Syllabus: Numerical Design Optimization

Course Information

Course Name: Numerical Design Optimization
Course Number: MANE 4280 (undergraduate) or MANE 6710 (graduate)
Section Number: 1
Credit Hours: 3 cr
Lecture: Tuesdays and Fridays, 10:00 ET – 11:20 ET
Mode of Delivery: In person, Troy 2012
Course Websites:

- Blackboard (LMS) for videos, handouts, assessment submission, and WebEx links
- Piazza for Q&A: `https://piazza.com/rpi/fall2024/mane42806710/info`

Prerequisites: MATH 2010 Multivariable Calculus and Matrix Algebra (or MATH 2011 and MATH 2012); and MANE 2110 Numerical Methods and Programming (or CSCI 1100 or permission of instructor). Students may not receive credit for both MANE 4280 and MANE 6710.

Instructor

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Course Description

This (co-listed) course introduces the theory and practical use of numerical design optimization methods. Topics include: gradient-based methods for unconstrained and constrained nonlinear optimization; numerical evaluation of derivatives; polynomial and kriging-based surrogate models; gradient-free optimization methods; optimization under uncertainty; multi-objective and multi-disciplinary optimization. Projects require the use of computer programs to generate numerical results; therefore, experience with programming is highly recommended.

Course Texts

J. R. R. A. Martins and A. Ning, "Engineering Design Optimization," free digital book.

Supplemental (Optional) References:

- J. S. Arora, "Introduction to Optimum Design," 3rd edition, Academic Press, 2012.
- J. Nocedal and Stephen J. Wright, "Numerical Optimization," 2nd edition, Springer, 2006.

Course Objectives

1. Identify and apply appropriate optimization algorithms/software for engineering design problems that are amenable to optimization.
2. Formulate design problems as optimization statements, selecting suitable mathematical models for the physical systems as necessary.
3. Prepare for relevant industrial positions that use, or could use, design optimization.

Learning Outcomes

Unconstrained Optimization of Smooth Objectives: After completing this subject area, students will be able to: explain local optima, global optima, and stationary points; state and explain the first-order necessary and second-order necessary/sufficient optimality conditions for a generic, unconstrained smooth objective; describe how the contours of an objective are related to its gradient and why the gradient is the direction of steepest descent; implement step computations for the steepest descent, Newton, and BFGS methods; describe the relative advantages and disadvantages of the steepest descent, Newton, and quasi-Newton methods; analyze the relative performance of two or more unconstrained optimization algorithm based on given data, and; formulate and solve unconstrained design optimization problems.

Computing and Analyzing Derivatives: After completing this subject area, students will be able to: state the advantages and disadvantages of 1) the finite-difference method; 2) the complex-step method, and; 3) algorithmic differentiation in the context of computing derivatives numerically; implement first- and second-order finite-difference formulae and the complex- step method in Matlab; apply algorithmic- differentiation software in both the forward and reverse modes; verify derivative accuracy using, e.g., simplified problems, and; identify the parameters that impact a design the most (sensitivity analysis).

Constrained Optimization of Smooth Objectives and Constraints: After completing this subject area, students will be able to: define the Lagrangian, and derive the first-order necessary conditions for a generic, constrained smooth problem; interpret the importance of a constraint based on its Lagrange multiplier; define and explain the feasible/infeasible spaces; implement and use penalty methods to find approximate solutions to constrained problems, and; use SQP/interior-point methods and assess their convergence.

Surrogate Modeling: After completing this subject area, students will be able to: state the advantages and disadvantages of surrogate models in the context of design optimization; in particular, explain the curse-of-dimensionality; employ sampling methods (e.g. Latin-hypercube sampling) to create the initial data for a surrogate model; find interpolants/fits based on linear and quadratic polynomials in n-dimensions; create Kriging-based (or GPR) surrogates for optimization, including the determination of parameters via maximization of the concentrated log-likelihood function, and; use surrogates in design optimization problems, including some form of adaptive sampling.

Gradient-free Optimization Methods: After completing this subject area, students will be able to: explain when gradient-free methods are appropriate, and when they are not; describe the Nelder-Mead simplex algorithm, the genetic algorithm, and the particle-swarm algorithm; apply gradient-free methods to solve optimization problems, either directly or on surrogate models; analyze the performance of two or more gradient-free optimization algorithms on the same problem, and; compare gradient-free and gradient- based algorithms on both smooth and non-smooth problems.

Optimization Under Uncertainty: After completing this subject area, students will be able to: explain the risks of using deterministic models in the context of design optimization; list sources of uncertainty that can impact design optimization, and explain the difference between aleatory and epistemic uncertainties; model random inputs using probability density functions, and apply Monte-Carlo and stochastic collocation methods for forward propagation of uncertainties, and; formulate and solve robust optimization and reliability-based optimization problems.

Other/Advanced Topics: After completing this subject area, students will be able to: select appropriate design-space parameterizations; select appropriate mathematical and/or computational models for engineering design problems, and implement them; explain Pareto optimality in the context of multi- objective optimization; explain multi-disciplinary analysis, and why it is critical in many fields of engineering design optimization, and; distinguish between high- and low-fidelity models, and when each is appropriate.

MANE 6710 Outcomes: In addition to the above, students enrolled in MANE 6710 are expected to; identify and read appropriate academic literature; write software for engineering analysis and/or combine analysis software with optimization software; present methodology and results in an academic-style report.

Course Assessment Measures

Assessment	Due Date	Learning Outcomes
In-class assignments	day of lecture	1–7
Test # 1	T Oct 1	1, 2
Test # 2	F Nov 1	3, 4
Test # 3	T Dec 10	5, 6, 7
Project # 1	T Sep 24	1, 2
Project # 2	F Oct 18	2, 3
Project # 3	T Nov 12	4, 5
Project # 4	T Dec 10	6
Analysis-model write-up #1	T Sep 10	7

Assessment	Due Date	Learning Outcomes
Analysis-model write-up #2	F Oct 4	7
Analysis-model write-up #3	F Oct 25	7
Analysis-model write-up #4	T Nov 19	7
Peer review #1	T Oct 1	7
Peer review #2	T Oct 29	7
Peer review #3	F Nov 22	7
Peer review #4	M Dec 16	7
Independent study report[1]	W Dec 18	8

Grading Criteria

MANE 4280:

- 64% projects ($4 \times 16\%$)
- 18% tests ($3 \times 6\%$)
- 6% in-class assignments
- 6% analysis-model write-ups ($4 \times 1.5\%$)
- 6% peer reviews ($4 \times 1.5\%$)

Note: The two in-class assignments on which a student scores lowest — including assignments not submitted — will not be included in a student's assignment grade. For example, a student who scores 100% on all assignments except for two will obtain a 100% assignment score.

MANE 6710:

- 64% projects ($4 \times 16\%$)
- 18% independent study report
- 12% tests ($3 \times 4\%$)
- 6% peer reviews ($4 \times 1.5\%$)

Letter Grade Determination

Your final letter grade will be calculated using the table below. The threshold refers to the numeric grade, as displayed in the LMS, at or above which you would obtain the corresponding letter grade.

Grade thresholds for MANE 4280:

Letter Grade	A	A-	B+	B	B-	C+	C	C-	D+	D	F
Threshold	94	90	87	84	80	77	74	70	67	60	< 60

Grade thresholds for MANE 6710:

[1] Only for students enrolled in MANE 6710

Letter Grade	A	A-	B+	B	B-	C+	C	C-	F
Threshold	94	90	87	84	80	77	74	70	< 70

Attendance Policy

Attendance is mandatory given the studio format of the lecture and the frequent in-class exercises.

Other Course Policies

- Projects will receive a 10% penalty if handed in within 24 hours of the deadline; a 25% penalty if handed in within a week of the deadline, and; a 100% penalty otherwise. In other words, projects handed in a week past the deadline will receive a grade of 0, notwithstanding excused absences.
- Extensions for assignments and analysis-model write-ups will *not* be given without a valid excused absence.
- Make-up tests will be provided with valid excused absence only.
- Grade challenges must be brought forward no more than one week after the grade is made available.

Academic Integrity

Student-teacher relationships are built on trust. For example, students must trust that teachers have made appropriate decisions about the structure and content of the courses they teach, and teachers must trust that the assignments that students turn in are their own. Acts that violate this trust undermine the educational process. The Rensselaer Handbook of Student Rights and Responsibilities and The Graduate Student Supplement define various forms of Academic Dishonesty and you should make yourself familiar with these. In this class, all assignments, projects, and tests that are turned in for a grade must represent the students own work. In cases where help was received, or collaboration was allowed, a notation on the assignment should indicate your collaboration.

- Submission of any assignment, project, or test that is in violation of this policy will result in a grade of zero on the first offense. If there is a subsequent infraction the student will receive a grade of F for the course.
- If you have any question concerning this policy before submitting an assignment, please ask for clarification.
- Collaboration and discussion is encouraged on the projects; *however, students must write their code and reports individually*.

Diversity and Inclusion Statement

I believe that diversity makes engineering teams stronger and more innovative, which is needed to have a positive impact on our world. Therefore, I strive to support full participation and success in this course for every student regardless of their background, experience, race, sexual and gender identity, religion, ability, or age. To honor such diversity, I aim to create a safe and welcoming environment, in and out of class, for respectful interactions and discourse. To that end, please let me know if there is information about you that will help me (e.g., preferred pronouns, accommodations, religious commitments). Concerns and feedback (also anonymously provided) are welcomed, respectfully considered, and will be used to improve the class and its atmosphere.

All participants in this course are encouraged to recognize the diversity around them and expected to treat their classmates with respect. Disrespectful, harmful, offensive, bigoted, or violent language or behavior will not be tolerated.

Schedule

In the schedule below, the column "Reading" refers to the relevant chapter from the Martins and Ning's ebook "Engineering Design Optimization." They present similar material to the videos, but in a different order. The readings are recommended because they complement the videos.

Date		Video and Lecture Content	Reading	What's Due?
F Aug 30	(1)	► introduction to optimization ► problem classification ► local versus global optima		Assignment #1
T Sep 3		Follow Monday schedule (no class)		
F Sep 6	(2)	► the gradient and level-set contours ► first-order optimality conditions ► *describe Project # 1*	Chap. 4 §4.1	Assignment #2
T Sep 10	(3)	► steepest descent method ► Wolfe conditions ► line-search algorithms ► *Project # 1 model discussion*	Chap. 4 §4.3–4.4.1	Project #1 Model Assignment #3
F Sep 13	(4)	► Sensitivity analysis ► finite-difference methods ► complex-step method	Chap. 6 §6.1–6.5	Assignment #4
T Sep 17	(5)	► second-order optimality conditions ► the Hessian and its eigenvalues ► *introduction to fmincon*	Chap. 4 §4.1	Assignment #5

Date		Video and Lecture Content	Reading	What's Due?
F Sep 20	(6)	▸ Newton's method and its globalization ▸ trust-region algorithms ▸ *work on project # 1*	Chap. 4 §4.4.3, 4.5	Assignment #6
T Sep 24	(7)	▸ Quasi-Newton methods ▸ BFGS	Chap. 4 §4.4.4	Project # 1 Assignment #7
F Sep 27	(8)	▸ algorithmic differentiation ▸ *describe Project # 2*	Chap. 6 §6.6	Assignment #8
T Oct 1		**Test 1: lectures 1–8**		Peer Review # 1
F Oct 4	(9)	▸ constrained optimization problems ▸ types of constraints ▸ feasible and infeasible design space ▸ *Project # 2 model discussion*	Chap. 1& 5 §1.2.3, 5.1	Project # 2 Model Assignment #9
T Oct 8	(10)	▸ constraint Jacobian ▸ Lagrangian and Lagrange multipliers ▸ first-order optimality: equality constraints ▸ *fmincon revisited*	Chap. 5 §5.3.1	Assignment #10
F Oct 11	(11)	▸ first-order optimality: inequality constraints ▸ interpretation of Lagrange multipliers ▸ *work on project # 2*	Chap. 5 §5.3.2–5.3.3	Assignment #11
T Oct 15	(12)	▸ penalty and barrier methods for constrained optimization ▸ SQP and interior point methods ▸ *work on project # 2*	Chap. 5 §5.4–5.6	Assignment #12
F Oct 18	(13)	▸ surrogate modeling overview ▸ data generation for surrogate models	Chap. 10 §10.1–10.2	Project # 2 Assignment #13

Date		Video and Lecture Content	Reading	What's Due?
T Oct 22	(14)	▸ regression and interpolation ▸ generalized linear models ▸ radial basis functions ▸ *describe Project # 3*	Chap. 10 §10.3.1, 10.3.5	Assignment #14
F Oct 25	(15)	▸ Gaussian process regression ▸ *Project # 3 model discussion*	Chap. 10 §10.4	Project # 3 Model Assignment #15
T Oct 29	(16)	▸ parameter estimation via max likelihood ▸ using surrogates in optimization ▸ *fminunc*	Chap. 10 §10.3.2, 10.6	Peer Review # 2 Assignment #16
F Nov 1		**Test 2: lectures 9–16**		
T Nov 5	(17)	▸ gradient-free optimization overview ▸ Nelder-Mead simplex method ▸ *work on project # 3*	Chap. 7 §7.1–7.3	Assignment #17
F Nov 8	(18)	▸ genetic/evolutionary algorithms ▸ *work on project # 3*	Chap. 7 §7.6	Assignment #18
T Nov 12	(19)	▸ particle-swarm optimization	Chap. 7 §7.7	Project # 3 Assignment #19
F Nov 15	(20)	▸ uncertainties in engineering analysis ▸ optimization under uncertainty ▸ *describe Project # 4*	Chap. 12 §12.1–12.2	Assignment #20
T Nov 19	(21)	▸ Monte-Carlo methods ▸ stochastic collocation ▸ *Project # 4 model discussion*	Chap. 12 §12.3.2– 12.3.3	Project # 4 Model Assignment #21
F Nov 22	(22)	▸ reliability analysis ▸ reliability analysis using Monte-Carlo ▸ first-order reliability method		Peer Review # 3 Assignment #22

Date		Video and Lecture Content	Reading	What's Due?
T Nov 26	(23)	► multi-objective optimization ► methods for multi-objective problems ► *work on project # 4*	Chap. 9 §9.1–9.4	Assignment #23
F Nov 29		Native American Heritage Day (no class)		
T Dec 3	(24)	► multi-disciplinary design optimization ► solving MDO problems ► *work on project # 4*	Chap. 13 §13.1–13.6	Assignment #24
F Dec 6	(25)	► choosing the right tool for the job ► *work on project # 4*	Chap. 1 §1.5	Assignment #25
T Dec 10		**Test 3: lectures 17–25**		Project # 4
M Dec 16				Peer Review # 4
W Dec 18				Project for MANE 6710