Notes on Local Maximum Entropy Approximation

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This notes is a summary of the Local Maximum Entropy (LME) approximation developed in [1]. The LME scheme has the Gaussian-like function,

$$f_i(\boldsymbol{y}_j) = \exp[-\|\boldsymbol{\beta}_i(\boldsymbol{y}_j - \boldsymbol{x}_i)\|^2 + \boldsymbol{\lambda}_j \cdot (\boldsymbol{y}_j - \boldsymbol{x}_i)] \tag{1}$$

where $\boldsymbol{x}_i$ and $\boldsymbol{y}_j$ are the positions of node i and material point j while $\boldsymbol{\beta}_i$ and $\boldsymbol{\lambda}_j$ are the corresponding parameters. Normalized by the partition function,

$$Z(\boldsymbol{y}_j) = \sum_i f_i(\boldsymbol{y}_j) \tag{2}$$

the shape function has the form,

$$p_i(\boldsymbol{y}_j) = \frac{f_i(\boldsymbol{y}_j)}{Z(\boldsymbol{y}_j)} \tag{3}$$

which is a smooth partition of unity. The parameters $\boldsymbol{\lambda}_j$ are Lagrangian multipliers satisfying the constraints,

$$\boldsymbol{y}_j = \langle \boldsymbol{x} \rangle_j \triangleq \sum_i p_i \boldsymbol{x}_i \tag{4}$$

its values are determined by minimizing the logarithm of partition function

$$\min_{\boldsymbol{\lambda}_j} \ln Z(\boldsymbol{\lambda}_j) \tag{5}$$

since $\mathbf{D} \ln Z \triangleq \frac{\partial \ln Z}{\partial \boldsymbol{\lambda}_j} = \mathbf{0}$ induces the constraints (4). Note that material points locate inside the convex hull with nodes as its vertices because $p_i \in [0, 1]$. Moreover, the Hessian of $\ln Z$, that is,

$$\mathbf{D}^2 \ln Z(\boldsymbol{\lambda}_j) = \langle [\boldsymbol{y}_j - \boldsymbol{x}_i - \langle \boldsymbol{y}_j - \boldsymbol{x}_i \rangle_j]^2 \rangle_j = \langle [\boldsymbol{x}_i - \boldsymbol{y}_j]^2 \rangle_j \geq 0 \tag{6}$$

ensures the unique solution of local minimization. Therefore, the Newton-Raphson method (Alg.1) can be applied to find the solution. It is suitable for the LME approximation because the Hessian matrix is easy to invert (e.g. 3×3 matrix for R^3).

$\boldsymbol{\lambda}_j^0 = \mathbf{0}$;
for $k = 0, 1, ...$ **do**
  $\boldsymbol{\lambda}_j^{k+1} = \boldsymbol{\lambda}_j^k - [\mathbf{D}^2 \ln Z]^{-1}(\boldsymbol{\lambda}_j^k) \cdot \mathbf{D} \ln Z(\boldsymbol{\lambda}_j^k)$;
  if $\|\mathbf{D} \ln Z(\boldsymbol{\lambda}_j^k)\| < \epsilon$ **then**
    return $\boldsymbol{\lambda}_j^k$;
  end
end

Algorithm 1: Newton-Raphson method for $\min_{\boldsymbol{\lambda}_j} \ln Z$

As remarked in [1], we interpret here the parameter $\boldsymbol{\beta}_i$ as the reciprocal primitive vectors at the nodal location $\boldsymbol{x}_i$, that is,

$$\boldsymbol{\beta}_i = 2\pi \boldsymbol{\alpha}_i^{-1} \tag{7}$$

where the column vectors of $\boldsymbol{\alpha}_i$ are the primitive vectors. Thus, $\boldsymbol{G}_i = \boldsymbol{\beta}_i^T \boldsymbol{\beta}_i$ defines a constant metric tensor at the node i. The gradient of shape function becomes,

$$\nabla p_i(\boldsymbol{y}_j) = \frac{\partial p_i}{\partial \boldsymbol{y}_j} = -p_i(\boldsymbol{G}_i + \boldsymbol{G}_i^T + [\mathbf{D}^2 \ln Z]^{-1} \cdot \nabla \mathbf{D} \ln Z)(\boldsymbol{y}_j - \boldsymbol{x}_i) \tag{8}$$

where the term $[\mathbf{D}^2 \ln Z]^{-1} \cdot \nabla \mathbf{D} \ln Z = \nabla \boldsymbol{\lambda}_j$ comes from the fact that $\mathbf{D} \ln Z = \mathbf{0}$. In detail,

$$\nabla \mathbf{D} \ln Z = \frac{\partial^2 \ln Z}{\partial \boldsymbol{\lambda}_j \partial \boldsymbol{y}_j} = -\mathbf{D}^2 \ln Z(\boldsymbol{\lambda}_j)(\boldsymbol{G}_i + \boldsymbol{G}_i^T) + \boldsymbol{I} \tag{9}$$

where $\boldsymbol{I}$ is the identity matrix. Assume a linear transformation of the nodal position defined by

$$\boldsymbol{x}_i^1 = \boldsymbol{\phi}_i(\boldsymbol{x}_i^0) = \boldsymbol{A}_i \boldsymbol{x}_i^0 + \boldsymbol{b}_i \tag{10}$$

where $\boldsymbol{A}_i$ is a non-singular matrix and the symbols 0 and 1 denote the reference configuration and the current configuration respectively. In consideration of the Cauchy-Born rule [2], the reciprocal primitive vectors deform accordingly,

$$\boldsymbol{\beta}_i^1 = \nabla \boldsymbol{\phi}_i(\boldsymbol{x}_i^0) = \boldsymbol{A}_i \boldsymbol{\beta}_i^0 \tag{11}$$

Since the positions of material points are interpolated by those of nodes, in the reference configuration,

$$\boldsymbol{y}_j^0 = \sum_i p_i^0 \boldsymbol{x}_i^0 \tag{12}$$

their new positions carried by the flow $\boldsymbol{\phi}$ are approximated by

$$\boldsymbol{y}_j^1 = \sum_i p_i^0 \boldsymbol{x}_i^1 \tag{13}$$

and the deformation gradient $\boldsymbol{F}_0^1$ is therefore given by

$$\boldsymbol{F}_0^1 \triangleq \nabla \boldsymbol{y}_j^1 = \sum_i \nabla p_i^0 \boldsymbol{x}_i^1 \tag{14}$$

In addition, the reciprocal primitive vectors $\boldsymbol{\beta}_j$ attached to the material point are deformed as well,

$$\boldsymbol{\beta}_j^1 = \boldsymbol{F}_0^1 \boldsymbol{\beta}_j^0 \tag{15}$$

We stress here the affine property (4) of the LME approximation. Assume an affine transformation $\boldsymbol{\phi}_a$,

$$\boldsymbol{x}_i^1 = \boldsymbol{\phi}_a(\boldsymbol{x}_i^0) = \boldsymbol{A}\boldsymbol{x}_i^0 + \boldsymbol{b} \tag{16}$$

Then, the LME approximation preserves the affine transformation,

$$\boldsymbol{y}_j^1 = \boldsymbol{\phi}_a(\boldsymbol{y}_j^0) = \sum_i p_i^0 \boldsymbol{x}_i^1 \tag{17}$$

Therefore the interpolation (13) preserves the homogeneous part of the flow $\boldsymbol{\phi}$ while smooths out its fluctuation part, which is more clear by subtracting (12) and (13). The displacements of material points $\boldsymbol{v}_j = \boldsymbol{y}_j^1 - \boldsymbol{y}_j^0$ and those of nodes $\boldsymbol{u}_i = \boldsymbol{x}_i^1 - \boldsymbol{x}_i^0$ are related by

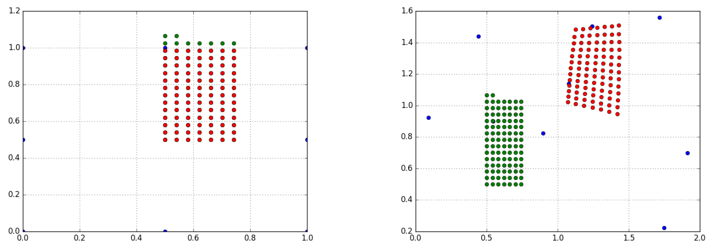
$$\boldsymbol{v}_j = \sum_i p_i^0 \boldsymbol{u}_i \tag{18}$$

If we put a material point at the center of convex hull, i.e., $\boldsymbol{y}^0 = \frac{1}{N}\sum_{i=1}^N \boldsymbol{x}_i^0$, the flow $\boldsymbol{\phi}$ carries the center $\boldsymbol{y}^0$ to the center $\boldsymbol{y}^1$ with pure displacement $\bar{\boldsymbol{v}}$. The material points other than the center fluctuate around the mean displacement $\bar{\boldsymbol{v}}$ and therefore these locations have smooth deformation. Here, we illustrate the properties of LME approximation by the random perturbation of nodes on a two dimensional grid shown in Fig.(1). Moreover, the deformations of reciprocal primitive vectors are illustrated in Fig.(2).

References

[1] Marino Arroyo and Michael Ortiz. Local maximum-entropy approximation schemes: a seamless bridge between finite elements and meshfree methods. *International journal for numerical methods in engineering*, 65(13):2167–2202, 2006.

[2] Morton Gurtin. *Phase transformations and material instabilities in solids.* Elsevier, 2012.



(a) Reference configuration (b) Current configuration

Figure 1: The LME approximation under the random perturbation of nodes. The blue dots are nodes, the green ones are material points at the reference configuration while the red ones are at the current configuration. Material points outside the convex hull of nodes cannot be achieved by the Newton-Raphson minimization.

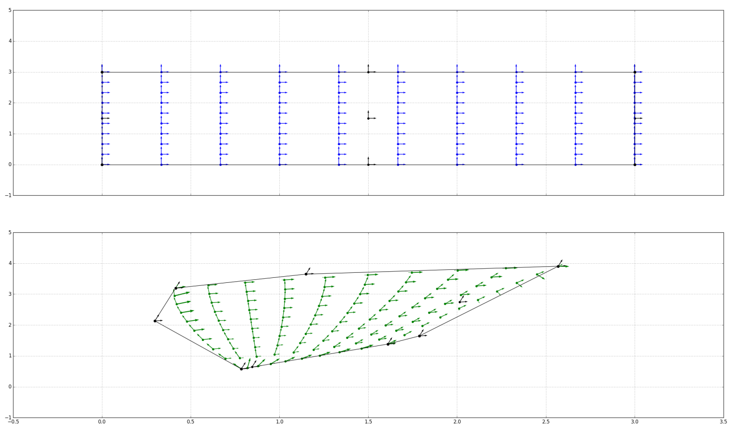


Figure 2: The LME approximation with the Cauchy-Born rule under the random perturbation of nodes. The black dots are nodes attached with its reciprocal primitive vectors, the blue ones are material points at the reference configuration while the green ones are at the current configuration