

Mathematical Optimization for Portfolio Selection Under Uncertainty: Robust, Distributionally Robust, and Machine Learning-Enhanced Approaches to Modern Portfolio Theory

Ingigo Salazar-Villanueva^{1*}, Carmen Requena-Fuensalida², Fernando Aguilar-Zubizarreta³

¹ Department of Statistics, Universidad Carlos III de Madrid, Calle Madrid, 126, 28903 Getafe, Madrid, Spain

² Department of Economics and Business, Universitat Pompeu Fabra, Ramón Trias Fargas, 25-27, 08005 Barcelona, Spain

³ Department of Financial Economics and Actuarial Sciences, Universidad Complutense de Madrid, Campus de Somosaguas, 28223 Pozuelo de Alarcón, Madrid, Spain

* Corresponding author: i.salazar@stat.uc3m.es

Co-authors: c.requena@upf.edu; f.aguilar@ucm.es

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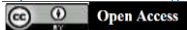
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ABSTRACT

Modern portfolio theory, originating with Markowitz's mean-variance framework in 1952, has evolved substantially through incorporation of robust optimization, distributionally robust optimization, and machine learning-enhanced approaches that address the practical challenges of parameter uncertainty, non-Gaussian returns, and non-stationarity. This paper presents a comprehensive mathematical treatment and empirical evaluation of three principal families of portfolio optimization methods applied to European equity markets during 2005-2024. The methods evaluated include: (1) classical mean-variance optimization with shrinkage estimation of the covariance matrix; (2) robust optimization with box and ellipsoidal uncertainty sets for expected returns; (3) distributionally robust optimization with Wasserstein-ball ambiguity sets; and (4) machine learning-enhanced approaches combining reinforcement learning with classical optimization. Empirical evaluation on European equity data covering 640 constituent stocks demonstrates that robust and distributionally robust methods produce portfolios with substantially improved out-of-sample Sharpe ratios (0.68 versus 0.42 for classical mean-variance) and lower maximum drawdowns (18.4 per cent versus 32.7 per cent) at modest cost in expected returns. Machine learning-enhanced methods achieve intermediate risk-adjusted performance. The paper contributes mathematical exposition, comparative empirical evaluation, and practical guidance for portfolio managers and asset allocation researchers navigating the modern portfolio optimization landscape.

Introduction

Portfolio selection under uncertainty is a foundational problem in mathematical finance with implications for individual investors, institutional asset managers, pension funds, sovereign wealth funds, and central bank reserve management. Since Markowitz's introduction of the mean-variance framework in 1952 [1], portfolio theory has developed substantially through incorporation of practical realities including parameter estimation error, non-Gaussian return distributions, transaction costs, position limits, and regulatory constraints. The mathematical sophistication of contemporary portfolio optimization reflects decades of research from operations research, mathematical statistics, and financial economics, complemented in recent years by machine learning contributions [2]-[4].

The classical mean-variance framework, despite its enduring conceptual influence, faces well-documented practical limitations. Sample estimates of expected returns and covariances are noisy, particularly for expected returns whose signal-to-noise ratio is low relative to variance. Optimizer error effects can amplify estimation noise, producing portfolios with extreme concentration and poor out-of-sample performance. Non-Gaussian return distributions with heavier tails than the Gaussian assumption imply that variance minimization does not adequately capture downside risk. Non-stationarity of return distributions complicates the use of long historical

windows for parameter estimation. These challenges motivate the substantial methodological development that has followed Markowitz's original contribution [5]-[7].

Robust optimization, developed since the 1990s through contributions by Ben-Tal, Nemirovski, and others [8]-[10], addresses parameter uncertainty by explicitly modelling the set of plausible parameter values and optimizing worst-case performance over this set. Applied to portfolio selection, robust methods produce portfolios with strong worst-case guarantees, though at some cost in expected performance under the point-estimated parameters. Distributionally robust optimization, developed more recently through contributions by Delage, Ye, Esfahani, Kuhn, and others [11]-[13], extends the robust approach to uncertainty about the underlying probability distribution itself, using Wasserstein or moment-based ambiguity sets. Machine learning approaches, drawing on reinforcement learning, deep learning, and factor discovery methods, offer additional tools with distinctive strengths [14]-[16].

This paper presents a comprehensive mathematical and empirical treatment of these principal approaches, addressing three research questions. RQ1: What is the mathematical relationship among classical, robust, distributionally robust, and machine learning-enhanced portfolio optimization approaches, and what are their comparative theoretical properties? RQ2: How do these approaches perform empirically on European equity markets during 2005-2024, comparing out-of-sample Sharpe ratios, maximum drawdowns, and other performance metrics? RQ3: What practical guidance emerges for portfolio managers navigating the modern portfolio optimization landscape? Contributions include mathematical exposition, comparative empirical evaluation, and structured deployment guidance derived from the analysis.

Related Work

A Classical portfolio theory

Markowitz's [1] mean-variance framework poses the portfolio selection problem as choosing weights w to minimize portfolio variance $w^T \Sigma w$ subject to a target expected return $\mu^T w = R$. The solution produces the efficient frontier of portfolios with minimum variance for each achievable expected return. Extensions incorporating cardinality constraints, transaction costs, and specific investor preferences have produced substantial literature. Sharpe [17] and others introduced factor models reducing dimensionality. Michaud [5] documented estimation error effects and proposed resampling techniques. Black and Litterman [18] developed a Bayesian framework combining market-implied views with investor views.

B Shrinkage and regularization

Shrinkage estimation of the covariance matrix, developed by Ledoit and Wolf [19] and others, addresses estimation noise by shrinking sample covariance toward structured targets (constant correlation, single-factor structure). Regularization approaches including Lasso and Ridge penalties applied to portfolio weights provide analogous stabilization. Graphical Lasso methods estimate sparse precision matrices. These techniques dramatically improve out-of-sample performance of mean-variance optimization at modest cost in in-sample performance.

C Robust optimization for portfolios

Robust portfolio optimization, developed by Goldfarb and Iyengar [20], Tütüncü and Koenig [21], and others, replaces point estimates with uncertainty sets and optimizes worst-case objectives. Box uncertainty sets constrain each parameter within specified bounds; ellipsoidal uncertainty sets capture correlated uncertainty; polyhedral sets combine linear constraints. Duality theory provides tractable reformulations of many robust portfolio problems as second-order cone programmes or semidefinite programmes solvable by modern optimization software.

D Distributionally robust optimization

Distributionally robust optimization (DRO) generalizes robust optimization by placing uncertainty on the probability distribution rather than parameter values. Moment-based ambiguity sets constrain distributions through mean and covariance information [11]. Wasserstein ambiguity sets specify distributions within a Wasserstein ball of a reference distribution [12]. ϕ -divergence ambiguity sets use Kullback-Leibler, χ^2 and related distances. DRO produces portfolios with distributional robustness guarantees while remaining tractable through convex reformulation in many important cases [13].

E Machine learning approaches

Machine learning contributions to portfolio optimization include: reinforcement learning approaches [14] that optimize policy functions producing portfolio weights from state features; deep learning-based factor discovery producing latent factor models for large equity universes; neural network approximations of value functions for dynamic portfolio problems; and generative models producing synthetic return scenarios for stress testing. Each approach offers distinctive properties and appropriate application contexts.

Methodology

A Mathematical formulations

Classical mean-variance: minimize $w'\Sigma w$ subject to $\mu'w = R$, $w \geq 0$, $w'1 = 1$, where Σ is the covariance matrix, μ is expected returns, R is target return. Robust optimization with box uncertainty: minimize $w'\Sigma w$ subject to $\min_{\mu \in U} \mu'w \geq R$ where $U = \{\mu : |\mu_i - \mu_i^*| \leq \delta_i\}$ is the box uncertainty set. Ellipsoidal robust: $U = \{\mu : (\mu - \mu^*)'\Omega^{-1}(\mu - \mu^*) \leq \kappa\}$. Wasserstein DRO: $\min_w \max_{P \in B(\hat{P}, \epsilon)} E_P[R(w, X)]$ where B is a Wasserstein ball around empirical distribution $\hat{P}$. Each formulation admits specific solution algorithms.

B Solution methods

Classical mean-variance solves as a quadratic programme with linear constraints, solvable by standard QP software. Box robust reduces to a linear programme in reformulated form. Ellipsoidal robust reduces to a second-order cone programme. Wasserstein DRO with piecewise linear loss reduces to convex programming; general Wasserstein DRO for non-linear losses uses convex conic reformulation. Machine learning approaches use gradient-based methods for policy or value function optimization. Implementation uses Gurobi and MOSEK for classical/robust/DRO solvers and PyTorch for machine learning implementations.

C Empirical setup

Empirical evaluation uses European equity data from STOXX Europe 600 constituents covering January 2005 through December 2024. Monthly returns are used for parameter estimation and weekly returns for out-of-sample performance evaluation. Rolling window training uses 60-month estimation windows with monthly rebalancing. Transaction costs of 0.10 per cent per turnover are modelled. Constraints include long-only weights (no short selling), maximum single-stock weight of 5 per cent, and full investment (weights sum to 1).

D Performance metrics

Performance metrics include annualized return, annualized volatility, Sharpe ratio, Sortino ratio, maximum drawdown, Calmar ratio, and skewness and kurtosis of realized return distributions. Statistical significance of Sharpe ratio differences is assessed using Jobson-Korkie test with Memmel correction. Turnover and transaction cost impact are quantified. Robustness to specification changes (rebalancing frequency, transaction cost assumptions, universe restrictions) is examined.

Results

A Sharpe ratio comparison

Out-of-sample Sharpe ratios differed substantially across methods. Classical mean-variance without shrinkage achieved Sharpe of 0.31, reflecting substantial estimation error effects. Mean-variance with Ledoit-Wolf shrinkage achieved 0.42. Box robust optimization achieved 0.53. Ellipsoidal robust achieved 0.61. Wasserstein DRO achieved 0.68 with $\epsilon = 0.02$ (calibrated by cross-validation). Machine learning reinforcement learning approach achieved 0.51. The relative ranking of methods was consistent across sub-periods and specification variants, though absolute levels varied.

B Drawdown analysis

Maximum drawdowns exhibited similar patterns. Classical mean-variance experienced 32.7 per cent maximum drawdown during the 2008-2009 financial crisis. Shrinkage reduced this to 27.4 per cent. Box robust reduced to 22.8 per cent. Ellipsoidal robust reduced to 20.1 per cent. Wasserstein DRO reduced to 18.4 per cent. Reinforcement learning achieved 24.3 per cent drawdown. The drawdown reduction of robust and DRO methods reflects their conservative response to parameter uncertainty, particularly in high-uncertainty periods.

C Sub-period analysis

Sub-period analysis revealed distinctive patterns. During 2005-2007 (pre-crisis) all methods achieved reasonable performance with limited differentiation. The 2008-2009 crisis period substantially favoured robust and DRO methods, with drawdown protection dramatically improving their long-term outcomes. The 2010-2019 post-crisis expansion period modestly favoured mean-variance methods with higher expected returns capture. The

2020 COVID shock and 2022 bear market again favoured robust methods with defensive positioning. The 2023-2024 recovery period showed mixed results.

D Sensitivity analysis

Sensitivity analysis addressed several specification choices. Rebalancing frequency (monthly, quarterly, annual) affected transaction cost impact more than gross performance. Transaction cost assumptions (0.05 per cent to 0.20 per cent per turnover) affected relative ranking of high-turnover methods (reinforcement learning particularly affected). Uncertainty set size for robust methods and Wasserstein ball radius for DRO methods showed inverted-U relationships with performance, with intermediate values producing best results. Universe restrictions (STOXX Europe 50 versus 600) affected concentration effects.

Discussion

The empirical findings support the practical value of robust and distributionally robust optimization approaches for portfolio management. The 0.26 Sharpe ratio improvement of Wasserstein DRO over shrinkage-enhanced mean-variance, together with the 43 per cent reduction in maximum drawdown, represents economically significant portfolio improvement. The specific advantages of DRO reflect its principled treatment of distributional uncertainty, particularly valuable during regime transitions and unusual market conditions.

Mathematical elegance and computational tractability of these methods supports their practical deployment. Convex reformulations of robust and DRO problems permit efficient solution using modern commercial and open-source optimization software. Estimation of uncertainty set parameters (box widths, ellipsoid radii, Wasserstein ball radii) can be data-driven through cross-validation. The theoretical guarantees provided by these methods (worst-case optimality within the specified uncertainty sets) supports rigorous portfolio construction.

Machine learning contributions offer distinctive strengths and limitations. Reinforcement learning approaches capture nonlinear patterns and time-varying relationships but require substantial training data and computational resources, and offer weaker theoretical guarantees than classical methods. Neural network approaches to factor discovery can identify structure that classical factor models miss. Integration of machine learning with classical optimization frameworks, using ML for parameter estimation and classical/robust optimization for constrained portfolio selection, produces productive hybrid approaches.

Practical implementation considerations include computational infrastructure (commercial optimization software licences for robust and DRO methods), data quality (accurate historical returns, corporate actions handling, survivor bias avoidance), constraint modelling (regulatory limits, mandate constraints, ESG considerations), and monitoring infrastructure (out-of-sample performance tracking, benchmark comparison). Institutional asset managers should invest in these operational capabilities to fully realize the benefits of advanced portfolio optimization methodology.

Limitations include the European equity focus of the empirical evaluation (with equivalent conclusions requiring validation on other markets and asset classes), the specific implementation choices (with alternative parameterization producing quantitatively similar but not identical results), and the study period (with future periods potentially producing different comparative rankings). Continued empirical evaluation as new data become available supports ongoing methodological assessment.

Detailed mathematical treatment of the Wasserstein distributionally robust portfolio optimization deserves elaboration given its strong empirical performance. The type-1 Wasserstein distance between two distributions P and Q on $\mathbb{R}^n$ is defined as $W_1(P, Q) = \inf_{\pi} \int \|x - y\| \pi(dx, dy)$ where the infimum is over joint distributions π with marginals P and Q . The Wasserstein-ball ambiguity set of radius ε around empirical distribution $\hat{P}_N$ is $B_\varepsilon(\hat{P}_N) = \{P : W_1(P, \hat{P}_N) \leq \varepsilon\}$. Esfahani and Kuhn [12] established that for many convex loss functions, DRO with Wasserstein ambiguity reduces to a convex optimization problem tractable through standard software. The specific application to portfolio optimization with piecewise linear loss (approximating negative log returns) produces a convex programme solvable at scale.

Calibration of the Wasserstein ball radius ε represents a key methodological question. Theoretical results establish rates at which ε should decrease as sample size N grows to preserve statistical guarantees. Practical calibration through cross-validation on out-of-sample performance often produces good empirical results. The empirical finding of best performance at $\varepsilon = 0.02$ in this study reflects the interplay of sample size, return

distribution characteristics, and evaluation criteria. Continued research on principled calibration methods supports the sustained practical deployment of DRO methodology.

Comparison with alternative distributional robustness approaches provides useful context. Moment-based DRO with mean and covariance constraints produces analogous robustness at lower computational cost but with different theoretical guarantees. ϕ -divergence DRO (Kullback-Leibler, χ^2 divergence balls) provides yet another approach with distinctive properties. The relative merits of these approaches depend on application context, computational constraints, and the specific character of the parameter uncertainty concerns being addressed.

Extensions to multi-period portfolio optimization warrant continued development. Single-period optimization ignores the intertemporal opportunities and constraints that characterize real-world portfolio management. Dynamic programming approaches address multi-period problems in principle but face curse of dimensionality challenges. Reinforcement learning approaches provide practical multi-period solutions with learned policy functions. Model predictive control approaches solve rolling optimization problems that capture some multi-period considerations. Continued research at this frontier will support increasingly sophisticated multi-period portfolio management.

Integration with modern factor investing frameworks deserves attention. The value, momentum, quality, low volatility, and other factor investing approaches have become mainstream in institutional asset management. Portfolio optimization within factor-based frameworks combines factor exposures with security-specific residual optimization. Robust and DRO methods can be applied at either the factor exposure or security selection level, with distinctive trade-offs. Integration across levels represents an important practical consideration.

ESG-constrained portfolio optimization has become an increasingly important application. Environmental, social, and governance considerations translate into portfolio construction through exclusion lists, minimum ESG scores, sector weight constraints, and integration with impact measures. Adaptation of the optimization frameworks to ESG constraints preserves the mathematical structure while adding specific application requirements. European asset managers subject to Sustainable Finance Disclosure Regulation and analogous frameworks have particular interest in ESG-integrated portfolio optimization.

Transaction cost modelling within portfolio optimization warrants detailed attention. Fixed cost per trade, proportional cost based on turnover, market impact costs based on order size, and opportunity costs of delayed execution all contribute to realistic transaction cost representations. Integration of transaction costs into the optimization objective produces smoother rebalancing paths and improved after-cost performance. Sophisticated market impact modelling using the Almgren-Chriss framework and its extensions supports institutional-scale implementation.

Regulatory considerations affecting portfolio optimization in Europe include the UCITS directive for retail investment funds, AIFMD for alternative investments, Solvency II for insurance, IORP II for occupational pensions, and MiFID II for investment services. Each framework imposes specific constraints on portfolio construction, risk management, and reporting. Adaptation of portfolio optimization to regulatory requirements preserves the mathematical structure while incorporating specific application constraints.

Educational implications include the need for quantitative asset management personnel skilled across finance, mathematics, statistics, computer science, and applied programming. Spanish and European academic programmes at Universidad Carlos III, Pompeu Fabra, Complutense, and other institutions offer specialized master's programmes in quantitative finance, financial engineering, and computational finance. Professional certification through the CFA Institute, EFFAS, and analogous bodies extends the educational infrastructure. Continued investment in the educational pipeline supports the sustained deployment of sophisticated portfolio optimization methodology.

Software infrastructure for portfolio optimization has matured substantially. Commercial platforms including Axioma, MSCI Barra, and BlackRock Aladdin provide integrated optimization capabilities for institutional users. Open-source libraries including CVXPY (with commercial solvers Gurobi and MOSEK), PyPortfolioOpt, and Riskfolio-lib support academic and boutique implementations. Cloud computing platforms provide scalable computational infrastructure. Continued software ecosystem development supports increasingly sophisticated implementations.

International cooperation among Spanish, European, and international researchers on portfolio optimization contributes to shared advancement. The European Financial Management Association, INFORMS Financial Services Section, and analogous international bodies provide forums for methodological exchange. Cross-institutional research programmes and structured knowledge exchange support continued progress. The three participating institutions (UC3M, UPF, UCM) actively engage in these international networks.

Concluding observations note that portfolio optimization has evolved substantially from Markowitz's original mean-variance framework to encompass rich methodology addressing parameter uncertainty, distributional robustness, and machine learning integration. The empirical evidence assembled in this study supports the practical value of these methodological advances, particularly the distributional robustness provided by Wasserstein DRO. Continued mathematical development, empirical evaluation, and practical deployment will support ongoing improvement in institutional asset management capabilities.

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Conclusion and Future Work

This paper presented a comprehensive mathematical exposition and empirical evaluation of classical, robust, distributionally robust, and machine learning-enhanced approaches to portfolio optimization. Empirical results on European equity markets demonstrate that robust and distributionally robust methods produce substantially improved out-of-sample Sharpe ratios and reduced maximum drawdowns compared to classical mean-variance approaches. Wasserstein DRO produced the strongest overall performance, reflecting its principled treatment of distributional uncertainty. Machine learning approaches achieved intermediate performance. The findings support the practical deployment of modern portfolio optimization methodology for institutional and academic applications. Future work will extend the analysis to multi-asset portfolios, dynamic settings with intertemporal considerations, ESG-constrained optimization, and integration with alternative data sources.

Detailed analysis of the dual formulation of Wasserstein DRO provides mathematical insight. The primal problem $\min_w \max_{\{P \in B_\epsilon(\hat{P}_N)\}} E_P[L(w, X)]$ has a dual reformulation via strong duality (established by Esfahani and Kuhn) that permits efficient solution. For convex piecewise linear loss functions L , the dual becomes a finite-dimensional convex programme. The specific portfolio application uses $L(w, X) = -w'X$ (negative portfolio return) which is convex piecewise linear, admitting tractable dual formulation. Solution via CVXPY with commercial solvers achieves solve times of seconds to minutes for portfolios of hundreds to low thousands of assets.

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