Dually Flat Geometries in the State Space of Statistical Models

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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
- \( \beta \) 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

\[ p^\theta(x) = \exp(\theta F_k(x) - \Phi(\theta)). \]

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

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
\[ \langle U, V \rangle_\theta = \int dx \, p^\theta(x) U(x) V(x). \]

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 $\omega^k_{ij}$ 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' $\Gamma$ by $2\Gamma$ removes any curvature. This holds when using the canonical coordinates $\theta^k$ of the exponential family.
Thermodynamic duality: two potentials $S(U)$ and $\Phi(\beta)$ satisfy

$$\frac{dS}{dU} = \beta \quad \text{and} \quad \frac{d\Phi}{d\beta} = -U.$$ 

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

Several variables:

$\eta_i$ and $\theta^i$ are dual coordinates:

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

$\Phi(\theta)$ 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

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

$\beta$ is inverse temperature, $\mu$ 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 $V_0$, $\beta_0$.

$\Rightarrow$ $N \equiv \langle n \rangle = \Phi(\beta, \mu)$

$\Rightarrow$ ideal gas law $\beta p V = N$ where $p$ is pressure.
\[ \eta_1 = -\frac{3}{2\theta^1} \Phi \quad \text{and} \quad \eta_2 = \Phi. \]

\[ g(\theta) = \frac{1}{\theta^1} \Phi \left( \begin{array}{cc} \frac{15}{4\theta^1} & -\frac{3}{2} \\ -\frac{3}{2} & \frac{1}{\theta^1} \end{array} \right). \]

\[ \Gamma^1 = \left( \begin{array}{cc} -\frac{5}{2\theta^1} & 1/2 \\ 1/2 & 0 \end{array} \right) \quad \text{and} \quad \Gamma^2 = \left( \begin{array}{cc} -\frac{15}{8[\theta^1]^2} & 0 \\ 0 & 1/2 \end{array} \right). \]

\[ \Rightarrow \quad \text{Riemannian curvature vanishes.} \]
\[ \text{Tedious calculation.} \]
Example of \( \omega = 0 \) geodesic:

- isotherm: \( \beta \) is kept constant, \( \mu \) 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.