

Managing Diversification¹

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Abstract

We propose a unified, fully general methodology to analyze and act on diversification in any environment, including long-short trades in highly correlated markets with complex derivatives. First, we build the diversification distribution, i.e. the distribution of the uncorrelated bets in the portfolio that are consistent with the portfolio constraints. Next, we summarize the wealth of information provided by the diversification distribution into one single diversification index, the effective number of bets, based on the entropy of the diversification distribution. Then, we introduce the mean-diversification efficient frontier, a diversification approach to portfolio optimization. Finally, we describe how to perform mean-diversification optimization in practice in the presence of transaction and market impact costs, by only trading a few optimally chosen securities. Fully documented code illustrating our approach can be downloaded from <http://www.mathworks.com/matlabcentral/fileexchange/23271>.

JEL Classification: C1, G11

Keywords: entropy, mean-diversification frontier, transaction costs, market impact, selection heuristics, systematic risk, idiosyncratic risk, principal component analysis, principal portfolios, r-square, risk contributions, random matrix theory, relative-value strategy, market-neutral strategy, bond immunization, long-short equity pairs.

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1 Introduction

The qualitative definition of diversification is very clear to portfolio managers: a portfolio is well-diversified if it is not heavily exposed to individual shocks.

Oddly enough, there exists no broadly accepted, unique, satisfactory methodology to precisely quantify and manage diversification. Commonly used measures of diversification include the percentage of risk explained by the systematic factors in a systematic-plus-idiosyncratic factor model; the difference between the weighted sum of the volatilities of each position and the total portfolio volatility; the Herfindal index and related measures based on portfolio weights. In addition to not applying in full generality in any market and with arbitrary positions, none of those measures highlights where diversification, or the lack thereof, arises in a given portfolio. We refer the reader to Meucci (2010) for a review and a discussion.

The contributions of this article are fourfold. First, instead of focusing on one single diversification number, we introduce the diversification distribution, a tool to analyze the fine structure of a portfolio's concentration profile in fully general markets and with fully general long-short positions. Second, we introduce the effective number of uncorrelated bets, an actionable index of diversification based on the entropy of the diversification distribution. Third, we introduce the mean-diversification frontier, a quantitative framework to manage the trade-off between the expected return and the effective number of uncorrelated bets. Fourth, we provide an efficient algorithm to implement in practice mean-diversification optimization in the presence of impact and transaction costs, by trading only a few securities.

To achieve the above, we first express a generic portfolio in terms of the exposures to uncorrelated sources of risk. The most natural choice for such sources are the principal components, but these might not be manageable in constrained portfolios: therefore we generalize the principal components to the conditional principal portfolios, whose volatilities fully describe the concentration profile of the trader's positions. Then we interpret these volatilities as a set of probability masses, the diversification distribution. The dispersion of this distribution, as measured by its entropy, becomes a summary index of diversification with a very natural interpretation, namely the effective number of uncorrelated bets in the portfolio. Finally, with this index we build the mean-diversification efficient frontier, which quantifies precisely the trade-off between expected returns, transaction and impact costs, and diversification.

In Section 2 we motivate and construct the diversification distribution, which is the foundation of diversification analysis. In Section 3 we introduce the entropy-based diversification index and use it to tackle diversification management. We illustrate our approach by means of practical examples throughout. Several technical results are thoroughly discussed in the appendix. A fully documented implementation of our approach can be downloaded from <http://www.mathworks.com/matlabcentral/fileexchange/23271>.

2 Diversification analysis

Consider a generic market of N securities. We denote the returns of these securities over the given investment horizon by the N -dimensional vector \mathbf{R} . We represent a generic portfolio in this market by the vector \mathbf{w} of the weights of each security. The return $R_{\mathbf{w}}$ on the portfolio reads:

$$R_{\mathbf{w}} \equiv \mathbf{w}'\mathbf{R}. \quad (1)$$

2.1 Total risk analysis

Since the pathbreaking work of Markowitz (1952), measuring risk in terms of variance has become standard practice in the financial industry. In uncorrelated markets the individual securities in a generic portfolio (1) constitute additive sources of risk:

$$\text{Var}\{R_{\mathbf{w}}\} \equiv \sum_{n=1}^N \text{Var}\{w_n R_n\}. \quad (2)$$

Therefore in uncorrelated markets maximum diversification corresponds to equal variance-adjusted weights.

In correlated markets this is not the case: for instance, a duration-weighted portfolio which is long each node of a government curve is fully concentrated on the curve shifts, see Litterman and Scheinkman (1991) and Appendix A.3 for all the details. However, although the securities in the market are correlated, it is always possible to determine sources of risk that are uncorrelated, and therefore additive.

The most natural choice of uncorrelated risk sources is provided by the principal component decomposition of the returns covariance Σ :

$$\mathbf{E}'\Sigma\mathbf{E} \equiv \Lambda. \quad (3)$$

In this expression the diagonal matrix $\Lambda \equiv \text{diag}(\lambda_1, \dots, \lambda_N)$ contains the eigenvalues of Σ , sorted in decreasing order, and the columns of the matrix $\mathbf{E} \equiv (\mathbf{e}_1, \dots, \mathbf{e}_N)$ are the respective eigenvectors. The eigenvectors define a set of N uncorrelated portfolios, the *principal portfolios*, whose returns $\tilde{\mathbf{R}} \equiv \mathbf{E}^{-1}\mathbf{R}$ are decreasingly responsible for the randomness in the market. Indeed, the eigenvalues Λ correspond to the variances of these uncorrelated portfolios.

In Figure 1 we display the geometrical interpretation of the decomposition (3): the eigenvectors $\mathbf{e}_1, \dots, \mathbf{e}_N$, i.e. the principal portfolios, are the directions of the principal axes of an ellipsoid; and the square root of the eigenvalues $\sqrt{\lambda_1}, \dots, \sqrt{\lambda_N}$, i.e. the volatilities of the principal portfolios, are the length of these axes, refer to Meucci (2005) for further details. We emphasize that the decomposition (3), which is the heart of the analysis to follow, holds for any market with a well-defined covariance, and not necessarily for normal markets only. For instance, the market in Figure 1 is log-normal as in Black and Scholes (1973), but the same interpretation holds also for non-parametric distributions,

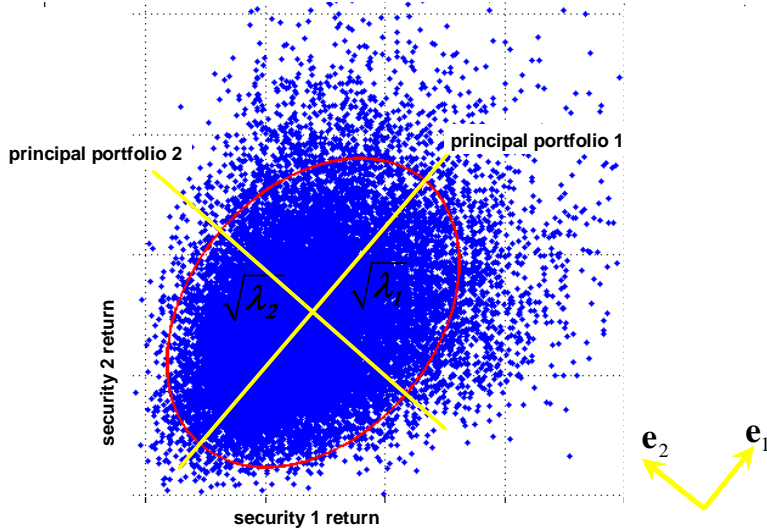


Figure 1: Geometric interpretation of principal component analysis

or for t -distributed markets, possibly skewed, where no two portfolios are ever independent, etc.

A generic portfolio can be seen either as a combination of the original securities with weights \mathbf{w} as in (1), or as a combination of the uncorrelated principal portfolios with weights $\tilde{\mathbf{w}} \equiv \mathbf{E}^{-1}\mathbf{w}$, see also Partovi and Caputo (2004). In terms of the latter we can introduce the *variance concentration curve*

$$v_n \equiv \tilde{w}_n^2 \lambda_n, \quad n = 1, \dots, N. \quad (4)$$

The generic entry v_n of this concentration curve represents the variance due to the n -th principal portfolio: much like (2), since the principal portfolios are uncorrelated, the total portfolio variance is the sum of these terms:

$$\text{Var}\{R_{\mathbf{w}}\} = \sum_{n=1}^N v_n. \quad (5)$$

Equivalently, we can consider the *volatility concentration curve*

$$s_n \equiv \frac{\tilde{w}_n^2 \lambda_n}{\text{Sd}\{R_{\mathbf{w}}\}}, \quad n = 1, \dots, N. \quad (6)$$

The volatility concentration curve does not simply represent a normalized decomposition of the variance concentration: as we prove in Appendix A.1, (6) represents the decomposition of volatility or tracking error into the contributions from each principal portfolio as in Litterman (1996).

Finally, we can normalize the variance and the volatility concentration curves further into the *diversification distribution*:

$$p_n \equiv \frac{\tilde{w}_n^2 \lambda_n}{\text{Var}\{R_{\mathbf{w}}\}}, \quad n = 1, \dots, N. \quad (7)$$

This is not simply a percentage version of the variance and the volatility concentration curves: as we show in Appendix A.2, the generic term p_n equals the r-square from a regression of the total portfolio return on the n -th principal portfolio.

This approach generalizes to correlated markets the methodology in Meucci (2007). We emphasize that the above analysis also applies to management against a benchmark with weights \mathbf{b} . Indeed, it suffices to replace the portfolio weights with the vector of the relative bets

$$\mathbf{w} \mapsto \mathbf{w} - \mathbf{b}. \quad (8)$$

Then (6) becomes the *tracking error concentration curve* and (7) becomes the *relative diversification distribution*.

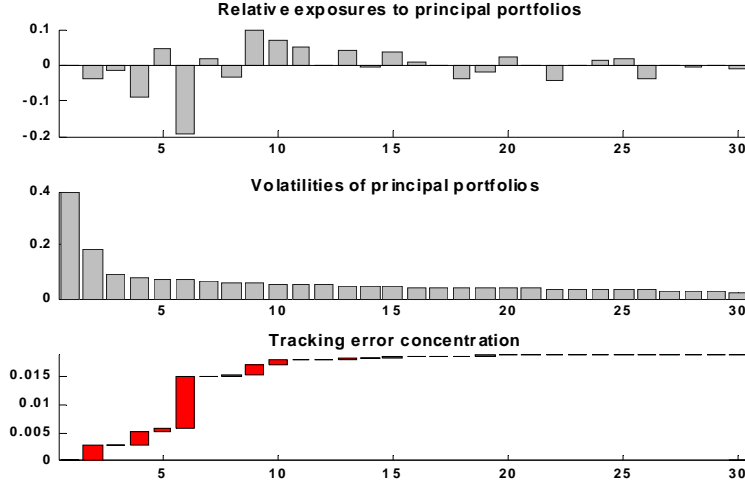


Figure 2: Diversification profile relative to a benchmark

To illustrate, we consider a simplified market of $N \equiv 30$ liquid mid-cap stocks in the Russel 3000 index. We assume that the manager tracks a benchmark in the same stocks with weights proportional to their market capitalization. We estimate the covariance matrix of the returns Σ by exponential smoothing daily observations. Then we analyze the relative diversification of the equally-weighted portfolio $\mathbf{w} \equiv \mathbf{1}/N$, which generates a tracking error of 1.89%. The

top plot in Figure 2 reports the relative exposures to the principal portfolios $\tilde{\mathbf{w}} \equiv \mathbf{E}^{-1}(\mathbf{w} - \mathbf{b})$; the middle plot reports the volatilities $\sqrt{\lambda_1}, \dots, \sqrt{\lambda_N}$ of the principal portfolios; the bottom plot displays the tracking error concentration curve. Notice how the exposure to the sixth principal portfolio is rather large and so is its contribution to the tracking error.

2.2 Conditional risk analysis

The first entry in the volatility or tracking error concentration curve (6) represents the exposure to the first principal portfolio, which represents the overall market.

Consider a portfolio of stocks in the same sector. As we show in Appendix A.4, the budget constraint fully determines the exposure to the overall market, but it has no effect on the exposure to the remaining principal portfolios. Since the market is the leading source of risk, the overall diversification level might be poor, but the manager might still be doing a great job at diversifying away the portion of risk under his control. In order to analyze this actionable portion of diversification, the manager simply renormalizes the remaining entries in the diversification distribution:

$$p_n \mapsto \tilde{p}_n \equiv \frac{p_n}{\sum_{m=2}^N p_m}, \quad n = 2, \dots, N. \quad (9)$$

Now, consider an investment in government bonds. Again, the budget constraint creates exposure to the overall market. However, as we show in Appendix A.3, unless the portfolio is duration-weighted, the budget constraint strongly influences but does not fully determine the exposure to the market. Furthermore, the budget constraint also has an effect on the exposures to the remaining principal portfolios. Therefore, a simple analysis such as (9) is no longer viable.

More in general, portfolios can be subject to a number of constraints that only allow for specific rebalancing directions. Alternatively, managers can wish to zoom into the fine structure of diversification along specific rebalancing directions that are not imposed by constraints, but rather by their personal choice. We represent the free directions for the rebalancing vector $\Delta \mathbf{w}$ through an implicit equation

$$\mathbf{A} \Delta \mathbf{w} \equiv \mathbf{0}, \quad (10)$$

where \mathbf{A} is a conformable $K \times N$ matrix whose each row represents a constraint.

The formulation (10) covers a variety of situations. For instance, the budget constraint reads $\mathbf{1}'\mathbf{w} \equiv 1$ and thus the respective row in \mathbf{A} is a vector of ones; a constant-delta exposure constraint to a given underlying implies that the respective row in \mathbf{A} are the securities' sensitivities to the chosen underlying; in a fund of funds, where the manager cannot rebalance within the funds, \mathbf{A} includes the null space of the funds' weights.

The formulation (10) also covers any rebalancing restriction on which the manager intends to condition the analysis, regardless of actual investment constraints. For instance, if we are analyzing a single-currency equity portfolio

using a multi-region, multi-asset covariance matrix, we do not wish to consider the additional securities as potential investment possibilities: then \mathbf{A} includes the rows of the identity matrix corresponding to those securities. Also, one might be skeptical about the statistical significance of the eigendirections relative to the smallest eigenvalues, as purported by random matrix theory, see e.g. Potters, Bouchaud, and Laloux (2005): in this case \mathbf{A} would include the suspicious eigenvectors, because reallocating those portfolios would not make statistical sense.

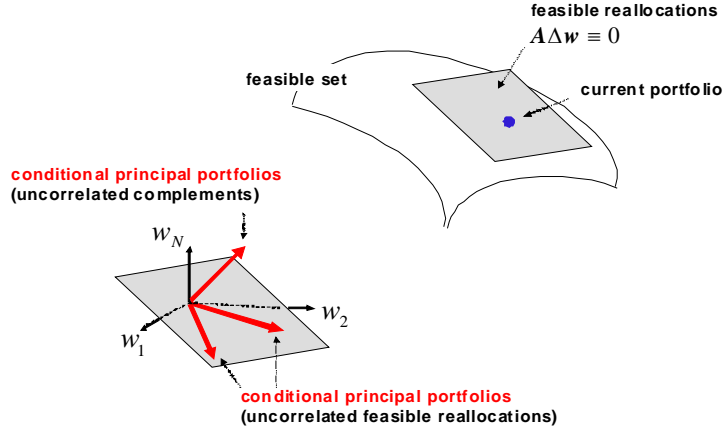


Figure 3: Conditional principal portfolios

Finally, (10) also covers non-linear constraints locally, by considering the space tangent to the constraint set, see Figure 3. For instance, a constraint on the value-at-risk corresponds to a row in \mathbf{A} which equals $-\mathbb{E}\{\mathbf{R}'\} - \mathbf{w}'\mathbf{R} \equiv \gamma$, where γ denotes the desired target VaR: this follows from a notable result in Hallerbach (2003) and Gourioux, Laurent, and Scaillet (2000), see Appendix A.5.

To analyze diversification in this context, instead of the standard principal portfolios (3), we decompose risk onto N *conditional principal portfolios*. Similarly to the standard principal portfolios, these are uncorrelated portfolios that are decreasingly responsible for the randomness in the market. However the conditional principal portfolios are adapted to the rebalancing constraints. More precisely, first we define recursively for $n = K + 1, \dots, N$ the portfolios that span the feasible reallocations

$$\begin{aligned} \mathbf{e}_n &\equiv \operatorname{argmax}_{\mathbf{e}'\mathbf{e}=1} \{\mathbf{e}'\Sigma\mathbf{e}\} \\ \text{such that } &\begin{cases} \mathbf{A}\mathbf{e} \equiv \mathbf{0} \\ \mathbf{e}'\Sigma\mathbf{e}_j \equiv 0, \quad \text{for all existing } \mathbf{e}_j, \end{cases} \end{aligned} \quad (11)$$

see also Figure 3. If \mathbf{A} is empty, this process generates the standard principal portfolios (3). For general matrices \mathbf{A} , the solutions $\mathbf{e}_{K+1}, \dots, \mathbf{e}_N$ still represent combinations of securities that are mutually uncorrelated and decreasingly responsible for the randomness in the market. However, the conditional principal portfolios are adapted to the desired directions (10), in that they can be freely added to the current allocation. Indeed, it is immediate to verify that a generic re-allocation $\Delta \mathbf{w} \equiv \alpha_{K+1} \mathbf{e}_{K+1} + \dots + \alpha_N \mathbf{e}_N$ satisfies (10) for arbitrary coefficients α . Next, we complement the above set of feasible reallocations to span the whole market. Hence, we define recursively for $n = 1, \dots, K$ the following uncorrelated portfolios, which are decreasingly responsible for the randomness in the inaccessible directions

$$\begin{aligned} \mathbf{e}_n &\equiv \underset{\mathbf{e}'\mathbf{e}=1}{\operatorname{argmax}} \{ \mathbf{e}'\Sigma\mathbf{e} \} \\ &\text{such that } \mathbf{e}'\Sigma\mathbf{e}_j \equiv 0, \quad \text{for all existing } \mathbf{e}_j. \end{aligned} \quad (12)$$

We refer the reader to Appendix A.6 for the computation of (11)-(12), which

only involves iterations of standard principal component analysis.

By collecting the conditional principal portfolios in a matrix $\mathbf{E} \equiv (\mathbf{e}_1, \dots, \mathbf{e}_N)$, we can express the returns covariance in the same format as (3)

$$\mathbf{E}'\Sigma\mathbf{E} \equiv \mathbf{\Lambda}. \quad (13)$$

In this expression $\mathbf{\Lambda}$ is a diagonal matrix whose non-zero entries represent the variances of the conditional principal portfolios:

$$\lambda_n \equiv \operatorname{Var} \{ \mathbf{e}_n' \mathbf{R} \}, \quad n = 1, \dots, N. \quad (14)$$

In Figure 4 we display the typical pattern of the generalized spectrum (14).

Proceeding as in the unconditional case, we can represent a generic allocation \mathbf{w} equivalently as a linear combination of the conditional principal portfolios with weights

$$\tilde{\mathbf{w}} \equiv \mathbf{E}^{-1} \mathbf{w}. \quad (15)$$

The total portfolio variance is the sum of the contributions from the conditional principal portfolios, since these are uncorrelated:

$$\operatorname{Var} \{ R_{\mathbf{w}} \} = \sum_{n=1}^N \tilde{w}_n^2 \lambda_n. \quad (16)$$

The conditioning equations (10) take on a very simple form in the new coordinates (15): indeed, the first K entries of $\tilde{\mathbf{w}}$ cannot be altered. Therefore instead of (7) we focus on the *conditional diversification distribution*

$$p_n | \mathbf{A} \equiv \frac{\tilde{w}_n^2 \lambda_n}{\sum_{m=K+1}^N \tilde{w}_m^2 \lambda_m}, \quad n = K+1, \dots, N, \quad (17)$$

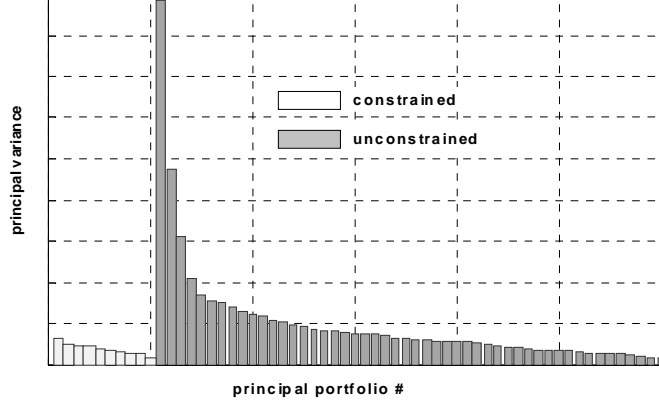


Figure 4: Generalized PCA spectrum: variances of conditional principal portfolios

where the notation emphasizes that the conditioning is enforced by the matrix \mathbf{A} in (10).

It is easy to check that if the rows of \mathbf{A} represent some unconditional principal portfolios then conditional and unconditional principal portfolios coincide. This is the case in the single-sector stock market with the budget constraint, where indeed $\mathbf{A} \equiv \mathbf{1}'$ and, as shown in Appendix A.4, $\mathbf{1}$ is a principal portfolio: then the conditional analysis $p_n|\mathbf{1}'$ in (17) is equivalent to the simple adjustment to the unconditional analysis (9).

The conditional diversification distribution provides a clear picture of the diversification structure of a portfolio when only specific rebalancing directions are allowed: by controlling the terms of this distribution the manager can efficiently manage diversification, hedging or leveraging the conditional principal portfolios based on his views on the market.

As in the unconditional case, the above conditional analysis also applies to management against a benchmark with weights \mathbf{b} : by replacing as in (8) the portfolio weights with the vector of the relative bets, (17) yields the *relative conditional diversification distribution*.

To illustrate, we consider our example of thirty liquid mid-cap stocks in the Russel 3000 index managed against a thirty-stock benchmark. First of all, we compute the relative diversification profile as it follows from conditioning the large 3000×3000 global matrix to only allow for trades in those thirty liquid stocks. As expected, the result is the same as the analysis in Figure 2.

Then we compute and display in Figure 5 the relative diversification profile that follows from further conditioning the analysis on the budget constraint. The load is now more evenly spread on two principal portfolios. Depending on

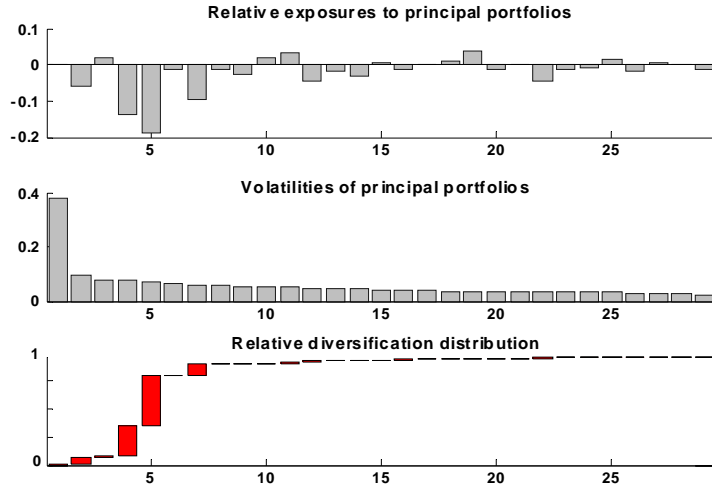


Figure 5: Diversification relative to a benchmark under budget constraint

his views on the market, the portfolio manager can proceed to either hedge these risks or to increase these exposures by means of a parsimonious set of trades as discussed further below.

3 Diversification management

Both the simple unconditional diversification distribution (7) and the conditional diversification distribution (17), whether absolute or relative to a benchmark, are always defined, are always positive and always add up to one. Therefore the diversification distribution can be interpreted as a set of probability masses associated with the principal portfolios.

The shape of the ensuing probability density provides a clear picture of the level of diversification of a given allocation: for a well-diversified portfolio the probability masses p_n are approximately equal and thus the diversification distribution is close to uniform; on the other hand, if the portfolio is concentrated in a specific conditional principal direction, the diversification distribution displays a sharp peak.

Therefore portfolio diversification can be represented as in Meucci (2007) by the dispersion of the diversification distribution, as summarized by its entropy, or equivalently by its exponential:

$$\mathcal{N}_{Ent} \equiv \exp \left(- \sum_{n=K+1}^N p_n \ln p_n \right), \quad (18)$$

where the unconditional case corresponds to $K = 0$.

The interpretation of \mathcal{N}_{Ent} is very intuitive. Indeed, it is easy to verify that $\mathcal{N}_{Ent} = 1$ in fully concentrated positions, i.e. when all the risk is completely due to one single principal portfolio. On the other hand, \mathcal{N}_{Ent} achieves its maximum value $N - K$ in portfolios whose risk is homogeneously spread among the $N - K$ available principal portfolios. In other words, \mathcal{N}_{Ent} represents the true number of uncorrelated bets in a fully general, potentially long-short, portfolio in a fully general market.

We remark that (18) is not the only measure of diversification based on entropy. However, other definitions such as Bera and Park (2004) act on the portfolio weights, and thus do not account for the volatilities and the correlations in the market. Also, (18) is not the only measure based on principal component analysis, see Rudin and Morgan (2006). However, the latter does not identify the causes of concentration. We discuss these and more related issues in Meucci (2010).

To illustrate, we consider our example of an equally weighted portfolio of $N \equiv 30$ liquid mid-cap stocks benchmarked to a market-capitalization weighted index of the same stocks.

We focus on the unconditional diversification number, i.e. $K \equiv 0$ in (18). Since the portfolio is managed against a benchmark we consider the relative diversification analysis, which corresponds to replacing in the construction of the index (18) the relative bets whenever the portfolio weights appear, as specified by (8). The result is $\mathcal{N}_{Ent} \approx 5.5$ effective relative bets, which is consistent with the bottom plot in Figure 2, see also Figure 6.

In order to optimize diversification, portfolio managers can compute the mean-diversification efficient frontier

$$\mathbf{w}_\varphi \equiv \underset{\substack{\mathbf{w} \in \mathcal{C} \\ \boldsymbol{\mu}'\mathbf{w} \geq \varphi}}{\operatorname{argmax}} \mathcal{N}_{Ent}(\mathbf{w}), \quad (19)$$

where $\boldsymbol{\mu}$ denotes the estimated expected returns and \mathcal{C} is a set of investment constraints. The parameter φ spans the set $[\underline{\varphi}, \overline{\varphi}]$ where

$$\underline{\varphi} \equiv \boldsymbol{\mu}' \underset{\mathbf{w} \in \mathcal{C}}{\operatorname{argmax}} \mathcal{N}_{Ent}(\mathbf{w}) \quad (20)$$

$$\overline{\varphi} \equiv \underset{\mathbf{w} \in \mathcal{C}}{\operatorname{argmax}} \boldsymbol{\mu}'\mathbf{w}. \quad (21)$$

When φ in (19) is close to $\underline{\varphi}$ diversification is the main concern, whereas as φ in (19) approaches $\overline{\varphi}$ the focus shifts on the expected returns.

For example, we consider our market of $N \equiv 30$ liquid stocks where as above \mathcal{N}_{Ent} in (19) is the unconditional number of relative bets. We set the expected returns $\boldsymbol{\mu}$ using a risk-premium argument as $\boldsymbol{\mu} \equiv 0.5\boldsymbol{\sigma}$, where $\boldsymbol{\sigma}$ are the square roots of the diagonal elements of $\boldsymbol{\Sigma}$. We assume that stock weights are bounded between -10% and 100% .

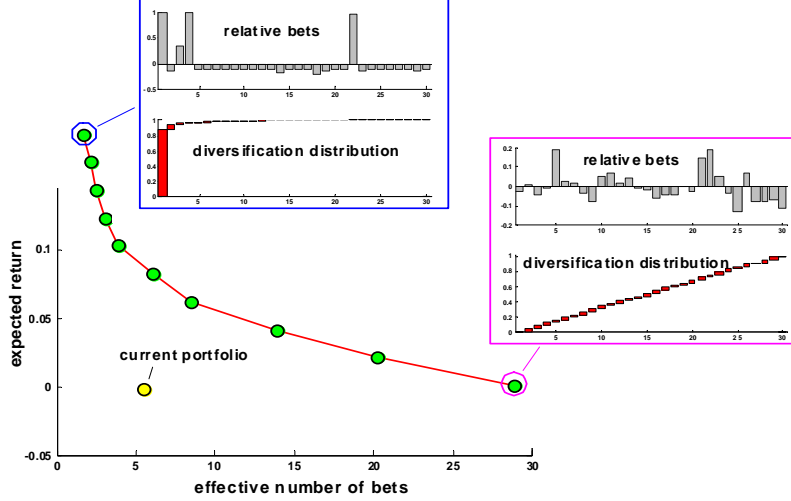


Figure 6: Mean-diversification efficient frontier

As we see in Figure 6, for small values of φ long-short positions alternate to increase diversification: the relative diversification distribution is highly uniform and the number of effective uncorrelated relative bets \mathcal{N}_{Ent} approaches thirty, i.e. the number of securities in this market. On the other hand, for large values of φ the relative diversification distribution concentrates on very few effective bets with higher expected returns: notice how the interplay of positions and correlations heavily concentrates risk, although the relative bets appear to be rather distributed. Also notice that the current equally weighted allocation is heavily suboptimal.

In practice, the expected returns should be adjusted for transaction and impact cost

$$\boldsymbol{\mu}'\mathbf{w} \mapsto \boldsymbol{\mu}'\mathbf{w} - \mathcal{T}(\mathbf{w}, \mathbf{w}_{cur}), \quad (22)$$

where \mathcal{T} is an empirically fitted function of the current allocation \mathbf{w}_{cur} and the target portfolio \mathbf{w} , see e.g. Torre and Ferrari (1999) and Almgren, Thum, Hauptmann, and Li (2005). Since \mathcal{T} is a discontinuous function of the weights, and thus it is not even convex, the diversification frontier cannot be computed exactly, because the optimization (19)-(22) can be solved numerically only in trivially small markets. Furthermore, it is operationally impractical to monitor the progress of a large number of trades.

Instead, it is better to pursue a parsimonious reallocation that gives rise to the largest possible increase in the mean-diversification trade-off with only a small number of trades. The exact combinatorial search for the best combination of trades is unfeasible, but it can be replaced by a recursive-acceptance selection algorithm, which converges in a matter of seconds. Intuitively, this routine adds

the best "team player" one at a time from among all the securities available in the market. Each time a player is tested, the optimization (19)-(22) runs on a very small number of variables and thus it can be solved. We discuss all the details of this algorithm in Appendix A.7.

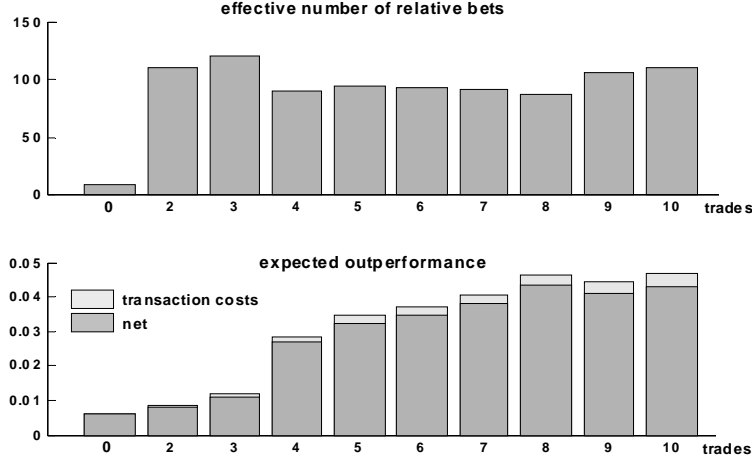


Figure 7: Mean-entropy trade-off management with few trades

To illustrate, we consider a mutual fund benchmarked to the full Russel 3000 index. Again, we consider \mathcal{N}_{Ent} in (19) to be the unconditional number of relative bets. We assume a transaction cost model

$$\mathcal{T}(\mathbf{w}; \mathbf{w}_{cur}) \equiv \sum_{n=1}^N \mathcal{T}_n(w_n - w_{n;cur}), \quad (23)$$

where \mathbf{w}_{cur} denotes the current equally weighted portfolio and

$$\mathcal{T}_n(v) \equiv \begin{cases} 0 & \text{if } v = 0 \\ \alpha_n & \text{if } 0 < |v| \leq \gamma_n \\ \beta_n |v|^\zeta & \text{if } |v| > \gamma_n. \end{cases} \quad (24)$$

In this expression $\zeta \approx 1.5$ and the security-specific coefficients α_n , β_n and γ_n are fitted empirically, refer to the above references for the rationale behind this specification. Notice the discontinuity in the origin, which makes (19)-(22) intractable with standard optimization techniques.

Instead, we run our optimization routine and we display in Figure 7 the results. The current equally weighed portfolio gives rise to only $\mathcal{N}_{Ent} \approx 9$ effective relative bets and less than 1% expected return over the benchmark. Given the

budget constraint, the minimum number of trades allowed is two. With only two trades the number of effective relative bets jumps to $\mathcal{N}_{Ent} \approx 110$. Three trades marginally increase both diversification and expected outperformance. With four trades, a dramatic improvement of expected outperformance is achieved at the expense of a little diversification. Adding trades beyond this point is not advisable.

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A Appendix

In this appendix we report results and computations that can be skipped at first reading.

A.1 Volatility concentration curve as contributions to risk

Assume

$$R_{\mathbf{w}} = \sum_{n=1}^N \tilde{w}_n \tilde{R}_n, \quad (25)$$

Then

$$\begin{aligned} \frac{\partial \text{Sd}\{R_{\mathbf{w}}\}}{\partial \tilde{\mathbf{w}}} &= \frac{\partial}{\partial \tilde{\mathbf{w}}} \left(\tilde{\mathbf{w}}' \text{Cov}\{\tilde{\mathbf{R}}\} \tilde{\mathbf{w}} \right)^{\frac{1}{2}} \\ &= \frac{1}{\text{Sd}\{R_{\mathbf{w}}\}} \left(\text{Cov}\{\tilde{\mathbf{R}}\} \tilde{\mathbf{w}} \right). \end{aligned} \quad (26)$$

Now recall that $\tilde{R}_1, \dots, \tilde{R}_N$ are uncorrelated, or $\text{Cov}\{\tilde{\mathbf{R}}\} \equiv \mathbf{\Lambda}$, a diagonal matrix. Then:

$$\frac{\partial \text{Sd}\{R_{\mathbf{w}}\}}{\partial \tilde{w}_n} = \frac{\lambda_n \tilde{w}_n}{\text{Sd}\{R_{\mathbf{w}}\}}. \quad (27)$$

A.2 R-square as contributions to risk

Consider a generic sub-set $\mathcal{N} \equiv \{n_1, \dots, n_K\}$ of the uncorrelated portfolios. Consider the following representation of the portfolio return:

$$R_{\mathbf{w}} \equiv \sum_{n \in \mathcal{N}} \tilde{w}_n \tilde{R}_n + \sum_{n \notin \mathcal{N}} \tilde{w}_n \tilde{R}_n, \quad (28)$$

where $\tilde{R}_1, \dots, \tilde{R}_N$ are uncorrelated, or $\text{Cov}\{\tilde{\mathbf{R}}\} \equiv \mathbf{\Lambda}$, a diagonal matrix. The r-square of the regression of $R_{\mathbf{w}}$ on the returns $\tilde{R}_{n_1}, \dots, \tilde{R}_{n_K}$ reads:

$$\begin{aligned} r^2 &\equiv 1 - \frac{\text{Var}\left\{\sum_{n \notin \mathcal{N}} \tilde{w}_n \tilde{R}_n\right\}}{\text{Var}\left\{\sum_{n \in \mathcal{N}} \tilde{w}_n \tilde{R}_n + \sum_{n \notin \mathcal{N}} \tilde{w}_n \tilde{R}_n\right\}} \\ &= \frac{\text{Var}\left\{\sum_{n \in \mathcal{N}} \tilde{w}_n \tilde{R}_n\right\}}{\text{Var}\{R_{\mathbf{w}}\}} = \frac{1}{\text{Sd}\{R_{\mathbf{w}}\}} \frac{\sum_{n \in \mathcal{N}} \tilde{w}_n^2 \lambda_n}{\text{Sd}\{R_{\mathbf{w}}\}} \end{aligned} \quad (29)$$

Using (27) we obtain:

$$\begin{aligned} r^2 &= \frac{1}{\text{Sd}\{R_{\mathbf{w}}\}} \sum_{n \in \mathcal{N}} \frac{\partial \text{Sd}\{R_{\mathbf{w}}\}}{\partial \tilde{w}_n} \tilde{w}_n \\ &= \frac{1}{\text{Sd}\{R_{\mathbf{w}}\}} \sum_{n \in \mathcal{N}} s_n. \end{aligned} \quad (30)$$

Using the definition (7) we obtain:

$$r^2 = \sum_{n \in \mathcal{N}} p_n. \quad (31)$$

A.3 Exposure management in the bond market

Consider the government bond market. The return of the generic n -th bond reads

$$R_n \approx -d_n \Delta y_n, \quad (32)$$

where d_n is the duration and Δy_n the change in the respective yield to maturity over the investment horizon.

We introduce the duration-adjusted weights

$$w_n \equiv \frac{\gamma}{d_n}, \quad (33)$$

where γ is defined by

$$\frac{1}{\gamma} \equiv \sum_{n=1}^N \frac{1}{d_n}. \quad (34)$$

The weights (33) add up to one and provide direct exposure to the market. Indeed, consider the PCA decomposition of the yield curve

$$\text{Cov} \{\Delta \mathbf{y}\} \equiv \mathbf{G} \mathbf{\Gamma} \mathbf{G}', \quad (35)$$

where $\mathbf{G} \equiv (\mathbf{g}_1, \dots, \mathbf{g}_N)$ is the eigenvector matrix and $\mathbf{\Gamma}$ is the diagonal matrix of the eigenvalues. Then as in Litterman and Scheinkman (1991) we obtain

$$\mathbf{g}_1 \approx \frac{\mathbf{1}}{\sqrt{N}}. \quad (36)$$

We can express the curve changes as

$$\Delta \mathbf{y} = \mathbf{g}_1 F_1 + \mathbf{g}_2 F_2 + \dots + \mathbf{g}_N F_N, \quad (37)$$

where the factors are defined as

$$\mathbf{F} \equiv \mathbf{G}' \Delta \mathbf{y}. \quad (38)$$

Then

$$\begin{aligned} R_{\mathbf{w}} &= \sum_{n=1}^N w_n R_n \approx - \sum_{n=1}^N w_n d_n \Delta y_n \stackrel{(33)-(32)}{\approx} -\gamma \mathbf{1}' \Delta \mathbf{y} \\ &\stackrel{(36)}{\approx} -\gamma \sqrt{N} \mathbf{g}_1' \Delta \mathbf{y} = \gamma \sqrt{N} \mathbf{g}_1' (\mathbf{g}_1 F_1 + \mathbf{g}_2 F_2 + \dots + \mathbf{g}_N F_N) \\ &= -\gamma \sqrt{N} \mathbf{g}_1' \mathbf{g}_1 F_1. \end{aligned} \quad (39)$$

In other words, the portfolio is fully exposed to the market, i.e. F_1 , but it is not exposed to the other factors. However this is only true for the specific duration-weighted allocation (33).

A.4 Exposure management in the stock market

Consider the equity market. Assume a one-factor model

$$\mathbf{R} = \beta R_M + \boldsymbol{\epsilon}, \quad (40)$$

where

$$\text{Cov} \{R_M, \boldsymbol{\epsilon}\} = \mathbf{0} \quad (41)$$

and

$$\boldsymbol{\Sigma}_\epsilon = \sigma_\epsilon^2 \mathbf{I} \quad (42)$$

Select stocks in the same sector, in such a way that

$$\boldsymbol{\beta} = \beta \mathbf{1}, \quad (43)$$

for a suitable scalar β .

Then the covariance matrix reads

$$\begin{aligned} \boldsymbol{\Sigma} &\equiv \text{Cov} \{\mathbf{R}\} = \beta \boldsymbol{\beta}' \sigma_M^2 + \boldsymbol{\Sigma}_\epsilon \\ &= \mathbf{1} \mathbf{1}' \beta^2 \sigma_M^2 + \sigma_\epsilon^2 \mathbf{I}, \end{aligned} \quad (44)$$

and $\mathbf{1}$ is an eigenvector:

$$\begin{aligned} \boldsymbol{\Sigma} \mathbf{1} &= \mathbf{1} \mathbf{1}' \beta^2 \sigma_M^2 + \sigma_\epsilon^2 \mathbf{1} \\ &= (N \beta^2 \sigma_M^2 + \sigma_\epsilon^2) \mathbf{1}. \end{aligned} \quad (45)$$

Furthermore, notice that $\mathbf{1}$ is the leading eigenvector. Indeed, by construction, the leading eigenvector satisfies

$$\begin{aligned} \mathbf{e}^* &\propto \underset{\mathbf{e}'\mathbf{e} \equiv 1}{\text{argmax}} \{ \mathbf{e}' \boldsymbol{\Sigma} \mathbf{e} \} \\ &= \underset{\mathbf{e}'\mathbf{e} \equiv 1}{\text{argmax}} \{ \mathbf{e}' [\mathbf{1} \mathbf{1}' \beta^2 \sigma_M^2 + \sigma_\epsilon^2 \mathbf{I}] \mathbf{e} \} \\ &= \underset{\mathbf{e}'\mathbf{e} \equiv 1}{\text{argmax}} \{ \mathbf{e}' \mathbf{1} \mathbf{1}' \beta^2 \sigma_M^2 \mathbf{e} + \sigma_\epsilon^2 \mathbf{e}' \mathbf{e} \} \\ &= \underset{\mathbf{e}'\mathbf{e} \equiv 1}{\text{argmax}} \{ (\mathbf{e}' \mathbf{1})^2 \} \\ &= \frac{1}{\sqrt{N}} \mathbf{1}. \end{aligned} \quad (46)$$

Therefore

$$\begin{aligned} R_{\mathbf{w}} &= \mathbf{w}' \mathbf{R} = \mathbf{w}' (\beta R_M + \boldsymbol{\epsilon}) \\ &= \mathbf{w}' (\beta \mathbf{1} R_M + \boldsymbol{\epsilon}) = \beta \mathbf{w}' \mathbf{1} R_M + \mathbf{w}' \boldsymbol{\epsilon} \\ &= \beta R_M + \mathbf{w}' \boldsymbol{\epsilon}. \end{aligned} \quad (47)$$

In other words the budget constraint fully determines the exposure to the first factor and has no effect on the remaining factors.

A.5 Tangent space of constraint set

Consider a generic non-linear constraint

$$g(\mathbf{w}) \equiv 0. \quad (48)$$

Differentiating this expression we obtain

$$(\Delta \mathbf{w})' \frac{\partial g(\mathbf{w})}{\partial \mathbf{w}} \equiv 0, \quad (49)$$

which locally is in the format (10) for

$$\mathbf{A}' \equiv \frac{\partial g(\mathbf{w})}{\partial \mathbf{w}} \quad (50)$$

For instance, consider the VaR constraint

$$\text{VaR}(\mathbf{w}) - \gamma \equiv 0. \quad (51)$$

Differentiating this expression we obtain locally

$$(\Delta \mathbf{w})' \frac{\partial \text{VaR}(\mathbf{w})}{\partial \mathbf{w}} \equiv 0. \quad (52)$$

Using a result in Hallerbach (2003) and Gouriéroux, Laurent, and Scaillet (2000), we can write

$$\frac{\partial \text{VaR}(\mathbf{w})}{\partial \mathbf{w}} \equiv -\mathbf{E}\{\mathbf{R} | -\mathbf{w}'\mathbf{R} \equiv \gamma\}, \quad (53)$$

which yields the expression in the main text.

A.6 Computation of conditional principal portfolios

Both (11) and (12) can be written as

$$\begin{aligned} \mathbf{e}^* &\equiv \underset{\|\mathbf{e}\| \equiv 1}{\text{argmax}} \{\mathbf{e}'\mathbf{\Sigma}\mathbf{e}\} \\ &\text{such that } \mathbf{B}\mathbf{e} \equiv \mathbf{0}, \end{aligned} \quad (54)$$

where $\|\mathbf{e}\|^2 \equiv \mathbf{e}'\mathbf{e}$ and \mathbf{B} is a conformable matrix. In particular, for (11)

$$\mathbf{B} \equiv \begin{pmatrix} \mathbf{A} \\ \mathbf{e}'_{K+1}\mathbf{\Sigma} \\ \vdots \\ \mathbf{e}'_{n-1}\mathbf{\Sigma} \end{pmatrix}; \quad (55)$$

and for (12)

$$\mathbf{B} \equiv \begin{pmatrix} \mathbf{e}'_1 \boldsymbol{\Sigma} \\ \vdots \\ \mathbf{e}'_{n-1} \boldsymbol{\Sigma} \\ \mathbf{e}'_{K+1} \boldsymbol{\Sigma} \\ \vdots \\ \mathbf{e}'_N \boldsymbol{\Sigma} \end{pmatrix}. \quad (56)$$

Therefore, we focus on the solution of the general formulation (54).

Define the Lagrangian

$$\mathcal{L} \equiv \mathbf{e}' \boldsymbol{\Sigma} \mathbf{e} - \lambda (\mathbf{e}' \mathbf{e} - 1) - \mathbf{e}' \mathbf{B}' \boldsymbol{\gamma} \quad (57)$$

The first order conditions read

$$\mathbf{0} \equiv \frac{\partial \mathcal{L}}{\partial \mathbf{e}} \equiv 2 \boldsymbol{\Sigma} \mathbf{e} - 2 \lambda \mathbf{e} - \mathbf{B}' \boldsymbol{\gamma}, \quad (58)$$

which implies

$$\begin{aligned} \mathbf{0} &\equiv \mathbf{B} \frac{\partial \mathcal{L}}{\partial \mathbf{e}} \equiv 2 \mathbf{B} \boldsymbol{\Sigma} \mathbf{e} - 2 \lambda \mathbf{B} \mathbf{e} - \mathbf{B} \mathbf{B}' \boldsymbol{\gamma} \\ &= 2 \mathbf{B} \boldsymbol{\Sigma} \mathbf{e} - \mathbf{B} \mathbf{B}' \boldsymbol{\gamma}. \end{aligned} \quad (59)$$

Hence

$$\boldsymbol{\gamma} = 2 (\mathbf{B} \mathbf{B}')^{-1} \mathbf{B} \boldsymbol{\Sigma} \mathbf{e}. \quad (60)$$

Substituting this in (58) we obtain

$$\mathbf{0} \equiv \boldsymbol{\Sigma} \mathbf{e} - \lambda \mathbf{e} - \mathbf{B}' (\mathbf{B} \mathbf{B}')^{-1} \mathbf{B} \boldsymbol{\Sigma} \mathbf{e}, \quad (61)$$

which shows that \mathbf{e}^* in (54) is an eigenvector of $\mathbf{P} \boldsymbol{\Sigma}$ where

$$\mathbf{P} \equiv \mathbf{I} - \mathbf{B}' (\mathbf{B} \mathbf{B}')^{-1} \mathbf{B}, \quad (62)$$

i.e. it solves

$$\mathbf{P} \boldsymbol{\Sigma} \mathbf{e}^* = \lambda \mathbf{e}^*, \quad (63)$$

or

$$\mathbf{e}^* \equiv \operatorname{argmax}_{\|\mathbf{e}\| \equiv 1} \{\mathbf{e}' \mathbf{P} \boldsymbol{\Sigma} \mathbf{e}\}. \quad (64)$$

Now consider the problem

$$\hat{\mathbf{e}} \equiv \operatorname{argmax}_{\|\mathbf{e}\| \equiv 1} \{\mathbf{e}' \mathbf{P} \boldsymbol{\Sigma} \mathbf{P}' \mathbf{e}\}. \quad (65)$$

Since $\mathbf{P} \boldsymbol{\Sigma} \mathbf{P}'$ is symmetric, it admits a basis of orthogonal eigenvectors. In particular $\hat{\mathbf{e}}$ satisfies

$$\mathbf{P} \boldsymbol{\Sigma} \mathbf{P}' \hat{\mathbf{e}} = \lambda \hat{\mathbf{e}}, \quad (66)$$

where λ is the maximum eigenvalue. Notice that \mathbf{P} as defined in (62) is symmetric

$$\mathbf{P} = \mathbf{P}' \quad (67)$$

and idempotent

$$\mathbf{P}\mathbf{P} = \mathbf{P}, \quad \mathbf{P}'\mathbf{P}' = \mathbf{P}'. \quad (68)$$

Hence, first of all

$$\begin{aligned} (\mathbf{P}\Sigma\mathbf{P}')(\mathbf{P}\hat{\mathbf{e}}) &= \mathbf{P}\Sigma\mathbf{P}'\mathbf{P}\hat{\mathbf{e}} \stackrel{(67)}{=} \mathbf{P}\Sigma\mathbf{P}'\mathbf{P}'\hat{\mathbf{e}} \\ &\stackrel{(67)}{=} \mathbf{P}\Sigma\mathbf{P}'\hat{\mathbf{e}} \stackrel{(67)}{=} \mathbf{P}\Sigma\mathbf{P}'\hat{\mathbf{e}} \stackrel{(66)}{=} \mathbf{P}\lambda\hat{\mathbf{e}} \\ &= \lambda\mathbf{P}\hat{\mathbf{e}}. \end{aligned} \quad (69)$$

In other words, $\mathbf{P}\hat{\mathbf{e}}$ is an eigenvector of $\mathbf{P}\Sigma\mathbf{P}'$ relative to the eigenvalue λ . but so is $\hat{\mathbf{e}}$, see (66). Since the eigenspace relative to a (unique) eigenvalue is unique it follows

$$\mathbf{P}\hat{\mathbf{e}} = \gamma\hat{\mathbf{e}}, \quad (70)$$

for a suitable scalar γ . Second, we verify

$$\begin{aligned} (\mathbf{P}\Sigma)(\mathbf{P}\hat{\mathbf{e}}) &= \mathbf{P}\Sigma\mathbf{P}\hat{\mathbf{e}} \stackrel{(67)}{=} \mathbf{P}\Sigma\mathbf{P}'\hat{\mathbf{e}} \stackrel{(68)}{=} \mathbf{P}\Sigma\mathbf{P}'\hat{\mathbf{e}} \stackrel{(66)}{=} \mathbf{P}\lambda\hat{\mathbf{e}} \\ &= \lambda\mathbf{P}\hat{\mathbf{e}}. \end{aligned} \quad (71)$$

In other words, $\mathbf{P}\hat{\mathbf{e}}$ is an eigenvector of $\mathbf{P}\Sigma$ relative to the eigenvalue λ . From (70) this implies that $\hat{\mathbf{e}}$ is an eigenvector of $\mathbf{P}\Sigma$ relative to the eigenvalue λ . Given the normalization $\|\mathbf{e}\| \equiv 1$, this means that $\hat{\mathbf{e}}$, as defined in (65) also solves

$$\hat{\mathbf{e}} \equiv \operatorname{argmax}_{\|\mathbf{e}\|=1} \{\mathbf{e}'\mathbf{P}\Sigma\mathbf{e}\}. \quad (72)$$

By comparing this with (64) it follows that $\hat{\mathbf{e}} \equiv \mathbf{e}^*$. The good feature of formulation (65) is that the matrix $\mathbf{P}\Sigma\mathbf{P}'$ is symmetric, and thus the formula represent the standard principal component analysis of a (not strictly) positive and symmetric matrix.

A.7 Trading selection algorithm

Suppose that we want to trade only M of the N securities, where M has to be larger than the number of portfolio constraints K .

First we introduce the set \mathcal{I}_M^N of all the possible trade combinations for a given number M of trades. Suppose that we have identified an M -dimensional potential combination of indices to trade $I_M \in \mathcal{I}_M^N$.

For instance, for $M \equiv 2$ trades and $N \equiv 3$ securities in the market, the set of all the possible combinations of tradable securities reads:

$$\mathcal{I}_2^3 \equiv \{\{1, 2\}, \{1, 3\}, \{2, 3\}\} \quad (73)$$

and a possible combination would be, say,

$$I_M \equiv \{1, 3\}. \quad (74)$$

We impose that transactions can only occur on those securities by enforcing

$$\Delta \mathbf{w} \equiv \mathbf{S}_{I_M} \mathbf{x}, \quad (75)$$

where \mathbf{x} is a yet-to-be defined M -dimensional vector of decision variables and \mathbf{S}_{I_M} is the $N \times M$ selection matrix for the trade index I .

In our example we have

$$\mathbf{S}_{\{1,3\}} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (76)$$

which ensures through (75) that only the first and the third entry of \mathbf{w} can change.

From (19) the actual amount to trade in the M securities indexed by I_M reads

$$\begin{aligned} \Delta \mathbf{w}_{I_M} \equiv & \mathbf{S}_{I_M} \operatorname{argmax}_{\mathbf{S}_{I_M} \mathbf{x} \in \tilde{\mathcal{C}}} \left\{ \lambda \left(\boldsymbol{\mu}' \mathbf{S}_{I_M} \mathbf{x} - \tilde{\mathcal{T}}(\mathbf{S}_{I_M} \mathbf{x}) \right) \right. \\ & \left. + (1 - \lambda) \tilde{\mathcal{N}}_{Ent}(\mathbf{S}_{I_M} \mathbf{x}) \right\}. \end{aligned} \quad (77)$$

where

$$\tilde{\mathcal{T}}(\mathbf{v}) \equiv \mathcal{T}(\mathbf{w}_0; \mathbf{w}_0 + \mathbf{v}) \quad (78)$$

$$\tilde{\mathcal{N}}_{Ent}(\mathbf{v}) \equiv \mathcal{N}_{Ent}(\mathbf{w}_0 + \mathbf{v}) \quad (79)$$

$$\tilde{\mathcal{C}} \equiv \mathcal{C} - \mathbf{w}_0. \quad (80)$$

This corresponds to the following optimal mean-diversification trade-off, which measures the goodness of trading the securities in I_M :

$$\mathcal{G}(I_M) \equiv \lambda \left(\boldsymbol{\mu}' \Delta \mathbf{w}_{I_M} - \tilde{\mathcal{T}}(\Delta \mathbf{w}_{I_M}) \right) + (1 - \lambda) \tilde{\mathcal{N}}_{Ent}(\Delta \mathbf{w}_{I_M}). \quad (81)$$

Notice that, regardless the number of securities N in the portfolio, the optimization (77) is performed on the low-dimension vector \mathbf{x} and thus this computation is very fast. In other words, the computation of (81), which represents the goodness of a generic index I_M is not a concern.

The amount (77) is optimal when the M securities indexed by I_M are traded. In order to find the best M -security trade we need to search through all possible combinations

$$\tilde{I}_M \equiv \operatorname{argmax}_{I_M \in \mathcal{I}_M^N} \{ \mathcal{G}(I_M) \}. \quad (82)$$

The optimal trade then follows from (77). Furthermore, since the best number of trades M is typically unknown a priori, one should compute the optimal trade-off as a function of the number of trades

$$\mathcal{G}(\tilde{I}_m), \quad m = \underline{M}, \dots, M, \quad (83)$$

where \underline{M} denotes the minimum possible number of trades, and stop at the number of trades M such that the marginal advantage of an extra trade becomes negligible.

However the combinatorial search (82) repeated as in (83) cannot be performed in practice, as the number of combinations to consider becomes quickly intractably large: indeed, the set \mathcal{I}_M^N contains $M!/(M! - (N - M)!)$ combinations, a formidable number even for relatively small M when N is of the order of at least, say, a few hundreds.

Therefore, to solve (82) we resort to a recursive acceptance selection heuristic as in Meucci (2005), which only requires MN calculations and thus converges in a matter of seconds. Intuitively, this routine adds one at a time the best "team player" from all the trades available in the market. More precisely, the routine proceeds as follows

A.7.1 The efficient recursive acceptance heuristics

Step 0. Initialize $M \equiv \underline{M}$, the lowest possible number of trades, typically $\underline{M} = 2$ in the presence of the budget constraint. Then set the current optimal choice

$$\tilde{I}_M \equiv \{n_1, \dots, n_M\} \quad (84)$$

as the indices of the M securities which give rise to the highest absolute sensitivity to the trade-off target in (19), namely

$$\mathbf{v} \equiv \left| \varphi \boldsymbol{\mu} + (1 - \varphi) \frac{\partial \mathcal{N}_{Ent}}{\partial \mathbf{w}} \right|. \quad (85)$$

Refer to Appendix A.7.2 for the computation of the derivative on the right hand side of (85).

Step 1. Consider all the augmented choices $\{n_1, \dots, n_M, q_j\}$ obtained by adding the generic j -th element q_j from the $N - M$ that populate the complement of the current choice.

Step 2. Evaluate for all $j = 1, \dots, N - M$ the goodness (81) of the above augmented choices

$$g_M^j \equiv \mathcal{G}(\{n_1, \dots, n_M, q_j\}) \quad (86)$$

Step 3. Determine the most effective new candidate, as the one which gives rise to the best augmented choice

$$j^* \equiv \operatorname{argmax}_{j \in \{1, \dots, N - M\}} \left\{ g_M^j \right\}. \quad (87)$$

Step 4. Add the best element to the current choice

$$\tilde{I}_{M+1} \equiv \left\{ \tilde{I}_M, q_{j^*} \right\} \quad (88)$$

Step 5. Set $M \equiv M+1$, i.e. set the current choice \tilde{I}_M as (88); if the goodness $\mathcal{G}(\tilde{I}_M)$ is satisfactory stop, otherwise go to Step 1.

A.7.2 Entropy sensitivities

Define

$$\mathbf{G} \equiv \mathbf{\Lambda}^{\frac{1}{2}} \mathbf{E}^{-1}, \quad (89)$$

and recall from (3) and (7) that

$$\mathbf{p} \equiv \frac{(\mathbf{G}\mathbf{w}) \circ (\mathbf{G}\mathbf{w})}{\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w}}, \quad (90)$$

where \circ denotes the Hadamard product:

$$(\mathbf{v} \circ \mathbf{w})_n \equiv v_n w_n, \quad n = 1, \dots, N. \quad (91)$$

Then

$$\begin{aligned} \frac{\partial \mathbf{p}}{\partial w_u} &= \frac{\partial}{\partial w_u} \frac{(\mathbf{G}\mathbf{w}) \circ (\mathbf{G}\mathbf{w})}{\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w}} \\ &= \frac{1}{\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w}} \frac{\partial (\mathbf{G}\mathbf{w}) \circ (\mathbf{G}\mathbf{w})}{\partial w_u} + (\mathbf{G}\mathbf{w}) \circ (\mathbf{G}\mathbf{w}) \frac{\partial}{\partial w_u} \left(\frac{1}{\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w}} \right) \\ &= \frac{2}{\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w}} \text{diag}(\mathbf{G}\mathbf{w}) \mathbf{G}_{:,u} - 2 \frac{(\mathbf{G}\mathbf{w}) \circ (\mathbf{G}\mathbf{w})}{(\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w})^2} (\mathbf{G}'\mathbf{G})_{u,:} \mathbf{w} \end{aligned} \quad (92)$$

and thus

$$\frac{\partial \mathbf{p}}{\partial \mathbf{w}} = 2 \left(\frac{\text{diag}(\mathbf{G}\mathbf{w}) \mathbf{G}}{\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w}} - \frac{[(\mathbf{G}\mathbf{w}) \circ (\mathbf{G}\mathbf{w})] (\mathbf{w}'\mathbf{G}'\mathbf{G})}{(\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w})^2} \right). \quad (93)$$

Using the chain rule and (93) we then obtain

$$\begin{aligned} \frac{\partial \mathcal{N}_{Ent}}{\partial \mathbf{w}} &= \frac{\partial}{\partial \mathbf{w}} e^{-\mathbf{p}' \ln \mathbf{p}} = -\mathcal{N}_{Ent} \frac{\partial (\mathbf{p}' \ln \mathbf{p})}{\partial \mathbf{w}} \\ &= -\mathcal{N}_{Ent} (\ln \mathbf{p} + \mathbf{1})' \frac{\partial \mathbf{p}}{\partial \mathbf{w}} \\ &= 2\mathcal{N}_{Ent} (\ln \mathbf{p} + \mathbf{1})' \left(\frac{[(\mathbf{G}\mathbf{w}) \circ (\mathbf{G}\mathbf{w})] (\mathbf{w}'\mathbf{G}'\mathbf{G})}{(\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w})^2} - \frac{\text{diag}(\mathbf{G}\mathbf{w}) \mathbf{G}}{\mathbf{w}'\mathbf{G}'\mathbf{G}\mathbf{w}} \right). \end{aligned} \quad (94)$$