Moment Problems and Polynomials

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Classical problem

Find a positive Borel measure μ on $\mathbf{R}$, with prescribed moments

$$s_k = \int x^k d\mu(x), \quad 0 \leq k < n.$$

With $n \leq \infty$.

Abstract version

X structured vector space, $f_1, ..., f_n$ linearly independent elements *standing for monomials*

Find $L \in X^*$ with prescribed values

$$L(f_k) = s_k, \ 0 \leq k < n,$$

and additional properties such as

minimal norm, L is positive on a specified cone, extremal among all solutions,...

Statisticians first

M. G. Kendall: *The Advanced Theory of Statistics*, London, 1945.

In prectice numerical moments of order higher than fourth are rarely required, being so sensitive to sampling fluctuations that values computed from moderate numbers of observations are subject to a large margin of error.

Cumulants

$$\sum_{k=0}^{\infty} \kappa_k \frac{z^n}{n!} = \log \sum_{\ell=0}^{\infty} s_\ell \frac{z^\ell}{\ell!}.$$

are invariants under the translation group.

Extremely simple for the classical probability distributions, additive for sums of independent random variables. The coefficients (Bell polynomials) have a high combinatorial significance.

Hald, Anders. *A History of Mathematical Statistics from 1750 to 1930*. New York: Wiley., 1998.

Best approximation

Chebyshev's problem (around 1860):

Given a C^1-function $F(x_1, ..., x_d; p_1, ...p_n)$ on a domain $\Omega \subset \mathbf{R}^d$, depending on parameters $p_1, ..., p_n$, find

$$\min_{p_1,...,p_n} \max_{x_1,...,x_d} |F(x_1, ..., x_d; p_1, ...p_n)|.$$

inspired by Poncelet's extremal problem for $\frac{p_1 x + p_2}{\sqrt{1+x^2}} - 1$.
Both Chebyshev and A. A. Markov have extensively worked on this subject, becoming masters of continued fractions, as a necessary technical tool.

Chebyshev polynomials

Consider the polynomial of minimal variation from zero, on an interval $[-h, h]$, of the form

$$f(x) = x^n + p_1 x^{n-1} + \ldots + p_n,$$

with $p_1, ..., p_n$ parameters to be determined.

Necessarily

$$f(x)^2 - L^2 = (x^2 - h^2)\frac{f'(x)^2}{n^2}$$

where L is the optimal value.

The division algorithm

$$f(x) - \sqrt{x^2 - h^2}\frac{f'(x)}{n} = \frac{L^2}{f(x) + \sqrt{x^2 - h^2}\frac{f'(x)}{n}}$$

hence

$$\frac{1}{\sqrt{x^2 - h^2}} - \frac{f'(x)}{nf(x)} = \frac{L^2}{\sqrt{x^2 - h^2}f(x)[f(x) + \sqrt{x^2 - h^2}f'(x)/n]}$$

that is

$$\frac{1}{\sqrt{x^2 - h^2}} - \frac{f'(x)}{nf(x)} = O(\frac{1}{x^{2n+1}}).$$

There is only one choice: $\frac{f'(x)}{nf(x)}$ is the n-th convergent of the coninued fraction expansion of $\frac{f'(x)}{nf(x)}$:

$$\frac{f'(x)}{nf(x)} = \cfrac{1}{x - \cfrac{h^2}{2x - \cfrac{h^2}{\ddots - \frac{h^2}{2x}}}}.$$

That is

$$f(x) = \frac{(x + \sqrt{x^2 - h^2})^n + (x - \sqrt{x^2 - h^2})^n}{2^n}.$$

Polynomial extrapolation

Chebyshev again

The real points $x_0, ..., x_n, X$ are given. Knowing the approximative values of a polynomial F of degree n at $n+1$ points x_k, find the errors in the values $F(x_k)$ which have minimal influence of the value $F(X)$.

As a matter of fact an extremal problem in square mean.

$$F(x) = \mu_0 q_0(x) f(x_0) + \ldots + \mu_m q_n(x) f(x_n)$$

with $q_k(x)$ unknown polynomials, such that

$$\mu_0 q_o(x)^2 + \ldots + \mu_n q_n(x)^2$$

is minimal.

Continued fractions

The solution exposed by Chebyshev reduces to a continued fraction argument. Given

$$\sum_{k=0}^{n} \frac{\mu_k}{x_k - z} = -\frac{s_0}{z} - \frac{s_1}{z^2} - \dots$$

find a polynomial $P(x)$ of degree m such that

$$P(x)(\frac{s_0}{z} + \frac{s_1}{z^2} + \dots)$$

begins with a term of highest order.

Bounds for integrals

Chebyshev 1833

Find bounds for $\int_0^a f(x)dx$, *from the known values*

$$s_0 = \int_0^A f(x)dx, s_1 = \int_0^A xf(x)dx, \ldots, s_n = \int_0^A x^n f(x)dx$$

where $A > a$ *and* $f(x) \geq 0$.

Major observation: if $q_m(x)/p_m(x)$ is the continued fraction convergent of the expansion of

$$\int_0^A \frac{f(x)dx}{x-z} = -\frac{s_0}{z} - \frac{s_1}{z^2} - \ldots$$

and $\lambda_1 < \lambda_2 < \ldots$ are the (simple) zeros of $p_n(x)$, then

$$\sum_{k=\ell+1}^{n-1} \frac{q_m(\lambda_k)}{p_n'(\lambda_k)} < \int_{\lambda_\ell}^{\lambda_n} f(x)dx < \sum_{k=\ell}^{n} \frac{q_m(\lambda_k)}{p_n'(\lambda_k)}$$

Limit Theorems in Probability Theory

Chebyshev 1887, Markov 1899:

Assume that the functions $f_n \geq 0$ satisfy

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} x^k f_n(x)dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x^k e^{-x^2/2} dx, \quad k \geq 0.$$

Then, for every $\alpha < \beta$

$$\lim_{n\to\infty} \int_{\alpha}^{\beta} f_n(x)dx = \frac{1}{\sqrt{2\pi}} \int_{\alpha}^{\beta} e^{-x^2/2} dx.$$

Stieltjes memoir, 1894-95

The sequence $(s_k)_{k=0}^{\infty}$ represents the moments of a positive measure supported on $[0, \infty)$ if and only if the continued fraction expansion

$$\frac{s_0}{z} + \frac{s_1}{z^2} + \ldots = \cfrac{1}{c_0 z - \cfrac{1}{c_1 - \cfrac{1}{c_2 z - \cfrac{1}{c_3 - \ldots}}}}$$

contains only non-negative terms $c_k \geq 0$.

Determinateness

If $\sum_{k=0}^{\infty} c_k = \infty$, then the convergents $\frac{P_m(z)}{Q_m(z)}$ converge in the upper-half plane to $\int_0^{\infty} \frac{d\sigma(x)}{z-x}$, and the measure $\sigma \geq 0$ is unique.

If $\sum_{k=0}^{\infty} c_k < \infty$, then the convergents satisfy in the upper-half plane:

$$P_{2k}(z) \to p(z), \quad Q_{2k}(z) \to q(z),$$

$$P_{2k+1}(z) \to p_1(z), \quad Q_{2k+1}(z) \to q_1(z),$$

where p, q, p_1, q_1 are entire functions of genus zero, satisfying

$$q(z)p_1(z) - q_1(z)p(z) = 1.$$

In that case the problem has infinitely many solutions, with distinct Cauchy transforms. Among these:

$$\frac{p(z)}{q(z)} = \sum_{k=1}^{\infty} \frac{\mu_k}{z - \lambda_k}, \quad \frac{p_1(z)}{q_1(z)} = \sum_{k=1}^{\infty} \frac{\mu'_k}{z - \lambda'_k}.$$

More on continued fractions

Hamburger 1919-1921

solves the power moment problem on the real axis, remarking (following Stieltjes) the positivity of the Hankel determinants

$$\det \begin{pmatrix} s_0 & s_1 & \cdots & s_n \\ s_1 & s_2 & \cdots & s_{n+1} \\ \vdots & & \ddots & \vdots \\ s_n & s_{n+1} & \cdots & s_{2n} \end{pmatrix} \geq 0$$

as necessary and sufficient conditions for solvability.

Recent references

Iosifescu, Kraaikamp: *Metrical Theory of Continued Fractions*, Springer 2002
Cuyt, Brevik Petersen, Verdonk, Waadeland, Jones: *Handbook of Continued Fractions*, Springer 2008
Khrushchev: *Orthogonal Polynomials and Continued Fractions*, Cambridge U. Press, 2008.

Bounded analytic interpolation

The moment problem as a tangential (i.e. boundary) interpolation problem for analytic functions of the form

$$f(z) = \int_{\mathbf{R}} \frac{d\sigma(x)}{x - z}, \quad f(z) \approx -\frac{s_0}{z} - \frac{s_1}{z^2} - \dots.$$

In this case $\Im z > 0 \;\Rightarrow\; \Im f(z) > 0$ and $\sup_{t \geq 1} |tf(it)| < \infty$.

The interpolation problem: *Find and describe $f : \Omega \to \omega$ analytic such that $f(\lambda) = c_\lambda$ for $\lambda \in \Delta$, discrete subset of Ω.*

has a glorious past and present, and MTNS is not disconnecetd from it:

Google citations, July 2014

Caratheodory-Fejér interpolation	13,000
Nevanlinna-Pick interpolation	39,000
Schur algorithm	284,000
H^∞-control	4,510,000

Nevanlinna parametrization

Obtained around 1922 by Hamburger and Nevanlinna:
free parametrization of all solutions to the power moment problem, in the indeterminate case

$$f(z) = \int_{\mathbf{R}} \frac{d\sigma(x)}{x - z} = -\frac{p(z)\phi(z) - p_1(z)}{q(z)\phi(z) - q_1(z)},$$

where $\phi(z)$ is any analytic function satisfying $\Im\phi(z) \geq 0$ whenever $\Im z > 0$.

Berg: *Indeterminate moment problems and the theory of entire functions*, J. Comput. Appl. Math. 65: 13(1995), 27 - 55.

Fourier transform

Known as the method of characteristic function in Probability

$$\hat{\sigma}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ix\xi} d\sigma(x)$$

uniquely determines σ (by known inversion formulae).

Bochner: $\sigma \geq 0$ if and only if $\hat{\sigma}(\xi_1 - \xi_2)$ is a positive semi-definite kernel.

If the moments exist $\hat{\sigma} \in C^\infty$ and

$$s_k = \sqrt{2\pi}(-i)^k \hat{\sigma}^{(k)}(0), \quad k \geq 0.$$

Carleman's approach

Quasi-analytic Functions (1926):

$u \in C^\infty[0,1]$ is fully determined by $(u^{(k)}(0))_{k=0}^\infty$ if and only if

$$\sum_{k=0}^{\infty} \frac{1}{L_k} = \infty$$

where

$$|u^{(k)}(x)| \leq K^{k+1} M_k, \quad 0 \leq x \leq 1, \quad k \geq 0,$$

and

$$L_k = \inf_{j \geq k} M_j^{1/j}.$$

Determinateness

via quasi-analyticity

$$\sum_{k=0}^{\infty} \frac{1}{s_{2k}^{1/(2k)}} = \infty$$

implies uniqueness of the positive measure on $\mathbf{R}$ with moments (s_k).

$$\sum_{k=0}^{\infty} \frac{1}{s_{k}^{1/(2k)}} = \infty$$

implies uniqueness of the positive measure on $[0, \infty)$ with moments (s_k).

Reconstruction

Carleman's reconstruction formula of a quasi-analytic function $u \in C_M^\infty$:

$$u(x) = \lim_{n\to\infty} \sum_{k=0}^{n-1} \omega_{n,k} u^{(k)}(0) x^k,$$

where the coefficients $\omega_{n,k}$ depend only on the class C_M^∞.

Laplace transform

$$g(t) = \mathcal{L}(\sigma)(t) = \int_0^\infty e^{-xt} d\sigma(x),$$

also satisfies

$$s_k = (-1)^k \mathcal{L}(\sigma)^{(k)}(0), \quad k \geq 0$$

whenever the moments exist.
Analytic extension

$$\mathcal{L}(\sigma)(z) = \int_0^\infty e^{-xz} d\sigma(x),$$

for $Rez > 0$ with known inversion formulae...

S. Bernstein (1929): characterization of transforms of positive measures

$$g \in C^\infty[0, \infty), \quad (-1)^k g^{(k)} \geq 0, \quad k \geq 0.$$

Abolutely continuous measures

$$d\sigma(x) = \tau(x)dx, \quad \tau \in L^p([0,\infty))$$

has Laplace transform in a Hardy class of the right half-plane, with an arsenal of function theory of a complex variable available.

Widder (1934) inversion: $g(t) = \mathcal{L}(\tau dx)(t)$ reads

$$\lim_{k\to\infty} (-1)^k g^{(k)}(\frac{k}{t})(\frac{k}{t})^{k+1} = \tau(t), \quad t > 0.$$

Summation of divergent series

Improving the convergence of series by average methods, induced by a regular summation scheme

$$t_n = \sum_{k=0}^{n} a_{nk} u_k,$$

so that

$$\lim u_n = u \quad \Rightarrow \lim t_n = u.$$

Hausdorff (1921) A sequence $(s_n)_{n=0}^{\infty}$ represents the moments of a probability measure on $[0,1]$ if and only if the matrix $D\mathrm{diag}(s_0, s_1, ...)D$ induces a regular summation scheme, where

$$D = ((-1)^n \begin{pmatrix} k \\ n \end{pmatrix}).$$

Extension of linear functionals

A positive Borel measure σ on $\mathbf{R}$, admitting all moments, is given by a positive linear functional $L : C_p(\mathbf{R}) \longrightarrow \mathbf{R}$, where C_p is the space of continuous functions of polynomial growth:

$$\int f d\sigma = L(f), \quad f \in C_p(\mathbf{R}).$$

M. Riesz (1922-23) Solving the moment problem by **linear extension** of positive linear functionals

$$L_d : \mathbf{R}_d[x] \longrightarrow \mathbf{R}$$

where

$$\mathbf{R}_d[x] = \{p \in \mathbf{R}[x];\ \deg p \leq d\}.$$

Convexity

M. Riesz method prompted to study the convex cones

$$\{p \in \mathbf{R}_d[x], \quad p(x) \geq 0, \quad x \in K\}$$

and

$$\{\sigma \in M_+(\mathbf{R}), \int x^k d\sigma(x) = s_k, \quad 0 \leq k \leq n\}.$$

Carathéodory (1911) carried earlier a similar analysis on the unit circle $\mathbf{T}$.

Classical Harmonic Analysis

On the unit circle $\mathbf{T}$, the moments of a measure are exactly its Fourier coefficients:

$$\hat{\sigma}(n) = \int_{-\pi}^{\pi} e^{-inx} d\sigma(x), \ n \in \mathbf{Z}.$$

Toeplitz and Carathéodory (1911): $\sigma \geq 0$ if and only if the kernel $\hat{\sigma}(n-m)$ is positive semi-definite.

F. Riesz and Herglotz (1911) establish a fundamental correspondence between non-negative harmonic functions in the unit disk and (moments of) positive measures on the circle.

Hilbert space

The moments of a positive measure σ are structured in a non-negative definite Gramm matrix

$$s_{k+m} = \int x^k x^m d\sigma(x) = \langle x^k, x^m \rangle_{2,\sigma}.$$

Hence an associated system of orthogonal polynomials

$$P_k(x) = \gamma_k z^k + O(z^{k-1}), \quad \langle P_k, P_m \rangle_{2,\sigma} = \delta_{km}.$$

The leading coefficient solves an extremal problem, à la Chebyshev-Markov:

$$\gamma_k^{-1} = \inf_{\deg q \leq k-1} \|z^k - q(z)\|_{2,\sigma}.$$

Christoffel functions

Given orthonormal polynomials P_n, the Christoffel function

$$C_n(z,z) = \sum_{k=0}^{n} |P_k(z)|^2$$

and its polarization

$$C_n(z,w) = \sum_{k=0}^{n} P_k(z)\overline{P_k(w)}$$

are essential in the study of the asymptotics of the polynomials P_n.

M. Riesz (1923): the solution to the extremal problem

$$\rho_n(\lambda) = \min\{\|q\|_{2,\sigma}^2, \quad \deg q \le n, \quad q(\lambda) = 1\}$$

is attained by the polynomial

$$\rho_n(z) = \frac{C(z,\lambda)}{C(\lambda,\lambda)}.$$

Weyl circle

Another parametrization of all solutions, obtained via the values of the Cauchy transforms

$$C(\sigma_n)(\lambda) = \int \frac{d\sigma_n(x)}{x-\lambda}, \quad \int x^k d\sigma_n(x) = s_k, \quad k \leq n.$$

They form a disk of radius ρ_n.

Parallel theory to the continuous case (Sturm-Liouville problem) studied by H. Weyl a decade before Riesz.

Jacobi matrices

The sequence of OP P_n satisfies a finite difference equation

$$zP_n(z) = b_{n+1}P_{n+1}(z) + a_nP_n(z) + b_nP_{n-1}(z), \quad P_{-1} = 0.$$

Hence the associated tri-diagonal symmetric matrix

$$J = \begin{pmatrix} a_0 & b_1 & 0 & 0 & \dots \\ b_1 & a_1 & b_2 & 0 & \dots \\ 0 & b_2 & a_2 & b_3 & \dots \\ \vdots & \ddots & \ddots & & \ddots \end{pmatrix}.$$

Just another remarkable free parametrization of a moment sequence, with uncountably many ramifications and applications.

OP literature

Herbert Stahl, Vilmos Totik: *General orthogonal polynomials*, Encyclopedia of Mathematics and its Applications, 43 Cambridge University Press, Cambridge, 1992. xii+250 pp.

Barry Simon: *Orthogonal poynomials on the unit circle*, 2. vol., Amer. Math. Soc. 2004.

The Oxford Handbook of Random Matrix Theory (Oxford Handbooks in Mathematics), (G. Akemann et al, eds.), Oxford Univ. Press, 2011.

The spectral theorem

Hilbert, Hellinger, Hahn, F. Riesz (around 1910)

Let U be a unitary transformation on a Hilbert space and let ξ be a fixed vector. The sequence $\langle U^n\xi, \xi\rangle, \quad n \in \mathbf{Z}$ is represented by a positive measure μ on the unit circle, because the kernel

$$s_{k-m} = \langle U^k\xi, U^m\xi\rangle$$

is positive semi-definite. Hence

$$\langle q(U)\xi, \xi\rangle = \int_{-\pi}^{\pi} q(e^{it})d\mu(t), \quad q \in \mathbf{C}[x].$$

With the known techniques of integration theory, one can define $f(U)$ for any bounded Borel function, so that

$$\langle f(U)\xi, \xi\rangle = \int_{-\pi}^{\pi} f(e^{it})d\mu(t).$$

Similarly

Given a bounded symmetric linear operator S, densely defined on a Hilbert space, and a vector ξ, the sequence

$$s_k = \langle S^k \xi, \xi \rangle, \quad k \geq 0$$

is a moment sequence, because the kernel $s_{k+m} = \langle S^k \xi, S^m \xi \rangle$ is positive semi-definite. Therefore there exists a positive measure on the line, such that

$$\langle f(A)\xi, \xi \rangle = \int f(x) d\sigma(x),$$

for every bounded Borel function on the line.

Self-adjointness

von Neumann (1929), Stone (1930)

The case of a symmetric linear operator S, densely defined but unbounded: even when all powers $S^n\xi$ are well defined and $s_{k+m} = \langle S^k\xi, S^m\xi\rangle$ is a moment sequence, the Borel functional calculus $f(S)$ may exist only on a larger Hilbert space. The self-adjoint condition

$$S = S^*$$

is necessary for having a spectral theorem/decomposition in the original Hilbert space.

Since then, this is the natural theoretical framework for quantum mechanics.

M. H. Stone: *Linear transformation in Hilbert space*, Amer. Math. Soc., 1932.

B. Simon: *The classical moment problem as a self-adjoint finite difference operator*, Adv. Math. , 137 (1998) pp. 82203.

Mark G. Krein (1907-1989)

Has incorporated the classical problem of moments in modern analysis, with great, original contributions. Master of the geometry of Hilbert space and function theory of a complex variable. A few of his topics of research:

Strings and spectral functions
Self-adjoint operators on Hilbert spaces of entire functions
Extremal problems related to the truncated moment problem
Convex analysis and duality
Prediction theory of stochastic processes
Stability and control of systems of differential equations
Representation theory of locally compact groups
Spectral analysis in spaces with an indefinite metric

Had 50 students, 805 descendants (many working today on moment problems) and was the uncontested mentor of the Ukrainian school of Functional Analysis.

Moment method in numerical mathematics

Given $f_0, ..., f_n$ linearly independent vectors in a Hilbert space, analyse the linear transformation $A_n : H_n \longrightarrow H_n$ such that

$$A_n f_k = \pi_n f_{k+1}, \quad 0 \leq k \leq n-1,$$

where $H_n = \mathrm{lin.span}(f_0, ..., f_{n-1})$ and π_n is the orthogonal projection onto H_n.

Yu. V. Vorobiov, *The method of moments in applied mathematics*, Fizmatgiz, Moscow, 1958.
Roger F. Harrington, *Field Computation by Moment Methods*, Wiley 1993.
L. Trefethen, M. Embree: *Spectra and pseudospectra*, Princeton, 2005.

Multivariate moments

Around for a century or so, still intriguing and occupying the recent generations. Challenges:

Algebraic structure of positive polynomials
Convex analysis of moment data
Matrix completion and extension of linear functionals
Function theory of several complex variables
Commuting systems of symmetric linear operatos
Determinateness

Some recent applications and ramifications

Global polynomial optimization
Geometric tomography
Bolzmann equation and max. entropy
Spectrum lowest bound for Schrödinger operators with rational potentials
Signal processing via wavelet transforms
Elliptic growth
Free probability theory

Structure of positive polynomials

Tarski's Ansatz (1930-ies) transformed into a precise real-algebra statement by Stengle (1970-ies) can be combined with the Hilbert space approach for obtaining simpler representations of positive polynomials as sums of squares (Schmüdgen, Putinar 1990-ies). With useless error bounds (Nie, Schweighofer, last decade).

Unexpected turn: due to the improvement of computational tools, working in the notoriously unstable space of higher moments is gratifying: Lasserre, Parrilo, Henrion, ...

Maximum entropy

Solve the truncated moment problem with densities of the form

$$\exp(P(x))dx$$

where deg P depends on the number of given moments and the geometry of the support.

Highly advocated by physicists and recently resurrected in continuum mechanics, reducing kinetic equations to moment systems, and *again* working in moment coordinates.

W. Dreyer, Maximization of the entropy in nonequilibrium, J. Phys. A: Math. Gen., 20, 1987, 65056517
C. D. Levermore, Moment Closure Hierarchies for Kinetic Theories, J. Stat. Phys., 83, 1996, 10211065.
W. Dreyer, M. Junk, M. Kunik, On the approximation of kinetic equations by moment systems, Nonlinearity, Vol. 14, 881-906, 200.

Phase transform

Allowing singular measures to be treated by the max entropy method:

Let μ be a finite positive measure supported on the cone on Γ^* in Euclidean space. For every $y \in \Gamma$ there exists a phase function $\xi_y \in L^1([0,\infty), dt)$, $0 \leq \xi_y \leq 1$, measurably depending on y, such that

$$1 + \int_\Gamma \frac{d\mu(x)}{x \cdot y - z} = \exp \int_0^\infty \frac{\xi_y(t)dt}{t - z}, \quad \Im z > 0. \tag{1}$$

Moreover, if $\int_{\Gamma^*} |x|^n d\mu(x) < \infty$ for some $n \in$, then $\int_0^\infty t^n \xi_y(t)dt < \infty$ for all $y \in \Gamma$.

M. Budisic, M. Putinar *Conditioning moments of singular measures for entropy optimization.I*, Indag. Math. 23(2012), 848-883.

Elliptic growth

Dynamics of domains $\Omega(t)$ in Euclidean space, modeling crystal growth, electrodeposition and some specific fluid motions. In the particular case of 2D, Stan Richardson observed that the harmonic moments satisfy

$$\int_{\Omega(t)} h dA = th(0), \quad \Delta h = 0.$$

Again the representation in moments of the dynamics is very rewarding.

M. Mineev-Weinstein, M. Putinar, R. Teodorescu, *Random Matrix Theory in 2D, Laplacian Growth and Operator Theory*, J. Phys. A: Math. Theor. **41** No 26 (4 July 2008) 263001 (74pp).

Conclusion

Identify the appropriate moments and use them as coordinates in your current mathematical endeavor.