The new method using Shannon entropy to decide the power exponents on JMAK equation

$$f(t, K, \beta) = \exp\left[-\left(\frac{t}{K}\right)^{\beta}\right]$$

$$H(\beta^*, \langle\xi\rangle) = \sup_{\beta} H(\beta, \langle\xi\rangle)$$

Kwansei Gakuin University,
Graduate School of Science and Technology
Osaki laboratory
mail(univ.): maruoka.hirokazu@kwansei.ac.jp
hmmaruoka1987@gmail.com

Hirokazu Maruoka

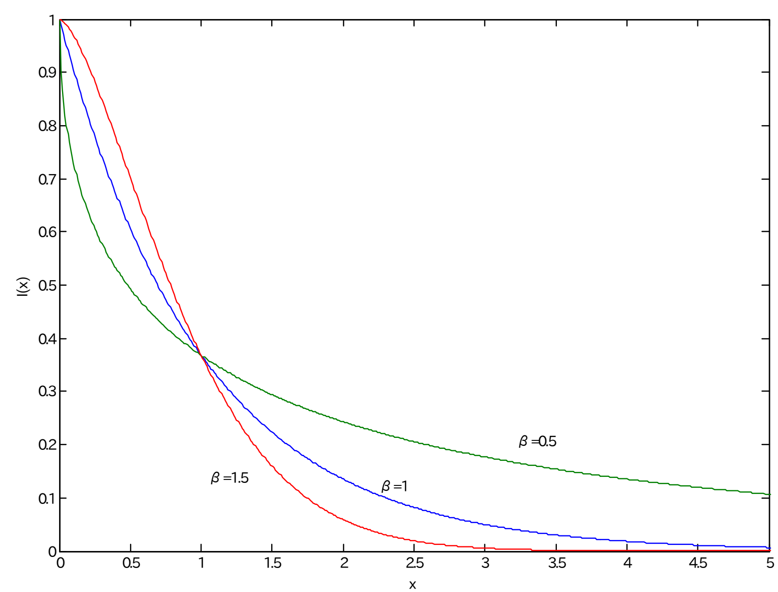
11 Nov. 2019

1. Introduction

JMAK (Johnson-Mehl-Avrami-Kolmogorov) equation

- JMAK (Johnson-Mehl-Avrami-Kolmogorov) equation is exponential equation inserted power-law behavior on the parameter, which is widely utilized to describe relaxation process, nucleation process, deformation of materials and so on.
- $\beta > 1$ corresponds to JMAK eq. And β is called Avrami constant which is associated with dimensionality of nucleus though anomalous β is frequently observed.
- Mathematically it corresponds to Weibull distribution.
- Another interpretation of β is still demanded.

$$f\left(t, K, \beta\right) = \exp\left[-\left(\frac{t}{K}\right)^{\beta}\right]$$



Shannon entropy of which first moment is fixed

$$e^{-\left(\frac{t}{\tau_K}\right)^{\beta}} = \int_0^{\infty} D(\tau)\, F(t-\tau) d\tau$$

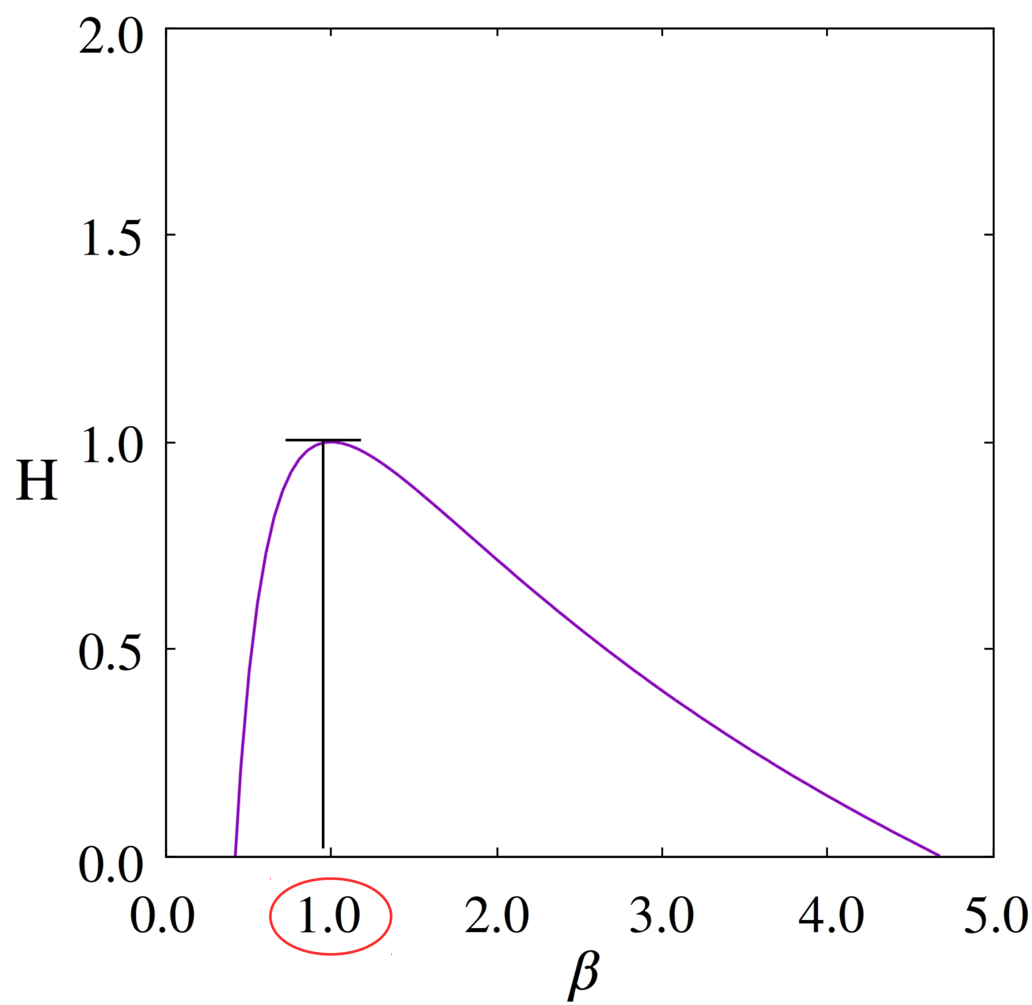
$$H = -\int_0^{\infty} D(\tau) \ln \frac{D(\tau)}{C} d\tau$$

$$H_W = \gamma\left(1-\frac{1}{\beta}\right) + \ln\frac{C\tau_K}{\beta} + 1$$

$$\langle\tau\rangle = \int_0^{\infty} \tau D(\tau) d\tau = \frac{\tau_K}{\beta}\Gamma\left(\frac{1}{\beta}\right)$$

$$\overline{H}_W = \gamma\left(1-\frac{1}{\beta}\right) - \ln\Gamma\left(\frac{1}{\beta}\right) + \ln C\langle\tau\rangle + 1$$

H. Maruoka et al. Chem. Phys. 2018



- Shannon entropy which first moment is introduce have supremum at β =1 ; it is a single exponential.

Purpose of this work

- This work intends to extend the method exercised previous work(Maruoka et al. Chem. Phys. 2018).

- This work intends to extend the previous method and attempt to explore the distributions of JMAK equation in which certain statistical quantities are fixed. Then we attempt to discuss the physical interpretation for obtained distributions.

Form of JMAK equation

$$f\left(t, K, \beta\right) = \exp\left[-\left(\frac{t}{K}\right)^{\beta}\right]$$

Constraint condition

$$\langle \xi \rangle = \Phi\left(K, \beta\right)$$

Maximum entropy estimation

$$H\left(\beta^{*}, \langle \xi \rangle\right) = \sup_{\beta} H\left(\beta, \langle \xi \rangle\right)$$

2. Method

Maximum entropy estimation method based on JMAK equation

Shannon entropy estimation

$$\exp\left[-\left(\frac{t}{K}\right)^{\beta}\right] = \int_0^{\infty} D(\tau)\, F(t-\tau)\, d\tau$$

$$D(\tau, K, \beta) = \frac{\beta}{K}\left(\frac{\tau}{K}\right)^{\beta-1} \exp\left[-\left(\frac{t}{K}\right)^{\beta}\right]$$

$$H(K, \beta) = \int_0^{\infty} D(\tau, K, \beta) \ln \frac{D(\tau, K, \beta)}{C} d\tau$$

$$H(K, \beta) = \gamma\left(1 - \frac{1}{\beta}\right) + \ln\frac{CK}{\beta} + 1$$

Constraint condition

$$\langle \xi \rangle = \Phi(K, \beta)$$

$$K = K(\langle \xi \rangle, \beta)$$

$$H[K(\langle \xi \rangle, \beta), \beta] = H(\beta, \langle \xi \rangle)$$

Maximum entropy estimation method based on JMAK equation

Shannon entropy estimation

$$H\left[K\left(\langle\xi\rangle,\beta\right),\beta\right]=H\left(\beta,\langle\xi\rangle\right)$$

↓

Maximum Shannon entropy estimation

$$H\left(\beta^{*},\langle\xi\rangle\right)=\sup_{\beta}H\left(\beta,\langle\xi\rangle\right)$$

- First step: Shannon entropy was estimated by assuming integral equation where F(t-τ) is step function
- Second step: Introducing statistical quantity i.e. constraint condition into Shannon entropy of step 1.
- H(β, <ξ>) is Shannon entropy of which statistical quantity <ξ> is fixed.
- β* gives the optimal distribution in which <ξ> is fixed.

3. Result and Discussion

3.1 Constraint condition of n-th moment

$$\langle K^n \rangle = \int_0^\infty \tau^n D(\tau, K, \beta)\, d\tau = \frac{K^n}{\beta}\Gamma\left(\frac{n}{\beta}\right)$$

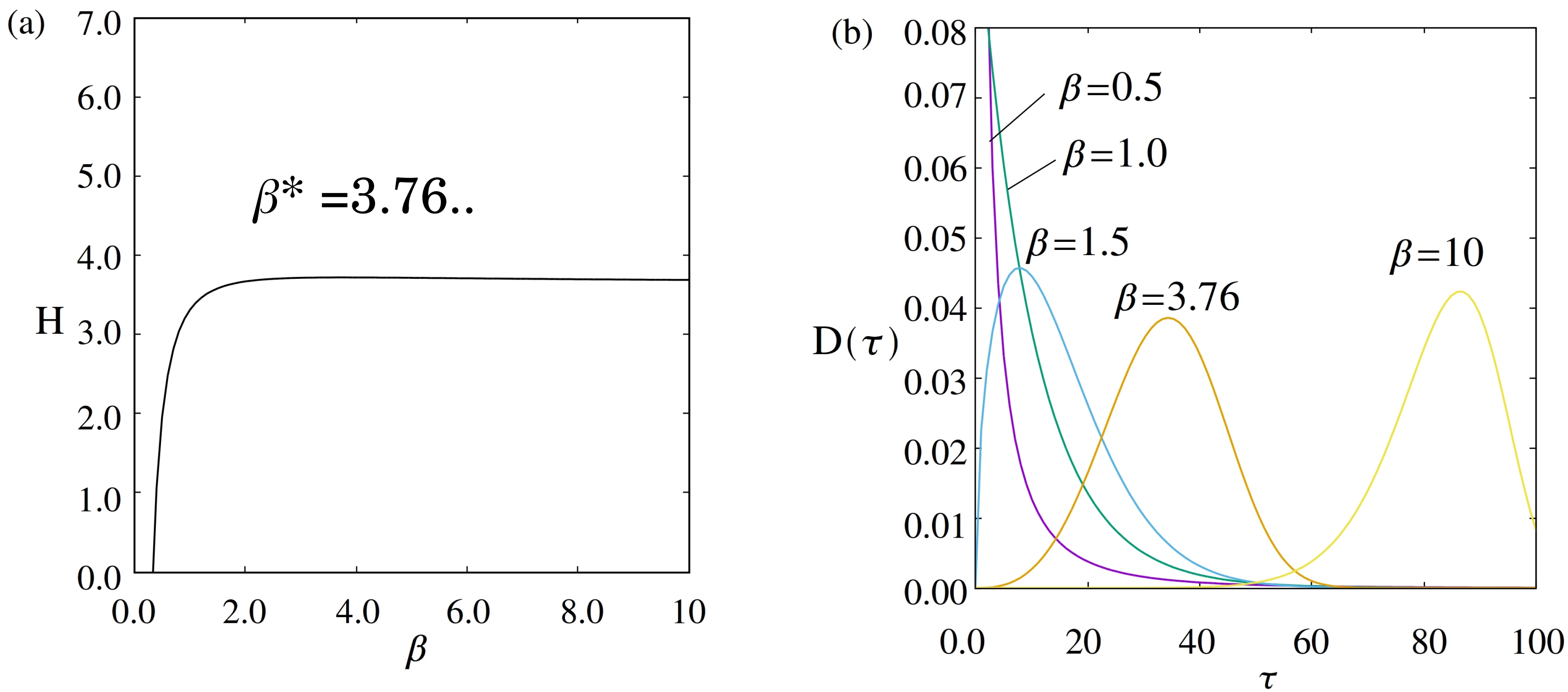
$$H(\beta, \langle K^n \rangle) = \gamma\left(1 - \frac{1}{\beta}\right) - \frac{1}{n}\ln\Gamma\left(\frac{n}{\beta}\right) + \left(\frac{1}{n} - 1\right)\ln\beta + \ln C\langle K^n \rangle^{1/n} + 1$$

n	β^*
1	1
2	1.2994
3	1.5
4	1.6533
5	1.7784
10	2.1981
100	3.8527
1000	5.7403

- β^* increases with n$and they are fractional number except for n=1 and 3.
- These results seem trivial but third moment can be related with volume in the case that *t* has space dimension. Rosin-Rammler distribution is applied for particle distributions.

3.2 Constraint condition of second cumulant : variance

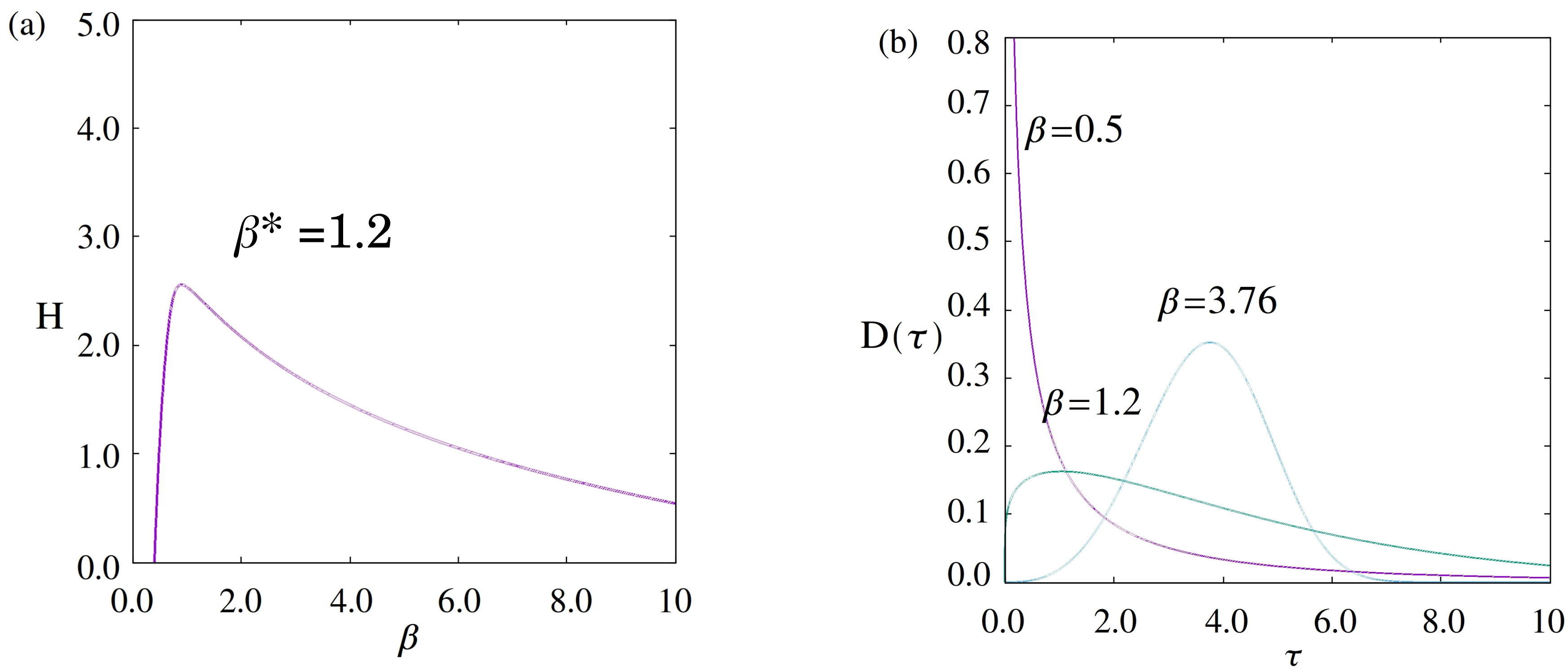
$$H\left(\beta,\sigma^2\right) = \gamma\left(1-\frac{1}{\beta}\right) - \ln\beta - \frac{1}{2}\ln\left[\Gamma\left(1+\frac{2}{\beta}\right) - \Gamma\left(1+\frac{1}{\beta}\right)^2\right] + \ln C\sqrt{\sigma^2} + 1$$



- The variance-introduced entropy seemingly gives symmetrical distribution?
- β observed in the shrink of PNIPA gels (Hashimoto et al. J. Phys.: Condens Matter. 2005) corresponds to the distributions that have larger entropy.

3.3 Constraint condition of third cumulant : skewness

$$H\left(\beta,c^{3}\right)=\gamma\left(1-\frac{1}{\beta}\right)-\frac{1}{3}\ln\beta^{3}\left[\frac{1}{\beta}\Gamma\left(\frac{3}{\beta}\right)-\frac{3}{\beta^{3}}\Gamma\left(\frac{2}{\beta}\right)\Gamma\left(\frac{1}{\beta}\right)+\frac{2}{\beta^{3}}\Gamma\left(\frac{1}{\beta}\right)^{3}\right]+\ln C\sqrt[3]{c^{3}}+1$$



- The maximum Shannon entropy of which skewness is fixed gives the positive-skewed distribution ($\beta^{*}=1.2$) .

4. Conclusion

Conclusive Summary

- The Shannon entropies which various statistical quantities i.e. constraint conditions are introduced gives different supremum β^*.
- The Shannon entropies which variance or skewness is introduced are quite interesting as its β^* seems to give the distribution in which its constraint condition, variance and skewness is typically fixed.
- Kolmogorov-Sinai theorem says that the partition obtained by maximum entropy gives smallest subsets of generator. The relation and interpretation based on the Kolmogorov-Sinai theorem should be pursued for further development.
- The method to decide β using Shannon entropy with Lagrange multipliers give the optimal distribution of which physical quantity is fixed. The phenomnena which are described by JMAK type equations may involve these constraint conditions.

Funding / Acknowledgement / Conflict of Interest

- Funding
  This research received no external funding.

- Acknowledgements
  The author wish to thank prof. K. Osaki, and K. Shigeoka for discussion of this research.

- Conflicts of Interest
  The author declares no conflict of interest.