial \theta_i} \right] \\ = & \frac{d}{2} \text{tr} \left(\Sigma^{-1} \frac{\partial K_\theta}{\partial \theta_i} \right) - \frac{1}{2} \text{tr} \left(\Sigma^{-1} G \Sigma^{-1} \frac{\partial K_\theta}{\partial \theta_i} \right) \\ = & \frac{d}{2} \text{tr} \left(\Sigma^{-1} \frac{\partial K_\theta}{\partial \theta_i} \right) - \frac{1}{2} \text{tr} \left(\alpha_\Sigma \Omega^{-1} \alpha_\Sigma^T \frac{\partial K_\theta}{\partial \theta_i} \right), \end{aligned} \tag{20}$$

where $G = (Y - M)\Omega^{-1}(Y - M)^T$ and $\alpha_\Sigma = \Sigma^{-1}(Y - M)$. The fourth equality is due to the symmetry of Σ .

Due to $\partial \Sigma / \partial \sigma_n^2 = \mathbf{I}_n$, the derivative with respect to σ_n^2 is:

$$\frac{\partial \mathcal{L}}{\partial \sigma_n^2} = \frac{d}{2} \text{tr}(\Sigma^{-1}) - \frac{1}{2} \text{tr}(\alpha_\Sigma \Omega^{-1} \alpha_\Sigma^T). \tag{21}$$

Letting $\alpha_\Omega = \Omega^{-1}(Y - M)^T$, the derivative with respect to ϕ_{ij} is

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \phi_{ij}} = & \frac{n}{2} \frac{\partial \ln \det(\Omega)}{\partial \phi_{ij}} + \frac{1}{2} \frac{\partial}{\partial \phi_{ij}} \text{tr}(\Sigma^{-1}(Y - M)\Omega^{-1}(Y - M)^T) \\ = & \frac{n}{2} \text{tr} \left(\Omega^{-1} \frac{\partial \Omega}{\partial \phi_{ij}} \right) \\ & - \frac{1}{2} \text{tr} \left[\left((\Omega^{-1}(Y - M)^T \Sigma^{-1}(Y - M)\Omega^{-1})^T \right)^T \frac{\partial \Omega}{\partial \phi_{ij}} \right] \\ = & \frac{n}{2} \text{tr} \left(\Omega^{-1} \frac{\partial \Omega}{\partial \phi_{ij}} \right) - \frac{1}{2} \text{tr} \left(\alpha_\Omega \Sigma^{-1} \alpha_\Omega^T \frac{\partial \Omega}{\partial \phi_{ij}} \right) \\ = & \frac{n}{2} \text{tr}[\Omega^{-1}(\mathbf{E}_{ij}\Phi^T + \Phi\mathbf{E}_{ji})] \\ & - \frac{1}{2} \text{tr}[\alpha_\Omega \Sigma^{-1} \alpha_\Omega^T (\mathbf{E}_{ij}\Phi^T + \Phi\mathbf{E}_{ji})], \end{aligned} \tag{22}$$

where the third equation is due to the symmetry of Ω . Similarly, the derivative with respect to φ_{ii} is

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \varphi_{ii}} = & \frac{n}{2} \frac{\partial \ln \det(\Omega)}{\partial \varphi_{ii}} \\ & + \frac{1}{2} \frac{\partial}{\partial \varphi_{ii}} \text{tr}(\Sigma^{-1}(Y - M)\Omega^{-1}(Y - M)^T) \\ = & \frac{n}{2} \text{tr}[\Omega^{-1}(\mathbf{J}_{ii}\Phi^T + \Phi\mathbf{J}_{ii})] \\ & - \frac{1}{2} \text{tr}[\alpha_\Omega \Sigma^{-1} \alpha_\Omega^T (\mathbf{J}_{ii}\Phi^T + \Phi\mathbf{J}_{ii})]. \end{aligned} \tag{23}$$

Multivariate Student-*t* process regression

The negative log likelihood of observations $Y \sim \mathcal{MT}_{n,d}(v, M, \Sigma, \Omega)$ where $M \in \mathbb{R}^{n \times d}$, $\Sigma \in \mathbb{R}^{n \times n}$, $\Omega \in \mathbb{R}^{d \times d}$ is

$$\begin{aligned} \mathcal{L} &= \frac{1}{2}(v + d + n - 1) \ln \det(\mathbf{I}_n + \Sigma^{-1}(Y - M)\Omega^{-1}(Y - M)^T) \\ &\quad + \frac{d}{2} \ln \det(\Sigma) + \frac{n}{2} \ln \det(\Omega) + \ln \Gamma_n\left(\frac{1}{2}(v + n - 1)\right) \\ &\quad + \frac{1}{2}dn \ln \pi - \ln \Gamma_n\left(\frac{1}{2}(v + d + n - 1)\right) \\ &= \frac{1}{2}(v + d + n - 1) \ln \det(\Sigma + (Y - M)\Omega^{-1}(Y - M)^T) \\ &\quad - \frac{v + n - 1}{2} \ln \det(\Sigma) + \ln \Gamma_n\left(\frac{1}{2}(v + n - 1)\right) \\ &\quad - \ln \Gamma_n\left(\frac{1}{2}(v + d + n - 1)\right) \\ &\quad + \frac{n}{2} \ln \det(\Omega) + \frac{1}{2}dn \ln \pi. \end{aligned}$$

Letting $U = \Sigma + (Y - M)\Omega^{-1}(Y - M)^T$ and $\alpha_\Omega = \Omega^{-1}(Y - M)^T$, the derivatives of U with respect to $\sigma_n^2, \theta_i, v, \phi_{ij}$ and φ_{ii} are

$$\frac{\partial U}{\partial \sigma_n^2} = \mathbf{I}_n, \quad \frac{\partial U}{\partial \theta_i} = \frac{\partial K_\theta}{\partial \theta_i}, \quad \frac{\partial U}{\partial v} = 0, \tag{24}$$

$$\begin{aligned} \frac{\partial U}{\partial \phi_{ij}} &= -(Y - M)\Omega^{-1} \frac{\partial \Omega}{\partial \phi_{ij}} \Omega^{-1}(Y - M)^T \\ &= -\alpha_\Omega^T \frac{\partial \Omega}{\partial \phi_{ij}} \alpha_\Omega, \end{aligned} \tag{25}$$

$$\begin{aligned} \frac{\partial U}{\partial \varphi_{ii}} &= -(Y - M)\Omega^{-1} \frac{\partial \Omega}{\partial \varphi_{ii}} \Omega^{-1}(Y - M)^T \\ &= -\alpha_\Omega^T \frac{\partial \Omega}{\partial \varphi_{ii}} \alpha_\Omega. \end{aligned} \tag{26}$$

Therefore, the derivative of negative log marginal likelihood with respect to θ_i is

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \theta_i} &= \frac{(\tau + d)}{2} \frac{\partial \ln \det(U)}{\partial \theta_i} - \frac{\tau}{2} \frac{\partial \ln \det(\Sigma)}{\partial \theta_i} \\ &= \frac{(\tau + d)}{2} \text{tr}\left(U^{-1} \frac{\partial K_\theta}{\partial \theta_i}\right) - \frac{\tau}{2} \text{tr}\left(\Sigma^{-1} \frac{\partial K_\theta}{\partial \theta_i}\right), \end{aligned} \tag{27}$$

where the constant $\tau = v + n - 1$.

The derivative with respect to σ_n^2 is

$$\frac{\partial \mathcal{L}}{\partial \sigma_n^2} = \frac{(\tau + d)}{2} \text{tr}(U^{-1}) - \frac{\tau}{2} \text{tr}(\Sigma^{-1}). \tag{28}$$

The derivative with respect to v is

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial v} &= \frac{1}{2} \ln \det(U) - \frac{1}{2} \ln \det(\Sigma) + \frac{1}{2} \psi_n\left(\frac{1}{2} \tau\right) \\ &\quad - \frac{1}{2} \psi_n\left[\frac{1}{2}(\tau + d)\right] \end{aligned} \tag{29}$$

where $\psi_n(\cdot)$ is the derivative of the function $\ln \Gamma_n(\cdot)$ with respect to v .

The derivative of \mathcal{L} with respect to ϕ_{ij} is

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \phi_{ij}} &= \frac{(\tau + d)}{2} \frac{\partial \ln \det(U)}{\partial \phi_{ij}} + \frac{n}{2} \frac{\partial \ln \det(\Omega)}{\partial \phi_{ij}} \\ &= -\frac{(\tau + d)}{2} \text{tr}[U^{-1} \alpha_\Omega^T (\mathbf{E}_{ij} \Phi^T + \Phi \mathbf{E}_{ji}) \alpha_\Omega] \\ &\quad + \frac{n}{2} \text{tr}[\Omega^{-1} (\mathbf{E}_{ij} \Phi^T + \Phi \mathbf{E}_{ji})]. \end{aligned} \tag{30}$$

Similarly, the derivative with respect to φ_{ii} is

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \varphi_{ii}} &= -\frac{(\tau + d)}{2} \text{tr}[U^{-1} \alpha_\Omega^T (\mathbf{J}_{ii} \Phi^T + \Phi \mathbf{J}_{ii}) \alpha_\Omega] \\ &\quad + \frac{n}{2} \text{tr}[\Omega^{-1} (\mathbf{J}_{ii} \Phi^T + \Phi \mathbf{J}_{ii})]. \end{aligned} \tag{31}$$

Appendix 2: Three Chinese stocks investment details

See Tables 12, 13, 14, 15, 16 and 17.

Table 12 The movement of invested \$100 for 200 days split in to 20 periods (Stock: BIDU)

Forecast terms	Buy&Sell decisions by prediction models				Buy&Hold stock/index			
	MV-GPR	MV-TPR	GPR	TPR	BIDU	INDU	NDX	SPX
Beginning (\$)	100				100			
Period 1	103.53	100.97	103.53	100.97	97.14	101.20	98.70	100.71
Period 2	109.80	106.09	115.60	102.03	94.87	99.55	94.10	98.44
Period 3	108.37	104.71	115.96	100.71	93.89	101.50	96.64	100.62
Period 4	117.17	113.22	125.37	108.89	95.21	101.70	96.94	100.87
Period 5	127.84	123.52	136.79	118.80	102.22	102.22	100.79	102.55
Period 6	137.94	130.14	147.59	128.18	107.39	102.44	101.54	103.09
Period 7	146.20	137.93	156.43	135.86	112.11	103.12	103.25	104.54
Period 8	155.97	147.15	166.88	144.94	113.57	103.72	105.34	105.09
Period 9	177.94	167.88	175.27	152.21	138.22	103.82	106.98	105.67
Period 10	179.83	174.07	177.13	153.83	131.26	101.33	104.90	103.17
Period 11	179.08	173.35	176.05	153.19	130.71	104.07	109.34	106.20
Period 12	190.96	184.85	187.73	163.35	137.58	104.75	110.49	106.91
Period 13	201.08	194.63	204.44	177.89	131.12	105.12	109.57	106.52
Period 14	207.28	200.64	210.75	183.38	132.54	104.01	108.35	104.94
Period 15	210.54	203.80	214.06	186.26	132.19	100.39	104.41	101.70
Period 16	233.92	226.43	237.83	206.95	144.35	106.31	112.48	107.77
Period 17	252.47	233.71	256.69	223.36	148.99	108.03	113.68	109.03
Period 18	250.38	227.57	254.56	221.51	143.25	109.45	116.17	110.38
Period 19	260.24	223.38	264.59	230.23	134.23	104.49	110.33	105.37
Period 20	270.29	233.29	274.81	239.13	139.12	109.10	114.29	109.97

Table 13 The movement of invested \$100 for 200 days split in to 20 periods (Stock: CTRP)

Forecast terms	Buy&Sell decisions by prediction models				Buy&Hold stock/index			
	MV-GPR	MV-TPR	GPR	TPR	CTRP	INDU	NDX	SPX
Beginning (\$)	100				100			
Period 1	105.67	105.67	105.67	105.67	100.78	101.20	98.70	100.71
Period 2	102.39	102.52	102.39	102.39	99.65	99.55	94.10	98.44
Period 3	102.77	102.90	102.77	102.77	91.63	101.50	96.64	100.62
Period 4	110.05	110.19	110.05	110.05	100.39	101.70	96.94	100.87
Period 5	121.51	121.66	121.51	121.51	108.33	102.22	100.79	102.55
Period 6	131.02	131.19	131.02	131.02	113.59	102.44	101.54	103.09
Period 7	138.90	139.08	144.25	138.90	120.90	103.12	103.25	104.54
Period 8	140.19	140.37	145.58	140.19	118.02	103.72	105.34	105.09
Period 9	150.29	146.38	151.82	146.20	131.35	103.82	106.98	105.67
Period 10	167.38	163.03	154.49	162.82	128.82	101.33	104.90	103.17
Period 11	166.33	162.01	154.28	161.80	127.37	104.07	109.34	106.20
Period 12	176.07	171.50	163.32	171.28	133.52	104.75	110.49	106.91
Period 13	176.00	171.43	163.25	171.21	117.53	105.12	109.57	106.52
Period 14	170.50	166.08	158.15	165.86	109.88	104.01	108.35	104.94
Period 15	178.68	174.04	165.73	173.82	108.35	100.39	104.41	101.70
Period 16	184.31	187.64	170.96	179.30	114.27	106.31	112.48	107.77
Period 17	183.77	191.85	176.72	180.87	115.96	108.03	113.68	109.03
Period 18	163.88	194.84	158.00	169.76	93.94	109.45	116.17	110.38
Period 19	169.89	201.99	163.80	176.73	80.69	104.49	110.33	105.37
Period 20	183.25	222.82	176.67	190.63	89.20	109.10	114.29	109.97

Table 14 The movement of invested \$100 for 200 days split in to 20 periods (Stock: NTES)

Forecast terms	Buy&Sell decisions by prediction models				Buy&Hold stock/index			
	MV-GPR	MV-TPR	GPR	TPR	NTES	INDU	NDX	SPX
Beginning (\$)	100				100			
Period 1	104.51	104.51	104.51	104.51	106.79	101.20	98.70	100.71
Period 2	106.19	106.19	106.19	106.19	106.35	99.55	94.10	98.44
Period 3	106.80	106.80	106.80	109.12	104.14	101.50	96.64	100.62
Period 4	115.90	115.90	115.90	114.28	108.66	101.70	96.94	100.87
Period 5	115.82	115.82	115.82	114.21	109.84	102.22	100.79	102.55
Period 6	120.96	117.65	120.73	115.20	116.55	102.44	101.54	103.09
Period 7	123.27	121.54	124.72	119.01	120.32	103.12	103.25	104.54
Period 8	127.77	125.33	128.62	122.73	117.34	103.72	105.34	105.09
Period 9	133.21	128.81	134.09	127.95	128.53	103.82	106.98	105.67
Period 10	133.36	128.96	134.24	128.09	127.40	101.33	104.90	103.17
Period 11	141.13	136.47	142.80	135.56	134.83	104.07	109.34	106.20
Period 12	141.45	136.78	139.44	135.87	137.23	104.75	110.49	106.91
Period 13	145.98	141.16	143.90	140.22	134.27	105.12	109.57	106.52
Period 14	147.95	144.00	145.84	143.04	129.90	104.01	108.35	104.94
Period 15	151.75	147.70	149.59	146.71	139.19	100.39	104.41	101.70
Period 16	158.59	154.36	156.33	153.33	144.80	106.31	112.48	107.77
Period 17	170.12	165.58	167.70	165.07	156.05	108.03	113.68	109.03
Period 18	177.19	171.24	174.67	171.93	162.04	109.45	116.17	110.38
Period 19	179.84	177.72	177.28	174.50	153.20	104.49	110.33	105.37
Period 20	188.32	176.70	180.31	177.48	153.52	109.10	114.29	109.97

Table 15 The detailed movement of invested \$100 for last 10 days period (Period 20, Stock: BIDU)

Day	Buy&Sell decisions by prediction models								Buy&Hold stock/index			
	MV-GPR		MV-TPR		GPR		TPR		BIDU	INDU	NDX	SPX
	Act	Dollar	Act	Dollar	Act	Dollar	Act	Dollar				
190	260.24		223.38		264.59		230.23		134.23	104.49	110.33	105.37
191	Buy	263.29	Buy	226.00	Buy	267.69	Buy	232.93	136.60	106.25	112.37	107.51
192	Keep	272.74	Keep	234.11	Keep	277.29	Keep	241.29	141.50	108.83	115.14	110.09
193	Keep	275.50	Keep	236.48	Keep	280.10	Keep	243.73	142.94	108.99	115.52	110.60
194	Keep	275.94	Keep	236.85	Keep	280.55	Keep	244.12	143.16	109.94	115.84	111.02
195	Sell	275.70	Sell	236.65	Sell	280.31	Sell	243.91	142.28	110.33	115.45	111.21
196	Buy	273.26	Buy	234.55	Buy	277.83	Buy	241.75	140.95	110.37	115.55	111.20
197	Keep	277.87	Keep	238.52	Keep	282.52	Keep	245.83	143.33	110.51	116.39	111.56
198	Keep	272.35	Keep	233.77	Keep	276.90	Keep	240.94	140.48	110.42	116.35	111.66
199	Sell	270.29	Keep	233.57	Sell	274.81	Sell	239.13	140.36	110.08	115.53	111.11
200	Keep	270.29	Sell	233.29	Keep	274.81	Keep	239.13	139.12	109.10	114.29	109.97

Table 16 The detailed movement of invested \$100 for last 10 days period (Period 20, Stock: CTRP)

Day	Buy&Sell decisions by prediction models								Buy&Hold stock/index			
	MV-GPR		MV-TPR		GPR		TPR		CTRTP	INDU	NDX	SPX
	Act	Dollar	Act	Dollar	Act	Dollar	Act	Dollar				
190	169.89		201.99		163.80		176.73		80.69	104.49	110.33	105.37
191	Buy	175.02	Buy	208.09	Buy	168.75	Buy	182.07	83.65	106.25	112.37	107.51
192	Keep	180.77	Keep	214.92	Keep	174.28	Keep	188.05	86.39	108.83	115.14	110.09
193	Keep	185.40	Keep	220.43	Keep	178.75	Keep	192.87	88.61	108.99	115.52	110.60
194	Sell	184.91	Sell	220.28	Sell	178.28	Sell	192.36	88.55	109.94	115.84	111.02
195	Keep	184.91	Buy	222.82	Keep	178.28	Keep	192.36	88.45	110.33	115.45	111.21
196	Keep	184.91	Keep	222.82	Keep	178.28	Keep	192.36	88.22	110.37	115.55	111.20
197	Buy	185.16	Keep	222.82	Buy	178.52	Buy	192.62	88.92	110.51	116.39	111.56
198	Keep	184.06	Keep	222.82	Keep	177.46	Keep	191.47	88.39	110.42	116.35	111.66
199	Sell	183.25	Keep	222.82	Sell	176.67	Sell	190.63	88.45	110.08	115.53	111.11
200	Keep	183.25	Keep	222.82	Keep	176.67	Keep	190.63	89.20	109.10	114.29	109.97

Table 17 The detailed movement of invested \$100 for last 10 days period (Period 20, Stock: NTES)

Day	Buy&Sell decisions by prediction models								Buy&Hold stock/index			
	MV-GPR		MV-TPR		GPR		TPR		NTES	INDU	NDX	SPX
	Act	Dollar	Act	Dollar	Act	Dollar	Act	Dollar				
190	179.84		177.72		177.28		174.50		153.20	104.49	110.33	105.37
191	Buy	176.57	Buy	174.49	Buy	174.06	Buy	171.33	151.35	106.25	112.37	107.51
192	Keep	184.84	Keep	182.66	Keep	182.21	Keep	179.36	158.44	108.83	115.14	110.09
193	Keep	184.16	Keep	181.98	Keep	181.54	Keep	178.69	157.86	108.99	115.52	110.60
194	Keep	185.46	Keep	183.27	Keep	182.82	Keep	179.95	158.97	109.94	115.84	111.02
195	Sell	185.33	Keep	179.25	Sell	182.69	Sell	179.83	155.49	110.33	115.45	111.21
196	Buy	187.22	keep	180.86	Buy	184.55	Buy	181.66	156.88	110.37	115.55	111.20
197	Keep	187.75	Keep	181.38	Keep	185.08	Keep	182.18	157.33	110.51	116.39	111.56
198	Sell	188.32	Keep	177.52	Keep	181.15	Keep	178.30	153.98	110.42	116.35	111.66
199	Keep	188.32	Sell	176.70	Sell	180.31	Sell	177.48	153.29	110.08	115.53	111.11
200	Keep	188.32	Keep	176.70	Keep	180.31	Keep	177.48	153.52	109.10	114.29	109.97

Appendix 3: Final investment details of stocks in Dow 30

See Tables 18 and 19.

Table 18 The detailed stock investment results under different strategies

Ticker	Industry	Buy&Sell strategy				Buy&Hold strategy			
		MV-GPR	MV-TPR	GPR	TPR	Stock	INDU	NDX	SPX
CVX	Oil and Gas	134.97	133.69	143.47	143.81	99.38	109.10	114.29	109.97
XOM	Oil and Gas	128.39	132.72	131.31	136.02	99.74			
MMM	Industrials	166.76	162.96	167.12	162.65	125.96			
BA	Industrials	160.12	159.98	158.60	157.38	106.39			
CAT	Industrials	142.58	138.45	146.13	151.75	97.16			
GE	Industrials	137.51	134.63	135.35	139.72	101.15			
UTX	Industrials	144.29	139.47	143.29	145.18	101.94			
KO	Consumer Goods	128.11	128.59	124.88	124.52	112.47			
MCD	Consumer Goods	120.69	117.09	122.19	119.59	98.81			
PG	Consumer Goods	126.62	123.32	127.14	127.10	117.04			
JNJ	Health Care	146.00	146.70	147.42	145.16	113.65			
MRK	Health Care	129.40	134.48	129.36	135.05	102.45			
PFE	Health Care	128.60	136.53	130.26	134.48	100.16			
UNH	Health Care	164.98	164.63	166.14	162.79	131.14			
HD	Consumer Services	171.46	165.74	169.55	170.18	133.33			
NKE	Consumer Services	147.17	146.13	142.36	148.26	122.27			
WMT	Consumer Services	136.50	132.59	133.77	135.67	117.31			
DIS	Consumer Services	168.19	168.43	168.51	168.12	115.97			
AXP	Financials	160.39	158.52	160.73	160.12	102.34			
GS	Financials	170.46	171.29	167.71	165.72	116.16			
JPM	Financials	174.90	170.07	176.48	172.12	110.09			
TRV	Financials	149.81	145.88	150.70	145.71	128.18			
V	Financials	161.50	153.48	157.04	158.70	116.37			
AAPL	Technology	201.82	206.64	203.45	208.07	147.34			
CSCO	Technology	159.13	164.88	158.61	155.92	131.34			
IBM	Technology	116.10	128.79	124.92	123.74	88.06			
INTC	Technology	183.80	179.45	185.52	188.22	149.24			
MSFT	Technology	173.61	166.09	176.57	172.76	120.01			

Table 19 The detailed industry portfolio investment results under different strategies

Industry Portfolio	Buy&Sell strategy				Buy&Hold strategy			
	MV-GPR	MV-TPR	GPR	TPR	Stock	INDU	NDX	SPX
Oil and Gas	131.68	133.20	137.39	139.92	99.56	109.10	114.29	109.97
Industrials	150.25	147.10	150.10	151.34	106.52			
Consumer Goods	125.14	123.00	124.73	123.73	109.44			
Health Care	142.24	145.59	143.30	144.37	111.85			
Consumer Services	155.83	153.22	153.55	155.56	122.22			
Financials	163.41	159.85	162.53	160.47	114.63			
Technology	166.89	169.17	169.81	169.74	127.20			

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