Constraint choice and model selection in the generalized maximum entropy principle (MEP)

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Introduction: A wide class of entropies can be used in the MEP

- Jos Uffink [1], generalizing the Shore and Johnson's axioms, proved that the functionals which are suitable to be used in the Maximum Entropy Principle (MEP) belong to a one-parameter family, which the Shannon entropy is a member of.
- Such functionals are monotonically increasing functions f of

$$U_q(P) = \left(\sum_G p^q(G)\right)^{1/(1-q)}$$

- For $q \to 1$, $U_q(P) \to$ Shannon entropy
- P. Jizba and J. Korbel discussed [2] that this generalized approach is suitable to study systems which do not respect standard hypothesis such as ergodicity, short-range interactions or exponential growth of the sample space: the resulting probability distributions take into account correlations that may not have been observed.
- Rényi entropy

$$S_R(P;q) = \log U_q(P)$$

- Constraint choice: mean vs normalized q-mean

$$\underline{\langle C\rangle_q} = \sum_G \frac{C(G)p^q(G)}{\sum_G p^q(G)}$$

Methods: Maximum entropy and maximum likelihood

- Constrained maximization of entropy through Lagrange multiplier technique.
- Parameter estimation through **Maximum likelihood** estimator: maximize the joint probability of the data in order to fix the parameters.
- Compare results for both constraint choices.

Mathematical formulation: Mean vs q-mean constraints

- Constrained maximization
  - $$\max_P \left[S_R(P;q) - \alpha'\left(\sum_G p(G) - 1\right) - \theta'\left(\langle C\rangle - C^*\right)\right]$$
  - $$\max_P \left[S_R(P;q) - \alpha\left(\sum_G p(G) - 1\right) - \theta\left(\underline{\langle C\rangle_q} - C^*\right)\right]$$
- Solutions
  - $$p(G) = \frac{1}{Z'}(1-(q-1)\,\hat{\theta}'\,C(G))^{\frac{1}{q-1}}$$
  - $$p(G) = \frac{1}{Z}(1-(1-q)\,\hat{\theta}\,C(G))^{\frac{1}{1-q}}$$
- Maximum likelihood
  - $$\sum_G C(G)p^{2-q}(G|\,\hat{\theta}'_{ML}) = \sum_G C(G)p^{1-q}(G|\,\hat{\theta}'_{ML})freq(G)$$
  - $$\sum_G C(G)p^{q}(G|\,\hat{\theta}_{ML}) = \sum_G f(G)p^{q-1}(G|\,\hat{\theta}_{ML})freq(G)$$

Discussion: Generaized mean is a better constraint in the MEP

- The solutions of the MEP show a power-law behavior: the mean could diverge, so it could be a bad constraint choice.
- If q is such that the distribution is normalizable, then all its q-moments converge.
- The q-mean allows us to characterize the power law for every possible value of the exponent.
- The q-mean, unlike the standard one, makes the Maximum entropy and Maximum likelihood consistent each other.
- Model selection, i.e. choice of the preferred parameters (q, θ) given the data, can be performed through the maximum likelihood approach.

Numerical simulations: Explanation

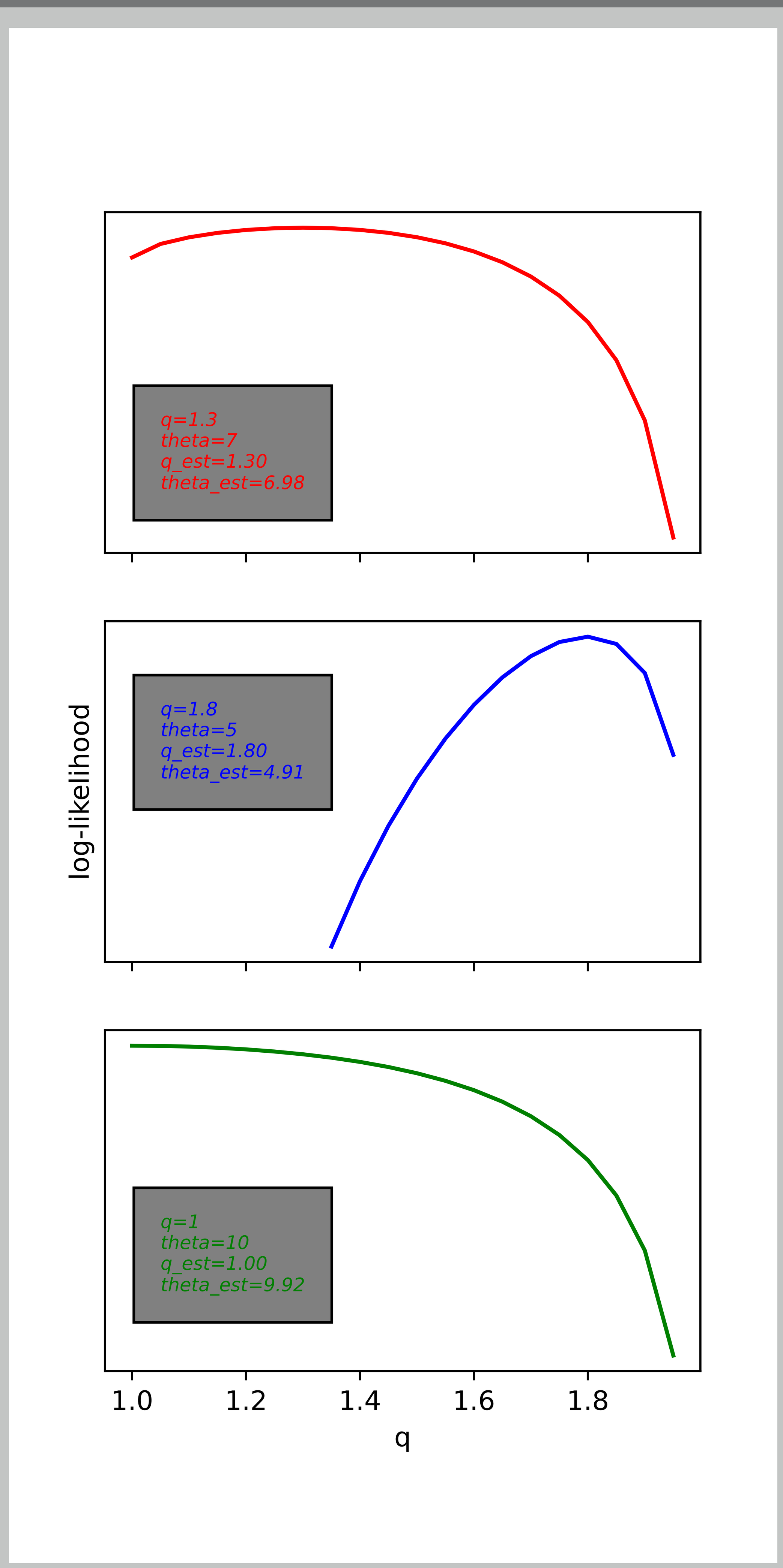
- Data sampled from p(G) in the simple case where $C(G) \in [0,+\infty)$ and $g(C) = 1$, for different values of q and θ ($q = 1$ being the exponential distribution)
- $P(C) = (2-q)\theta(1-(1-q)\theta C)^{\frac{1}{1-q}}$
- Parameters estimated through maximum likelihood model selection

Numerical results: Parameter estimation

- Number of points sampled $N = 10^5$...
- ...for each of three PDFs (r, b, g) with different parameters

Probability density	q	θ	q_{est}	θ_{est}
(r), 1st moment converge	1.3	7	1.30	6.98
(b), 1st moment diverge	1.8	5	1.80	4.91
(g), exponential PDF	1	10	1.00	9.92

Numerical results: Log-likelihood vs q plot



Log-likelihood vs q plot. The log-likelihood, for each q, is evaluated in the point $(q,\theta) = (q, \hat{\theta}_{ML}(q))$

References

[1] Jos Uffink.
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Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics, 26(3):223–261, 1995.

[2] Petr Jizba and Jan Korbel.
Maximum entropy principle in statistical inference: Case for non-shannonian entropies.
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