Lectures for Mathematical Modeling

Chapter 5: Experimental Modeling

Your Name

Your Institution

Chapter Overview

The Foundation of Scientific Knowledge

Theory Meets Reality

When we think about how scientific knowledge advances, we often imagine brilliant theorists working in isolation. While theoretical work is crucial, most understanding comes from the careful interplay between theory and experimentation.

Historical Examples:

- Newton's gravity theory gained acceptance through successful predictions
- Einstein's relativity validated through carefully designed experiments
- Modern medicine relies on experimental validation of theoretical models

The Foundation of Scientific Knowledge

Theory Meets Reality

When we think about how scientific knowledge advances, we often imagine brilliant theorists working in isolation. While theoretical work is crucial, most understanding comes from the careful interplay between theory and experimentation.

Modern Applications:

- Developing new medical treatments
- Designing more efficient engines
- Understanding social behaviors
- Optimizing manufacturing processes

The Foundation of Scientific Knowledge

Theory Meets Reality

When we think about how scientific knowledge advances, we often imagine brilliant theorists working in isolation. While theoretical work is crucial, most understanding comes from the careful interplay between theory and experimentation.

Key Insight

Mathematical models, no matter how elegant, must ultimately be tested against reality through systematic experimentation.

This chapter bridges the gap between mathematical theory and practical application through experimental modeling.

A Simple Example: Understanding Plant Growth

Example (Sunlight and Plant Growth)

Imagine you're trying to understand how sunlight affects plant growth. You start with a simple question: "Do plants grow taller with more sunlight?"

The System:

- **Input variable**: Amount of sunlight (hours per day)
- **Output variable**: Plant height after fixed time
- **Goal**: Develop mathematical relationship between sunlight and growth

A Simple Example: Understanding Plant Growth

Example (Sunlight and Plant Growth)

Imagine you're trying to understand how sunlight affects plant growth. You start with a simple question: "Do plants grow taller with more sunlight?"

A Naive Approach:

- Simply observe plants in nature
- Measure heights in different locations
- Look for correlations

Problems with this approach:

- Plants in sunny locations might have better soil
- Different genetic varieties
- Varying water availability
- Cannot isolate causal factors

A Simple Example: Understanding Plant Growth

Example (Sunlight and Plant Growth)

Imagine you're trying to understand how sunlight affects plant growth. You start with a simple question: "Do plants grow taller with more sunlight?"

The Experimental Approach:

- Create controlled conditions
- Systematically vary only sunlight
- Keep everything else constant
- Use multiple groups: 2, 4, 6, 8 hours per day

Mathematical Model:

$$\text{Height} = a + b \times \text{Sunlight Hours} + \text{Error}$$

This controlled approach enables reliable causal inference.

Key Elements of Experimental Modeling

Fundamental Components

Our simple plant growth example illustrates key concepts that apply to all experimental modeling:

Controlled Manipulation:

- Deliberately change the input (sunlight)
- Keep other factors constant (soil, water, temperature)
- Create conditions that don't occur naturally

Key Elements of Experimental Modeling

Fundamental Components

Our simple plant growth example illustrates key concepts that apply to all experimental modeling:

Systematic Design:

- Choose specific levels of input to test
- Ensure adequate coverage of the range of interest
- Balance experimental effort with information gain

Key Elements of Experimental Modeling

Fundamental Components

Our simple plant growth example illustrates key concepts that apply to all experimental modeling:

Replication:

- Include multiple plants in each group
- Account for natural variation
- Enable statistical inference

Key Elements of Experimental Modeling

Fundamental Components

Our simple plant growth example illustrates key concepts that apply to all experimental modeling:

Mathematical Modeling:

- Use data to develop quantitative relationships
- Express results in mathematical form
- Enable prediction and optimization

Definition (Experimental Modeling)

Experimental modeling is the systematic use of controlled manipulation to understand systems and build mathematical descriptions of their behavior.

Why Control Matters: The Confounding Problem

Experimental vs. Observational Studies

The difference between experimental and observational studies is crucial for developing reliable mathematical models.

Example (Study Time and Test Scores)

Observational Study: You notice students who study more get higher scores. Strong positive correlation found in 100 students.
Question: Can you conclude studying causes higher scores?

Why Control Matters: The Confounding Problem

Experimental vs. Observational Studies

The difference between experimental and observational studies is crucial for developing reliable mathematical models.

Potential Confounding Factors:

- Students who study more might be naturally more motivated
- Better study environments at home
- Taking easier courses
- Better prior preparation
- Different learning abilities

These alternatives make it impossible to isolate the causal effect of study time.

Why Control Matters: The Confounding Problem

Experimental vs. Observational Studies

The difference between experimental and observational studies is crucial for developing reliable mathematical models.

Experimental Approach:

- Randomly assign students to different study time requirements
- Control for confounding factors
- Measure results under controlled conditions

Definition (Experimental vs. Observational Studies)

Observational: Observe without manipulation. Discovers associations but cannot establish causation.
Experimental: Deliberately manipulate factors. Enables causal relationships and predictive models.

The Three Pillars of Good Experimental Design

Fundamental Principles

Three principles apply to all experimental modeling, from simple to sophisticated:

Replication: Why You Need Multiple Units

- Using one plant per condition would be unreliable
- Natural variation requires multiple observations
- Enables estimation of experimental error
- Provides statistical foundation for inference
- Distinguishes real effects from random noise

The Three Pillars of Good Experimental Design

Fundamental Principles

Three principles apply to all experimental modeling, from simple to sophisticated:

Randomization: Why Assignment Should Be Random

- Prevents unconscious bias in assignment
- Ensures representative distribution across groups
- Makes statistical analysis methods valid
- Insurance against known and unknown sources of bias

The Three Pillars of Good Experimental Design

Fundamental Principles

Three principles apply to all experimental modeling, from simple to sophisticated:

Control: Why Everything Else Must Stay the Same

- Isolates the effect of the factor being studied
- Holds potentially confounding variables constant
- Enables attribution of effects to manipulated variables
- Foundation for causal inference

Universal Application

These principles apply whether studying plants, engineering systems, social behaviors, or any other system.

Mathematical Representation of Experiments

From Intuition to Formalism

Every experiment can be described mathematically, enabling rigorous design and analysis.

Definition (Experimental System (Basic))

An experimental system consists of:

- **Input variables** (factors): $x_1, x_2, \ldots, x_k$ that we control
- **Output variable** (response): y that we observe
- **System function**: f that relates inputs to outputs
- **Error term**: ϵ that captures uncontrolled variation

The basic experimental model: $y = f(x_1, x_2, \ldots, x_k) + \epsilon$

Mathematical Representation of Experiments

From Intuition to Formalism

Every experiment can be described mathematically, enabling rigorous design and analysis.

Plant Growth Example Revisited:

- Input variable: $x =$ hours of sunlight
- Output variable: $y =$ plant height
- System function: $f(x) = a + bx$ (linear relationship)
- Error term: $\epsilon =$ genetics, measurement error, other factors

Complete model: $y = a + bx + \epsilon$

Mathematical Representation of Experiments

From Intuition to Formalism

Every experiment can be described mathematically, enabling rigorous design and analysis.

Benefits of Mathematical View:

- Forces precision about what we're studying
- Helps identify what needs to be controlled
- Guides choice of analytical methods
- Enables predictions about new conditions

Transformation

Mathematical framework transforms experimental design from art to science.

Experimental Design as Optimization

The Design Problem

Once we have mathematical representation, experimental design becomes an optimization problem: How do we choose input values to learn as much as possible?

Definition (Design Space and Design Points)

- **Design space** $\mathcal{X}$: Set of all possible input combinations
- **Design points**: Specific combinations $\mathbf{x}_i$ that we test
- **Experimental design**: Collection of n design points $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$

Experimental Design as Optimization

The Design Problem

Once we have mathematical representation, experimental design becomes an optimization problem: How do we choose input values to learn as much as possible?

Plant Example Design Choices:

- Design space: $\mathcal{X} = [0, 12]$ hours of sunlight
- Design option 1: $\{2, 4, 6, 8\}$ hours
- Design option 2: $\{1, 3, 7, 11\}$ hours
- Design option 3: $\{0, 4, 8, 12\}$ hours

Crucial Question: Which design is better?

Experimental Design as Optimization

The Design Problem

Once we have mathematical representation, experimental design becomes an optimization problem: How do we choose input values to learn as much as possible?

What Makes a Design "Better"?

- More precise parameter estimates
- Better prediction accuracy
- Greater ability to detect effects
- Robustness to assumptions

This leads us toward optimal design theory and systematic approaches to design selection.

Precision and Bias in Parameter Estimation

Quality Metrics for Experiments

Experimental quality depends on how well we can estimate unknown parameters in our mathematical model.

Definition (Bias and Precision)

For parameter θ and estimate $\hat{\theta}$:

- **Bias**: $\text{Bias}(\hat{\theta}) = E[\hat{\theta}] - \theta$
- **Precision**: Measured by $\text{Var}(\hat{\theta})$ (smaller = more precise)
- **Mean Squared Error**: $\text{MSE}(\hat{\theta}) = \text{Bias}^2(\hat{\theta}) + \text{Var}(\hat{\theta})$

Precision and Bias in Parameter Estimation

Quality Metrics for Experiments

Experimental quality depends on how well we can estimate unknown parameters in our mathematical model.

Practical Interpretation:

- **Unbiased estimator**: Correct parameter value on average
- **Precise estimator**: Similar results when experiment repeated
- **Good estimator**: Both unbiased and precise (low MSE)

Precision and Bias in Parameter Estimation

Quality Metrics for Experiments

Experimental quality depends on how well we can estimate unknown parameters in our mathematical model.

How Design Affects Quality:

- Poor spacing of design points $\rightarrow$ bias in estimates
- Too few replicates $\rightarrow$ low precision
- Clustering points in one region $\rightarrow$ reduced precision
- Extreme points $\rightarrow$ better precision for linear models

Understanding these relationships enables optimal experimental design.

Studying Multiple Factors Systematically

Beyond One Factor at a Time

Real systems rarely depend on just one factor. Plants need both sunlight and water; drug effectiveness depends on dose and timing; engineering performance depends on multiple design parameters.

One-Factor-at-a-Time Approach:

- Fix water, study sunlight effect
- Fix sunlight, study water effect
- Seems logical and systematic

Serious Limitations:

- Assumes factors don't interact
- Inefficient use of experimental resources
- Can miss important interaction effects

Studying Multiple Factors Systematically

Beyond One Factor at a Time

Real systems rarely depend on just one factor. Plants need both sunlight and water; drug effectiveness depends on dose and timing; engineering performance depends on multiple design parameters.

The Factorial Approach:

- Study both factors simultaneously
- Use all combinations of factor levels
- More efficient and informative
- Reveals interaction effects

Key Advantage

Factorial designs enable discovery of interactions that would be completely missed by one-factor-at-a-time approaches.

2×2 Factorial Design Example

Example (Plant Growth with Sunlight and Water)

Two factors: Sunlight (4 vs. 8 hours) and Water (100ml vs. 200ml daily)

Four Experimental Conditions:

- Low sunlight, low water
- Low sunlight, high water
- High sunlight, low water
- High sunlight, high water

This design tests all possible combinations systematically.

2×2 Factorial Design Example

Example (Plant Growth with Sunlight and Water)

Two factors: Sunlight (4 vs. 8 hours) and Water (100ml vs. 200ml daily)

Information Obtained:

- **Main effect of sunlight**: Average difference between high and low sunlight
- **Main effect of water**: Average difference between high and low water
- **Interaction effect**: Whether sunlight effect depends on water level

2×2 Factorial Design Example

Example (Plant Growth with Sunlight and Water)

Two factors: Sunlight (4 vs. 8 hours) and Water (100ml vs. 200ml daily)

Mathematical Model:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \epsilon$$

where:

- x_1 = sunlight level (coded as -1, +1)
- x_2 = water level (coded as -1, +1)
- β_{12} = interaction coefficient

If $\beta_{12} \neq 0$, factors interact.

Mathematical Structure of Factorial Designs

Elegant Mathematical Properties

Factorial designs have mathematical structure that makes them particularly powerful for experimental modeling.

Definition (2^k Factorial Design)

A 2^k factorial design studies k factors, each at 2 levels (coded as -1 and +1). This creates 2^k experimental conditions corresponding to all possible combinations.

General Model:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i<j} \beta_{ij} x_i x_j + \ldots + \beta_{123\ldots k} x_1 x_2 \cdots x_k + \epsilon$$

Mathematical Structure of Factorial Designs

Elegant Mathematical Properties

Factorial designs have mathematical structure that makes them particularly powerful for experimental modeling.

Theorem (Orthogonality in 2^k Designs)

In a 2^k factorial design with coded variables, all model terms are orthogonal, meaning:

- *Each effect can be estimated independently*
- *Parameter estimates have minimum variance*
- *Statistical tests for different effects are independent*

Mathematical Structure of Factorial Designs

Elegant Mathematical Properties

Factorial designs have mathematical structure that makes them particularly powerful for experimental modeling.

Why Orthogonality Matters:

- Makes mathematics simpler and more elegant
- Ensures estimates are as precise as possible
- Can interpret each effect separately
- Design is robust to missing data

Mathematical elegance translates to practical advantages for experimental analysis.

Interaction Effects: When $1 + 1 \neq 2$

Beyond Additive Effects

One of the most important advantages of factorial designs is detecting interactions—situations where factors influence each other.

Definition (Interaction Effect)

An interaction exists between factors A and B if the effect of factor A depends on the level of factor B. Mathematically: $\beta_{AB} \neq 0$ in the model.

Types of Interactions:

- **No interaction**: Parallel lines when plotting response vs. A for different B levels
- **Moderate interaction**: Lines with different slopes
- **Strong interaction**: Lines that cross

Interaction Effects: When $1 + 1 \neq 2$

Beyond Additive Effects

One of the most important advantages of factorial designs is detecting interactions—situations where factors influence each other.

Example (Drug Interaction)

Two drugs for treating a condition:

- Drug A alone: Moderate effectiveness
- Drug B alone: Moderate effectiveness
- Drugs A and B together: Could be highly effective (synergy) or dangerous (antagonism)

Factorial design reveals whether drugs work additively or interact—potentially life-saving information.

Interaction Effects: When $1 + 1 \neq 2$

Beyond Additive Effects

One of the most important advantages of factorial designs is detecting interactions—situations where factors influence each other.

Real-World Significance:

- Engineering: Material properties depend on temperature AND pressure
- Medicine: Drug effectiveness depends on dose AND timing
- Agriculture: Fertilizer response depends on soil type AND weather
- Manufacturing: Quality depends on multiple process parameters

Critical Point

Interactions are everywhere in real systems. One-factor-at-a-time approaches miss them completely.

Modeling Complex Relationships

Beyond Linear Models

While factorial designs excel for understanding effects and interactions, they assume specific model forms. When we need more complex relationships or optimization, we turn to Response Surface Methodology (RSM).

Philosophy of RSM:

- Focus on building accurate empirical models
- Emphasize prediction and optimization over mechanism understanding
- Use local approximation rather than global modeling
- Employ sequential learning strategies

Modeling Complex Relationships

Beyond Linear Models

While factorial designs excel for understanding effects and interactions, they assume specific model forms. When we need more complex relationships or optimization, we turn to Response Surface Methodology (RSM).

Key Ideas:

- **Local approximation**: Build accurate models in regions of interest
- **Polynomial models**: Flexible local approximations using Taylor series
- **Sequential design**: Use each experiment to guide the next
- **Optimization focus**: Design experiments to support performance optimization

Modeling Complex Relationships

Beyond Linear Models

While factorial designs excel for understanding effects and interactions, they assume specific model forms. When we need more complex relationships or optimization, we turn to Response Surface Methodology (RSM).

Definition (Response Surface Model)

A response surface model approximates the unknown function $\eta(\mathbf{x})$:

$$y(\mathbf{x}) = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j} \beta_{ij} x_i x_j + \epsilon$$

Components:

- Linear terms: Main effects
- Quadratic terms: Curvature
- Cross-product terms: Interactions

Why Polynomial Models Work

Theoretical and Practical Advantages

Polynomial response surfaces are the workhorses of empirical modeling for several reasons:

Theoretical Justification:

- Taylor's theorem: Any smooth function can be approximated locally by polynomials
- Higher-order terms can be added as needed
- Flexibility increases with polynomial degree

Why Polynomial Models Work

Theoretical and Practical Advantages

Polynomial response surfaces are the workhorses of empirical modeling for several reasons:

Practical Advantages:

- Easy to fit using linear regression methods
- Computationally efficient
- Provide interpretable mathematical relationships
- Enable analytical optimization using calculus
- Parameters have clear physical meaning

Why Polynomial Models Work

Theoretical and Practical Advantages

Polynomial response surfaces are the workhorses of empirical modeling for several reasons:

Optimization Capability: For optimization, we can find critical points analytically:

$$\frac{\partial y}{\partial x_i} = \beta_i + 2\beta_{ii}x_i + \sum_{j \neq i} \beta_{ij}x_j = 0$$

This system of equations locates optima directly from the fitted model.

Central Composite Designs

Efficient Designs for Response Surfaces

To fit second-order polynomial models, we need designs that provide information about curvature. Central Composite Designs (CCDs) achieve this efficiently.

Definition (Central Composite Design)

A CCD combines:

- **Factorial points**: 2^k or 2^{k-p} factorial design (corners of hypercube)
- **Axial points**: Points at distance α from center along coordinate axes
- **Center points**: Multiple points at origin for error estimation

Central Composite Designs

Efficient Designs for Response Surfaces

To fit second-order polynomial models, we need designs that provide information about curvature. Central Composite Designs (CCDs) achieve this efficiently.

Design Parameters:

- α = axial distance from center
- n_c = number of center points
- These choices determine design properties

Theorem (Rotatability Condition)

A CCD is rotatable (constant prediction variance at equal distances from center) if and only if:

$$\alpha = (2^k)^{1/4}$$

Central Composite Designs

Efficient Designs for Response Surfaces

To fit second-order polynomial models, we need designs that provide information about curvature. Central Composite Designs (CCDs) achieve this efficiently.

Why Rotatability Matters:

- Design performs equally well in all directions
- Balanced information about response surface
- No directional bias in exploration
- Particularly valuable when optimum location is unknown

Design Philosophy

Rotatability ensures the design doesn't favor exploration in particular directions, providing balanced coverage of the local region.

Sequential Response Surface Methods

Moving Toward Optimum Conditions

One of RSM's most powerful aspects is its sequential nature—systematically moving toward optimal regions rather than trying to explore everything at once.

Sequential RSM Process:

- **Phase I**: Use first-order designs to identify improvement direction
- **Steepest ascent/descent**: Move toward better regions
- **Phase II**: When improvement slows, use second-order designs
- **Optimization**: Locate optimum precisely

Sequential Response Surface Methods

Moving Toward Optimum Conditions

One of RSM's most powerful aspects is its sequential nature—systematically moving toward optimal regions rather than trying to explore everything at once.

Definition (Steepest Ascent Method)

Using first-order model $\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i$, move along:

$$\mathbf{x}_{new} = \mathbf{x}_{center} + \lambda \frac{\nabla \hat{y}}{\|\nabla \hat{y}\|}$$

where λ determines step size and $\nabla \hat{y} = (\hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_k)$.

Sequential Response Surface Methods

Moving Toward Optimum Conditions

One of RSM's most powerful aspects is its sequential nature—systematically moving toward optimal regions rather than trying to explore everything at once.

When Sequential RSM is Valuable:

- Experimental region is large and optimum location unknown
- Experiments are expensive—want to minimize number needed
- System is complex and local exploration more practical than global modeling
- Real-time optimization where conditions can change

Sequential approach enables efficient exploration while minimizing experimental effort.

Engine Optimization Example

Example (Automotive Performance Optimization)

An automotive engineer wants to optimize engine performance by adjusting fuel injection timing and air-fuel ratio. Response: fuel efficiency (mpg).

Central Composite Design:

- **Factorial points**: All combinations of high/low timing and ratio
- **Axial points**: Extreme timing (ratio at center), extreme ratio (timing at center)
- **Center points**: Several runs at nominal settings

Engine Optimization Example

Example (Automotive Performance Optimization)

An automotive engineer wants to optimize engine performance by adjusting fuel injection timing and air-fuel ratio. Response: fuel efficiency (mpg).

Response Surface Model:

$$\text{MPG} = \beta_0 + \beta_1 T + \beta_2 R + \beta_{11} T^2 + \beta_{22} R^2 + \beta_{12} T R$$

where T = timing, R = air-fuel ratio.

Engine Optimization Example

Example (Automotive Performance Optimization)

An automotive engineer wants to optimize engine performance by adjusting fuel injection timing and air-fuel ratio. Response: fuel efficiency (mpg).

Information Gained:

- Optimal settings for maximum efficiency
- Sensitivity of efficiency to each factor
- Interaction effects between timing and ratio
- Robustness analysis for varying operating conditions

This enables both optimization and robust design that performs well under uncertainty.

Mathematical Foundations for Efficient Experimentation

When Resources are Limited

As experiments become more expensive and systems more complex, it becomes crucial to design experiments that extract maximum information from minimum effort.

The Optimization Question: Given limited experimental resources, how do we choose design points to maximize information about our system?

This leads to mathematical optimization problems:

- What criterion should we optimize?
- How do we quantify "information"?
- What constraints must we consider?

Mathematical Foundations for Efficient Experimentation

When Resources are Limited

As experiments become more expensive and systems more complex, it becomes crucial to design experiments that extract maximum information from minimum effort.

Why Optimal Design Matters:

- Experimental resources are often expensive (time, money, materials)
- Poor designs waste resources and provide poor information
- Systematic approaches can dramatically improve efficiency
- Mathematical theory provides principled solutions

Impact

Optimal designs can often provide the same information as standard designs using 30-50

Information Matrix and Optimality Criteria

Quantifying Information

The mathematical foundation for optimal design comes from the information matrix and various optimality criteria.

Definition (Information Matrix)

For linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, the information matrix is:

$$\mathbf{M} = \mathbf{X}^T\mathbf{X}$$

This matrix quantifies how much information the design provides about the parameters.

Information Matrix and Optimality Criteria

Quantifying Information

The mathematical foundation for optimal design comes from the information matrix and various optimality criteria.

Common Optimality Criteria:

- **D-optimality**: Maximize $\det(\mathbf{M})$ (minimize volume of confidence ellipsoid)
- **A-optimality**: Minimize trace$(\mathbf{M}^{-1})$ (minimize average parameter variance)
- **E-optimality**: Maximize $\lambda_{\min}(\mathbf{M})$ (minimize maximum parameter variance)
- **G-optimality**: Minimize maximum prediction variance

Information Matrix and Optimality Criteria

Quantifying Information

The mathematical foundation for optimal design comes from the information matrix and various optimality criteria.

Intuitive Interpretations:

- **D-optimal**: Make parameter estimates as precise as possible overall
- **A-optimal**: Minimize average uncertainty in parameters
- **E-optimal**: Ensure no parameter is estimated very poorly
- **G-optimal**: Provide good predictions everywhere in design region

Choice depends on primary goal: parameter estimation, prediction, or robustness.

The General Equivalence Theorem

Remarkable Mathematical Result

One of the most elegant results in design theory connects different optimality criteria.

Theorem (Equivalence of D- and G-Optimality)

For polynomial regression models, D-optimal and G-optimal designs are equivalent.

Implications:

- Designs that minimize parameter uncertainty also minimize prediction uncertainty
- Provides both theoretical insight and computational advantages
- Unifies different design objectives

The General Equivalence Theorem

Remarkable Mathematical Result

One of the most elegant results in design theory connects different optimality criteria.

Practical Consequences:

- Can optimize for parameter estimation and get good prediction properties automatically
- Computational algorithms can focus on one criterion
- Provides theoretical justification for D-optimality
- Simplifies design choice decisions

This remarkable connection between seemingly different objectives highlights the deep mathematical structure underlying experimental design.

Computing Optimal Designs

From Theory to Practice

Finding optimal designs requires solving constrained optimization problems. Several algorithms make this practical.

Exchange Algorithms:

1. Start with initial design
2. For each candidate point, calculate improvement if added
3. Add point giving maximum improvement
4. Examine each current design point
5. Remove point causing minimum degradation
6. Repeat until convergence

Computing Optimal Designs

From Theory to Practice

Finding optimal designs requires solving constrained optimization problems. Several algorithms make this practical.

Algorithm Properties:

- Iterative improvement approach
- Guaranteed to improve design at each step
- Converge to designs satisfying optimality conditions
- Computationally efficient for moderate-sized problems

Theorem (Convergence of Exchange Algorithms)

Under mild regularity conditions, exchange algorithms converge to designs satisfying optimality conditions.

Computing Optimal Designs

From Theory to Practice

Finding optimal designs requires solving constrained optimization problems. Several algorithms make this practical.

Practical Considerations:

- Global optimality not guaranteed, but results typically excellent
- Multiple starting points can improve results
- Modern software makes optimal design accessible
- Computational cost scales with problem size

Exchange algorithms have made optimal design practical for real experimental problems.

Modern Experimental Modeling

Beyond Fixed Designs

Modern experimental modeling increasingly relies on adaptive strategies that use information from previous experiments to guide future choices.

Why Adaptive Strategies?

- Experimental resources are often limited
- Large experimental spaces make exhaustive exploration impossible
- Prior knowledge is often incomplete or uncertain
- Real-time learning can improve efficiency dramatically

Modern Experimental Modeling

Beyond Fixed Designs

Modern experimental modeling increasingly relies on adaptive strategies that use information from previous experiments to guide future choices.

Key Concepts:

- **Sequential design**: Use results from each experiment to plan the next
- **Adaptive strategies**: Modify experimental approach based on accumulating evidence
- **Real-time optimization**: Continuously update models and optimize choices
- **Uncertainty-guided exploration**: Focus experiments where uncertainty is highest

Modern Experimental Modeling

Beyond Fixed Designs

Modern experimental modeling increasingly relies on adaptive strategies that use information from previous experiments to guide future choices.

Definition (Sequential Design Strategy)

A sequential design strategy is a function ϕ that maps current data $\mathcal{D}_n$ and models $\mathcal{M}$ to the next experimental condition:

$$\mathbf{x}_{n+1} = \phi(\mathcal{D}_n, \mathcal{M})$$

This mathematical framework enables systematic adaptive experimentation.

Common Sequential Strategies

Different Approaches for Different Goals

Various sequential strategies embody different experimental philosophies and perform better in different situations.

Uncertainty Sampling:

- Choose points where model uncertainty is highest
- Reduces overall model uncertainty efficiently
- Good for parameter estimation and model building
- May not focus on regions of practical importance

Common Sequential Strategies

Different Approaches for Different Goals

Various sequential strategies embody different experimental philosophies and perform better in different situations.

Expected Improvement:

- Choose points likely to improve best observed response
- Balances exploration of uncertain regions with exploitation of promising areas
- Excellent for optimization problems
- Requires careful balance between exploration and exploitation

Common Sequential Strategies

Different Approaches for Different Goals

Various sequential strategies embody different experimental philosophies and perform better in different situations.

Entropy Reduction:

- Choose points that reduce uncertainty about model parameters most
- Information-theoretic foundation
- Good for discriminating between competing models
- Can be computationally intensive

Each strategy optimizes different aspects of experimental learning and suits different experimental objectives.

Bayesian Optimization Example

Example (Drug Discovery Optimization)

Pharmaceutical companies use sequential design to optimize drug compounds through systematic exploration of chemical space.

The Process:

1. Test small number of initial compound variations
2. Fit Gaussian process model to predict effectiveness across chemical space
3. Use acquisition function to identify most promising untested compounds
4. Synthesize and test compound with highest expected improvement
5. Update model and repeat

Bayesian Optimization Example

Example (Drug Discovery Optimization)

Pharmaceutical companies use sequential design to optimize drug compounds through systematic exploration of chemical space.

Mathematical Framework:

- **Gaussian process model**: Provides predictions with uncertainty
- **Acquisition function**: Balances exploration and exploitation
- **Expected improvement**: $EI(x) = \sigma(x)\phi(Z) + (\mu(x) - f_{best})\Phi(Z)$
- where $Z = \frac{\mu(x) - f_{best}}{\sigma(x)}$

Bayesian Optimization Example

Example (Drug Discovery Optimization)

Pharmaceutical companies use sequential design to optimize drug compounds through systematic exploration of chemical space.

Results:

- Can find highly effective compounds with far fewer experiments
- Systematic exploration of chemical space
- Balances discovery of new regions with optimization of known good regions
- Dramatically reduces time and cost of drug development

This approach represents the cutting edge of experimental efficiency in high-stakes applications.

Multi-Objective Experimental Design

When You Want Multiple Things

Real experimental problems often involve multiple, potentially conflicting objectives requiring careful balance.

Definition (Multi-Objective Design Problem)

Optimize multiple criteria simultaneously:

$$\max_{\mathbf{x}}\{f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_m(\mathbf{x})\}$$

where $f_i(\mathbf{x})$ represents different experimental objectives.

Example: Drug development wants to maximize effectiveness while minimizing side effects.

Multi-Objective Experimental Design

When You Want Multiple Things

Real experimental problems often involve multiple, potentially conflicting objectives requiring careful balance.

Solution Approaches:

- **Weighted combinations**: Combine objectives using weights $\sum_i w_i f_i(\mathbf{x})$
- **Pareto optimization**: Find designs that cannot be improved in one objective without degrading another
- **Constraint methods**: Optimize one objective while constraining others

Multi-Objective Experimental Design

When You Want Multiple Things

Real experimental problems often involve multiple, potentially conflicting objectives requiring careful balance.

Choosing Approaches:

- **Weighted**: When you can quantify trade-offs clearly
- **Pareto**: When you want to explore trade-off space
- **Constraint**: When some objectives have hard limits

The choice depends on how well you understand preferences among objectives and whether you want to explore trade-offs or optimize specific combinations.

Agent-Based Models in Social Psychology

Virtual Laboratories for Social Systems

Modern experimental modeling has expanded beyond traditional laboratories to include virtual environments where researchers can control complex social systems.

The Challenge:

- Real social systems are difficult to control experimentally
- Ethical constraints limit manipulation possibilities
- Long time scales make observation difficult
- Complex interactions are hard to isolate

Agent-Based Models in Social Psychology

Virtual Laboratories for Social Systems

Modern experimental modeling has expanded beyond traditional laboratories to include virtual environments where researchers can control complex social systems.

Example (Social Learning and Behavior Spread)

How do behaviors spread through social networks? Agent-based models provide virtual laboratories for systematic experimentation.

Mathematical Framework:

$$A_i(t+1) = f(A_i(t), \mathcal{N}_i(t), E(t), \boldsymbol{\theta})$$

where $A_i(t)$ is agent i's state, $\mathcal{N}_i(t)$ represents neighbors, and $E(t)$ is environment.

Agent-Based Models in Social Psychology

Virtual Laboratories for Social Systems

Modern experimental modeling has expanded beyond traditional laboratories to include virtual environments where researchers can control complex social systems.

Experimental Design:

- **Factors**: Network topology, learning rates, environmental dynamics
- **Responses**: Time to adoption, final adoption rates, spread patterns
- **Design**: Factorial experiments varying network and agent parameters

Advantages:

- Perfect experimental control impossible in real social systems
- Can test theoretical predictions systematically
- Enables exploration of extreme scenarios safely

Cyber-Physical Systems Engineering

Integrating Computational and Physical Components

Modern engineering systems integrate computation and physics in ways that make traditional design approaches inadequate.

Example (Autonomous Vehicle Control Systems)

Designing control systems for autonomous vehicles requires understanding interactions between:

- **Computational**: Decision algorithms, sensor processing, communication
- **Physical**: Vehicle dynamics, sensor characteristics, environmental conditions

Cyber-Physical Systems Engineering

Integrating Computational and Physical Components

Modern engineering systems integrate computation and physics in ways that make traditional design approaches inadequate.

Experimental Framework:

- **Virtual experiments**: Simulation environments modeling both cyber and physical aspects
- **Design variables**: Control parameters, sensor configurations, algorithm choices
- **Responses**: Safety metrics, efficiency measures, robustness indicators

Cyber-Physical Systems Engineering

Integrating Computational and Physical Components

Modern engineering systems integrate computation and physics in ways that make traditional design approaches inadequate.

Sequential Design Strategy:

1. Initial screening using factorial designs to identify important factors
2. Response surface modeling for detailed characterization
3. Robust optimization to find settings performing well under uncertainty
4. Physical validation testing final designs on real vehicles

This reduces expensive real-world testing while ensuring robust, reliable designs.

Neural Network Models of Brain Function

Understanding Computational Principles of the Brain

Experimental modeling enables precise testing of theoretical predictions about neural computation.

Example (Working Memory Mechanisms)

How does the brain maintain and manipulate information over short periods?
Three Competing Hypotheses:

- **Persistent activity**: Sustained neural firing
- **Synaptic storage**: Changes in synaptic strength
- **Oscillatory coding**: Patterns of neural oscillations

Neural Network Models of Brain Function

Understanding Computational Principles of the Brain

Experimental modeling enables precise testing of theoretical predictions about neural computation.

Mathematical Models:

$$\text{Model 1:} \quad \frac{dA_i}{dt} = -\gamma A_i + \sum_j W_{ij} f(A_j) + I_i(t) \tag{1}$$

$$\text{Model 2:} \quad \frac{dW_{ij}}{dt} = \eta A_i A_j - \delta W_{ij} \tag{2}$$

$$\text{Model 3:} \quad A_i(t) = \bar{A}_i + \tilde{A}_i \cos(\omega t + \phi_i) \tag{3}$$

Neural Network Models of Brain Function

Understanding Computational Principles of the Brain

Experimental modeling enables precise testing of theoretical predictions about neural computation.

Experimental Design for Model Discrimination:

- **T-optimal designs**: Maximize differences between model predictions
- **Sequential experiments**: Use results to refine subsequent tests
- **Multi-modal measurements**: EEG, fMRI, and behavioral data simultaneously

Result: Evidence supports oscillatory coding through theta-alpha coupling, demonstrating how systematic experimental design can discriminate among competing theoretical frameworks.

The Journey We've Taken

From Simple Examples to Sophisticated Applications

This comprehensive exploration has taken us from basic experimental concepts to advanced mathematical frameworks for optimal design and sequential learning.

Foundation Principles:

- Replication, randomization, and control remain fundamental
- These principles ensure reliable causal inference
- Apply regardless of system complexity
- Enable mathematical models that accurately represent reality

The Journey We've Taken

From Simple Examples to Sophisticated Applications

This comprehensive exploration has taken us from basic experimental concepts to advanced mathematical frameworks for optimal design and sequential learning.

Mathematical Structure:

- Factorial designs reveal elegant orthogonality properties
- Optimal parameter estimation through systematic design
- Interaction effects captured that would be missed otherwise
- Mathematical elegance translates to practical advantages

The Journey We've Taken

From Simple Examples to Sophisticated Applications

This comprehensive exploration has taken us from basic experimental concepts to advanced mathematical frameworks for optimal design and sequential learning.

Advanced Methods:

- Response surface methods enable optimization and complex modeling
- Optimal design theory provides principled resource allocation
- Sequential strategies adapt to accumulating information
- Modern applications extend to virtual and cyber-physical systems

Key Insights and Principles

Fundamental Lessons

Several key insights emerge that reflect the maturity of modern experimental modeling.

Integration of Theory and Practice:

- Mathematical models must be tested against reality
- Experimentation validates and refines theoretical understanding
- Systematic design principles ensure efficient learning
- Theory guides experimental choices while data informs theory

Key Insights and Principles

Fundamental Lessons

Several key insights emerge that reflect the maturity of modern experimental modeling.

Efficiency Through Mathematics:

- Mathematical frameworks enable optimal resource use
- Poor experimental designs waste valuable resources
- Systematic approaches can improve efficiency by 30-50
- Theory provides principled solutions to design problems

Key Insights and Principles

Fundamental Lessons

Several key insights emerge that reflect the maturity of modern experimental modeling.

Adaptive Learning:

- Modern approaches emphasize sequential and adaptive strategies
- Each experiment should inform the design of the next
- Real-time learning enables exploration of complex systems
- Uncertainty-guided exploration maximizes information gain

Key Insights and Principles

Fundamental Lessons

Several key insights emerge that reflect the maturity of modern experimental modeling.

Expanding Frontiers:

- Virtual experimentation opens new possibilities
- Cyber-physical systems require integrated approaches
- Complex social and biological systems become accessible
- Computational methods enable previously impossible studies

Future Direction

The boundary between physical and virtual experimentation continues to blur, creating new opportunities for systematic investigation.

Practical Implications

Lessons for Applied Work

The principles developed have profound implications for how we approach real-world experimental problems.

Design Before You Experiment:

- Invest time in careful experimental planning
- Use mathematical principles to guide design choices
- Consider multiple objectives and constraints
- Plan for sequential learning and adaptation

Practical Implications

Lessons for Applied Work

The principles developed have profound implications for how we approach real-world experimental problems.

Embrace Systematic Approaches:

- Factorial designs reveal interactions missed by ad hoc approaches
- Optimal design theory maximizes information per experiment
- Sequential methods enable efficient exploration
- Mathematical frameworks provide reliability and reproducibility

Practical Implications

Lessons for Applied Work

The principles developed have profound implications for how we approach real-world experimental problems.

Integration is Key:

- Combine multiple experimental approaches
- Use virtual and physical experiments synergistically
- Integrate experimental and computational modeling
- Balance exploration with exploitation of knowledge

Practical Implications

Lessons for Applied Work

The principles developed have profound implications for how we approach real-world experimental problems.

Quality Over Quantity:

- Well-designed experiments are worth more than many poorly-designed ones
- Systematic approaches often require fewer total experiments
- Investment in design pays dividends in results
- Mathematical rigor ensures reliable conclusions

Core Message

Experimental modeling transforms scientific investigation from art to systematic science while maintaining the creativity essential for discovery.

Looking Forward

Future Directions and Opportunities

The principles and methods developed provide foundation for emerging areas of experimental modeling.

Emerging Technologies:

- Virtual and augmented reality for immersive experiments
- AI-guided experimental design and real-time adaptation
- Automated laboratory systems enabling high-throughput experimentation
- Advanced sensors and measurement capabilities

Looking Forward

Future Directions and Opportunities

The principles and methods developed provide foundation for emerging areas of experimental modeling.

New Application Domains:

- Digital social systems and online experiments
- Personalized medicine and adaptive clinical trials
- Smart cities and urban system optimization
- Climate intervention and geoengineering research

Looking Forward

Future Directions and Opportunities

The principles and methods developed provide foundation for emerging areas of experimental modeling.

Methodological Advances:

- Integration of causal inference with experimental design
- Multi-fidelity modeling combining different experimental approaches
- Robust design under deep uncertainty
- Real-time experimental optimization and control

The mathematical principles remain relevant as experimental capabilities expand, ensuring that new possibilities are exploited efficiently and reliably.

Your Experimental Modeling Journey

Applying These Principles

The comprehensive foundation provided enables you to tackle increasingly complex experimental challenges while maintaining scientific rigor.

Questions for Reflection:

- How will you apply systematic experimental design principles in your field of interest?
- What complex systems could benefit from the advanced methods we've explored?
- How can you balance experimental efficiency with thoroughness in your research?
- What ethical responsibilities accompany the power of systematic experimental manipulation?
- How will emerging technologies change experimental possibilities in your domain?

Remember: The most profound scientific advances often come from asking the right questions and designing the right experiments to answer them.

Thank You

Questions and Discussion

Systematic experimentation: Where mathematical theory meets practical discovery

Next Chapter Preview:

Simulation Modeling

Building on experimental foundations to explore computational modeling