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Design and Analysis of Computer Experiments

PhD in Statistics & Computer Science
Bocconi University

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Course Objectives. Researchers, private entities, and public organizations are increasingly turning to mathematical models— machine learning algorithms, artificial intelligence tools, and computer simulators — to inform decision-making. As concerns about explainability, interpretability, and responsible AI continue to grow, there is a pressing need for tools that clarify input–output relationships and ensure robust, transparent, and interpretable results. Tools from the design of computer experiments literature then become essential to address these challenges. The course offers students an in-depth journey into the use of computer simulations. It illustrates designs based on finite changes, with a connection to the functional ANOVA expansion and Shapley Values. It proposes an in depth theoretical investigation of the links between measures of statistical association and global sensitivity analysis, with attention to properties such as zero-independence and max-functionality. It connects these methods to post-hoc explainability in machine learning. The link between design of experiments, interpretability and sensitivity is analysed in depth. A variety of sensitivity methods (from measures of association based on optimal transport to Breiman's permuation importance) is discussed and illustrated with applications in simulation (deterministic and stochastic) and artificial intelligence (neural networks). The course emphasizes intuition and step-by-step examples drawn from real-world applications. The analysis of recent research papers on these topics conclude the course.

Course Outline

1. Explainability and Interpretability in Context (Borgonovo et al., 2023)
   - The Decision Analysis Process
   - Models of Phenomena and Models of Data
   - Families of Sensitivity Measures
2. Deterministic Methods
   - Tornado Diagrams (Howard, 1988)
   - Spider Plots (Eschenbach, 1992)

Finite-Change Indices and Generalized Tornado Diagrams (Borgonovo and Smith, 2011; Borgonovo, 2017)

Value of Information (Howard, 1966)

3. Global Sensitivity Analysis

   Properties of Measures of Statistical Association (Chatterjee and Harrison, 1988; Wiesel, 2022; Deb and Sen, 2021; Borgonovo et al., 2025b)

   Variance-Based Sensitivity Measures (Saltelli and Tarantola, 2002)

   Moment-Independent Measures (Borgonovo et al., 2014)

   Optimal-Transport Indices (Borgonovo et al., 2025c)

   Value of Information and Information Density (Hazen et al., 2023)

4. Explainability and Machine Learning

   Explainability and Sensitivity Analysis in Machine Learning (Rudin, 2019)

   Direction of Impact

   Partial Dependence Plots (Friedman, 2001)

   Individual Conditional Expectations (Goldstein et al., 2015)

   Accumulated Local Effects (ALE) Plots (Apley and Zhu, 2020)

   Trend Consistency and Diagnostic Indices (Borgonovo et al., 2025a)

   Variable Importance in Machine Learning (Fischer et al., 2017)

   Permutation Importance Breiman (2001)

   Shapley Values (Borgonovo et al., 2024)

5. . Into the future: Research Exercises

Exam The exam consists in a seminar presentation at the end of the course.

Course Material The course material shall consist of the readings and class notes provided by the teacher. All material shall be made available electronically.

References

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