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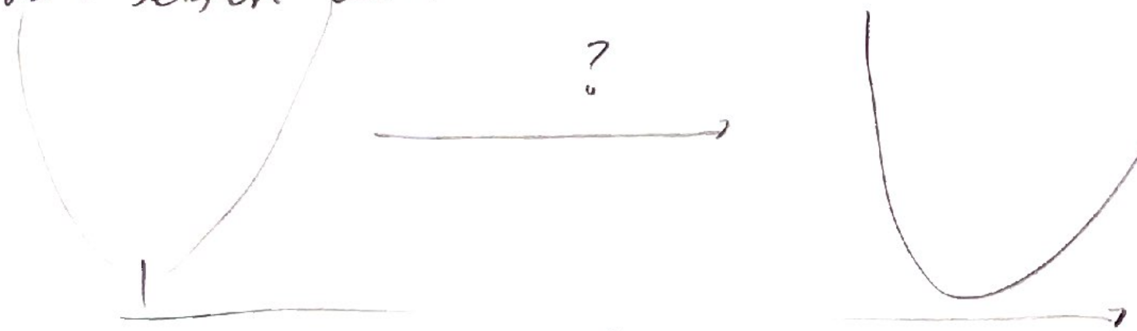
Optimal Processes & The Geometries of Thermodynamics.

(1)

Schmiedl & Seifert 2007



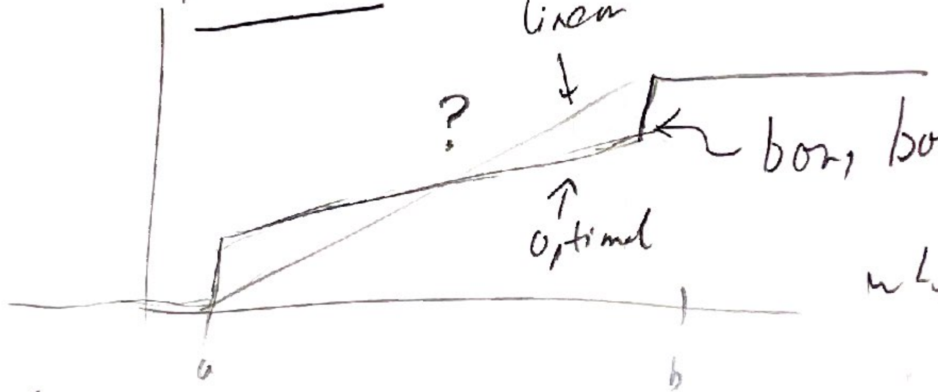
$$\dot{x} = -\mu \frac{\partial U}{\partial x} + \sqrt{\frac{2\mu}{\beta}}\,\xi$$

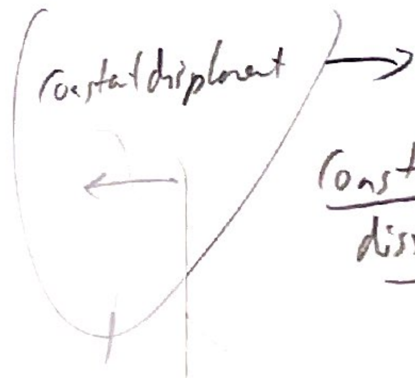
μ = mobility

$$U = \frac{1}{2}\left(x - \lambda(\tau)\right)^2$$

↑ control center of trap

Finite time





Constant dissipation

Minimal dissipation Protocols

1) Intrinsic
2) FEP
3) Molecular Motors/Machines

Fisher Information $p(x;\lambda)$ ← defined over a family of distribution.

$$I(\lambda) = \int dx \; p(x|\lambda) \left[\frac{\partial \ln P(x|\lambda)}{\partial \lambda}\right]^2$$

$$= \mathrm{var}\left(\frac{\partial}{\partial \lambda} \ln P(x|\lambda)\right] = \mathrm{Var}[\text{score}]$$

If λ vector   Bounds variance of unbiased estimator $T(x)$ unbiased estimator of λ

$\langle T \rangle = \lambda$

CRAMER-RAO bound $\mathrm{var}(T) \geq \frac{1}{I(\lambda)}$

$$\cancel{P(y/x|\lambda) = e^{+\beta F(\lambda) - \beta E(x,\lambda)}}$$

~~score~~ $\cancel{\frac{\partial \ln P(x|\lambda)}{\partial \lambda} = \beta}$

$P(x:\lambda) = e^{+\beta F - \beta E(x,\lambda)}$

Fisher information at Eq

$$\frac{\partial \ln P(x|\lambda)}{\partial \lambda} = \beta \frac{\partial F}{\partial \lambda} - \beta \frac{\partial E}{\partial \lambda}$$

$$\beta F = -\ln \sum e^{-\beta E(x,\lambda)}$$

$$\beta \frac{\partial F}{\partial \lambda} = \sum e^{+\beta F} e^{-\beta E(x,\lambda)} \beta \frac{\partial E}{\partial \lambda} = \beta \left\langle \frac{\partial E}{\partial \lambda} \right\rangle$$

$$I(\lambda) = \left\langle \left(\frac{\partial E}{\partial \lambda} - \left\langle \frac{\partial E}{\partial \lambda} \right\rangle \right)^2 \right\rangle$$

$I(\lambda)$ = variance of fluctuations (at Thermodynamic equilibrium)

(B)

Fisher Information multidimensional λ^i vector of parameters.

$$g_{ij} = \int dx\ p(x|\lambda) \left(\frac{\partial \ln P(x|\lambda)}{\partial \lambda^i}\right)\left(\frac{\partial \ln P(x|\lambda)}{\partial \lambda^j}\right)$$

positive semi-definite

varies smoothly with λ
(except at phase-transitions)

why Raised index

$$g_{ij} = \left\langle (x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle) \right\rangle^2$$

covariance matrix

λ^i "column vector" vector

λ_i co-vector
Dual space!

"$x^T A y$" $= x_i A^i{}_j y^j$

Matrix notation can't destinguish between A_{ij} $A^i{}_j$ & A^{ij}

Fisher Information Riemannian ~~Me~~ Metric

Distance

1) $d(a,b) \geq 0$ $[d(a,b) = 0$ only when $a = b]$
   non-negative
2) symmetric $d(a,b) = d(b,a)$ (length to there same as there to here)
3) triangle inequality $d(a,b) + d(b,c) \geq d(a,c)$ (going direct is never longer than going via intermediate point)

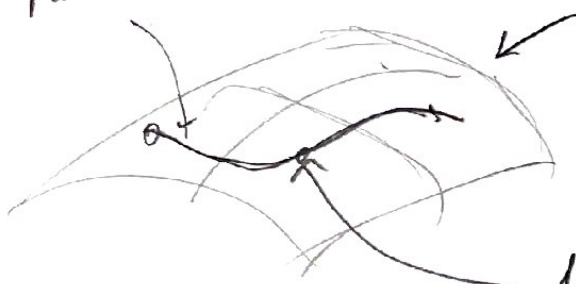
$$\mathcal{L} = \int_0^T \sqrt{\frac{\partial \lambda^i}{\partial t} \, g_{ij} \, \frac{\partial \lambda^j}{\partial t}} \, dt$$

Fisher Information distance

metric tensor

Riemannian Geometry

(Not about embedding
Klein bottle, 4 dimensions)



Manifold "surface"

smoothly

locally at each point a metric tensor g_{ij}
that tells you how far apart local points are

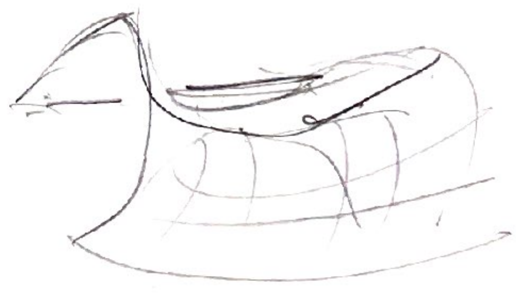
Intrinsic curvature (A piece of paper is not curved)
Not about embedding into space.

"Scalar Curvature"
Ricci Scalar

Positive sphere

0 flat

negative hyperbolic



Complexity!

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Ricci Scalar curvature

$$S = tr_g R \quad \equiv \quad g^{ij} R_{ij}$$

← Ricci tensor

↑ inverse metric

$$= g^{\mu\nu} \left(\partial_\lambda \Gamma^\lambda_{\mu\nu} - \partial_\nu \Gamma^\lambda_{\mu\lambda} + \Gamma^\sigma_{\mu\nu} \Gamma^\lambda_{\lambda\sigma} - \Gamma^\sigma_{\mu\lambda} \Gamma^\lambda_{\nu\sigma} \right)$$

↑ Christoffel symbols

$$\Gamma_{cab} = \frac{1}{2} \left(\partial_b g_{ca} + \partial_a g_{cb} - \partial_c g_{ab} \right)$$

$$\Gamma_{cab} = g_{cd} \Gamma^d{}_{ab}$$

Shortest Path → "straight lines" Geodesics

distance
$$\mathcal{L} = \int_0^{\tau} \sqrt{\frac{\partial x^i}{\partial t} g_{ij} \frac{\partial x^j}{\partial t}}\, dt$$

action or path energy
$$\mathcal{J} = \tau \int_0^{\tau} \frac{\partial x^i}{\partial t} g_{ij} \frac{\partial x^j}{\partial t}\, dt$$

$$\mathcal{J} \geq \mathcal{L}^2$$

Because of Cauchy - Schwarz inequality,

(let $h = 1$)

$$\int_0^{\tau} f^2\, dt \int_0^{\tau} h^2\, dt \geq \left[\int_0^{\tau} f h\, dt\right]^2$$

$$\langle f, f\rangle \langle h, h\rangle \geq |\langle f, h\rangle|^2$$

inner product

Thermodynamic Geometry

Eq. Thermodynamics has Riemannian Geometry

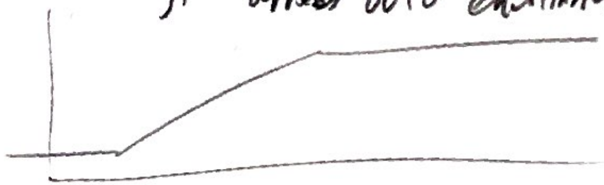
Weinhold 1975 } Macroscopic Thermodynamics.
Ruppeiner 1979 }
Salamon & Berry 1983 ← connected to minimum dissipation
Geodesic

Minimum

Linear Response Metric

Sivak 2012

$\dot{\lambda}$ drives out of equilibrium



$A \equiv \dfrac{\partial \beta E}{\partial \lambda}$ $\delta A = A(t) - \langle A \rangle_{\lambda(t)}$ "excess" deviation from equilibrium

$$\langle \delta B(t_b) \rangle_{\Lambda} \overset{LR}{=} \int_{-\infty}^{t_b} \langle \delta B(t_b)\, \delta A(t) \rangle_{\lambda} \frac{\partial \lambda}{\partial t}\, dt$$

time correlation function

$$\langle \delta B(t_b) \rangle_{\Lambda} \overset{MLR}{=} \left[\frac{\partial \lambda}{\partial t}\right]_{\lambda_b} \underbrace{\int_{-\infty}^{t_1} \langle \delta B(t_b)\, \delta A(t) \rangle_{\lambda}\, dt}_{\zeta_{BA}(\lambda)}$$

Kirkwood 1946

$\zeta_{BA}(\lambda)$ Friction coefficient [zeta]

(11)

$\Rightarrow$ Minimum dissipation Paths are Geodesics in Linear Response Metric

$\Rightarrow$ Constant ex. Power

$$\text{Work} = \int \underbrace{\frac{\partial E}{\partial \lambda}}_{-A} \frac{\partial \lambda}{\partial t}\, dt$$

Mean Power $\langle \beta P \rangle = -\frac{\partial \lambda}{\partial t} \langle A \rangle_\Lambda$

excess Power

$\langle \beta \delta P \rangle = -\frac{\partial \lambda}{\partial t} \langle \delta A \rangle_\Lambda$

P_{ex} mean excess power

$$\langle \delta \beta P \rangle \overset{\text{MCR}}{\equiv} \left[\frac{\partial \lambda^i}{\partial t}\right] \zeta_{ij} \frac{\partial \lambda^j}{\partial t}$$

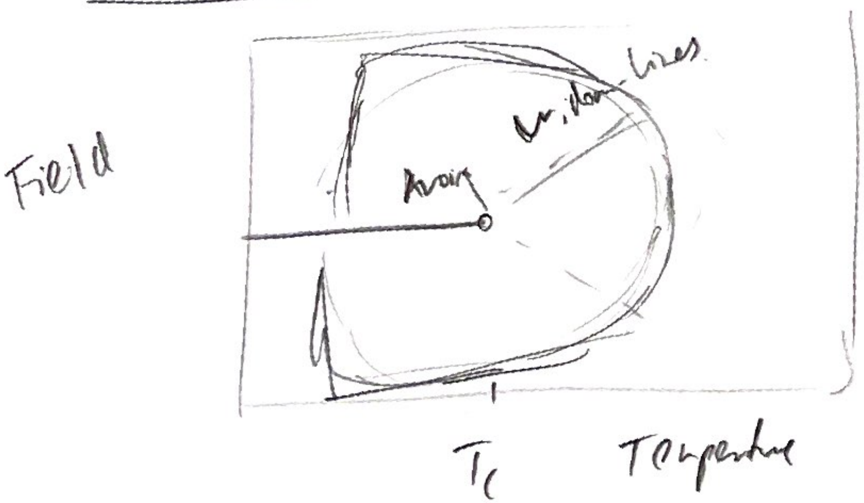
positive semi definite!

dissipation $\langle W_{ex} \rangle = \int dt\, P_{ex}$ $\quad \langle W_{ex} \rangle \geq \frac{\mathcal{L}^2}{\Delta t}$ $\leftarrow$ distance on metric

$J = \Delta t \langle W_{ex} \rangle \geq \mathcal{L}^2$

Optimal Paths are Geodesics in various geometries.

2D ising Model → Computation of friction tensor. Rotskoff 2015



⇒ see also Mike DeWeese paper.

Linear Response metric, approximation to Earth mover distance

Wasserstein Metric

Chennakesavalu & Rotskoff 2023