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# Predictive Stochastic Programming: A New Class of Models and Algorithms

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This research project is intended to build fundamental mathematical concepts which arise in very large stochastic optimization, which happens to provide the foundations for developments in Artificial Intelligence and Machine learning (AI/ML). Because uncertainty is ubiquitous in several DoD applications, this project goes beyond AI/ML applications. In particular, this project focuses on designing optimization methods which employ AI/ML to improve both data science and decision-making supported by optimization. Our approach enables the use of previously observed Action/Reaction pairs (observations among adversaries) to enable optimization models to learn adversarial relationships and use such understanding to improve decision-making by incorporating a “look-ahead” feature within optimization models. By incorporating such recognition capabilities, our project can provide decision-support which is cognizant of potential reactions from adversaries. Predictive Stochastic Programming (PSP) is a formal mathematical approach which allows decision models to learn from prior engagements with an adversary, and to use that knowledge to recommend decisions which are more responsive, and more agile than is possible with previously known approaches such as ordinary stochastic programming (SP). While the latter paradigm (i.e., SP), provides the basis for our work, in its original form, it lacks the agility required to learn from previous experiences (i.e., observations). By adding this new predictive feature to SP, we can close-the-loop between decision cycles, thus enabling a more responsive set of recommendations.

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Final Report for 2024
Predictive Stochastic Programming
AFOSR Grant **FA9550-20-1-0006**
PI: Suvrajeet Sen, University of Southern California

## 1. Project Overview

This research project is intended to build fundamental mathematical concepts which arise in very large *stochastic* optimization, which happens to provide the foundations for developments in Artificial Intelligence and Machine learning (AI/ML). Because uncertainty is ubiquitous in several DoD applications, this project goes beyond AI/ML applications. In particular, this project focuses on designing optimization methods which employ AI/ML to improve both data science and decision-making supported by optimization. Our approach enables the use of previously observed Action/Reaction pairs (observations among adversaries) to enable optimization models to learn adversarial relationships and use such understanding to improve decision-making by incorporating a "look-ahead" feature within optimization models. By incorporating such recognition capabilities, our project can provide decision-support which is cognizant of potential reactions from adversaries. Predictive Stochastic Programming (PSP) is a formal mathematical approach which allows decision models to *learn* from prior engagements with an adversary, and to use that knowledge to recommend *decisions* which are more responsive, and more agile than is possible with previously known approaches such as ordinary stochastic programming (SP). While the latter paradigm (i.e., SP), provides the basis for our work, in its original form, it lacks the agility required to learn from previous experiences (i.e., observations). By adding this new predictive feature to SP, we can close-the-loop between decision cycles, thus enabling a more responsive set of recommendations.

## 2. Publications which have already appeared in print or accepted (Names in italics below represent graduate student or post-doc at the time of paper submission)

- *H. Gangammanavar* and S. Sen, "Stochastic Dynamic Linear Programming: A Sequential Sampling-Based Multi-Stage Stochastic Programming Algorithm," *SIAM J. on Optimization*, vol. 31#3, pp. 2111-2140, 2021. https://doi.org/10.1137/19M12907
    - Just as SDDP (by Periera and Pinto, *Mathematical Programming*, 1991) is a multi-stage extension of two-stage Benders' Decomposition, our paper, entitled SDLP, is a stochastic multi-stage extension of Stochastic Decomposition (by Higle and Sen, *Math. of Operations Research*, 1991). However, unlike SDDP, the SDLP approach responds to stochastic phenomenon in real-time, by learning from past data and decision outcomes. This extension allows a user to interface outcomes of a stochastic discrete-time simulation *directly* into a multi-stage decision algorithm, so that *reactions* to previously observed *actions* can be accommodated on a real-time basis. This approach accommodates linear decision constraints under the assumption that the stochastic processes are stagewise independent. This work should be considered as a more easily implemented version of the "Multi-stage Stochastic Decomposition Algorithm" (S. Sen and Z. Zhou, "Multi-stage Stochastic Decomposition: A Bridge Between Stochastic

Programming and Approximate Dynamic Programming" *SIAM Journal on Optimization*, 2014.)

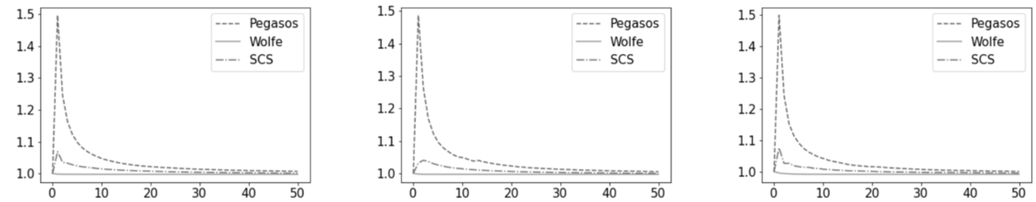
- *J. Liu, G. Li,* and S. Sen, "Coupled Learning Enabled Stochastic Programming with Endogenous Uncertainty," *Mathematics of Operations Research*, vol. 47# pp. 1681-1705, 2021. https://doi.org/10.1287/moor.2021.1185
    - Predictive analytics, empowered by machine learning, is usually followed by decision-making problems in prescriptive analytics. In this paper, we extend the above sequential prediction-optimization paradigm to a coupled scheme such that the prediction model can guide the decision problem to produce coordinated decisions yielding higher levels of performance. Specifically, for stochastic programming (SP) models with latently decision-dependent uncertainty, without any parametric assumption of the latent dependency, we develop a coupled learning enabled optimization (CLEO) algorithm in which the learning step of predicting the local dependency and the optimization step of computing a candidate decision are conducted interactively. The CLEO algorithm automatically balances the exploration and exploitation via the trust region method with active sampling. Under certain assumptions, we show that the sequence of solutions provided by CLEO converges to a directional stationary point of the original nonconvex and non-smooth SP problem with probability 1. In addition, we present preliminary experimental results which demonstrate the computational potential of this data-driven approach.
- *Y. Deng* and S. Sen, "Predictive Stochastic Programming" *Computational Management Science*, (Special Issue of 15th ICSP), vol. 19, pp. 65–98, 2022. https://doi.org/10.1007/s10287-021-00400-0
    - Unlike ordinary SP, PSP models work with datasets which represent random covariates, often referred to as predictors (or features) and responses (or labels) in the machine learning literature. As a result, these PSP models call for methodologies which borrow relevant concepts from both learning and optimization. We refer to such a methodology as Learning Enabled Optimization (LEO). This paper sets forth the foundation for such a framework by introducing several novel concepts such as statistical optimality, hypothesis tests for model-fidelity, generalization error of PSP, and finally, a non-parametric methodology for model selection. These new concepts, which are collectively referred to as LEO, provide a formal framework for modeling, solving, validating, and reporting solutions for PSP models. We illustrate the LEO framework by applying it to a production-marketing coordination model based on combining a pedagogical production planning model with an advertising dataset intended for sales prediction.
- *J. Xu*, and S.Sen, "Ensemble Variance Reduction Methods for Stochastic Mixed-Integer Programming and their Application to the Stochastic Facility Location Problem," *INFORMS Journal on Computing, 2023*. https://doi.org/10.1287/ijoc.2021.0324
    - Sample average approximation (SAA), the standard approach to Stochastic Mixed Integer Programming, does not provide guidance for cases with limited computational budgets. In such settings, variance reduction is critical in identifying good decisions. This paper explores two closely related ensemble methods to determine effective decisions with a probabilistic guarantee: a) The

first approach recommends a decision by coordinating aggregation in the space of decisions, as well as aggregation of objective values. This combination of aggregation methods generalizes the bagging method and the "compromise decision" of stochastic linear programming. Combining these concepts, we propose a stopping rule which provides an upper bound on the probability of early termination. b) The second approach applies efficient computational budget allocation for objective function evaluation and contributes to identifying the best solution with a predicted lower bound on the probability of correct selection. It also reduces the variance of the upper bound estimate at optimality. Furthermore, it adaptively selects the evaluation sample size. Both approaches provide approximately optimal solutions even in cases with a huge number of scenarios, especially when scenarios are generated by using oracles/simulators. Finally, we demonstrate the effectiveness of these methods via extensive computational results for "megascale" (extremely large scale) stochastic facility location problems.

- *J. Xu* and S. Sen, "Compromise policy for multi-stage stochastic linear programming: Variance and Bias Reduction," *Computers and Operations Research*, vol. 153, pp. 106-132, *2023*. https://doi.org/10.1287/ijoc.2021.0324
    - This paper focuses on algorithms for multi-stage stochastic linear programming (MSLP). We propose an ensemble method named the ''compromise policy'', which not only reduces the variance of the function approximation but also reduces the bias of the estimated optimal value. It provides a tight lower bound estimate with a confidence interval. By exploiting parallel computing, the compromise policy provides demonstrable advantages in performance and stability with marginally extra computational time. We further propose a meta-algorithm to solve the MSLP problems based on in-sample and out-of-sample optimality tests. Our meta-algorithm is incorporated within an SDDP-type algorithm for MSLP and significantly improves the reliability of the decisions suggested by SDDP. These advantages are demonstrated via extensive computations, which illustrate the effectiveness of our approach.
- *S. Diao* and S. Sen, "Distribution-free Algorithms for Predictive Stochastic Programming (PSP) in the Presence of Streaming Data" *Computational Optimization and Applications*. https://doi.org/10.1007/s10589-023-00529-5
    - Predictive analytics, empowered by machine learning, is usually followed by decision-making problems in prescriptive analytics. In this paper, we extend the above sequential prediction-optimization paradigm to a coupled scheme such that the prediction model can guide the decision problem to produce coordinated decisions yielding higher levels of performance. This paper studies a fusion of concepts from stochastic programming and non-parametric statistical learning in which data is available in the form of covariates interpreted as predictors and responses. Such models are designed to impart greater agility, allowing decisions under uncertainty to adapt to the knowledge of predictors (leading indicators). This paper studies two classes of methods for such joint prediction-optimization models. One of the methods may be classified as a first-order method, whereas the other studies piecewise linear approximations. Both methods are based on coupling non-parametric estimation for

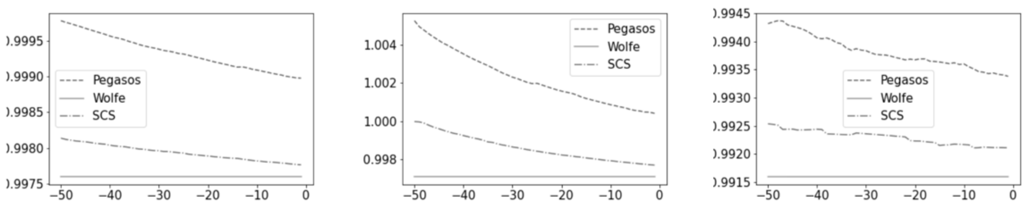
predictive purposes, and optimization for decision-making within one unified framework. In addition, or study incorporates several non-parametric estimation schemes, including k nearest neighbors (kNN) and other standard kernel estimators. Our computational results demonstrate that the new algorithms proposed in this paper outperform traditional approaches which were not designed for streaming data applications requiring simultaneous estimation and optimization as important design features for such algorithms. Such computational results motivate a paradigm shift in optimization algorithms that are intended for modern streaming applications.

- *D. Zhang* and S. Sen, "A Stochastic Conjugate Subgradient Algorithm for Kernelized Support Vector Machines: The Evidence" presented at a workshop in *NeurIPS, 2022*. A full and revised version is currently under review at *SIAM J. on Optimization*. (https://order-up-ml.github.io/papers/)
    - Kernel Support Vector Machines (Kernel SVM) provide a powerful class of tools for classifying data whose classes are best identified via a nonlinear function. While a Kernel SVM is traditionally treated as a Quadratic Program (QP), the current methods of choice belong to the category of first-order algorithms typified by stochastic gradient descent (SGD). In this paper we treat the Kernel SVM as a Stochastic Quadratic Linear Programming (SQLP) problem which motivates a decomposition-based algorithm which separates parameter choice from error estimation, with the latter being separable by data points. To take advantage of the quadratic structure due to the kernel matrix we introduce a stochastic conjugate subgradient approach which retains many of the advantages of first-order methods, while accommodating nonlinearity as well as non-smoothness. In this sense, it goes beyond first order algorithms for non-smooth convex optimization. Convergence rate of the new method is established in this paper.
    - ***Our computational experiments with this decomposition approach reveal that we can surpass the scalability of first order methods while improving both the speed and accuracy of optimization.*** This computational evidence is expected to be a game-changer because it appears to be the first algorithm which is beats a well-known first-order method (known as PEGASOS) across the spectrum of instances (for Kernel SVM) which have been solved. The PEGASOS algorithm has long reigned as one of the best first-order methods for Kernel SVMs because of its speed. However, as shown in Figures 1 and 2 below, the accuracy of SCS is far superior, although the first-order method can be faster on smaller instances. As the size of the data set increases however, PEGASOS is unable to match either the speed, accuracy, or scalability of the SCS method. To drive this point home, we present Table 1 which shows that as the size of the data set (no. of samples) increases to two million (Skin-Nonskin), PEGASOS is *not only slower, it is also less accurate*. Because the evidence is so compelling, we provide some graphs below. While this algorithm uses only first-order information, its clever use of the deterministic approach of Wolfe (1974) allows us to obtain a stochastic (online) version with very strong convergence properties.




Breast Cancer | Heart Failure | Wine Quality

Figure 1: First 50 iterations objective values for different combinations (data,algorithm).




Breast Cancer | Heart Failure | Wine Quality

Figure 2: Last 50 iterations objective values for different combinations (data,algorithm).

Table 1: Classification performance for different data sets

| | | heart attack | breast cancer | wine quality | avila Bible | magic telescope | room occupancy | Skin-Nonskin |
|---|---|---|---|---|---|---|---|---|
| | samples | 273 | 500 | 680 | 2000 | 5000 | 7500 | 200000 |
| | | | | | | | | |
| Pegasos | accuracy | 0.833 | 0.95 | 0.855 | 0.714 | 0.735 | 0.974 | 0.93 |
| | time(s) | 0.750 | 1.147 | 3.933 | 5.602 | 25.992 | 56.549 | 176.454 |
| | | | | | | | | |
| SCS | accuracy | 0.833 | 0.97 | 0.86 | 0.718 | 0.740 | 0.976 | 0.97 |
| | time(s) | 6.121 | 4.921 | 12.497 | 38.266 | 33.256 | 39.887 | 19.684 |
| | | | | | | | | |
| Wolfe | accuracy | 0.833 | 0.97 | 0.87 | 0.726 | N/A | N/A | N/A |
| | time(s) | 1.481 | 2.289 | 4.195 | 32.978 | N/A | N/A | N/A |

A full length paper on the theory and computations of the above paper has been submitted to *SIAM J. on Optimization*, and is currently in its second review (after a *positive first review*).

- ***Our computational experiments with this decomposition approach reveal that we can surpass the scalability of first order methods while improving both the speed and accuracy of optimization.*** This computational evidence is expected to be a game-changer because it appears to be the first algorithm which is beats a well-known first-order method (known as PEGASOS) across the spectrum of instances (for Kernel SVM) which have been solved. The PEGASOS algorithm has long reigned as one of the best first-order methods for Kernel SVMs because of its speed. However, as shown in Figures 1 and 2 below, the accuracy of SCS is far superior, although the first-order method can be faster on smaller instances. As the size of the data set increases however, PEGASOS is unable to match either the speed, accuracy, or scalability of the SCS method. To drive this point home, we present Table 1 which shows that as the size of the data set (no. of samples) increases to two million (Skin-Nonskin), PEGASOS is *not only slower, it is also less accurate*. Because the evidence is so compelling, we provide some graphs below. While this algorithm uses only first-order information, its clever use of the deterministic approach of Wolfe (1974) allows us to obtain a stochastic (online) version with very strong convergence properties.

- S. Diao and S. Sen, "A Unifying Theory for the Reliability of Stochastic Programming Solutions using Compromise Decisions," to be submitted to *Mathematical Programming*, 2024

  - This paper studies the reliability of stochastic programming solutions by using the notion of compromise decisions. A compromise decision is obtained by minimizing an aggregation of objective function approximations across replications with regularizing the candidate decisions of all replications. We refer to the post-parallel-processing problem as the problem of Compromise Decisions. We quantify the reliability of compromise decisions by estimating the expectation and variance of the pessimistic distance of sampled instances from the set of true optimal decisions. The Rademacher average of families of functions is used to bound the sample complexity of the compromise decision.

- D. Zhang, Y. Zhang and S. Sen *"A Sampling-based Progressive Hedging Algorithm for Stochastic Programming",* to be submitted to *Mathematical Programming*, 2024.

  - The Progressive Hedging Algorithm (PHA) is a cornerstone in tackling large-scale stochastic programming (SP) challenges. However, its traditional implementation is hindered by several limitations, including the requirement to solve all scenario subproblems in each iteration, reliance on an explicit probability distributions, and a convergence process that is highly sensitive to the choice of penalty parameters. This paper introduces a sampling-based PHA that aims to overcome these limitations. Our approach employs a dynamic selection process for the number of scenario subproblems solved per iteration. It incorporates adaptive sequential sampling for determining sample sizes, stochastic conjugate subgradient methods for direction finding, and a line-search technique to update the dual variables. Experimental results demonstrate that this novel algorithm not only addresses the bottlenecks of the conventional PHA but also potentially surpasses its scalability, representing a substantial improvement in the field of stochastic programming.

## 3. Student and Post-doc Funding and Placement

Thanks to the funding provided by this grant, we were able to support several students and post-doctoral scholars who have gone on to become post-doctoral scholars or faculty members at some of the top universities in the world (e.g., Northwestern University, Southern Methodist University, Tsinghua University), and some others have gone on to become applied scientists at some of the top "Tech" companies in the world (e.g., Google, Facebook, and Amazon).