統計力学における Gauß原理とその拡張
Gauß principle in statistical mechanics and its parameter extension

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Outline

Motivation

In the standard textbooks of statistical physics:

- Gibbs (Shannon) entropy $S^{\mathrm{GS}} \equiv -k_{\mathrm{B}} \sum_i p_i \ln p_i$, is given.
- For the case in which all $p_i = 1/W = \mathrm{const.}$, $S^{\mathrm{GS}} \to k_{\mathrm{B}} \ln W = S^{\mathrm{B}}$, i.e., Boltzmann entropy.

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However, it seems not so conceptually reasonable!
In this talk:
Boltzmann relation $S^{\mathrm{B}} \equiv k_{\mathrm{B}} \ln W$, Gauß principle + something
$\Rightarrow$ the appropriate statistical entropy functional.

Outline

Tsallis' nonextensive thermostatistics

C. Tsallis, *Introduction to Nonextensive Statistical Mechanics: Approaching a Complex World* , Springer, New York, 2009.

Tsallis' generalized entropy:

$$S_q \equiv \frac{\sum_i p_i^q - 1}{1 - q} \quad \underset{q \to 1}{\longrightarrow} \quad S^{\mathrm{GS}} = -\sum_i p_i \ln p_i,$$

Introducing the so-called escort probabilities, w.r.t. p_i,

$$P_i \equiv \frac{p_i^q}{\sum_j p_j^q},$$

and the escort average of energy

$$U_q \equiv \sum_i E_i P_i,$$

Power law distribution

MaxEnt

$$\frac{\partial}{\partial p_i}\left(S_q - \beta^{\mathrm{T}} U_q - \gamma^{\mathrm{T}} \sum_j p_j\right) = 0.$$

leads to the asymptotic power-law distribution:

$$p_i \propto \exp_q\left[-\frac{\beta^{\mathrm{T}}}{\sum_j p_j^q}\left(E_i - U_q\right)\right], \quad \underset{E_i >> U_q}{\longrightarrow} E_i^{\frac{1}{1-q}}, \text{ power law!}$$

Tsallis' q-logarithmic and q-exponential functions:

$$\ln_q(x) \equiv \frac{x^{1-q} - 1}{1-q} \quad \underset{q\to 1}{\longrightarrow} \quad \ln(x).$$

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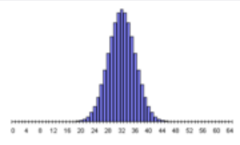
Gaussian functions:
ubiquitous and fundamental in many fields.



Gauß principle (Gauß' law of error)

- Gauß' original derivation of Gaussian error functions
- Maximum Likelihood estimator = arithmetic mean

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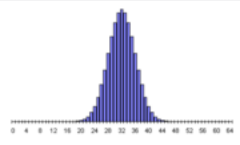

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Statistical (or thermodynamic) ensembles

- Micro-canonical ensemble:
  $p = 1/W(E)$, Principle of equal a priori probability
  $W(E) = \Omega(E)dE$, where $\Omega(E)$ is the energy density of state of a thermal system.
  Boltzmann entropy: $S^{\mathrm{B}}(E) = k_{\mathrm{B}} \ln W(E) \approx k_{\mathrm{B}} \ln \Omega(E)$.
- Canonical ensemble:

$$p_i = \frac{1}{Z(\beta)} \exp(-\beta E_i), \quad \beta \equiv \frac{1}{k_{\mathrm{B}} T},$$

  Gibbs entropy: $S = -k_{\mathrm{B}} \sum_i p_i \ln p_i$,
  energy expectation: $U = \sum_i E_i p_i, \quad \Rightarrow \quad S = S(U)$.

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Greene and Callen Principle

Statistical mechanics are based on the entropies:

- Boltzmann entropy $S^{\mathrm{B}}(E)$ in micro-canonical ensemble and;
- Gibbs entropy $S(U)$ in canonical ensemble.

where U is the average energy.

Greene and Callen principle

The functional dependence of $S(U)$ on U is same as that of $S^{\mathrm{B}}(E)$ on energy E.

$\Rightarrow$ Otherwise there would be a separate thermodynamics for each ensemble in statistical mechanics.

R.F. Greene, H.B. Callen, Phys. Rev. **83** (1951) 1231-1235.

Lavenda's works

B.H. Lavenda, *Statistical Physics: A Probabilistic Approach*, Wiley-Interscience, New York, 1991.

Based on both Greene-Callen and Gauß' principles, Lavenda established:

A route which determines uniquely the statistical entropy function from a stationary probability distribution casting into the form of the normal law of error.

Outline

Review: Gauß principle

We want to determine a functional form of the probability function, $f(x_i; a)$ of given data $x_i (i = 1, \cdots, n)$ and the location parameter a.

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1) $\mathcal{L}(a)$ has a single maximum at $\hat{a}$:

$$\frac{d}{da} \ln \mathcal{L}(a)\Big|_{a=\hat{a}} = 0,$$

and simultaneously,
2) the $\hat{U}$ equals to the arithmetic mean:

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We finally obtain the Gaussian error function

$$f(x;\hat{a}) \propto \exp\left[-\frac{(x-\hat{a})^2}{2\sigma^2}\right].$$

Outline

Some parameter extensions

The q-logarithmic and q-exponential functions:

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q-extension of Gauß principle

H. Suyari and M. Tsukada, *Law of Error in Tsallis Statistics*, IEEE Trans. Inform. Theory, **51** (2005) 753-757.

The log-likelihood is replaced with q-log-likelihood

$$\ln \mathcal{L} \equiv \sum_{i=1}^{n} \ln f(x_i; \hat{a}) \quad \Rightarrow \quad \ln_q \mathcal{L}_q = \sum_{i=1}^{n} \ln_q f(x_i; \hat{a}_q).$$

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We can obtain q-Gaussian function:

$$f(x; \hat{a}_q) \propto \exp_q \left[-\frac{(x-\hat{a}_q)^2}{2\sigma_q^2} \right].$$

Some parameter extensions

The κ-logarithmic and κ-exponential functions:

$$\ln_{\{\kappa\}}(x) \equiv \frac{x^{\kappa} - x^{-\kappa}}{2\kappa} \quad \underset{\kappa\to 0}{\longrightarrow} \quad \ln(x).$$

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Introducing κ-log-likelihood

$$\ln_{\{\kappa\}} \mathcal{L}_{\kappa} = \sum_{i=1}^{n} \ln_{\{\kappa\}} f(x_i; \hat{a}_{\kappa}).$$

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As a proportional constant we choose

$$-\frac{d^2 s(\hat{a})}{d\hat{a}^2},$$

where $s(\hat{a})$ is a twice differentiable concave function. Then

Gauß Principle

$$\frac{d\ln f(x;\hat{a})}{d\hat{a}} = -\frac{d^2 s(\hat{a})}{d\hat{a}^2}(x-\hat{a})$$
$$= -\frac{d}{d\hat{a}}\left\{\frac{ds(\hat{a})}{d\hat{a}}(x-\hat{a}) + s(\hat{a})\right\}.$$

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Integrating it, we have

A form of the law of error

$$\ln f(x; \hat{a}) = \Sigma(x) - s(\hat{a}) - \frac{ds(\hat{a})}{d\hat{a}}(x - \hat{a}),$$

where $\Sigma(x)$ is a constant of integration.

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$$\ln f(x;\hat{a}) = \Sigma(x) - s(\hat{a}) - \frac{ds(\hat{a})}{d\hat{a}}(x-\hat{a}),$$

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This form implies that $x = \hat{a}$ is the most probable value.
Because $\frac{ds(\hat{a})}{d\hat{a}} > 0$, and

$$\ln f(\hat{a};\hat{a}) = \Sigma(\hat{a}) - s(\hat{a}),$$

we see that

$$f(x;\hat{a}) = f(\hat{a};\hat{a}) \exp\left[-\frac{ds(\hat{a})}{d\hat{a}}(x-\hat{a})\right].$$

Outline

Gauß principle in statistical mechanics

The relevant pdf of a thermal system is

$$f(E;U) = \Omega(E)\, p(E;U),$$

- $p(E;U)$ is the statistical factor, i.e., a probability of a single state with energy E.
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The statistical factor is Gibbs pdf:

$$p(E;\beta(U)) = \frac{1}{Z(\beta(U))} \exp\left[-\beta(U)\, E\right],$$

and then

$$f(E;U) = \Omega(E)\, \exp\Big[-\Phi(\beta(U)) - \beta(U)E \Big],$$

where we introduced Massieu function $\Phi(\beta) = \ln Z(\beta)$.

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$$f(E; U) = \Omega(E) \exp\Big[-\Phi(\beta(U)) - \beta(U)E \Big],$$

where we introduced Massieu function $\Phi(\beta) = \ln Z(\beta)$.
Taking the logarithm of the both sides, we have

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Utilizing the associated Legendre relations

$$\Phi(\beta) = S(U) - \beta U, \quad \beta(U) = \frac{dS(U)}{dU},$$

and Boltzmann's relation (in $k_{\mathrm{B}} = 1$ unit)

$$S^{\mathrm{B}}(E) = \ln \Omega(E),$$

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we have

$$\ln f(E;\hat{U}) = S^{\mathrm{B}}(E) - S(\hat{U}) - \frac{dS(\hat{U})}{d\hat{U}}(E - \hat{U}).$$

This is just the form of the law of error, hence the expectation value of energy $\hat{U}$ is the most probable value.

Gauß principle in statistical mechanics 2

$$\ln f(E;\hat{U}) = S^{\mathrm{B}}(E) - S(\hat{U}) - \frac{dS(\hat{U})}{d\hat{U}}\big(E - \hat{U}\big).$$

Expanding $S^{\mathrm{B}}(E)$ around $E = \hat{U}$, we have

$$S^{\mathrm{B}}(E) \approx S^{\mathrm{B}}(\hat{U}) + \frac{dS^{\mathrm{B}}(E)}{dE}\Big|_{E=\hat{U}}(E - \hat{U}) + \frac{1}{2}\frac{d^2 S^{\mathrm{B}}(E)}{dE^2}\Big|_{E=\hat{U}}(E - \hat{U})^2.$$

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Since $S(\hat{U})$ is concave, we can introduce the positive quantity

$$\frac{1}{\sigma_1^2} \equiv -\frac{d^2S(U)}{dU^2}\Big|_{U=\hat{U}} > 0,$$

and we finally obtain Gaussian error function

$$f(E;\hat{U}) = f(\hat{U};\hat{U})\exp\left[-\frac{(E-\hat{U})^2}{2\sigma_1^2}\right].$$

Outline

Entropy functional

Next we focus on the functional form of the statistical entropy. Rearranging Eq. gives

$$-\ln \frac{f(E;\hat{U})}{\Omega(E)} = S(\hat{U}) + \beta(\hat{U})(E - \hat{U}).$$

The statistical entropy can be defined by the expectation value of the log-likelihood ratio $-\ln f(E;\hat{U})/\Omega(E)$, i.e.,

$$-\int_0^\infty dE\, f(E;\hat{U}) \ln \frac{f(E;\hat{U})}{\Omega(E)} = \quad S(\hat{U}) + \beta(\hat{U}) \left(\int dEf(E;\hat{U})\, E - \hat{U} \right).$$

Since $\hat{U}$ is equal to the expectation value of energy, we confirm the well known fact that the statistical entropy is equal to $S(\hat{U})$ and its functional form is

$$\begin{aligned} S(\hat{U}) &= -\int dE\, \Omega(E)\, p(E;\beta(\hat{U})) \ln p(E;\beta(\hat{U})) \\ &= -\int d\Gamma\, p(E;\beta(\hat{U})) \ln p(E;\beta(\hat{U})). \end{aligned}$$

Outline

S_{2-q}-formalism

T. Wada, A.M. Scarfone, Phys. Lett. A **335** (2005) 351.

Starting from the q-exponential probability distribution:

$$p_i = \alpha_q \exp_q[-\gamma - \beta E_i],$$

where α_q is a q-dependent constant,

$$\alpha_q \equiv \left(\frac{1}{2-q}\right)^{1-q} = \frac{1}{\exp_q(1)}.$$

the useful identity:

$$\frac{d}{dx}(x \ln_q x) = \ln_q \frac{x}{\alpha_q}.$$

S_{2-q}-formalism

From the q-distribution, we have

$$-\ln_q \frac{p_i}{\alpha_q} - \beta E_i - \gamma = 0.$$

Utilizing the identity it follows

$$\frac{\partial}{\partial p_i}\Big(-\sum_j p_j \ln_q p_j - \beta \sum_j E_j p_j - \gamma \sum_j p_j \Big) = 0,$$

which is equivalent to the maximization of S_{2-q}

$$S_{2-q} = -\sum_i p_i \ln_q p_i,$$

under the constraints of

$$\sum_i E_i p_i = U\ , \quad \text{and} \quad \sum_i p_i = 1.$$

Legendre structures 1

The q-exponential distribution can be written as

$$p_i = \alpha_q \exp_q \left[-\beta E_i - \gamma\right]$$
$$= \exp_q \left[-\frac{\beta}{2-q} E_i - \left(\frac{\gamma+1}{2-q}\right)\right]$$

Here we introduced

$$\beta^N \equiv \frac{\beta}{2-q}$$
$$\Phi_q^N \equiv \frac{\gamma+1}{2-q}, \quad \text{generalized Massiue potential}$$

Legendre structures 1

$$p_i = \exp_q\left[-\beta^N E_i - \Phi_q^N\right].$$

By differentiating $\sum_i p_i = 1$ w.r.t. β^N, and using $d\exp_q(x)/dx = \exp_q(x)^q$, we have

$$0 = \sum_i \frac{dp_i}{d\beta^N} = -\sum_i (E_i + \frac{d\Phi_q^N}{d\beta^N}) p_i^q, \quad \Rightarrow \quad \frac{d\Phi_q^N}{d\beta^N} = -\frac{\sum_i E_i p_i^q}{\sum_j p_j^q}.$$

which leads to the Legendre relation:

$$\frac{d\Phi_q^N}{d\beta^N} = -U_q.$$

Note that the escort probabilities P_i are naturally appeared!

Legendre structures 1

The normalized Tsallis entropy

$$S_q^N = -\sum_i P_i \ln_q p_i.$$

Substituting

$$p_i = \exp_q \left[-\beta^N E_i - \Phi_q^N \right]$$

into S_q^N leads to

$$S_q^N = \sum_i P_i \left(\beta^N E_i + \Phi_q^N \right) = \beta^N U_q + \Phi_q^N.$$

S_q^N and Φ_q^N are Legendre duals each other.

Outline

q-extension

The relevant q-generalized statistical factor is a q-exponential pdf,

$$p_q(E;\beta^N) = \exp_q\Big[-\beta^N E - \Phi_q^N(\beta^N)\Big].$$

Here Φ_q^N is the generalized Massieu function

$$\Phi_q^N(\beta^N) = S_q^N - \beta^N U_q,$$

which is the Legendre dual of the normalized Tsallis entropy S_q^N, and

$$\beta^N(\hat{U}_q) = \frac{dS_q^N(U_q)}{dU_q}\Big|_{U_q=\hat{U}_q}.$$

q-extension

Then the associated pdf for a thermal system is

$$f_q(E; U_q) = \Omega(E)\, p_q(E; \beta^N) = \Omega(E)\ \exp_q\Big[-\beta^N E - \Phi_q^N(\beta^N)\Big],$$

Taking the q-logarithm, we have

$$\ln_q f_q(E; \hat{U}_q) = \ln_q \Omega(E) \Big[1 - (1-q)\Big(\beta^N E + \Phi_q^N\Big)\Big] - \beta^N E - \Phi_q^N(\beta^N).$$

q-extension

Taking the q-logarithm, we have

$$\ln_q f_q(E;\hat{U}_q) = \ln_q \Omega(E)\left[1-(1-q)\left(\beta^N E + \Phi_q^N\right)\right] - \beta^N E - \Phi_q^N(\beta^N).$$

Using the Legendre relations and introducing the q-generalization of "stochastic" entropy as

$$\Sigma_q(E) = \ln_q \Omega(E)\left[1-(1-q)\left(S_q^N + \beta^N(E-\hat{U}_q)\right)\right],$$

we obtain

$$\ln_q f_q(E;\hat{U}_q) = \Sigma_q(E) - S_q^N(\hat{U}_q) - \frac{dS_q^N(U_q)}{dU_q}\Big|_{U_q=\hat{U}_q}(E-\hat{U}_q).$$

This is just an error law of the type.

we obtain

$$\ln_q f_q(E;\hat{U}_q) = \Sigma_q(E) - S_q^N(\hat{U}_q) - \frac{dS_q^N(U_q)}{dU_q}\Big|_{U_q=\hat{U}_q}(E-\hat{U}_q).$$

This is just an error law of the type.
Then, by Greene-Callen principle,if the functional dependence of $\Sigma_q(E)$ on E is same as that of $S_q^N(U_q)$ on U_q, we obtain the q-Gaussian error function

$$f_q(E;\hat{U}_q) = f_q(\hat{U}_q;\hat{U}_q)\exp_q\left[-\frac{1}{2\sigma_q^2}(E-U_q)^2\right],$$

where we introduced the positive quantity σ_q^2 defined as

$$\frac{1}{\sigma_q^2} \equiv -\frac{d^2 S_q^N(U_q)}{dU_q^2}\Big|_{U_q=\hat{U}_q} > 0.$$

Outline

q-entropy functional

From the normalization condition of the pdf, we have

$$0 = \frac{d}{d\beta^N} \int_0^\infty \Omega(E) p_q(E; \beta^N) dE$$
$$= -\int_0^\infty \Omega(E) dE \Big(E + \frac{d\Phi_q^N(\beta^N)}{d\beta^N} \Big) \Big[p_q(E; \beta^N) \Big]^q .$$

Then it leads to

$$U_q(\beta^N) \equiv \int_0^\infty F_q(E; U_q) E dE = -\frac{d\Phi_q^N(\beta^N)}{d\beta^N}.$$

Here we introduced a variant $F_q(E; U_q)$ of escort pdf with respect to $f_q(E; U_q)$ as

$$F_q(E; U_q) = \frac{\Omega(E) \left[p_q(E; \beta^N) \right]^q}{\int d\Gamma \left[p_q(E; \beta^N) \right]^q} = \Omega(E) P_q(E; U_q),$$

where P_q is the escort pdf of p_q.

Rearranging and taking q-logarithm we have

$$\ln_q \frac{f_q(E; \hat{U}_q)}{\Omega(E)} = -S_q^N - \beta^N (E - \hat{U}_q).$$

As a q-generalization, let us choose the q-expectation value of the q-log likelihood ratio, i.e.,

$$-\int dE\, F_q(E; \hat{U}_q) \ln_q \frac{f_q(E; \hat{U}_q)}{\Omega(E)}$$
$$= S_q^N(\hat{U}_q) + \beta^N \left(\int dE F_q(E; \hat{U}_q) E - \hat{U}_q \right).$$

Since $\hat{U}_q$ is equal to the escort average of energy, we thus found the q-generalized statistical entropy is the normalized Tsallis entropy,

$$S_q^N(\hat{U}_q) = -\int dE\, \Omega(E)\, P_q(E; \beta^N) \ln_q p_q(E; \beta^N)$$
$$= -\int d\Gamma\, P_q(E; \beta^N) \ln_q p_q(E; \beta^N).$$

Outlook

For the details, please see the following paper:
T. Wada, "Nonextensive entropies derived from Gauss' principle",
Phys. Lett. A **375**, (2011) 2037-2040.

- Further study on the *q*-generalized "stochastic" entropy is needed.
- What is the relation with information geometry?
- How does Bayes' theorem relate with?

Collaboration is welcome!