Dually Flat Geometries in the State Space of Statistical Models

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Outline

1. A manifold of equilibrium states
2. Dually flat geometries
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1. A manifold of equilibrium states

Application of differential geometry to thermodynamics initiated by

Weinhold (1975)

Metric space (Hilbert space) spanned by extensive variables X_i

such as internal energy, total magnetization, number of particles, ...

Present work: uses canonical ensemble of statistical mechanics.

Relevant potential: $\Phi = \log Z$, (Z is the partition sum)

instead of energy, entropy, free energy, ...

Scalar product defines metric tensor g: $g_{ij} = \langle X_i, X_j \rangle$.

Ruppeiner (1979)

The metric tensor g is determined by fluctuations + correlations.

Riemannian curvature, determined by g, implies interactions.

No curvature for the ideal gas model.

Boltzmann-Gibbs distribution

$$p(x) = \frac{1}{Z} e^{-\beta[H(x) - hM(x)]}$$

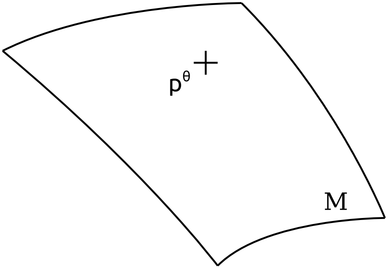
$H(x)$ is Hamiltonian, $M(x)$ is total magnetization
β is inverse temperature, h is external magnetic field
$Z = Z(\beta, h)$ the normalization.

Statistics: the BG distribution belongs to the *exponential family* because it can be written into the form

$$p^\theta(x) \quad = \quad \exp(\theta^k F_k(x) - \Phi(\theta)).$$

$$\theta^1 = -\beta,\ F_1(x) = -H(x),\ \theta^2 = \beta h,\ F_2(x) = M(x),\ \Phi(\theta) = \log Z(\beta, h).$$

Derivatives of $\Phi(\theta)$ yield expectation values: $\partial_k \Phi(\theta) = \langle F_k \rangle_\theta$.



The $p^\theta(x)$ form a *differentiable manifold* $\mathbb{M}$.

The variables X_k with $X_k = F_k - \langle F_k \rangle_\theta$ span a tangent plane.

The obvious scalar product is $\langle U, V \rangle_\theta = \int \mathrm{d}x\, p^\theta(x) U(x) V(x)$.

The metric tensor g is given by $g_{ij}(\theta) = \langle X_i, X_j \rangle$.

The Christoffel symbols are defined by

$$\Gamma^k_{ij} = \frac{1}{2} g^{ks} \left(\partial_i g_{sj} + \partial_j g_{is} - \partial_s g_{ij} \right),$$

They determine the Riemannian curvature of the manifold.

2. Dually flat geometries

Geometry: metric tensor $g(\theta)$ plus geodesics

Geodesics are solutions of Euler-Lagrange eq. $\ddot{\theta}^k + \omega^k_{ij}\dot{\theta}^i\dot{\theta}^j = 0.$

The coefficients ω^k_{ij} determine the *connection*.

Riemannian curvature : Levi-Civita connection : $\omega = \Gamma$

(Amari 1985) A model belonging to the exponential family
has dually flat geometries $\omega = 0$ and $\omega = 2\Gamma$.

Duality of connections is related to
the duality known from thermodynamics.

Replacing 'acceleration' Γ by 2Γ removes any curvature.
This holds when using the canonical coordinates θ^k of the exponential family.

Thermodynamic duality: two potentials $S(U)$ and $\Phi(\beta)$ satisfy

$$\frac{\mathrm{d}S}{\mathrm{d}U} = \beta \qquad \text{and} \qquad \frac{\mathrm{d}\Phi}{\mathrm{d}\beta} = -U.$$

Entropy $S(U)$ is the Legendre transform of $\Phi(\beta)$ (Massieu 1869).

Several variables:
η_i and θ^j are dual coordinates:

$$\eta_i = \frac{\partial \Phi}{\partial \theta^i} = \langle F_i \rangle_\theta \quad \text{and} \quad \theta^j = -\frac{\partial S}{\partial \eta_j}.$$

$\Phi(\theta)$ and $S(\eta)$ are dual potentials:

$$\Phi(\theta) = \sup_\eta \{S(\eta) + \theta^k \eta_k\}, \quad \text{and} \quad S(\eta) = \inf_\theta \{\Phi(\theta) - \theta^k \eta_k\}.$$

3. Thermodynamic length

Geodesics for $\omega = 0$: $\theta^k(t) = (1-t)\theta^k(t=0) + t\theta^k(t=1)$.

Geodesics for $\omega = 2\Gamma$: $\theta^k(t) = \theta^k[(1-t)\eta(t=0) + t\eta(t=1)]$,
with $\theta[\eta]$ inverse function of $\eta(\theta)$.

Thermodynamic length: integrate $\mathrm{d}s = \sqrt{g_{ij}\theta^i\theta^j}$ along geodesic.

Easy calculation when coordinates known in which the geodesic is a straight line.

4. The ideal gas

Probability density for x in n-particle phase space

$$f(x, n) = \frac{1}{Z} e^{-\beta(H_n(x) - \mu n)}.$$

β is inverse temperature, μ is chemical potential,
H_n is Hamiltonian for n free particles, enclosed in volume V.

Let $\theta^1 = \beta/\beta_0$, $\theta^2 = \beta\mu$, $F_1(x, n) = -H_n(x)$, $F_2(x, n) = n$.
$\Rightarrow$ ideal gas model belongs to the exponential family.

Calculations $\Rightarrow$ $\Phi(\beta, \mu) = \log Z = \frac{V}{V_0} e^{\beta\mu} \left(\frac{\beta_0}{\beta}\right)^{3/2}$,
with numerical constants V_0, β_0.
$\Rightarrow$ $N \equiv \langle n \rangle = \Phi(\beta, \mu)$
$\Rightarrow$ ideal gas law $\beta p V = N$ where p is pressure.

$$\Rightarrow \qquad \eta_1 = -\frac{3}{2\theta^1}\Phi \quad \text{and} \quad \eta_2 = \Phi.$$

$$\Rightarrow \qquad g(\theta) = \frac{1}{\theta^1}\Phi \begin{pmatrix} \frac{15}{4\theta^1} & -\frac{3}{2} \\ -\frac{3}{2} & \theta^1 \end{pmatrix}.$$

$\Rightarrow$ Christoffel symbols:

$$\Gamma^1 = \begin{pmatrix} -5/2\theta^1 & 1/2 \\ 1/2 & 0 \end{pmatrix} \quad \text{and} \quad \Gamma^2 = \begin{pmatrix} -15/8[\theta^1]^2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$

$\Rightarrow$ Riemannian curvature vanishes.
Tedious calculation.

Example of $\omega = 0$ geodesic:

isotherm: β is kept constant, μ varies linearly.
Thermodynamic length $= 2|\sqrt{N^{(2)}} - \sqrt{N^{(1)}}|$

Example of $\omega = 2\Gamma$ geodesic:

pV is kept constant, N varies linearly.
Thermodynamic length proportional to change in N.

5. Conclusions

Application of differential geometry to thermodynamics is considered here for models belonging to the exponential family.

Amari's dually flat geometries are also meaningful in a thermodynamical context.

Future work: application to models of interacting particles.