

English Summary

$$\text{Information gain } K(P, P') = \sum_{i=1}^N P_i \ln \frac{P_i}{P'_i}$$

generalized canonical distribution

Jaynes' Principle of unbiased guess:

maximize missing information

$$I(P) = \sum_{i=1}^N P_i \ln P_i = \text{Min}$$

under constraints $\sum_i P_i = 1$

$$\Rightarrow P_i = \exp(\psi - \lambda_\nu M_i^\nu)$$

$\langle M^\nu \rangle_{\text{macro}} = \sum_i P_i M_i^\nu \quad \nu = 1, \dots, m$
micro-observable

normalization \Rightarrow $e^{-\psi} = \sum_i \exp(-\lambda_\nu M_i^\nu) \equiv Z$ partition fun.

Legendre transform $I(M) = \psi(t) - Mt, \quad M \equiv \frac{d\psi}{dt} \Rightarrow \frac{dI}{dM} = -t$

Shannon-Information:

$$I(P) = \sum_i P_i \ln P_i = \sum_i P_i (\psi - \lambda_\nu M_i^\nu) = \psi - \lambda_\nu \sum_i P_i M_i^\nu$$

$$I = \psi(\lambda_1, \dots, \lambda_m) - \lambda_\nu \langle M^\nu \rangle$$

Ans $\psi(\lambda_1, \dots, \lambda_m) = -\ln \sum_i \exp(-\lambda_\nu M_i^\nu)$ folgt

$$\frac{\partial \psi}{\partial \lambda_\nu} = - \frac{\sum_i (-M_i^\nu) \exp(-\lambda_\nu M_i^\nu)}{\sum_i \exp(-\lambda_\nu M_i^\nu)} = \sum_i M_i^\nu \underbrace{\exp(\psi - \lambda_\nu M_i^\nu)}_{P_i}$$

$$\frac{\partial \psi}{\partial \lambda_\nu} = \langle M^\nu \rangle$$

Damit können wir die Legendre-Transform identifizieren:

$$\begin{aligned} \varphi(t) &\rightarrow \varphi(\lambda_1, \dots, \lambda_m) && \text{Var. } \lambda_\nu \\ M &\rightarrow \langle M^\nu \rangle = \frac{\partial \varphi}{\partial \lambda_\nu} && \text{neue Var. } \langle M^\nu \rangle \\ I(M) &\rightarrow I = \varphi - \lambda_\nu \langle M^\nu \rangle && \text{Legendre-Transform. von } \varphi \end{aligned}$$

Es folgt $\frac{\partial I}{\partial \langle M^\nu \rangle} = -\lambda_\nu$

wegen $\frac{\partial I}{\partial \langle M^\nu \rangle} = \frac{\partial \varphi}{\partial \lambda_\nu} \frac{\partial \lambda_\nu}{\partial \langle M^\nu \rangle} - \frac{\partial \lambda_\nu}{\partial \langle M^\nu \rangle} \langle M^\nu \rangle - \lambda_\nu$

Zusammengefasst:

$$dI = -\lambda_\nu d\langle M^\nu \rangle$$

(Thermodyn.: Gibbs'sche Fundamentalgl.)

Betrachte Variation

$$\begin{aligned} \langle M^\nu \rangle &\rightarrow \langle M^\nu \rangle + \delta \langle M^\nu \rangle \\ \lambda_\nu &\rightarrow \lambda_\nu + \delta \lambda_\nu \\ \varphi &\rightarrow \varphi + \delta \varphi \\ P_i &\rightarrow P_i + \delta P_i \end{aligned}$$

Informationsgewinn:

$$\begin{aligned} K(P + \delta P, P) &= \sum_i (P_i + \delta P_i) \ln(P_i + \delta P_i) - \sum_i (P_i + \delta P_i) \ln P_i \\ &= \underbrace{\sum_i (P_i + \delta P_i) \ln(P_i + \delta P_i)}_{I(P + \delta P)} - \sum_i (P_i + \delta P_i) \ln P_i \\ &= (\varphi + \delta \varphi) - (\lambda_\nu + \delta \lambda_\nu) (\langle M^\nu \rangle + \delta \langle M^\nu \rangle) - \sum_i (P_i + \delta P_i) (\varphi - \lambda_\nu M_i^\nu) \\ &= \delta \varphi - \delta \lambda_\nu (\langle M^\nu \rangle + \delta \langle M^\nu \rangle) - \underbrace{\sum_i (P_i + \delta P_i) M_i^\nu}_{\langle M^\nu \rangle + \delta \langle M^\nu \rangle} (\varphi - \lambda_\nu) \end{aligned}$$

Entwicklung für kleine Var $\delta\lambda_\nu$:

$$\delta\psi = \frac{\partial\psi}{\partial\lambda_\nu} \delta\lambda_\nu + \frac{1}{2} \frac{\partial^2\psi}{\partial\lambda_\nu \partial\lambda_\mu} \delta\lambda_\nu \delta\lambda_\mu + \dots$$

$$\delta\langle M^\nu \rangle = \frac{\partial\langle M^\nu \rangle}{\partial\lambda_\mu} \delta\lambda_\mu + \dots$$

$$\begin{aligned} \Rightarrow K(P+\delta P, P) &= \underbrace{\left(\frac{\partial\psi}{\partial\lambda_\nu} - \langle M^\nu \rangle\right)}_0 \delta\lambda_\nu + \left[\frac{1}{2} \frac{\partial}{\partial\lambda_\mu} \left(\frac{\partial\psi}{\partial\lambda_\nu}\right) - \frac{\partial\langle M^\nu \rangle}{\partial\lambda_\mu} \right] \delta\lambda_\nu \delta\lambda_\mu \\ &= -\frac{1}{2} \frac{\partial\langle M^\nu \rangle}{\partial\lambda_\mu} \delta\lambda_\mu \delta\lambda_\nu \\ &\quad ! \\ &\geq 0 \end{aligned}$$

Also $\frac{\partial\langle M^\nu \rangle}{\partial\lambda_\mu} \delta\lambda_\mu \delta\lambda_\nu \leq 0$ negativ semidefinite
Bilinearform $\forall \delta\lambda_\mu$

Definiere Suszeptibilitätsmatrix

$$\underline{\underline{\chi}}^{\mu\nu} := \frac{\partial\langle M^\mu \rangle}{\partial\lambda_\nu} = \frac{\partial^2\psi}{\partial\lambda_\nu \partial\lambda_\mu} \quad \left(\begin{array}{l} \text{Änderung von } \langle M^\nu \rangle \\ \text{bei Var. von } \lambda_\nu \\ \delta\langle M \rangle = \underline{\underline{\chi}} \delta\lambda \end{array} \right)$$

$$\underline{\underline{\chi}}_{\delta\lambda}^{\nu} := \frac{\delta\lambda_\nu}{\delta\langle M^\nu \rangle} = -\frac{\partial^2 I}{\partial\langle M^\nu \rangle \partial\langle M^\nu \rangle} \quad (\delta\lambda = \underline{\underline{\chi}}_{\delta\lambda}^{\nu} \delta\langle M \rangle)$$

$$\underline{\underline{\chi}}_{\delta\lambda}^{\nu} = \underline{\underline{\chi}}^{\nu-1}$$

$$\text{Wegen } \underbrace{\frac{\partial}{\partial\lambda_\mu} \left(\frac{\partial\psi}{\partial\lambda_\nu}\right)}_{\chi^{\nu\mu}} = \underbrace{\frac{\partial}{\partial\lambda_\nu} \left(\frac{\partial\psi}{\partial\lambda_\mu}\right)}_{\chi^{\mu\nu}}$$

Symmetrische Matrix

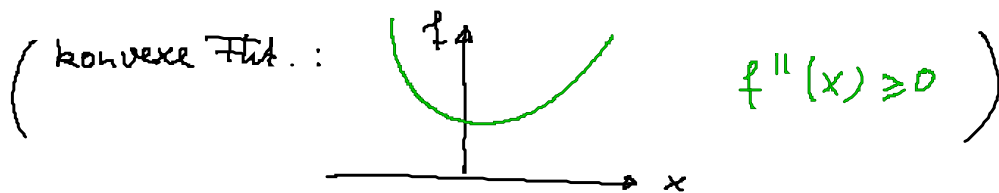
Aus $K(P+\delta P, P) \geq 0$ folgt

$$\sum_{\nu} M^{\nu} \delta \lambda_{\nu} \delta \lambda_{\nu} = \delta \langle M^{\nu} \rangle \delta \lambda_{\nu} = \sum_{\nu} \delta \langle M^{\nu} \rangle \delta \langle M^{\nu} \rangle \leq 0$$

negativ-semidefinite quadrat. Form

$$\Rightarrow \sum_{\nu} \delta \lambda_{\nu}^2 \leq 0, \quad \sum_{\nu} \delta \langle M^{\nu} \rangle^2 \leq 0$$

NB : $\Rightarrow \mathbb{I}(\langle M^{\nu} \rangle)$ und $-\varphi(\lambda_{\nu})$ konvex!



Zusammenhang mit Korrelationsmatrix :

$$Q^{\mu\nu} := \langle \Delta M^{\mu} \Delta M^{\nu} \rangle \quad \text{Korrelationsmatrix}$$

$$= \langle M^{\mu} M^{\nu} \rangle_c \quad \text{2. Kumulante}$$

$$= \left. \frac{\partial^2 \Gamma(\kappa)}{\partial \alpha_{\mu} \partial \alpha_{\nu}} \right|_{\alpha=0} \quad \text{mit Kumulanten erzeugenden}$$

$$\Gamma(\kappa) = \ln \langle \exp(\alpha_{\nu} M^{\nu}) \rangle$$

$$= \ln \sum_i P_i \exp(\alpha_{\nu} M_i^{\nu})$$

$$= \ln \sum_i e^{\varphi - (\lambda_{\nu} - \alpha_{\nu}) M_i^{\nu}}$$

$$= \ln[e^{\varphi}] + \ln \sum_i \exp(-(\lambda_{\nu} - \alpha_{\nu}) M_i^{\nu})$$

$$= \varphi(\lambda) \quad \underbrace{- \varphi(\lambda - \alpha)}$$

$$(e^{-\varphi} = Z)$$

$$\Gamma(\alpha) = \varphi(\lambda) - \varphi(\lambda - \alpha) :$$

$$Q^{\mu\nu} = - \frac{\partial^2 \psi(\lambda - \kappa)}{\partial \alpha_\mu \partial \alpha_\nu} \Big|_{\alpha=0} = - \frac{\partial^2 \psi(\lambda)}{\partial \lambda_\mu \partial \lambda_\nu} = - \chi^{\mu\nu}$$

Korr.

Suszeptibilität

Also

$$\langle \Delta M^\mu \Delta M^\nu \rangle = - \frac{\partial \langle M^\mu \rangle}{\partial \lambda_\nu} = - \frac{\partial \langle M^\nu \rangle}{\partial \lambda_\mu}$$

Fluktuations - Dissipations - Theorem

↓
zufällige Schwankung
um Mittelwert

↙
systematische Änderung
der Mittelwerte

$$\Delta M^\mu = M^\mu - \langle M^\mu \rangle$$