Estimation of Covariance Matrices for Portfolio Optimization using Gaussian Processes

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June 11, 2018

Abstract

Estimating covariances between financial assets plays an important role in risk management and optimal portfolio allocation. In practice, when the sample size is small compared to the number of variables, i.e. when considering a wide universe of assets over just a few years, this poses considerable challenges and the empirical estimate is known to be very unstable. Here, we propose a novel covariance estimator based on the Gaussian Process Latent Variable Model (GP-LVM). Our estimator can be considered as a non-linear extension of standard factor models with readily interpretable parameters reminiscent of market betas. Furthermore, our Bayesian treatment naturally shrinks the sample covariance matrix towards a more structured matrix given by the prior and thereby systematically reduces estimation errors.

1 Introduction

Many financial problems require the estimation of covariance matrices between given assets. This may be useful to optimize one’s portfolio, i.e.: maximize the portfolio returns $w^T r$ and/or minimize the volatility $\sqrt{w^T K w}$. Indeed, Markowitz received a Noble Price in economics for his treatment of modern portfolio theory[1]. In practice, estimating historical returns and high-dimensional covariance matrices is challenging and often times equally weighted portfolio outperforms the portfolio constructed from sample estimates[2].

The estimation of covariance matrices is especially hard, if the number of assets is large compared to the number of observations. Sample estimations in those cases are very unstable or can even become singular. To cope with this problem, a wide range of estimators, e.g. factor models such as the single-index model[3] or shrinkage estimators [4], have been developed and employed in portfolio optimization.

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With today’s machine learning techniques we can even further improve those estimates. Machine learning has already arrived in finance and there are many applications based on it. Nevmyvalov et al. [5] trained an agent via reinforcement learning to optimally execute trades. Gately et al. [6] forecast asset prices with neural networks and Chapados et al. [7] with Gaussian processes and recently, Heaton et al. [8] made an ansatz to optimally allocate portfolios using deep autoencoders.

Also Bayesian machine learning methods are used more and more in this domain. The fact, that in Bayesian framework parameters are not treated as true values, but as random variables, accounts for estimation uncertainties and can even alleviate the unwanted impacts of outliers. Furthermore, one can easily incorporate additional information and/or personal views by selecting suitable priors.

In this paper, we propose a Bayesian covariance estimator based on the Gaussian Process Latent Variable Model (GP-LVM) [9], which can be considered as a non-linear extension of standard factor models with readily interpretable parameters reminiscent of market betas. Our Bayesian treatment naturally shrinks the sample covariance matrix (which maximizes the likelihood function) towards a more structured matrix given by the prior and thereby systematically reduces estimation errors.

We evaluated our model on the stocks of S&P500 from 2000 to 2017 and found significant improvements in terms of model fit, as well as portfolio performance compared to current state-of-the-art covariance estimators.

In Section 2 we begin with an introduction to the Bayesian non-parametric Gaussian Processes and discuss the associated requirements for inference and learning. Section 3 introduces the financial background needed for portfolio optimization and how to relate it to Gaussian Processes. In Section 4 we conduct experiments on covariance matrix estimations and discuss the results. We conclude in Section 5.

2 Background

In this paper, we utilize a Bayesian non-parametric machine learning approach based on Gaussian Processes (GPs). Combining those with latent variable models leads to Gaussian Process Latent Variable Models (GP-LVMs), that we use to estimate the covariance between different assets. These approaches have been described in detail in [9, 10]. We provide a brief review here. Subsequently, we show, how to relate those machine learning approaches to the known models in finance, e.g. the single-index model [3].

2.1 Gaussian Processes

A Gaussian process (GP) is a generalization of the Gaussian distribution. Using a GP, we can define a distribution over functions \( f(x) \), where \( x \in \mathbb{R}^D \) and \( f \in \mathbb{R} \). Like a Gaussian distribution, the GP is specified by a mean and a covariance. In the GP case, however, the mean is a function of the input variable \( m(x) \) and the covariance is a function of two variables \( k(x, x') \), which contains information about how the GP evaluated at \( x \) and \( x' \) covary

\[
m(x) = \mathbb{E}[f(x)]
\]

\[
k(x, x') = \text{cov}(f(x), f(x')).
\]

We write \( f \sim \text{GP}(m(\cdot), k(\cdot, \cdot)) \). Any finite collection of function values, at \( x_1, \ldots, x_N \), is jointly Gaussian distributed

\[
p(f(x_1), f(x_2), \ldots, f(x_N)) = \mathcal{N}(\mu, K),
\]
where \( \mu = (m(x_1), \ldots, m(x_N))^T \) is the mean vector and \( K \in \mathbb{R}^{N \times N} \) is the Gram matrix with entries \( K_{ij} = k(x_i, x_j) \). We refer to the covariance function as kernel function. The properties of the function \( f \) (i.e. smoothness, periodicity) are determined by the choice of this kernel function. Popular choices include the linear kernel
\[
k_{\text{Lin}}(x, x') = \sigma^2 x^T x',
\]
the squared-exponential (SE) kernel
\[
k_{\text{SE}}(x, x') = \sigma^2 \exp(-0.5||x - x'||_2^2/l^2)
\]
as well as the exponential kernel
\[
k_{\text{OU}}(x, x') = \sigma^2 \exp(-||x - x'||_2/l).
\]
Depending on the kernel, sample functions from a GP are then either linear (\( k_{\text{Lin}} \)), smoothly varying with length scale \( l \) and infinitely often differentiable (\( k_{\text{SE}} \)) or draws from an Ornstein-Uhlenbeck process (\( k_{\text{OU}} \)).

Given a data set \( D \) of \( N \) input points \( X = \{x_1, \ldots, x_N\} \) and \( N \) corresponding targets \( y = \{y_1, \ldots, y_N\} \) the predictive distribution for a zero mean GP at \( N^* \) new locations \( X^* \) reads
\[
y^* | X^*, y, X \sim N(f^*, K^*),
\]
where
\[
f_* = K_{XX} K^{-1}_{XX} y
\]
\[
K_* = K_{XX} - K_{X*} K^{-1}_{XX} K_{X*}.
\]
\( K_{XX} \in \mathbb{R}^{N \times N} \) is the covariance matrix between the GP evaluated at \( X \) and \( X \), \( K_{XX} \in \mathbb{R}^{N \times N} \) is the covariance matrix of the GP evaluated at \( X \). As we can see in equations (2.8) and (2.9), the kernel function plays a very important role in the GP framework and will be important for our financial model as well.

### 2.2 Gaussian Process Latent Variable Model

Principal component analysis (PCA) is one of the most used techniques for reducing the dimensions of the data, which has also been motivated as the maximum likelihood solution to a particular form of Gaussian latent variable model \([11]\). Given a data matrix \( Y \in \mathbb{R}^{N \times D} \) the goal is to find a lower dimensional representation \( X \), without losing too much information. From a generative point of view, \( Y \) is created by the latent variable \( X \) via a linear mapping \( W \)
\[
Y = XW^T + \epsilon,
\]
where \( X \in \mathbb{R}^{N \times Q} \) represents the \( N \) data points in the \( Q \)-dimensional latent space and \( W \in \mathbb{R}^{D \times Q} \) is the mapping of each point \( X_n \) to \( Y_n \) (\( X_n \) and \( Y_n \) are the \( n \)-th rows of \( X \) and \( Y \)). For \( Q = D \) we can exactly fit the data. Meaning, we can find \( W \) and \( X \) so that \( \epsilon \) in equation (2.10) is zero (trivial case: \( W = 1 \) and \( X = Y \)). For \( Q < D \) the question is not that trivial anymore. Here we are looking for \( W \) and \( X \), so that \( \epsilon \) stays as small as possible. In the probabilistic PCA (PPCA), we put a standard Gaussian prior on \( X \) and assume the noise \( \epsilon \) to be Gaussian with variance \( \sigma^2 \) as well. Thus, we can integrate out \( X \) analytically and get the following marginal likelihood
\[
p(Y|W) = \prod_{n=1}^{N} \mathcal{N}(Y_n|0, WW^T + \sigma^2 I).
\]
We can optimize (2.11) with respect to $W$ and get the classical PCA solution \cite{11}.

The same can be done in the dual space, where instead of putting a standard Gaussian prior on $X$, we put it on $W$ and get

\[
p(Y|X) = \prod_{d=1}^{D} \mathcal{N}(Y_d|0, XX^T + \sigma^2I)
= \prod_{d=1}^{D} \mathcal{N}(Y_d|0, K),
\]

(2.12)

here $Y_d \in \mathbb{R}^N$ is the $d$-th row of $Y$.

Compared to equation (2.3), this equation can be seen as a Gaussian process with zero mean and a linear kernel function with noise $k(X_q, X_q') = X_q^T X_q' + \sigma^2 \delta_{qq'}$. Since we do not know the $X_q$’s, we treat them as latent variables and identify the linear model as a linear subclass of the more general Gaussian Process Latent Variable Model (GP-LVM). Indeed, in \cite{9} Lawrence introduced the GP-LVM as a non-linear extension of probabilistic PCA in this fashion.

Thus, choosing a non-linear kernel for the mapping from latent to observed space, equation (2.10) for each of the $N$ data points becomes

\[
Y_n = f(X_n) + \epsilon,
\]

(2.13)

where $f = (f_1, ..., f_D)^T$ is a group of $D$ samples from a GP with a covariance function $k$. By this we assume the rows of $Y$ (indexed by $Y_n \in \mathbb{R}^D$) to be jointly Gaussian distributed with the covariance given by $k$ and the columns of $Y$ (indexed by $Y_d \in \mathbb{R}^N$) to be independent. For a zero mean Gaussian random noise $\epsilon$ with variance $\sigma^2$ and with a GP prior on $f \sim \text{GP}(0, K \otimes 1)$, the marginal likelihood of $Y$ becomes \cite{9}

\[
p(Y|X) = \prod_{d=1}^{D} \mathcal{N}(Y_d|0, K)
= \frac{1}{(2\pi)^{ND/2}|K|^{D/2}} \exp\left(-\frac{1}{2} \text{tr}(K^{-1}YY^T)\right),
\]

(2.15)

where $K = k(X, X) + \sigma^2I$. Note that the dependency on the latent positions $X$ is given through the kernel matrix $K$, which also depends on the kernel hyperparameters. As suggested in \cite{9}, we can optimize the log marginal likelihood $\log p(Y|X)$ with respect to the latent positions and the hyperparameters.

Optimization can easily lead to overfitting. Therefore, a fully Bayesian treatment of the model would be preferable but is intractable. Titsian and Lawrence introduced in \cite{12} a variational inference framework, which not only handles the problem of overfitting but also allows to automatically select the dimensionality of the latent space.

### 2.3 Variational Inference

For our linear model $Y = XW^T + \epsilon$ we can either marginalize $W$ or marginalize $X$ but not both. We decided to marginalize $W$, leading to equation (2.15). Optimization of (2.15) can easily overfit.\footnote{We use operator overloading here. For $Y \in \mathbb{R}^{N \times D}$, we refer to the $n$-th row by $Y_n \in \mathbb{R}^D$ and the $d$-th column by $Y_d \in \mathbb{R}^N$. The same is true for $X \in \mathbb{R}^{N \times Q}$. $X_n$ and $X_q$ refer to the row and the column of $X$ respectively.}
To account for overfitting, we treat it in a Bayesian manner as well. Therefore, we assign a prior density \( p(X) \) to \( X \) and its posterior becomes

\[
p(X|Y) = \frac{p(Y|X)p(X)}{p(Y)}, \tag{2.16}
\]

which is analytically intractable.

The idea behind variational Bayes is to approximate the true posterior \( p(X|Y) \) by another distribution \( q(X) \) selected from a tractable family. The goal is to select the one distribution \( q(X) \), that is closest to the true posterior \( p(X|Y) \) in some sense. A natural choice to quantify the closeness is given by the Kullback-Leibler divergence \( ^2 \)

\[
\text{KL}[q(X) || p(X|Y)] = \int q(X) \log \frac{q(X)}{p(X|Y)} dx. \tag{2.17}
\]

By defining \( \tilde{p}(X|Y) = p(Y|X)p(X) \) as the unnormalized posterior, equation (2.17) can be rewritten as

\[
\text{KL}[q(X) || p(X|Y)] = \int q(X) \log \frac{q(X)}{p(X|Y)} dx + \log p(Y) = -\mathbb{E}_{q(X)} \left[ \log \frac{\tilde{p}(X|Y)}{q(X)} \right] + \log p(Y) \tag{2.18}
\]

with the first term on the right hand side being known as the evidence lower bound (ELBO).

Equation (2.18) is the objective function we want to minimize with respect to \( q(X) \) to get a good approximation to the true posterior. Note, on the left hand side only the ELBO is \( q \) dependent. So, in order to minimize (2.18), we can just as well maximize the ELBO.

Because the Kullback-Leibler divergence is non-negative, the ELBO is a lower bound on the evidence \( \log p(Y) \). Therefore, this procedure not only gives the best approximation to the posterior, but it also bounds the evidence, which serves as a measure of the goodness of our fit. The number of latent dimensions \( Q \) can be chosen to be the one, which maximizes the ELBO.

So, GP-LVM is an algorithm, which reduces the dimensions of our data-matrix \( Y \in \mathbb{R}^{N \times D} \) from \( D \) to \( Q \) in a non-linear way and at the same time estimates the covariance matrix between the \( N \) points. The estimated covariance matrix can then be used for further analysis.

### 3 Finance

Now we have a procedure to estimate the covariance matrix between different data points. This section discusses, how we can use this in finance to build optimal portfolios.

#### 3.1 CAPM

The Capital Asset Pricing Model (CAPM) describes the relationship between the expected returns for an asset \( r_n \in \mathbb{R}^D \) for \( D \) days and its risk \( \beta_n \)

\[
\mathbb{E}[r_n] = r_f + \beta_n \mathbb{E}[r_m - r_f], \tag{3.1}
\]

\(^3\text{Note that the Kullback-Leibler divergence is non-negative, but nevertheless not a true distance measure as it is in general neither symmetric nor satisfies the triangle inequality.}\)

\(^3\text{The evidence \( \log p(Y) \) is also referred to as \( \log \) marginal likelihood in the literature. The term marginal likelihood is already used for \( p(Y|X) \), in this paper. Therefore, we will refer to \( \log p(Y) \) as the evidence.}\)
where \( r_f \in \mathbb{R}^D \) is the risk free return on \( D \) different days, \( r_m \) is the market return on \( D \) different days.

The main idea behind CAPM is, that an investor needs to be compensated for the risk of his holdings. For a risk free asset with \( \beta_n = 0 \), the expected return \( \mathbb{E}[r_n] \) is just the risk free rate \( r_f \). If an asset is risky with a risk \( \beta_n \neq 0 \), the expected return \( \mathbb{E}[r_n] \) is increased by \( \beta_n \mathbb{E}[\tilde{r}_m] \), where \( \tilde{r}_m \) is the excess return of the market \( \tilde{r}_m = r_m - r_f \).

We can write down equation (3.1) in terms of the excess return \( \tilde{r}_n \) and get

\[
\mathbb{E}[\tilde{r}_n] = \beta_n \mathbb{E}[\tilde{r}_m], \tag{3.2}
\]

where \( \tilde{r}_n \) is the excess return of a given asset and \( \tilde{r}_m \) is the excess return of the market (also called a risk factor). Arbitrage pricing theory\(^\text{[14]}\) generalizes the above model by allowing multiple risk factors \( F \) beside the market \( \tilde{r}_m \). In particular, it assumes that asset returns follow a factor structure

\[
r_n = \alpha_n + F \beta_n + \epsilon_n, \tag{3.3}
\]

with \( \epsilon_n \) denoting some independent zero mean noise with variance \( \sigma_n^2 \). Here \( F \in \mathbb{R}^{D \times Q} \) is the matrix of \( Q \) factor returns on \( D \) days and \( \beta_n \in \mathbb{R}^Q \) is the loading of stock \( n \) to the \( Q \) factors. Arbitrage pricing theory then shows that the expected excess returns adhere to

\[
\mathbb{E}[\tilde{r}_n] = \mathbb{E}[\tilde{F}] \beta_n, \tag{3.4}
\]

i.e. the CAPM is derived as special case when assuming a single risk factor (single-index model).

As done in the GP-LVM, we can rewrite equation (3.3) as

\[
\tilde{r}_d = B f_d + \epsilon_d, \tag{3.5}
\]

where the subscript \( d \) refers to the dual-space. \( \tilde{r}_d \in \mathbb{R}^N \) is now the vector of returns on day \( d \) for \( N \) different stocks, \( f_d \in \mathbb{R}^Q \) is the \( d \)-th row of \( F \) and \( B = (\beta_1, ..., \beta_N)^T \) is a matrix of the couplings \( \beta_n \). We assumed the variance of the noise \( \epsilon_n \) for each stock to be fixed over the days. But we don’t need to fix it over different stocks. Thus, \( \epsilon_d \sim \mathcal{N}(0, \Psi) \), where \( \Psi \) is a diagonal matrix and the \( n \)-th entry on the diagonal corresponds to the variance of the noise of stock \( n \). Equation (3.5) is the dual-space representation of equation (3.3).

Assuming a standard Gaussian prior on the \( f_d \)’s, we can marginalize them out and get

\[
\tilde{r}_d \sim \mathcal{N}(\tilde{r}_d | 0, K + \Psi), \tag{3.6}
\]

where \( K = BB^T \), \( (K)_{ij} = \beta_i^T \beta_j \) is the covariance between stock \( i \) and \( j \). Assuming independence over returns on different days leads to

\[
p(\tilde{r} | B) = p(\tilde{r}_1, ..., \tilde{r}_D | B) = \prod_{d=1}^D \mathcal{N}(\tilde{r}_d | 0, K + \Psi), \tag{3.7}
\]

which we have earlier referred to as the marginal likelihood. We can get \( B = (\beta_1, ..., \beta_N)^T \) by maximizing the marginal likelihood. In the case of non-isotropic noise \( (\Psi \neq \sigma^2 I) \) there is no analytic solution for this optimization problem. If the noise is isotropic, the solution to equation (3.7) is given by \(^\text{[11]}\)

\[
B = U (\Lambda - \sigma^2 I)^{1/2}, \tag{3.8}
\]

where \( U \in \mathbb{R}^{N \times Q} \) is the matrix composed of the principal eigenvectors of \( K \), with corresponding eigenvalues \( \lambda_1, ..., \lambda_Q \) in the diagonal matrix \( \Lambda \).
This procedure can be seen as a linear dimensionality reduction, where we reduce the \(N \times D\) matrix \(\tilde{r}\) to a low rank matrix \(B\) of size \(N \times Q\). For fixed \(Q\) we can even capture more structure by making the dimensionality reduction procedure non-linear. This is done by making \((K)_{ij}\) a non-linear function of \(\beta_i\) and \(\beta_j\). By choosing a proper kernel function \(k(\cdot, \cdot)\), the resulting matrix will be a valid covariance matrix. However, the solution is then not tractable anymore and we need approximation methods. We chose to use variational inference as described in section 2.3. After inferring \(\beta\) and the hyperparameters of the kernel, we can calculate the covariance matrix \(K\) and use it for further analysis.

### 3.2 Modern Portfolio Theory

In his paper from 1952, Markowitz provided the foundation for modern portfolio theory\,[1], for which he received a Nobel Price in economics. The method analyses how good a given portfolio is, based on the mean and the variance of the returns of the assets contained in the portfolio, which can also be formulated as an optimization problem for selecting an optimal portfolio, given the covariance between the assets and the risk tolerance \(q\) of the investor.

Given the covariance matrix \(K \in \mathbb{R}^{N \times N}\), we can calculate the optimal portfolio weights \(w\) by

\[
w_{\text{opt}} = \min_{w} (w^T K w - q r^T w),
\]

where \(r\) is the mean return vector. Risk friendly investors have a higher \(q\) than risk averse investors. The model is constrained by \(\sum_{w} = 1\). Since, in general \(r\) is very hard to estimate and we are primarily interested in the estimation of the covariance matrix \(K\), we set \(q\) to zero and get

\[
W_{\text{opt}} = \min_{w} (w^T K w).
\]

This portfolio is called the minimal risk portfolio, i.e. the solution to equation (3.10) provides the weights for the portfolio, which minimizes the overall risk, assuming the estimated \(K\) is the true covariance matrix.

### 4 Experiments

In this section we discuss the performance of the GP-LVM on financial data. First, we evaluate the model on the daily return series of the S&P500 stocks. The return \(r_{nd}\) of stock \(n\) on day \(d\) is calculated by \((p_{n,d} - p_{n,d-1}) / p_{n,d-1}\), where \(p\) is the \(N \times (D+1)\) price matrix.

In the second part, we learn a stable covariance matrix \(K\) from past data and look at the future performance of the suggested portfolio. The learning and the prediction period can be varied. We are using a learning period of one year and predict optimal weights for the next six months, i.e., we rebalance our portfolio every six months.

#### 4.1 Data Collection and Modeling

For a given time period, we take all the stocks from the S&P500, whose daily close prices were available for the whole period\,\,[4] The data were downloaded from Yahoo Finance.

After having the close prices in a matrix \(\tilde{p} \in \mathbb{R}^{N \times (D+1)}\), we calculate the return matrix \(r\), where \(r_{nd} = (p_{n,d} - p_{n,d-1}) / p_{n,d-1}\) builds the basis of our analysis.

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\[\text{Survivorship Bias - Only stocks which survived the complete period are included with this type of data collection.}\]
We can feed $r$ into the GP-LVM. The GP-LVM procedure, as described in Section 2, assumes
the likelihood to be Gaussian with the covariance given by the kernel function for each day and
assumes independence over different days. We use the following kernel functions

$$
\begin{align*}
    k_{\text{noise}}(\beta_i, \beta_j) &= \sigma_{\text{noise}}^2 \delta_{i,j}, \\
    k_{\text{linear}}(\beta_i, \beta_j) &= \sigma^2 \beta_i^T \beta_j,
\end{align*}
$$

and the stationary kernels

$$
\begin{align*}
    k_{\text{SE}}(\beta_i, \beta_j) &= k_{\text{SE}}(d_{ij}) = \sigma^2 \exp\left(-\frac{1}{2l^2}d_{ij}^2\right), \\
    k_{\text{OU}}(\beta_i, \beta_j) &= k_{\text{OU}}(d_{ij}) = \sigma^2 \exp\left(-\frac{1}{2l}d_{ij}\right), \\
    k_{\text{MS2}}(\beta_i, \beta_j) &= k_{\text{MS2}}(d_{ij}) = \sigma^2 \left(1 + \frac{\sqrt{5}d_{ij}}{l} + \frac{5d_{ij}^2}{3l^2}\right) \exp\left(-\frac{\sqrt{5}}{2l}d_{ij}\right),
\end{align*}
$$

where $d_{ij} = \|\beta_i - \beta_j\|_2$ is the Euclidean distance between $\beta_i$ and $\beta_j$. $\sigma^2$ is the kernel variance
and $l$ kernel length scale. The full kernel function $k(\cdot, \cdot)$ at the end is the sum of the noise kernel
$k_{\text{noise}}$ and one of the other kernels. From now on, if we refer to the $SE$-kernel for example, we
mean $k = k_{\text{SE}} + k_{\text{noise}}$.

We fixed the kernel length scale $l = 1$ and assigned a zero mean Cauchy prior with scale equal
to one to the $\beta$‘s. The constraint on the kernel length scale $l$ is justified by the Cauchy prior on $\beta$, since the Cauchy distribution allows for variable length scale in the $\beta$-space. $\sigma$ and $\sigma_{\text{noise}}$ are
assigned a half Gaussian prior with variance of 0.5, which is a really flat prior, since the returns
are rarely above 0.1 for a day.

These are the specifications for the full model (likelihood for the data and prior for $\beta$ and all
kernel hyperparameters, which we denote by $\theta$) and we can infer the posterior over all parameters.

As described in Section 2.3, we make a variational approximation to the posterior. The inference
procedure can be performed by any probabilistic programming language, we chose Stan\textsuperscript{15}.\textsuperscript{5} For given $\beta$ and $\theta$, we can reconstruct the covariance matrix $K$ by the function $k(\cdot, \cdot)$. Thereafter, we
only need to minimize equation (3.10), which provides the weights $w$ for our portfolio in the future.

Minimization of (3.10) is done under the following constraints: $\sum_n w_n = 1$ and $0 < w_n < 0.1, \forall n$.
The first constraint makes sure we are fully invested and the second leads to a long only portfolio
and prohibits too much weight for a single asset.

### 4.2 Model Comparison

The GP-LVM, which provides us the covariance matrix between the stocks, can be evaluated in
many different ways. Since it projects the data from a $D$-dimensional space to a $Q$-dimensional
latent space, we can look at the reconstruction error. A suitable measure of the reconstruction
error is the R-squared ($R^2$) score, which equals one if there is no reconstruction error and decreases
if the reconstruction error increases. It is defined by

$$
R^2 = 1 - \frac{\sum_i(y_i - f_i)^2}{\sum_i(y_i - \bar{y})^2},
$$

where $y = (y_1, ..., y_N)^T$ are the true values, $f = (f_1, ..., f_N)^T$ are the predicted values and $\bar{y}$ is
the mean of $y$. $R^2$ is directly related to the variance explained by the model. E.g. an $R^2$ of 0.7
captures 70% of the variance of the data and explains the rest as noise.

\textsuperscript{5}Code is available on github: https://github.com/RSNirwan/PortfolioAllocationUsingGPLVM

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In the following we look at the $R^2$ as a function of the latent dimension $Q$ for different kernels. Figure 4.1 shows the results for three non-linear kernels and a linear kernel. Only a single dimension in the non-linear case can already capture almost 50% of the structure, whereas the linear kernels is at 30%. As one would expect, the higher $Q$ is, the more structure can be learned. But at some point the model will also start learning the noise and overfit.

As explained in Section 2.3, the evidence lower bound (ELBO) is a good measure to evaluate different models and already incorporates models complexity (overfitting). Figure 4.1 shows the ELBO as a function of the latent dimension $Q$. Here we see, that the model selects just a few latent dimensions. Depending on the used kernel, latent dimensions from three to five are already enough to capture the structure. If we further increase the dimensions, the ELBO starts dropping, which is a sign of overfitting.

In Figure 4.1, we randomly chose 100 stocks from the S&P500 and made the analysis on returns from Jan 2017 to Dez 2017. Each of the stocks is captured differently by the model. Thus, each one has its own $R^2$-score. Figure 4.1 shows the mean of the $R^2$’s of different stocks. Figure 4.2 shows the $R^2$-score for each of the 30 randomly chosen stocks in the same period. We switched to 30 stocks and only show the result for two kernels to keep the plot neat.

![Figure 4.1](image1.png)

**Figure 4.1:** Left: $R^2$-score as a function of the latent dimension $Q$ for different kernel functions. Right: ELBO as a function of the latent dimension $Q$.

![Figure 4.2](image2.png)

**Figure 4.2:** Comparison of $R^2$-score of each individual stock for exponential and linear kernel.
As can be seen from Figure 4.1, we don’t need to go to higher dimensions. \( Q \) between two and five is already good enough and captures the structure that can be captured by the model. After getting the covariance matrix \( K \) by the GP-LVM, we can get the optimal weights \( w \) by solving equation (3.10).

To get the real world performance of the model, we will learn the optimal weight vector \( w \) from the historical stock data and keep stocks for a short period in the future according to \( w \).

4.3 Predictive Performance

For our tests, the procedure is the following: First we get stock data from the S&P500 from Jan 2000 to Dez 2017. Then we learn \( w \) from the past year and buy accordingly for the next six months. After six months, we again learn the new portfolio weights \( w \) from the past year, rebalance the portfolio and keep it for the next six months and so on. Figure 4.3 shows the performance of the portfolio for different kernels for \( Q = 4 \). The dates, where we rebalanced the portfolio, are highlighted by the vertical black line in the background. For the GP-LVM we chose the linear, SE and exponential kernel functions. We also included the performance given by the sample covariance matrix, i.e. \( K = \frac{1}{T} (r - \hat{\mu})(r - \hat{\mu})^T \) where \( \hat{\mu}_n = \frac{1}{T} \sum_{d=1}^D r_{nd} \), the shrunk Ledoit-Wolf covariance matrix\(^6\) and the equally weighted portfolio, where \( w = (1, 1, ..., 1)/N \).

![Figure 4.3: Price performance of our model on real stock data form the S&P500. The weights are learned from the past year and the portfolio is rebalanced every six months. Since only the relative performance between the models is important, we show the performance of the total returns, not the excess returns.](image)

The model with the exponential kernels performs best. It might be due to the market structure, which is captured best by the exponential kernel. It even performs better than the equally weighted portfolio, which is known to be a good portfolio as well. To preclude, that the exponential case has been just lucky in this setting, we run the simulation many times, where we randomly choose 100 stocks from the S&P500 from 2000 to 2017. Almost always the GP-LVM with exponential kernel performs best.

4.4 Interpretation of the Latent Space

Even though the performance for \( Q \) between three and five is the best, it helps to visualize results for \( Q = 1 \) and \( Q = 2 \), to get a better understanding of the model.

\(^6\)Here, we have used the implementation in the Python toolbox scikit-learn [16].
Equation (3.7) is a distribution over functions, that fit the daily returns best given the latent space $\beta$. The prior over these functions is dependent on our choice of the kernel function. For the linear kernel the samples from the posterior distribution are linear functions, for the SE they are not linear anymore and are infinitely often differentiable and for the exponential kernel they are non-linear as well but they are not differentiable at all. To get an intuition of the learned distribution, we will plot the mean function of the distribution for a random day for the three kernel functions. Figure 4.4 shows the results.

Figure 4.4: Mean function of the posterior Gaussian process for 50 stock returns on two randomly chosen days from the S&P500.

Here, we see how the model tries to capture the structure. It places the stocks according to their correlation somewhere on the abscissa and then tries to fit them with a function. The form of the function is given by the choice of the kernel. The linear model tries to fit the points by a linear function and has to explain the rest as noise. It is obvious, that if we allow non-linear functions, we can capture more structure and thereby reducing the part stated as noise.

The same happens in higher dimensions, but we cannot visualize the functions anymore. The 2-dimensional latent space can be visualized as a scatter plot. For a stationary kernel function like the SE, the distance between the stocks is directly related to their correlation. In Figure 4.5 we see the latent space for some selected stocks from the US and find clusters of sub sectors. The tech-companies are on the right side of the plot. Banks and Hedge funds are in the lower left part.
Telecommunication companies like Verizon (VZ) and AT&T (T) are on the left side and the car companies like General Motors (GM) and Ford Motor (F) are in the middle. We note, that even though Tesla (TSLA) is a car company, it is not where GM and F are, but more on the side of the tech-companies.

![Figure 4.5: Scatterplot of the 2-dimensional latent space for the SE kernel.](image)

5 Conclusion

We applied the Gaussian Process Latent Variable Model (GP-LVM) to estimate the covariance matrix between different assets given their time series. We then showed how the GP-LVM can be seen as a non-linear extension to the CAPM with latent factors. The $R^2$ score is an indicator of the structure captured by the model. We saw that for fixed latent space dimension $Q$, every non-linear kernel can capture more structure than the linear one. Best results are given for the exponential kernel.

The estimated covariance matrix helps us to build a minimal risk portfolio according to Markowitz Portfolio theory. We evaluated the performance of different models on the S&P500 from year 2000 to 2017. All tested kernels beat the performance of the empirical covariance. Again, the exponential kernel performed best, even better than the equally weighted portfolio, that is known to have a good performance.

Furthermore, we discussed the role of the latent positions of the assets. In the future, one could also put a Gaussian process on the latent positions and allow them to vary in time, which would lead to a time-dependent covariance matrix.
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