Portfolio Optimization

Graph-Based Portfolios

Daniel P. Palomar (2025). *Portfolio Optimization: Theory and Application*. Cambridge University Press.

port folio optimization book.com

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Outline

- Introduction
- 2 Hierarchical Clustering and Dendrograms
- 3 Hierarchical Clustering-Based Portfolios
 - Hierarchical 1/N Portfolio
 - Hierarchical Risk Parity (HRP) Portfolio
 - Hierarchical Equal Risk Contribution (HERC) Portfolio
- Mumerical Experiments
- Summary

Executive Summary

- Graph representation compresses big data for efficient analysis of large networks and pattern extraction.
- Asset graphs capture critical relationships in financial data for modern portfolio design.
- **Potential enhancement** to traditional mean-variance formulation through graph information.
- Open research question: How to optimally incorporate graph structure into portfolio optimization.
- Overview: These slides explore several approaches to include graph information (Palomar 2025, chap. 12).

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Introduction

Markowitz's Mean-Variance Portfolio

- Balances expected return and risk.
- Optimization problem:

maximize
$$\mathbf{w}^{\mathsf{T}} \boldsymbol{\mu} - \frac{\lambda}{2} \mathbf{w}^{\mathsf{T}} \boldsymbol{\Sigma} \mathbf{w}$$
 subject to $\mathbf{w} \in \mathcal{W}$,

where λ is risk-aversion hyper-parameter and \mathcal{W} denotes the constraint set (e.g., $\mathcal{W} = \{ \mathbf{w} \mid \mathbf{1}^\mathsf{T} \mathbf{w} = 1, \mathbf{w} \geq \mathbf{0} \}$).

Challenges With Estimation Errors

- ullet Mean vector μ and covariance matrix Σ are prone to errors.
- Estimation errors significantly impact portfolio performance.

Improvement Using Graph of Assets

- Potential for enhancement by incorporating asset graph connectivity.
- Graph connectivity patterns may reveal key investment insights.

Graphs and Distance Matrices

Graph-Based Portfolio Construction

- Utilizes graph information encoded as a distance matrix **D**.
- Distance reflects the relationship between asset pairs.

Correlation-Based Distance Matrix

$$D_{ij} = \sqrt{rac{1}{2}(1-
ho_{ij})}$$

where ρ_{ij} is the correlation between assets i and j.

Connection With Euclidean Distance

- Standardized data columns: $\tilde{\mathbf{x}}_i = (\mathbf{x}_i \mu_i)/\sigma_i$.
- Empirical correlation: $\rho_{ij} = \frac{1}{T} \tilde{\mathbf{x}}_i^{\mathsf{T}} \tilde{\mathbf{x}}_j$.
- Normalized squared Euclidean distance: $\frac{1}{T} \| \tilde{\mathbf{x}}_i \tilde{\mathbf{x}}_j \|_2^2 = 2(1 \rho_{ij})$.

Graphs and Distance Matrices

Other Distance Functions

Minkowski metric based on p-norm:

$$D_{ij} = \|\tilde{\boldsymbol{x}}_i - \tilde{\boldsymbol{x}}_j\|_p$$

where
$$\| \boldsymbol{a} \|_{p} = \left(\sum_{t=1}^{T} |a_{i}|^{p} \right)^{1/p}$$
.

- Manhattan distance (p = 1).
- Euclidean distance (p = 2).

Holistic Distance Matrix Approach

Euclidean distance between distance vectors:

$$\tilde{D}_{ij} = \|oldsymbol{d}_i - oldsymbol{d}_j\|_2$$

- d_i : ith column of D.
- Reflects similarity of assets with the entire asset universe.
- Overcomes the limitation of pairwise-only information.

Toy Example

Correlation Matrix C:

$$\mathbf{C} = \begin{bmatrix} 1 & 0.7 & 0.2 \\ 0.7 & 1 & -0.2 \\ 0.2 & -0.2 & 1 \end{bmatrix}$$

Correlation-Based Distance Matrix *D*:

$$\mathbf{D} = \begin{bmatrix} 0 & 0.3873 & 0.6325 \\ 0.3873 & 0 & 0.7746 \\ 0.6325 & 0.7746 & 0 \end{bmatrix}$$

Euclidean Distance Matrix of Correlation Distances \tilde{D} :

$$\tilde{\boldsymbol{D}} = \begin{bmatrix} 0 & 0.5659 & 0.9747 \\ 0.5659 & 0 & 1.1225 \\ 0.9747 & 1.1225 & 0 \end{bmatrix}$$

Graphs and Distance Matrices

Other advanced graph estimation methods (Palomar 2025, chap. 5):

Heavy-Tailed Markov Random Field (MRF) With Degree Control

where

- gdet(·): generalized determinant.
- w: graph weight vector.
- $\mathcal{L}(\mathbf{w})$: Laplacian operator.
- $\mathfrak{d}(w)$: degree operator.
- ν : controls heavy-tailness.

Graphs and Distance Matrices

k-Component Heavy-Tailed MRF With Degree Control

Aims for a k-component graph (graph with k clusters):

where

- ullet γ : regularization hyper-parameter.
- F: enforces low-rank property.

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Hierarchical Clustering and Dendrograms

Clustering Overview

- Multivariate statistical analysis technique.
- Used in machine learning, data mining, pattern recognition, bioinformatics, finance, etc.
- Groups elements into clusters based on similar characteristics.
- Unsupervised classification method.

Hierarchical Clustering

- Forms a recursive nested clustering.
- Builds a binary tree of data points representing nested groups.
- Allows data exploration at different levels of granularity.
- Contrasts with partitional clustering, which finds all clusters simultaneously without a hierarchical structure.

Dendrogram

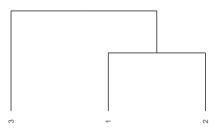
- Visual representation of the hierarchical clustering tree.
- Encodes the successive or hierarchical clustering process.
- Provides a complete, interpretable description of the clustering in graphical format.
- Popular due to its high interpretability.

Hierarchical Clustering and Dendrograms

Consider a toy example with distance matrix:

$$\tilde{\mathbf{D}} = \begin{bmatrix} 0 & 0.5659 & 0.9747 \\ 0.5659 & 0 & 1.1225 \\ 0.9747 & 1.1225 & 0 \end{bmatrix}$$

The dendrogram groups first the first and second elements since they have the smallest distance:



Basic Procedure

Hierarchical Clustering Process

- Requires a distance matrix **D**.
- Sequentially clusters items based on distance.

Methods for Hierarchical Clustering

- **Agglomerative (bottom-up):** starts with each item as a singleton cluster, merges the closest clusters sequentially, and continues until one cluster remains.
- **Divisive (top-down):** starts with all items in one cluster and recursively divides each cluster into smaller ones.

Levels of Hierarchy

- Each level represents a grouping into disjoint clusters.
- The entire hierarchy is an ordered sequence of groupings.

Basic Procedure

Linkage Clustering Methods

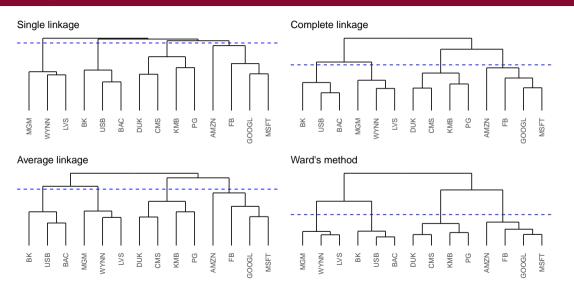
Measure of dissimilarity between clusters:

- **Single linkage:** distance is the minimum distance between any two points in the clusters (related to the minimum spanning tree (MST)).
- Complete linkage: distance is the maximum distance between any two points in the clusters.
- Average linkage: distance is the average distance between any two points in the clusters.
- Ward's method: distance is the increase in squared error when merging clusters (related to distances between cluster centroids).

Effects of Linkage Method

- Significantly impacts the resulting hierarchical clustering.
- Single linkage may cause a "chaining" effect and imbalanced groups.
- Complete linkage tends to produce more balanced groups.
- Average linkage is an intermediate case.
- Ward's method often yields results similar to average linkage.

Dendrograms of S&P 500 Stocks



Number of Clusters

Determining the Number of Clusters

- Traversing the dendrogram from top to bottom transitions from one giant cluster to N singleton clusters.
- In practice, dealing with N singleton clusters may lead to overfitting.

Simplification vs. Detail

- Fewer clusters simplify the data but lose fine details, too many clusters might identify spurious patterns.
- The challenge lies in choosing the optimal number of clusters.

Automatic Detection of Optimal Clusters

- Essential to avoid overfitting.
- Aids in identifying the most appropriate number of clusters.

Gap Statistic

- Determines the optimal number of clusters.
- Compares empirical within-cluster dissimilarity to uniformly distributed data.
- Identifies the balance between simplification and preserving significant patterns.

Quasi-Diagonalization of Correlation Matrix

Quasi-Diagonalization of Correlation Matrix

- Hierarchical clustering reorders items in the correlation matrix.
- Groups similar assets closer and dissimilar assets farther apart.
- Known as matrix seriation or matrix quasi-diagonalization.
- An old statistical technique for revealing inherent clusters.

Benefits of Quasi-Diagonalization

- Rearranges the correlation matrix into a quasi-diagonal form.
- Reveals similar assets as blocks along the main diagonal.
- Enhances visual pattern recognition compared to a randomly ordered matrix.

Visualization Through Heatmaps

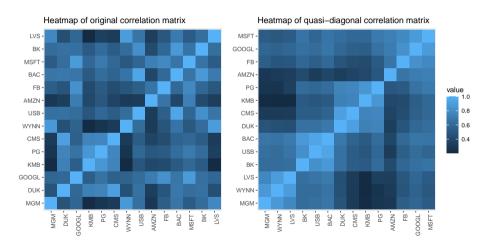
- Heatmaps can display the original and quasi-diagonal correlation matrices.
- Original matrix with randomly ordered stocks shows no clear pattern.
- Quasi-diagonal matrix, after reordering, shows correlated stocks in diagonal blocks.

Identification of Clusters

- Quasi-diagonal matrix allows for easy identification of asset clusters.
- Corresponding dendrograms can confirm the number and composition of these clusters.

Quasi-Diagonalization of Correlation Matrix

Effect of seriation in the correlation matrix of S&P 500 stocks:



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Hierarchical Clustering-Based Portfolios

Portfolio Design Based on Graph of Assets

- Aims to create robust, diversified portfolios with better risk-adjusted performance.
- ullet Less reliance on noisy estimates of mean vector μ and covariance matrix Σ .

Hierarchical Clustering for Diversification

- Distributes capital weights across hierarchically nested clusters.
- Identifies isolated stocks contributing to diversification.
- Visualized using the hierarchical tree layout.

Capital Allocation in Hierarchical Clustering-Based Portfolios

- Total capital starts at the top of the dendrogram.
- Capital is allocated top-down through the hierarchy.
- Each division of a cluster into sub-clusters splits the capital accordingly.
- Portfolios for sub-clusters are designed at each split.

Hierarchical Clustering-Based Portfolios

Characteristics of Hierarchical Clustering-Based Portfolios

- Distance matrix: Defines the graph (e.g., correlation-based, distance matrix of columns, sophisticated graph learning).
- 2 Linkage method: Employed in the clustering process (e.g., single, complete, average, Ward).
- Clustering stopping criterion: Determines when to stop clustering (e.g., single-item clusters, gap statistic).
- **Splitting criterion:** Recursively splits the assets (e.g., bisection, dendrogram-based).
- Intra-weight allocation: Allocation of weights within clusters.
- Inter-weight allocation: Allocation of weights across clusters.

We Will Explore

- Hierarchical 1/N portfolio.
- Hierarchical risk parity portfolio.
- Hierarchical equal risk contribution portfolio.

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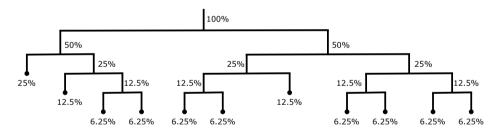
Cluster-Based Waterfall Portfolio Overview

- Introduced by (Papenbrock 2011) in his PhD thesis.
- Utilizes hierarchical tree from correlation-based distance matrix.
- Allocation process splits weights equally at each dendrogram split.

Allocation Process

- Proceeds in a top-down manner through the dendrogram.
- Splits weights equally at each splitting point.
- Illustration provided in the next figure.

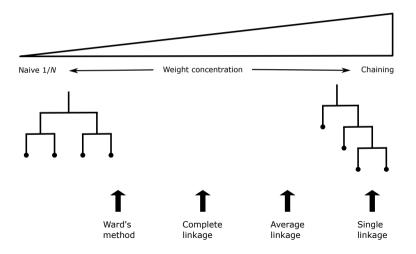
Illustration of the hierarchical 1/N portfolio construction in a top-down manner:



Impact of Linkage Method on Weight Allocation:

- Single linkage: suffers from "chaining" effect, leading to high weights on some stocks.
- Complete linkage: produces more even groups and weights.
- Average linkage: intermediate between single and complete linkage.
- Ward's method: similar to complete linkage but with even more balanced groups and weights.
- Regular 1/N portfolio: represents equalized weights without using graph information, termed *naive* 1/N portfolio.

Chaining effect of different linkage methods on the hierarchical 1/N allocation:



Summary:

- **①** Distance matrix: correlation-based: $D_{ij} = \sqrt{\frac{1}{2}(1 \rho_{ij})}$.
- Linkage method: single linkage for high-risk investors; Ward's method for risk-averse investors.
- Olustering stopping criterion: continues to single-item clusters.
- **Splitting criterion:** follows the dendrogram.
- Intra-weight allocation: 1/N portfolio strategy.
- **Inter-weight allocation:** 1/N portfolio with N=2, i.e., 50% 50% split at each branching.

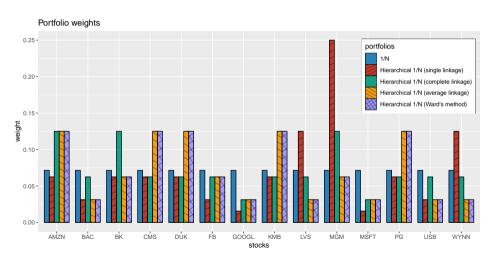
Comparing Hierarchical 1/N Portfolios with Different Linkage Methods

- ullet Hierarchical 1/N portfolios are compared using single, complete, average, and Ward's linkage methods.
- Naive 1/N portfolio serves as a benchmark.

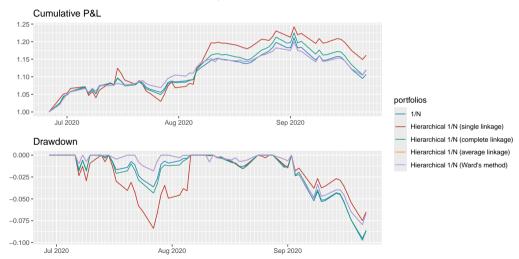
Backtest Results

- ullet Ward's method seems to be a good choice for hierarchical 1/N portfolio construction.
- The original publication (Papenbrock 2011) supports the use of Ward's method for subsequent analysis.

Portfolio allocation of hierarchical 1/N portfolios with different linkage methods:



Backtest performance of hierarchical 1/N portfolios with different linkage methods:



Comparison of Hierarchical 1/N Portfolio Using Different Distance Matrices

① Correlation-based distance matrix: as per (Papenbrock 2011):

$$D_{ij} = \sqrt{rac{1}{2}(1-
ho_{ij})}$$

Orrelation-based distance-of-distance matrix: as used in (López de Prado 2016):

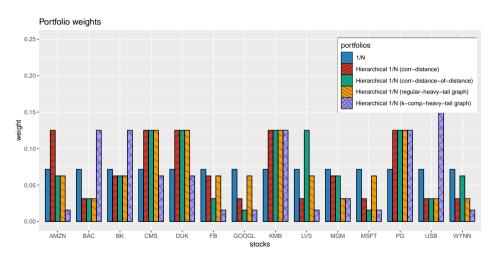
$$\tilde{D}_{ij} = \|\boldsymbol{d}_i - \boldsymbol{d}_j\|_2$$

Graphs estimated via heavy-tailed MRF: regular heavy-tailed MRF; *k*-component heavy-tailed MRF.

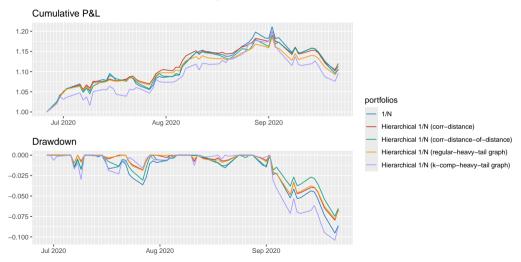
Backtest Observations

- The simple correlation-based distance-of-distance matrix appears to have a better drawdown profile.
- More exhaustive backtests are recommended to draw definitive conclusions.

Portfolio allocation of hierarchical 1/N portfolios with different distance matrices:



Backtest performance of hierarchical 1/N portfolios with different distance matrices:



Final Comparison of Hierarchical 1/N Portfolio

- Selected version uses Ward's method for linkage and correlation-based distance-of-distance matrix.
- Benchmarks: naive 1/N portfolio, global minimum variance portfolio (GMVP), and Markowitz mean-variance portfolio (MVP).

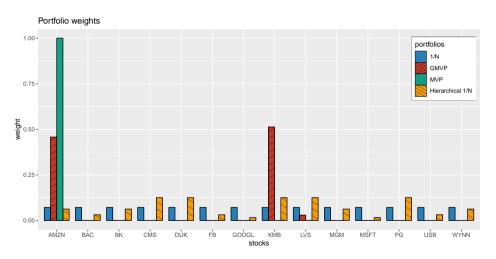
Observations

- Hierarchical 1/N portfolio emphasizes diversification.
- MVP exhibits the worst drawdown due to sensitivity in estimating μ .
- \bullet GMVP and naive 1/N portfolio show better performance than MVP.
- ullet Hierarchical 1/N portfolio shows mildest drawdown, indicating good risk management.

Considerations and Further Evaluation

- The presented backtest is anecdotal and not sufficient for definitive conclusions.
- A proper empirical evaluation requires multiple randomized backtests.
- ullet Further analysis is necessary to robustly assess the performance of the hierarchical 1/N portfolio against benchmarks.

Portfolio allocation of hierarchical 1/N portfolio along benchmarks:



Backtest performance of hierarchical 1/N portfolio along benchmarks:



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Hierarchical Risk Parity (HRP) Portfolio Overview

- Introduced by López de Prado (2016).
- Based on hierarchical tree from correlation-based distance-of-distance matrix.
- Utilizes single linkage method for clustering.
- Allocation process uses inverse-variance portfolio (IVarP) for weight splitting.

Global Minimum Variance Portfolio (GMVP) Recap

- Minimizes portfolio variance subject to budget constraint.
- ullet Solution simplifies to IVarP if covariance matrix $oldsymbol{\Sigma}$ is diagonal:

$$\mathbf{w} = \frac{\mathbf{\sigma}^{-2}}{\mathbf{1}^{\mathsf{T}}\mathbf{\sigma}^{-2}}.$$

Inverse-Variance Portfolio (IVarP) for N=2 Assets

• Weight allocation based on inverse of variances:

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} \sigma_2^2/(\sigma_1^2 + \sigma_2^2) \\ \sigma_1^2/(\sigma_1^2 + \sigma_2^2) \end{bmatrix}.$$

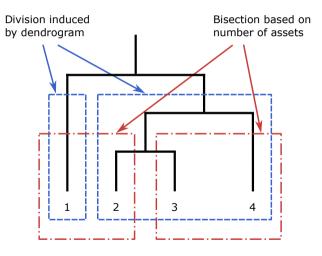
HRP Portfolio Design Process

- ullet Similar to hierarchical 1/N portfolio, allocation proceeds top-down through the dendrogram.
- **Differences:** uses bisection for splitting, not the dendrogram's natural structure; weight splitting based on IVarP for N=2 assets.
- ullet Empirical evaluation required to compare performance with hierarchical 1/N portfolio.

Interpretation and Connection to GMVP

- HRP can be seen as a refined version of the IVarP.
- At each step, weights are scaled based on inverse variances, ignoring correlations between subsets.
- Correlations considered only in variance computation of subsets.
- When covariance matrix is diagonal, IVarP, GMVP, and HRP coincide.
- Connection between HRP and GMVP explored further in subsequent sections.

Comparison of bisection splitting and dendrogram-based splitting:



Summary:

- **Distance matrix:** correlation-based distance-of-distance matrix.
- Linkage method: single linkage.
- Olustering stopping criterion: continues to single-item clusters.
- Splitting criterion: bisection, ignoring dendrogram grouping sizes.
- Intra-weight allocation: IVarP.
- **10 Inter-weight allocation:** IVarP for N = 2.

Comparison of HRP Portfolios with Benchmarks

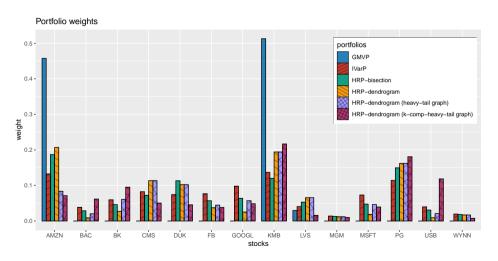
- HRP portfolios compared with global minimum variance portfolio (GMVP) and inverse-variance portfolio (IVarP).
- Two versions of HRP: one with bisection split and another with dendrogram split.

Observations

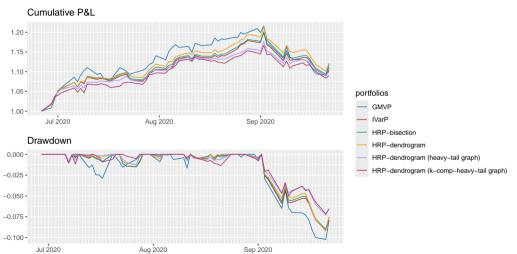
- GMVP shows concentration in two assets, while others are more diversified.
- HRP portfolios show similar diversification to IVarP.
- HRP portfolios exhibit slight improvement over IVarP.
- Graphs estimated via heavy-tailed MRF methods may offer better performance than correlation-based methods.
- HRP portfolios aim to balance diversification and risk management.
- The choice of splitting method in HRP (bisection vs. dendrogram) may not significantly alter the diversification profile compared to IVarP.
- The performance of HRP portfolios in terms of drawdown and P&L suggests potential advantages over traditional IVarP, especially when using advanced graph estimation methods.

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Portfolio allocation of HRP portfolios and benchmarks:



Backtest performance of HRP portfolios and benchmarks:



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Hierarchical Equal Risk Contribution (HERC) Portfolio Overview

- Introduced by Raffinot (2018).
- \bullet Refines and extends the hierarchical 1/N and HRP portfolios.
- Incorporates early stopping based on the gap statistic for cluster selection.
- Utilizes equal risk contribution (ERC) for weight allocation among clusters.

Key Differences from Previous Approaches

- Early stopping with gap statistic: automatically selects the appropriate number of clusters; avoids clustering down to single assets.
- **General equal risk contribution:** splits weights based on alternative risk measures (e.g., standard deviation, conditional value-at-risk); formula for two clusters:

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} \mathsf{RC}_1/(\mathsf{RC}_1 + \mathsf{RC}_2) \\ \mathsf{RC}_2/(\mathsf{RC}_1 + \mathsf{RC}_2) \end{bmatrix},$$

where RC_i is the risk contribution of the *i*th cluster.

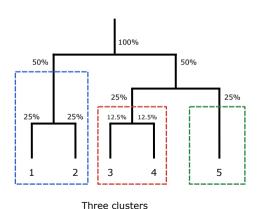
Main Findings

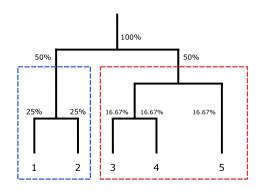
- Hierarchical 1/N portfolio is a strong baseline.
- HERC portfolios based on downside risk measures (especially conditional drawdown-at-risk) show statistically better risk-adjusted performances.

Illustration of Early Stopping

- The next figure demonstrates early stopping in hierarchical clustering with a toy dendrogram.
- Groups assets into clusters based on the gap statistic, avoiding overly granular clustering.

Effect of early stopping in the hierarchical clustering process:





Summary:

- **① Distance matrix:** correlation-based distance-of-distance matrix.
- Linkage method: Ward's method.
- **Olustering stopping criterion:** gap statistic for optimal cluster selection.
- Splitting criterion: follows the dendrogram structure.
- **1** Intra-weight allocation: 1/N portfolio strategy.
- **1 Inter-weight allocation:** equal risk contribution based on various risk measures.

Conclusion

HERC portfolio represents a sophisticated approach to portfolio construction, balancing risk across clusters for improved risk-adjusted returns.

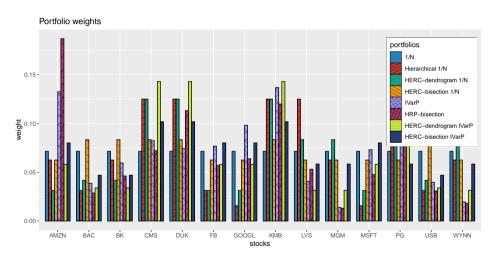
Simplification in Weight Splitting for HERC Portfolios

- For weight allocation, two risk contribution measures are considered:
 - RC_i = 1: leads to a 50% 50% split, similar to the hierarchical 1/N portfolio.
 - RC_i = $1/\sigma_i^2$: aligns with the inverse-variance portfolio (IVarP) formula, akin to the HRP portfolio.

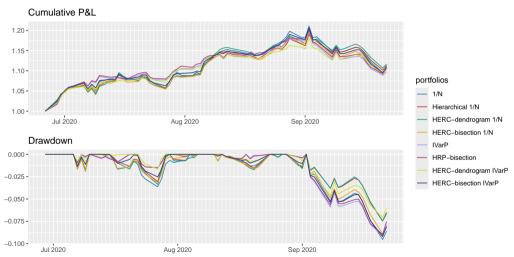
Comparison of HERC Portfolios with Benchmarks

- Benchmarks include: 1/N portfolio, hierarchical 1/N portfolio, inverse-variance portfolio (IVarP), and HRP portfolio.
- Two versions of HERC portfolios are evaluated: one with bisection split and another with dendrogram split.

Portfolio allocation of HERC portfolios and benchmarks:



Backtest performance of HERC portfolios and benchmarks:



Observations and Further Evaluation

- Difficult to draw definitive conclusions from a single backtest.
- More exhaustive backtests are necessary to robustly assess the performance of HERC portfolios.
- Future analysis should aim to evaluate the risk-adjusted returns and drawdown characteristics of HERC portfolios in various market conditions.

Conclusion

- The HERC portfolio introduces a nuanced approach to portfolio construction by incorporating risk contributions and early stopping based on the gap statistic.
- Its performance relative to traditional and hierarchical portfolio strategies warrants further empirical investigation to fully understand its benefits and limitations.

From Portfolio Risk Minimization to Hierarchical Portfolios

- The basic structure of hierarchical portfolios is heuristic and suboptimal, which is understandable since the motivation was not optimality but stability against estimation errors.
- On the other hand, portfolios designed based on the minimization of some properly chosen measure of risk are not heuristic by definition but optimal according to the design criterion.
- Can we make an explicit connection between the two paradigms?
- Indeed, it is possible to design a continuum between hierarchical portfolios and optimally designed portfolios (Palomar 2025, sec. 12.3.4).

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Numerical Experiments

Overview

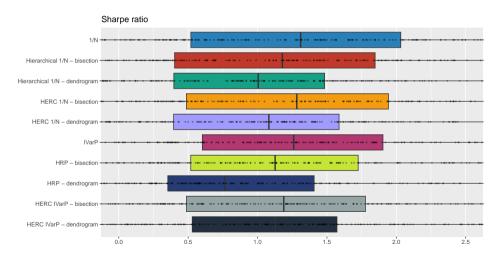
- Conducted multiple randomized backtests using S&P 500 stocks from 2015-2020.
- Generated 200 resamples with N = 50 stocks and a random two-year period.
- Walk-forward backtest with a 1-year lookback, reoptimizing monthly.
- Caution: results are indicative and should be supplemented with more exhaustive backtests.

Observations

- **Splitting:** natural dendrogram splits might be expected to outperform, but it seems that bisection might provide more balanced clusters (while utilizing dendrogram ordering).
- **Graph learning:** sophisticated methods do not clearly outperform simple graph-based approaches.

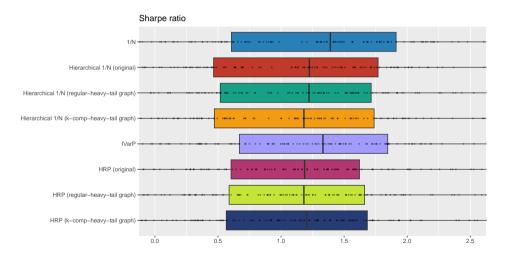
Numerical Experiments – Splitting: Visection vs. Dendrogram

Comparison of graph-based portfolios: bisection vs. dendrogram splitting:



Numerical Experiments – Graph Estimation: Simple vs. Sophisticated

Comparison of graph-based portfolios: simple vs. sophisticated graph learning methods:



Numerical Experiments - Final Comparison

Portfolios Compared

- Hierarchical 1/N portfolio.
- HERC 1/N portfolio.
- HRP portfolio.
- HERC IVarP.

Benchmarks

- 1/N portfolio.
- IVarP.

Empirical Results

The following table and figures show no significant differences among methods.

Conclusion

- Further exhaustive comparison needed to draw clear conclusions.
- Current analysis does not favor one graph-based portfolio method over others.

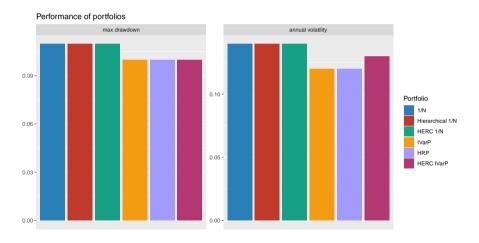
Numerical Experiments – Final Comparison

Comparison of selected graph-based portfolios: performance measures:

Portfolio	Sharpe ratio	annual return	annual volatility	max drawdown
1/N	1.01	14%	14%	11%
Hierarchical $1/N$	0.81	12%	14%	11%
HERC 1/N	0.99	14%	14%	11%
IVarP	1.04	13%	12%	10%
HRP	0.91	11%	12%	10%
HERC IVarP	0.89	12%	13%	10%

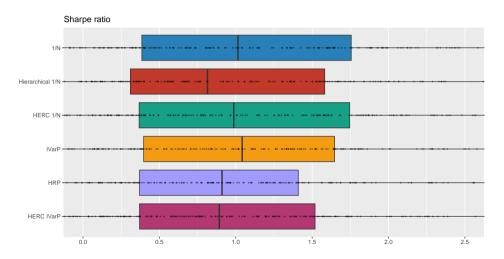
Numerical Experiments – Final Comparison

Comparison of selected graph-based portfolios: barplots of maximum drawdown and annualized volatility:



Numerical Experiments – Final Comparison

Comparison of selected graph-based portfolios: boxplots of Sharpe ratio:



Outline

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Summary

Graphs compactly represent big data, revealing underlying structure and patterns.

Key takeaways for portfolio design using graphs:

- Graphs represent asset relationships: nodes are assets, edges are pairwise relationships.
- Financial graphs can be learned from data, e.g., based on heavy-tailed Markov random fields or k-component versions for clustered graphs (Palomar 2025, chap. 5).
- Hierarchical clustering partitions assets into clusters at different levels of detail.
- Graph information should be incorporated into portfolio formulation, with notable examples being hierarchical 1/N, risk parity, and equal risk contribution portfolios.

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