CALIBRATION OF DISTRIBUTIONALLY ROBUST EMPIRICAL OPTIMIZATION MODELS

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Abstract. In this paper, we study the out-of-sample properties of robust empirical optimization and develop a theory for data-driven calibration of the “robustness parameter” for worst-case maximization problems with concave reward functions. Building on the intuition that robust optimization reduces the sensitivity of the expected reward to errors in the model by controlling the spread of the reward distribution, we show that the first-order benefit of “little bit of robustness” is a significant reduction in the variance of the out-of-sample reward while the corresponding impact on the mean is almost an order of magnitude smaller. One implication is that a substantial reduction in the variance of the out-of-sample reward (i.e. sensitivity of the expected reward to model misspecification) is possible at little cost if the robustness parameter is properly calibrated. To this end, we introduce the notion of a robust mean-variance frontier to select the robustness parameter and show that it can be approximated using resampling methods like the bootstrap. Our examples also show that “open loop” calibration methods (e.g. selecting a 90% confidence level regardless of the data and objective function) can lead to solutions that are very conservative out-of-sample.

1. Introduction

Robust optimization is an approach to account for model misspecification in a stochastic optimization problem. Misspecification can occur because of incorrect modeling assumptions or estimation uncertainty, and decisions that are made on the basis of an incorrect model can perform poorly out-of-sample if misspecification is ignored. Distributionally robust optimization (DRO) accounts for misspecification in the in-sample problem by optimizing against worst-case perturbations from the “nominal model”, and has been an active area of research in a number of academic disciplines including Economics, Finance, Electrical Engineering and Operations Research/Management Science.
DRO models are typically parameterized by an “ambiguity parameter” \( \delta \) that controls the size of the deviations from the nominal model in the worst-case problem. The ambiguity parameter may appear as the confidence level of an uncertainty set or a penalty parameter that multiplies some measure of deviation between alternative probability distributions and the nominal in the worst-case objective, and parameterizes a family of robust solutions \( \{x_n(\delta) : \delta \geq 0\} \), where \( \delta = 0 \) is empirical/sample-average optimization (i.e. no robustness) with solutions becoming “increasingly conservative” as \( \delta \) increases. The choice of \( \delta \) clearly determines the out-of-sample performance of the robust solution, and the goal of this paper is to understand this relationship in order to develop a data-driven approach for choosing \( \delta \). (Here, \( n \) denotes the size of the historical data set used to construct the robust optimization problem.)

The problem of calibrating \( \delta \) is analogous to that of the free parameters in various Machine Learning algorithms (e.g. the penalty parameter in LASSO, Ridge regression, SVM, etc). Here, free parameters are commonly tuned by optimizing an estimate of out-of-sample loss (e.g. via cross-validation, bootstrap or some other resampling approach), so it is natural that we consider doing the same for the robust model. The following examples show, however, that this may not be the correct thing to do.

Consider first the problem of robust logistic regression which we apply to the WDBC breast cancer dataset \[34\]. We adopt the “penalty version” of the robust optimization model with relative entropy as the penalty function \[29, 35, 36, 41\] and the robustness parameter/multiplier \( \delta \) being such that \( \delta = 0 \) is empirical optimization (which in this case coincides with the maximum likelihood estimator) with the “amount of robustness” increasing in \( \delta \). A rigorous formulation of the model is given in Section \[3\] Estimates of the out-of-sample expected loss for solutions \( \{x_n(\delta) : \delta \geq 0\} \) of the robust regression problem for different values of the ambiguity parameter \( \delta \) can be generated using the bootstrap and are shown in Figure \[11\] (i).

For this example, the out-of-sample expected log-likelihood (reward) of the robust solution with \( \delta = 0.2 \) outperforms that of the maximum likelihood estimator (the solution of sample average optimization with \( \delta = 0 \)), though the improvement is a modest 1.1%. Similar observations have been made elsewhere (e.g. \[10, 30\]), and one might hope that it is always possible to find a robust solution that generates higher out-of-sample expected reward than empirical optimization, and that there are examples where the improvement is significant. It turns out, however, that this is not the case. In fact, we show that such an improvement cannot in general be guaranteed even when mis-specification is substantial and will also be small if it happens to occur.
Figure 1.1. Simulated mean reward—usual practice for calibration. The figures (i) and (ii) show the average of reward (log-likelihood and utility) of bootstrap samples for robust versions of logistic regression and portfolio selection, respectively. The logistic regression (i) is applied to the WDBC breast cancer data set, which consists of \( n = 569 \) samples and (the first) 10 covariates of the original data set at [34], and the average of the log-likelihood (y-axis) is taken over 25 bootstrap samples, attaining the maximum at \( \delta = 0.2 \). The data set for portfolio selection (ii) consists of \( n = 50 \) (historical) samples of 10 assets and the average of the investor’s utility function values is taken over 50 bootstrap samples, attaining the maximum at \( \delta = 0 \), i.e., non-robust optimizer.

As a case in point, Figure 1.1 (ii) shows the expected out-of-sample utility of solutions of a robust portfolio selection problem is lower than that of empirical optimization (\( \delta = 0 \)) for every level of robustness. This is striking because the nominal joint distribution of monthly returns for the 10 assets in this example was constructed non-empirically using only 50 monthly data points, so model uncertainty is large by design and one would hope that accounting for misspecification in this example would lead to a significant improvement in the out-of-sample expected reward.

In summary, the logistic regression example shows that it may be possible for DRO to produce a solution that out-performs empirical optimization in terms of the out-of-sample expected reward. However, this improvement is small and cannot be guaranteed even when model uncertainty is substantial (as shown by the portfolio choice example). While the underwhelming performance of DRO in both examples might raise concerns about its utility relative to empirical optimization, it may also be the case that robust optimization is actually doing well, but requires an interpretation of out-of-sample performance that goes beyond expected reward in order to be appreciated. Should this be the case, the practical implication is that \( \delta \) should be calibrated using considerations in addition to the expected reward.
With this in mind, suppose that we expand our view of out-of-sample performance to include not just the expected reward but also its variance. Intuitively, robust decision making should be closely related to controlling the variance of the reward because the expected value of a reward distribution with a large spread will be sensitive to misspecification errors that affect its tail. In other words, calibrating the in-sample DRO problem so that the resulting solution has a reasonable expected reward while also being robust to misspecification boils down to making an appropriate trade-off between the mean and the variance of the reward, and it makes sense to account for both these quantities when selecting the robustness parameter $\delta$. This relationship between DRO and mean-variance optimization is formalized in [25] and discussed in Section 3, while a closely related result on the relationship between DRO and empirical optimization with the standard deviation of the reward as a regularizer is studied in [17, 33]. We note, however, that none of these papers study the impact of robustness on the distribution of the out-of-sample reward nor the implications for calibration.

![Bootstrap robust mean-variance frontiers of the two examples.](image)

**Figure 1.2.** Bootstrap robust mean-variance frontiers of the two examples. The above plots show the relation between the mean and the variance of the simulated reward through bootstrap. In contrast with Fig.1.1, the two examples show similar curves, implying larger variance reduction and limited improvement of mean. As will be shown, these properties are generic.

Figure 1.2 shows the mean and variance of the out-of-sample reward for our two examples for different values of $\delta$. A striking feature of both frontier plots is that the change in the (estimated) out-of-sample mean reward is small relative to that of the variance when $\delta$ is small. For example, while $\delta = 0.2$ optimizes the out-of-sample log-likelihood (expected reward) for the logistic regression problem, an improvement of about 1.1% when compared to the maximum likelihood estimator and reduces the variance by about 33.0%, $\delta = 0.4$ has about the same log-likelihood as maximum
likelihood with almost 40% variance reduction. In the case of portfolio choice, \( \delta = 3 \) reduces the (estimated) out-of-sample variance by 42% at the cost of only 0.07% expected utility.

More generally, while substantial out-of-sample variance reduction is observed in both examples, we show that this is a generic property of DRO with concave rewards. We also show that variance reduction is almost an order of magnitude larger than the change in the expected reward when \( \delta \) is small (indeed, as we have seen, expected reward can sometimes improve), so the frontier plots in Figure 1.2 are representative of those for all DRO problems with concave rewards. This suggest, as we have illustrated, that the robustness parameter should be calibrated by trading off between the mean and variance of the out-of-sample reward, and not just by optimizing the mean alone, and that substantial variance reduction can be had at very little cost.

Our contributions can be summarized as follows:

1. We characterize the distributional properties of robust solutions and show that for small values of \( \delta \), the reduction in the variance of the out-of-sample reward is (almost) an order of magnitude greater than the loss in expected reward;
2. We show that Jensen’s inequality can be used to explain why the expected reward associated with robust optimization sometimes exceeds that of empirical optimization and provide conditions when this occurs. We also show that this “Jensen effect” is relatively small and disappears as the number of data points \( n \to \infty \);
3. We introduce methods of calibrating \( \delta \) using estimates of the out-of-sample mean and variance of the reward using resampling methods like the bootstrap.

While free parameters in many Machine Learning algorithms are commonly tuned by optimizing estimates of out-of-sample expected reward, DRO reduces sensitivity of solutions to model misspecification by controlling the variance of the reward. Both the mean and variance of the out-of-sample reward should be accounted for when calibrating \( \delta \).

Our results say nothing about large \( \delta \) though our experiments suggest that the benefits of DRO are diminishing as \( \delta \) increases (i.e. increasingly fast loss in expected reward and the rate of variance reduction rate going to zero), so the solutions associated with a robustness parameter that is too large may be “overly pessimistic”.
2. Literature Review

Decision making with model ambiguity is of interest in a number of fields including Economics, Finance, Control Systems, and Operations Research/Management Science. Notable contributions in Economics include the early work of Knight [32] and Ellsberg [19], Gilboa and Schmeidler [24], Epstein and Wang [20], Hansen and Sargent [26], Klibanoff, Marinacci and Mukerji [31], Bergemann and Morris [6], Bergemann and Schlag [7], and the monograph by Hansen and Sargent [27], while papers in finance include Garlappi, Uppal and Wang [23], Liu, Pan and Wang [38], Maenhout [39], and Uppal and Wang [43]. In particular, solutions of the Markowitz portfolio choice model are notoriously sensitive to small changes in the data and robust optimization has been studied as an approach to addressing this issue [21, 23, 37, 43].

The literature on robust control is large and includes Jacobson [29], Doyle, Glover, Khargonekar and Francis [15], and Petersen, James and Dupuis [41], whose models have been adopted in the Economics literature [27], while early papers in Operations Research and Management Science include Ben-Tal and Nemirovski [4], El Ghaoui and Lebret [13], Bertsimas and Sim [11], and more recently Ben-Tal, den Hertog, Waegenaere and Melenberg [3], Delage and Ye [14] (see also Lim, Shanthikumar and Shen [36] for a survey and the recent monograph Ben-Tal, El Ghaoui and Nemirovski [5]).

Calibration methods in robust optimization. We briefly summarize calibration methods that have been suggested in the robust optimization literature.

High confidence uncertainty sets. One approach that is proposed in a number of papers advocates the use of uncertainty sets that include the true data generating model with high probability, where the confidence level (typically 90%, 95%, or 99%) is a primitive of the model [3, 9, 14, 17, 33]. This has been refined by [8] who develop methods for finding the smallest uncertainty set that guarantee the desired confidence level, but the confidence level itself remains a primitive. One concern with this approach is that it is “open loop” in that confidence levels are chosen independent of the data and the objective function, but there is no reason, as far as we are aware, to expect that these particular confidence levels have anything to do with good out-of-sample performance. In the portfolio example we discuss (see Section 8.2), solutions associated with these traditional confidence levels lie at the conservative end of the performance-robustness frontier.

Optimizing estimates of out-of-sample expected reward by resampling. Here, the robustness parameter $\delta$ is chosen to optimize an estimate of out-of-sample expected reward that is generated through
a resampling procedure (bootstrap, cross-validation), extending the methods used to calibrate regularized regression models in Machine Learning [28]. While different from the previous approach in that confidence levels now depend on the data and the objective function (it is no longer “open loop”), this approach ignores variability reduction which, as we will show, plays a central role in the effectiveness of robust optimization. While this can produce a robust solution, for some examples, that out-performs empirical optimization in terms of out-of-sample expected reward (e.g. the logistic regression example with $\delta = 0.2$, and the robust bandit application in [30]), this is not guaranteed. For example, it leads to the choice of $\delta = 0$ in the portfolio selection example which is just the empirical solution and comes with no robustness benefits. Moreover, there are larger values of the robustness parameter than 0.2 in the logistic regression example that further reduce out-of-sample variance with negligible impact on the expected reward. In contrast to the “high-confidence” approach where classical confidence levels of 90%, 95%, or 99% produce overly conservative solutions in the portfolio choice example, this approach produces a solution that is insufficiently robust.

*Satisficing approach.* This is an in-sample approach where the decision maker specifies a target level $T$ and finds the “most robust” decision that achieves this target in the worst case [12]. That is, he/she chooses the largest robustness parameter $\delta$ under which the worst-case expected reward exceeds the target $T$. In the satisficing approach, the target $T$ is a primitive of the problem and the confidence level $\delta$ is optimized. This is opposite to the “high confidence” approach where the confidence level is a model primitive and the worst case expected performance is optimized.

**Other related literature.** Several recent papers discuss DRO from the perspective of regularizing empirical optimization with the variance, including [17], [25] and [33]. The paper [17] provides confidence intervals for the optimal objective value and shows consistency of solutions using Owen’s empirical likelihood theory, while [33] studies the sensitivity of estimates of the expected value of random variables to worst-case perturbations of a simulation model. The paper [25] studies the connection between robust optimization and variance regularization by developing an expansion of the robust objective, which we discuss in Section 3, but is an in-sample analysis. We also note the paper [44] which studies the asymptotic properties of stochastic optimization problems with risk-sensitive objectives.

Also related is [16] which develops finite sample probabilistic guarantees for the out-of-sample expected reward generated by robust solutions. Compared to our paper, one important difference is that the focus of [16] is the out-of-sample expected reward whereas ours is on the variance
reduction properties of DRO and the implications for calibration, neither of which is discussed in [16]. We also note that while the probabilistic guarantees in [16] formalize the relationship between data size, model complexity, robustness, and out-of-sample expected reward, these results as with others of this nature depend on quantities that are difficult to compute (e.g. the covering number or the VC Dimension), require a bounded objective function, and come with the usual concerns that performance bounds of this nature are loose [1]. Note too that [16] is a finite sample analysis whereas ours is asymptotic (large sample size), though calibration experiments for small data sets produce results that are consistent with our large sample theory.

3. Robust empirical optimization

Suppose we have historical data $Y_1, \ldots, Y_n$ generated i.i.d. from some population distribution $P$. Assume $f(x, Y)$ is strictly jointly concave and sufficiently smooth in the decision variable $x \in \mathbb{R}^m$ as required in all subsequent analysis. Let $P_n$ denote the empirical distribution associated with $Y_1, \ldots, Y_n$ and

$$x_n(0) = \arg \max_x \left\{ \mathbb{E}_{P_n} [f(x, Y)] = \frac{1}{n} \sum_{i=1}^n f(x, Y_i) \right\} \quad (3.1)$$

be the solution of the empirical optimization problem. Let $\delta > 0$ be a positive constant and

$$x_n(\delta) = \arg \max_x \min_{Q} \left\{ \mathbb{E}_Q [f(x, Y)] + \frac{1}{\delta} \mathcal{H}_{\phi}(Q | P_n) \right\} \quad (3.2)$$

be the solution of the robust empirical optimization problem where

$$\mathcal{H}_{\phi}(Q | P_n) := \begin{cases} \sum_{i:p_i^n > 0} p_i^n \phi \left( \frac{q_i}{p_i^n} \right), & \sum_{i:p_i^n > 0} q_i = 1, q_i \geq 0, \\
+\infty, & \text{otherwise}, \end{cases} \quad (3.3)$$

is the $\phi$-divergence of $Q = [q_1, \ldots, q_n]$ relative to $P_n = [p_1^n, \ldots, p_n^n]$. As is standard, we assume that $\phi$ is a convex function satisfying

$$\text{dom } \phi \subset [0, \infty), \quad \phi(1) = 0, \quad \phi'(1) = 0, \quad \text{and } \phi''(1) > 0. \quad (3.4)$$

The constant $\delta$ can be interpreted as the “amount of robustness” in the robust model (3.2). The robust problem coincides with the empirical model when $\delta = 0$, and delivers “more conservative” solutions as $\delta$ increases.

It is shown in [25] that if $\phi(z)$ is sufficiently smooth, then solving the robust optimization problem (3.2) is almost the same as solving an empirical mean-variance problem. Specifically, if $\phi$ is also
twice continuously differentiable, then
\[
\min_Q \left\{ \mathbb{E}_Q[f(x, Y)] + \frac{1}{\delta} \mathcal{H}_\phi(Q \mid \mathbb{P}_n) \right\} = \mathbb{E}_{\mathbb{P}_n}[f(x, Y)] - \frac{\delta}{2\phi''(1)} \nu_{\mathbb{P}_n}[f(x, Y)] + o(\delta), \tag{3.5}
\]
where
\[
\nu_{\mathbb{P}_n}[f(x, Y)] := \frac{1}{n} \sum_{i=1}^{n} \left( f(x, Y_i) - \mathbb{E}_{\mathbb{P}_n}[f(x, Y_i)] \right)^2
\]
is the variance of the reward under the empirical distribution.

The expansion (3.5) shows that DRO is closely related to mean-variance optimization. Intuitively, a decision is sensitive to model misspecification if smaller errors in the model have a big impact on the expected reward, which can happen if the reward distribution (in-sample) has a large spread and model errors affect its tail. To protect against this, it makes sense to reduce this spread, which is exactly what robust optimization is doing in (3.5). It is also shown in [25] that the higher order terms in the expansion (3.5) are the skewness and a generalized notion of the kurtosis of the reward distribution. Robust optimization also controls these elements of the reward distribution but they are less important than the mean and variance when the robustness parameter is small.

Robust optimization (3.2) defines a family of policies \( \{x_n(\delta), \delta \geq 0\} \) with “robustness” increasing in \( \delta \), and our eventual goal is to identify values of the parameter \( \delta \) such that the corresponding solution \( x_n(\delta) \) performs well out-of-sample. While it is common practice to select \( \delta \) by optimizing some estimate of the out-of-sample expected reward (e.g. via the bootstrap or cross-validation), the characterization (3.5) suggests that estimates of the mean and variance of the out-of-sample reward should be used to select \( \delta \). Much of this paper is concerned with making this intuition rigorous, a big part of which is characterizing the impact of robustness on the mean and the variance.

The dual characterization of \( \phi \)-divergence implies that the worst-case objective
\[
\min_Q \left\{ \mathbb{E}_Q[f(x, Y)] + \frac{1}{\delta} \mathcal{H}_\phi(Q \mid \mathbb{P}_n) \right\} = -\min_c \left\{ c + \frac{1}{\delta} \mathbb{E}_{\mathbb{P}_n}[\phi^*(\delta(-f(x, Y) - c))] \right\},
\]
where
\[
\phi^*(\zeta) := \sup_z \{ z\zeta - \phi(z) \}
\]
is the convex conjugate of \( \phi(z) \), so the robust solution (3.2) can be obtained by solving
\[
(x_n(\delta), c_n(\delta)) = \arg \min_{x, c} \left\{ c + \frac{1}{\delta} \mathbb{E}_{\mathbb{P}_n}[\phi^*(\delta(-f(x, Y) - c))] \right\}. \tag{3.6}
\]
This will be used to characterize the distributional properties of the robust solution.
4. Statistics of robust solutions

The results in Section 3 highlight the close relationship between robust optimization and controlling the spread of the reward distribution. We now study the statistical properties of the robust solution \((x_n(\delta), c_n(\delta))\), which will be used to study properties of the out-of-sample reward that form the basis of our calibration procedure.

4.1. Consistency.

Let
\[
x^*(0) = \arg\max_x \left\{ \mathbb{E}_P[f(x, Y)] \right\},
\]
\[
(x^*(\delta), c^*(\delta)) = \arg\min_{x, c} \left\{ c + \frac{1}{\delta} \mathbb{E}_P[\phi^*\left(\delta(-f(x, Y) - c)\right)] \right\}
\]

(4.1) (4.2)

denote the solutions of the nominal and robust optimization problems under the data generating model \(P\). Note that \(x^*(\delta)\) also solves the robust optimization problem under the data generating model \(P\).

Observe that (3.6) is a standard empirical optimization so it follows from Theorem 5.4 in [42] that \(x_n(0)\) and \((x_n(\delta), c_n(\delta))\) are consistent.

**Proposition 4.1.** \(x_n(0) \xrightarrow{P} x^*(0)\) and \((x_n(\delta), c_n(\delta)) \xrightarrow{P} (x^*(\delta), c^*(\delta))\).

**Proof.** Let
\[
g(x, c, Y) := c + \frac{1}{\delta} \phi^*\left(\delta(-f(x, Y) - c)\right).
\]

We can write the objective functions in (3.6) and (4.2) as
\[
G_n(x, c) := \mathbb{E}_{P_n}[g(x, c, Y)],
\]
\[
G(x, c) := \mathbb{E}_{P}[g(x, c, Y)].
\]

Since \(\phi^*(\xi)\) is convex and non-decreasing in \(\xi\) and \(\delta(-f(x, Y) - c)\) is jointly convex in \((x, c)\) for \(P\)-a.e. \(Y\), \(g(x, c, Y)\) is jointly convex in \((x, c)\). It now follows from Theorem 5.4 in [42] that \((x_n(\delta), c_n(\delta)) \xrightarrow{P} (x^*(\delta), c^*(\delta))\). Consistency of \(x_n(0)\) also follows from Theorem 5.4 in [42]. \(\square\)

4.2. Asymptotic normality.
4.2.1. *Empirical optimization.* Consider first the case of empirical optimization. The following result follows from Theorem A.1 in the Appendix.

**Proposition 4.2.** Let $x^*(0)$ be the solution of the optimization problem (4.1). Then the solution $x_n(0)$ of the empirical optimization problem (3.1) is asymptotically normal

$$
\sqrt{n} \left( x_n(0) - x^*(0) \right) \xrightarrow{D} N \left( 0, \xi(0) \right), \ n \to \infty,
$$

where

$$
\xi(0) = \mathbb{V}_P \left[ \mathbb{E}_P \left[ \nabla_x^2 f(x^*(0), Y) \right]^{-1} \nabla_x f(x^*(0), Y) \right].
$$

4.2.2. *Robust optimization.* We consider now the asymptotic distribution of the solution $(x_n(\delta), c_n(\delta))$ of the robust optimization problem (3.6). For every $n$, $(x_n(\delta), c_n(\delta))$ is characterized by the first order conditions

$$
\begin{align*}
\mathbb{E}_{P_n} \left[ (\phi^*)' \left( - \delta (f(x, Y) + c) \right) \nabla_x f(x, Y) \right] &= \frac{1}{n} \sum_{i=1}^{n} \left( (\phi^*)' \left( - \delta (f(x, Y_i) + c) \right) \nabla_x f(x, Y_i) \right) = 0, \\
\mathbb{E}_{P_n} \left[ (\phi^*)' \left( - \delta (f(x, Y) + c) \right) - 1 \right] &= \frac{1}{n} \sum_{i=1}^{n} \left( (\phi^*)' \left( - \delta (f(x, Y_i) + c) \right) - 1 \right) = 0.
\end{align*}
$$

(4.3)

Equivalently, if we define the vector-valued function $\psi : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^{n+1}$ where

$$
\psi(x, c) := \begin{bmatrix}
(\phi^*)' \left( - \delta (f(x, Y) + c) \right) \nabla_x f(x, Y) \\
- \frac{\phi^{(2)}(1)}{\delta} \left( (\phi^*)' \left( - \delta (f(x, Y) + c) \right) - 1 \right)
\end{bmatrix},
$$

(4.4)

then the first order conditions (4.3) can be written as $\mathbb{E}_{P_n} [\psi(x, c)] = 0$. Let $(x^*(\delta), c^*(\delta))$ denote the solution of the robust optimization problem (4.2) under the data generating model $\mathbb{P}$, which is characterized by the first order conditions

$$
\mathbb{E}_P [\psi(x, c)] = \begin{bmatrix}
\mathbb{E}_P \left[ (\phi^*)' \left( - \delta (f(x, Y) + c) \right) \nabla_x f(x, Y) \right] \\
\mathbb{E}_P \left[ - \frac{\phi^{(2)}(1)}{\delta} \left( (\phi^*)' \left( - \delta (f(x, Y) + c) \right) - 1 \right) \right]
\end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.
$$

(4.5)

Asymptotic normality of $(x_n(\delta), c_n(\delta))$ follows from consistency (Proposition 4.1) and Theorem A.1.

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1We have added a scaling constant $- \frac{\phi^{(2)}(1)}{\delta}$ in the second equation. Note that this constant does not affect the solution of the first order conditions, but does make subsequent analysis more convenient.
Proposition 4.3. Let \((x_n(\delta), c_n(\delta))\) solve the robust empirical optimization problem (3.6) and \((x^*(\delta), c^*(\delta))\) solve the robust problem (4.2) under the data generating model \(\mathbb{P}\). Define

\[
A := \mathbb{E}_{\mathbb{P}}[-J_\psi(x^*(\delta), c^*(\delta))] \in \mathbb{R}^{(m+1) \times (m+1)},
\]

\[
B := \mathbb{E}_{\mathbb{P}}[\psi(x^*(\delta), c^*(\delta)) \psi(x^*(\delta), c^*(\delta))'] \in \mathbb{R}^{(m+1) \times (m+1)},
\]

where \(\psi(x, c)\) is given by (4.4) and \(J_\psi\) denotes the Jacobian matrix of \(\psi\), and

\[
V(\delta) := A^{-1}BA^{-1}' \in \mathbb{R}^{(m+1) \times (m+1)}.
\]

Then \((x_n(\delta), c_n(\delta))\) is jointly asymptotically normal where

\[
\sqrt{n} \begin{bmatrix}
x_n(\delta) - x^*(\delta) \\
c_n(\delta) - c^*(\delta)
\end{bmatrix} \xrightarrow{D} N(0, V(\delta)),
\]

as \(n \to \infty\).

We obtain further insight into the structure of the asymptotic distribution of \((x_n(\delta), c_n(\delta))\) by expanding the limiting mean \((x^*(\delta), c^*(\delta))\) and covariance matrix \(V(\delta)\) in terms of \(\delta\). Specifically, if we define \(\xi(\delta) \in \mathbb{R}^{m \times m}, \eta(\delta) \in \mathbb{R}\) and \(\kappa(\delta) \in \mathbb{R}^{m \times 1}\) as the entries of the matrix

\[
V(\delta) \equiv \begin{bmatrix}
\xi(\delta) & \kappa(\delta) \\
\kappa(\delta)' & \eta(\delta)
\end{bmatrix} = A^{-1}BA^{-1}',
\]

associated with the asymptotic covariance matrix of \((x_n(\delta), c_n(\delta))\) then we have the following.

Theorem 4.4. The solution \((x_n(\delta), c_n(\delta))\) of the robust problem (3.6) is jointly asymptotically normal with

\[
\sqrt{n} \left( x_n(\delta) - x^*(\delta) \right) \xrightarrow{D} N(0, \xi(\delta)),
\]

\[
\sqrt{n} \left( c_n(\delta) - c^*(\delta) \right) \xrightarrow{D} N(0, \eta(\delta)),
\]

\[
n \text{Cov}_{\mathbb{P}}[x_n(\delta), c_n(\delta)] \xrightarrow{} \kappa(\delta),
\]

as \(n \to \infty\). Furthermore, we can write

\[
x^*(\delta) = x^*(0) + \pi \delta + o(\delta),
\]

\[
c^*(\delta) = -\mathbb{E}_{\mathbb{P}}[f(x^*(0), Y)] - \delta \frac{\phi_1(1)}{2} \mathbb{V}_{\mathbb{P}}[f(x^*(0), Y)] + o(\delta),
\]
where
\[ \pi := \frac{1}{\phi''(1)} \left( \mathbb{E}_P[\nabla_x^2 f(x^*(0), Y)] \right)^{-1} \text{Cov}_P[\nabla_x f(x^*(0), Y), f(x^*(0), Y)] \]  
(4.6)

and
\[ V(\delta) = \begin{bmatrix} \xi(\delta) & \kappa(\delta) \\ \kappa'(\delta) & \eta(\delta) \end{bmatrix} = \begin{bmatrix} \xi(0) & \kappa(0) \\ \kappa'(0) & \eta(0) \end{bmatrix} + O(\delta), \]

with
\[ \xi(0) = \mathbb{V}_P \left( \mathbb{E}_P[\nabla_x^2 f(x^*(0), Y)] \right)^{-1} \nabla_x f(x^*(0), Y), \]
\[ \eta(0) = \mathbb{V}_P[f(x^*(0), Y)], \]
\[ \kappa(0) = \left( \mathbb{E}_P[\nabla_x^2 f(x^*(0), Y)] \right)^{-1} \text{Cov}_P[\nabla_x f(x^*(0), Y), f(x^*(0), Y)]. \]

**Proof.** The first part of the Theorem follows immediately from Proposition 4.3. To derive the expansions for \( \pi(\delta) \) and \( c^*(\delta) \), note firstly that
\[ \phi^*(\zeta) = \zeta + \frac{\alpha_2}{2!} \zeta^2 + \frac{\alpha_3}{3!} \zeta^3 + o(\zeta^3), \]  
(4.7)

where
\[ \alpha_2 = \frac{1}{\phi''(1)}, \quad \alpha_3 = -\frac{\phi^{(3)}(1)}{[\phi''(1)]^3}. \]

It follows that
\[ (\phi^*)'(\zeta) = 1 + \alpha_2 \zeta + \frac{\alpha_3}{2!} \zeta^2 + o(\zeta^2), \]

so the first order conditions for the optimization problem (4.6) are
\[ \mathbb{E}_P \left[ (\phi^*)' \left( -\delta (f(x, Y) + c) \right) \nabla_x f(x, Y) \right] = \mathbb{E}_P \left[ \left( 1 - \frac{\delta}{\phi^{(2)}(1)} (f(x, Y) + c) \right) \nabla_x f(x, Y) \right] = 0, \]  
(4.8)
\[ \mathbb{E}_P \left[ \frac{\phi^{(2)}(1)}{\delta} \left( 1 - (\phi^*)' \left( -\delta (f(x, Y) + c) \right) \right) \right] = \mathbb{E}_P \left[ f(x, Y) + c - \frac{\alpha_3 \delta}{2! \alpha_2} (f(x, Y) + c)^2 + o(\delta) \right] = 0. \]  
(4.9)

Let \( x \) be arbitrary and \( c(x) \) denote the solution of (4.9). Writing
\[ c(x) = c_0(x) + c_1(x) \delta + o(\delta) \]
and substituting into (4.9) gives
\[ E_P \left[ \left( f(x, Y) + c_0 \right) + \delta \left\{ c_1 - \frac{\alpha_3}{2! \alpha_2} \left( f(x, Y) + c_0 \right)^2 \right\} + o(\delta) \right] = 0. \]

It now follows that
\[ c_0(x) = -E_P[f(x, Y)], \quad c_1(x) = -\frac{1}{2} \frac{\phi(3)(1)}{[\phi(2)(1)]^2} V_P[f(x, Y)]. \]

Similarly, we can write
\[ x^*(\delta) = x^*(0) + \pi \delta + o(\delta). \]

To compute \( \pi \), we substitute into (4.8) which gives
\[ E_P \left[ \nabla_x f(x^*(\delta), Y) - \frac{\delta}{\phi(2)(1)} \left( f(x^*(\delta), Y) + c(x^*(\delta)) \right) \nabla_x f(x^*(\delta), Y) \right] \]
\[ = E_P \left[ \nabla_x f(x^*(0), Y) + \delta \nabla_x^2 f(x^*(0), Y) \pi + o(\delta) \right] \]
\[ - \frac{\delta}{\phi(2)(1)} E_P \left[ \nabla_x f(x^*(0), Y) \left( f(x^*(0), Y) - E_P[f(x^*(0), Y)] \right) \right] + o(\delta) \]
\[ = \delta \left\{ E_P \left[ \nabla_x^2 f(x^*(0), Y) \right] \pi - \frac{1}{\phi(2)(1)} \text{Cov}_P \left[ f(x^*(0), Y), \nabla_x f(x^*(0), Y) \right] \right\} \]
\[ = 0, \]

where the first equality follows from
\[ c(x^*(\delta)) = -E_P[f(x^*(\delta), Y)] - \frac{\delta}{2} \frac{\phi(3)(1)}{[\phi(2)(1)]^2} V_P[f(x^*(\delta), Y)] + o(\delta) \]
\[ = -E_P[f(x^*(0), Y)] - \frac{\delta}{2} \frac{\phi(3)(1)}{[\phi(2)(1)]^2} V_P[f(x^*(0), Y)] + o(\delta), \quad (4.10) \]

(note that \( E_P[\nabla_x f(x^*(0), Y)] = 0 \)). We can now solve for \( \pi \) which gives (4.6) while (4.10) gives the expression for \( c_1 \).

To obtain the expression for \( V(\delta) \) observe from (4.7) that we can write (4.4) as
\[
\psi(x, c) = \begin{bmatrix}
\nabla_x f(x, Y) - \frac{\delta}{\phi(2)(1)} \left( f(x, Y) + c \right) \nabla_x f(x, Y) + o(\delta)

f(x, Y) + c + O(\delta)
\end{bmatrix}
\equiv \begin{bmatrix}
\psi_1(x, c) \\
\psi_2(x, c)
\end{bmatrix}.
\]
This implies that $J_\psi$, the Jacobian matrix of $\psi(x, c)$, has

$$
\begin{bmatrix}
\nabla_{x_1} \psi_1 & \cdots & \nabla_{x_m} \psi_1 \\
\nabla_{x_2} \psi_2 & \cdots & \nabla_{x_m} \psi_2 \\
\nabla_{c_1} \psi_1 & & \nabla_{c_1} \psi_2 \\
\end{bmatrix}
$$

and hence

$$
A = E_P [-J_\psi(x^*(\delta), c^*(\delta))] = \begin{bmatrix} -E_P[\nabla^2_x f(x^*(0), Y)] & 0 \\
0 & -1 \end{bmatrix} + O(\delta),
$$

so

$$
A^{-1} = - \begin{bmatrix} E_P[\nabla^2_x f(x^*(0), Y)]^{-1} & 0 \\
0 & 1 \end{bmatrix} + O(\delta) = A^{-1}'.
$$

Likewise

$$
\psi(x^*(\delta), c^*(\delta)) = \begin{bmatrix} \nabla_x f(x^*(0), Y) \\
f(x^*(0), Y) - E_P[f(x^*(0), Y)] \end{bmatrix} + O(\delta),
$$

so

$$
B = E_P[\psi(x^*(\delta), c^*(\delta)) \psi(x^*(\delta), c^*(\delta))']
\begin{bmatrix}
\nabla_P[\nabla_x f(x^*(0), Y)] & \text{Cov}_P[\nabla_x f(x^*(0), Y), f(x^*(0), Y)] \\
\text{Cov}_P[\nabla_x f(x^*(0), Y), f(x^*(0), Y)]' & \nabla_P[f(x^*(0), Y)] \end{bmatrix} + O(\delta).
$$

The expression for $V(\delta) = A^{-1} B (A^{-1})'$ now follows. \qed

Theorem 4.3 shows (asymptotically) that robust optimization adds a bias $\pi$ to the empirical solution where the magnitude of the bias is determined by the robustness parameter $\delta$. It can be shown that the direction of the bias $\pi$ optimizes a trade-off between the loss of expected reward and the reduction in variance:

$$
\pi = \arg \max_{\pi} \left\{ \frac{\delta^2}{2} \left| \pi' E_P \left[ \nabla^2_x f(x^*(0), Y) \right] \pi - \frac{1}{\phi(2)(1)} \pi' \text{Cov}_P[f(x^*(0), Y), \nabla_x f(x^*(0), Y)] \right| \right\} 
\begin{align*}
&\equiv E_P[f(x^*(0) + \delta \pi, Y)] - E_P[f(x^*(0), Y)] \\
&- \frac{\delta}{2\phi(2)(1)} \left( \nabla_P[f(x^*(0) + \delta \pi, Y)] - \nabla_P[f(x^*(0), Y)] \right) + o(\delta^2). 
\end{align*}
$$

5. **Out of sample performance: Empirical optimization**

5.1. **Preliminaries.** Let $D = \{Y_1, \cdots, Y_n\}$ be data generated i.i.d. under $P$, $x_n(0)$ be the solution of the empirical optimization problem (5.1) constructed using $D$, and $Y_{n+1}$ be an additional sample
generated under $\mathbb{P}$ independent of the original sample. Theorem A.1 and Proposition 4.2 imply

$$x_n(0) = x^*(0) + \frac{\sqrt{\xi(0)}}{\sqrt{n}} Z + oP\left(\frac{1}{\sqrt{n}}\right),$$

(5.1)

where $\sqrt{\xi(0)}$ is an $m \times m$ matrix such that $\sqrt{\xi(0)}\sqrt{\xi(0)'} = \xi(0)$ and $Z$ is an $m$-dimensional standard normal random vector. In particular, $x_n(0)$ deviates from $x^*(0)$ because of data variability which is captured by the term involving $Z$. Note that $Z$ depends only on the data $D$ used to construct the in-sample problems and is therefore independent of $Y_{n+1}$. We study out-of-sample performance of $x_n(0)$ by evaluating the mean and variance of the reward $f(x_n(\delta), Y_{n+1})$ over random samples of the data $D$ and $Y_{n+1}$.

The following result is helpful. The proof can be found in the Appendix.

**Proposition 5.1.** Let $Y_1, \ldots, Y_n, Y_{n+1}$ be independently generated from the distribution $\mathbb{P}$. Let $x$ be constant and $\Delta \in \sigma\{Y_1, \ldots, Y_n\}$. Then for any constant $\delta$

$$\mathbb{E}_\mathbb{P}[f(x + \delta \Delta, Y_{n+1})]$$

(5.2)

$$= \mathbb{E}_\mathbb{P}[f(x, Y_{n+1})] + \delta \mathbb{E}_\mathbb{P}[\Delta'] \mathbb{E}_\mathbb{P}[\nabla_x f(x, Y_{n+1})] + \frac{\delta^2}{2} \text{tr}\left(\mathbb{E}_\mathbb{P}[\Delta\Delta'] \mathbb{E}_\mathbb{P}[\nabla_x^2 f(x, Y_{n+1})]\right) + o(\delta^2),$$

$$\mathbb{V}_\mathbb{P}[f(x + \delta \Delta, Y_{n+1})]$$

(5.3)

$$= \mathbb{V}_\mathbb{P}[f(x, Y_{n+1})] + \delta \mathbb{V}_\mathbb{P}[\Delta'] \nabla_x \mathbb{V}_\mathbb{P}[f(x, Y_{n+1})]$$

$$+ \frac{\delta^2}{2} \text{tr}\left(\mathbb{E}_\mathbb{P}[\Delta\Delta'] \nabla_x^2 \mathbb{V}_\mathbb{P}[f(x, Y_{n+1})] + 2 \mathbb{V}_\mathbb{P}[\Delta] \mathbb{E}_\mathbb{P}[\nabla_x f(x, Y_{n+1})] \mathbb{E}_\mathbb{P}[\nabla_x f(x, Y_{n+1})']\right) + o(\delta^2),$$

where the first and second derivatives of the variance of the reward with respect to decision $x$ satisfy

$$\nabla_x \mathbb{V}_\mathbb{P}[f(x, Y_{n+1})] = 2 \text{Cov}_\mathbb{P}[f(x, Y_{n+1}), \nabla_x f(x, Y_{n+1})],$$

(5.4)

$$\nabla_x^2 \mathbb{V}_\mathbb{P}[f(x, Y_{n+1})] = 2 \mathbb{V}_\mathbb{P}[\nabla_x f(x, Y_{n+1})] + 2 \text{Cov}_\mathbb{P}[f(x, Y_{n+1}), \nabla_x^2 f(x, Y_{n+1})].$$

(5.5)

5.2. **Empirical optimization.** We now derive an expansion of the out-of-sample expected reward and variance under the empirical optimal solution, which will serve as a baseline case when studying the out-of-sample performance of robust optimization.

**Proposition 5.2.**

$$\mathbb{E}_\mathbb{P}[f(x_n(0), Y_{n+1})] = \mathbb{E}_\mathbb{P}[f(x^*(0), Y_{n+1})] + \frac{1}{2n} \text{tr}\left(\xi(0) \mathbb{E}_\mathbb{P}[\nabla_x^2 f(x^*(0), Y_{n+1})]\right) + o\left(\frac{1}{n}\right),$$

(5.6)
\[ \mathbb{V}_P[f(x_n(0), Y_{n+1})] = \mathbb{V}_P[f(x^*(0), Y_{n+1})] + \frac{1}{2n} \text{tr} \left( \xi(0) \nabla^2_x \mathbb{V}_P[f(x^*(0), Y_{n+1})] \right) + o\left(\frac{1}{n}\right). \]  \hspace{1cm} (5.7)

where \( \nabla^2_x \mathbb{V}_P[f(x^*(0), Y_{n+1})] \) is defined in (5.5).

Proposition 5.2 shows that the expected reward under the empirical solution \( x_n(0) \) equals the optimal expected reward under the data generating model and a loss due to the variability of the empirical solution around \( x^*(0) \) (the “gap” in Jensen’s inequality). Likewise, the variance of the out-of-sample reward has a contribution from the variability of the new sample \( Y_{n+1} \) and a contribution from the variability of the empirical solution. The terms related to the variability \( \xi(0) \) of the empirical solution are scaled by the number of data points and disappear as \( n \to \infty \).

**Proof.** We know from Theorem A.1 and Proposition 4.2 that (5.1) holds. It now follows from Proposition 5.1 (with \( \Delta \equiv \sqrt{\xi(0)} Z \) and \( \delta = \frac{1}{\sqrt{n}} \)) that

\[
\begin{align*}
\mathbb{V}_P[f(x_n(0), Y_{n+1})] &= \mathbb{V}_P[f\left(x^*(0) + \sqrt{\frac{\xi(0)}{n}} (Z + o_P(1)), Y_{n+1}\right)] \\
&= \mathbb{V}_P[f(x^*(0), Y_{n+1})] \\
&\quad + \frac{2}{\sqrt{n}} \mathbb{E}_P \left[ \left( \sqrt{\frac{\xi(0)}{n}} Z \right)' \mathbb{Cov}_P[f(x^*(0), Y_{n+1}), \nabla_x f(x^*(0), Y_{n+1})] \right] \\
&\quad + \frac{1}{2n} \text{tr} \left( \mathbb{E}_P \left[ \sqrt{\frac{\xi(0)}{n}} ZZ' \sqrt{\frac{\xi(0)}{n}} \right] \nabla^2_x \mathbb{V}_P[f(x^*(0), Y_{n+1})] \right) \\
&\quad + 2 \mathbb{V}_P \left[ \sqrt{\frac{\xi(0)}{n}} Z \right] \mathbb{E}_P \left[ \nabla_x f(x^*(0), Y_{n+1}) \right] \mathbb{E}_P \left[ \nabla_x f(x^*(0), Y_{n+1}) \right]' + o\left(\frac{1}{n}\right).
\end{align*}
\]

Noting that \( Z \) is standard normal, \( \mathbb{E}_P \left[ \sqrt{\xi(0)} ZZ' \sqrt{\xi(0)} \right] = \xi(0) \), and \( \mathbb{E}_P[\nabla_x f(x^*(0), Y_{n+1})] = 0 \) (by the definition of \( x^*(0) \)), we obtain (5.7). The expression (5.6) for the expected out-of-sample profit under the empirical optimal can be derived in the same way. \[\square\]

### 6. Out-of-sample performance: Robust optimization

We now study the mean and variance of the out-of-sample reward generated by solutions of robust optimization problems \( x_n(\delta) \). We are particularly interested to characterize the impact of the robustness parameter \( \delta \).

#### 6.1. Expected reward.

Recall from Theorem 4.4 that the robust solution is asymptotically normal

\[ x_n(\delta) = x^*(\delta) + \frac{\sqrt{\xi(\delta)}}{\sqrt{n}} Z + o_P\left(\frac{1}{\sqrt{n}}\right) \]
with mean

\[ x^*(\delta) = x^*(0) + \delta \pi + o(\delta) \]  

(6.1)

where the asymptotic bias \( \pi \) is given by (4.6). It follows that the out-of-sample expected reward

\[
\mathbb{E}_P \left[ f(x_n(\delta), Y_{n+1}) \right] = \mathbb{E}_P \left[ f \left( x^*(\delta) + \frac{\sqrt{\xi(\delta)}}{\sqrt{n}} (Z + o_P(1)), Y_{n+1} \right) \right]
\]

\[
= \mathbb{E}_P \left[ f(x^*(\delta), Y_{n+1}) \right] + \frac{1}{2n} \text{tr} \left( \xi(\delta) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right) + o \left( \frac{1}{n} \right).
\]

The first term is the expected reward around the asymptotic mean \( x^*(\delta) \) while the second term reflects the reduction in the out-of-sample reward from Jensen’s inequality that comes from the concavity of the objective function and fluctuations of the (finite sample) robust solution around the asymptotic mean with variance \( \xi(\delta)/n \). We saw analogous terms for the out-of-sample mean reward under the empirical optimizer (5.6). A key difference with the robust optimizer is the impact of the bias \( \pi \), which affects both the mean \( x^*(\delta) \) and the covariance \( \xi^*(\delta) \) of the robust solution. We now study the impact of this bias on the reward.

By (6.1) and Proposition 5.1 (with \( \Delta = \pi \)) we have

\[
\mathbb{E}_P \left[ f(x^*(\delta), Y_{n+1}) \right] = \mathbb{E}_P \left[ f(x^*(0), Y_{n+1}) \right] + \frac{\delta^2}{2} \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \pi + o(\delta^2). \tag{6.2}
\]

Asymptotically, adding bias \( \pi \) reduces the out-of-sample expected reward, which is intuitive because it perturbs the mean of the solution away from the optimal \( x^*(0) \) under the data generating model. However, the reduction is of order \( \delta^2 \) which is small when \( \delta \) is small.

To evaluate the impact of the bias (6.1) on the Jensen effect, observe that the second term in (6.2) can be written

\[
\frac{1}{2n} \text{tr} \left( \xi(\delta) \mathbb{E}_P \left[ \nabla^2_x f(x^*(\delta), Y_{n+1}) \right] \right)
\]

\[
= \frac{1}{2n} \text{tr} \left( \xi(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right) + \frac{1}{2n} \text{tr} \left( (\xi(\delta) - \xi(0)) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right)
\]

\[
+ \frac{1}{2n} \text{tr} \left( \xi(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(\delta), Y_{n+1}) - \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right)
\]

\[
+ \frac{1}{2n} \text{tr} \left( (\xi(\delta) - \xi(0)) \mathbb{E}_P \left[ \nabla^2_x f(x^*(\delta), Y_{n+1}) - \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right).
\]

The first term is the Jensen loss associated with the empirical solution (5.6), while the remaining terms are adjustments to the Jensen effect due to changes in the variability of the robust solution.
and the change in the curvature of the reward. Since

$$\xi(\delta) = \xi(0) + \delta \xi'(0) + o(\delta),$$

(see Theorem 4.4 where $\xi'(0)$ is the derivative of $\xi(\delta)$ with respect to $\delta$ at $\delta = 0$) we can write

$$\frac{1}{2n} \text{tr} \left( \xi(\delta) \mathbb{E}_P \left[ \nabla^2_x f(x^*(\delta), Y_{n+1}) \right] \right)$$

$$= \frac{1}{2n} \text{tr} \left( \xi(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right)$$

$$+ \frac{\delta}{2n} \left\{ \text{tr} \left( \xi'(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right) + \pi' \nabla_x \text{tr} \left( \xi(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right) \right\} + o(\delta),$$

where the sum of the second and third terms

$$\frac{\delta}{2n} \left\{ \text{tr} \left( \xi'(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right) + \pi' \nabla_x \text{tr} \left( \xi(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right) \right\}$$

measures the adjustment to the Jensen effect after robustification. An asymptotic expansion of the out-of-sample reward is obtained by combining (6.2), (6.2) and (6.3).

6.2. Variance of the reward. Expanding $x_n(\delta)$ around $x^*(\delta)$ using (5.3) with $\delta = \frac{1}{\sqrt{n}}$ and $\Delta = \sqrt{\xi(\delta)}(Z + o_P(1))$ gives

$$\mathbb{V}_P[f(x_n(\delta), Y_{n+1})]$$

$$= \mathbb{V}_P[f(x^*(\delta) + \frac{\sqrt{\xi(\delta)}}{\sqrt{n}}(Z + o_P(1)), Y_{n+1})]$$

$$= \mathbb{V}_P[f(x^*(\delta), Y_{n+1})]$$

$$+ \frac{1}{2n} \text{tr} \left( \xi(\delta) \left\{ \nabla^2_x \mathbb{V}_P[f(x^*(\delta), Y_{n+1})] + 2 \mathbb{E}_P[\nabla_x f(x^*(\delta), Y_{n+1})] \mathbb{E}_P[\nabla_x f(x^*(\delta), Y_{n+1})'] \right\} \right)$$

$$+ o\left(\frac{1}{n}\right),$$

where $\nabla^2_x \mathbb{V}_P[f(x^*(0), Y_{n+1})]$ is given in (5.5). As in (6.2) this decomposes the variance of the reward into a contribution due to variability in $Y_{n+1}$, and another from the variability of the robust solution $x_n(\delta)$ from data variability. Noting (6.1), it follows from Proposition 5.1 that the first term in (6.5)

$$\mathbb{V}_P[f(x^*(\delta), Y_{n+1})] = \mathbb{V}_P[f(x^*(0), Y_{n+1})] + \delta \pi' \nabla_x \mathbb{V}_P[f(x^*(0), Y_{n+1})] + o(\delta^2).$$

Robustifying empirical optimization has an order $\delta$ effect on the variance. In comparison the impact of bias on the mean reward is of order $\delta^2$ (see (6.2)) while the order $\delta$ terms from Jensen’s inequality
in (6.4) diminish like $1/n$. This suggests that the potential impact of robust optimization on the variance can be substantially greater than its impact on the mean when $\delta$ is small.

It will be shown below that the second term
\[
\frac{1}{2n} \text{tr} \left( \xi(0) \nabla^2 \nabla_P [f(x^*(0), Y_{n+1})] \right) \tag{6.7}
\]
\[
= \frac{1}{2n} \text{tr} \left( \xi(0) \nabla^2 \nabla_P [f(x^*(0), Y_{n+1})] \right) \\
+ \frac{\delta}{2n} \left\{ \text{tr} \left( \xi'(0) \nabla^2 \nabla_P [f(x^*(0), Y_{n+1})] \right) + \pi' \nabla_x \text{tr} \left( \xi(0) \nabla^2 \nabla_P [f(x^*(0), Y_{n+1})] \right) \right\} \\
+ \frac{1}{n} O(\delta^2).
\]
The first term is from the empirical optimizer (5.7) while the remaining terms reflect the impact of robustness on solution variability. These higher order terms are of order $\delta/n$ so are dominated by the order $\delta$ term from (6.6) and disappear as $n \to \infty$.

6.3. Main Result. Taken together, the results from Sections 6.1 and 6.2, which we summarize below, tell us that when the robust parameter $\delta$ is small, the reduction in the variance of the out-of-sample reward is (almost) an order-of-magnitude larger than the impact on the expected reward. To ease notation, let
\[
\mu_f := \text{Cov}_P \left[ \nabla_x f(x^*(0), Y_{n+1}), f(x^*(0), Y_{n+1}) \right],
\]
\[
\Sigma_f := \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right].
\]
Observe that $f(x, Y)$ is concave in $x$ so $\mu_f^{\top} \Sigma_f^{-1} \mu_f < 0$.

**Theorem 6.1.** The expected value of the out-of-sample reward under the robust solution is
\[
\mathbb{E}_P \left[ f(x_n(\delta), Y_{n+1}) \right] = \mathbb{E}_P \left[ f(x^*(0), Y_{n+1}) \right] + \frac{1}{2n} \text{tr} \left( \frac{\xi(0)}{n} \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right) \\
+ \frac{\delta^2}{2} \frac{\delta^2}{\phi'(1)} \mu_f^{\top} \Sigma_f^{-1} \mu_f + \frac{\delta}{2n} \rho + \frac{1}{n} O(\delta^2) + o\left( \frac{1}{n} \right) + o(\delta^2),
\]
where the constant
\[
\rho = \text{tr} \left( \xi'(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right) + \pi' \nabla_x \text{tr} \left( \xi(0) \mathbb{E}_P \left[ \nabla^2_x f(x^*(0), Y_{n+1}) \right] \right),
\]
and $\pi$ is given by (4.6). The variance of the out-of-sample reward is

$$\mathbb{V}_P[f(x_n(\delta), Y_{n+1})] = \mathbb{V}_P[f(x^*(0), Y_{n+1})] + \frac{1}{2n} \text{tr} \left( \xi(0) \nabla_x^2 \mathbb{V}_P[f(x^*(0), Y_{n+1})] \right) + \frac{2\delta}{\phi'(1)} \mu_f' \Sigma_f^{-1} \mu_f + \frac{\delta}{2n} \theta + \frac{1}{n} O(\delta^2) + O(1/n) + O(\delta^2),$$

(6.9)

where $\nabla_x \mathbb{V}_P[f(x^*(0), Y_{n+1})]$ and $\nabla_x^2 \mathbb{V}_P[f(x^*(0), Y_{n+1})]$ are given in (5.4)–(5.5) and

$$\theta = \text{tr} \left( \xi'(0) \nabla_x^2 \mathbb{V}_P[f(x^*(0), Y_{n+1})] \right) + \pi' \nabla_x \text{tr} \left( \xi(0) \nabla_x^2 \mathbb{V}_P[f(x^*(0), Y_{n+1})] \right).$$

Proof. It follows from (6.2), (6.2) and (6.3) and the expression (4.6) for $\pi$ that the out-of-sample expected reward is given by (6.8). The out-of-sample variance is given by (6.5), (6.6) and (6.7). All that remains is to justify (6.7), which we initially stated without proof.

Noting the definition of $\nabla_x^2 \mathbb{V}_P[f(x^*(\delta), Y_{n+1})]$ in (5.5) observe firstly that

$$\text{tr} \left( \xi(\delta) \nabla_x f(x^*(\delta), Y_{n+1}) \right)$$

$$= \sum_{i,j} \xi_{ij}(\delta) \text{Cov}_P[f_{x_i}(x^*(\delta), Y_{n+1}), f_{x_j}(x^*(\delta), Y_{n+1})]$$

$$= \text{tr} \left( \xi(\delta) \nabla_x f(x^*(0), Y_{n+1}) \right)$$

$$+ \delta \pi' \sum_{i,j} \xi_{ij}(\delta) \nabla_x \text{Cov}_P[f_{x_i}(x^*(0), Y_{n+1}), f_{x_j}(x^*(0), Y_{n+1})] + o(\delta)$$

$$= \text{tr} \left( \xi(0) \nabla_x f(x^*(0), Y_{n+1}) \right)$$

$$+ \delta \left\{ \text{tr} \left( \xi'(0) \nabla_x f(x^*(0), Y_{n+1}) \right) + \pi' \nabla_x \text{tr} \left( \xi(0) \nabla_x f(x^*(0), Y_{n+1}) \right) \right\} + o(\delta)$$

$$+ \frac{2\delta}{\phi'(1)} \mu_f' \Sigma_f^{-1} \mu_f + \frac{\delta}{2n} \theta + \frac{1}{n} O(\delta^2) + O(1/n) + O(\delta^2),$$

(6.9)
Finally, we also have

\[
\text{tr}\left(\xi(\delta) \text{Cov}_P \left[ f(x^*(\delta), Y_{n+1}), \nabla_x^2 f(x^*(\delta), Y_{n+1}) \right] \right) = \sum_{i,j} \xi_{ij}(\delta) \text{Cov}_P \left[ f(x^*(\delta), Y_{n+1}), f_{x_i x_j}(x^*(\delta), Y_{n+1}) \right] - \delta \pi' \sum_{i,j} \xi_{ij}(\delta) \nabla_x \text{Cov}_P \left[ f(x^*(\delta), Y_{n+1}), f_{x_i x_j}(x^*(\delta), Y_{n+1}) \right] + o(\delta)
\]

\[
\text{tr} \left( \xi(0) \text{Cov}_P \left[ f(x^*(0), Y_{n+1}), \nabla_x^2 f(x^*(0), Y_{n+1}) \right] \right) + \delta \left\{ \text{tr} \left( \xi'(0) \text{Cov}_P \left[ f(x^*(0), Y_{n+1}), \nabla_x^2 f(x^*(0), Y_{n+1}) \right] \right) + \delta \pi' \nabla_x \text{tr} \left( \xi(0) \text{Cov}_P \left[ f(x^*(0), Y_{n+1}), \nabla_x^2 f(x^*(0), Y_{n+1}) \right] \right) \right\} + o(\delta).
\]

Finally, we also have

\[
\mathbb{E}_P \left[ \nabla_x f(x^*(\delta), Y_{n+1}) \right] = \mathbb{E}_P \left[ \nabla_x f(x^*(0), Y_{n+1}) \right] + \delta \mathbb{E}_P \left[ \nabla_x^2 f(x^*(0), Y_{n+1}) \right] \pi + o(\delta)
\]

\[
= \delta \mathbb{E}_P \left[ \nabla_x^2 f(x^*(0), Y_{n+1}) \right] \pi + o(\delta),
\]

(recall \( \mathbb{E}_P \left[ \nabla_x f(x^*(0), Y_{n+1}) \right] = 0 \)) so

\[
\mathbb{E}_P \left[ \nabla_x f(x^*(\delta), Y_{n+1}) \right] \mathbb{E}_P \left[ \nabla_x f(x^*(\delta), Y_{n+1}) \right]' = O(\delta^2).
\]

Equation (6.7) follows. \( \square \)

Proposition 5.2 and Theorem 6.1 allow us to write the asymptotic mean and variance of the reward under the robust solution in terms of that of the empirical solution.

**Corollary 6.2.** Let \( \rho \) and \( \theta \) be defined as in Theorem 6.1. Then

\[
\mathbb{E}_P \left[ f(x_n(\delta), Y_{n+1}) \right] = \mathbb{E}_P \left[ f(x_n(0), Y_{n+1}) \right] \quad (6.10)
\]

\[
+ \frac{1}{2} \frac{\delta^2}{\phi'(1)^2} \mu_f' \Sigma_f^{-1} \mu_f + \frac{\delta}{2n} \rho + o(\delta^2) + \frac{1}{n} O(\delta^2) + o \left( \frac{1}{n} \right),
\]

\[
\mathbb{V}_P \left[ f(x_n(\delta), Y_{n+1}) \right] = \mathbb{V}_P \left[ f(x_n(0), Y_{n+1}) \right] \quad (6.11)
\]

\[
+ \frac{2\delta}{\phi'(1)} \mu_f' \Sigma_f^{-1} \mu_f + \frac{\delta}{2n} \theta + \frac{1}{n} O(\delta^2) + o \left( \frac{1}{n} \right) + O(\delta^2).
\]
We see from (6.2) and (6.10) that robust optimization reduces the expected out-of-sample reward by order $\delta^2$, while the adjustment from the Jensen effect is of order $\delta/n$. On the other hand, the dominant term in the out-of-sample variance (equations (6.9) and (6.11)) is of order $\delta$, which comes from the asymptotic bias $\delta \pi$ that is added to the empirical optimal (6.6), which dominates the order $\delta^2$ and $\delta/n$ adjustments to the mean. In other words, the robust mean-variance frontier \{(\mu(\delta), \sigma^2(\delta)), \delta \geq 0\} where

$$
\mu(\delta) := \mathbb{E}_P[f(x_n(\delta), Y)], \quad \sigma^2(\delta) := \mathbb{V}_P[f(x_n(\delta), Y)]
$$

always looks like the plots shown in Figure 1.2 with the reduction in variance being large relative to the loss of reward when $\delta$ is small.

We also note that the adjustment to the mean reward (6.2) and (6.10) from the Jensen effect can be positive or negative, depending on the sign of $\rho$, which dominates the $O(\delta^2)$ reduction that comes from the bias when $\delta$ is small. This has one interesting implication: though robust optimization is a worst-case approach, the out-of-sample expected reward under the optimal robust decision will exceed that of the empirical optimal if $\rho$ is positive and the robustness parameter $\delta$ is sufficiently small. This was seen in the logistic regression example in Section 1. We note however, that the Jensen effect is small because it is scaled by $n$ and disappears as $n \to \infty$, and is likely to be dominated by other effects when $\delta$ gets large.

7. Calibration of Robust Optimization Models

Theorem 6.1 shows that when the ambiguity parameter $\delta$ is small, variance reduction is the first order benefit of robust optimization while the impact on the mean is (almost) an order of magnitude smaller. This implies that $\delta$ should be calibrated by trading off between the out-of-sample mean and variance and not just by optimizing the mean alone, as is commonly done when tuning the free parameters (e.g. in Machine Learning applications).

Observe, however, that the robust mean-variance frontier (6.12) can not be computed by the decision maker because he/she does not know the data generating model $P$, so it is natural to approximate the frontier using resampling methods. One such approach uses the well known bootstrap procedure [18], which we now describe, and formally state in Algorithm 1.

Specifically, suppose the decision maker has a data set $D = \{Y_1, \cdots, Y_n\}$ and the associated empirical distribution $P_n$. To approximate the out-of-sample behavior of different possible data sets (of size $n$), one may generate a so-called bootstrap data set, call it $D^{(1)}$, by simulating $n$ new
i.i.d. data points from the empirical distribution \( P_n \). Associated with this bootstrap data set is the bootstrap empirical distribution \( P_n^{(1)} \). This process can be repeated as many times as desired, with \( D^{(j)} \) and \( P_n^{(j)} \) denoting the bootstrap data set and bootstrap empirical distribution generated at repeat \( j \). We denote the number of bootstrap samples by \( k \) in Algorithm 1.

For each \( D^{(j)} \) and \( P_n^{(j)} \), we can compute (a family of) robust decisions \( x^{(j)}(\delta) \) by solving the robust optimization problem defined in terms of the bootstrap empirical distribution \( P_n^{(j)} \) over a specified set of \( \delta \) (step 5). The mean and variance of the reward for \( x^{(j)}(\delta) \) under the original empirical distribution \( P_n \), which we denote by \( m_j(\delta) \) and \( v_j(\delta) \) in steps 6 and 7, can then be computed. The \( k \) bootstrap samples produces the mean-variance pairs \((m_j(\delta), v_j(\delta)) \), \( j = 1, \cdots, k \). Averaging these gives an estimate of the out-of-sample mean-variance frontier (steps 8 and 9).

**Algorithm 1: Bootstrap Estimate of the Out-of-Sample Mean-Variance Frontier Generated by Robust Solutions**

| Input: Data set \( D = \{Y_1, \ldots, Y_n\} \); ambiguity parameter grid \( G = [\delta_1, \ldots, \delta_m] \in \mathbb{R}_+^m \). |
| Output: Mean and variance of out-of-sample reward parametrized by \( \delta \in G \). |

1. for \( j \leftarrow 1 \) to \( k \) do  
   2. \( D^{(j)} \leftarrow \) bootstrap data set (sample \( n \) i.i.d. data points from \( P_n \))  
   3. for \( i \leftarrow 1 \) to \( m \) do  
      4. \( x^{(j)}(\delta_i) \leftarrow \arg\max_x \{ E_Q[f(x, Y)] + \frac{1}{\delta_i} \mathcal{H}_\phi(Q || P_n^{(j)}) \} \),  
      5. \( m_j(\delta_i) \leftarrow E_{P_n}[f(x^{(j)}(\delta_i), Y)] \),  
      6. \( v_j(\delta_i) \leftarrow V_{P_n}[f(x^{(j)}(\delta_i), Y)] \).  
   7. \( \mu(\delta_i) \leftarrow \frac{1}{k} \sum_{j=1}^k m_j(\delta_i) \), for all \( \delta_i \in G \)  
   8. \( \sigma^2(\delta_i) \leftarrow \frac{1}{k} \sum_{j=1}^k v_j(\delta_i) + \frac{1}{k^2} \sum_{j=1}^k \left( m_j(\delta_i) - \mu(\delta_i) \right)^2 \), for all \( \delta_i \in G \)  
   9. return \( \{(\mu(\delta_i), \sigma^2(\delta_i)) : i = 1, \ldots, m\} \)

In the next section, we consider three applications, inventory control, portfolio optimization and logistic regression. We illustrate various aspects of our theory and show how the bootstrap robust mean-variance frontier given in Algorithm 1 can be used to effectively calibrate ambiguity parameters in such settings.

### 8. Applications

We consider three examples. The first is a simulation experiment in the setting of robust inventory control. The data generating model is known to us and we use this example to illustrate key elements of our theory. The second and third examples are out-of-sample tests with real data. The
first of these is a portfolio choice example, where model uncertainty (by design) is extreme, while the final example is that of robust maximum likelihood estimation. Substantial variance reduction relative to the loss in mean is seen in all three examples, and the use of the bootstrap frontier to calibrate the robustness parameter is also illustrated.

8.1. Application 1: Inventory Control. We first consider a simulation example with reward

\[ f(x, Y) = r \min\{x, Y\} - cx. \]  

This is a so-called inventory problem where \( x \) is the order quantity (decision), \( Y \) is the random demand, and \( r \) and \( c \) are the revenue and cost parameters.

The demand distribution \( \mathbb{P} \) is a mixture of two exponential distributions \( \text{Exp}(\lambda_L) \) and \( \text{Exp}(\lambda_H) \), where \( \lambda_L \) and \( \lambda_H \) are the rate parameters. This may correspond to two demand regimes (high and low) with different demand characteristics. For this numerical example, we set the mean values as \( \lambda_L^{-1} = 10 \) and \( \lambda_H^{-1} = 100 \), and revenue and cost parameters \( r = 30 \) and \( c = 2 \). The probability that demand is drawn from the low segment is 0.7 (or equivalently, the probability that demand is drawn from the high segment is 0.3).

We run the following experiment. The decision maker is initially shown \( n \) data points \( Y_1, \ldots, Y_n \) drawn i.i.d. from the mixture distribution \( \mathbb{P} \). The decision maker then optimizes the robust objective function under the empirical distribution \( \mathbb{P}_n \) to produce the optimal robust order quantity \( x_n^*(\delta) \). Another data point \( Y_{n+1} \) is then generated from \( \mathbb{P} \), independent of the previous data points, and the objective value \( f(x_n^*(\delta), Y_{n+1}) \) is recorded. The out-of-sample mean and variance \( \mathbb{E}_\mathbb{P}[f(x_n^*(\delta), Y_{n+1})] \) and \( \mathbb{V}_\mathbb{P}[f(x_n^*(\delta), Y_{n+1})] \) are approximated by running the experiment \( K \) times, where \( K \) is some large number, each time using a newly generated data set \( Y_1, \ldots, Y_n, Y_{n+1} \sim \mathbb{P} \); the sample mean and variance are computed over the \( K \) repeats.

In Figure 8.1 we plot the pair \( (\mathbb{E}_\mathbb{P}[f(x_n^*(\delta), Y_{n+1})], \mathbb{V}_\mathbb{P}[f(x_n^*(\delta), Y_{n+1})]) \) for different sample sizes \( n = 10, 30, 50 \). Each line in the figure corresponds to a different sample size (e.g. the dotted line with \(-\)marks corresponds to a sample size \( n = 10 \)), and the marks on a given line correspond to different values of \( \delta \); the right-most mark corresponds to \( \delta = 0 \) (empirical). In this figure, we also plot the “true” robust mean variance frontier, i.e., the pair \( (\mathbb{E}_\mathbb{P}[f(x^*(\delta), Y)], \mathbb{V}_\mathbb{P}[f(x^*(\delta), Y)]) \), which is independent of \( n \).

Figure 8.1 shows that as the sample size \( n \) increases, the gap between the out-of-sample mean-variance frontiers and the “true” robust mean variance frontier gets smaller. This gap can be explained by Theorem 6.1, which shows that the difference between these frontiers should go to zero.
Figure 8.1. Out-of-sample robust mean variance frontiers for \( n = 10, 30 \) and 50 data points, and the true frontier generated by solutions of DRO under the data generating model for different values of the robustness parameter \( \delta \).

like \( O(n^{-1}) \). This is shown in Figure 8.2 which plots the maximum gap (over \( \delta \)) between the out-of-sample frontier and the true frontier under the true frontier for different values of \( n \).

Recall, in the previous section, we proposed the bootstrap frontier as an approximation to the out-of-sample frontier. We next investigate how well the bootstrap frontier approximates the out-of-sample frontier for various sample sizes \( n \). From the perspective of calibration, it is not necessary for
the bootstrap frontier to equal the out-of-sample frontier exactly, it need only preserve the \textit{relative shape} of the out-of-sample frontier. As an example, suppose the bootstrap frontier matched the out-of-sample frontier with the only difference being that it was double its size (in both the mean and variance axis). In this scenario, the choice of $\delta$ should be the same when using either frontier since the relative trade-off between mean and variance is identical. In light of this observation, in Figures 8.3 (A), (B), and (C) we plot the \textit{normalized} bootstrap and out-of-sample frontiers, where the change in the mean and variance has been normalized to 1, for various sample sizes $n = 10, 30, 50$, respectively. It is clear that as the sample size increases, the bootstrap frontier more closely approximates the relative shape of the out-of-sample frontier.

8.2. \textbf{Application 2: Portfolio Optimization.} In our second application, we consider real monthly return data from the “10 Industry Portfolios” data set of French \cite{22}. The reward function is exponential utility of returns

\[ f(x, R) = -\exp(-\gamma R^\top x), \tag{8.2} \]

where $x \in \mathbb{R}^d$ is the portfolio vector (decision variables), $R \in \mathbb{R}^d$ is the vector of random returns, and $\gamma$ is the risk-aversion parameter. To simplify the experiments, we choose a risk-aversion parameter $\gamma = 1$. For the purposes of this example, we impose a budget constraint $1^\top x = 1$ and assume that asset holdings are bounded, $-1 \leq x_i \leq 1$, $i = 1, \ldots, d$.

We conduct the following experiment. We have $d = 10$ assets and are interested to see how robust optimization and our approach for calibrating $\delta$ perform when we estimate the 10-dimensional joint distribution with relatively few data points ($n = 50$, for the time period April 1968 to June 1972). The robust portfolios will be tested on the empirical distributions for monthly returns of future 50 month windows, July 1972 to September 1976, October 1976 to December 1980 and January 1981 to March 1985 that do not overlap with the training set.

To begin, we solve the robust portfolio choice problem using the 50 monthly returns for the period April 1968 to June 1972 for different values of $\delta$ and construct the robust mean-variance frontier using the bootstrap procedure described in Algorithm \ref{alg:bootstrap}. Figure 8.4 shows the associated bootstrap robust mean-variance frontier, around which we also mark the $+/−$ one standard deviations of the bootstrap samples in both the mean and variance dimensions. Empirical optimization corresponds to the point $\delta = 0$, and as predicted by Theorem \ref{thm:robust_mean_variance} there is significantly more reduction in the variance as compared to the mean when $\delta$ is close to 0.
Figure 8.3. Bootstrap frontier vs out-of-sample frontier (with normalization).
Both frontiers are scaled and normalized so that both the mean and variance equal 1 when $\delta = 0$ (i.e., empirical optimization) and 0 in the most robust case ($\delta = 100$).
We see that as $n$ increases, the points on the frontier corresponding to the same values of $\delta$ converge.

**Calibration and Out-of-sample Tests:** The bootstrap frontier estimates the the out-of-sample mean and variance for different decisions and can be used to calibrate $\delta$. For this example, the rate of variance reduction relative to the loss in the mean is substantial for $\delta \leq 5$, but this begins to diminish (and the cost of robustness increases) once $\delta$ exceeds 5. A value of $\delta$ between 2 and 5 seems reasonable. While values of $\delta > 10$ may be preferred by some, the balance clearly tips towards loss in mean reward relative to variance reduction/robustness improvement. Note also that a classical approach to calibration which optimizes expected reward (and ignores objective variability) would
select $\delta = 0$ which corresponds to empirical optimization and completely nullifies all the benefits of the robust optimization model.

It is also interesting to compare calibration using the bootstrap frontier with the decisions obtained by solving robust optimization problems with “high confidence uncertainty sets”. The basic idea behind this approach is to use uncertainty sets that include the true data generating model with high probability, where the confidence level $1 - \alpha$ (typically 90%, 95%, or 99%) is a primitive of the model. The use of uncertainty sets with these confidence levels is commonly advocated in the robust optimization literature.

For a given statistical significance level $0 < \alpha < 1$, define an uncertainty set of the form

$$\mathcal{U}_\alpha = \{ Q : \mathcal{H}(Q | P_n) \leq Q_n(\alpha) \},$$  \hspace{1cm} (8.3)

where $\mathcal{H}$ is some statistical distance measure and the threshold $Q_n(\alpha)$ is the $(1 - \alpha)$-quantile of the distribution of $\mathcal{H}(Q | P_n)$ under the assumption that the data have the distribution $P_n$, i.e., the probability that the true data generating model lies in $\mathcal{U}_\alpha$ is $(1 - \alpha)$. The $\alpha$-parameterized “high confidence uncertainty set” problem is then given by

$$\max_x \min_{Q \in \mathcal{U}_\alpha} \left\{ \mathbb{E}_Q[f(x, Y)] \right\}. \hspace{1cm} (8.4)$$

For this experiment, the statistical distance measure is relative entropy, i.e., $\mathcal{H}(Q | P_n) = \mathcal{R}(Q | P_n)$. 

---

**Figure 8.4.** Bootstrap robust mean-variance frontier for portfolio optimization generated using 50 months of monthly return data between April 1968 and June 1972.
It can be shown that for any \( \alpha \) there is a unique ambiguity parameter value \( \delta_{\alpha} > 0 \), for which the solution of (8.4) coincides with our robust solution \( x^{*}(\delta_{\alpha}) \). In Table 8.1 we report the corresponding ambiguity parameter values \( \delta_{\alpha} \) for typical values of the significance level \( \alpha \).

**Table 8.1.** Corresponding ambiguity parameter values \( \delta_{\alpha} \) for various traditional values of the significance level \( \alpha \)

| Significance level \( \alpha \) | Ambiguity values \( \delta_{\alpha} \) |
|---------------------------------|----------------------------------|
| 0.10                           | 55                               |
| 0.05                           | 58                               |
| 0.01                           | 63                               |

While robust decisions associated with the significance levels in Table 8.1 may or may not perform well out-of-sample in this or any given application, it is clear that the range of \( \delta_{\alpha} \) associated with these significant levels is limited. This directly impacts the range of possible solutions available to the decision maker, which in this example are concentrated on the “extremely conservative” region of the bootstrap frontier (Figure 8.4). This approach cannot access a broad range of reasonable solutions due to the nature of its parameterization.

We next analyze the out-of-sample performance of the robust solutions corresponding to \( \delta = 1, 2, 3, 5, 10 \) obtained from our bootstrap frontier in Figure 8.4, the three “high confidence uncertainty set” solutions of corresponding to \( \delta_{\alpha} = 55 \ (\alpha = 0.10) \), \( \delta_{\alpha} = 58 \ (\alpha = 0.05) \), \( \delta_{\alpha} = 63 \ (\alpha = 0.01) \), and the empirical optimization solution corresponding to \( \delta = 0 \). In particular, we test each of the solutions on the empirical distributions for three out-of-sample test sets of data size \( n = 50 \) that do not overlap with the training data; Figure 8.5 shows the out-of-sample performance. Note that in the figure we report the mean and variance of the utility function \( f(x, R) \) defined in (8.2), which is consistent with the framework of the robust optimization model in this paper.

Figure 8.5 consistently shows that as the value of \( \delta \) (“robustness”) increases from zero, the mean performance degrades but the objective variability reduces, which is expected from our theory. Consistent with the bootstrap frontier (Figure 8.4), the portfolios associated with “high confidence uncertainty sets” have low variance though the impact on expected utility is substantial.

### 8.3. Application 3: Logistic Regression

As final application we apply robust optimization to logistic regression which we evaluate on the WDBC breast cancer diagnosis data set [34].

The reward function for logistic regression is given by

\[
f((x, x_0), (Y, Z)) = \ln(1 + \exp(-Y(x^T Z + x_0))), \tag{8.5}
\]
where $Y \in \{-1, 1\}$ is the binary label, $Z$ is the vector of covariates, and $x$ and $x_0$ are decision variables representing coefficients and intercept, respectively, of the linear model for classification. Ordinary logistic regression is formulated as the maximization of the sample average of (8.5).

To demonstrate the out-of-sample behavior of robust maximum likelihood, we solve the ordinary/robust likelihood maximization problem using the first half of the WDBC breast cancer diagnosis data set [34], i.e., 285 out of the 569 samples, and compute the log-likelihood and the variance of the log-likelihood of the resulting model using the remaining half of the samples, i.e., 284 out of 569. Figure 8.6 shows both the the bootstrap frontier and the frontier obtained from the out-of-sample test. Once again, that choices of $\delta$ that deliver good out-of-sample log-likelihood can be obtained using the bootstrap estimate of the robust frontier.

9. Conclusions

Proper calibration of DRO models requires a principled understanding of how the distribution of the out-of-sample reward depends on the “robustness parameter”. In this paper, we studied out-of-sample properties of robust empirical optimization and developed a theory for data-driven calibration of the robustness parameter. Our main results showed that the first-order benefit of
Figure 8.6. Bootstrap frontier vs. out-of-sample test frontier with WDBC breast cancer diagnosis data set.

The out-of-sample test frontier shows the mean and variance of the log-likelihood of the second-half of the samples of the WDBC data set (i.e., 284 samples) on the basis of solutions obtained by using the first-half of those (i.e., 285 samples). Here, we used three attributes: no.2, no.24, and no.25 (out of 30 available covariates), which are found to be best possibly predictive in the paper [40]. To solve the optimization problems, we used RNUOPT (NTT DATA Mathematical Systems Inc.), a nonlinear optimization solver package.

“little bit of robustness” is a significant reduction in the variance of the out-of-sample reward while the impact on the mean is almost an order of magnitude smaller. Our results imply that the robustness parameter should be calibrated by making trade-offs between estimates of the out-of-sample mean and variance and that substantial variance reduction is possible at little cost when the robustness parameter is small. To calibrate the robustness parameter, we introduced the robust mean-variance frontier and showed that it can be approximated using resampling methods like the bootstrap. We applied the robust mean-variance frontiers to three applications: inventory control, portfolio optimization and logistic regression. Our results showed that classical calibration methods that match “standard” confidence levels (e.g. 95%) are typically associated with an excessively large robustness parameter and overly pessimistic solutions that perform poorly out-of-sample, while ignoring the variance and calibrating purely on the basis of the mean (a second-order effect) can lead to a robustness parameter that is too small and a solution that misses out on the first-order benefits of robust optimization.
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A. Asymptotic normality: General results. We summarize results from [45] on the theory of $M$-estimation that we use to characterize the asymptotic properties of robust optimization.

Let

\[ x^* := \arg\max_x \left\{ \mathbb{E}_P [g(x, Y)] \right\}, \]
\[ x_n := \arg\max_x \left\{ \mathbb{E}_{P_n} [g(x, Y)] \equiv \frac{1}{n} \sum_{i=1}^{n} g(x, Y_i) \right\}. \]

The following result from [45] gives conditions under which $x_n$ is asymptotically normal.

**Theorem A.1.** For every $x$ in an open subset of Euclidean space, let $x \mapsto \nabla_x g(x, Y)$ be a measurable vector-valued function such that, for every $x^1$ and $x^2$ in a neighborhood of $x^*$ and a measurable function $F(Y)$ with $\mathbb{E}_P [F(Y)^2] < \infty$

\[ \|\nabla_x g(x^1, Y) - \nabla_x g(x^2, Y)\| \leq F(Y)\|x^1 - x^2\|. \]

Assume that $\mathbb{E}_P [\nabla_x^2 g(x^*, Y)]^2 < \infty$ and that the map

\[ x \mapsto \mathbb{E}_P [\nabla_x g(x, Y)] \]

is differentiable at a solution $x^*$ of the equation $\mathbb{E}_P [\nabla_x g(x, Y)] = 0$ with non-singular derivative matrix

\[ \Sigma(x^*) := \nabla_x \mathbb{E}_P [\nabla_x g(x, Y)]. \]

If $\mathbb{E}_{P_n} [\|\nabla_x g(x_n, Y)\|] = o_P(n^{-1/2})$, and $x_n \xrightarrow{P} x^*$, then

\[ \sqrt{n}(x_n - x^*) = \Sigma(x^*)^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_x g(x^*, Y_i) + o_P(1). \]

In particular, the sequence $\sqrt{n}(x_n - x^*)$ is asymptotically normal with mean 0 and covariance matrix

\[ \Sigma(x^*)^{-1} \mathbb{E}_P [\nabla_x g(x^*, Y') \nabla_x g(x^*, Y')] (\Sigma(x^*)^{-1})'. \]

Under conditions that allow for exchange of the order of differentiation with respect to $x$ and integration with respect to $Y$, we have

\[ \Sigma(x) := \nabla_x^2 \mathbb{E}_P [g(x, Y)] = \nabla_x \mathbb{E}_P [\nabla_x g(x, Y)] = \mathbb{E}_P [\nabla_x^2 g(x, Y)]. \]
Note however that Theorem A.1 does not require that \( x \mapsto g(x, Y) \) is twice differentiable everywhere for \( \Sigma(x) \) to exist.

### A.2. Proof of Proposition 5.1

Taylor series implies

\[
f(x + \delta \Delta, Y_{n+1}) = f(x, Y_{n+1}) + \delta \Delta' \nabla_x f(x, Y_{n+1}) + \frac{1}{2} \delta^2 \operatorname{tr} \left( \Delta \Delta' \nabla^2_x f(x, Y_{n+1}) \right) + o(\delta^2).
\]

We obtain (5.2) by taking expectations and noting that \( \Delta \) and \( Y_{n+1} \) are independent. To derive (5.3) observe firstly that

\[
\mathbb{E}_P \left[f(x + \delta \Delta, Y_{n+1}) \right] = \mathbb{E}_P \left[f(x, Y_{n+1}) \right] + \delta \mathbb{E}_P \left[\nabla_x f(x, Y_{n+1}) \right] + \frac{1}{2} \delta^2 \mathbb{E}_P \left[\nabla^2_x f(x, Y_{n+1}) \right] + o(\delta^2).
\]

while expectations on both sides of a Taylor series expansion of \( f(x + \delta \Delta, Y_{n+1})^2 \) gives

\[
\mathbb{E}_P \left[f(x + \delta \Delta, Y_{n+1})^2 \right] = \mathbb{E}_P \left[f(x, Y_{n+1})^2 \right] + 2 \delta \mathbb{E}_P \left[\nabla_x f(x, Y_{n+1}) \right] \mathbb{E}_P \left[\nabla_x f(x, Y_{n+1}) \right] + \frac{1}{2} \delta^2 \mathbb{E}_P \left[\nabla^2_x f(x, Y_{n+1}) \right] + o(\delta^2).
\]

It now follows that

\[
\mathbb{V}_P \left[f(x + \delta \Delta, Y_{n+1}) \right] = \mathbb{V}_P \left[f(x, Y_{n+1}) \right] + 2 \delta \mathbb{E}_P \left[\nabla_x f(x, Y_{n+1}) \right] \mathbb{Cov}_P \left[f(x, Y_{n+1}), \nabla_x f(x, Y_{n+1}) \right] + \frac{1}{2} \delta^2 \left\{ \mathbb{E}_P \left[\nabla^2_x f(x, Y_{n+1}) \right] + 2 \mathbb{Cov}_P \left[f(x, Y_{n+1}), \nabla^2_x f(x, Y_{n+1}) \right] \right\} + o(\delta^2).
\]

When \( \Delta \) is constant, the definition of a derivative implies (5.4) and the expansion of \( \mathbb{V}_P \left[f(x + \delta \Delta, Y_{n+1}) \right] \) can be written as (5.3).