PART III. Optimal design theory
(LECTURE 3)

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Comments

In this lecture, we begin the formal study of the design of experiments within the framework of optimal design theory. After outlining the historical background and motivation, we introduce the regression model, its standard assumptions, and the role of least squares estimation in experimental planning. We define an experimental design as a probability measure and discuss how approximate designs can be discretized. Central to this theory is the information matrix, whose statistical meaning and key properties are carefully examined, supported by rigorous proofs of foundational theorems and lemmas.

We then develop the geometric underpinnings of design theory, making use of convex hulls, Carathéodory's theorem, and integral representations to describe the structure of feasible designs. Building on this foundation, we introduce optimality criteria for experimental design, including D-, L-, E-, G-, and e_k-optimality, and present their general formulation. The lecture concludes with the equivalence theorem for D-optimality, supported by auxiliary results such as determinant inequalities, concavity of the log-determinant function, and its differentiation, laying the groundwork for modern optimization-based approaches to experimental design.

Design of Experiments: Historical Background and Motivation

Motivation

Up to now, we have studied estimation methods for model parameters, most notably the least squares method. According to the Gauss–Markov theorem, the covariance matrix of the parameter estimates depends on the design matrix X. Thus, the precision of estimation can be improved by adjusting this matrix.

- Rows of the matrix X correspond to experimental conditions or measurement points.
- Choosing these points optimally is the main objective of optimal design theory.

Historical Development

- Early experiments lacked formal planning; setups were chosen intuitively.
- **R. Fisher** pioneered formal design theory in the 1930s using combinatorial tools (e.g., Latin squares).
- In the 1950s, **G. Box** and **J. Kiefer** developed the theory of optimal design for regression models.

Comments

Until now, we have discussed parameter estimation methods for linear models, focusing on the least squares approach. According to the Gauss–Markov theorem, the covariance matrix of the least squares estimator depends on the design matrix X. Therefore, the accuracy of our estimates can be improved by modifying this matrix. In practical terms, the rows of matrix X correspond to specific experimental conditions or measurement points. Selecting these points in a mathematically optimal way becomes a central task of optimal experimental design.

Historically, statistical data collection was performed without systematic planning. Experimenters would decide where, when, and how to conduct measurements largely based on intuition. However, as the cost of experiments grew with scientific and technological progress, the need emerged for a mathematical framework that could justify experimental choices.

This framework is known as the theory of experimental design. Its origin is usually attributed to Ronald Fisher, whose foundational book was published in 1935. His approach, largely based on combinatorial tools such as Latin squares, laid the groundwork for modern design methods. In the 1950s, statisticians George Box and Jack Kiefer introduced a new direction — the theory of optimal design for regression experiments. In this setting, the goal is to model the relationship between observed outputs and controllable conditions, and to choose measurement points that yield the most informative data. Kiefer's contributions are considered the foundation of classical optimal regression design theory.

Model Structure

$$y_j = \eta(t_j, \theta) + \epsilon_j, \quad j = 1, \ldots, N, \tag{1o}$$

- y_j: observed responses,
- $t_j \in \chi$: experimental conditions (design points),
- $\theta = (\theta_0, \ldots, \theta_{m-1})^T$: unknown parameters,
- $\eta(t, \theta)$: known function up to θ,
- ϵ_j: observation errors.

Standard Assumptions

(a) Unbiasedness: $E[\epsilon_j] = 0 \Rightarrow E[y_j] = \eta(t_j, \theta)$
(b) Uncorrelated errors: $E[\epsilon_i \epsilon_j] = 0$ for $i \neq j$
(c) Homoscedasticity: $E[\epsilon_j^2] = \sigma^2 > 0$
(d) Linearity in θ: $\eta(t, \theta) = \theta^T f(t)$
(e) Basis: $f_i(t)$, $i = 0, \ldots, m-1$ continuous and linearly independent on χ
(f) Design space: χ is compact and topological

Comments

We now introduce the general structure of a parametric regression model used in experimental design. Suppose we observe a sequence of real-valued responses, denoted by y_1 through y_N. These are modeled as $y_j = \eta(t_j, \theta) + \epsilon_j$, for j from 1 to N. Here, η is a known function up to a parameter vector θ, which consists of m components. The variables t_1 through t_N represent the design points, that is, the conditions under which each measurement is taken. These belong to a design space denoted by the symbol χ. The terms ϵ_j are random errors of observation.

We make several standard assumptions about the model.

First, the errors are unbiased: the expectation of ϵ_j is zero, which implies that the expected value of y_j is equal to $\eta(t_j, \theta)$. Second, we assume the errors are uncorrelated, meaning the expectation of the product $\epsilon_i \epsilon_j$ is zero whenever i is not equal to j. Third, the errors are homoscedastic — they all have the same variance σ^2, which is strictly positive. Fourth, the model is linear in the parameters, meaning that $\eta(t, \theta)$ equals the scalar product of θ with a known vector function $f(t)$. Fifth, the components of $f(t)$ are continuous and linearly independent on the design space χ.

Finally, we assume that χ is a fixed, compact topological space, meaning that its structure is stable and allows for analysis using limits and continuity.

Note: Assumptions (a)–(e) reflect features of real experiments and can be relaxed.

Experimental Objective

- Estimate parameters $\theta_0, \ldots, \theta_{m-1}$,
- Estimate the regression function $\eta(t, \theta)$,
- Test hypotheses on parameter values.

Estimator and Optimization Criterion

- Estimator $\widehat{\theta} = \widehat{\theta}(t_1, \ldots, t_N,\ y_1, \ldots, y_N)$
- Method of estimation depends on both data and design points
- Under assumptions (a)–(e), least squares is a well-established method:

$$\sum_{j=1}^{N} (y_j - \eta(t_j, \theta))^2 \longrightarrow \min_{\theta}$$

Comments

The assumptions labeled (a) through (e) reflect typical features of real-world experimental setups. While these assumptions can be relaxed — for instance, allowing heteroscedastic or correlated errors — we will not consider such generalizations in our course.

In practice, the goals of experimentation usually fall into three related categories. First, we aim to estimate the unknown parameters θ_0 through θ_{m-1}. Second, we may be interested in estimating the regression function $\eta(t, \theta)$, which is determined by these parameters. And third, we often need to test hypotheses about the values of the individual parameters.

The precision of any estimates obtained depends on two factors: the method used to estimate the parameters, and the choice of design points — that is, the values of t_1 through t_N at which the observations y_1 through y_N are made.

The estimator, denoted $\widehat{\theta}$, is a statistic that depends on both the observation values and the design points. Formally, $\widehat{\theta} = \widehat{\theta}(t_1, \ldots, t_N,\ y_1, \ldots, y_N)$. Choosing an appropriate form of this statistic is a separate task studied in estimation theory.

Under assumptions (a) through (e), the least squares method is a well-established and effective estimation procedure. It defines $\widehat{\theta}$ as the solution to the optimization problem of minimizing, over θ, the sum from $j = 1$ to N of the squared differences $y_j - \eta(t_j, \theta)$, quantity squared.

This least squares criterion was discussed earlier in detail.

Experimental Design as a Probability Measure

Discrete Design

$$\xi_N = \begin{pmatrix} t_1 & \dots & t_N \\ 1/N & \dots & 1/N \end{pmatrix}, \quad t_i \in \chi, \quad i = 1, \dots, N$$

- Total number of observations: N
- t_i may repeat for different i
- Equal weights 1/N

Approximate Design

$$\xi = \begin{pmatrix} t_1 & \dots & t_n \\ \omega_1 & \dots & \omega_n \end{pmatrix}, \quad t_i \in \chi, \quad \omega_i \geq 0, \quad \sum_{i=1}^{n} \omega_i = 1$$

- n = number of distinct support points
- $t_i \neq t_j$ for $i \neq j$
- Weights ω_i represent relative frequencies

Comments

As mentioned earlier, the accuracy of the resulting parameter estimates can be improved by choosing appropriate conditions for conducting the experiment. These conditions are encoded in the structure of the experimental design.

In the discrete setting, the design is represented by a two-row table denoted by ξ_N. The first row consists of the design points t_1 through t_N, where each t_i belongs to the set χ. The second row contains weights, all equal to 1/N, where N is the total number of measurements. It is important to note that in this formulation, individual design points may repeat; that is, t_i can be equal to t_j even when i is not equal to j. This representation reflects the classical setup of repeating measurements at some points.

This two-row array is commonly referred to as a discrete or normalized design.

Building on this concept, J. Kiefer introduced a generalization that allowed a broader class of optimization problems to be addressed. According to Kiefer's idea, the design can be viewed as a probability measure over the design space. This leads to the notion of approximate design, denoted simply by ξ.

In this generalized formulation, the design consists of n distinct support points t_1 through t_n, again chosen from the set χ. Each point is assigned a nonnegative weight ω_i, which indicates its relative importance or frequency. The weights must sum to one, forming a proper probability measure. Unlike in the discrete design, the points in an approximate design must be distinct — that is, t_i is not equal to t_j when i is not equal to j.

This formalism lays the foundation for the theory of optimal design, where the aim is to select the measure ξ that yields the most precise estimates according to a given criterion.

From Approximate to Exact Designs

In practice, only discrete designs can typically be implemented.
Given an approximate design

$$\xi = \begin{pmatrix} t_1 & \dots & t_n \\ \omega_1 & \dots & \omega_n \end{pmatrix},$$

one conducts approximately $N\omega_i$ measurements at each point t_i, for $i = 1, \dots, n$.
Rounding rule (example): Use integer allocations $N_i = \lfloor N\omega_i + \delta_i \rfloor$ where $\delta_i \in [0, 1)$ are chosen so that $\sum_{i=1}^{n} N_i = N$.

Convex Structure of Design Space

Let Ξ_n be the set of approximate designs with exactly n support points. Define the full design space:

$$\Xi = \bigcup_{n=1}^{\infty} \Xi_n.$$

Remark

The set Ξ is convex: if $\xi_1, \xi_2 \in \Xi$, then $\xi = \alpha\xi_1 + (1-\alpha)\xi_2 \in \Xi$ for all $\alpha \in [0, 1]$.

Comments

Although approximate experimental designs are the primary objects of theoretical optimization, in practical settings only discrete designs can be implemented.

Suppose we are given an approximate design ξ with n support points t_1 through t_n and corresponding weights ω_1 through ω_n. If we plan to conduct a total of N measurements, the natural approach is to perform approximately $N\omega_i$ measurements at point t_i. This is called discretization or rounding of the approximate design.

A standard method is deterministic rounding. To do this, we define the integer number of measurements at each support point as $N_i = \lfloor N\omega_i + \delta_i \rfloor$ where $\delta_i \in [0, 1)$ are chosen so that $\sum_{i=1}^{n} N_i = N$. This avoids over- or under-shooting the planned sample size. Specific rounding schemes and corrections are well documented in design literature, such as in the books by Fedorov, Pukelsheim, and Atkinson–Donev.

Next, we consider the geometric structure of the space of all approximate designs. Denote by Ξ_n the set of all designs with exactly n support points with nonzero weights. The total space Ξ is the union over all such Ξ_n.

A key property of this space is convexity. That is, for any two designs ξ_1 and ξ_2 in Ξ, any convex combination of them — meaning $\alpha\xi_1 + (1-\alpha)\xi_2$ — also belongs to Ξ for any α between 0 and 1. This makes the use of convex optimization techniques possible when searching for optimal designs.

The convex combination of designs

Let

$$\xi_1 = \begin{pmatrix} t_1 & t_2 & \cdots & t_n \\ \overline{\omega}_1 & \overline{\omega}_2 & \cdots & \overline{\omega}_n \end{pmatrix}, \quad \xi_2 = \begin{pmatrix} t_1 & t_2 & \cdots & t_n \\ \widetilde{\omega}_1 & \widetilde{\omega}_2 & \cdots & \widetilde{\omega}_n \end{pmatrix},$$

where the supports are extended with zero weights if necessary.
Then their convex combination is

$$\xi = \alpha\xi_1 + (1-\alpha)\xi_2 = \begin{pmatrix} t_1 & t_2 & \cdots & t_n \\ \omega_1 & \omega_2 & \cdots & \omega_n \end{pmatrix}, \quad \text{with } \omega_i = \alpha\overline{\omega}_i + (1-\alpha)\widetilde{\omega}_i.$$

Information Matrix

The information matrix of a design ξ is

$$M(\xi) = \int_{\chi} f(t) f^T(t)\, \xi(dt) \in \mathbb{R}^{m\times m},$$

where $f(t)$ is the regressor vector and χ is the design space.
Define the class of all such matrices:

$$\mathcal{M} = \{M : M = M(\xi),\ \xi \in \Xi\}.$$

Comments

We now clarify what we mean by the convex combination of designs. Let us consider two designs ξ_1 and ξ_2, defined on the same set of support points, possibly after extending them by adding zero-weighted points to match their domains. Their convex combination with coefficient α is defined by combining the weights linearly: the new weight ω_i is equal to $\alpha\overline{\omega}_i + (1-\alpha)\widetilde{\omega}_i$.

This operation defines a new design ξ, whose structure is crucial in convex optimization of experiments.

Next, we define the information matrix of a design. Given a regressor vector function $f(t)$, the information matrix of design ξ is defined as the integral over the design space χ of the outer product $f(t)f^T(t)$ with respect to the design measure ξ. In essence, this matrix summarizes the precision of parameter estimation under design ξ.

We denote by $\mathcal{M}$ the set of all information matrices that correspond to all possible approximate designs ξ from the space Ξ.

Discrete Uniform Design

Consider the discrete design $\xi_N = \begin{pmatrix} x_1, \dots, x_N \\ \frac{1}{N}, \dots, \frac{1}{N} \end{pmatrix}$.

Then the information matrix is $M(\xi_N) = \frac{1}{N} F^T F = \frac{1}{N} \sum_{i=1}^{N} f(x_i) f^T(x_i)$,

where each row of F

is the regressor vector $f^T(x_i)$: $F = \begin{pmatrix} f_0(x_1) & f_2(x_1) & \cdots & f_{m-1}(x_1) \\ f_0(x_2) & f_2(x_2) & \cdots & f_{m-1}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_0(x_N) & f_2(x_N) & \cdots & f_{m-1}(x_N) \end{pmatrix}$.

If $F^T F$ is nonsingular, the least squares estimator is $\widehat{\theta} = (F^T F)^{-1} F^T Y$, with dispersion matrix

$$D\widehat{\theta} = \sigma^2 (F^T F)^{-1} = \frac{\sigma^2}{N} (M(\xi_N))^{-1}.$$

Conclusion: the information matrix $M(\xi_N)$ is proportional to the inverse of the covariance matrix of $\widehat{\theta}$.

Comments

Let us now clarify the statistical meaning of the information matrix by focusing on the discrete case. Consider the uniform discrete design ξ_N i.e. the design which consists of N equally weighted points x_1 through x_N.

The information matrix of such a design is given by $1/N$ times $F^T F$.

The matrix F generalizes the classical design matrix X. Its rows are formed from the values of the regressor vector f evaluated at each point: the entry in row i, column j of F is equal to function f_j evaluated at point x_i. Thus, F is an N by m matrix, where m is the number of parameters in the model.

If the matrix $F^T F$ is invertible, then the least squares estimator for the parameter vector θ is given by $(F^T F)^{-1} F^T Y$. The dispersion matrix of this estimator is equal to $\sigma^2 (F^T F)^{-1}$, which is also equal to σ^2/N times the inverse of the information matrix.

Hence, the information matrix is proportional to the inverse of the covariance matrix of the estimator vector $\widehat{\theta}$.

Theorem 7: Properties of Information Matrices

The following statements hold:

(1) Every information matrix is positive semidefinite;
(2) If $n < m$, then for any design $\xi \in \Xi_n$, we have $\det M(\xi) = 0$;
(3) The set $\mathcal{M}$ of all information matrices is convex;
(4) Under regularity conditions (a)–(e), the set $\mathcal{M}$, considered as a set of vectors composed of diagonal and upper triangular elements, is compact in $\mathbb{R}^{(m)(m+1)/2}$;
(5) Under the same conditions, for any desing $\xi \in \Xi$, there exists a plan $\widetilde{\xi} \in \Xi_n$ with $n \le (m)(m+1)/2 + 1$, such that

$$M(\widetilde{\xi}) = M(\xi).$$

Proof:

1. Positive Semidefiniteness. For any vector $l \in \mathbb{R}^m$,

$$l^T M(\xi) l = \int_\chi l^T f(t) f^T(t) l \, \xi(dt) = \int_\chi (l^T f(t))^2 \, \xi(dt) \ge 0.$$

Hence, $M(\xi)$ is positive semidefinite.

Comments

This theorem summarizes five key structural properties of the set of information matrices associated with approximate experimental designs. First, every such matrix is positive semidefinite. This reflects the fact that the expression defining the matrix — namely, the integral of the outer product of the regressor vector with itself — yields a nonnegative definite result.

Second, if a design is concentrated in fewer than m points, where m is the dimension of the parameter vector θ, then the determinant of the information matrix equals zero. In such cases, the design does not provide enough independent information to estimate all parameters.

Third, the set of all information matrices, denoted by $\mathcal{M}$, is convex. That is, if we take any two matrices in this set and form their weighted average, the result is again an information matrix.

The fourth point states that under regularity conditions, this set is not only convex but also compact when viewed as a subset of Euclidean space with dimension equal to $m(m+1)/2$. This dimension corresponds to the number of distinct entries in a symmetric matrix of size m.

Finally, any information matrix can be represented by a design supported at a finite number of points — specifically, at most $m(m+1)/2+1$ points. This result is crucial in practice: it justifies searching for optimal designs within a finite-dimensional class.

Let us prove the statements of the theorem.

First, we show that the information matrix is always positive semidefinite. By definition, for any vector l from the m-dimensional real space, the quadratic form $l^T M(\xi) l$ equals the integral over the design space of the square of $l^T f(t)$, all multiplied by the measure $\xi(dt)$. Since squares of real numbers are always nonnegative, the result is greater than or equal to zero. Hence, the matrix $M(\xi)$ is positive semidefinite.

2. Singularity for $n < m + 1$. Using the subadditivity property of matrix rank:

$$\operatorname{rank}(M(\xi)) \le \sum_{i=1}^{n} \operatorname{rank}\bigl(f(x_i)f^{T}(x_i)\bigr).$$

Each term has rank 1, since

$$f(t)f^{T}(t) = \begin{pmatrix} f_0(t)f^{T}(t) \\ f_1(t)f^{T}(t) \\ \vdots \\ f_{m-1}(t)f^{T}(t) \end{pmatrix},$$

i.e., all rows are scalar multiples of $f^{T}(t)$. Thus,

$$\operatorname{rank}(M(\xi)) \le n.$$

If $n < m$, then $\operatorname{rank}(M(\xi)) < m$, so $\det M(\xi) = 0$.

Comments

Here we proceed to the proof of the second statement. Suppose the design ξ is supported on n points. Then, the information matrix is a sum of n matrices of the form $f(x_i)f^{T}(x_i)$. Each such matrix has rank one, because all its rows are proportional to the vector $f^{T}(x_i)$. Therefore, the rank of the total matrix $M(\xi)$ is at most n.

Now, if n is strictly less than m, then the rank of $M(\xi)$ is strictly less than m, meaning that the matrix is singular and its determinant is zero.

3. Convexity of the Set $\mathcal{M}$. Let $\mathrm{M}_1 = \mathrm{M}(\xi_1), \mathrm{M}_2 = \mathrm{M}(\xi_2) \in \mathcal{M}$, and $\alpha \in [0,1]$. Then

$$\begin{aligned}\mathrm{M} &= \alpha \mathrm{M}_1 + (1-\alpha)\mathrm{M}_2 \\ &= \alpha \int \mathrm{f}(\mathrm{t})\mathrm{f}^{\mathrm{T}}(\mathrm{t})\, \xi_1(\mathrm{dt}) + (1-\alpha) \int \mathrm{f}(\mathrm{t})\mathrm{f}^{\mathrm{T}}(\mathrm{t})\, \xi_2(\mathrm{dt}) \\ &= \int \mathrm{f}(\mathrm{t})\mathrm{f}^{\mathrm{T}}(\mathrm{t})\, [\alpha\xi_1(\mathrm{dt}) + (1-\alpha)\xi_2(\mathrm{dt})] \\ &= \int \mathrm{f}(\mathrm{t})\mathrm{f}^{\mathrm{T}}(\mathrm{t})\, \xi(\mathrm{dt}),\end{aligned}$$

where $\xi = \alpha\xi_1 + (1-\alpha)\xi_2 \in \Xi$, since this set is convex. Hence, $\mathrm{M} \in \mathcal{M}$. Thus the set $\mathcal{M}$ of all information matrices generated by designs $\xi \in \Xi$ is convex.

Note: This result is foundational for optimal design theory, enabling use of convex optimization techniques.

Comments

Let us now verify part three of the theorem, which asserts that the set of all information matrices is convex.

To do this, we consider two information matrices, denoted by M_1 and M_2, each corresponding to some designs ξ_1 and ξ_2. We take a convex combination of these matrices, with weights α and $1-\alpha$, where α lies between 0 and 1 inclusive.

By linearity of integration, we can combine the two integrals defining M_1 and M_2 into a single integral involving the convex combination of the design measures. That is, $\alpha\mathrm{M}_1 + (1-\alpha)\mathrm{M}_2$ equals the integral of the outer product $\mathrm{f}(\mathrm{t})\mathrm{f}^{\mathrm{T}}(\mathrm{t})$ with respect to the new measure, which is $\alpha\xi_1 + (1-\alpha)\xi_2$.

According to a previous remark, this new measure is again a valid design measure, and therefore the resulting matrix is also an element of the set of information matrices.

Thus, we have shown that the set of all such matrices is closed under convex combinations, meaning it is convex.

This property is fundamental in optimal design theory. It ensures that optimization problems over information matrices can be tackled using powerful tools from convex analysis.

Let $V \subset \mathbb{R}^k$. We introduce several basic notions:

Convex Combination

A vector $\alpha v_1 + (1-\alpha)v_2$ is called a convex combination of v_1 and v_2 if $0 < \alpha < 1$.

Convex Set

A set $V \subset \mathbb{R}^k$ is called convex if it contains all convex combinations of any two of its vectors:

$$v_1, v_2 \in V \;\Rightarrow\; \alpha v_1 + (1-\alpha)v_2 \in V.$$

Convex Hull

The convex hull $\operatorname{conv} V$ of a set V is the intersection of all convex sets containing V.

We define:

$$\widehat{V}_n = \left\{ v \in \mathbb{R}^k \,\middle|\, v = \sum_{i=1}^{n} \alpha_i v_i,\ \alpha_i > 0,\ \sum \alpha_i = 1,\ v_i \in V \right\}, \quad \widehat{V} = \bigcup_{n=1}^{\infty} \widehat{V}_n.$$

Comments

To proceed with the proof of parts four and five of the theorem, we introduce several auxiliary definitions concerning convexity in Euclidean space.

First, we define a convex combination of two vectors as any linear combination where the coefficients are strictly between zero and one, and add up to one. Specifically, $\alpha v_1 + (1-\alpha)v_2$, with α strictly between 0 and 1.

Second, we define a convex set as a set that contains all convex combinations of any two of its elements. That is, if v_1 and v_2 belong to V, then every convex combination of them also lies in V.

Third, the convex hull of a set V is defined as the smallest convex set that contains V, or equivalently, the intersection of all convex sets containing V.

We now introduce notations that will be used shortly. The set $\widehat{V}_n$ consists of all convex combinations of n elements from V with positive coefficients summing to one. The union over all such n defines the set $\widehat{V}$. These sets are useful for characterizing the convex hull and expressing matrix combinations in vector form.

Lemma 8

The set $\widehat{\mathrm{V}}$ is the convex hull of V:

$$\widehat{\mathrm{V}} = \operatorname{conv} \mathrm{V}.$$

Proof: We split the proof into two parts. First, we show that $\widehat{\mathrm{V}} \subset \operatorname{conv} \mathrm{V}$; then we show the converse inclusion $\operatorname{conv} \mathrm{V} \subset \widehat{\mathrm{V}}$.

1. $\widehat{\mathrm{V}} \subset \operatorname{conv} \mathrm{V}$. We prove this by induction.
Clearly, $\widehat{\mathrm{V}}_1 \subset \operatorname{conv} \mathrm{V}$.
Assume that $\widehat{\mathrm{V}}_n \subset \operatorname{conv} \mathrm{V}$. We show that $\widehat{\mathrm{V}}_{n+1} \subset \operatorname{conv} \mathrm{V}$.
Let $\mathrm{v} \in \widehat{\mathrm{V}}_{n+1}$, then

$$\mathrm{v} = \sum_{i=1}^{n+1} \alpha_i \mathrm{v}_i = \sum_{i=1}^{n} \alpha_i \mathrm{v}_i + \alpha_{n+1} \mathrm{v}_{n+1}.$$

Without loss of generality, we may assume $\alpha_{n+1} > 0$.

Comments

We now state and begin the proof of an important lemma: the set denoted by $\widehat{\mathrm{V}}$ is equal to the convex hull of the set V. That is, every element in $\widehat{\mathrm{V}}$ can be written as a convex combination of vectors from the original set V, and vice versa.

To prove this, we divide the argument into two parts. First, we prove that the set $\widehat{\mathrm{V}}$ is a subset of the convex hull of V. Then we will prove the opposite inclusion.

To establish the first part, we use mathematical induction. In the base case, $\widehat{\mathrm{V}}_1$ clearly lies within the convex hull of V, since it consists of a single point from V.

For the induction step, suppose that $\widehat{\mathrm{V}}_n$ is contained in the convex hull of V. Consider an arbitrary element v from the set $\widehat{\mathrm{V}}_{n+1}$. This vector v can be written as the sum over i from 1 to $n+1$ of $\alpha_i \mathrm{v}_i$. We rearrange this sum by grouping the first n terms together, and separating the term with index $n+1$. That is, we write v as the sum over i from 1 to n of $\alpha_i \mathrm{v}_i$, plus $\alpha_{n+1} \mathrm{v}_{n+1}$.

Without loss of generality, we may assume that the last coefficient α_{n+1} is strictly greater than zero.

Proof of Lemma 8: Inclusion

Let us denote $\alpha = 1 - \alpha_{n+1} = \sum_{i=1}^{n} \alpha_i$.
Define the vectors:

$$\overline{v}_1 = v_{n+1}, \quad \overline{v}_2 = \sum_{i=1}^{n} \frac{\alpha_i}{\sum_{i=1}^{n} \alpha_i} v_i = \sum_{i=1}^{n} \alpha_i' v_i, \quad \text{where } \sum_{i=1}^{n} \alpha_i' = 1.$$

Then:

- $\overline{v}_1 \in V \subset \text{conv}V$,
- $\overline{v}_2 \in \widehat{V}_n \subset \text{conv}V$ (by the induction hypothesis),
- Since convV is convex, we conclude:

$$(1 - \alpha)\,\overline{v}_1 + \alpha\,\overline{v}_2 \in \text{conv}V.$$

Hence, by mathematical induction, we have proved the inclusion $\widehat{V} \subset \text{conv}\, V$.

Comments

To complete the inductive step, we now express the vector v in terms of two auxiliary vectors. Let α be defined as $1 - \alpha_{n+1}$, which is equal to the sum of α_i from i = 1 to n.

We then define two vectors. First, we let $\overline{v}_1$ be equal to v_{n+1}. Second, we define $\overline{v}_2$ as the weighted sum over i from 1 to n of α_i divided by the sum of α_i, times v_i. In other words, $\overline{v}_2$ equals the sum of $\alpha_i' v_i$, where the sum of all α_i' equals one.

By construction, the first vector $\overline{v}_1$ belongs to the original set V, and therefore lies in the convex hull of V. The second vector $\overline{v}_2$ lies in the set $\widehat{V}_n$. By the induction hypothesis, this also lies in the convex hull of V.

Since the convex hull is closed under convex combinations, the weighted sum of these two vectors — namely, $(1 - \alpha)\overline{v}_1 + \alpha\overline{v}_2$ — also lies in the convex hull of V.

This completes the inductive step. We have shown that any element of $\widehat{V}_{n+1}$ also belongs to the convex hull of V. Therefore, by mathematical induction, the entire set $\widehat{V}$ is contained in the convex hull of V.

Proof of Lemma 8: Converse inclusion

Clearly, $V \subset \widehat{V}$ since $\widehat{V}_1 = V$.
We now verify that $\widehat{V}$ is convex:

- Let $\widehat{v}_1, \widehat{v}_2 \in \widehat{V}$.
- Suppose $\widehat{v}_1 = \sum_{i=1}^{n_1} \alpha_i v_i$ and $\widehat{v}_2 = \sum_{i=1}^{n_2} \alpha'_i v'_i$.
- Then for any $\alpha \in [0,1]$ we have:

$$v = \alpha\widehat{v}_1 + (1-\alpha)\widehat{v}_2 = \sum_{i=1}^{n_1} \alpha\alpha_i v_i + \sum_{i=1}^{n_2} (1-\alpha)\alpha'_i v'_i = \sum_{i=1}^{n_1+n_2} \widetilde{\alpha}_i \widetilde{v}_i,$$

where:

$$\widetilde{v}_i = v_i, \quad \widetilde{\alpha}_i = \alpha\alpha_i, \quad i \le n_1;$$
$$\widetilde{v}_i = v'_{i-n_1}, \quad \widetilde{\alpha}_i = (1-\alpha)\alpha'_{i-n_1}, \quad i > n_1.$$

- Then $\sum_{i=1}^{n_1+n_2} \widetilde{\alpha}_i = 1$, and all $\widetilde{\alpha}_i \ge 0$, hence $v \in \widehat{V}$.

Since $\widehat{V}$ is convex and contains V, we conclude:

$$\operatorname{conv} V \subset \widehat{V}.$$

The Lemma is proved. □

Comments

We now complete the proof of the lemma by establishing the reverse inclusion, namely that the convex hull of V is contained in the set $\widehat{V}$.

First, we observe that the set V is a subset of $\widehat{V}$. This follows directly from the definition, since $\widehat{V}_1$ is equal to V.

Next, we show that the set $\widehat{V}$ is convex. To do this, consider two arbitrary elements of $\widehat{V}$, denoted $\widehat{v}_1$ and $\widehat{v}_2$. Suppose that $\widehat{v}_1$ is a convex combination of vectors v_i, for i from 1 to n_1, and that $\widehat{v}_2$ is a convex combination of other vectors v'_i, for i from 1 to n_2.

We now consider a convex combination of $\widehat{v}_1$ and $\widehat{v}_2$ with weights α and $1-\alpha$. Expanding this expression, we obtain a single convex combination of the vectors v_i and v'_i, with new weights defined as $\alpha\alpha_i$ and $(1-\alpha)\alpha'_i$ respectively.

All these new weights are non-negative, and their sum equals one. Therefore, the resulting vector again belongs to $\widehat{V}$. This confirms that $\widehat{V}$ is convex.

Since the convex hull of V is, by definition, the smallest convex set containing V, and since $\widehat{V}$ is convex and contains V, it must contain the entire convex hull of V.

We thus conclude that the convex hull of V is a subset of $\widehat{V}$. This completes the proof of the lemma.

Lemma 9

Let $v_1, \ldots, v_{k+2} \in \mathbb{R}^k$. Then there exist scalars $\beta_1, \ldots, \beta_{k+2}$, not all zero, such that

$$\sum_{i=1}^{k+2} \beta_i v_i = 0, \quad \sum_{i=1}^{k+2} \beta_i = 0.$$

Proof: Consider the lifted vectors $\overline{v}_i = (v_i^T,\ 1)^T \in \mathbb{R}^{k+1}$. Since we have $k+2$ vectors in a $(k+1)$-dimensional space, they are linearly dependent. Therefore, there exist scalars $\beta_1, \ldots, \beta_{k+2}$, not all zero, such that

$$\sum_{i=1}^{k+2} \beta_i \overline{v}_i = 0.$$

Writing this out, we have:

$$\sum_{i=1}^{k+2} \beta_i v_i = 0, \quad \sum_{i=1}^{k+2} \beta_i = 0.$$

This proves the lemma. □

Comments

We now prove a basic linear algebra lemma. Suppose we are given $k+2$ vectors in k-dimensional space. Then there exists a nontrivial linear combination of these vectors that sums to the zero vector, and at the same time, the sum of the coefficients in this combination is zero.

To show this, we use the standard lifting technique. For each vector v_i in k-dimensional space, construct a new vector by appending a one at the end. The resulting vector is denoted $\overline{v}_i$ and lives in $k+1$ dimensional space.

Now we have $k+2$ vectors in a space of dimension $k+1$. Therefore, these vectors must be linearly dependent. That means there exist scalars β_1 through β_{k+2}, not all equal to zero, such that the sum over i of $\beta_i \overline{v}_i$ equals zero.

Writing this sum explicitly, we separate it into two parts: the sum over $\beta_i v_i$, and the sum over β_i times the constant one. These two parts must both vanish, which yields the desired result: the sum over i of $\beta_i v_i$ equals zero, and the sum over i of β_i equals zero.

This completes the proof of the lemma.

Carathéodory's Theorem

Let V be a compact subset of $\mathbb{R}^k$. Then every point $v \in \text{conv}(V)$ can be written as a convex combination of at most k+1 points from V:

$$v = \sum_{i=1}^{m} \alpha_i v_i, \quad v_i \in V,\ \alpha_i \geq 0,\ \sum_{i=1}^{m} \alpha_i = 1,\ m \leq k+1.$$

Proof: Let $v \in \text{conv}(V)$ be arbitrary. By Lemma 9, it can be written as a convex combination:

$$v = \sum_{i=1}^{n} \alpha_i v_i, \quad v_i \in V,\ \alpha_i > 0,\ \sum_{i=1}^{n} \alpha_i = 1.$$

If $n \leq k+1$, the statement holds. Suppose instead that $n \geq k+2$.
By Lemma 9, the vectors $v_1, \ldots, v_n$ satisfy a nontrivial relation of the form:

$$\sum_{i=1}^{n} \beta_i v_i = 0, \quad \sum_{i=1}^{n} \beta_i = 0, \quad \text{not all } \beta_i = 0.$$

We will use this relation to eliminate one point from the combination while keeping the result unchanged.

Comments

We now state and begin proving Carathéodory's theorem, which is fundamental in convex analysis. It asserts that any point in the convex hull of a compact set in k-dimensional space can be expressed as a convex combination of at most $k+1$ elements from that set.

Let V be a compact subset of k-dimensional Euclidean space. Let v be any point in the convex hull of V. According to the previous lemma, any such point can be written as a convex combination of a finite number of points from V, say v_i with weights α_i, which are strictly positive and sum to one.

If the number of such points is less than or equal to $k+1$, then the claim holds directly. But suppose the number is greater than or equal to $k+2$. Then we can apply the second lemma we proved earlier.

This lemma guarantees that the set of vectors v_1 through v_n satisfies a nontrivial linear dependence, meaning that there exists a set of coefficients β_i, not all zero, such that the sum over i of $\beta_i v_i$ equals zero, and the sum of the β_i equals zero as well.

We will use this relation to eliminate one of the points from the convex combination without changing the result, and we will continue this process iteratively until no more than $k+1$ points remain.

To reduce the number of terms, define the index

$$i_0 = \arg\min_i \left\{ \frac{\alpha_i}{\beta_i} \ : \ \beta_i > 0 \right\}.$$

Let the updated weights be

$$\overline{\alpha}_i = \alpha_i - \frac{\alpha_{i_0}}{\beta_{i_0}} \beta_i, \quad \text{for all } i = 1, \ldots, n.$$

Then clearly:

$$v = \sum_{i=1}^{n} \overline{\alpha}_i v_i, \quad \sum \overline{\alpha}_i = 1, \quad \overline{\alpha}_i \geq 0,$$

and at least one of the new coefficients is zero, namely $\overline{\alpha}_{i_0} = 0$.
Repeating this reduction process, we ultimately obtain a representation

$$v = \sum_{i=1}^{k+1} \widetilde{\alpha}_i v_i, \quad \widetilde{\alpha}_i \geq 0, \quad \sum \widetilde{\alpha}_i = 1.$$

The Theorem is proved. □

Comments

To complete the proof of Carathéodory's theorem, we reduce the number of vectors in the convex combination. Suppose that the point v is represented as a convex combination of n points from the set V, with n greater than or equal to $k + 2$. According to the lemma, there exists a nontrivial linear dependence among any $k + 2$ vectors in Euclidean space of dimension k. That means there exist real numbers β_1 through β_n, not all zero, such that the sum of $\beta_i v_i$ is equal to zero, and the sum of β_i is zero.

We then define the index i_0 as the value of i which minimizes the ratio α_i/β_i among those i for which β_i is strictly positive. Using this, we define new coefficients $\overline{\alpha}_i$ as $\alpha_i - (\alpha_{i_0}/\beta_{i_0})\beta_i$. These modified coefficients remain nonnegative and sum to one.

Importantly, one of the coefficients, namely the one corresponding to i_0, becomes zero. Thus, the number of terms with nonzero weights is reduced by at least one. Repeating this process iteratively, we eventually reduce the representation to a convex combination involving at most $k + 1$ points. This proves the theorem.

To apply Carathéodory's theorem to sets of information matrices, we need one more technical result.

Let

$$\widetilde{\mathrm{V}} = \left\{ \int \mathrm{v}(\mathrm{x})\, \xi(\mathrm{dx}) \,:\, \mathrm{v} \in \mathrm{V} \right\},$$

where ξ is a probability measure on the measurable space $(\mathrm{X}, \mathcal{B})$, and V is a set of continuous vector-valued functions on X.

Lemma 10

If the set X is compact, then $\widetilde{\mathrm{V}} = \operatorname{conv} \mathrm{V}$.

Proof:

- Since the functions $\mathrm{v}(\mathrm{x}) \in \mathrm{V}$ are continuous and X is compact, the convex hull convV is also compact.
- It is easy to see that $\mathrm{convV} \subset \widetilde{\mathrm{V}}$, because $\widetilde{\mathrm{V}}$ is convex and contains V.
- Assume, for contradiction, that $\widetilde{\mathrm{V}} \neq \mathrm{convV}$. Then there exists a probability measure ξ^* such that

$$\mathrm{v}^* = \int \mathrm{v}\, \xi^*(\mathrm{dv}), \quad \mathrm{v}^* \notin \mathrm{convV}.$$

Comments

This part of the lecture prepares a technical result that is essential for applying Carathéodory's theorem to sets of information matrices. The main object introduced here is the set $\widetilde{\mathrm{V}}$, which consists of all integrals of the form: the integral of v(x) with respect to $\xi(\mathrm{dx})$, where v belongs to the set V, and ξ is a probability measure defined on the measurable space X with sigma-algebra $\mathcal{B}$.

The lemma claims that if the set X is compact, then the set $\widetilde{\mathrm{V}}$ coincides exactly with the convex hull of V. In other words, all such integrals can be represented as convex combinations of elements in V.

To prove this, we proceed step by step. First, since the functions v(x) are continuous and the set X is compact, the convex hull of V is also compact. Next, we observe that the convex hull is contained in $\widetilde{\mathrm{V}}$ because $\widetilde{\mathrm{V}}$ is convex and includes the original set V.

Now we suppose, for contradiction, that $\widetilde{\mathrm{V}}$ is strictly larger than the convex hull. Then there must exist a probability measure ξ^* such that the integral of v with respect to ξ^* equals some vector v^* that lies outside the convex hull of V.

End of proofs of Lemma 10 and Theorem 7

To reach a contradiction, we apply the separation theorem:

- Since $v^* \notin \text{conv}V$ and convV is compact, there exists a hyperplane separating v^* from convV.
- That is, there exists a vector α such that

$$\alpha^{\mathrm{T}} v \le C < \alpha^{\mathrm{T}} v^* \quad \text{for all } v \in \text{conv}V.$$

- On the other hand, since $v^* = \int v\, \xi^*(dv)$, we have:

$$\alpha^{\mathrm{T}} v^* = \int \alpha^{\mathrm{T}} v\, \xi^*(dv) \le \int C\, \xi^*(dv) = C.$$

- Contradiction. Thus, $\widetilde{V} = \text{conv}V$.

□

Consequence

Item (4) and (5) of Theorem 7 follows directly from this lemma and Carathéodory's Theorem.

Theorem 7 is proved. □

Comments

To complete the proof, we invoke the separation theorem from convex analysis. This theorem states that if a point lies outside a compact convex set, then there exists a hyperplane that separates the point from the set.

In our case, the vector v^* does not belong to the convex hull of V. Since the convex hull is compact, the separation theorem ensures that there exists a vector α such that, for all vectors v in the convex hull of V, the scalar product $\alpha^{\mathrm{T}} v$ is less than or equal to a constant C, which is strictly less than $\alpha^{\mathrm{T}} v^*$.

This inequality provides the key contradiction. Recall that v^* is defined as the integral of v with respect to the measure ξ^*. Therefore, $\alpha^{\mathrm{T}} v^*$ equals the integral over $\alpha^{\mathrm{T}} v$ with respect to ξ^*.

Because $\alpha^{\mathrm{T}} v$ is at most C for all v in the convex hull, the integral is also bounded above by C. Hence, $\alpha^{\mathrm{T}} v^*$ is less than or equal to C.

But earlier we concluded that $\alpha^{\mathrm{T}} v^*$ is strictly greater than C. This contradiction proves that our initial assumption was false, and thus v^* must belong to the convex hull of V.

This completes the proof of the lemma.

As an immediate consequence, items four and five of Theorem 7 — concerning the compactness of the information matrix and the number of design's support points— follows directly from this lemma and Carathéodory's Theorem. This completes the proof of Theorem 7.

Corollary

If conditions (a)–(e) are satisfied, then the information matrix of any design ξ can be written as a convex combination of at most $m(m+1)/2+1$ matrices of the form $f(x_i)f^T(x_i)$. That is,

$$M(\xi) = \sum_{i=1}^{n} w_i f(x_i) f^T(x_i), \; w_i \geq 0, \; \sum w_i = 1, \quad \text{where } n \leq m(m+1)/2+1.$$

Remark

Since the information matrix is symmetric, it is fully determined by $m(m+1)/2$ elements. In other words, it can be associated with a vector in $\mathbb{R}^{m(m+1)/2}$.

Remark

We have obtained the following important consequence: continuous optimal designs can be constructed from designs of the form

$$\xi = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \\ w_1 & w_2 & \cdots & w_n \end{pmatrix}, \quad n \leq m(m+1)/2+1.$$

Comments

This slide presents a corollary and two remarks that follow from the previously established representation theorem for information matrices under conditions (a) through (e). The corollary states that for any design ξ, the information matrix $M(\xi)$ can be written as a convex combination of at most $m(m+1)/2+1$ rank-one symmetric matrices of the form $f(x_i)f^T(x_i)$. In other words, there exist support points x_1 through x_n and nonnegative weights w_1 through w_n summing to one, such that the information matrix equals the sum over i of $w_i f(x_i)f^T(x_i)$, with the number of support points n not exceeding the stated bound.

The first remark emphasizes a geometric interpretation. Since the matrix M is symmetric, it is uniquely determined by its distinct entries, namely $m(m+1)/2$ parameters. Hence, M can be identified with a point in a Euclidean space of corresponding dimension.

The second remark highlights a constructive implication for optimal design. Any approximate design that is optimal in a given sense can be replaced by a design with no more than $m(m+1)/2+1$ support points. Thus, we have obtained an upper bound for the number of support points of the optimal design.

Key Definitions

- A design ξ is called ***nonsingular*** if its information matrix $M(\xi)$ is invertible.
- For any nonsingular design ξ, the matrix
$$D(\xi) = M(\xi)^{-1}$$
is defined as the ***inverse information matrix***.

- There is generally ***no single optimal design*** ξ^* that minimizes the inverse information matrix for all other designs ξ, i.e.,
$$D(\xi^*) \leq D(\xi) \quad \text{for all } \xi \in \Xi.$$
- This means we cannot find a design that is "better" than all others in every possible way.

- To solve this, we define optimality using specific functions that have a clear statistical meaning.
- These are typically either:
  - ***Concave functions*** on $M(\xi)$.
  - ***Convex functions*** on $D(\xi)$.

Comments

In regression design theory, a fundamental concept is that of a nonsingular design. A design is called nonsingular if its information matrix is invertible. This condition is essential: only for such designs can we uniquely and unbiasedly estimate all the parameters of the regression model. If the information matrix is singular, then the parameter vector is not fully identifiable based on the experiment.

For any nonsingular design ξ, we define the matrix $D(\xi)$ as the inverse of its information matrix, that is, $D(\xi) = M(\xi)^{-1}$. This matrix characterizes the precision of parameter estimation: smaller entries in D correspond to more accurate estimates.

However, in most practical situations, there does not exist a design ξ^* such that $D(\xi^*) \leq D(\xi)$ for every other nonsingular design ξ. In other words, the set of nonsingular designs does not contain a universally best element in terms of the matrix ordering.

Therefore, to compare and rank designs in a meaningful way, one introduces so-called optimality criteria. These are real-valued functions defined either on the set of information matrices or on their inverses. Concave functions on information matrices — or equivalently, convex functions on their inverses — are typically used. These criteria have clear statistical meaning: for example, minimizing the average variance of parameter estimates or minimizing the volume of confidence ellipsoids. They allow us to formally define what we mean by the “best” design under specific optimality goals.

D-criterion

The name derives from "determinant." The D-optimality criterion is written as:

$$\log\det \mathrm{M}(\xi) \to \sup_{\xi\in\Xi} \quad \text{or} \quad \log\det \mathrm{D}(\xi) \to \inf_{\xi\in\Xi}.$$

It corresponds to minimizing the volume of the confidence ellipsoid:

$$\left\{\widetilde{\theta} : (\widetilde{\theta}-\widehat{\theta})^{\mathrm{T}}\mathrm{D}\widehat{\theta}(\widetilde{\theta}-\widehat{\theta}) \le \alpha\right\},$$

where α is a constant depending only on the confidence level.

L-criterion

The L-optimality criterion is:

$$\operatorname{tr}\mathrm{LD}(\xi) \to \inf_{\xi\in\Xi_{\text{н}}},$$

where $\Xi_{\mathrm{NS}} = \{\xi \in \Xi : \det \mathrm{M}(\xi) \neq 0\}$, and $\mathrm{L} \in \mathbb{R}^{(\mathrm{d}+1)\times(\mathrm{d}+1)}$ is a fixed nonnegative definite matrix.
Its statistical meaning is minimization of generalized quadratic loss:

$$\mathbb{E}(\widehat{\theta}-\theta)^{\mathrm{T}}\mathrm{L}(\widehat{\theta}-\theta).$$

Comments

We now turn to specific optimality criteria used to compare and choose among different designs. The most classical of these is the D-optimality criterion. The letter "D" refers to the determinant of the information matrix. According to this criterion, the optimal design is the one that maximizes the logarithm of the determinant of the information matrix $\mathrm{M}(\xi)$ over all admissible designs. Equivalently, one can minimize the logarithm of the determinant of the inverse matrix $\mathrm{D}(\xi)$. In mathematical terms, the criterion is written as: $\log\det \mathrm{M}(\xi) \to \sup_{\xi\in\Xi}$, or, alternatively, $\log\det \mathrm{D}(\xi) \to \inf_{\xi\in\Xi}$.

This criterion has a clear geometric interpretation. It corresponds to minimizing the volume of the confidence ellipsoid for the parameter vector. The ellipsoid is defined as the set of all parameter values $\widetilde{\theta}$ such that the quadratic form of the deviation, with respect to the matrix $\mathrm{D}(\xi)$, does not exceed a fixed constant α. This constant α depends only on the chosen confidence level. Thus, the D-criterion aims to minimize the uncertainty region for the estimated parameters.

Another widely used criterion is the L-optimality criterion. It is defined as the trace of the product of a fixed symmetric nonnegative definite matrix L and the matrix $\mathrm{D}(\xi)$. The goal is to minimize this trace over all nonsingular designs. The statistical meaning of this criterion is minimization of the expected value of the quadratic loss, where the loss is defined with respect to the matrix L. Specifically, it minimizes the expected value of the scalar product of the estimation error with the matrix L. This framework allows tailoring the criterion to emphasize certain parameters or combinations thereof.

e_k-criterion

A design $\xi \in \Xi$ is called e_k-optimal if

$$e_k^T M^-(\xi) e_k \to \inf_{\xi \in \Xi_{e_k}}, \quad \Xi_{e_k} = \{\xi \in \Xi : e_k^T M^-(\xi) M(\xi) = e_k^T\}.$$

This criterion minimizes the variance of the estimator $\widehat{\theta}_k$.

E-criterion

A design $\xi \in \Xi_{NS}$ is called E-optimal if

$$\lambda_{\min}(M(\xi)) \to \sup_{\xi \in \Xi_{NS}} \quad \text{or} \quad \lambda_{\max}(D(\xi)) \to \inf_{\xi \in \Xi_{NS}}.$$

This criterion maximizes the smallest eigenvalue of the information matrix.

G-criterion

A design $\xi \in \Xi_{NS}$ is called G-optimal if

$$\max_{t \in \chi} d(t, \xi) \to \inf_{\xi \in \Xi_{NS}}, \quad d(t, \xi) =$$

This criterion minimizes the maximum prediction variance over the design space.

Comments

On this slide we discuss three important optimality criteria used in the theory of experimental designs: the e_k-criterion, the E-criterion, and the G-criterion.

First, the e_k-criterion focuses on minimizing the variance of the estimator for the single parameter coordinate θ_k. In other words, it aims to reduce the k-th diagonal element of the covariance matrix, which corresponds to the uncertainty in estimating θ_k. It is important to note that e_k-optimal designs are generally degenerate, meaning that not all parameters can be estimated unbiasedly from such designs. However, these designs are useful when only a subset of parameters is of interest. Additionally, the e_k-criterion is a special case of the more general L-optimality criterion when the weighting matrix L is chosen as the outer product of the k-th standard basis vector with itself.

The E-criterion aims to improve the overall worst-case precision by maximizing the smallest eigenvalue of the information matrix. Equivalently, it minimizes the largest eigenvalue of the covariance matrix. This means that the longest axis of the confidence ellipsoid is shortened, leading to a more balanced estimation accuracy across all parameters.

Finally, the G-criterion is concerned with prediction accuracy. It minimizes the maximum variance of predicted values over the entire design space. This criterion ensures that the worst prediction variance at any point is as small as possible, which is crucial for reliable response surface estimation.

Together, these criteria provide different perspectives and tools to design experiments depending on the specific goals: precise estimation of individual parameters, balanced overall estimation, or reliable prediction.

General Form of Optimality Criteria

Optimality criteria in general form

All discussed optimality criteria can be expressed as

$$\Psi(\mathrm{M}^{-}(\xi)) \to \inf_{\xi} \quad \text{or} \quad \Phi(\mathrm{M}(\xi)) \to \sup_{\xi}.$$

Here, the functions Ψ and Φ satisfy the following properties:

(a) Monotonicity:

$$\Phi(\mathrm{M}(\xi_1)) \le \Phi(\mathrm{M}(\xi_2)) \quad \text{if} \quad \mathrm{M}(\xi_1) \le \mathrm{M}(\xi_2).$$

(b) Homogeneity:

$$\Phi(\theta\mathrm{M}(\xi)) \le \gamma(\theta)\Phi(\mathrm{M}(\xi)),$$

where $\gamma(\theta)$ is a non-decreasing function.

(c) Concavity (convexity for Ψ):

$$\Phi(\mathrm{M}((1-\alpha)\xi_1 + \alpha\xi_2)) \ge (1-\alpha)\Phi(\mathrm{M}(\xi_1)) + \alpha\Phi(\mathrm{M}(\xi_2)).$$

Remark

A more complete list of criteria can be found in the experimental design literature.

Comments

This slide presents the general mathematical form in which most optimality criteria for experimental design can be expressed. These criteria are usually written either in terms of the inverse information matrix or the information matrix itself. More precisely, we try to minimize a function Ψ of the inverse information matrix — that is, $\Psi(\mathrm{M}^{-}(\xi))$ — or equivalently, to maximize a function Φ of the information matrix — that is, $\Phi(\mathrm{M}(\xi))$.

For these functions to define reasonable and meaningful criteria, they are typically required to satisfy three important properties.

First is monotonicity. This means that if one design has an information matrix smaller than another in the matrix ordering sense, then the value of the function Φ for that design must also be smaller. In other words, if $\mathrm{M}(\xi_1) \le \mathrm{M}(\xi_2)$, then $\Phi(\mathrm{M}(\xi_1)) \le \Phi(\mathrm{M}(\xi_2))$. This guarantees that better information matrices give better criterion values.

Second is homogeneity. If we scale the information matrix by a positive factor θ, then the criterion Φ scales no faster than some corresponding function $\gamma(\theta)$, which itself is non-decreasing. That is, $\Phi(\theta\mathrm{M}(\xi)) \le \gamma(\theta)\Phi(\mathrm{M}(\xi))$.

Third is concavity. This means that if we mix two designs — say, ξ_1 and ξ_2 — with weights $1-\alpha$ and α, then the criterion value for the mixed design is at least as large as the weighted average of the criterion values for the individual designs. Mathematically, $\Phi(\mathrm{M}((1-\alpha)\xi_1 + \alpha\xi_2)) \ge (1-\alpha)\Phi(\mathrm{M}(\xi_1)) + \alpha\Phi(\mathrm{M}(\xi_2))$. This property is crucial for optimization because it guarantees that local maxima are also global.

Taken together, these properties ensure that the function Φ behaves in a predictable and mathematically nice way, which allows us to formulate and solve design optimization problems efficiently. There are many other optimality criteria that are used in practice, but their study is beyond the scope of our course.

Kiefer–Wolfowitz Equivalence Theorem

For the model (1o) under assumption (a) – (f) if the set of information matrices is compact, then the following conditions are equivalent for a design ξ^*:

(a) ξ^* is ***D-optimal***;

(b) ξ^* is ***G-optimal***;

(c) $\mathbf{max}_{x\in\mathcal{X}} d(x, \boldsymbol{\xi^*}) = m$,

where $d(x, \xi^*) = f^T(x)M^{-1}(\xi^*)f(x)$.

Moreover, if ξ^* has finite support, this maximum is attained at the support points x_i^*. All D-optimal designs share the same information matrix. Under the conditions of the theorem $\xi^* \in \Xi$.

Notation

$D(\xi) = M(\xi)^{-1}$ is the inverse information matrix; m is the number of parameters.

Comments

This slide introduces one of the central results in the theory of optimal experimental design — the Kiefer–Wolfowitz Equivalence Theorem. It establishes a deep connection between different optimality criteria and provides a powerful tool for verifying the optimality of a given design.

According to the theorem, if the set of possible information matrices is compact — which is a standard regularity assumption — then three conditions are equivalent for a design denoted ξ^*.

First, condition (a): the design ξ^* is D-optimal. This means it maximizes the determinant of the information matrix, or equivalently, minimizes the volume of the confidence ellipsoid for the parameter estimates.

Second, condition (b): the same design ξ^* is also G-optimal. That is, it minimizes the maximum variance of the predicted response over the entire experimental region.

Third, condition (c): the maximum value of the function $d(x, \xi^*)$, taken over all points x in the design space, is equal to m, where m is the number of parameters in the model. Here, the function $d(x, \xi)$ is defined as the transpose of the regression vector at x times the inverse information matrix times the regression vector at x. This quantity represents the variance of the predicted response at point x.

Importantly, if the optimal design ξ^* is concentrated on a finite set of points, then this maximum value of the function d is achieved exactly at the support points of the design. These are the points where the design assigns positive weight.

Another significant implication of the theorem is that all D-optimal designs — even if they differ in their specific support points — share the same information matrix. This means the precision of estimation is the same across all such designs.

This theorem is extremely useful because it allows us to check D-optimality by verifying a simpler G-optimality condition or by calculating the function d and checking whether its maximum equals m.

Lemma 11

Let A be an arbitrary positive definite matrix of size $m \times m$. Then the following integral representation for its determinant holds:

$$(\det A)^{-1/2} = \frac{1}{\pi^{m/2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-x^T Ax}\, dx_1 \dots dx_m.$$

Proof:

- We use the ***classical identity*** from real analysis:
$$\int_{-\infty}^{\infty} e^{-z^2}\, dz = \sqrt{\pi}.$$
- First, assume that A is a ***diagonal matrix***, where $A = \mathbf{\Lambda}$ with nonzero diagonal elements λ_i. Then, the integral becomes:
$$\int_{\mathbb{R}^m} e^{-x^T Ax}\, dx = \int_{\mathbb{R}^m} e^{-\sum_{i=1}^m \lambda_i x_i^2}\, dx = \prod_{i=1}^m \int_{-\infty}^{\infty} e^{-\lambda_i x_i^2}\, dx_i.$$
- Each one-dimensional integral evaluates to $\sqrt{\pi/\lambda_i}$, so the result is:
$$\int_{\mathbb{R}^m} e^{-x^T Ax}\, dx = \prod_{i=1}^m \sqrt{\frac{\pi}{\lambda_i}} = \pi^{m/2} (\det A)^{-1/2}.$$

Comments

To prove the Kiefer–Wolfowitz equivalence theorem, we need several auxiliary results. This slide presents the first such lemma — a classic identity from multivariate calculus.

The lemma states that for any positive definite matrix A of size $m \times m$, we can express the reciprocal square root of the determinant of A as a Gaussian integral over $\mathbb{R}^m$. Specifically, the formula involves the exponential of minus one-half times $x^T Ax$, integrated over the whole space.

This result is not just an elegant analytical identity — it plays an important role in optimal design theory because it connects determinants with Gaussian densities, which frequently appear in statistical estimation, particularly in maximum likelihood and Bayesian contexts.

The proof is straightforward for diagonal matrices. We start by recalling the classical Gaussian integral: the integral of e^{-z^2} over the real line equals $\sqrt{\pi}$. Then, if the matrix A is diagonal, say with elements λ_1 through λ_m, the quadratic form reduces to the sum of $\lambda_i x_i^2$ for each component. The multivariate integral then splits into a product of independent one-dimensional integrals, each of which evaluates to $\sqrt{\pi/\lambda_i}$. Multiplying these together yields the final formula.

In the next step, we will generalize this to arbitrary positive definite matrices.

Proof of the Lemma (continued)

- If A is an arbitrary ***positive definite matrix***, we can use the ***spectral decomposition theorem*** to write:

$$A = P^T \mathbf{\Lambda} P, \quad \text{where } P^T P = I \text{ and } \mathbf{\Lambda} \text{ is diagonal.}$$

- Let's make a change of variables: $x = Py$. This simplifies the quadratic form:

$$x^T A x = (Py)^T A P y = y^T \mathbf{\Lambda} y = \sum_{i=1}^{m} \lambda_i y_i^2.$$

- Since the columns of P form an orthonormal basis, the ***Jacobian*** of this transformation is equal to one. Therefore, the integral becomes:

$$\int_{\mathbb{R}^m} e^{-x^T A x} dx = \int_{\mathbb{R}^m} e^{-y^T \mathbf{\Lambda} y} dy = \pi^{m/2} (\det A)^{-1/2}.$$

This completes the proof. □

Comments

To complete the proof of the lemma, we now consider the case when matrix A is arbitrary but still positive definite. In this more general setting, we apply the spectral decomposition theorem. According to this result, matrix A can be written as $P^T \Lambda P$, where P is an orthogonal matrix ($P^T P = I$) and Λ is a diagonal matrix containing the eigenvalues of A on its main diagonal.

We now make a change of variables: let vector $x = Py$. This transformation corresponds to a rotation of the coordinate system. Since P is an orthogonal matrix, this change preserves volume, and therefore the Jacobian of the transformation is equal to one.

Substituting this new variable into the quadratic form $x^T A x$, we get: $y^T \Lambda y$. Because Λ is diagonal, this reduces to a sum of $\lambda_i y_i^2$, where i runs from 1 to m.

Thus, the multivariate integral of the exponential of $-x^T A x$ becomes the same as in the diagonal case. The integral over y is then the product of m one-dimensional Gaussian integrals, each evaluating to $\sqrt{\pi/\lambda_i}$. Therefore, we again arrive at the expression $\pi^{m/2} (\det A)^{-1/2}$.

This confirms that the lemma holds for any positive definite matrix A.

Lemma 12

Let A and B be arbitrary positive definite matrices of size $m \times m$. Then the following inequality holds:

$$\det(\alpha A + (1-\alpha)B) \geq (\det A)^{\alpha}(\det B)^{1-\alpha}, \quad \text{for all } \alpha \in [0,1],$$

with equality if and only if $A = B$.

Proof: The proof is based on Hölder's inequality.

- Let $p > 1$ and define $q = \frac{p}{p-1}$. Let $f \in L^p$, $g \in L^q$ be functions on a measurable set $X \subset \mathbb{R}^n$.
- Then:

$$\int_X f(x)g(x)dx \leq \left(\int_X f(x)^p dx\right)^{1/p} \left(\int_X g(x)^q dx\right)^{1/q},$$

with equality if and only if

$$\frac{f(x)^p}{\int_X f(x)^p dx} = \frac{g(x)^q}{\int_X g(x)^q dx}.$$

Comments

To advance the proof of the Kiefer–Wolfowitz Equivalence Theorem, we need another auxiliary result: for any two positive definite matrices A and B, both of size $m \times m$, the determinant of their convex combination, $\alpha A + (1-\alpha)B$, is at least the product of $(\det A)^{\alpha}$ and $(\det B)^{1-\alpha}$, for any α between 0 and 1.

Equality holds only when $A = B$. This inequality will allow us to further establish concavity of the determinant function, which is critical for linking D-optimality, maximizing the determinant of the information matrix, to G-optimality, minimizing the maximum prediction variance.

The proof hinges on Hölder's inequality. For functions f in L^p and g in L^q, where $q = p/(p-1)$ and $p > 1$, the integral of $f(x)g(x)$ over a measurable set X is bounded by the p-norm of f times the q-norm of g. Equality holds only when the normalized p-th power of f equals the normalized q-th power of g. Applying Hölder's inequality, we derive the determinant inequality by expressing the determinant in terms of integrals, building on the Gaussian integral from the previous lemma.

Completion of the Proof (Determinant Inequality)

- Let $p = \frac{1}{\alpha}, \quad q = \frac{1}{1-\alpha}, \quad f(x) = e^{-\alpha x^T A x}, \quad g(x) = e^{-(1-\alpha)x^T B x}.$
- Then:
$$\int_{\mathbb{R}^n} e^{-z^T(\alpha A+(1-\alpha)B)z}\,dz = \int f(z)g(z)\,dz$$
- Applying Hölder's inequality:
$$\int f(z)g(z)\,dz \le \left(\int f^{1/\alpha}(z)\,dz\right)^{\alpha}\left(\int g^{1/(1-\alpha)}(z)\,dz\right)^{1-\alpha}$$
- Using the Gaussian integral formula:
$$\frac{\pi^{n/2}}{\sqrt{\det(\alpha A+(1-\alpha)B)}} \le \left(\frac{\pi^{n/2}}{\sqrt{\det A}}\right)^{\alpha}\left(\frac{\pi^{n/2}}{\sqrt{\det B}}\right)^{1-\alpha}$$
- Therefore:
$$\det(\alpha A+(1-\alpha)B) \ge (\det A)^{\alpha}(\det B)^{1-\alpha}$$

Equality holds if and only if $A = B$. □

Comments

To complete the proof of the determinant inequality, we apply Hölder's inequality directly to the Gaussian integral involving the convex combination of matrices A and B. First, we define two functions: $f(z) = e^{-\alpha z^T A z}$, and $g(z) = e^{-(1-\alpha)z^T B z}$. We also set the exponents $p = 1/\alpha$ and $q = 1/(1-\alpha)$.

With these definitions, the integral of the exponential of $-z^T(\alpha A + (1-\alpha)B)z$ becomes the integral of $f(z)g(z)$. Hölder's inequality now tells us that this integral is less than or equal to the product of the L^p-norm of f raised to α and the L^q-norm of g raised to $1-\alpha$.

The norms of f and g correspond to Gaussian integrals. From the previous lemma, we know that the integral of $e^{-z^T Az}$ over all of Euclidean space is equal to $\pi^{n/2}/\sqrt{\det A}$. Applying this fact to f and g, we arrive at an inequality for the integral involving the convex combination of A and B.

Finally, rearranging the inequality gives us the determinant inequality: $\det(\alpha A + (1-\alpha)B) \ge (\det A)^{\alpha}(\det B)^{1-\alpha}$. Equality holds only if $A = B$. This concludes the proof of the lemma.

Lemma 13

The function $f(A) = \ln\det A$ is strictly concave on the set of positive definite matrices of size $m \times m$.

Proof: By definition, it suffices to show that for any $0 < \alpha < 1$ and $A \neq B$, the inequality

$$\ln\det(\alpha A + (1-\alpha)B) > \alpha \ln\det A + (1-\alpha)\ln\det B$$

holds. This follows immediately by taking the logarithm of the inequality from the previous lemma. □

Lemma 14

For any differentiable matrix function $A(\alpha)$ with $A(\alpha) > 0$ (the matrix of size $m \times m$), the following identity holds:

$$\frac{\partial}{\partial\alpha}\ln\det A(\alpha) = \operatorname{tr}\left(A^{-1}(\alpha)\frac{\partial A(\alpha)}{\partial\alpha}\right)$$

Comments

In this slide, we present two important lemmas that play a central role in the analysis of optimality criteria and the proof of the equivalence theorem.

The first lemma states that the function $f(A) = \ln\det A$ is strictly concave on the set of positive definite matrices of size $m \times m$. That is, if we take any two distinct positive definite matrices A and B, and form their convex combination weighted by α and $1-\alpha$, then the logarithm of the determinant of this combination is strictly greater than the weighted sum of the logarithms of the determinants. This is a classic result in matrix analysis, and it follows directly by taking the logarithm of the determinant inequality we proved earlier. That inequality stated that the determinant of the convex combination of A and B is at least the product of their determinants raised to the corresponding weights. Taking the logarithm transforms the multiplicative inequality into an additive one, and the strict inequality holds whenever A and B are not equal.

The second lemma provides a useful identity for differentiating the log-determinant function. If we have a matrix-valued function $A(\alpha)$, and this matrix is positive definite for all values of α, then the derivative of $\ln\det A(\alpha)$ with respect to α is equal to the trace of $A^{-1}(\alpha)$ times the derivative of $A(\alpha)$. This result comes from matrix calculus and is widely used in optimization, especially in contexts where we differentiate likelihood functions or objective functions involving log determinants. It provides an efficient way to compute gradients without directly differentiating the determinant itself, which would be more complicated.

These lemmas will be used in the next steps of the proof.

Proof of Lemma on Derivative of log-det

Proof: We use the rule for the derivative of the logarithm:

$$\frac{\partial}{\partial\alpha}\ln\det \mathrm{A}(\alpha) = \frac{1}{\det \mathrm{A}(\alpha)}\cdot\frac{\partial}{\partial\alpha}\det \mathrm{A}(\alpha)$$

Using the expansion of the determinant:

$$\det \mathrm{A} = \sum_{i,j=1}^{m}(-1)^{i+j}a_{ij}A_{ij}, \quad \text{where } A_{ij} \text{ are cofactors}$$

Since cofactors do not depend on the element a_{ij}, we get:

$$\frac{\partial \det \mathrm{A}}{\partial a_{ij}} = (-1)^{i+j}A_{ij}$$

Using the identity:

$$a^{ij} = \frac{(-1)^{i+j}A_{ji}}{\det \mathrm{A}} \quad (\text{entries of } \mathrm{A}^{-1})$$

We obtain:

$$\frac{\partial}{\partial\alpha}\ln\det \mathrm{A}(\alpha) = \sum_{i,j=1}^{m}\underbrace{\frac{(-1)^{i+j}A_{ij}}{\det \mathrm{A}}}_{a^{ji}}\frac{\partial a_{ij}(\alpha)}{\partial\alpha} = \operatorname{tr}\left(\mathrm{A}^{-1}\cdot\frac{\partial \mathrm{A}}{\partial\alpha}\right) \qquad \square$$

Comments

To prove the identity for the derivative of the log determinant, we begin by applying the standard calculus rule for differentiating a logarithmic function. The derivative of $\ln\det \mathrm{A}(\alpha)$ with respect to α is equal to $1/\det \mathrm{A}(\alpha)$ times the derivative of $\det \mathrm{A}(\alpha)$ with respect to α.

Next, we recall the classical formula for the determinant of a square matrix. It can be written as a sum over all elements a_{ij} multiplied by their corresponding cofactors A_{ij}, each weighted by the sign factor $(-1)^{i+j}$. This expansion allows us to compute the partial derivative of the determinant with respect to any element a_{ij}, which equals the signed cofactor.

Then, we recall the standard expression for the entries of the inverse matrix. The entry in position (i,j) of the inverse matrix A^{-1} is equal to the signed cofactor A_{ji} divided by the determinant of A. Using this identity, we rewrite the derivative of the determinant as a sum over i and j of the derivative of a_{ij} times the corresponding entry of the inverse matrix.

Combining all these steps, the derivative of $\ln\det \mathrm{A}(\alpha)$ becomes the trace of the product of A^{-1} and $\partial \mathrm{A}/\partial\alpha$. This completes the proof of the lemma.