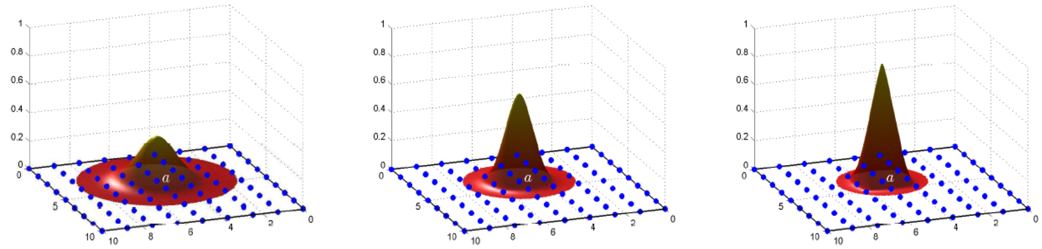
## MAXIMUM-ENTROPY (MAX-ENT) BASIS FUNCTIONS



Maximum-Entropy basis functions are used to construct approximants for partial differential equations. Since construction of max-ent basis functions does not depend on a mesh, they can be employed to formulate meshfree methods. This has led to the *maximum-entropy meshfree (MEM) method*:

- Ortiz A, Puso MA, Sukumar N. Maximum-entropy meshfree method for compressible and near-incompressible elasticity. *Computer Methods in Applied Mechanics and Engineering* 2010; **119**(25-28):1859-1871.

- Ortiz A, Puso MA, Sukumar N. Maximum-entropy meshfree method for incompressible media problems. *Finite Elements in Analysis and Design* 2010; (in press), doi:10.1016/j.finel.2010.12.009.

### WHAT IS MAX-ENT?

The *principle of maximum entropy* (max-ent) was formulated by Jaynes [1] based on the Shannon's principle of entropy [2] as a means for least-biased statistical inference when insufficient information is available. The *principle of maximum entropy* is suitable to find the least-biased probability distribution when there is insufficient data to set it up. In the context of meshfree approximants, the probability distribution represents the set of basis functions associated to a scattered set of nodes in a given domain. Thus, basis functions are viewed as the probability of influence of node ***i*** at coordinate ***x***.

The connection between max-ent basis functions and linear approximation was proposed by Sukumar [3]. In Ref. [3] the principle of maximum entropy was employed to construct linear approximants on arbitrary polygonal domains. In an later work by Arroyo and Ortiz [4], max-ent basis functions were proposed as meshfree approximants with emphasis on establishing a smooth transition between finite element and meshfree methods. In a forthcoming work by Sukumar and Wright [5] generalized the construction of max-ent meshfree basis functions by using the relative (Shannon-Jaynes) entropy functional with a prior [6,8]. In particular, when a Gaussian prior is employed the approach in Ref. [4] is recovered.

In order to compute max-ent basis functions, let us consider a *prior* denoted by $m_i(\mathbf{x})$. The distribution of max-ent basis functions $\phi_i(\mathbf{x})$ is the solution of the following optimization problem (*principle of relative entropy* [8]):

(Eq. 1)

$$\max\left[H(\phi_1,\phi_2,\dots,\phi_n,m_1,m_2,\dots,m_n) = -\sum_{i=1}^{n}\phi_i(\mathbf{x})\log\left(\frac{\phi_i(\mathbf{x})}{m_i(\mathbf{x})}\right)\right]$$

Subject to:

(Eq. 2a)
$\sum_{i=1}^{n} \phi_i(\mathbf{x}) = 1$

(Eq. 2b)
$\sum_{i=1}^{n} \phi_i(\mathbf{x})\mathbf{x}_i = \mathbf{x}$

In Equations (2a) and (2b), $\mathbf{x}^{\mathrm{T}} = [x \; y \; z]$. Applying the procedure of Lagrange multipliers and using the shifted coordinates $\widetilde{\mathbf{x}}_j = \mathbf{x}_j - \mathbf{x}$, the following expression for maximum-entropy basis functions is obtained:

(Eq. 3)
$$\phi_i = \frac{\widetilde{Z}_i}{\sum_{j=1}^{n} \widetilde{Z}_j} = \frac{\widetilde{Z}_i}{\widetilde{Z}}$$

and

(Eq. 4)
$$\widetilde{Z}_j = m_j(\mathbf{x}) e^{-\widetilde{\mathbf{x}}_j^{\mathrm{T}} \lambda(\mathbf{x})}$$

In Equation (4), the set of Lagrange multipliers $\lambda(\mathbf{x})$ is the minimizer of the dual of the optimization problem posed in Equation (1), $\log \widetilde{Z}$, which gives rise to the following system of nonlinear equations:

(Eq. 5)
$$f(\lambda) = \nabla \log \widetilde{Z}(\lambda) = -\sum_i^n \phi_i \widetilde{\mathbf{x}}_i = 0$$

which in three dimensions is given as

(Eq. 6)
$$\begin{aligned} f_1(\lambda) &= -\sum_i^n \phi_i \widetilde{x}_i \\ f_2(\lambda) &= -\sum_i^n \phi_i \widetilde{y}_i \\ f_3(\lambda) &= -\sum_i^n \phi_i \widetilde{z}_i \end{aligned}$$

## WHY MAXENT AS A MESHFREE APPROXIMANT?

Finite elements are constructed with piecewise basis functions that possess Kronecker-delta property. Basis functions that are endowed with the Kronecker-delta property automatically vanish on the boundary. The latter allows the direct imposition of essential boundary conditions on the nodes. However, most meshfree methods are constructed with basis functions that may take on negative values. As a consequence, the Kronecker-delta property is lost and vanishing of basis functions on the boundary is not met. Due to the latter, special techniques need to be employed to enforce essential boundary conditions [7,9]. Maximum-entropy basis functions are obtained from a convex optimization problem and thus they satisfy the non-negative constraint:

(Eq. 7)

$$\phi_i(\mathbf{x}) \geq \ 0 \qquad \forall\ i, \mathbf{x}$$

The convex character renders the following properties to max-ent basis functions [4]: variation diminishing property; positive-definite mass matrices and weak Kronecker-delta property on the boundary. The latter property is noteworthy since it enables the direct imposition of essential boundary conditions as in finite elements.

### ON PRIOR FUNCTIONS

There are several choices for a *prior* function. Three of them are *Gaussian*, *Cubic spline* and *Quartic spline*.

*Gaussian prior:*

(Eq. 8)

$$m_i(\mathbf{x}) = m_i(\tilde{\mathbf{x}}_i) = e^{-\beta_i \|\mathbf{x}_i - \mathbf{x}\|^2} = e^{-\beta_i \|\tilde{\mathbf{x}}_i\|^2}$$

where $\beta_i = \frac{\gamma}{h_i}$ and $\boldsymbol{h_i}$ is a characteristic nodal spacing that may vary for each node ***i***.

*Cubic spline:*

(Eq. 9)

$$m(r_i) = m_i(\tilde{\mathbf{x}}_i) = \begin{cases} \frac{2}{3} - 4r_i^2 + 4r_i^3 & r_i \leq \frac{1}{2} \\ \frac{4}{3} - 4r_i + 4r_i^2 - \frac{4}{3}r_i^3 & \frac{1}{2} < r_i \leq \ 1 \\ 0 & r_i \ \ 1 \end{cases}$$

where $r_i = \frac{\|\mathbf{x}_i - \mathbf{x}\|}{d_i} = \frac{\|\tilde{\mathbf{x}}_i\|}{d_i}$ and $d_i = \gamma\ h_i$ is the radius of the basis function support at node ***i*.**

*Quartic spline:*

(Eq. 10)

$$m(r_i) = m_i(\tilde{\mathbf{x}}_i) = \begin{cases} 1 - 6r_i^2 + 8r_i^3 - 3r_i^4 & 0 \leq \ r_i \leq \ 1 \\ 0 & r_i > \ 1 \end{cases}$$

where $r_i = \frac{\|\mathbf{x}_i - \mathbf{x}\|}{d_i} = \frac{\|\tilde{\mathbf{x}}_i\|}{d_i}$ and $d_i = \gamma\ h_i$ is the radius of the basis function support at node ***i*.**

In Equations (8) to (10), $\gamma$ is a constant dimensionless parameter that controls the support-width of the basis function at node ***i***.

### MAXENT DERIVATIVES

The gradient of max-ent basis functions for any prior is given as

(Eq. 11)

$$\nabla\phi_i = \phi_i \left[ \tilde{\mathbf{x}}_i \cdot (\mathbf{H}^{-1} - \mathbf{H}^{-1} \cdot \mathbf{A}) + \frac{\nabla m_i}{m_i} - \sum_{j=1}^{n} \phi_j \frac{\nabla m_j}{m_j} \right]$$

where

(Eq. 12)

$$\mathbf{A} = \sum_{j=1}^{n} \phi_j \tilde{\mathbf{x}}_j \otimes \frac{\nabla m_j}{m_j}$$

and $\mathbf{H}$ is the hessian matrix defined as

$$\mathbf{H} = \nabla_{\boldsymbol{\lambda}} f = \nabla_{\boldsymbol{\lambda}} \nabla_{\boldsymbol{\lambda}} \ln \tilde{Z} = \sum_{j=1}^{n} \phi_j \tilde{\mathbf{x}}_j \otimes \tilde{\mathbf{x}}_j$$

## REFERENCES


[1] Jaynes ET. Information theory and statistical mechanics. *Physical Review* 1957; **106**(4):620-630.

[2] Shannon CE. A mathematical theory of communication. *The Bell Systems Technical Journal* 1948; **27**(4):379-423.

[3] Sukumar N. Construction of polygonal interpolants: a maximum entropy approach. *International Journal for Numerical Methods in Engineering* 2004; **61**(12):2159-2181.

[4] Arroyo M., Ortiz M. Local maximum-entropy approximation schemes: a seamless bridge between finite elements and meshfree methods. *International Journal for Numerical Methods in Engineering* 2006; **65**(13):2167-2202.

[5] Sukumar N., Wright RW. Overview and construction of meshfree basis functions: From moving least squares to entropy approximants. *International Journal for Numerical Methods in Engineering* 2007; **70**(2):181-205.

[6] Jaynes ET. Probability theory the logic of science. *Cambridge University Press* 2003.

[7] Fernández-Méndez S, Huerta A. Imposing essential boundary conditions in mesh-free methods. *Computer Methods in Applied Mechanics and Engineering* 2004; **193**(12–14):1257–1275.

[8] Shore JE, Johnson RW. Axiomatic derivation of the principle of maximum entropy and the principle of minimum cross-entropy. *IEEE Transactions on Information Theory* 1980; **26**(1):26–36.

[9] Fries TP, Matthies HG. Classification and overview of meshfree methods. *Technical Report Informatikbericht-Nr. 2003-03*, Institute of Scientific Computing, Technical University Braunschweig, Braunschweig, Germany, 2004.