Quantum Mechanics and Information Geometry

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- Information Geometry
- Hamilton-Jacobi theory
- Quantum Mechanics and Information Geometry

- $\mathcal{P}(\chi)$: Space of probability distributions on χ
- Θ: Family of parameters $\subset \mathbb{R}^n$
- Statistical manifold

$$\mathcal{S} = \{p : \Theta \to \mathcal{P}(\chi)\}$$

  - Injective
  - $p(\Theta) \subset \mathcal{P}(\chi)$
  - $\operatorname{supp}(p(\boldsymbol{\theta})) = \chi \ , \quad \boldsymbol{\theta} \in \Theta \qquad \Big(p(x|\boldsymbol{\theta}) > 0\Big)$

Fisher-Rao metric

$$\boldsymbol{\theta} = (\theta^1, \ldots, \theta^n) \in \Theta$$

$$g_{ij}(\boldsymbol{\theta}) := \int_{\mathcal{X}} \mathrm{d}x\, p(x|\boldsymbol{\theta}) \frac{\partial}{\partial \theta^i} \log p(x|\boldsymbol{\theta}) \frac{\partial}{\partial \theta^j} \log p(x|\boldsymbol{\theta})$$

- Metric defined on any statistical manifold
- Important results
  - Cramér-Rao Inequality

$$\hat{\boldsymbol{\theta}} \ : \text{Estimator}$$

$$V_{\boldsymbol{\theta}}[\hat{\boldsymbol{\theta}}] - g^{-1}(\boldsymbol{\theta}) \geq 0$$

  - Chentsov's Theorem

Example: Family of gaussian distributions

$$\chi = \mathbb{R} \qquad \Theta = \left\{ (\mu, \sigma) \mid -\infty < \mu < \infty; 0 < \sigma < \infty \right\}$$

$$p : \Theta \to \mathcal{P}(\chi)$$

$$p(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{(x-\mu)^2}{2\sigma^2} \right\}$$

Fisher-Rao metric: $$g_{ij}(\mu, \sigma) = \begin{pmatrix} \frac{1}{\sigma^2} & 0 \\ 0 & \frac{2}{\sigma^2} \end{pmatrix}$$

- $\mathcal{S}$: Differentiable Manifold (not necessarily statistical)

$$\mathcal{D} : \mathcal{S} \times \mathcal{S} \to \mathbb{R}$$

$$\mathcal{D}(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) \geq 0 \ \ ; \ \ \mathcal{D}(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) = 0 \Leftrightarrow \boldsymbol{\theta} = \tilde{\boldsymbol{\theta}}$$

  - Distance like measure
  - First derivatives vanish on the diagonal

$$\mathcal{D}\big|_{\mathrm{diag}} = 0$$

$$\left.\frac{\partial \mathcal{D}}{\partial \theta^i}\right|_{\mathrm{diag}} = \left.\frac{\partial \mathcal{D}}{\partial \tilde{\theta}^i}\right|_{\mathrm{diag}} = 0$$

$$\theta^i \to \xi^i \qquad \tilde{\theta}^i \to \tilde{\xi}^i$$

$$\frac{\partial^2 \mathcal{D}}{\partial \xi^k \partial \xi^l} = \frac{\partial \theta^j}{\partial \xi^k} \frac{\partial \theta^i}{\partial \xi^l} \frac{\partial^2 \mathcal{D}}{\partial \theta^j \partial \theta^i} + \frac{\partial^2 \theta^i}{\partial \xi^k \partial \xi^l} \frac{\partial \mathcal{D}}{\partial \theta^i}$$

$$\theta^i \to \xi^i \qquad \tilde{\theta}^i \to \tilde{\xi}^i$$

$$\left.\frac{\partial^2 \mathcal{D}}{\partial \xi^k \partial \xi^l}\right|_{\mathrm{diag}} = \underbrace{\frac{\partial \theta^j}{\partial \xi^k}\frac{\partial \theta^i}{\partial \xi^l}\left.\frac{\partial^2 \mathcal{D}}{\partial \theta^j \partial \theta^i}\right|_{\mathrm{diag}}}_{\text{Covariant Tensor}} + \frac{\partial^2 \theta^i}{\partial \xi^k \partial \xi^l}\left.\overset{=0}{\cancel{\frac{\partial \mathcal{D}}{\partial \theta^i}}}\right|_{\mathrm{diag}}$$

$$\theta^i \to \xi^i \qquad \tilde{\theta}^i \to \tilde{\xi}^i$$

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$$\left.\frac{\partial^2 \mathcal{D}}{\partial \theta^j \partial \theta^i}\right|_{\text{diag}} = \left.\frac{\partial^2 \mathcal{D}}{\partial \tilde{\theta}^j \partial \tilde{\theta}^i}\right|_{\text{diag}} = -\left.\frac{\partial^2 \mathcal{D}}{\partial \theta^j \partial \tilde{\theta}^i}\right|_{\text{diag}} = g_{ij}(\boldsymbol{\theta})$$

- Example: Relative entropy (Kullback-Leibler divergence)

$$\mathcal{D}(p,q) = \int_{\mathcal{X}} p(x) \log\left(\frac{p(x)}{q(x)}\right) \mathrm{d}x$$

- Many others: Rényi, Hellinger, Tsallis,...
- In all these cases:

$$\frac{\partial^2 \mathcal{D}}{\partial\theta^j \partial\theta^i} = C \times \text{Fisher-Rao metric}$$

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- Question: Given a metric is there a canonical divergence function?

- Information Geometry
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- Variational formulation of dynamics

$$I(\gamma) = \int_{t_0}^{t_f} \mathcal{L}(\gamma, \dot{\gamma})\mathrm{d}t \qquad \gamma(t_0) = \boldsymbol{\theta} \quad \gamma(t_f) = \tilde{\boldsymbol{\theta}}$$

- Evaluation at the solution γ_s gives a two point function

$$S(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) = I(\gamma_s)$$ Hamilton's characteristic function

- Solution of Hamilton-Jacobi equation

$$H(\boldsymbol{\theta}, \frac{\partial S}{\partial \boldsymbol{\theta}}) = E$$

- S is called complete when $\det \left\| \frac{\partial^2 S}{\partial \theta^i \partial \theta^j} \right\| \neq 0$

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{v}) = \frac{1}{2} g_{ij}(\boldsymbol{\theta}) v^i v^j$$

Thm: A complete solution S of the Hamilton-Jacobi equation associated with this Lagrangian is a divergence function that generates the metric g.

- Particular case: $g_{ij} = constant$
- Euler-Lagrange equations: $\dot{v} = 0 \quad \Rightarrow \quad \theta^i(t) = v^i t + \theta^i$
- Time one map: $\theta^i(1) = \tilde{\theta}^i \Rightarrow v^i = (\tilde{\theta}^i - \theta^i)$
- Evaluation of the action functional:

$$S(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) = I(\gamma_s) = \int_0^1 \frac{1}{2} g_{ij} v^i v^j \mathrm{d}t$$

$$= \frac{1}{2} g_{ij} v^i v^j = \frac{1}{2} g_{ij} (\tilde{\theta}^i - \theta^i)(\tilde{\theta}^j - \theta^j)$$

- The divergence function is not unique
- The structure is fixed up to second order
- There are other proposals to reconstruct a divergence function
  - Ref: *N. Ay and S. Amari*, Entropy **2015**, 17, 8111-8129
- Identification with H-J problem allows to identify and characterise global and local conditions for its existence.

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Complex separable Hilbert space $\mathcal{H}$ Scalar product $\langle \cdot \,, \cdot \rangle$

$$T\mathcal{H} \simeq \mathcal{H} \times \mathcal{H} \quad \Rightarrow$$

Hermitean structure

$$h(\cdot \,, \cdot) = g(\cdot \,, \cdot) + i\omega(\cdot \,, \cdot)$$

The space of states is complex projective space: $\mathcal{PH}$

The Riemannian metric g is not invariant under the transformation:

$$\Psi \to e^{i\alpha}\Psi$$

Fubini-Study metric:

$$g_{ij} = \frac{1}{\|\psi\|^2}\mathrm{Re}\langle \frac{\partial \psi}{\partial \theta^i} \,, \frac{\partial \psi}{\partial \theta^j} \rangle - \frac{1}{\|\psi\|^4}\langle \psi \,, \frac{\partial \psi}{\partial \theta^i} \rangle \langle \frac{\partial \psi}{\partial \theta^j} \,, \psi \rangle$$

- Θ: Family of parameters $\subset \mathbb{R}^n$
- Quantum Statistical manifold
  - Particular realisation of $\mathcal{H}$: Square integrable functions.

$$\mathcal{S} = \{\psi : \Theta \to \mathcal{PH}\} \qquad \psi(x|\boldsymbol{\theta}) = \sqrt{p(x|\boldsymbol{\theta})}e^{i\alpha(x|\boldsymbol{\theta})}$$

- Pull-back of the Fubini-Study metric:

$$\begin{aligned} g_{ij}(\boldsymbol{\theta}) := \frac{1}{4}\int_{\chi} \mathrm{d}x\, p(x|\boldsymbol{\theta}) \frac{\partial}{\partial\theta^i} \log p(x|\boldsymbol{\theta}) \frac{\partial}{\partial\theta^j} \log p(x|\boldsymbol{\theta}) \\ + \int_{\chi} \mathrm{d}x\, p(x|\boldsymbol{\theta}) \frac{\partial\alpha(x|\boldsymbol{\theta})}{\partial\theta^i} \frac{\partial\alpha(x|\boldsymbol{\theta})}{\partial\theta^j} \\ - \int_{\chi} \mathrm{d}x\, p(x|\boldsymbol{\theta}) \frac{\partial\alpha(x|\boldsymbol{\theta})}{\partial\theta^i} \int_{\chi} \mathrm{d}x\, p(x|\boldsymbol{\theta}) \frac{\partial\alpha(x|\boldsymbol{\theta})}{\partial\theta^j} \end{aligned}$$

  - Ref: *P. Facchi et al.*, Physics letters A **374**, 48, 4801-4803 (2010)

Example: Family of gaussian distributions

$$\chi = \mathbb{R} \qquad \Theta = \{(\mu, \sigma, \alpha) | -\infty < \mu \infty; 0 < \sigma \infty; \alpha \in \mathbb{R}\}$$

$$\psi : \Theta \to \mathcal{PH}$$

$$\psi(x|\mu, \sigma, \alpha) = \frac{1}{(\sigma(\sqrt{2\pi}))^{1/2}} e^{-\frac{(x-\mu)^2}{4\sigma^2}} e^{i\alpha x}$$

Quantum Fisher-Rao metric:

$$g_{ij}(\mu, \sigma, \alpha) = \begin{pmatrix} \frac{1}{\sigma^2} & 0 & 0 \\ 0 & \frac{2}{\sigma^2} & 0 \\ 0 & 0 & \sigma^2 \end{pmatrix}$$

The classical statistical manifold is a totally geodesic submanifold of the quantum statistical manifold

- Example: Relative entropy

$$S(\rho,\sigma) = \mathrm{Tr}\rho(\log\rho - \log\sigma)$$

  - Quantum Rényi entropy, Quantum Tsallis entropy...

- Importance:
  - Measure separation of quantum states (Quantum information)
  - Measure entanglement

- There is a natural ambiguity in defining them.

Logarithmic derivative $\boxed{\mathrm{d}\rho\rho^{-1} \neq \rho^{-1}\mathrm{d}\rho}$

- Relation with Information Geometry might help choosing all these structures consistently

- Dualistic Structure: (g, ∇, ∇^*)

$$Z(g(X,Y)) = g(\nabla_Z X, Y) + g(X, \nabla^*_Z Y)$$

  - Trivial case: Levi-Civita Connection. $(g, \nabla_{(L-C)}, \nabla_{(L-C)})$

- Given g, ∇ (not necessarily Riemannian) $\exists!\ \nabla^*$
  - Examples in Satistical models: α-connections, exponential connection, mixture connection

- Relation with divergence functions:

$$\left.\frac{\partial^2 \mathcal{D}}{\partial \theta^j \partial \theta^i}\right|_{\mathrm{diag}} = \left.\frac{\partial^2 \mathcal{D}}{\partial \tilde{\theta}^j \partial \tilde{\theta}^i}\right|_{\mathrm{diag}} = g_{ij}(\boldsymbol{\theta})$$

$$\left.\frac{\partial^3 \mathcal{D}}{\partial \tilde{\theta}^k \partial \theta^i \partial \theta^j}\right|_{\mathrm{diag}} = \Gamma^{(D)}_{ij,k} \qquad \left.\frac{\partial^3 \mathcal{D}}{\partial \theta^k \partial \tilde{\theta}^i \partial \tilde{\theta}^j}\right|_{\mathrm{diag}} = \Gamma^{*(D)}_{ij,k}$$

$$\left.\frac{\partial^3 \mathcal{D}}{\partial\tilde{\theta}^k \partial\theta^i \partial\theta^j}\right|_{\mathrm{diag}} - \left.\frac{\partial^3 \mathcal{D}}{\partial\theta^k \partial\tilde{\theta}^i \partial\tilde{\theta}^j}\right|_{\mathrm{diag}} = 2T_{ijk}$$

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{v}) = \frac{1}{2} g_{ij}(\boldsymbol{\theta}) v^i v^j + \frac{1}{6} T_{ijk} v^i v^j v^k$$

Thm: A complete solution S of the Hamilton-Jacobi equation associated with this Lagrangian is a divergence function that generates the dualistic structure.

- Open Questions:
  - Role of the antisymmetric structure.
  - Role of the dual connections in Q.M.

- Camerino (Italy):
  - Domenico Felice
  - Stefano Mancini
- Naples (Italy):
  - Florio M. Ciaglia
  - Fabio di Cosmo
  - Giuseppe Marmo
- References:
  - *Hamilton-Jacobi approach to Potential Functions in Information Geometry.* **arXiv:1608.06584**
  - *Quantum & Classical Information Geometric Dynamics.* **arXiv:1608.06105**