4.1.2 Discretization Scheme

Using D dimensional, 3 point, Gauss-Hermite quadrature (see §2.1.6) once more we can discretize the entropy,

$$\begin{aligned} H_{KL}[f|\rho q] &= \frac{1}{\rho}\int_{\mathbb{R}^D} f(\mathbf{v}) \ln\left(\frac{f(\mathbf{v})}{\rho q(\mathbf{v})}\right) d\mathbf{v} \\ &\approx \frac{1}{\rho}\sum_{i=1}^{3^D} f_i \ln\left(\frac{f_i}{\rho q_i}\right), \\ &:= \mathcal{H}_{\mathbf{q}}[\mathbf{f}] \end{aligned} \tag{4.4}$$

where $f(\mathbf{v})$ and $\mathbf{f}$ are related via (2.19), as are $q(\mathbf{v})$ and $\mathbf{q}$.

This leads us to the general MinxEnt-LBM collision step,

$$\begin{aligned} \text{MinxEnt-LBM Collision Step:} \qquad \mathbf{f}^{\text{post}} &= \underset{\mathbf{f}\in\gamma}{\operatorname{argmin}} \quad \mathcal{H}_{\mathbf{q}}[\mathbf{f}] \\ \gamma &= \left\{\mathbf{f} \mid \mathbf{f} > \mathbf{0},\ \widetilde{C_1}(\mathbf{f}/\rho) = c_1, ..., \widetilde{C_K}(\mathbf{f}/\rho) = c_K\right\} \end{aligned} \tag{4.5}$$

where the $\widetilde{C}_k$ are the discretized versions of the constraint functionals, C_K. For example if $C_1(p) = \int p(\mathbf{v})\, d\mathbf{v}$, then $\widetilde{C}_1(\mathbf{p}) = \sum_i \mathbf{p}_i$.

Two further problem specific steps are needed. They are, the choice of $q(\mathbf{v})$ and the minimization method.

Regarding the choice of $q(\mathbf{v})$, it will typically differ depending on the system under study, however it must at least meet the requirement,

$$\int_{\mathbb{R}^D} q(\mathbf{v})\, d\mathbf{v} = 1.$$

Addressing the issue of minimization method, we will describe two possible methods here but in principle one could apply any method for constrained optimization. Of course some methods may be more suitable than others for a given problem.

4.1.3 Minimization Method: Newton-Raphson

The first method we consider is Newton-Raphson Minimization. We first convert the constrained minimization problem into an unconstrained one.

Though in principle the MinxEnt-LBM does not explicitly require any specific form on the constraints (except that they are self-consistent), we will limit our discussion here to constraints that are linear in p_i. This may require making linear approximations of nonlinear constraints. In such a case, we can write the discretized constraint functionals as,

$$\widetilde{C}_k(\mathbf{p}) = \sum_{j=1}^{3^D} \mathcal{T}_{kj}\mathbf{p}_j = c_k \qquad k = 1, ..., K$$

and equivalently,

$$\widetilde{C}_k(\mathbf{f}) = \sum_{j=1}^{3^D} \mathcal{T}_{kj}\mathbf{f}_j = \rho c_k \qquad k = 1, ..., K$$

for some $\mathcal{T}_{kj}$ and where $K < 3^D$ (since otherwise we have more constraints than free variables).

Since our constraints are linear in $\mathbf{f}$ we will find it useful to move from distribution space into

"moment space." This will enable us to implement the constraints in a much more straightforward manner during the minimization.

To move into moment space, consider an invertible 3^D by 3^D matrix, $\mathbf{T}$, and define the vector of moments, $\mathbf{M}$,

$$\mathbf{M} := \mathbf{T}\mathbf{f} \tag{4.6}$$

We select $\mathbf{T}$ such that $T_{kj} = \mathcal{T}_{kj}$ for $k \leq K, 1 \leq j \leq 3^D$. In principle the choices for the remaining $K - k$ rows of $\mathbf{T}$ are arbitrary, provided that $\mathbf{T}$ remains invertible and well conditioned. By construction the first K moments are constrained:

$$\begin{aligned} M_1 =& (\mathbf{T}\mathbf{f})_1 = \rho c_1, \\ M_2 =& (\mathbf{T}\mathbf{f})_2 = \rho c_2, \\ &\vdots \\ M_K =& (\mathbf{T}\mathbf{f})_K = \rho c_K, \end{aligned}$$

We define the vector of unconstrained moments by

$$\mathbf{m} = \langle M_{K+1}, M_{K+2}, ..., M_{3^D} \rangle \in \mathbb{R}^{3^D - K}.$$

With this notation, the *full* vector of moments (including constraints) is written,

$$\mathbf{M} = \langle \rho c_1, \ldots, \rho c_K, \mathbf{m} \rangle.$$

Using the definition of $\mathbf{T}$ in (4.6), we now seek the vector $\mathbf{m}$ that minimizes the discretized entropy (4.4) in moment space:

$$\begin{aligned} \mathcal{H}_{\mathbf{q}}[\mathbf{T}^{-1}\mathbf{M}] =& \sum_{i=1}^{3^D} (\mathbf{T}^{-1}\mathbf{M})_i \ln\left((\mathbf{T}^{-1}\mathbf{M})_i \frac{\omega(\mathbf{v}_i)}{\rho\, q_i} \right) \\ :=& \mathcal{S}_{\mathbf{q}}(\mathbf{M}). \end{aligned} \tag{4.7}$$

With the first K components of $\mathbf{M}$ fixed by the K constraints, the constrained minimization problem has become an unconstrained minimization over $3^D - K$ dimensions. The Newton-Raphson minimization procedure involves the gradient of $\mathcal{S}_{\mathbf{q}}$ with respect to $\mathbf{m}$:

$$\begin{aligned} \nabla_k \mathcal{S}(\mathbf{m}) =& \frac{\partial \mathcal{S}_q}{\partial m_k}(\mathbf{M}) \\ =& \sum_{i=1}^{3^D} (\mathbf{T}^{-1})_{ik} \left[\ln\left((\mathbf{T}^{-1}\mathbf{M})_i \frac{\omega(\mathbf{v}_i)}{\rho\, \mathbf{q}_i} \right) + 1 \right] \quad k \in \{K+1, \ldots, 3^D\}. \end{aligned} \tag{4.8}$$

The minmization problem involves finding $\mathbf{m}$ so that $\nabla \mathcal{S}(\mathbf{m}) = \mathbf{0}$.

The Hessian is

$$\begin{aligned} \mathbf{H}_{jk}(\mathbf{m}) =& \frac{\partial^2 \mathcal{S}_q}{\partial m_j \partial m_k}(\mathbf{M}) \\ =& \sum_{i=1}^{3^D} \frac{(T^{-1})_{ik}(T^{-1})_{ij}}{(\mathbf{T}^{-1}\mathbf{M})_i} \quad j, k \in \{K+1, \ldots, 3^D\}. \end{aligned} \tag{4.9}$$

The $n+1$st step of the Newton-Raphson method is

$$\mathbf{m}^{n+1} = \mathbf{m}^n - \mathbf{H}(\mathbf{m}^n)^{-1}\,\nabla\mathcal{S}(\mathbf{m}^n). \tag{4.10}$$

For the initial moments, $\mathbf{m}^0$ we compute the moments of the discretized equilibrium distribution,

$$\mathbf{M}^0 = \mathbf{T}\mathbf{f}^{\mathrm{eq}}.$$

and then take,

$$\mathbf{m}^0 = \langle \mathbf{M}^0_{K+1}, \mathbf{M}^0_{K+1}, ..., \mathbf{M}^0_{3^D} \rangle.$$

Continuing the Newton-Raphson until some convergence criteria is met, and labeling the final distribution $\mathbf{m}^{n_{\mathrm{end}}}$ we construct,

$$\mathbf{M}^{\mathrm{post}} := \langle \rho c_1, \rho c_2, ..., \rho c_K, \mathbf{m}^{n_{\mathrm{end}}} \rangle.$$

and subsequently define the post-collision probability distribution,

$$\mathbf{f}^{\mathrm{post}} = \mathbf{T}^{-1}\mathbf{M}^{\mathrm{post}}$$

This procedure can be summarized by the following algorithm,

1. Calculate pre-collision moments $\mathbf{M}^0 = \mathbf{T}\mathbf{f}^{\mathrm{eq}}$ and constraints $\rho c_1, \rho c_2, ..., \rho c_K$ and calculate $\mathbf{m}^0$.
   (a) Calculate the gradient vector $\nabla\mathcal{S}(\mathbf{m}^n)$ (4.8) and Hessian $\mathbf{H}(\mathbf{m}^n)$ (4.9)
   (b) Perform a Newton-Raphson step, (4.10), for the unconstrained moments, creating $\mathbf{m}^{n+1}$. Construct $\mathbf{M}^{n+1}$.
   (c) Repeat steps (a)-(b) until convergence criteria is met
2. Define the full post-collision moment vector, $\mathbf{M}^{\mathrm{post}} = \mathbf{M}^{\mathrm{end}}$
3. Return to distribution space $\mathbf{f}^{\mathrm{post}} = \mathbf{T}^{-1}\mathbf{M}^{\mathrm{post}}$

Most of the computational overhead of this method involves calculating the Hessian.

4.1.4 Minimization Method: "Iterative Interpolation"

An alternative to the Newton-Raphson is a method we call "Iterative Interpolation" though to our knowledge it has no explicit name. See Figure 4.1. We make no claims about the theoretical properties of the procedure (such as convergence rate, optimal choices of parameters, etc). This is merely a formal description of a possible minimization procedure.

Assume that $q(\mathbf{v})$ is suitably chosen to ensure that the discretized entropy (4.4) is strictly convex in $\mathbf{f}$. Since $\mathcal{H}_{\mathbf{q}}$ is a strictly convex function we know that given $\mathbf{f}$ and $\mathbf{f}'$, and for any $\beta \in (0,1)$,

$$\mathcal{H}_{\mathbf{q}}((1-\beta)\mathbf{f} + \beta\mathbf{f}') < (1-\beta)\mathcal{H}_{\mathbf{q}}(\mathbf{f}) + \beta\mathcal{H}_{\mathbf{q}}(\mathbf{f}'). \tag{4.11}$$

In particular, given a $\mathbf{f}_0$, if we can find a $\mathbf{f}_*$ such that,

$$\mathcal{H}_{\mathbf{q}}(\mathbf{f}_0) = \mathcal{H}_{\mathbf{q}}(\mathbf{f}_*) \quad \forall\beta \in (0,1), \tag{4.12}$$

then (4.11) becomes,