

Risk Budgeting and Diversification Based on Optimized Uncorrelated Factors ^{1,2}

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this revision: 10 November 2015
latest revision and code: symmys.com/node/599

Abstract

We measure the contributions to risk of a set of factors, strategies, or investments, based on "Minimum-Torsion Bets", namely a set of uncorrelated factors, optimized to closely track the factors used to allocate the portfolio. We then introduce a novel definition of contributions to risk, which generalizes the "marginal contributions to risk", traditionally used in banks for risk budgeting and in asset management to build risk parity strategies.

The Minimum-Torsion Bets allow us to also introduce a natural diversification score, the Effective Number of Minimum-Torsion Bets, which we use to measure and manage diversification.

We discuss the advantages of the Minimum-Torsion Bets over the traditional approach to diversification based on marginal contributions to risk. We present two case studies, a security-based investment in the stocks of the S&P 500, and a factor-based investment in the five Fama-French factors.

Fully documented code is available at symmys.com/node/599.

JEL Classification: C1, G11

Keywords: Effective Number of Bets, principal component analysis, Diversification Distribution, marginal contributions to risk, Procrustes problem

¹The authors are grateful to Marcello Colasante, David Elliott, Bruno Dupire, Yashin Gopi, Lionel Martellini, Sergei Polevikov, Thierry Roncalli, and two anonymous referees.

²This article appears as: Meucci, A. and Santangelo, A. and Deguest, R. (2015) "Risk budgeting and diversification based on optimized uncorrelated factors", Risk, Volume 11, Issue 29, 70-75

1 Introduction

In recent years finance practitioners and academics have witnessed a surge in interest in two different, yet related, areas: *risk budgeting*, namely the fair attribution of the total risk of an enterprise to the different business lines (see a review and references in [Tasche, 2008]); and *risk parity*, namely the investment in strategies that equally contribute to the risk of the total portfolio (see a review and references in [Roncalli, 2013]).

In traditional risk budgeting and risk parity, the contributions to risk of business lines or strategies are measured by means of the Euler principle as marginal risk contributions. Such contributions are spurious, because in reality they contain effects from all the factors at once. Furthermore, there exists no clear metric to quantify the diversification represented by the marginal risk contributions.

In this article we propose an alternative approach to risk budgeting and risk parity based on the Effective Number of Bets in [Meucci, 2009a]: instead of the marginal contributions from correlated factors, we measure the true contributions from uncorrelated bets. Then the Effective Number of Bets precisely quantify the diversification level, summarizing in one number the fine structure of diversification contained in the set of uncorrelated bets in our portfolio.

In the original paper, the uncorrelated bets are the market's principal components. The Principal Components Bets have spurred interest and called for extensive empirical analysis, see [Frahm and Wiechers, 2011], [DFine, 2011], [Lohre et al., 2011], [Lohre et al., 2012], [Deguest et al., 2013]. However, the principal components are suboptimal, because they are purely statistical entities, not related to the investment process.

In this article we introduce a natural set of uncorrelated bets to manage diversification, the Minimum-Torsion Bets, which are the uncorrelated factors closest ("minimum-torsion") to the factors used by the portfolio manager. The contributions to risk from the Minimum-Torsion Bets constitutes a generalization of the marginal contributions to risk used in traditional risk budgeting and risk parity.

The remainder of the paper is organized as follows: in Section 2 we revisit the general Effective Number of Bets framework in the context of factor-based risk budgeting, risk parity, and diversification management. In Section 3 we review the suboptimal implementation of the Effective Number of Bets, namely when the bets are represented by the principal components. In Section 4 we introduce the natural implementation of the Effective Number of Bets, namely when the bets are the Minimum-Torsion Bets. In Section 5 we highlight the key advantages of our approach to risk budgeting and risk parity, based on Effective Number of Minimum-Torsion Bets, and the traditional approach based on marginal contributions to risk. In Sections 6-7 we test our approach in two practical case studies, one security-based investment in the stocks of the S&P 500, and one factor-based investment in the five Fama-French factors. In Section 8 we conclude. In the appendix we detail all the technical proofs.

2 Effective Number of Bets

Here we review the Effective Number of Bets approach in [Meucci, 2009a], using a notation more suitable for the generalizations to follow. Refer to the original paper for all the details.

Consider an arbitrary portfolio which gives rise to a yet to be realized projected return R . In asset-based portfolio management, a portfolio is a combination of \bar{n} correlated assets (stocks, options, bonds, futures, ...), and the portfolio return is a weighted average of the return of each asset $R = \sum_{n=1}^{\bar{n}} w_n R_n$, where w_n represent the weight of the n -th asset in the portfolio.

More in general, in factor-based portfolio management, and in factor-based risk budgeting and risk parity, a portfolio is a combination of \bar{k} correlated factors, such as momentum, value, etc. Then, the portfolio return is a combination of the factor returns

$$R = \sum_{k=1}^{\bar{k}} b_k F_k, \quad (1)$$

where b_k represent the exposure of the portfolio to the k -th factor. We stress that (1) is a linear factor model for the return of a *portfolio*, where the factors may include a portfolio-specific residual, as in

the case study in Section 7.

Typically, but not necessarily \bar{k} (the number of factors) is much smaller than \bar{n} (the number of assets). Furthermore, clearly, asset-based portfolio management represents a special case of factor-based management (1), where $\bar{n} \equiv \bar{k}$, the factors are the asset returns $F_n = R_n$ and the exposures are the portfolio weights $b_n = w_n$.

Let us assume for now an ideal, apparently non-realistic scenario, where we can express the portfolio return as a combination of \bar{k} **Bets**, or *uncorrelated* factors

$$R = \sum_{k=1}^{\bar{k}} \hat{b}_k \hat{F}_k, \quad (2)$$

where $\mathbb{C}r\{\hat{F}_j, \hat{F}_k\} = 0$ if $j \neq k$. Then, we can compute the **Diversification Distribution**, namely true relative contributions to total risk from each bet

$$p_k \equiv \frac{\mathbb{V}\{\hat{b}_k \hat{F}_k\}}{\mathbb{V}\{R\}}, \quad k = 1, \dots, \bar{k}, \quad (3)$$

where \mathbb{V} denotes the variance. Notice that, as for any distribution, the masses p_k sum to one and are non-negative

$$\sum_{k=1}^{\bar{k}} p_k = 1, \quad p_k \geq 0, \quad k = 1, \dots, \bar{k}, \quad (4)$$

The Diversification Distribution (3) provides a detailed picture of the portfolio concentration structure. A portfolio is well diversified among the \bar{k} factors, and thus achieves risk parity, if the masses $p_1, \dots, p_{\bar{k}}$ are equal, or equivalently if the Diversification Distribution is uniform. To quantify diversification precisely, we use the exponential of the entropy, a tool from information theory, that measures the uniformity of a distribution. Accordingly, we define the **Effective Number of Bets** as follows

$$\mathbb{N} \equiv e^{-\sum_{k=1}^{\bar{k}} p_k \ln p_k}. \quad (5)$$

In the case of full concentration, i.e. when all the risk loads on one single factor, that factor's risk contribution (3) is 1, while all the other contributions are 0, and therefore $\mathbb{N} = 1$, the lowest possible value. At the opposite extreme, in the case of full diversification, the contributions to risk (3) from all the factors are equal, and $\mathbb{N} = \bar{k}$, the maximum possible value. For the intermediate cases $1 \leq \mathbb{N} \leq \bar{k}$.

As stated in [Meucci, 2012], the exponential of the entropy (5) is not the only possible choice for a function that satisfies the above intuitive properties. More in general $\mathbb{N}_\gamma \equiv (\sum_{k=1}^{\bar{k}} p_k^\gamma)^{\frac{1}{1-\gamma}}$, where $\gamma \geq 1$, satisfies the same properties. The case $\gamma = 1$ (in the limit sense) is the exponential of the entropy (5); the case $\gamma = 2$ is the inverse Herfindahl–Hirschman Index [W].

3 Principal Components bets

To measure diversification via the Effective Number of Bets, we need to express our portfolio returns as a combination of uncorrelated terms, as in (2). To do so, one option is to use the principal components of the original factors \mathbf{F} in (1), as suggested in [Meucci, 2009a].

Accordingly, we compute the covariance matrix of the factors $\Sigma_F \equiv \mathbb{C}v\{\mathbf{F}\}$. Next, we perform the principal component decomposition $\mathbf{e}\boldsymbol{\lambda}^2\mathbf{e}' = \Sigma_F$, where $\boldsymbol{\lambda}$ is the diagonal matrix of the singular values (square-root of eigenvalues) of Σ_F and \mathbf{e} is the matrix whose columns are the eigenvectors of Σ_F , which are orthogonal, and are normalized with length one $\mathbf{e}\mathbf{e}' = \mathbf{e}'\mathbf{e} = \mathbf{I}$, the identity matrix.

The eigenvectors generate \bar{k} uncorrelated factors called **Principal Components Bets** $\hat{\mathbf{F}}_{PC}$ and \bar{k} new portfolio exposures called **Principal Components Exposures** $\hat{\mathbf{b}}_{PC}$, which allow us to express the portfolio return (1) in the uncorrelated format (2), as follows

$$\hat{\mathbf{F}}_{PC} \equiv \mathbf{e}'\mathbf{F}, \quad \hat{\mathbf{b}}_{PC} \equiv \mathbf{e}'\mathbf{b}, \quad R = \hat{\mathbf{b}}_{PC}'\hat{\mathbf{F}}_{PC}, \quad (6)$$

where the last equality follows from $\mathbf{b}'\mathbf{F} = \hat{\mathbf{b}}_{PC}'\hat{\mathbf{F}}_{PC}$.

Then given the exposures \mathbf{b} , we can compute the **Principal Components Diversification Distribution** and the **Effective Number of Principal Components Bets**

$$\mathbf{p}_{PC}(\mathbf{b}) = \frac{(\mathbf{e}'\mathbf{b}) \circ (\mathbf{e}'\Sigma_F\mathbf{b})}{\mathbf{b}'\Sigma_F\mathbf{b}} \Rightarrow \mathbb{N}_{PC}(\mathbf{b}) = e^{-\mathbf{p}_{PC}(\mathbf{b})' \ln \mathbf{p}_{PC}(\mathbf{b})}, \quad (7)$$

where \circ denotes the term-by-term product, see Appendix A.1.

The principal components approach provides a formal set of uncorrelated factors from which to compute the Effective Number of Bets. However, it presents several problems.

First, the principal components bets tend to be statistically unstable, especially those relative to the lowest eigenvalues.

Second, the principal components bets are not invariant under simple scale transformations, as provided by a diagonal matrix \mathbf{d} with positive entries

$$\begin{array}{ccc} \mathbf{F} & \xrightarrow{\text{PCA decorrelation}} & \hat{\mathbf{F}}_{PC} \\ \text{scaling} \downarrow & & \downarrow \text{scaling} \\ \mathbf{dF} & \xrightarrow{\text{PCA decorrelation}} & (\mathbf{dF})_{PC} \neq \mathbf{d}\hat{\mathbf{F}}_{PC} \end{array} \quad (8)$$

To illustrate the above diagram, suppose that we want to measure the uncorrelated sources of risk in a portfolio in terms of P&L, rather than in terms of returns. The returns are the P&L normalized by a constant, so we expect the uncorrelated sources of risk to be the same. However, the Effective Number of Bets based on principal components of the P&L and of the return are different. To illustrate with a second example, suppose that we wish to measure some returns in basis points, instead of percentage points. The ensuing principal components bets will change dramatically, which is unacceptable.

Third, the principal components bets are not unique. Indeed, as discussed in [Deguest et al., 2013], if \mathbf{e}_k is one of the \bar{k} eigenvectors, so is its opposite $-\mathbf{e}_k$, and thus there are basically $2^{\bar{k}}$ possible combinations of principal components bets.

Fourth, the principal components bets are in general not easy to interpret, and hence disconnected from the decision process. In particular, in a dynamic setting, the meaning of the PCA factors changes from one date to another date, except possibly for the very first few factors.

Fifth, the principal components bets give rise to counter-intuitive results.

Example 1 *To illustrate the counter-intuitive results obtained with the principal component framework, consider the equal-load (equal-weight, in asset-based allocation) portfolio $\mathbf{b}_{eq} \equiv (\frac{1}{\bar{n}}, \dots, \frac{1}{\bar{n}})'$. Also, consider an idealized, though non-realistic, market where all the factors have equal volatility and equal, positive pair-wise correlation*

$$[\Sigma_F]_{m,n} \equiv \mathbb{C}v\{F_m, F_n\} = \begin{cases} \rho\sigma^2 & \text{for all } m \neq n \\ \sigma^2 & \text{for } m = n \end{cases} \quad (9)$$

In such a homogeneous market, if the correlation $\rho > 0$ is very small, we would expect the equal-load portfolio to be highly diversified, giving rise to a number of uncorrelated bets close to the number of factors $\mathbb{N}_{PC}(\mathbf{b}_{eq}) \approx \bar{n}$. Instead, the equal-load portfolio always displays maximum concentration, i.e. only one (!) bet

$$\mathbb{N}_{PC}(\mathbf{b}_{eq}) = 1. \quad (10)$$

The counter-intuitive full-concentration effect (10) follows because the equal-load portfolio is fully exposed to the first principal component and not exposed to any other principal component, see the proof in Appendix A.2.

4 Minimum-Torsion Bets

The Effective Number of Bets approach to risk budgeting and risk parity builds on the *uncorrelated* decomposition (2). Hence, unlike the standard approach to risk parity based on *marginal* contributions to risk, the Effective Number of Bets approach highlights the contributions from truly separate sources of risk.

However, if the uncorrelated portfolio decomposition (2) is achieved via the principal components bets (6), we obtain suboptimal results for the several reasons highlighted in Section 3.

Fortunately, the principal components bets are not the only zero-correlation transformation of the original factors \mathbf{F} that allows to express the portfolio as in the uncorrelated decomposition (2). There exist several alternative factor rotations, or *torsions* $\tilde{\mathbf{F}} = \tilde{\mathbf{t}}\mathbf{F}$, of the original factors \mathbf{F} , that are uncorrelated, and that are represented by a suitable $\tilde{k} \times \tilde{k}$ decorrelating torsion matrix $\tilde{\mathbf{t}}$.

For instance, one could think of independent component analysis, see [Back and Weigend, 1997], or more simply we could use the lower-triangular Cholesky decomposition $\Sigma_F \equiv \mathbb{C}v\{\mathbf{F}\} \equiv \mathbf{U}'$, where $\tilde{\mathbf{t}} \equiv \mathbf{U}^{-1}$. Indeed $\mathbb{C}v\{\mathbf{U}^{-1}\mathbf{F}\} = \mathbf{U}^{-1}\mathbf{U}'\mathbf{U}^{-1'} = \mathbf{I}$, and thus $\tilde{\mathbf{F}} = \mathbf{U}^{-1}\mathbf{F}$ are uncorrelated. However, such transformations display the same problems as the principal component approach. Most notably, the resulting uncorrelated factors $\tilde{\mathbf{F}}$ are not interpretable, as in general they bear no relationship with the original factors \mathbf{F} that are used to manage the portfolio.

4.1 Problem formulation

Here, we propose a natural, interpretable definition for the de-correlating transformation and the resulting uncorrelated factors: we choose the *minimum torsion* linear transformation that least disrupts the original factors \mathbf{F} . More precisely, among all the torsions $\tilde{\mathbf{t}}$ that ensure that the new factors are uncorrelated, we select the **Minimum-Torsion transformation**, i.e. the transformation that minimizes the tracking error with respect to the original factors

$$\tilde{\mathbf{t}}_{MT} \equiv \underset{\mathbb{C}r\{\tilde{\mathbf{t}}\mathbf{F}\}=\mathbf{I}_{\tilde{k} \times \tilde{k}}}{\operatorname{argmin}} NTE\{\tilde{\mathbf{t}}\mathbf{F}\|\mathbf{F}\}, \quad (11)$$

where NTE denotes the multi-entry normalized tracking error

$$NTE\{\mathbf{Z}\|\mathbf{F}\} \equiv \sqrt{\frac{1}{\tilde{k}} \sum_k \mathbb{V}\left\{\frac{Z_k - F_k}{\mathbb{S}d\{F_k\}}\right\}}. \quad (12)$$

Suppose that we can solve the minimum torsion optimization (11), which we do further below in this section. Then we introduce the **Minimum-Torsion Bets** $\tilde{\mathbf{F}}_{MT}$ and the respective **Minimum-Torsion Exposures** $\tilde{\mathbf{b}}_{MT}$, and use them to express the portfolio return (1) in the uncorrelated format (2), as follows

$$\tilde{\mathbf{F}}_{MT} \equiv \tilde{\mathbf{t}}_{MT}\mathbf{F}, \quad \tilde{\mathbf{b}}_{MT} \equiv \tilde{\mathbf{t}}_{MT}'^{-1}\mathbf{b}, \quad R = \tilde{\mathbf{b}}_{MT}'\tilde{\mathbf{F}}_{MT}. \quad (13)$$

The interpretation of the Minimum-Torsion Bets $\tilde{\mathbf{F}}_{MT}$ is easily visualized geometrically in Figure 1, by equating factors to vectors, and no-correlation to orthogonality. Whereas the Minimum-Torsion Bets $\tilde{\mathbf{F}}_{MT}$ are the closest to the original factors \mathbf{F} used to manage the portfolio, the PCA bets $\tilde{\mathbf{F}}_{PC}$ defined in (6) bear no close relationship to the management factors \mathbf{F} .

Then, the Minimum-Torsion Bets and exposures (13) allow us to compute the **Minimum-Torsion Diversification Distribution** and the **Effective Number of Minimum-Torsion Bets**, as follows

$$\mathbf{p}_{MT}(\mathbf{b}) = \frac{(\tilde{\mathbf{t}}_{MT}'^{-1}\mathbf{b}) \circ (\tilde{\mathbf{t}}_{MT}\Sigma_F\mathbf{b})}{\mathbf{b}'\Sigma_F\mathbf{b}} \Rightarrow \mathbb{N}_{MT}(\mathbf{b}) = e^{-\mathbf{p}_{MT}(\mathbf{b})' \ln \mathbf{p}_{MT}(\mathbf{b})}, \quad (14)$$

see Appendix A.1.

The Minimum-Torsion Bets (13) address all the problems of the principal components bets (6). In particular, the normalization in the tracking error (12) allows us not to worry about non-homogenous

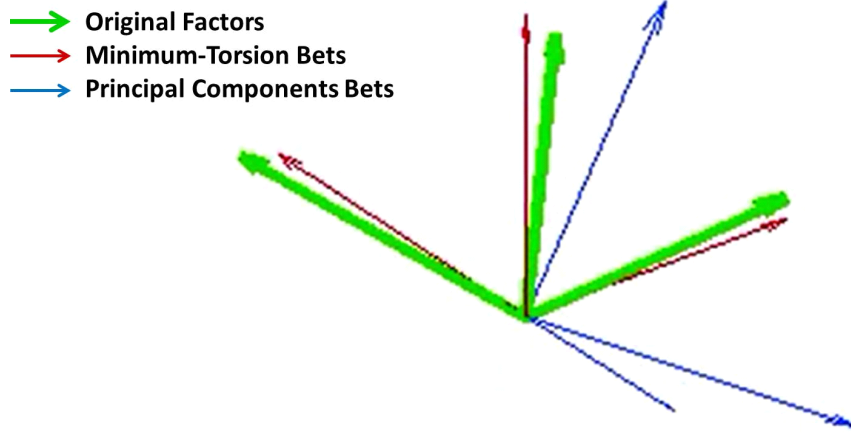


Figure 1: Minimum-Torsion Bets are the uncorrelated (orthogonal) factors closest to the original factors, Principal Component Bets are uncorrelated (orthogonal) factors with no clear connection to the original factors

factors \mathbf{F} measured in completely different units, such as interest rates and implied volatilities. In other words, unlike in the case of uncorrelated bets defined by the principal components (8), for the Minimum-Torsion Bets the following diagram holds

$$\begin{array}{ccc}
 \mathbf{F} & \xrightarrow{\text{MT decorrelation}} & \hat{\mathbf{F}}_{MT} \\
 \text{scaling} \downarrow & & \downarrow \text{scaling} \\
 d\mathbf{F} & \xrightarrow{\text{MT decorrelation}} & (d\hat{\mathbf{F}})_{MT} = d\hat{\mathbf{F}}_{MT}
 \end{array} \tag{15}$$

Example 2 To provide a first taste of the intuitive nature of the Minimum-Torsion Bets, let us consider again the idealized homogeneous market with equal volatilities and arbitrary small homogeneous correlations (9). Furthermore, let us consider again the equal-load (equal-weight, in asset-based allocation) portfolio $\mathbf{b}_{eq} \equiv (\frac{1}{\bar{n}}, \dots, \frac{1}{\bar{n}})'$. Unlike with Principal Components Bets (10), the Number of Minimum-Torsion Effective Bets (14) for the equal-load portfolio is, as intuition suggests, the largest possible

$$\mathbb{N}_{MT}(\mathbf{b}_{eq}) = \bar{n}, \tag{16}$$

see Appendix A.2. This result is very intuitive: in an uncorrelated market each position of equal size represents a separate bet.

4.2 Problem solution

The solution of the minimum torsion optimization (11) is a special instance of a quadratically constrained quadratic program [W], related to the solution of the orthogonal Procrustes problem [W]. Adapting from [Everson, 1997], we obtain the solution by first computing analytically a starting guess, and then perturbing the starting guess via an efficient recursive algorithm, as follows.

Let us denote by σ_F the vector of the factors standard deviations, extracted with the correlation matrix C_F from the covariance matrix $\Sigma_F \equiv \mathbb{C}v\{\mathbf{F}\}$, as follows

$$\Sigma_F \equiv dg(\sigma_F) C_F dg(\sigma_F), \quad (17)$$

where the operator $dg(\mathbf{v})$ embeds the $\bar{k} \times 1$ vector \mathbf{v} into the principal diagonal of a square matrix which is zero anywhere else.

Then, let us factor as in [Meucci, 2009b] the correlation matrix via its Riccati root \mathbf{c} , namely the symmetric positive definite matrix such that

$$C_F = \mathbf{c}\mathbf{c}' = \mathbf{c}^2. \quad (18)$$

The Riccati root of the correlation matrix C_F is easily computed in terms of the PCA decomposition $C_F = \mathbf{g}\gamma^2\mathbf{g}'$, where γ is the diagonal matrix of the singular values (square-root of eigenvalues) of the correlation matrix C_F and \mathbf{g} is the matrix whose columns are the respective eigenvectors, which are orthogonal, and are normalized with length one $\mathbf{g}\mathbf{g}' = \mathbf{g}'\mathbf{g} = \mathbf{I}$, the identity matrix. Then the Riccati root of the correlation matrix (18) reads explicitly

$$\mathbf{c} = \mathbf{g}\gamma\mathbf{g}'. \quad (19)$$

Next, we compute a perturbation matrix π recursively with the algorithm below (refer to Appendix A.3.2 for the rationale)

$\boldsymbol{\pi} = \text{Perturb}(\boldsymbol{c})$		(20)
Minimum-Torsion recursion		
0. Initialize	$\boldsymbol{d} \leftarrow \boldsymbol{I}$	
1. Riccati root	$\boldsymbol{u} \leftarrow (\boldsymbol{d}\boldsymbol{c}^2\boldsymbol{d})^{\frac{1}{2}}$	
2. Rotation	$\boldsymbol{q} \leftarrow \boldsymbol{u}^{-1}\boldsymbol{d}\boldsymbol{c}$	
3. Stretching	$\boldsymbol{d} \leftarrow dg(dg^{-1}(\boldsymbol{q}\boldsymbol{c}))$	
4. Perturbation	$\boldsymbol{\pi} \leftarrow \boldsymbol{d}\boldsymbol{q}$	
5. If convergence, output $\boldsymbol{\pi}$; else go to 1		

where the operator $dg^{-1}(\mathbf{m})$ extracts the $\bar{k} \times 1$ vector on the principal diagonal of the $\bar{k} \times \bar{k}$ matrix \mathbf{m} .

Example 3 For instance from a correlation matrix

$$C_F = \begin{pmatrix} 1 & 0.5 & 0.3 \\ 0.5 & 1 & 0.1 \\ 0.3 & 0.1 & 1 \end{pmatrix}$$

we obtain

$$\mathbf{c} = \begin{pmatrix} 0.9544 & 0.2580 & 0.1503 \\ 0.2580 & 0.9656 & 0.0313 \\ 0.1503 & 0.0313 & 0.9881 \end{pmatrix}, \quad \pi = \begin{pmatrix} 0.9535 & -0.0016 & -0.0026 \\ 0.0017 & 0.9661 & -0.0001 \\ 0.0027 & 0.0001 & 0.9886 \end{pmatrix}$$

The algorithm (20) converges extremely fast, within a dozen iterations, or fractions of a second, even when π has $\bar{k}^2 \approx 150,000$ entries (!), the dimensions required to handle the S&P case study in Section 6.

The solution of the minimum torsion problem (11) then reads

$$\mathring{\mathbf{t}}_{MT} = dg(\sigma_F) \pi \mathbf{c}^{-1} dg(\sigma_F)^{-1}, \quad (21)$$

where we emphasize that the factors cannot be collinear, or else the inverse Riccati root \mathbf{c}^{-1} is not defined.

The minimum torsion transformation (21) defines the Minimum-Torsion Bets and the Minimum-Torsion Exposures, as in (13); and the Minimum-Torsion Diversification Distribution and the Effective Number of Minimum-Torsion Bets, as in (14).

Furthermore, we can solve analytically the original minimum-torsion problem (11) under the additional constraint that the volatilities of the new factors be the same as the volatilities of the original factors

$$\mathbb{S}d\{\mathring{\mathbf{t}}\mathbf{F}\} = \boldsymbol{\sigma}_F. \quad (22)$$

As we show in see Appendix A.3, the solution is close to the minimum torsion (21)

$$\mathring{\mathbf{t}} \equiv dg(\boldsymbol{\sigma}_F) \mathbf{c}^{-1} dg(\boldsymbol{\sigma}_F)^{-1} \approx \mathring{\mathbf{t}}_{MT}. \quad (23)$$

The approximate minimum-torsion (23) is essentially the solution of the orthogonal Procrustes problem first derived by [Schoenemann, 1966]. Geometrically, the approximate minimum-torsion generates orthogonal bets $\mathring{\mathbf{t}}\mathbf{F}$ by rotating the original factors \mathbf{F} . However, we verified numerically that the discrepancy between the approximate minimum-torsion bets $\mathring{\mathbf{t}}\mathbf{F}$ and the true Minimum-Torsion Bets $\mathring{\mathbf{t}}_{MT}\mathbf{F}$ can become relevant in highly correlated markets.

We note that the approximate minimum torsion transformation (23) resembles the decorrelating solution in [Klein and Chow, 2010]. However, such solution i) applies to the empirical distribution of the factors, rather than arbitrary distributions; ii) it applies to the covariance matrix, rather than the correlation matrix, thereby being sensitive to the units in which the factors are measured; iii) it does not account for the perturbation term $\boldsymbol{\pi}$ as the exact solution (21) does.

5 Minimum-Torsion Bets versus Marginal Contributions to Risk

In Table (24) we represent the main conceptual differences between the traditional approach to risk budgeting and risk parity, based on marginal contributions to risk, and the present approach, based on the Effective Number of Minimum-Torsion Bets

	Marginal Contributions	Minimum-Torsion
Risk contrib.	Marginal contributions	Diversification Distributions
Expression	$\mathbf{m} \equiv \frac{\mathbf{b} \circ (\boldsymbol{\Sigma}_F \mathbf{b})}{\mathbf{b}' \boldsymbol{\Sigma}_F \mathbf{b}}$	$\mathbf{p} \equiv \frac{(\mathring{\mathbf{t}}_{MT}^{-1} \mathbf{b}) \circ (\mathring{\mathbf{t}}_{MT} \boldsymbol{\Sigma}_F \mathbf{b})}{\mathbf{b}' \boldsymbol{\Sigma}_F \mathbf{b}}$
Meaning	spurious contributions from original factors	proper contributions from Minimum-Torsion Bets
Properties	$\sum_k m_k = 1, \quad m_k \leq 0$	$\sum_k p_k = 1, \quad p_k \geq 0$

In traditional risk budgeting and risk parity the key are the **marginal contributions to risk**

$$\mathbf{m} \equiv \frac{\mathbf{b} \circ (\boldsymbol{\Sigma}_F \mathbf{b})}{\mathbf{b}' \boldsymbol{\Sigma}_F \mathbf{b}}, \quad (25)$$

see e.g. [Roncalli, 2013]. In traditional risk budgeting and risk parity, a portfolio is diversified if the marginal contributions to risk \mathbf{m} are uniform.

In our approach to risk budgeting and risk parity the key is the Diversification Distribution of the Minimum-Torsion Bets \mathbf{p} , defined in (14): a portfolio is diversified if \mathbf{p} is close to uniform.

The generic k -th marginal contribution to risk is the sum of a true k -related term and a spurious term that contains correlations $\rho_{j,k}$ with all the other $\bar{k} - 1$ factors, volatilities σ_j of all but the k -th factor, and exposures b_j to all but the k -th factor

$$m_k \propto \underbrace{\sigma_k^2 b_k^2}_{\text{pure } k\text{-related}} + \underbrace{b_k \sigma_k \sum_{j \neq k} \rho_{j,k} \sigma_j b_j}_{\text{spurious } k\text{-related}}, \quad (26)$$

where $[\Sigma_F]_{j,k} \equiv \rho_{j,k} \sigma_j \sigma_k$. Unlike for the marginal contributions to risk (26), the generic k -th term p_k in the Diversification Distribution is by construction the most "pure k -related" contribution to total risk.

Furthermore, the marginal contributions to risk \mathbf{m} sum to one, just like the Diversification Distribution \mathbf{p} . However, unlike the Diversification Distribution \mathbf{p} , the marginal contributions to risk \mathbf{m} are not necessarily positive, due to either negative correlations or the presence of negative exposures to factors. As a result, when enforcing traditional risk budgeting and risk parity, one focuses on the absolute values of the marginal contributions to risk $|m_k|$, which no longer sum to one. On the other hand, the Diversification Distribution of the Minimum-Torsion Bets \mathbf{p} has always non-negative entries and thus represents a pie-chart of risk.

Finally, notice that if the factors \mathbf{F} are uncorrelated, then the Minimum-Torsion transformation $\hat{\mathbf{t}}_{MT}$ is the identity, and thus the marginal contributions to risk and the Diversification Distribution are one and the same, $\mathbf{m} = \mathbf{p}$.

To summarize, both traditional risk budgeting/parity and Effective Number of Minimum-Torsion Bets apply in full generality across markets with arbitrary factors. When the factors in traditional risk budgeting/parity are uncorrelated, the marginal contributions to risk display all the palatable features of the Diversification Distribution: they sum to one, they are positive, and they are the true contributors to risk. In the more general case where the factors are correlated, the traditional risk parity approach incurs problems.

Hence, we can interpret the Effective Number of Minimum-Torsion Bets approach as a generalization of the traditional risk parity approach, which addresses the issues of the latter approach.

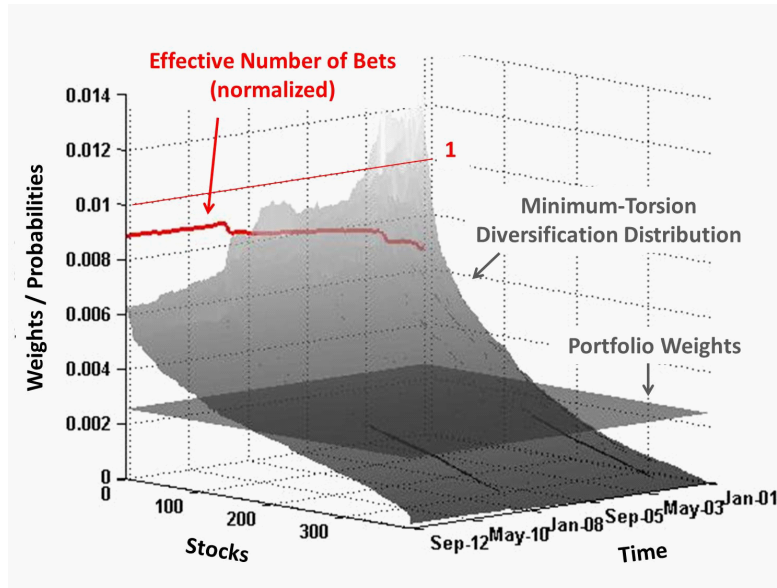


Figure 2: Diversification through time of an equal-weight portfolio of stocks

6 Case study: security-based investment

We consider an investment in $\bar{n} = 392$ stocks in the S&P 500 Index (for simplicity, we consider the stocks alive through the whole analysis period). In this case the factors \mathbf{F} and respective exposures \mathbf{b} in (1) are the \bar{n} stock returns and the \bar{n} portfolio weights respectively.

Let us consider a simple equal-load portfolio $\mathbf{b}_{eq} \equiv (\frac{1}{\bar{n}}, \dots, \frac{1}{\bar{n}})'$. We estimate every month the covariance matrix of the S&P stock returns Σ_F using a one-year rolling window of daily ob-

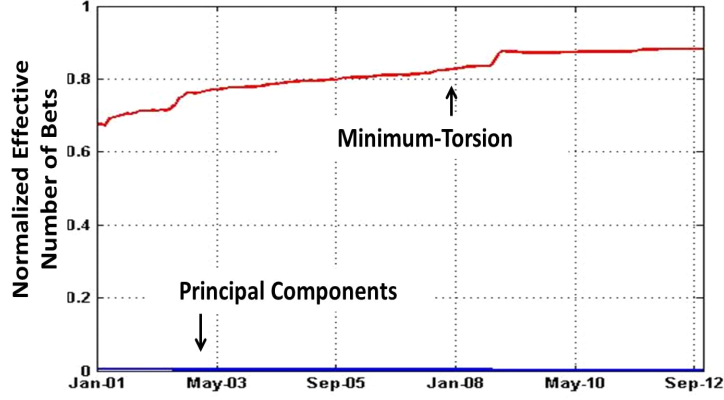


Figure 3: Intuitive diversification measure via Minimum-Torsion versus counter-intuitive diversification measure via principal components

servations, and filtering the smallest eigenvalues to ensure positive definiteness. Using the portfolio loadings and the returns covariance we compute the Minimum-Torsion Diversification Distribution $p_{MT}(\mathbf{b}_{eq})$ and the Minimum-Torsion Effective Number of Bets $N_{MT}(\mathbf{b}_{eq})$ of the equal-load portfolio, as in (14).

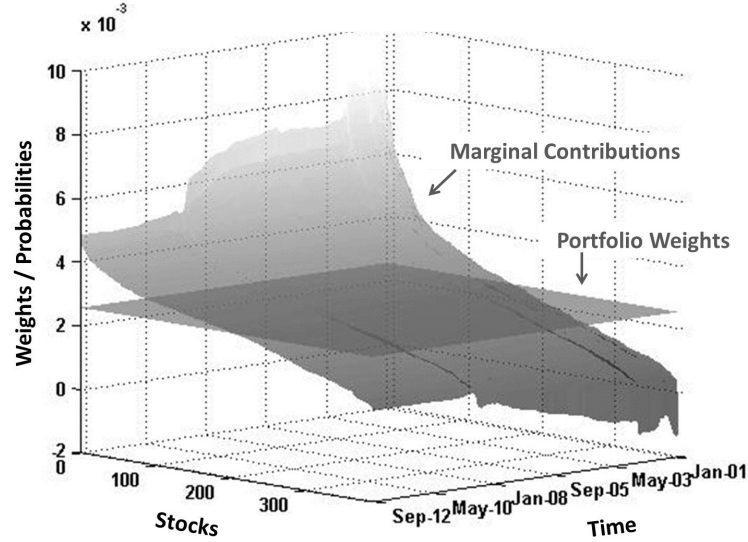


Figure 4: Marginal contributions to risk through time of an equal-weight portfolio of stocks

In Figure 2 we display the results. Each month, we sort the bets in decreasing order of risk contribution, as measured by the Minimum-Torsion Diversification Distribution $p_{MT}(\mathbf{b}_{eq})$. The fairly homogeneous structure of the S&P 500 stocks and the equal-load allocation provide a portfolio that is not as diversified as one would expect. Unlike the portfolio weights, the Minimum-Torsion Diversification Distribution is not flat: some stocks are riskier than others, a fact well known to portfolio managers.

The fine structure of diversification represented by the Minimum-Torsion Diversification Distrib-

ution is summarized into the Effective Number of Minimum-Torsion Bets $\mathbb{N}_{PC}(\mathbf{b}_{eq})$. The Effective Number of Bets is strictly less than the number of stocks \bar{n} , because of the non-homogeneous contributions to risk from each stock. However, as intuition suggests, the Effective Number of Bets is of the order of a few hundreds, given that the Minimum-Torsion Diversification Distribution is not too steep:

$$0 \ll \frac{\mathbb{N}_{MT}(\mathbf{b}_{eq})}{\bar{n}} < 1. \quad (27)$$

The intuitive result (27) is the empirical counterpart of the similar theoretical full-diversification result (16).

For comparison, we also compute the principal component Diversification Distribution $\mathbf{p}_{PC}(\mathbf{b}_{eq})$ and the principal component Effective Number of Bets $\mathbb{N}_{PC}(\mathbf{b}_{eq})$ of the equal-load portfolio, as in (7). The Diversification Distribution is now too steep to display, loading basically in full on the first entry (which is no longer interpretable and not directly comparable with the portfolio weights). As a result, as we see in Figure 3, the normalized Effective Number of Bets is almost zero

$$0 \approx \frac{\mathbb{N}_{PC}(\mathbf{b}_{eq})}{\bar{n}} \ll 1. \quad (28)$$

The counter-intuitive result (28) is the empirical counterpart of the similar, extreme, theoretical full-concentration result (10).

Finally, we compute the marginal risk contributions of the equal-load portfolio $\mathbf{m}(\mathbf{b}_{eq})$, as in (25) and display them in Figure 4. The overall risk profile is similar to the Diversification Distribution $\mathbf{p}_{MT}(\mathbf{b}_{eq})$ in Figure 2. However, even with such a homogeneous market and portfolio, we notice negative contributions at the beginning of the sample. A likely explanation for the observed negative volatility contributions is that the correlations among S&P500 stocks was lowest around 2000-2001. At very low average correlation, it is likely that there are stocks which exhibit negative correlations with other stocks or the index.

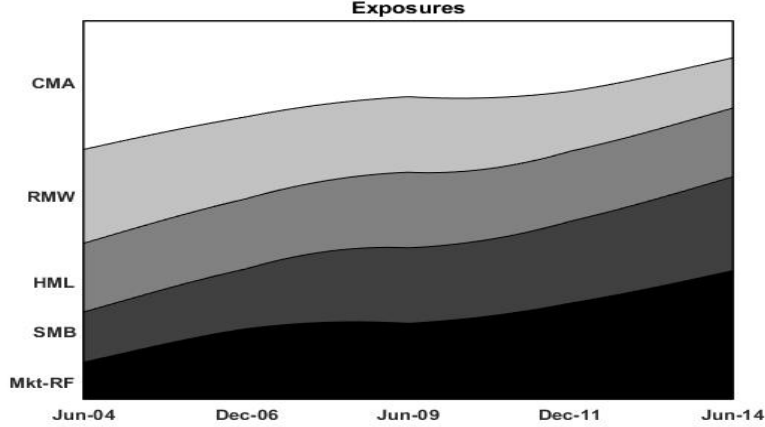


Figure 5: Exposures in the five Fama-French factors

7 Case study: factor-based investment

As a second application, we consider an equity strategy based on a linear factor model

$$R = \sum_{k=1}^5 b_k F_k + U, \quad (29)$$

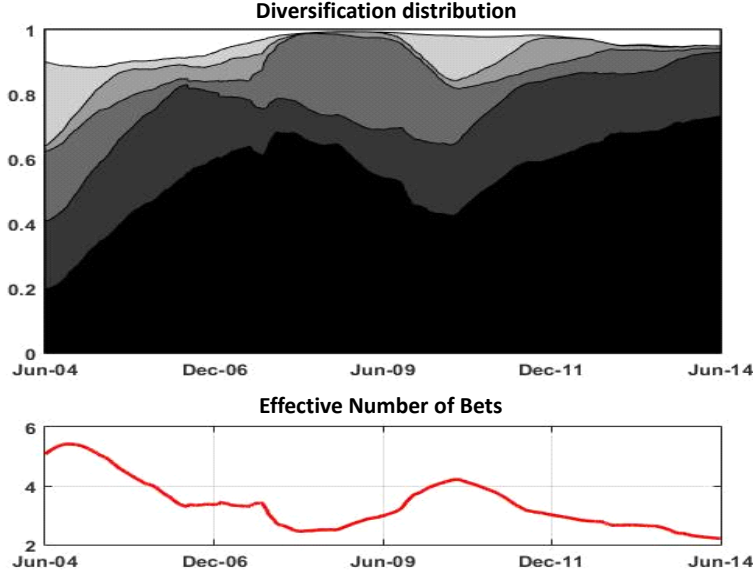


Figure 6: Minimum-Torsion Diversification Distribution (top plot) and Effective Number of Minimum-Torsion Bets (bottom plot) of the factor-based investment strategy through time

where the factors are as in [Fama and French, 2014]: $F_1 \equiv F^{mkt-rf}$ is the market portfolio excess return; $F_2 \equiv F^{SMB}$ is the Small-Minus-Big market capitalization factor; $F_3 \equiv F^{HML}$ is the High-Minus-Low book-to-market value factor; $F_4 \equiv F^{RMW}$ is the difference between the returns on diversified portfolios of stocks with robust and weak profitability, $F_5 \equiv F^{CMA}$ is the difference between the returns on diversified portfolios of the stocks of low and high investment firm. The portfolio-specific residual U is uncorrelated with the factors, i.e.

$$\mathbb{C}v\{U, F_k\} = 0, \text{ for } k = 1, \dots, 5. \quad (30)$$

In our factor-based portfolio management framework (1), the residual is a sixth factor $F_6 \equiv U$ with unit exposure $b_6 \equiv 1$.

We consider the time series for the factors \mathbf{F} in the period from 26-Jun-2003 to 30-Jun-2015, available at http://mba.tuck.dartmouth.edu/pages/faculty/ken.french/data_library. We built the exposures \mathbf{b} in such a way that the first factors weight the most at the beginning and as time goes by their importance decrease in favor of the last factors, keeping fixed the unit exposure in the residual, as summarized in Figure 5.

We estimate the covariance matrix of the factors $\Sigma_{\mathbf{F}}$ using a two-years rolling window of weekly observations by a forward-backward exponential smoothing procedure. Using the exposures and the estimated factors covariance matrix we compute the Minimum-Torsion Diversification Distribution $\mathbf{p}_{MT}(\mathbf{b})$ and the Minimum-Torsion Effective Number of Bets $\mathbb{N}_{MT}(\mathbf{b})$, as in (14), see Figure 6.

We also compute the marginal risk contributions $\mathbf{m}(\mathbf{b})$, as in (25) and display their absolute values in Figure 7. As in the case study on security-based investment, the overall risk profile is similar to the Minimum-Torsion Diversification Distribution $\mathbf{p}_{MT}(\mathbf{b})$ in Figure 6. Again, we notice negative contributions, as highlighted by the fact that the sum of absolute marginal contributions is higher than one.

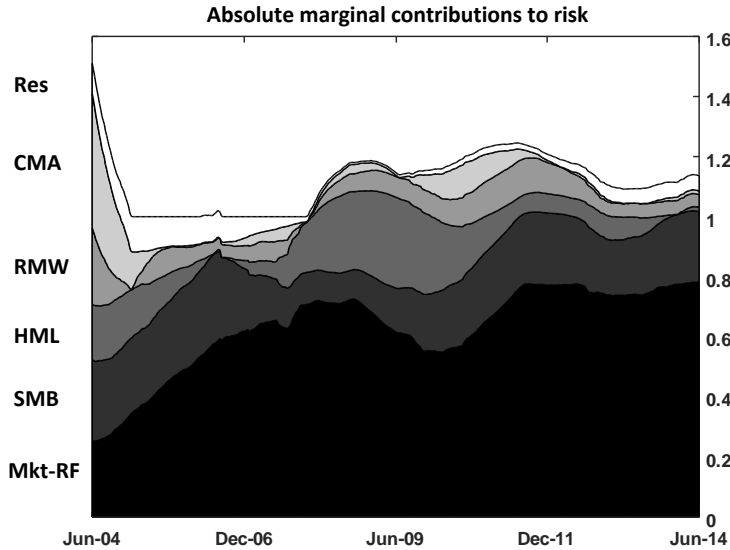


Figure 7: Absolute value of marginal contributions to risk through time of a factor-based investment in five Fama-French factors and an uncorrelated residual

8 Conclusions

We have introduced the Minimum-Torsion Bets, the set of uncorrelated factors which closely tracks the factors used in the allocation process. With the Minimum-Torsion Bets we have given new life to the Effective Number of Bets approach to risk budgeting and risk parity and, more in general, diversification management. Indeed, unlike the Principal Component Bets originally used to measure the Effective Number of Bets, the Minimum-Torsion Bets are easily interpretable and give rise to intuitive results.

We have highlighted the improvements of the Effective Number of Minimum-Torsion Bets over the standard approach to risk budgeting/parity, which relies on marginal contributions to risk.

We have illustrated how to use the Effective Number of Minimum-Torsion Bets to measure the diversification of a portfolio of stocks in the S&P500 and of an equity strategy built as a portfolio of five systematic Fama-French factors and one idiosyncratic residual.

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A Appendix

In this appendix we discuss technical results that can be skipped at first reading.

A.1 Explicit expressions for Effective Number of Bets

The denominator in the Diversification Distribution (3) follows from the expression of the portfolio return as a combination of factors (1) and reads

$$\mathbb{V}\{R\} = \mathbb{V}\{\mathbf{b}'\mathbf{F}\} = \mathbf{b}'\mathbb{V}\{\mathbf{F}\}\mathbf{b} = \mathbf{b}'\Sigma_F\mathbf{b}. \quad (31)$$

Assume that the Bets are an uncorrelated linear transformation of the factors

$$\mathring{\mathbf{F}} \equiv \mathbf{t}\mathbf{F}, \quad \mathring{\mathbf{b}} \equiv \mathring{\mathbf{t}}'^{-1}\mathbf{b}. \quad (32)$$

Then numerator of the Diversification Distribution (3) reads

$$\begin{aligned} \mathbb{V}\{\mathring{\mathbf{b}} \circ \mathring{\mathbf{F}}\} &= \mathring{\mathbf{b}} \circ \mathbb{V}\{\mathring{\mathbf{F}}\} \circ \mathring{\mathbf{b}} = \mathring{\mathbf{b}} \circ (\mathbb{C}v\{\mathring{\mathbf{F}}\}\mathring{\mathbf{b}}) \\ &= (\mathring{\mathbf{t}}'^{-1}\mathbf{b}) \circ (\mathring{\mathbf{t}}\Sigma_F\mathring{\mathbf{t}}'\mathring{\mathbf{t}}'^{-1}\mathbf{b}) = (\mathring{\mathbf{t}}'^{-1}\mathbf{b}) \circ (\mathring{\mathbf{t}}\Sigma_F\mathbf{b}) \end{aligned} \quad (33)$$

Dividing the numerator (33) by the denominator (31) we obtain the explicit formula Diversification Distribution (3), as follows

$$\mathbf{p} = \frac{(\mathring{\mathbf{t}}'^{-1}\mathbf{b}) \circ (\mathring{\mathbf{t}}\Sigma_F\mathbf{b})}{\mathbf{b}'\Sigma_F\mathbf{b}}. \quad (34)$$

The Principal Components expression (7) follows from setting $\mathring{\mathbf{t}} = \mathbf{e}'$ in the Diversification Distribution (34), as prescribed by the Principal Components transformation (6), which is a special case of (32).

The Minimum-Torsion expression (14) follows from setting $\mathring{\mathbf{t}} = \mathring{\mathbf{t}}_{MT}$ in the Diversification Distribution (34), as prescribed by the Minimum-Torsion transformation (13), which is a special case of (32).

A.2 Number of bets in homogeneous markets

Consider $\bar{n} \equiv \bar{k}$ factors $\mathbf{F} \equiv (F_1, \dots, F_{\bar{n}})'$. Assume that the variances are all equal to σ^2 and all the pair-wise correlations are equal to $\rho > 0$, as in (9).

As proved in Appendix A.4 of [Meucci, 2009a], the equally-loading portfolio \mathbf{b}_{eq} is the eigenvector of the covariance matrix Σ_F relative to the largest eigenvalue λ_1^2 , or $\Sigma_F\mathbf{b}_{eq} = \lambda_1^2\mathbf{b}_{eq}$ (the eigenvectors are defined modulo a scale factor, so \mathbf{b}_{eq} need not satisfy $\mathbf{b}_{eq}'\mathbf{b}_{eq} = 1$). As a result, the Diversification Distribution (7) reads $\mathbf{p}_{PC}(\mathbf{b}_{eq}) = (1, 0, \dots, 0)'$ and thus $\mathbb{N}_{PC}(\mathbf{b}_{eq}) = 1$, as in (10).

On the other hand, the minimum torsion transformation acts equally on all the factors, which are indistinguishable. Hence, for symmetry reasons $(\mathring{\mathbf{t}}_{MT}'^{-1}\mathbf{b}_{eq}) \propto \mathbf{1}$ is a vector of equal entries, and so is $(\mathring{\mathbf{t}}_{MT}'\Sigma_F\mathbf{b}_{eq}) \propto \mathbf{1}$. Therefore the Diversification Distribution (14) reads $\mathbf{p}_{MT} = (\frac{1}{\bar{n}}, \dots, \frac{1}{\bar{n}})'$ and thus $\mathbb{N}_{MT}(\mathbf{b}_{eq}) = \bar{n}$, as in (16).

A.3 Minimum-torsion optimization

Let us denote the vector of the standard deviations in the covariance matrix Σ_F by $\boldsymbol{\sigma} \equiv (dg^{-1}\Sigma_F)^{1/2}$, where the operator $dg^{-1}\mathbf{x}$ extracts the diagonal from a matrix \mathbf{x} . Let us denote by $dg(\mathbf{v})$ a diagonal matrix with the vector \mathbf{v} on the diagonal.

Solving (11) is equivalent to solving

$$\mathring{\mathbf{t}}_{MT} \equiv \underset{\mathbb{C}r\{\mathbf{t}\mathbf{F}\}=\mathbf{I}}{\operatorname{argmin}} \operatorname{tr}(\mathbb{C}v\{dg(\boldsymbol{\sigma})^{-1}(\mathbf{t}\mathbf{F}) - dg(\boldsymbol{\sigma})^{-1}\mathbf{F}\}). \quad (35)$$

Let us define the normalized factors $\mathbf{Z} \equiv dg(\boldsymbol{\sigma})^{-1}\mathbf{F}$, whose covariance is the correlation matrix

$$\mathbb{C}v\{\mathbf{Z}\} = \mathbf{C}_F \equiv dg(\boldsymbol{\sigma})^{-1} \boldsymbol{\Sigma}_F dg(\boldsymbol{\sigma})^{-1}. \quad (36)$$

Noting that $\mathbb{C}r\{tdg(\boldsymbol{\sigma})\mathbf{Z}\} = \mathbf{I} \Leftrightarrow \mathbb{C}r\{dg(\boldsymbol{\sigma})^{-1}tdg(\boldsymbol{\sigma})\mathbf{Z}\} = \mathbf{I}$, we write (35) as follows

$$\hat{\mathbf{t}}_{MT} \equiv \underset{\mathbb{C}r\{dg(\boldsymbol{\sigma})^{-1}tdg(\boldsymbol{\sigma})\mathbf{Z}\}=\mathbf{I}}{\operatorname{argmin}} tr(\mathbb{C}v\{dg(\boldsymbol{\sigma})^{-1}\mathbf{t}dg(\boldsymbol{\sigma})\mathbf{Z} - \mathbf{Z}\}). \quad (37)$$

Equivalently, we can write

$$\hat{\mathbf{t}}_{MT} = dg(\boldsymbol{\sigma}) \hat{\mathbf{x}} dg(\boldsymbol{\sigma})^{-1}, \quad (38)$$

where $\hat{\mathbf{x}}$ solves

$$\begin{aligned} \hat{\mathbf{x}} &\equiv \underset{\mathbb{C}r\{\mathbf{x}\mathbf{Z}\}=\mathbf{I}}{\operatorname{argmin}} tr(\mathbb{C}v\{(\mathbf{x} - \mathbf{I})\mathbf{Z}\}) \\ &= \underset{\mathbb{C}r\{\mathbf{x}\mathbf{Z}\}=\mathbf{I}}{\operatorname{argmin}} tr((\mathbf{x} - \mathbf{I})\mathbf{C}_F(\mathbf{x}' - \mathbf{I})) \\ &= \underset{\mathbb{C}r\{\mathbf{x}\mathbf{Z}\}=\mathbf{I}}{\operatorname{argmin}} tr(\mathbf{x}\mathbf{C}_F\mathbf{x}' - \mathbf{x}\mathbf{C}_F - \mathbf{C}_F\mathbf{x}' + \mathbf{C}_F) \\ &= \underset{\mathbb{C}r\{\mathbf{x}\mathbf{Z}\}=\mathbf{I}}{\operatorname{argmin}} tr(\mathbf{x}\mathbf{C}_F\mathbf{x}' - 2\mathbf{x}\mathbf{C}_F) + \bar{k} \end{aligned} \quad (39)$$

where the last equality follows from the symmetry of \mathbf{C}_F .

Let us denote by \mathcal{D} the set of diagonal matrices with full rank, and let us introduce the Riccati root of the correlation matrix

$$\mathbf{c} = \mathbf{c}' \equiv (\mathbf{C}_F)^{\frac{1}{2}}. \quad (40)$$

Then $\hat{\mathbf{x}}$ in (38) is the solution of

$$\hat{\mathbf{x}} = \underset{\mathbf{x}\mathbf{c}\mathbf{c}'\mathbf{x}' \in \mathcal{D}}{\operatorname{argmin}} tr(\mathbf{x}\mathbf{c}\mathbf{c}'\mathbf{x}' - 2\mathbf{x}\mathbf{c}\mathbf{c}) \quad (41)$$

A.3.1 Constrained analytical solution

Let us impose the stronger constraint that volatilities are preserved (22), which amounts to

$$\mathbb{C}v\{\mathbf{x}\mathbf{Z}\} = \mathbf{x}\mathbf{C}_F\mathbf{x}' = \mathbf{I}. \quad (42)$$

We emphasize that the constraint (42) does restrict the solution, see (A.3.2) below. From the constraint (42) we obtain $tr(\mathbf{x}\mathbf{C}_F\mathbf{x}') = tr(\mathbf{I}) = \bar{k}$. As a result, the minimization (41) becomes

$$\hat{\mathbf{x}} = \underset{\mathbf{x}\mathbf{c}\mathbf{c}'\mathbf{x}'=\mathbf{I}}{\operatorname{argmax}} tr(\mathbf{x}\mathbf{c}\mathbf{c}), \quad (43)$$

Defining $\mathbf{y} \equiv \mathbf{x}\mathbf{c}$, we can write

$$\hat{\mathbf{x}} \equiv [\operatorname{argmax}_{\mathbf{y}\mathbf{y}'=\mathbf{I}} tr(\mathbf{y}\mathbf{c})]\mathbf{c}^{-1} = \mathbf{c}^{-1}, \quad (44)$$

where $\operatorname{argmax}_{\mathbf{y}\mathbf{y}'=\mathbf{I}} tr(\mathbf{y}\mathbf{c}) = \mathbf{I}$ because \mathbf{c} is symmetric with positive eigenvalues, see (67) below.

A.3.2 Unconstrained numerical solution

To solve the general problem (41) without the additional constraint on volatilities (42), let us define $\boldsymbol{\pi} \equiv \mathbf{x}\mathbf{c}$. Then

$$\hat{\mathbf{x}} = \hat{\boldsymbol{\pi}}\mathbf{c}^{-1}, \quad (45)$$

where

$$\hat{\boldsymbol{\pi}} \equiv \underset{\boldsymbol{\pi}\boldsymbol{\pi}' \in \mathcal{D}}{\operatorname{argmin}} tr(\boldsymbol{\pi}\boldsymbol{\pi}' - 2\boldsymbol{\pi}\mathbf{c}). \quad (46)$$

Adapting from [Everson, 1997], we can address the optimization (46) with an iterative algorithm that solves two alternating steps. Let us write

$$\boldsymbol{\pi} \equiv \mathbf{d}\mathbf{q}, \quad (47)$$

where \mathbf{d} is diagonal with full rank and \mathbf{q} is orthonormal, in such a way that the constraint $\boldsymbol{\pi}\boldsymbol{\pi}' = \mathbf{d}\mathbf{q}\mathbf{q}'\mathbf{d}' = \mathbf{d}^2 \in \mathcal{D}$ is satisfied.

Step 1. Assume we know the diagonal matrix $\mathbf{d} \in \mathcal{D}$ such that $\boldsymbol{\pi}\boldsymbol{\pi}' = \mathbf{d}^2$. Then (46) becomes

$$\hat{\boldsymbol{\pi}} \equiv \underset{\boldsymbol{\pi}\boldsymbol{\pi}' = \mathbf{d}^2}{\operatorname{argmin}} \operatorname{tr}(\boldsymbol{\pi}\boldsymbol{\pi}' - 2\boldsymbol{\pi}\mathbf{c}) = \underset{\boldsymbol{\pi}\boldsymbol{\pi}' = \mathbf{d}^2}{\operatorname{argmax}} \operatorname{tr}(\mathbf{c}\boldsymbol{\pi}), \quad (48)$$

where we used the symmetry of the Riccati root \mathbf{c} . The problem (48) is in the same format as (55) below. The solution then follows from (66) and reads

$$\hat{\boldsymbol{\pi}} = \mathbf{d}((\mathbf{d}\mathbf{c}^2\mathbf{d})^{\frac{1}{2}})^{-1}\mathbf{d}\mathbf{c}. \quad (49)$$

Since \mathbf{d} is invertible, from (47) we obtain

$$\hat{\mathbf{q}} = \mathbf{d}^{-1}\hat{\boldsymbol{\pi}} = ((\mathbf{d}\mathbf{c}^2\mathbf{d})^{\frac{1}{2}})^{-1}\mathbf{d}\mathbf{c}. \quad (50)$$

Step 2. Assume we know the orthogonal matrix \mathbf{q} such that $\mathbf{q}\mathbf{q}' = \mathbf{I}$ and $\boldsymbol{\pi} = \mathbf{d}\mathbf{q}$. Then (46) becomes

$$\hat{\mathbf{d}} \equiv \underset{\mathbf{d}\mathbf{q}\mathbf{q}'\mathbf{d} \in \mathcal{D}}{\operatorname{argmin}} \operatorname{tr}(\mathbf{d}\mathbf{q}\mathbf{q}'\mathbf{d} - 2\mathbf{d}\mathbf{q}\mathbf{c}) = \underset{\mathbf{d}^2 \in \mathcal{D}}{\operatorname{argmin}} \operatorname{tr}(\mathbf{d}^2 - 2\mathbf{d}\mathbf{q}\mathbf{c}). \quad (51)$$

In order to solve (51), we differentiate its objective function

$$f(\mathbf{d}) \equiv \operatorname{tr}(\mathbf{d}^2) - 2\operatorname{tr}(\mathbf{d}\mathbf{q}\mathbf{c}) = \operatorname{tr}(\mathbf{d}^2) - 2\operatorname{tr}(\mathbf{c}\mathbf{d}\mathbf{q}) \quad (52)$$

with respect to each entries on the diagonal of $\mathbf{d} = dg(d_1, \dots, d_{\bar{k}})$

$$\begin{aligned} \frac{\partial f}{\partial d_k} &= \frac{\partial}{\partial d_k} (\sum_j d_j^2 - 2\sum_{j,i} c_{j,i} d_i q_{ij}) \\ &= 2(d_k - \sum_j q_{k,j} c_{j,k}) \\ &= 2(d_k - [\mathbf{q}\mathbf{c}]_{k,k}), \end{aligned} \quad (53)$$

Setting to zero the derivatives we obtain $\hat{d}_k = [\mathbf{q}\mathbf{c}]_{k,k}$ for all $k = 1, \dots, \bar{k}$, or

$$\hat{\mathbf{d}} = dg(dg^{-1}(\mathbf{q}\mathbf{c})). \quad (54)$$

Alternating (50) and (54) we arrive at the algorithm (20), which we initialized with $\mathbf{d} \equiv \mathbf{I}$.

A.4 The constrained Procrustes problem

Adapting from [Schoenemann, 1966], here we present the solution to the orthogonal Procrustes problem

$$\hat{\mathbf{z}} \equiv \underset{\mathbf{z}\mathbf{z}' = \mathbf{d}^2}{\operatorname{argmax}} \operatorname{tr}(\mathbf{k}\mathbf{z}), \quad (55)$$

where \mathbf{k} is a real matrix and \mathbf{d}^2 is diagonal with full rank.

Consider the singular value decomposition of the product

$$\mathbf{k}\mathbf{d} \equiv \mathbf{p}dg(\boldsymbol{\theta})\mathbf{s}', \quad (56)$$

where \mathbf{p} and \mathbf{s} are orthonormal matrices and $\boldsymbol{\theta}$ is a vector with nonnegative entries. Using (56) and since \mathbf{d} is invertible, we can define the change of variables

$$\mathbf{y} \equiv \mathbf{s}' \mathbf{d}^{-1} \mathbf{z} \mathbf{p}. \quad (57)$$

Then the optimization target in (55) reads

$$\begin{aligned} \text{tr}(\mathbf{k} \mathbf{z}) &= \text{tr}(\mathbf{p} \text{dg}(\boldsymbol{\theta}) \mathbf{s}' \mathbf{d}^{-1} \mathbf{d} \mathbf{s} \mathbf{y} \mathbf{p}') = \text{tr}(\mathbf{p} \text{dg}(\boldsymbol{\theta}) \mathbf{y} \mathbf{p}') \\ &= \text{tr}(\text{dg}(\boldsymbol{\theta}) \mathbf{y} \mathbf{p}' \mathbf{p}) = \text{tr}(\text{dg}(\boldsymbol{\theta}) \mathbf{y}) = \sum_{k=1}^{\bar{k}} \theta_{k,k} y_{k,k}, \end{aligned} \quad (58)$$

and the constraint in (55) is equivalent to

$$\mathbf{y} \mathbf{y}' = \mathbf{s}' \mathbf{d}^{-1} \mathbf{z} \mathbf{p} \mathbf{p}' \mathbf{z}' \mathbf{d}^{-1} \mathbf{s} = \mathbf{s}' \mathbf{d}^{-1} \mathbf{z} \mathbf{z}' \mathbf{d}^{-1} \mathbf{s} = \mathbf{s}' \mathbf{d}^{-1} \mathbf{d}^2 \mathbf{d}^{-1} \mathbf{s} = \mathbf{s}' \mathbf{s} = \mathbf{I}. \quad (59)$$

Hence the solution of (55) is

$$\hat{\mathbf{z}} = \mathbf{d} \mathbf{s} \hat{\mathbf{y}} \mathbf{p}', \quad (60)$$

where

$$\hat{\mathbf{y}} \equiv \underset{\mathbf{y} \mathbf{y}' = \mathbf{I}}{\text{argmax}} \sum_{n=1}^{\bar{n}} \theta_{k,k} y_{k,k}. \quad (61)$$

Since $\theta_{k,k} \geq 0$ for all $k = 1, \dots, \bar{k}$, the maximum is attained by $\hat{y}_{k,k} = 1$ for all $k = 1, \dots, \bar{k}$, which implies $\hat{\mathbf{y}} = \mathbf{I}$. Substituting this in (60) we obtain the solution to (55)

$$\hat{\mathbf{z}} = \mathbf{d} \mathbf{s} \mathbf{p}'. \quad (62)$$

Notice that if \mathbf{k} is invertible, then we can simplify the solution (62). Indeed, we can write

$$\mathbf{s} \mathbf{p}' = \mathbf{s} \text{dg}(\boldsymbol{\theta})^{-1} \underbrace{\mathbf{s}' \mathbf{s}}_{\mathbf{I}} \text{dg}(\boldsymbol{\theta}) \mathbf{p}' \stackrel{(56)}{=} \mathbf{s} \text{dg}(\boldsymbol{\theta})^{-1} \mathbf{s}' \mathbf{d} \mathbf{k}' \stackrel{(64)}{=} \mathbf{u}^{-1} \mathbf{d} \mathbf{k}', \quad (63)$$

where

$$\mathbf{u} \equiv \mathbf{s} \text{dg}(\boldsymbol{\theta}) \mathbf{s}'. \quad (64)$$

It is easy to see that \mathbf{u} is the Riccati root of

$$\begin{aligned} \mathbf{U} &\equiv \mathbf{d} \mathbf{k}' \mathbf{k} \mathbf{d} \stackrel{(56)}{=} \mathbf{s} \text{dg}(\boldsymbol{\theta}) \mathbf{p}' \mathbf{p} \text{dg}(\boldsymbol{\theta}) \mathbf{s}' = \mathbf{s} \text{dg}(\boldsymbol{\theta}) \text{dg}(\boldsymbol{\theta}) \mathbf{s}' = \mathbf{s} \text{dg}(\boldsymbol{\theta}) \underbrace{\mathbf{s}' \mathbf{s}}_{\mathbf{I}} \text{dg}(\boldsymbol{\theta}) \mathbf{s}' \\ &= \mathbf{u} \mathbf{u}' = \mathbf{u}^2. \end{aligned} \quad (65)$$

Hence, from the non singularity of \mathbf{k} we obtain the solution to (55) as follows

$$\hat{\mathbf{z}} \stackrel{(62)-(63)}{=} \mathbf{d} \mathbf{u}^{-1} \mathbf{d} \mathbf{k}' \stackrel{(65)}{=} \mathbf{d} ((\mathbf{d} \mathbf{k}' \mathbf{k} \mathbf{d})^{\frac{1}{2}})^{-1} \mathbf{d} \mathbf{k}'. \quad (66)$$

Notice that if \mathbf{k} is symmetric with positive eigenvalues, then \mathbf{k} is the Riccati root of $\mathbf{k}' \mathbf{k}$. Hence

$$\left. \begin{array}{l} \mathbf{k} = \mathbf{k}' \\ \mathbf{d} = \mathbf{I} \end{array} \right\} \Rightarrow \hat{\mathbf{z}} = ((\mathbf{k}' \mathbf{k})^{\frac{1}{2}})^{-1} \mathbf{k}' = (\mathbf{k})^{-1} \mathbf{k} = \mathbf{I}. \quad (67)$$