Information Geometry on q-Gaussian Densities and Behaviors of Solutions to Related Diffusion Equations*

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Introduction (1)

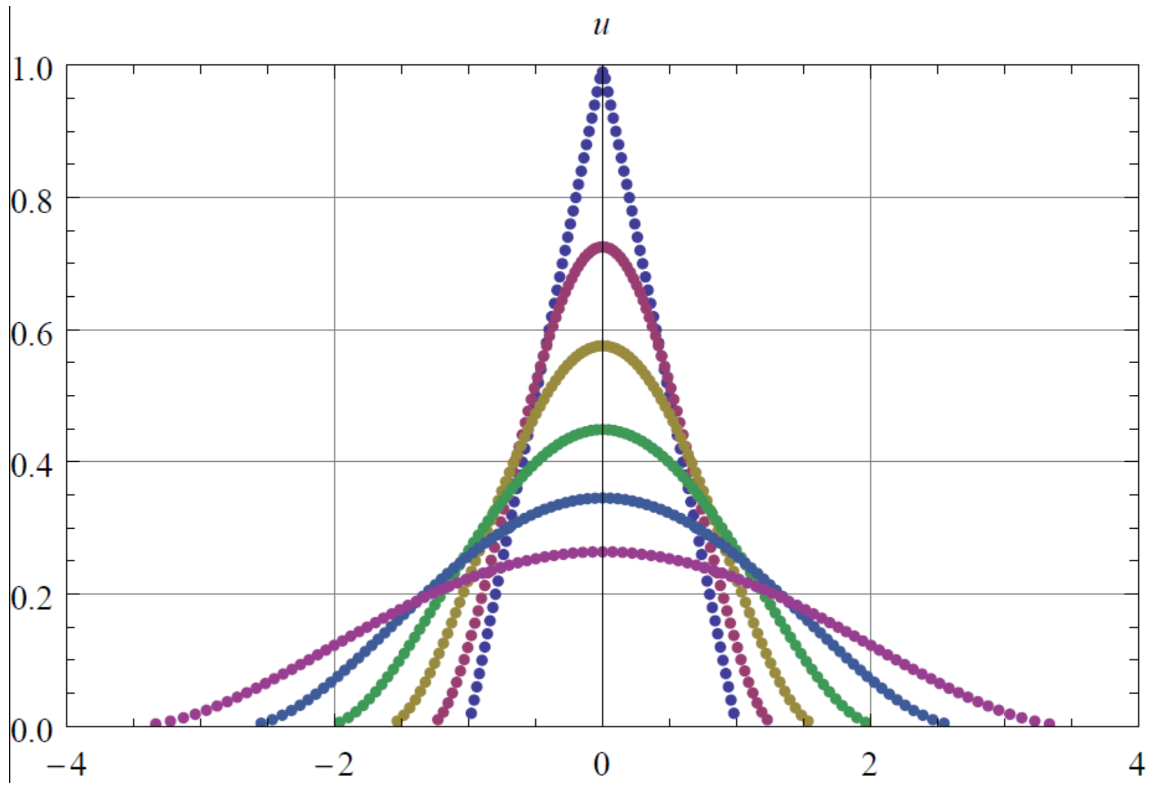
- Porous medium equation (PME)

$$\frac{\partial u}{\partial t} = \Delta u^m, \quad m > 1$$

  - Example: Diffusion coefficient depending on the power of u
    - Percolation in porous medium,
    - intensive thermal wave, …
  - Slow diffusion (anomalous diffusion):
    - Finite propagation speed
    - m=1 (normal diffusion): Infinite propagation speed

Solution of the PME for 1D case (initial function with bounded support)

m =1.5



propagation speed is finite

Introduction (2)

- Nonlinear Fokker-Planck equation (NFPE)

$$\frac{\partial p}{\partial \tau} = \nabla \cdot (\beta x p + D \nabla p^m), \quad \beta > 0$$

- Corresponding physical phenomena ➔ Slow diffusion + drift force (by quadratic potential)
  - equilibrium density exists
- Nonlinear transformation between the PME and the NFPE

Previous work

[Aronson], [Vazquez], [Toscani] and many others…

- Existence, uniqueness & mass conservation
  - W.l.o.g. we consider probability densities
- Special solution: self-similar solution
- Convergence rate to the self-similar solution
- Lyapunov functional (free energy) technique

Introduction (3)

- The purpose of the presentation:
  - Behavioral analysis of the PME type diffusion eq. focusing on a <u>stable invariant manifold</u>

    the family of q-Gaussian densities

    $\Downarrow$

  - A new point of view
  - Technique and concepts from Information Geometry can be applied

Outline

- 1.Generalized entropy and exponential family
- 2.Information geometry on the q-Gaussian family and analytical tools
- 3.Behavioral analysis of the PME and NFPE
  - Invariant manifold
  - The second moments, m-projection, geodesic
  - Peculiar phenomena to slow diffusion
  - Convergence rate to the q-Gaussian family

1. Generalized entropy and exp family (1) [Naudts 02 & 04], [Eguchi04]

- $\phi(s)$:strictly increasing and positive on $(0,\infty)$
- generalized logarithmic function

$$\ln_\phi(t) := \int_1^t \frac{1}{\phi(s)} ds, \quad t > 0.$$

- Strictly inc.
- Concave
- $\ln_\phi(1) = 0$

- generalized exponential function

  $\exp_\phi$: the inverse of $\ln_\phi(t)$

- convex function $F_\phi(s)$ for $s > 0$

to define entropy

$$F_\phi(s) := \int_1^s \ln_\phi t dt, \quad F_\phi(0) < +\infty \text{ :assumed.}$$

Generalized entropy and exp family (2)

- Bregman divergence

$$\mathcal{D}_\phi[p\|q] = \int F_\phi(p(x)) - F_\phi(q(x)) - \ln_\phi q(x)(p(x) - q(x))d\mu,$$

- Generalized entropy

$$\mathcal{I}_\phi[p] := \int -F_\phi(p(x)) + (1 - p(x))F_\phi(0)dx$$

- Generalized exponential model

$$\mathcal{M}_\phi = \{p_\theta(x) = \exp_\phi(\underline{\theta}^T h(x) - \underline{\kappa_\phi(\theta)}) | \theta \in \Omega \subset \mathbf{R}^d\} \subset L^1(\mathbf{R}^n)$$

θ: canonical paramtr., $\kappa_\phi(\theta)$: normalizing const

$h(x)$: vector of stochastic variables (Hamiltonian)

Remark [Naudts 02, 04]

- Requirements to the generalized entropy:
  - 1. For a certain χ , the entropy should be of the form:

$$\int p \ln_\chi(1/p)dx$$

  - 2. $\exp_\phi$-family achieves an ME for $\mathcal{I}_\phi[p]$

Then $\mathcal{I}_\phi[p]$ in the previous slide is determined.

- $\ln_\chi$ is called the deduced log func of $\ln_\phi$

Another representation of $\mathcal{D}_\phi[p||q]$

- Conjugate function of F_ϕ

$$U_\phi(t) := t \exp_\phi t - F_\phi(\exp_\phi t).$$

- U-divergence [Eguchi 04]

$$\mathcal{D}_\phi[p||q] := \int U_\phi(\ln_\phi q) - U_\phi(\ln_\phi p) - p(\ln_\phi q - \ln_\phi p)dx$$

Example (1) (to be used later)

- Generalized log ➔ q-logarithm q: real

$$\ln_q t \quad := \quad (t^{1-q} - 1)/(1-q),$$

- Generalized exp ➔ q-exponential

$$\exp_q t \quad := \quad [1 + (1-q)t]_+^{1/(1-q)}$$

  - $\phi(u) = u^q, q > 0, q \neq 1$ ⟺ PME

- Generalized entropy

$$\mathcal{I}[p] = \frac{1}{2-q} \int \frac{p(x)^{2-q} - p(x)}{q-1} dx$$

(2-q)-Tsallis entropy

Example (2) (to be used later)

- Bregman divergence

$$\mathcal{D}[p\|q] = \int \frac{q(x)^{2-q} - p(x)^{2-q}}{2-q} - p(x)\frac{q(x)^{1-q} - p(x)^{1-q}}{1-q} dx,$$

- Gen. exp family ➔ q-Gaussian family

$$\mathcal{M} := \left\{ f(x;\theta,\Theta) \middle| \theta \in \mathbf{R}^n,\ 0 > \Theta = \Theta^T \in \mathbf{R}^{n\times n} \right\}$$

q-Gaussian density

$$f(x;\theta,\Theta) = \exp_q\left(\overbrace{\theta^T x + x^T \Theta x}^{\theta^T h(x)} - \kappa(\theta,\Theta)\right),$$

$$\theta = (\theta^i) \in \mathbf{R}^n, \Theta = (\theta^{ij}) \in \mathbf{R}^{n\times n},$$

- When q goes to 1, all of them recover to the standard ones.

2. Information geometry [Amari,Nagaoka00] on q-Gaussian family $\mathcal{M}$

- $\mathcal{M}$:finite dimensional manifold in $L^1(\mathbf{R}^n)$
- Potential function on $\mathcal{M}$

$$\Psi_\phi(\theta) := \int U_\phi(\ln_\phi p_\theta) + (1 - p_\theta)F_\phi(0)dx + \kappa_\phi(\theta)$$

  - $U_\phi(t)$:Legendre transform of $F_\phi(s)$
- Legendre structure on $\mathcal{M}$ compatible with statistical physics
  - Riemannian metric, covariant derivatives, geodesics and so on.

Important tools from IG (1)

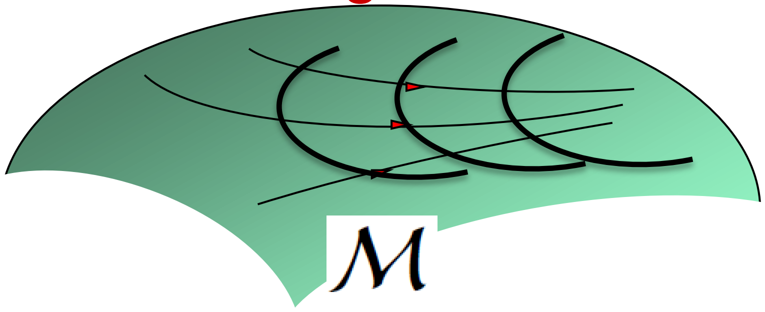
- 1. dual coordinates (Expectation parameters)

$$\eta_i(\theta) := \partial_i \Psi_\phi(\theta) = \int h_i(x) p_\theta(x) d\mu = \mathbf{E}_{p_\theta}[h_i(x)],$$

  - Expectation of each $h_i(x)$

    (= the 1st and 2nd moments for q-Gaussian)

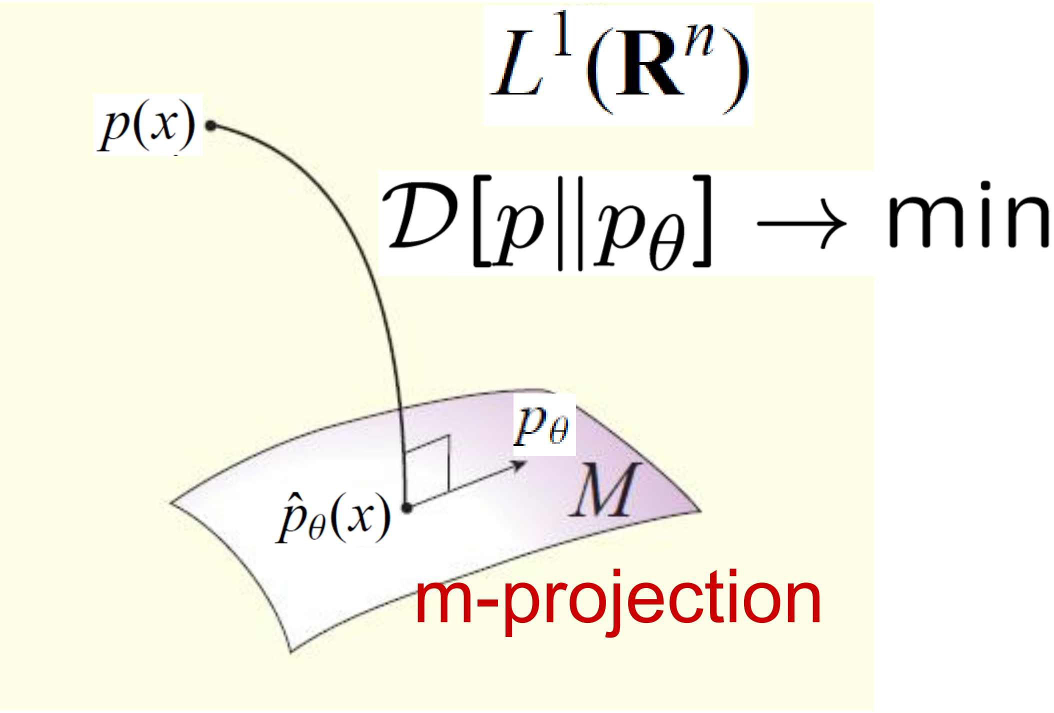
- 2. m-geodesic
  - a curve on $\mathcal{M}$ represented as a straight line in the η-coordinates



Important tools from IG (2)

- 3. m-projection of $p(x)$

$$\hat{p}_\theta := \text{arg min}_{p_\theta \in \mathcal{M}} \mathcal{D}[p \| p_\theta]$$



Useful properties of the m-projection

Proposition 2 *Let* $\hat{p}_\theta \in \mathcal{M}_\phi$ *be the m-projection of* p*. Then the following properties hold:*

i) *The expectation of* $h(x)$ *is conserved by the m-projection, i.e.,* $\mathbf{E}_p[h(x)] = \mathbf{E}_{\hat{p}_\theta}[h(x)]$,

ii) *The following triangular equality holds:* $\mathcal{D}_\phi[p||p_\theta] = \mathcal{D}_\phi[p||\hat{p}_\theta] + \mathcal{D}_\phi[\hat{p}_\theta||p_\theta]$ *for all* $p_\theta \in \mathcal{M}_\phi$.

- Rem: The property i) claims that the 1st and 2nd moments are conserved.

3. Behavioral analysis of PME and NFPE

- PME: $$\frac{\partial u}{\partial t} = \Delta u^m, \quad m > 1$$
- NFPE: $$\frac{\partial p}{\partial \tau} = \nabla \cdot (\beta x p + D \nabla p^m), \quad \beta > 0$$
- Relation between u and p [Vazquez 03]

$$p(z,\tau) := (t+1)^{\alpha} u(x,t), \quad z := (t+1)^{-\beta} R x, \ \tau := \ln(t+1)$$

$$D = RR^T$$

$$\beta = \frac{1}{n(m-1)+2}, \quad \alpha = n\beta$$

Key preliminary result

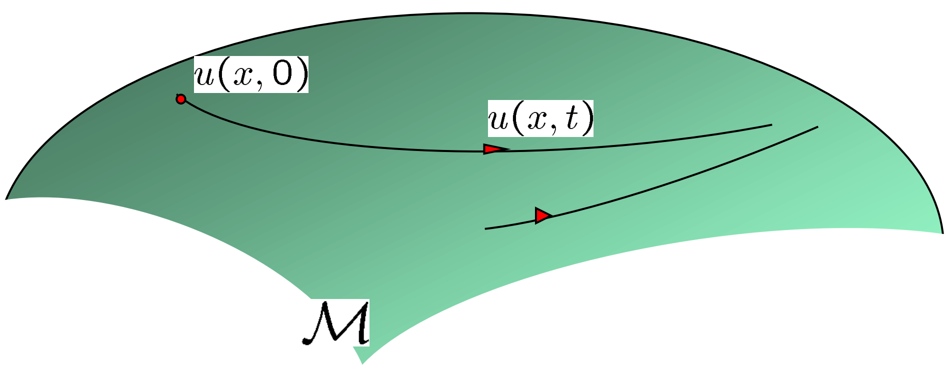
<u>Assumption:</u> $1<m=2-q<2$

<u>Proposition</u>

The q-Gaussian family $\mathcal{M}$ is a stable invariant manifold of the PME and NFPE.

Idea of the proof)

Show the R.H.S. of the PME Δu^m is tangent to $\mathcal{M}$ when u is on $\mathcal{M}$.



Trajectories of m-projections (PME)

- The 1st and 2nd moments of $u(t)$

$$\eta^{\mathrm{PM}} = (\eta_i^{\mathrm{PM}}) \text{ and } H^{\mathrm{PM}} = (\eta_{ij}^{\mathrm{PM}})$$

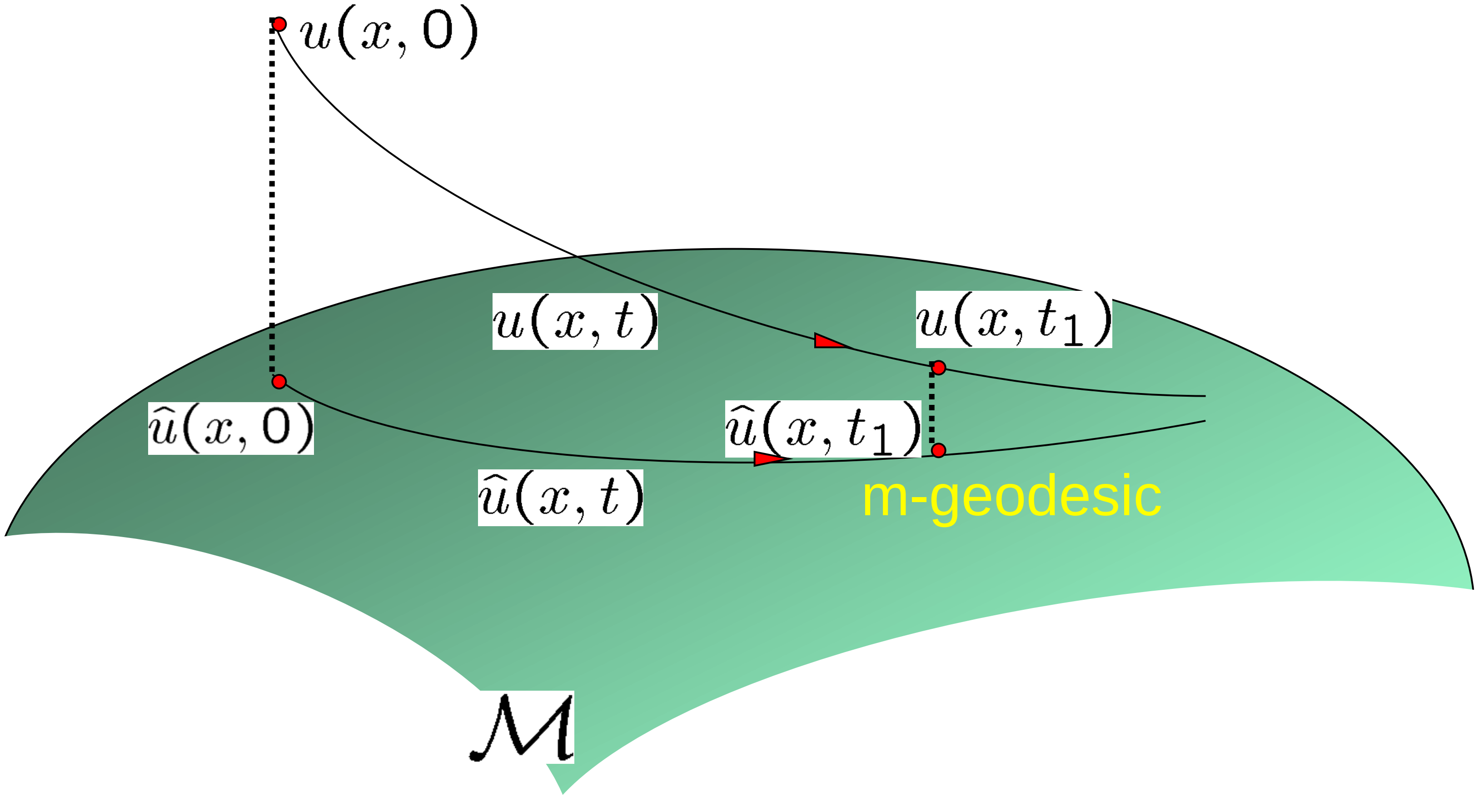
where

$$\eta_i^{\mathrm{PM}}(t) := \mathbf{E}_u[x_i] = \int x_i u(x,t)dx, \quad \eta_{ij}^{\mathrm{PM}}(t) := \mathbf{E}_u[x_i x_j].$$

<u>Thm</u>

The m-projection of the solution to the PME evolves following an m-geodesic curve, i.e., its expectation coordinate is a straight line.

Properties of the m-projection and behavioral analysis



Idea of the proof

- Time derivatives of the moments:

$$\dot{\eta}_i^{\mathrm{PM}} = 0, \quad \dot{\eta}_{ij}^{\mathrm{PM}} = 2\delta_{ij} \int u^m d\mu.$$

$$\begin{aligned} \eta^{\mathrm{PM}}(t) &= \eta^{\mathrm{PM}}(0), \\ H^{\mathrm{PM}}(t) &= H^{\mathrm{PM}}(0) + \sigma_u^{\mathrm{PM}}(t) I. \end{aligned}$$

$$\sigma_u^{\mathrm{PM}}(t) := 2 \int_0^t dt' \int u(x,t')^m dx.$$

straight line in the η-coordinates

Implication of the theorem (1)

- The theorem implies the existence of nontrivial N-1 constants of motions. N=dim $\mathcal{M}$

$$
\begin{aligned}
I_0 &= \int u(x,t)dx, \quad I_i = \int x_i u(x,t)dx, \quad i = 1,\cdots,n, \\
I_{ij} &= \int x_i x_j u(x,t)dx, \quad i = 1,\cdots,n, \; j = 1,\cdots,n, \; i \neq j, \\
I_{kk} &= \sum_{i=1}^{n} e_i^{(k)} \left(\int x_i^2 u(x,t)dx - \eta_{ii}(0) \right), \quad k = 1,\cdots,n-1,
\end{aligned}
$$

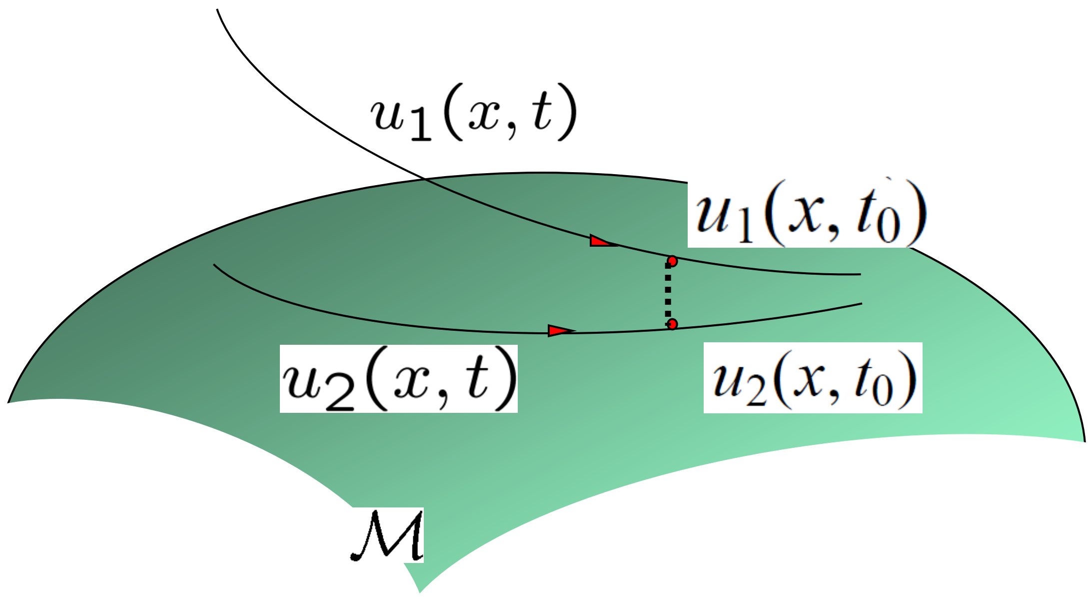
- A solution to the PME on the invariant manifold $\mathcal{M}$ is possibly solvable by quadratures.

Implication of the theorem (2)

Corollary: Let $u_1(x,t)$ and $u_2(x,t) \in \mathcal{M}$ be solutions of the PME.

If $\hat{u}_1(x,t_0) = u_2(x,t_0)$ at $t = t_0$, then

$$\dot{H}_1^{\mathrm{PM}}(t_0) - \dot{H}_2^{\mathrm{PM}}(t_0) = 2m(m-1)\mathcal{D}[u_1(x,t_0) \| u_2(x,t_0)]I$$

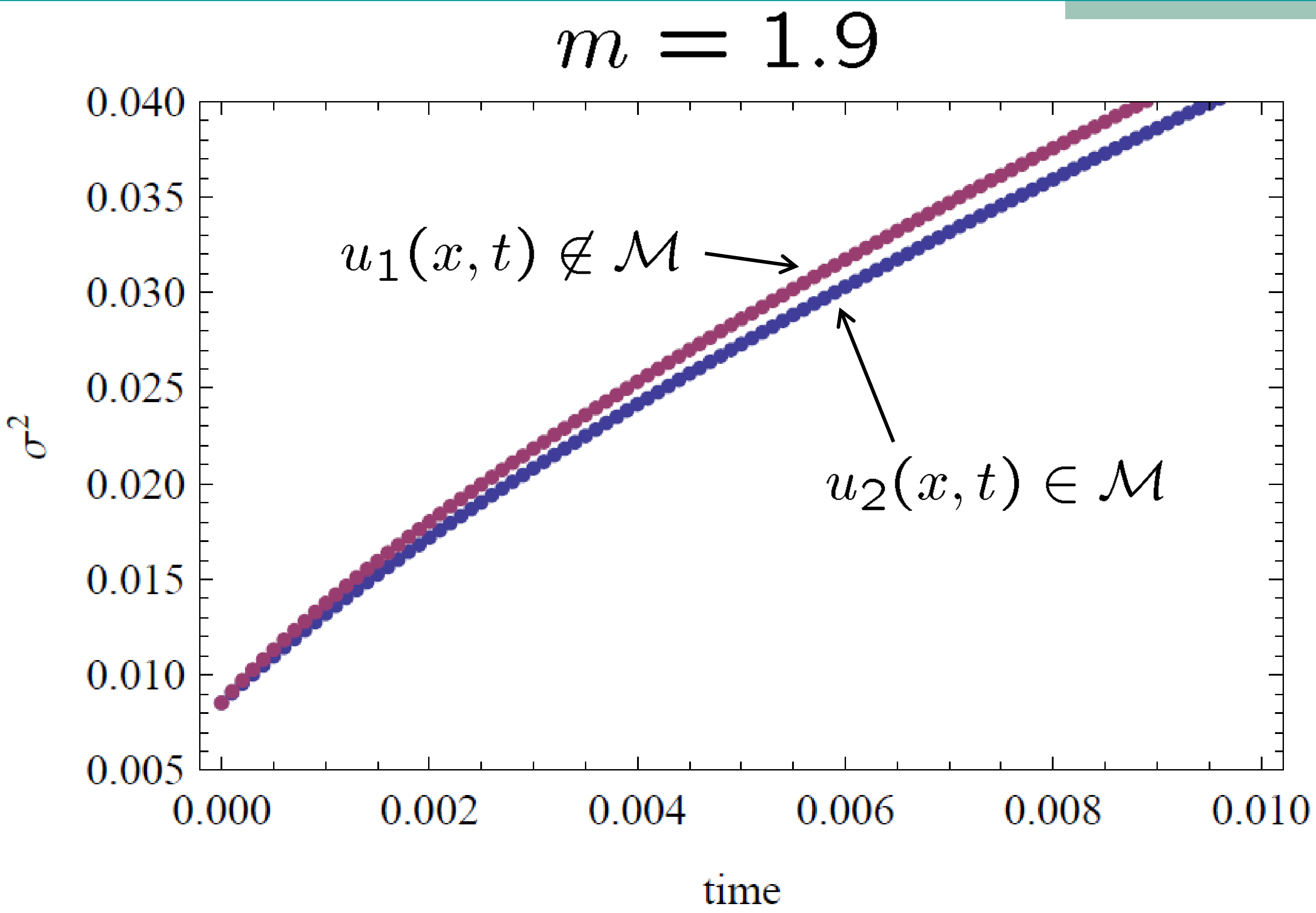


Implication of the theorem (3)

- Idea of the proof
  - The formula of the 2^{nd} moments + the property i) of the m-projection
- The corollary shows that the evolutional speed of each solution depends on the Bregman divergence from $\mathcal{M}$.

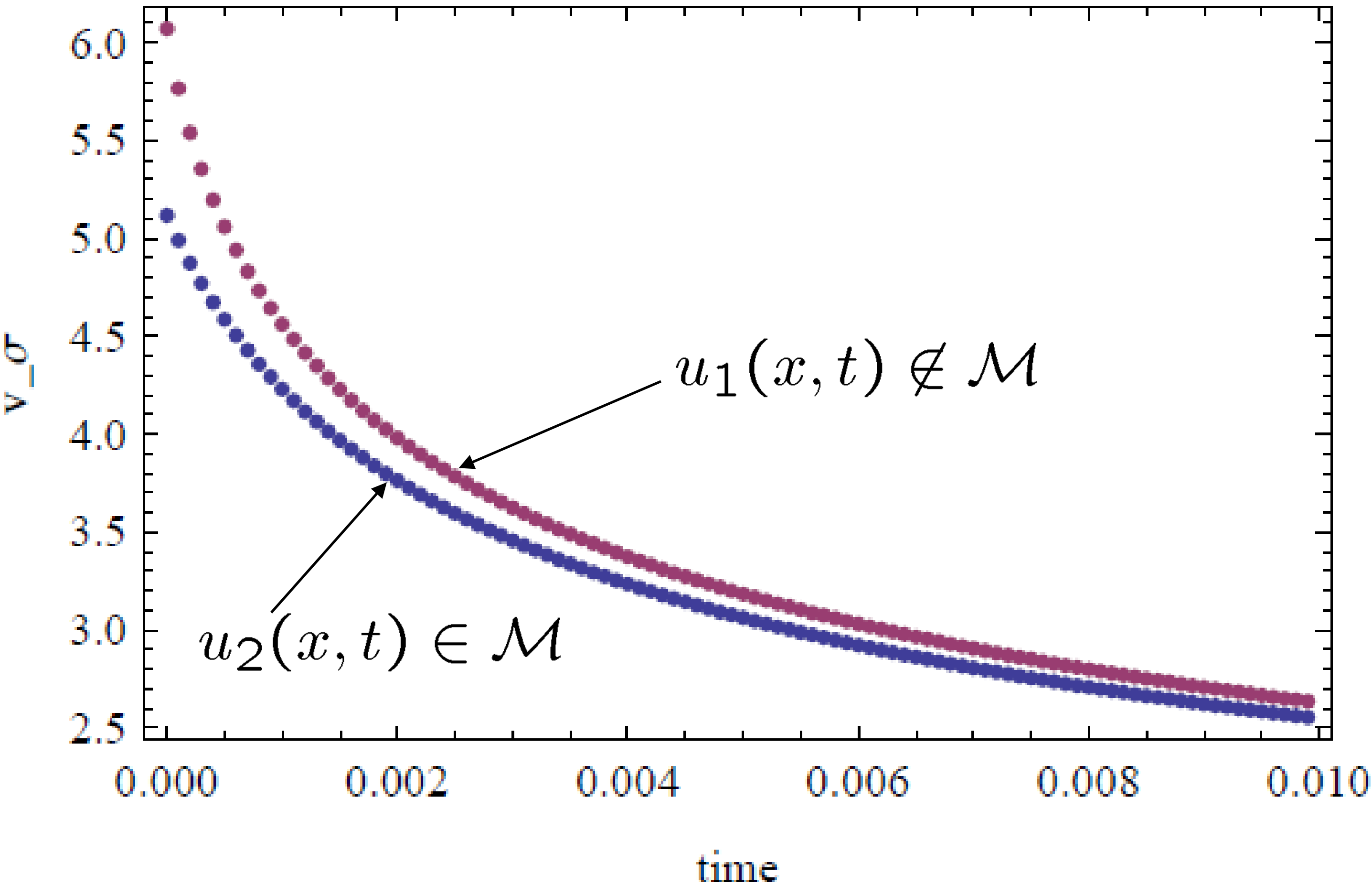
  (=the difference of the entropies)
- When m=1 (normal diffusion), such a phenomenon does not occur.

Difference of the second moments



Difference of the evolutional speed

$m = 1.9$



Convergence analysis for the NFPE and its application to the PME

- Generalized free energy

$$\mathcal{F}[p] := \int \frac{\beta}{2m} x^T D^{-1} x p(x) dx - \mathcal{I}[p]$$

- It works as a Lyapunov functional for the NFPE:

$$\frac{d\mathcal{F}[p(x,\tau)]}{d\tau} = -\frac{1}{2-q}\int p|\beta R^{-1}x + (2-q)p^{-q}R\nabla p|^2 dx \leq 0.$$

- The equilibrium density is a q-Gaussian:

$$p_\infty(x) = f(x; 0, \Theta_\infty) = \exp_q(x^T\Theta_\infty x - \kappa(0, \Theta_\infty)),$$

$$\theta_\infty = 0, \quad \Theta_\infty = -\frac{\beta}{2m}D^{-1}.$$

Convergence analysis for the NFPE and its application to the PME

- Difference of the free energy from the equilibrium density:

$$\begin{aligned}\mathcal{D}[p\|p_\infty] &= \Psi(0,\Theta_\infty) - \mathcal{I}[p] - \Theta_\infty \cdot \mathbf{E}_p[xx^T] \\ &= \mathcal{F}[p] - \mathcal{F}[p_\infty].\end{aligned}$$

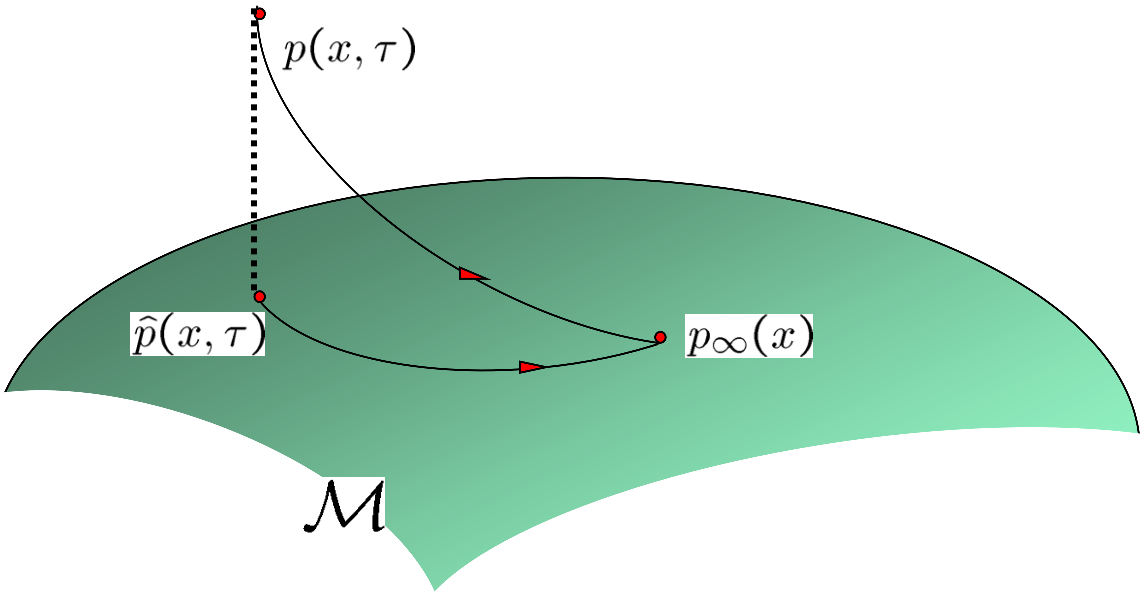
- Thus, $\mathcal{D}[p(x,\tau)\|p_\infty(x)]$ is monotone decreasing.

⇒ Interpreted as a generalized H-theorem

Convergence analysis for the NFPE and its application to the PME

- 1. The property ii) of the m-projection:

$$\mathcal{D}[p(x,\tau)||p_\infty(x)]$$
$$= \mathcal{D}[p(x,\tau)||\widehat{p}(x,\tau)] + \mathcal{D}[\widehat{p}(x,\tau)||p_\infty(x)]$$



Convergence analysis for the NFPE and its application to the PME

- 2. The known convergence result [Toscani05]

$$\mathcal{D}[p(x,\tau)||p_\infty(x)] = \mathcal{F}[p(x,\tau)] - \mathcal{F}[p_\infty(x)] \leq \mathcal{D}[p(x,0)||p_\infty(x)]e^{-2\beta\tau}.$$

- 3. The property of the transformation between the PME and the NFPE

  If $\widehat{u}$ is a transform of $\widehat{p}$, then

  - $\widehat{u}$ is an m-projection of u

    $\Longleftrightarrow$ $\widehat{p}$ is an m-projection of p

  -

$$\det(R)\int \hat{u}(x,t)^m - u(x,t)^m dx = (1+t)^{\alpha(1-m)}\int \hat{p}(x,\tau)^m - p(x,\tau)^m dx$$

Convergence analysis for the NFPE and its application to the PME

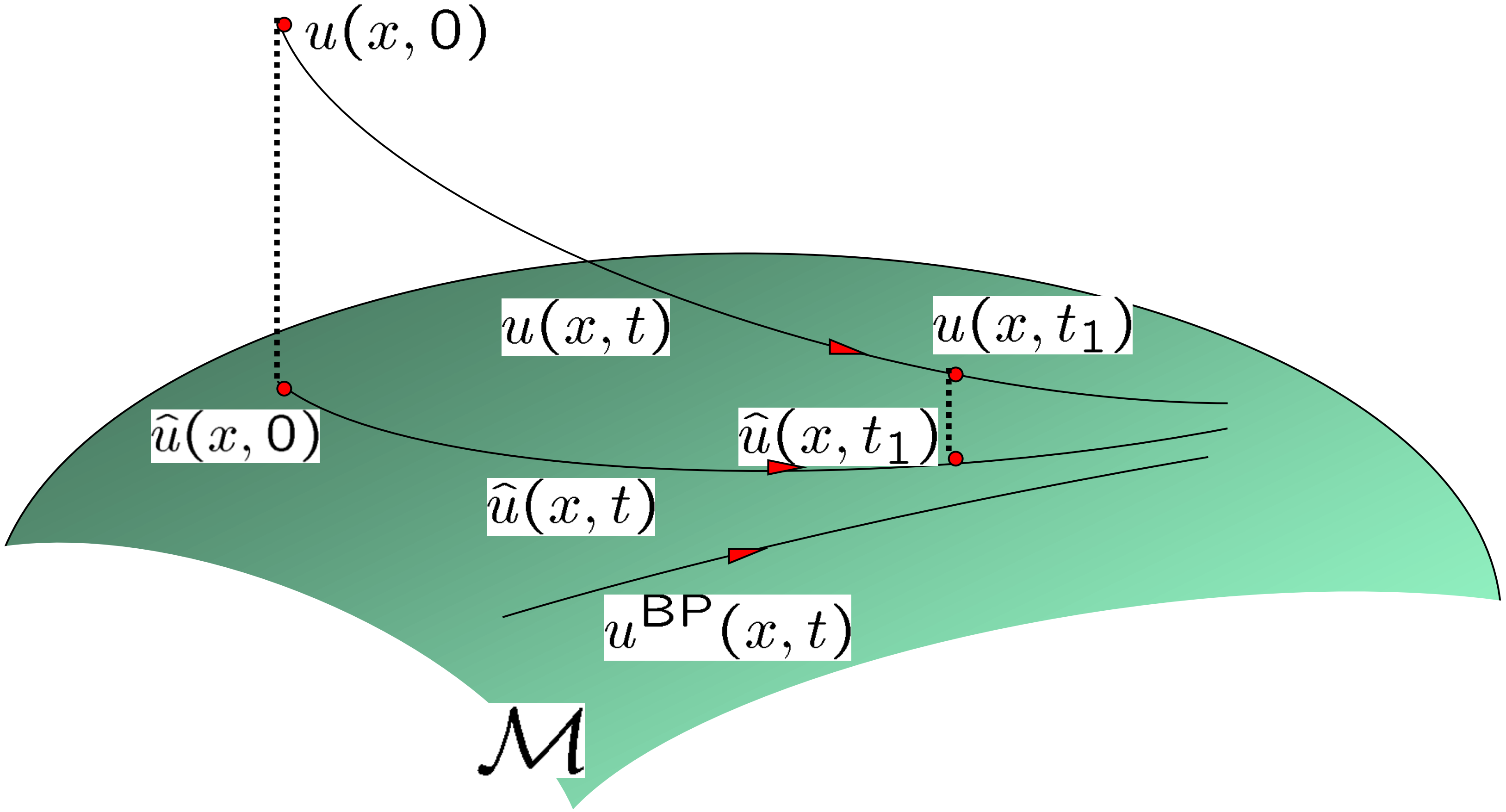
- Using 1, 2 and 3, we have the following:

Proposition 5 *Let $u(x,t)$ be a solution of the PME and $\hat{u}(x,t)$ be the m-projection of $u(x,t)$ to the q-Gaussian family $\mathcal{M}$ at each t. Then $u(x,t)$ asymptotically approaches to $\mathcal{M}$ with*

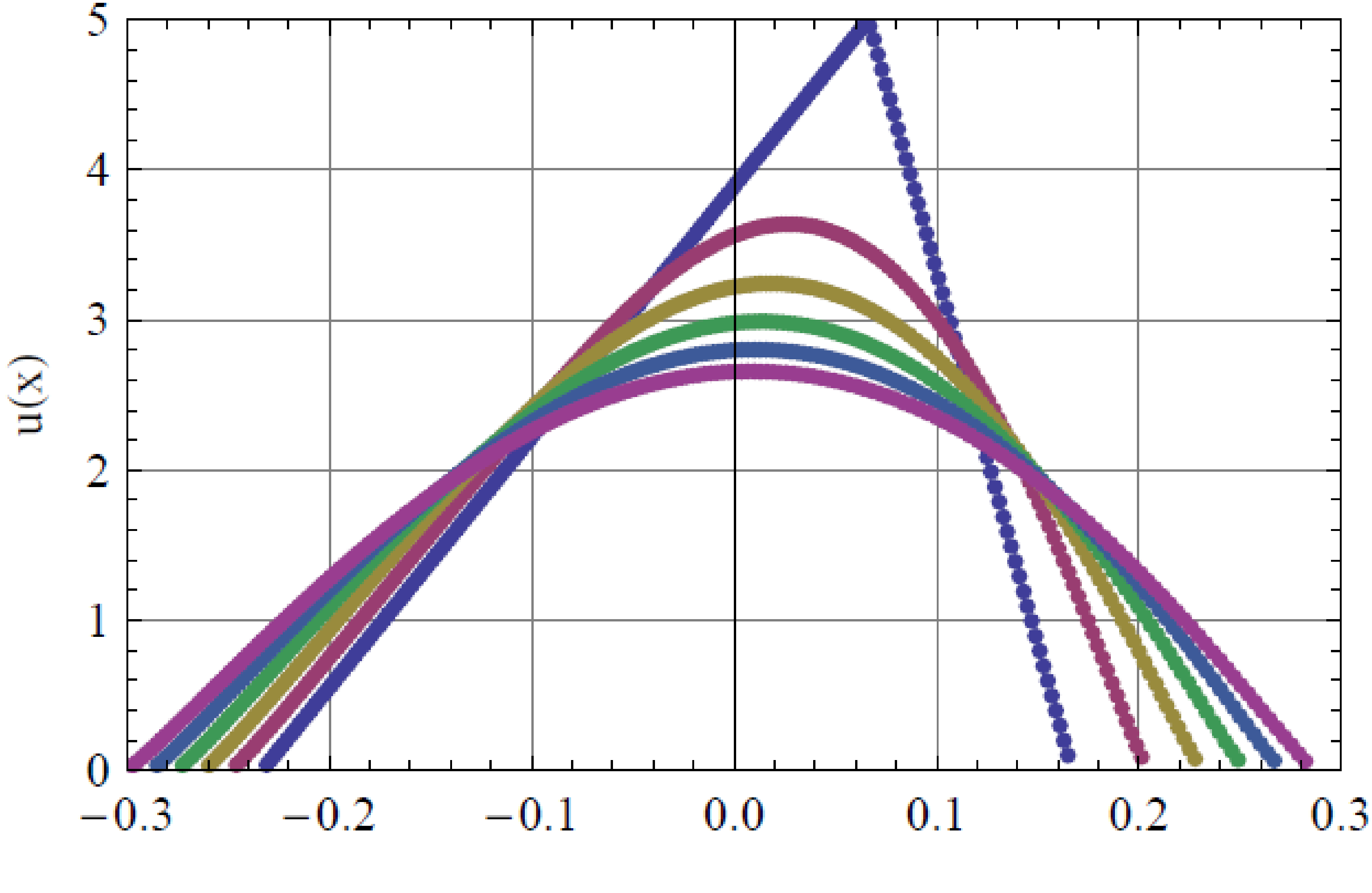
$$\mathcal{D}[u(x,t)||\hat{u}(x,t)] \leq \frac{C_0}{1+t},$$

- Convergence rate to the q-Gaussian family
- $L1$-norm convergence rate is derived from this result via the Csiszar-Kullback inequality.

Convergence analysis for the NFPE and its application to the PME



Convergence analysis for the NFPE and its application to the PME



Remark: $L1$-norm convergence rate

- Csiszar-Kullback inequality [Carrillo & Toscani 00]

$$\|f_1 - f_2\|_1^2 \leq C\mathcal{D}[f_1\|f_2], \ \exists C > 0$$

- The proposition implies that

  $L1$ convergence rate to $\mathcal{M}$ is $1/\sqrt{1+t}$

  faster than $1/t^{\beta}$ $\quad (\beta < 1/2$ if $m > 1)$

$L1$ convergence rate to the self-similar solution u^{BP}

[Toscani 05]

Self-similar solution u^{BP}

- Proposition

  Self-similar solution is an m- and e-geodesic

$$u^{\mathsf{BP}}(x,t) = t^{-\alpha}\,\mathrm{exp}_q\left(x^T\Theta(t)x - \psi(0,\Theta(t))\right)$$

$$\Theta(t) = -t^{-1}\frac{\beta}{2m}I$$

Conclusions

- Behavioral analysis of solutions to the PME and NFPE focusing on the q-Gaussian family.
  - Constants of motions, evolutional speeds, convergence rate to $\mathcal{M}$.
  - Generalized concepts of statistical physics
- Future work
  - Relation with Otto's result (Wasserstein geometry)
  - The other parameter range: m<1 (fast diffusion), 2<m, or the other type of diffusion equation

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