

Machine Learning Risk Models

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Abstract

We give an explicit algorithm and source code for constructing risk models based on machine learning techniques. The resultant covariance matrices are not factor models. Based on empirical backtests, we compare the performance of these machine learning risk models to other constructions, including statistical risk models, risk models based on fundamental industry classifications, and also those utilizing multilevel clustering based industry classifications.

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1 Introduction and Summary

In most practical quant trading applications⁴ one faces an old problem when computing a sample covariance matrix of returns: the number N of returns (e.g., the number of stocks in the trading universe) is much larger than the number T of observations in the time series of returns. The sample covariance matrix C_{ij} ($i, j = 1, \dots, N$) in this case is badly singular: its rank is at best $T - 1$. So, it cannot be inverted, which is required in, e.g., mean-variance optimization (Markowitz, 1952). In fact, the singularity of C_{ij} is only a small part of the trouble: its off-diagonal elements (more precisely, sample correlations) are notoriously unstable out-of-sample.

The aforesaid “ills” of the sample covariance matrix are usually cured via multifactor risk models,⁵ where stock returns are (linearly) decomposed into contributions stemming from some number K of common underlying factors plus idiosyncratic “noise” pertaining to each stock individually. This is a way of dimensionally reducing the problem in that one only needs to compute a factor covariance matrix Φ_{AB} ($A, B = 1, \dots, K$), which is substantially smaller than C_{ij} assuming $K \ll N$.⁶

In statistical risk models⁷ the factors are based on the first K principal components of the sample covariance matrix C_{ij} (or the sample correlation matrix).⁸ In this case the number of factors is limited ($K \leq T - 1$), and, furthermore, the principal components beyond the first one are inherently unstable out-of-sample. In contrast, factors based on a granular fundamental industry classification⁹ are much more ubiquitous (in hundreds), and also stable, as stocks seldom jump industries. Heterotic risk models (Kakushadze, 2015c) based on such industry classifications sizably outperform statistical risk models.¹⁰ Another alternative is to replace the fundamental industry classification in the heterotic risk model construction by a

⁴ Similar issues are also present in other practical applications unrelated to trading or finance.

⁵ For a general discussion, see, e.g., (Grinold and Kahn, 2000). For explicit implementations (including source code), see, e.g., (Kakushadze and Yu, 2016a), (Kakushadze and Yu, 2017a).

⁶ This does not solve all problems, however. Thus, unless $K < T$, the sample factor covariance matrix is still singular (albeit the model covariance matrix Γ_{ij} that replaces C_{ij} need not be). Furthermore, the out-of-sample instability is still present in sample factor correlations. This can be circumvented via the heterotic risk model construction (Kakushadze, 2015c); see below.

⁷ See (Kakushadze and Yu, 2017a), which gives complete source code, and references therein.

⁸ The (often misconstrued) “shrinkage” method (Ledoit and Wolf, 2004) is nothing but a special type of statistical risk models; see (Kakushadze, 2016), (Kakushadze and Yu, 2017a) for details.

⁹ E.g., BICS (Bloomberg Industry Classification System), GICS (Global Industry Classification Standard), ICB (Industry Classification Benchmark), SIC (Standard Industrial Classification), etc.

¹⁰ In the heterotic risk model construction the sample factor covariance matrix at the most granular level in the industry classification typically would be singular. However, this is rectified by modeling the factor covariance matrix by another factor model with factors based on the next-less-granular level in the industry classification, and this process of dimensional reduction is repeated until the resultant factor covariance matrix is small enough to be nonsingular and sufficiently stable out-of-sample (Kakushadze, 2015c), (Kakushadze and Yu, 2016a). Here one can also include non-industry style factors. However, their number is limited (especially for short horizons) and, contrary to an apparent common misconception, style factors generally are poor proxies for modeling correlations and add little to no value (Kakushadze and Yu, 2016a).

statistical industry classification based on clustering (using machine learning techniques) the return time series data (Kakushadze and Yu, 2016b),¹¹ without any reference to a fundamental industry classification. Risk models based on statistical industry classifications outperform statistical risk models but underperform risk models based on fundamental industry classifications (Kakushadze and Yu, 2016b).

In this paper we discuss a different approach to building a risk model using machine learning techniques. The idea is simple. A sample covariance matrix C_{ij} is singular (assuming $T \ll N$), but it is semi-positive definite. Imagine that we could compute a large number M of “samplings” of C_{ij} , call them $C_{ij}^{(m)}$, $m = 1, \dots, M$, where each “sampling” is semi-positive definite. Consider their mean¹²

$$\Gamma_{ij} = \frac{1}{M} \sum_{m=1}^M C_{ij}^{(m)} \quad (1)$$

By construction Γ_{ij} is semi-positive definite. In fact, assuming $C_{ij}^{(m)}$ are all (sizably) different from each other, Γ_{ij} generically will be positive definite and invertible (for large enough M). So, the idea is sound, at least superfluously, but the question is, what should these “samplings” $C_{ij}^{(m)}$ be? Note that each element of the sample covariance matrix C_{ij} ($i \neq j$) only depends on the time series of the corresponding two stock returns $R_i(t)$ and $R_j(t)$, and not on the universe of stocks, so any cross-sectional “samplings” cannot be based on sample covariance matrices. In principle, serial “samplings” could be considered if a long history were available. However, here we assume that our lookback is limited, be it due to a short history that is available, or, more prosaically, due to the fact that data from a while back is not pertinent to forecasting risk for short horizons as market conditions change.

A simple way around this is to consider cross-sectional “samplings” $C_{ij}^{(m)}$ that are not sample covariance matrices but are already dimensionally reduced, even though they do not have to be invertible. Thus, given a clustering of N stocks into K clusters, we can build a multifactor risk model, e.g., via an incomplete heterotic construction (see below). Different clusterings then produce different “samplings” $C_{ij}^{(m)}$, which we average via Eq. (1) to obtain a positive definite Γ_{ij} , which is *not* a factor model. However, as usual, the devil is in the detail, which we discuss in Section 2. E.g., the matrix (1) can have nearly degenerate or small eigenvalues, which requires further tweaking Γ_{ij} to avert, e.g., undesirable effects on optimization.

In Section 3 we discuss backtests to compare the machine learning risk models of this paper to statistical risk models, and heterotic risk models based on fundamental industry classification and statistical industry classification. We briefly conclude in Section 4. Appendix A provides R source code¹³ for machine learning risk models, and some important legalese relating to this code is relegated to Appendix B.

¹¹ Such statistical industry classifications can be multilevel and granular.

¹² In fact, instead of the arithmetic mean, here we can more generally consider a weighted average with some positive weights w_m (see below). Also, in this paper $C_{ij}^{(m)}$ are nonsingular.

¹³ The code in Appendix A is not written to be “fancy” or optimized for speed or otherwise.

2 Heterotic Construction and Sampling

So, we have time series of returns (say, daily close-to-close returns) R_{is} for our N stocks ($i = 1, \dots, N$, $s = 1, \dots, T$, and $s = 1$ corresponds to the most recent time in the time series). Let us assume that we have a clustering of our N stocks into K clusters, where K is sizably smaller than N , and each stock belongs to one and only one cluster. Let the clusters be labeled by $A = 1, \dots, K$. So, we have a map

$$G : \{1, \dots, N\} \mapsto \{1, \dots, K\} \quad (2)$$

Following (Kakushadze, 2015c), we can model the sample correlation matrix $\Psi_{ij} = C_{ij}/\sigma_i\sigma_j$ (here $\sigma_i^2 = C_{ii}$ are the sample variances) via a factor model:

$$\tilde{\Psi}_{ij} = \xi_i^2 \delta_{ij} + \sum_{A,B=1}^K \Omega_{iA} \Phi_{AB} \Omega_{jB} = \xi_i^2 \delta_{ij} + U_i U_j \Phi_{G(i),G(j)} \quad (3)$$

$$\Omega_{iA} = U_i \delta_{G(i),A} \quad (4)$$

$$\xi_i^2 = 1 - \lambda(G(i)) U_i^2 \quad (5)$$

$$\Phi_{AB} = \sum_{i \in J(A)} \sum_{j \in J(B)} U_i \Psi_{ij} U_j \quad (6)$$

Here the N_A components of U_i for $i \in J(A)$ are given by the first principal component of the $N(A) \times N(A)$ matrix $[\Psi(A)]_{ij} = \Psi_{ij}$, $i, j \in J(A)$, where $J(A) = \{i | G(i) = A\}$ is the set of the values of the index i corresponding to the cluster labeled by A , and $N_A = |J(A)|$ is the number of such i . Also, $\lambda(A)$ is the largest eigenvalue (corresponding to the first principal component) of the matrix $[\Psi(A)]_{ij}$. The matrix Ω_{iA} is the factor loadings matrix, ξ_i^2 is the specific variance, and the factor covariance matrix Φ_{AB} has the property that $\Phi_{AA} = \lambda(A)$. By construction, $\tilde{\Psi}_{ii} = 1$, and the matrix $\tilde{\Psi}_{ij}$ is positive-definite. However, Φ_{AB} is singular unless $K \leq T - 1$.

This is because the rank of Ψ_{ij} is (at most) $T - 1$. Let $V_i^{(a)}$ be the principal components of Ψ_{ij} with the corresponding eigenvalues $\lambda^{(a)}$ ordered decreasingly ($a = 1, \dots, N$). More precisely, at most $T - 1$ eigenvalues $\lambda^{(a)}$, $a = 1, \dots, T - 1$ are nonzero, and the others vanish. So, we have

$$\Phi_{AB} = \sum_{a=1}^{T-1} \lambda^{(a)} \tilde{U}_A^{(a)} \tilde{U}_B^{(a)} \quad (7)$$

$$\tilde{U}_A^{(a)} = \sum_{i \in J(A)} U_i V_i^{(a)} \quad (8)$$

So, the rank of Φ_{AB} is (at most) $T - 1$, and the above incomplete heterotic construction provides a particular regularization of the statistical risk model construction based on principal components. In the complete heterotic construction Φ_{AB} itself is modeled via another factor model, and this nested “Russian-doll” embedding is continued until at the final step the factor covariance matrix (which gets smaller and smaller at each step) is nonsingular (and sufficiently stable out-of-sample).

2.1 Sampling via Clustering

However, there is another way, which is what we refer to as “machine learning risk models” here. Suppose we have M different clusterings. Let $\tilde{\Psi}_{ij}^{(m)}$ be the model correlation matrix (3) for the m -th clustering ($m = 1, \dots, M$). Then we can construct a model correlation matrix as a weighted sum

$$\tilde{\Psi}_{ij} = \sum_{m=1}^M w_m \tilde{\Psi}_{ij}^{(m)} \quad (9)$$

$$\sum_{m=1}^M w_m = 1 \quad (10)$$

The simplest choice for the weights is to have equal weighting: $w_m = 1/M$. More generally, so long as the weights w_m are positive, the model correlation matrix $\tilde{\Psi}_{ij}$ is positive-definite. (Also, by construction $\tilde{\Psi}_{ii} = 1$.) However, combining a large number M of “samplings” $\tilde{\Psi}_{ij}^{(m)}$ accomplishes something else: each “sampling” provides a particular regularization of the sample correlation matrix, and combining such samplings covers many more directions in the risk space than each individual “sampling”. This is because $\tilde{U}_A^{(a)}$ in Eq. (7) are different for different clusterings.

2.2 K-means

We can use k-means (Forgy, 1965), (Lloyd, 1957), (Lloyd, 1982), (Hartigan, 1975), (Hartigan and Wong, 1979), (MacQueen, 1967), (Steinhaus, 1957) for our clusterings. Since k-means is nondeterministic, it automatically produces a different “sampling” with each run. The idea behind k-means is to partition N observations into K clusters such that each observation belongs to the cluster with the nearest mean. Each of the N observations is actually a d -vector, so we have an $N \times d$ matrix X_{is} , $i = 1, \dots, N$, $s = 1, \dots, d$. Let C_a be the K clusters, $C_a = \{i | i \in C_a\}$, $a = 1, \dots, K$. Then k-means attempts to minimize

$$g = \sum_{a=1}^K \sum_{i \in C_a} \sum_{s=1}^d (X_{is} - Y_{as})^2 \quad (11)$$

where

$$Y_{as} = \frac{1}{n_a} \sum_{i \in C_a} X_{is} \quad (12)$$

are the cluster centers (i.e., cross-sectional means),¹⁴ and $n_a = |C_a|$ is the number of elements in the cluster C_a . In Eq. (11) the measure of “closeness” is chosen to be the Euclidean distance between points in \mathbf{R}^d , albeit other measures are possible.¹⁵

¹⁴ Throughout this paper “cross-sectional” refers to “over the index i ”.

¹⁵ E.g., the Manhattan distance, cosine similarity, etc.

2.3 What to Cluster?

Here we are not going to reinvent the wheel. We will simply use the prescription of (Kakushadze and Yu, 2016b). Basically, we can cluster the returns, i.e., take $X_{is} = R_{is}$ (then $d = T$). However, stock volatility is highly variable, and its cross-sectional distribution is not even quasi-normal but highly skewed, with a long tail at the higher end – it is roughly log-normal. Clustering returns does not take this skewness into account and inadvertently we might be clustering together returns that are not at all highly correlated solely due to the skewed volatility factor. A simple “machine learning” solution is to cluster the normalized returns $\tilde{R}_{is} = R_{is}/\sigma_i$, where $\sigma_i^2 = \text{Var}(R_{is})$ is the serial variance ($\sigma_i^2 = C_{ii}$). However, as was discussed in detail in (Kakushadze and Yu, 2016b), this choice would also be suboptimal and this is where quant trading experience and intuition trumps generic machine learning “lore”. It is more optimal to cluster $\hat{R}_{is} = R_{is}/\sigma_i^2$ (see (Kakushadze and Yu, 2016b) for a detailed explanation). A potential practical hiccup with this is that if some stocks have very low volatilities, we could have large \hat{R}_{is} for such stocks. To avoid any potential issues with computations, we can “smooth” this out via “Winsorization” of sorts (MAD = mean absolute deviation):¹⁶

$$\hat{R}_{is} = \frac{R_{is}}{\sigma_i u_i} \quad (13)$$

$$u_i = \frac{\sigma_i}{v} \quad (14)$$

$$v = \exp(\text{Median}(\ln(\sigma_i)) - 3 \text{MAD}(\ln(\sigma_i))) \quad (15)$$

and for all $u_i < 1$ we set $u_i = 1$. This is the definition of \hat{R}_{is} that is used in the source code internally. Furthermore, $\text{Median}(\cdot)$ and $\text{MAD}(\cdot)$ above are cross-sectional.

2.4 A Tweak

The number of clusters K is a hyperparameter. In principle, it can be fixed by adapting the methods discussed in (Kakushadze and Yu, 2016b). However, in the context of this paper, we will simply keep it as a hyperparameter and test what we get for its various values. As K increases, in some cases it is possible to get relatively small eigenvalues in the model correlation matrix $\tilde{\Psi}_{ij}$, or nearly degenerate eigenvalues. This can cause convergence issues in optimization with bounds (see below). To circumvent this, we can slightly deform $\tilde{\Psi}_{ij}$ for such values of K .

Here is a simple method that deals with both of the aforesaid issues at once. To understand this method, it is helpful to look at the eigenvalue graphs given in Figures 1, 2, 3, 4, which are based on a typical data set of daily returns for $N = 2000$ stocks and $T = 21$ trading days. These graphs plot the eigenvalues for a single “sampling” $\tilde{\Psi}_{ij}^{(m)}$, as well as $\tilde{\Psi}_{ij}$ based on averaging $M = 100$ “samplings” (with equal weights), for $K = 150$ and $K = 40$ (K is the number of clusters). Unsurprisingly, there are

¹⁶ This is one possible tweak. Others produce similar results.

some small eigenvalues. However, their fraction is small. Furthermore, these small eigenvalues get even smaller for larger values of K , but increase when averaging over multiple “samplings”, which also smoothes out the eigenvalue graph structure.

What we wish to do is to deform the matrix $\tilde{\Psi}_{ij}$ by tweaking the small eigenvalues at the tail. We need to define what we mean by the “tail”, i.e., which eigenvalues to include in it. There are many ways of doing this, some are simpler, some are more convoluted. We use a method based on eRank or effective rank (Roy and Vetterli, 2007), which can be more generally defined for any subset S of the eigenvalues of a matrix, which (for our purposes here) is assumed to be symmetric and semi-positive-definite. Let

$$\text{eRank}(S) = \exp(H) \quad (16)$$

$$H = - \sum_{a=1}^L p_a \ln(p_a) \quad (17)$$

$$p_a = \frac{\lambda^{(a)}}{\sum_{b=1}^L \lambda^{(b)}} \quad (18)$$

where $\lambda^{(a)}$ are the L positive eigenvalues in the subset S , and H has the meaning of the (Shannon a.k.a. spectral) entropy (Campbell, 1960), (Yang *et al*, 2005).

If we take S to be the full set of N eigenvalues of $\tilde{\Psi}_{ij}$, then the meaning of $\text{eRank}(S)$ is that it is a measure of the effective dimensionality of the matrix $\tilde{\Psi}_{ij}$. However, this is not what we need to do for our purposes here. This is because the large eigenvalues of $\tilde{\Psi}_{ij}$ contribute heavily into $\text{eRank}(S)$. So, we define S to include all eigenvalues $\tilde{\lambda}^{(a)}$ ($a = 1, \dots, N$) of $\tilde{\Psi}_{ij}$ that do not exceed 1: $S = \{\tilde{\lambda}^{(a)} | \tilde{\lambda}^{(a)} \leq 1\}$. Then we define (here $\text{floor}(\cdot) = \lfloor \cdot \rfloor$ can be replaced by $\text{round}(\cdot)$)

$$n_* = |S| - \text{floor}(\text{eRank}(S)) \quad (19)$$

So, the tail is now defined as the set S_* of the n_* smallest eigenvalues $\tilde{\lambda}^{(a)}$ of $\tilde{\Psi}_{ij}$.

We can now deform $\tilde{\Psi}_{ij}$ by (i) replacing the n_* tail eigenvalues in S_* by $\tilde{\lambda}_* = \max(S_*)$, and (ii) then correcting for the fact that the so-deformed matrix no longer has a unit diagonal. The resulting matrix $\hat{\Psi}_{ij}$ is given by:

$$\hat{\Psi}_{ij} = \sum_{a=1}^{N-n_*} \tilde{\lambda}^{(a)} \tilde{V}_i^{(a)} \tilde{V}_j^{(a)} + z_i z_j \sum_{a=N-n_*+1}^N \tilde{\lambda}_* \tilde{V}_i^{(a)} \tilde{V}_j^{(a)} \quad (20)$$

$$z_i^2 = y_i^{-2} \sum_{a=N-n_*+1}^N \tilde{\lambda}^{(a)} [\tilde{V}_i^{(a)}]^2 \quad (21)$$

$$y_i^2 = \sum_{a=N-n_*+1}^N \tilde{\lambda}_* [\tilde{V}_i^{(a)}]^2 \quad (22)$$

Here $\tilde{V}_i^{(a)}$ are the principal components of $\tilde{\Psi}_{ij}$. This method is similar to that of (Rebonato and Jäckel, 1999). The key difference is that in (Rebonato and Jäckel,

1999) the “adjustments” z_i are applied to all principal components, while here they are only applied to the tail principal components (for which the eigenvalues are deformed). This results in a smaller distortion of the original matrix. The resultant deformed matrix $\widehat{\Psi}_{ij}$ has improved tail behavior (see Figure 5). Another bonus is that, while superfluously we only modify the tail, the eigenvectors of the deformed matrix $\widehat{\Psi}_{ij}$ are no longer $\widetilde{V}_i^{(a)}$ for all values of a , and the eigenvalues outside of the tail are also deformed. In particular, in some cases there can be some (typically, a few) nearly degenerate¹⁷ eigenvalues $\widetilde{\lambda}^{(a)}$ in the densely populated region of $\widetilde{\lambda}^{(a)}$ (where they are of order 1), i.e., outside of the tail and the higher-end upward-sloping “neck”. The deformation splits such nearly degenerate eigenvalues, which is a welcome bonus. Indeed, the issue with nearly degenerate eigenvalues is that they can adversely affect convergence of the bounded optimization (see below) as the corresponding directions in the risk space have almost identical risk profiles.

3 Backtests

Here we discuss some backtests. We wish to see how our machine learning risk models compare with other constructions (see below). For this comparison, we run our backtests exactly as in (Kakushadze, 2015c), except that the model covariance matrix is build as above (as opposed to the full heterotic risk model construction of (Kakushadze, 2015c)). To facilitate the comparisons, the historical data we use in our backtests here is the same as in (Kakushadze, 2015c)¹⁸ and is described in detail in Subsections 6.2 and 6.3 thereof. The trading universe selection is described in Subsection 6.2 of (Kakushadze, 2015c). We assume that i) the portfolio is established at the open with fills at the open prices; and ii) it is liquidated at the close on the same day (so this is a purely intraday strategy) with fills at the close prices (see (Kakushadze, 2015a) for pertinent details). We include strict trading bounds

$$|H_i| \leq 0.01 A_i \quad (23)$$

Here H_i are the portfolio stock holdings ($i = 1, \dots, N$), and A_i are the corresponding historical average daily dollar volumes computed as in Subsection 6.2 of (Kakushadze, 2015c). We further impose strict dollar-neutrality on the portfolio, so that

$$\sum_{i=1}^N H_i = 0 \quad (24)$$

The total investment level in our backtests here is $I = \$20\text{M}$ (i.e., $\$10\text{M}$ long and $\$10\text{M}$ short), same as in (Kakushadze, 2015c). For the Sharpe ratio optimization with bounds we use the R function `bopt.calc.opt()` in Appendix C of (Kakushadze,

¹⁷ They are not degenerate even within the machine precision. However, they are spaced much more closely than other eigenvalues (on average, that is).

¹⁸ The same data is also used in (Kakushadze and Yu, 2016b), (Kakushadze and Yu, 2017a).

2015c). Table 1 gives summaries of the eigenvalues for various values of K . Considering that the algorithm is nondeterministic, the results are stable against reruns. Table 2 summarizes the backtest results. Here we can wonder whether the following would produce an improvement. Suppose we start from the sample correlation matrix Ψ_{ij} and run the algorithm, which produces the model correlation matrix $\tilde{\Psi}_{ij}$. Suppose now we rerun the algorithm (with the same number of “samplings” M) but use $\tilde{\Psi}_{ij}$ instead of Ψ_{ij} in Eq. (6) to build “sampling” correlation matrices $\Psi_{ij}^{(m)}$. In fact, we can do this iteratively, over and over again, which we refer to as multiple iterations in Table 3. The results in Table 3 indicate that we do get some improvement on the second iteration, but not beyond. Let us note that for $K \geq 100$ with iterations (see Table 3) the method of Subsection 2.4 was insufficient to deal with the issues with small and nearly degenerate eigenvalues, so we used the full method of (Rebonato and Jäckel, 1999) instead (see Subsection 2.4 and Table 3 for details), which distorts the model correlation matrix more (and this affects performance).

4 Concluding Remarks

So, the machine learning risk models we discuss in this paper outperform statistical risk models (Kakushadze and Yu, 2017a). They have the performance essentially similar to the heterotic risk models based on statistical industry classifications using multilevel clustering (Kakushadze and Yu, 2016b). However, here we have single-level clustering, and there is no aggregation of clusterings as in (Kakushadze and Yu, 2016b). Also, the resultant model correlation matrix $\tilde{\Psi}_{ij}$ is *not* a factor model, whereas the models of (Kakushadze and Yu, 2016b) are factor models. Note that both the machine learning risk models of this paper and the models of (Kakushadze and Yu, 2016b) still underperform the heterotic risk models based on fundamental industry classifications; see (Kakushadze, 2015c), (Kakushadze and Yu, 2016a).

In this regard, let us tie up a few “loose ends”, so to speak. Suppose we take just a single “sampling” $\Psi_{ij}^{(m)}$. This is an incomplete, single-level heterotic risk model. However, $\Psi_{ij}^{(m)}$ by construction is positive-definite, so we can invert it and use it in optimization. So, does averaging over a large number M of “samplings” (as in the machine learning risk models of this paper), or implementing a multilevel “Russian-doll” embedding (Kakushadze, 2015b) as in (Kakushadze and Yu, 2016b), add value? It does. Thus, two runs based on a single “sampling” with $K = 40$ and $M = 1$ produced the following results: (i) ROC = 42.434%, SR = 15.479, CPS = 2.044; and (ii) ROC = 42.735%, SR = 15.51, CPS = 2.054 (see Table 2 for notations). Also, what if, instead of using a single k-means to compute $\Psi_{ij}^{(m)}$, we aggregate a large number P of k-means clusterings as in (Kakushadze and Yu, 2016b)? This does not appear to add value. Here are the results from a typical run with $K = 30$, $M = 100$ and $P = 100$: ROC = 42.534%, SR = 15.764, CPS = 2.09. Apparently, and perhaps unsurprisingly, aggregating multiple clusterings and averaging over multiple “samplings” has similar effects. This, in fact, is reassuring.

A R Code

In this appendix we give R (R Project for Statistical Computing, <https://www.r-project.org/>) source code for constructing machine learning risk models discussed in the main text. The code is straightforward and self-explanatory. The sole function is `qrm.calc.ml.cor.mat()` with the following inputs: `r1` is the $N \times T$ matrix of returns (N is the number of stocks, T is the number of points in the time series); `k` is the number of clusters K ; `nn` is the number of iterations (see Section 3); `calc.num` is the number of “samplings” M ; `iter.num` is the maximum number of iterations (which we always set to 100, and which was never saturated in any of our hundreds of thousands of `kmeans()` calls) used by the built-in R function `kmeans()` internally called via the function `qrm.stat.ind.class()` given in Appendix A of (Kakushadze and Yu, 2016b); `num.try` is the number of clusterings `qrm.stat.ind.class()` aggregates internally, with `num.try = 1` (which is the value we use) corresponding to a single k-means clustering; `reg.tail` is the Boolean for regularizing (when set to `TRUE`) the tail of the eigenvalues as in Subsection 2.4. The output of `qrm.calc.ml.cor.mat()` is the inverse Γ_{ij}^{-1} of the model covariance matrix $\Gamma_{ij} = \sigma_i \sigma_j \tilde{\Psi}_{ij}$ (or $\Gamma_{ij} = \sigma_i \sigma_j \hat{\Psi}_{ij}$, when `reg.tail = TRUE` – see Subsection 2.4), where σ_i^2 are the sample variances. The weights with which the M “samplings” are combined are internally set to be uniform. However, this can be modified if so desired. The weights can be based on the Euclidean or some other distance, the sum over the specific variances ξ_i^2 , the average correlations, etc. In our simulations nontrivial weights did not add value.

```
qrm.calc.ml.cor.mat <- function (r1, k, nn = 1,
  calc.num = 100, iter.max = 100,
  num.try = 1, reg.tail = F)
{
  calc.mod.erank <- function(x)
  {
    take <- log(x) > 0
    n <- sum(take)
    x <- x[!take]
    p <- x / sum(x)
    h <- - sum(p * log(p))
    er <- exp(h)
    er <- er + n
    return(er)
  }

  calc.het.cor <- function(p, ind)
  {
    u <- rep(0, nrow(ind))
    for(a in 1:ncol(ind))
```

```

{
  tt <- ind[, a] == 1
  p1 <- p[tt, tt]
  p1 <- eigen(p1)
  u[tt] <- p1$vectors[, 1]
}
flm <- u * ind
q <- t(flm) %*% p %*% flm
g <- flm %*% q %*% t(flm)
diag(g) <- 1
return(g)
}

calc.cor.mat <- function(p, r1, k, iter.max, num.try)
{
  ww <- 0
  gg <- 0
  for(j in 1:calc.num)
  {
    ind <- qrm.stat.ind.class(r1, k,
      iter.max = iter.max, num.try = num.try,
      demean.ret = F)
    g <- calc.het.cor(p, ind)
    w <- 1 ### uniform weighting
    gg <- gg + g * w
    ww <- ww + w
  }
  gg <- gg / ww
  return(gg)
}

gg <- cor(t(r1), t(r1))
for(a in 1:nn)
  gg <- calc.cor.mat(gg, r1, k, iter.max, num.try)
if(reg.tail)
{
  xx <- eigen(gg)
  vv <- xx$values
  uu <- xx$vectors
  er <- trunc(calc.mod.erank(vv))
  tt <- (er + 1):length(vv)
  zz <- colSums(t(uu[, tt]^2) *
    vv[tt]) / vv[er] / rowSums(uu[, tt]^2)

```

```

    zz <- sqrt(zz)
    vv[tt] <- vv[er]
    uu <- t(t(uu) * sqrt(vv))
    uu[, tt] <- zz * uu[, tt]
    gg <- uu %*% t(uu)
  }
  gg <- solve(gg)
  ss <- apply(r1, 1, sd)
  gg <- t(gg / ss) / ss
  return(gg)
}

```

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References

- Campbell, L.L. (1960) Minimum coefficient rate for stationary random processes. *Information and Control* 3(4): 360-371.
- Forgy, E.W. (1965) Cluster analysis of multivariate data: efficiency versus interpretability of classifications. *Biometrics* 21(3): 768-769.
- Grinold, R.C. and Kahn, R.N. (2000) *Active Portfolio Management*. New York, NY: McGraw-Hill.
- Hartigan, J.A. (1975) *Clustering Algorithms*. New York, NY: John Wiley & Sons, Inc.
- Hartigan, J.A. and Wong, M.A. (1979) Algorithm AS 136: A K-Means Clustering Algorithm. *Journal of the Royal Statistical Society, Series C (Applied Statistics)* 28(1): 100-108.
- Kakushadze, Z. (2015a) Mean-Reversion and Optimization. *Journal of Asset Management* 16(1): 14-40. Available online: <https://ssrn.com/abstract=2478345>.
- Kakushadze, Z. (2015b) Russian-Doll Risk Models. *Journal of Asset Management* 16(3): 170-185. Available online: <https://ssrn.com/abstract=2538123>.
- Kakushadze, Z. (2015c) Heterotic Risk Models. *Wilmott Magazine* 2015(80): 40-55. Available online: <https://ssrn.com/abstract=2600798>.
- Kakushadze, Z. (2016) Shrinkage = Factor Model. *Journal of Asset Management* 17(2): 69-72. Available online: <https://ssrn.com/abstract=2685720>.
- Kakushadze, Z. and Yu, W. (2016a) Multifactor Risk Models and Heterotic CAPM. *Journal of Investment Strategies* 5(4): 1-49. Available online: <https://ssrn.com/abstract=2722093>.
- Kakushadze, Z. and Yu, W. (2016b) Statistical Industry Classification. *Journal of Risk & Control* 3(1): 17-65. Available online: <https://ssrn.com/abstract=2802753>.
- Kakushadze, Z. and Yu, W. (2017a) Statistical Risk Models. *Journal of Investment Strategies* 6(2): 11-40. Available online: <https://ssrn.com/abstract=2732453>.
- Ledoit, O. and Wolf, M. (2004) Honey, I Shrunk the Sample Covariance Matrix. *Journal of Portfolio Management* 30(4): 110-119.

- Lloyd, S.P. (1957) Least square quantization in PCM. *Working Paper*. Bell Telephone Laboratories, Murray Hill, NJ.
- Lloyd, S.P. (1982) Least square quantization in PCM. *IEEE Transactions on Information Theory* 28(2): 129-137.
- MacQueen, J.B. (1967) Some Methods for classification and Analysis of Multivariate Observations. In: LeCam, L. and Neyman, J. (eds.) *Proceedings of the 5th Berkeley Symposium on Mathematical Statistics and Probability*. Berkeley, CA: University of California Press, pp. 281-297.
- Markowitz, H.M. (1952) Portfolio Selection. *Journal of Finance* 7(1): 77-91.
- Rebonato, R. and Jäckel, P. (1999) The Most General Methodology to Create a Valid Correlation Matrix for Risk Management and Option Pricing Purposes. *Journal of Risk* 2(2): 17-28.
- Roy, O. and Vetterli, M. (2007) The effective rank: A measure of effective dimensionality. In: *European Signal Processing Conference (EUSIPCO)*. Poznań, Poland (September 3-7, 2007), pp. 606-610.
- Sharpe, W.F. (1994) The Sharpe Ratio. *Journal of Portfolio Management* 21(1): 49-58.
- Steinhaus, H. (1957) Sur la division des corps matériels en parties. *Bull. Acad. Polon. Sci.* 4(12): 801-804.
- Yang, W., Gibson, J.D. and He, T. (2005) Coefficient rate and lossy source coding. *IEEE Transactions on Information Theory* 51(1): 381-386.

Table 1: Summary of eigenvalues of the model correlation matrix $\tilde{\Psi}_{ij}$ for the indicated values of the number K of clusters. All runs are for the number of “samplings” $M = 100$ except for the second entry with $K = 100$ marked with an asterisk, for which $M = 1000$. 1st Qu. = first quartile; 3rd Qu. = third quartile. Mean is always 1 as $\tilde{\Psi}_{ij}$ is a correlation matrix with a unit diagonal (and the sum of eigenvalues equals the sum of the diagonal elements).

K	Min	1st Qu.	Median	Mean	3rd Qu.	Max
10	0.078	0.4795	0.6579	1	0.8318	514.9
20	0.0684	0.45	0.6114	1	0.7856	503.6
30	0.0695	0.4221	0.5662	1	0.7533	499.7
40	0.07	0.3895	0.5346	1	0.7295	497.8
50	0.0684	0.3722	0.515	1	0.7025	496
60	0.0685	0.3574	0.4979	1	0.6841	495.9
70	0.0661	0.3469	0.4838	1	0.6686	497.1
70	0.0665	0.3477	0.4848	1	0.6701	496.9
70	0.0653	0.3464	0.483	1	0.6686	496.9
70	0.0652	0.3467	0.4825	1	0.6663	497.4
70	0.0642	0.3474	0.4835	1	0.67	496.6
70	0.0662	0.3477	0.4843	1	0.6679	496.7
70	0.064	0.3473	0.4853	1	0.6691	496.9
80	0.0614	0.3393	0.4739	1	0.6532	497.6
90	0.0355	0.3298	0.4626	1	0.641	497.6
100	0.015	0.3241	0.4532	1	0.6307	498.3
100*	0.0152	0.3318	0.4618	1	0.6276	498.1
101	0.0184	0.3217	0.4515	1	0.6278	498.6
102	0.0203	0.3219	0.4512	1	0.6255	498.6
103	0.0197	0.321	0.4496	1	0.6268	498.4
104	0.0153	0.319	0.4482	1	0.6245	498.5
105	0.0088	0.3204	0.4491	1	0.6236	498.2
106	0.0116	0.3191	0.447	1	0.6213	498.4
107	0.009	0.3176	0.4466	1	0.6215	498.2
108	0.0067	0.3165	0.4441	1	0.6187	498.4
109	0.0105	0.319	0.4447	1	0.6182	498.2
110	0.0032	0.3149	0.4432	1	0.6176	498.3
120	0.0026	0.3103	0.4355	1	0.6081	499
130	0.0051	0.3023	0.4259	1	0.5986	499.7
140	0.0022	0.2976	0.4209	1	0.5917	499.4
150	0.002	0.292	0.4132	1	0.5839	499.8

Table 2: Backtest results for machine learning risk models for the indicated number K of clusters (here and in Tables 3 and 4 the number of “samplings” $M = 100$). ROC = annualized Return-on-Capital (in %). SR = annualized daily Sharpe Ratio (Sharpe, 1994). CPS = Cents-per-Share. The cases marked “tail” correspond to using the deformed model correlation matrix $\hat{\Psi}_{ij}$; see Subsection 2.4 for details. Also see Figures 6, 7, 8 for graphs of ROC, SR and CPS based on these results.

K	ROC (%)	SR	CPS
10	42.643	15.524	2.059
20	43.135	16.089	2.093
30	43.11	16.337	2.095
40	43.025	16.409	2.094
40	42.961	16.366	2.091
50	42.895	16.43	2.091
50	42.891	16.486	2.091
60	42.647	16.414	2.084
70	42.449	16.358	2.08
80	42.131	16.313	2.071
90	41.842	16.236	2.064
100	41.387	16.096	2.051
110	40.958	16.057	2.041
120, tail	40.726	15.902	2.033
130, tail	40.215	15.838	2.019
140, tail	39.894	15.819	2.011
150, tail	39.162	15.668	1.986

Table 3: Backtest results for machine learning risk models for the indicated number K of clusters with iterations (see Section 3 for details). X2, X3, X4 stand for 2, 3, 4 iterations, respectively. The cases marked “tail” correspond to using the deformed model correlation matrix $\hat{\Psi}_{ij}$ based on the method of (Rebonato and Jäckel, 1999) (and *not* on the method of Subsection 2.4), whereby $\hat{\Psi}_{ij} = \Theta_{ij}/\sqrt{\Theta_{ii}}\sqrt{\Theta_{jj}}$, $\Theta_{ij} = \sum_{a=1}^{N-n_*} \tilde{\lambda}^{(a)} \tilde{V}_i^{(a)} \tilde{V}_j^{(a)} + \sum_{a=N-n_*+1}^N \tilde{\lambda}_* \tilde{V}_i^{(a)} \tilde{V}_j^{(a)}$; see Subsection 2.4 for notations. For comparison purposes, also see Table 4, which gives backtest results for machine learning risk models *without* iterations using the deformed model correlation matrix $\hat{\Psi}_{ij}$ based on the method of (Rebonato and Jäckel, 1999).

K	ROC (%)	SR	CPS
10, X2	42.614	15.213	2.036
10, X2	42.609	15.204	2.036
10, X2	42.627	15.236	2.037
20, X2	43.468	15.82	2.087
30, X2	43.64	16.054	2.099
40, X2	43.672	16.207	2.102
40, X2	43.668	16.186	2.102
40, X3	43.643	16.026	2.091
40, X4	43.508	15.899	2.08
50, X2	43.676	16.296	2.103
60, X2	43.75	16.398	2.109
70, X2	43.714	16.396	2.112
80, X2	43.62	16.41	2.113
90, X2	43.501	16.418	2.113
90, X3	43.654	16.33	2.109
90, X4	43.537	16.22	2.097
100, X2, tail	43.216	16.213	2.086
110, X2, tail	43.153	16.198	2.087
120, X2, tail	43.091	16.244	2.088
130, X2, tail	43.001	16.214	2.089
140, X2, tail	42.944	16.249	2.09
150, X2, tail	42.91	16.267	2.093

Table 4: Backtest results for machine learning risk models for the indicated number K of clusters, all *without* iterations, and using the deformed model correlation matrix $\hat{\Psi}_{ij}$ based on the method of (Rebonato and Jäkel, 1999); see Table 3 for details.

K	ROC (%)	SR	CPS
10	42.421	15.337	2.033
20	42.824	15.853	2.062
30	42.845	16.027	2.066
40	42.805	16.187	2.068
50	42.567	16.186	2.06
60	42.425	16.171	2.057
70	42.263	16.121	2.054
80	42.191	16.155	2.055
90	42.096	16.117	2.054
100	41.854	16.079	2.047
110	41.645	15.991	2.041
120	41.431	15.967	2.035
130	41.44	15.966	2.04
140	41.344	15.989	2.038
150	41.156	15.995	2.033

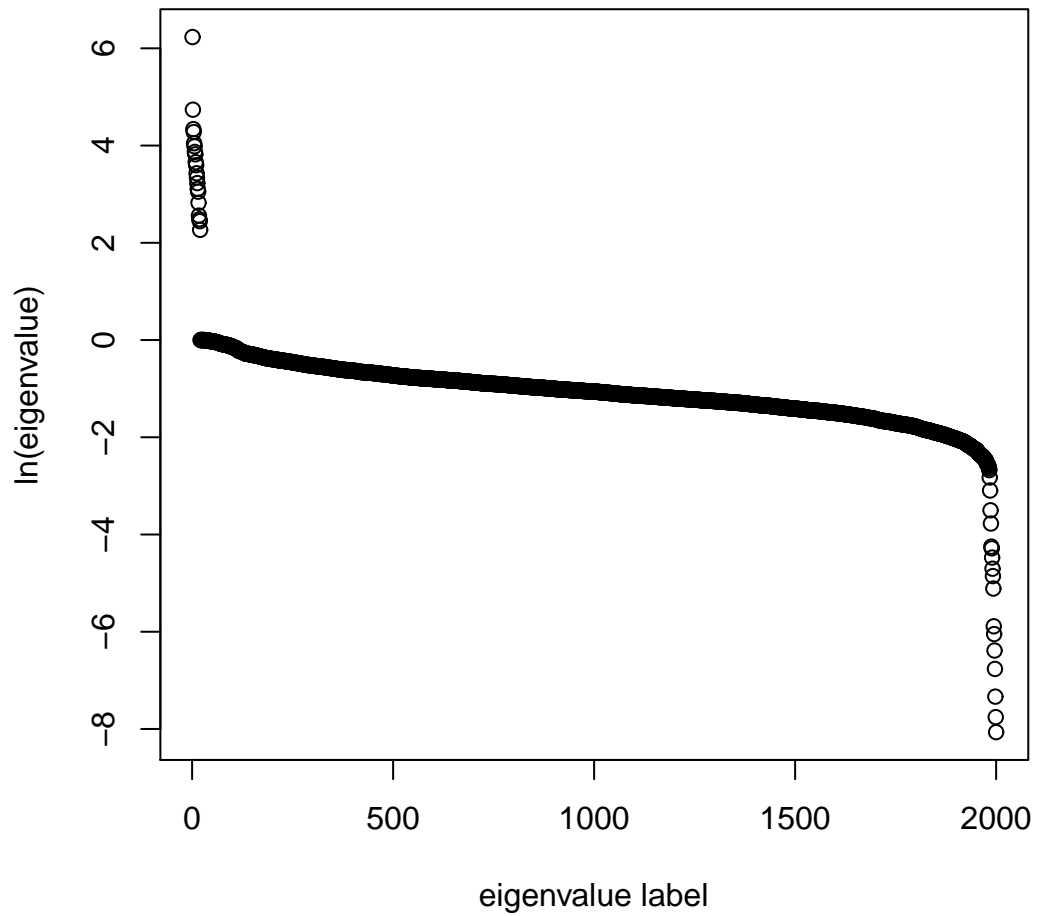


Figure 1: A typical graph of the log of the eigenvalues (ordered decreasingly) of the model correlation matrix $\tilde{\Psi}_{ij}^{(m)}$ for a single “sampling” ($M = 1$). The number of clusters $K = 150$. See Subsection 2.4 for details.

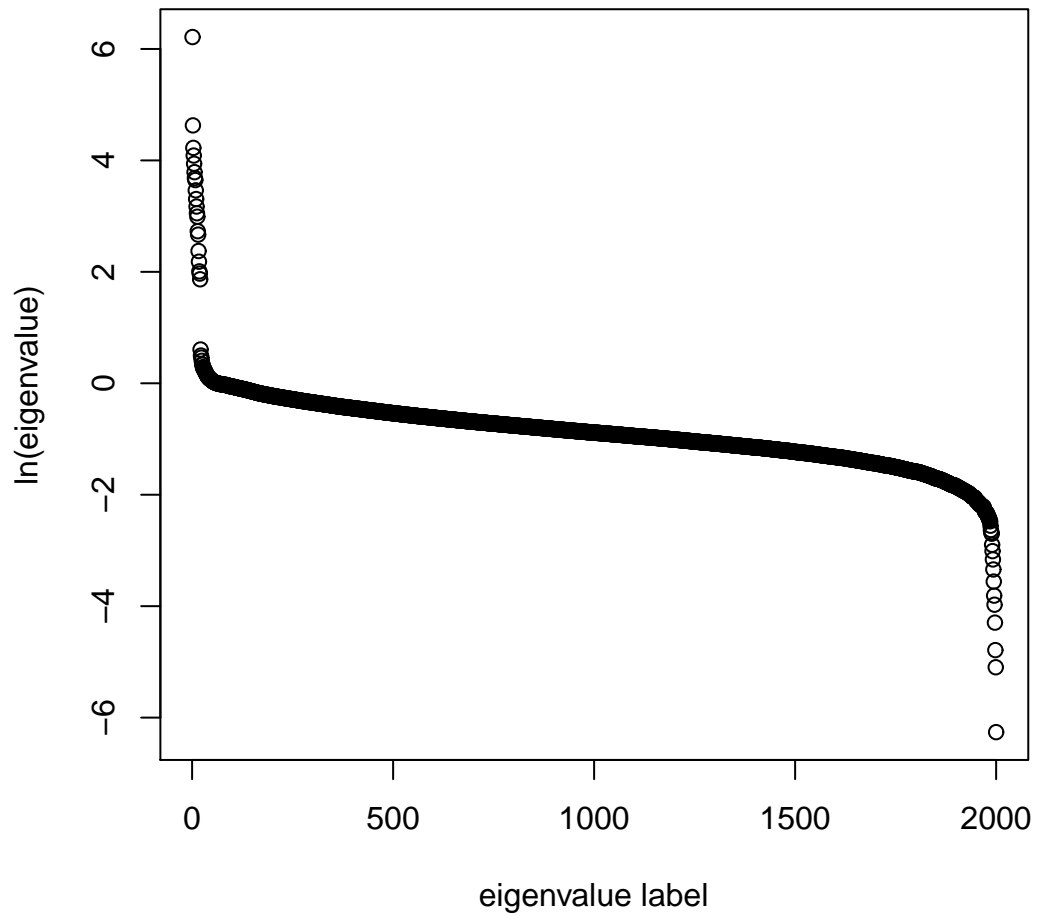


Figure 2: A typical graph of the log of the eigenvalues (ordered decreasingly) of the model correlation matrix $\tilde{\Psi}_{ij}$ obtained by combining $M = 100$ “samplings” (with equal weights). The number of clusters $K = 150$. See Subsection 2.4 for details.

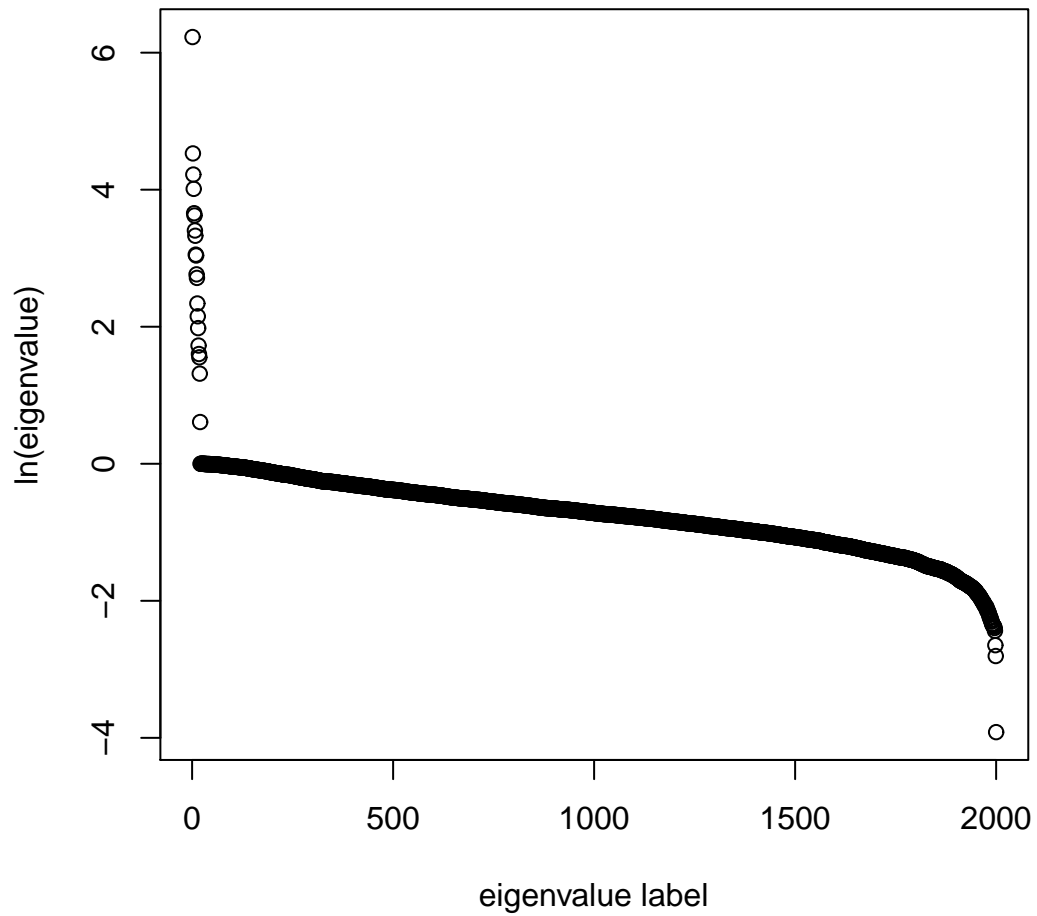


Figure 3: A typical graph of the log of the eigenvalues (ordered decreasingly) of the model correlation matrix $\tilde{\Psi}_{ij}^{(m)}$ for a single “sampling” ($M = 1$). The number of clusters $K = 40$. See Subsection 2.4 for details.

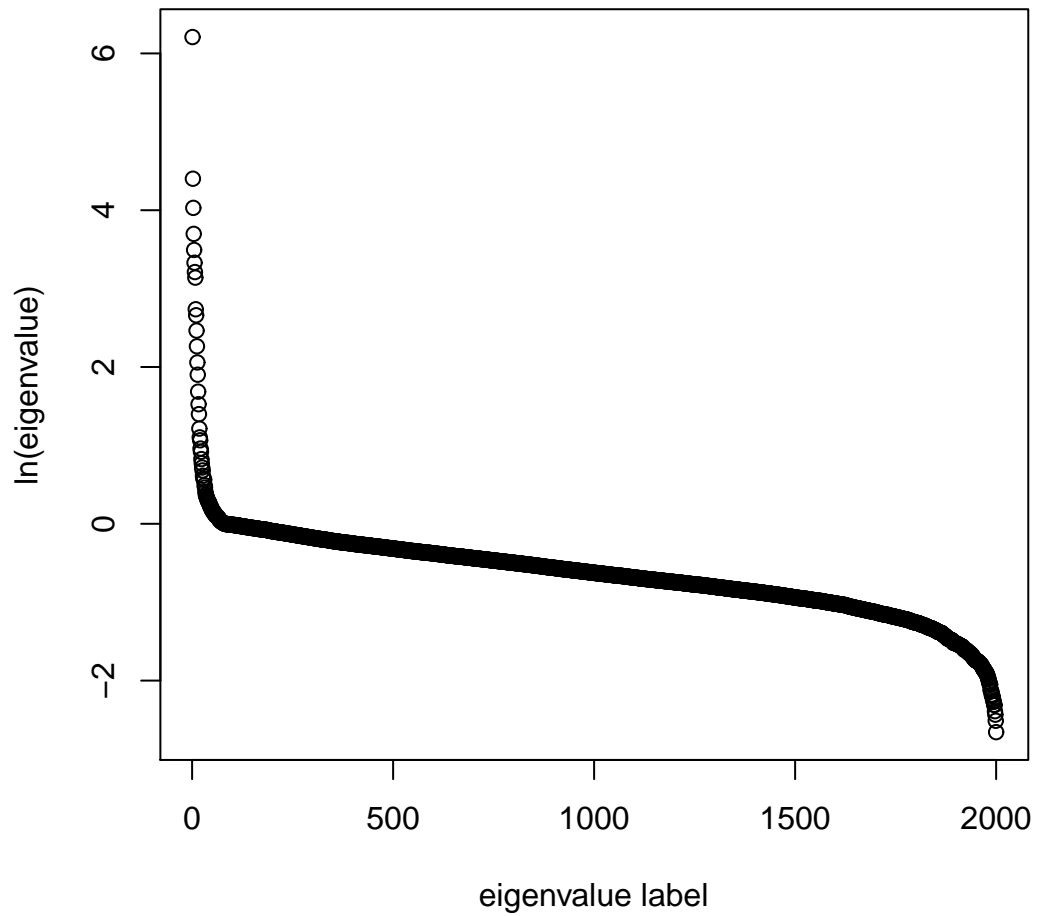


Figure 4: A typical graph of the log of the eigenvalues (ordered decreasingly) of the model correlation matrix $\tilde{\Psi}_{ij}$ obtained by combining $M = 100$ “samplings” (with equal weights). The number of clusters $K = 40$. See Subsection 2.4 for details.

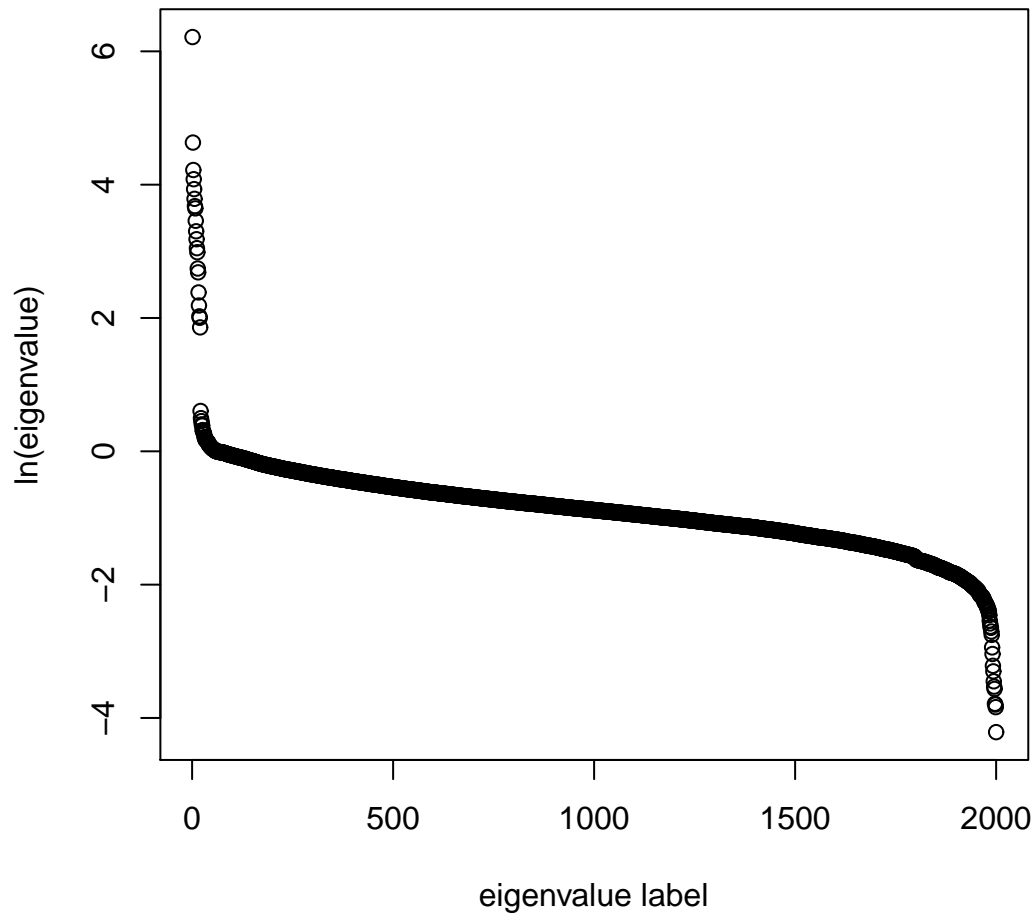


Figure 5: A typical graph of the log of the eigenvalues (ordered decreasingly) of the deformed (by adjusting the low-end “tail” eigenvalues) model correlation matrix $\hat{\Psi}_{ij}$ obtained by combining $M = 100$ “samplings” (with equal weights). The number of clusters $K = 150$. See Subsection 2.4 for details.

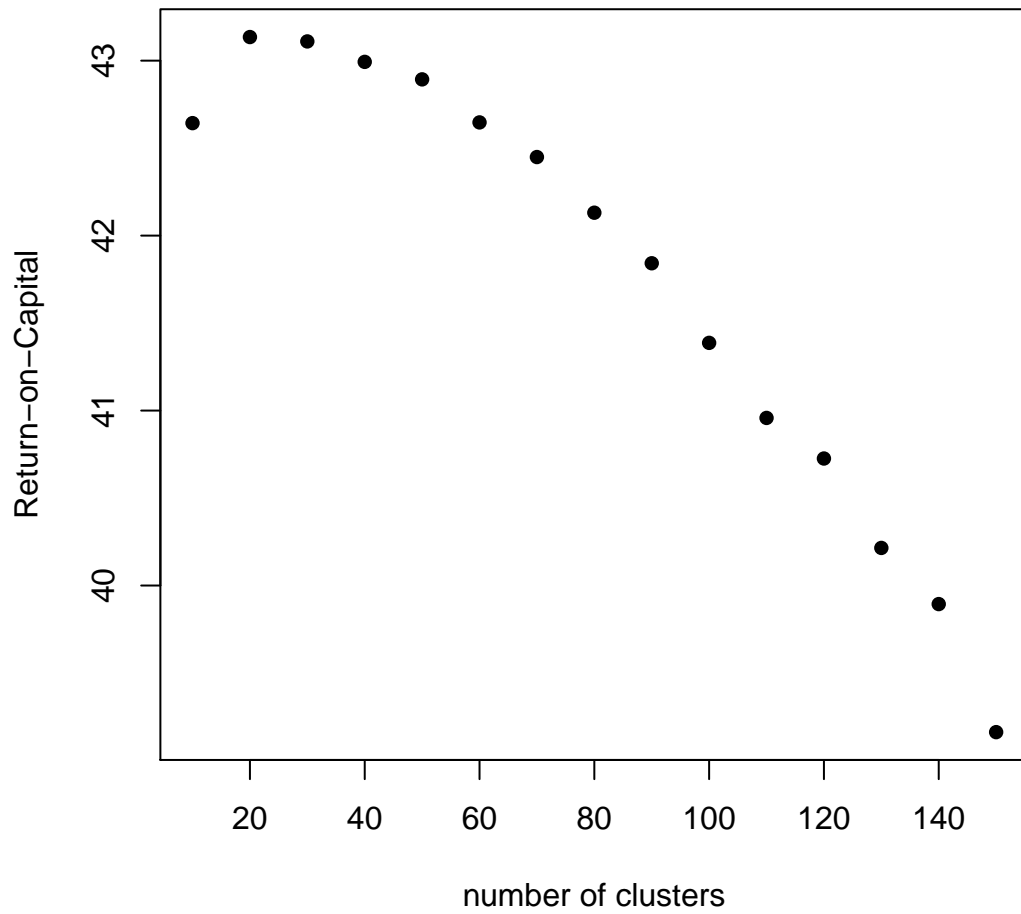


Figure 6: Return-on-Capital (ROC) vs. K (the number of clusters) based on simulations from Table 2. For multiple simulations per K , the average ROC is shown.

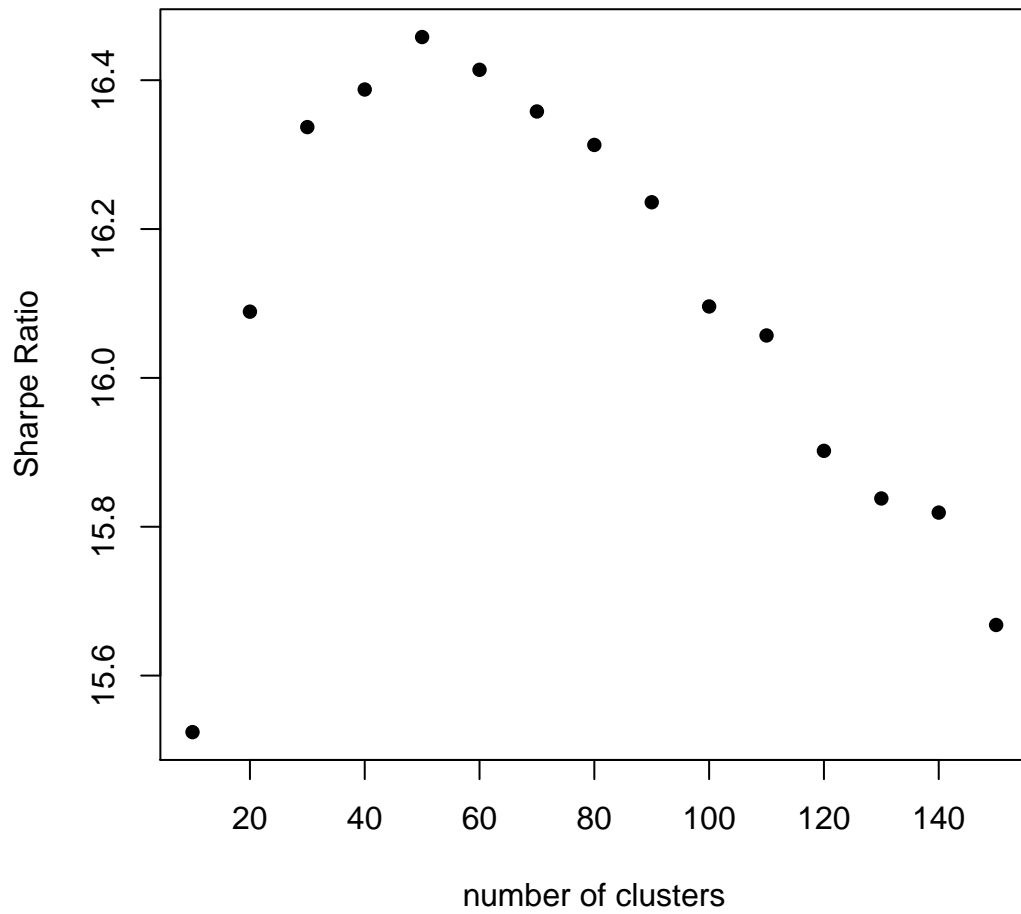


Figure 7: Sharpe Ratio (SR) vs. K (the number of clusters) based on simulations from Table 2. For multiple simulations per K , the average SR is shown.

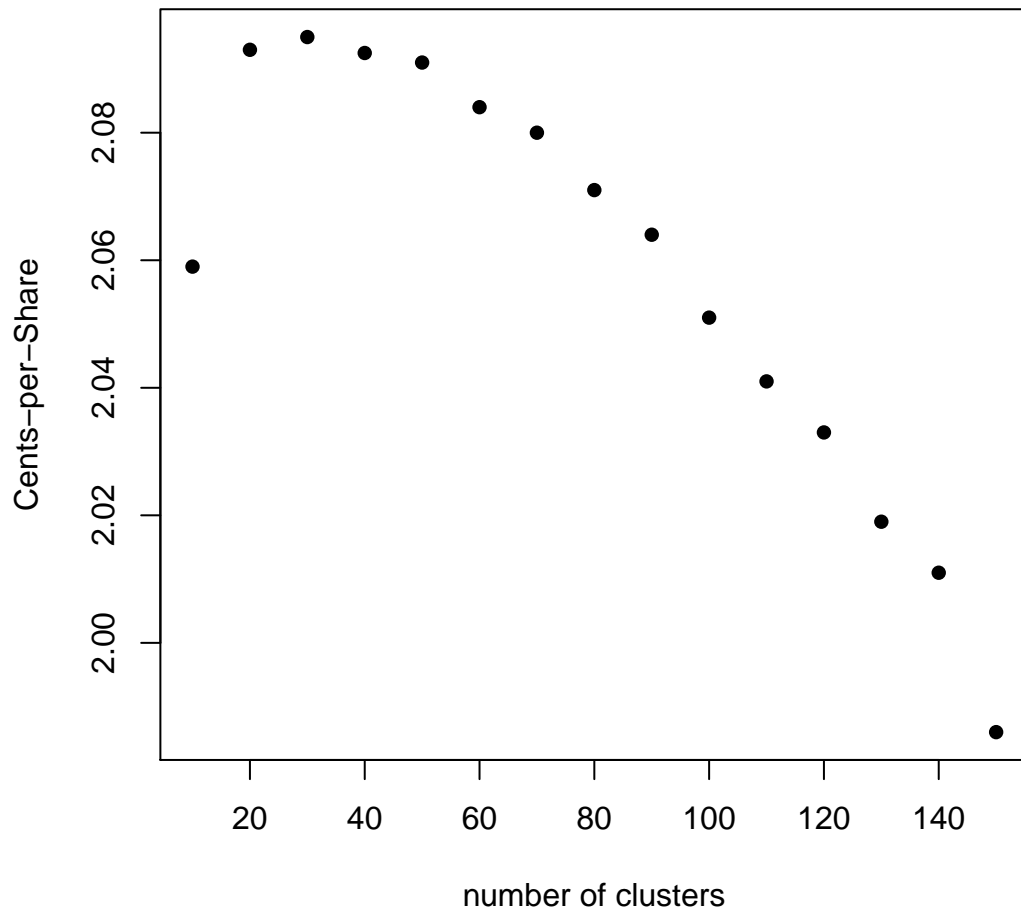


Figure 8: Cents-per-Share (CPS) vs. K (the number of clusters) based on simulations from Table 2. For multiple simulations per K , the average CPS is shown.