Maximum Entropy Reconstruction for Discrete Distributions with Unbounded Support

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Abstract. The classical problem of moments is addressed by the maximum entropy approach for one-dimensional discrete distributions. The numerical technique of adaptive support approximation is proposed to reconstruct the distributions in the region where the main part of probability mass is located.

Keywords: maximum entropy, moment problem

1 Introduction

In the stochastic chemical kinetics prior information regarding the properties of the distribution (e.g. approximately normally distributed) is not directly accessible and in such a case regaining the probability distribution from the moment description is non-trivial. In fact it turns out that this problem, known as the classical moment problem, has a long history in other application domains and only recently very efficient methods for the reconstruction of the distribution became available.

Given a number of moments of a random variable, there is in general no unique solution for the corresponding distribution. However it is possible to define a sequence of distributions that converges to the true one whenever the number of constraints approaches infinity [19]. Conditions for the existence of a solution are well-elaborated (such as Krein’s and Carleman’s conditions) but they do not provide a direct algorithmic way to create the reconstruction. Therefore, Padé approximation [18] and inverse Laplace transform [6] have been considered but turned out to work only in restricted cases and require a large number of constraints. Similar difficulties are encountered when lower and upper bounds for the probability distribution are derived [9,23,14]. Kernel-based approximation methods have been proposed where one restricts to a particular class of distributions [8,19,7]. The numerically most stable methods are, however, based on the maximum entropy principle which has its roots in statistical mechanics and information theory. The idea is to choose from all distributions that fulfill the moment constraints the distribution that maximizes the entropy. The maximum entropy reconstruction is the least biased estimate that fulfills the moment constraints and it makes no assumptions about the missing information. No additional knowledge about the shape of the distribution neither a large number of moments is necessary. For instance, if only the first moment (mean) is provided the result of applying the maximum entropy principle is exponential distribution. In case of two moments (mean and variance) the reconstruction is given by normal distribution. Additionally, if experimental data (or simulation traces) is available, data-driven maximum entropy methods can be applied [26,3]. Recently, notable progress has been made in the development of numerical methods for the moment constrained maximum entropy problem [11,18], where the main effort is put to the transformation of the problem in order to overcome the numerical difficulties that arise during the optimization procedure.

In this paper we propose a combination of the classical Newton-based technique to numerically solve the maximum entropy problem with the procedure of distribution support approximation.

2 Maximum Entropy Reconstruction

The moment closure is usually used to approximate the moments of a stochastic dynamical system over time. The numerical integration of the correspondent ODE system is usually faster than a direct integration of the probability distribution or an estimation of the moments based on Monte-Carlo simulations of the system.
However, if one is interested in certain events and only the moments of the distribution are known, the corresponding probabilities are not directly accessible and have to be reconstructed based on the moments. Here, we shortly review standard approaches to reconstruct one-dimensional marginal probability distributions $\pi_i(x_i, t) = P(X_i(t) = x_i)$ of a Markov chain that describes the dynamics of chemical reactions network. The task of approximating multi-dimensional distributions follows the same line however for our case these techniques revealed to be not effective due to numerical difficulties in the optimization procedure. Thus, we have given (an approximation of) the moments of the $i$-th population and obviously, the corresponding distribution is in general not uniquely determined for a finite set of moments. In order to select one distribution from this set, we apply the maximum entropy principle. In this way we minimize the amount of prior information about the distribution and avoid any other latent assumption about the distribution. Taking its roots in statistical mechanics and thermodynamics, the maximum entropy approach was successfully applied to solve moment problems in the field of climate prediction, econometrics, performance analysis and many others.

2.1 Maximum Entropy Approach

The maximum entropy principle says that among the set of allowed discrete probability distributions $G$ we choose the probability distribution $q$ that maximizes the entropy $H(g)$ over all distributions $g \in G$, i.e.,

$$q = \arg \max_{g \in G} H(g) = \arg \max_{g \in G} \left( -\sum_x g(x) \ln g(x) \right).$$

(1)

where $x$ ranges over all possible states of the discrete state space. Note that we assume that all distributions are defined on the same state space. In our case the set $G$ consists of all discrete probability distributions that satisfy the moment constraints. Given a sequence of $M$ non-central moments $E(X^k) = \mu_k$, $k = 0, 1, \ldots, M$,

the following constraints are considered

$$\sum_x x^k g(x) = \mu_k, k = 0, 1, \ldots, M.$$  

(2)

Here, we choose $g$ to be a non-negative function and add the constraint $\mu_0 = 1$ in order to ensure that $g$ is a distribution. The above problem is a nonlinear constrained optimization problem, which is usually addressed by the method of Lagrange. Consider the Lagrangian functional

$$L(g, \lambda) = H(g) - \sum_{k=0}^{M} \lambda_k \left( \sum_x x^k g(x) - \mu_k \right),$$

where $\lambda = (\lambda_0, \ldots, \lambda_M)$ are the corresponding Lagrangian multipliers. It is possible to show that maximizing the unconstraint Lagrangian $L$ gives a solution to the constrained maximum entropy problem The variation of the functional $L$ according to the unknown distribution provides the general form of $g(x)$

$$\frac{\partial L}{\partial g(x)} = 0 \implies g(x) = \exp \left( -1 - \sum_{k=0}^{M} \lambda_k x^k \right) = \frac{1}{Z(x)} \exp \left( -\sum_{k=1}^{M} \lambda_k x^k \right),$$

where

$$Z(x) = e^{1+\lambda_0} \sum_x \exp \left( -\sum_{k=1}^{M} \lambda_k x^k \right)$$  

(3)

is a normalization constant. In the dual approach we insert the above equation for $g(x)$ into the Lagrangian thus we can transform the problem into an unconstrained convex minimization problem of the dual function w.r.t to the dual variable $\lambda$

$$\Psi(\lambda) = \ln Z(x) + \sum_{k=1}^{M} \lambda_k \mu_k,$$

According to the Kuhn-Tucker theorem, the solution $\lambda^* = \arg \min \Psi(\lambda)$ of the minimization problem for the dual function equals the solution $q$ of the original constrained optimization problem.
2.2 Maximum Entropy Numerical Approximation

It is possible to solve the constrained maximization problem in Eq. (1) for \( M \leq 2 \) analytically. For \( M > 2 \) numerical methods have to be applied to incorporate the knowledge of moments of order three and more. Here we use the Levenberg-Marquardt method \([24]\) to minimize the dual function \( \Psi(\lambda) \). An approximate solution \( \tilde{q} \) is given by

\[
\tilde{q}(x) = \exp \left( -1 - \sum_{k=0}^{M} \hat{\lambda}_k x^k \right),
\]

where \( \hat{\lambda} \) is the result of the iteration

\[
\lambda^{(t+1)} = \lambda^{(t)} - \left( H + \gamma^{(t)} \cdot \text{diag}(H) \right)^{-1} \frac{\partial \Psi}{\partial \lambda}.
\]

The damping factor \( \gamma \) is updated according to the strategy suggested in \([24]\) and \( \lambda^{(t)} = (\lambda_1^{(t)}, \ldots, \lambda_M^{(t)}) \) is an approximation of the vector \( \lambda = (\lambda_1, \ldots, \lambda_M) \) in the \( t \)-th step of the iteration. We compute \( \lambda_0 \) as \( \lambda_0 = \ln Z - 1 \) (see Eq. (3)). Initially we choose \( \lambda^{(0)} = (0, \ldots, 0) \) and stop when the solution converges, i.e. when the condition \( |\lambda^{(t+1)} - \lambda^{(t)}| < \delta \lambda \) is satisfied for a small threshold \( \delta \lambda > 0 \). In the \( t \)-th iteration the components of the gradient vector are approximated by \( \frac{\partial \Psi}{\partial \lambda} \approx \mu_i - \frac{1}{Z} \bar{\mu}_i \) and the entries of the Hessian matrix are computed as

\[
H_{i,j} = \frac{\partial^2 \Psi}{\partial \lambda_i \partial \lambda_j} \approx \frac{Z \cdot \bar{\mu}_{i+j} - \bar{\mu}_i \bar{\mu}_j}{Z^2}, \quad i, j = 1, \ldots, M.
\]

The approximation \( \bar{\mu}_i \) of the \( i \)-th moment is given by

\[
\bar{\mu}_i = \sum_x x^i \exp \left( - \sum_{k=1}^{M} \lambda_k^{(t)} x^k \right), \quad i = 1, \ldots, 2M,
\]

In order to approximate the moments we need to truncate the infinite sum in Eq. (5). We refer to Section A for a detailed description of how the distribution support can be approximated.

The convexity \([18]\) of the dual function \( \Psi(\lambda) \) guarantees the existence of a unique minimum \( \lambda^* \) approximated by \( \hat{\lambda} \). Theoretical conditions for the existence of the solution are discussed in detail in \([23,22,17]\). A similar analysis for the multivariate case is provided in \([16]\). The iterative procedure in Eq. (4) might however fail due to numerical instabilities when the inverse of the Hessian is calculated. The iterative minimization presented in \([4]\) and the Broyden-Fletcher-Goldfarb-Shanno (BFGS) procedure \([5]\) can be used to improve the numerical stability. In the sequel we denote by \( \tilde{\pi}_i(x,t) \) the reconstructed distribution of the \( i \)-th species for a given sequence of moments \( \mu_0, \ldots, \mu_M \), i.e. the marginal probability distribution \( \pi_i(x,t) = P(X_i = x) \). Note that the reconstruction approach presented above provides a reasonable approximation of the probabilities only in high-probability regions. In order to accurately approximate the tails of the distribution special methods have been developed \([8]\).

3 Conclusions

As future work, we plan to extend the reconstruction procedure in several ways. First, we want to consider moments of higher order than five. Since in this case the concrete values become very large it might be advantageous to consider central moments instead which implies that the reconstruction procedure has to be adapted. Alternatively, we might (instead of algebraic moments) consider other functions of the random variables such as exponential functions \([20]\), Fup functions \([10]\), and Chebyshev polynomials \([4]\). Another possible extension could address the problem of truncating the support of the distribution such that the reconstruction is applied to a finite support. We expect that in this case the reconstruction will become more accurate since we will not have to rely on the Gauss-Hermite quadrature formula. For instance, the theory of Christoffel functions \([8]\) could be used to determine the region where the main part of the probability mass is located.

Finally, we want to improve the approximation for species that are present in very small quantities, since for those species a direct representation of the probabilities is more appropriate than a moment representation. Therefore, we plan to consider the conditional moments approach \([12]\), where we only integrate the moments of species having large molecular counts but keep the discrete probabilities for the species with small populations.
A Approximation of the Support

During the iteration procedure we need to approximate one-dimensional moments by summing up over all states \( x \in \mathbb{Z}^+ \) that have positive probability mass. However our case studies possess the infinite number of such states and the appropriate truncation has to be done. Instead of considering whole state space \( \mathbb{Z}^+ \) we consider a subset \( D = \{ x_L, \ldots, x_R \} \subset \mathbb{Z}^+ \), where we have to choose such values for \( x_L \) and \( x_R \) that the iteration procedure converges. It might fail to converge if the difference \( (x_R - x_L) \) is very large so that the conditional number of the matrix \( (\hat{H} + \gamma^{(\ell)} \cdot \text{diag}(H)) \) is very large. To find a reasonable initial guess \( D^{(0)} = \{ x^{(0)}_L, \ldots, x^{(0)}_R \} \) we use the results in [23] and consider the roots of the function \( \Delta^0_k(w) \)

\[
\Delta^0_k(w) = \begin{vmatrix}
\mu_0 & \mu_1 & \cdots & \mu_k \\
\vdots & \vdots & \ddots & \vdots \\
\mu_{k-1} & \mu_k & \cdots & \mu_{2k-1} \\
1 & w & \cdots & w^k \\
\end{vmatrix},
\]

where \( k = \lfloor \frac{M}{2} \rfloor \), and \( M \) is even. The initial guess \( D^{(0)} \) is defined by \( x^{(0)}_L = \lfloor w_1 \rfloor \) and \( x^{(0)}_R = \lceil w_k \rceil \), where \( w_1 < \cdots < w_k \) are real and simple roots of the equation \( \Delta^0_k(w) = 0 \). In the \( \ell \)-th iteration we check if the probability of the right-most state \( x^{(\ell)}_R \) is reasonably small in comparison to the maximum value of \( \tilde{q}^{(\ell)}(x) \) for \( x \in D^{(\ell)} \), i.e.

\[
\tilde{q}^{(\ell)}(x^{(\ell)}_R) < \delta_{\text{prob}} \cdot \max_{x \in D^{(\ell)}} \tilde{q}^{(\ell)}(x),
\]

where \( \delta_{\text{prob}} \) is a small threshold (for all our experiments we chose \( \delta_{\text{prob}} = 10^{-3} \)). We extend the support until inequality (7) is satisfied by adding new state on each iteration

\[
geq \begin{cases}
\{ \max(0, x^{(\ell)}_L), x^{(\ell)}_R \}, & \ell \text{ is even} \\
\{ x^{(\ell)}_L, x^{(\ell)}_R + 1 \}, & \ell \text{ is odd} 
\end{cases}
\]

The final results \( \hat{\lambda} \) and \( \hat{D} \) of the iteration yields the distribution \( \tilde{q}(x) \) that approximates the marginal distribution of interest.

Please note that \( M \) is assumed to be even when we use the function \( \Delta^0_k \). Tari et. al also provide the extension of this technique that allows to account for the case when odd number of moments is known (\( M \) is odd) by considering the function \( \Delta^1_z(\eta) \)

\[
\Delta^1_z(\eta) = \begin{vmatrix}
\mu_1 - w_1 \mu_0 & \mu_2 - w_1 \mu_1 & \cdots & \mu_z - w_1 \mu_{z-1} \\
\vdots & \vdots & \ddots & \vdots \\
\mu_{z-1} - w_1 \mu_{z-2} & \mu_z - w_1 \mu_{z-1} & \cdots & \mu_{2z-2} - w_1 \mu_{2z-3} \\
1 & \eta & \cdots & \eta^{z-1} \\
\end{vmatrix},
\]

where \( z = \lfloor \frac{M}{2} \rfloor + 1 \). Let \( W = \{ w_1, \ldots, w_k \} \) be the set of the solutions of \( \Delta^0_k(w) = 0 \) and \( H = \{ \eta_1, \ldots, \eta_z \} \) be the set of solutions of \( \Delta^1_z(\eta) = 0 \), where all the elements of \( W \) and \( H \) are real and simple. The first approximation \( D^{(0)} \) is then defined by \( x^{(0)}_L = \lfloor \min(w_1, \eta_1) \rfloor \) and \( x^{(0)}_R = \lceil \max(w_k, \eta_z) \rceil \).

**Alternative method for support approximation extension.** Instead of adding only one state to the support approximation \( D^{(\ell+1)} \) we can use the following heuristics on Chebyshev’s inequality \( P\{|X - \mu_1| \geq z, \xi = \mu_2/z\} \leq \xi, \xi = \mu_2/z \). We compute \( z = \mu_2/0.1 \) (where we fix \( \xi = 0.1 \)) such that the correspondent set \( \tilde{D} = \{ \lfloor \mu_1 - z \rfloor, \ldots, \lceil \mu_1 + z \rceil \} \) shall include at least 90% of the probability mass.

The initial approximation \( D^{(0)} \) is compared to \( \tilde{D} \) by computing the difference \( l = |z - x^{(0)}_R| \). The latter serves as an increment in support extension procedure, i.e. the approximation of the support on iteration \( (i+1) \) is given by \( D^{(i+1)} = \{ x^{(i+1)}_L, \ldots, x^{(i+1)}_R \} \), where \( x^{(i+1)}_L = \max \left( 0, x^{(i)}_L - \lfloor l/2 \rfloor \right) \) and \( x^{(i+1)}_R = x^{(i)}_R + \lceil l/2 \rceil \).
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