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Maximum Entropy Approximation



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Outline

- Motivation and Objectives
- Meshfree Approximations
- Construction of Polygonal Interpolants
- Principle of Maximum Uncertainty/Entropy
- Numerical Results
- Concluding Remarks



Inputs	Simulator	Output
(Parameters)	(Function)	(Response)
$\mathbf{x} \equiv (x_1, x_2, \dots, x_d)$	$u: \mathbf{R}^d \to \mathbf{R}$	y

Seek
$$u^h$$
 s.t.

$$u^h(\mathbf{x}_i) = y_i$$

- Polynomial interpolants
 Splines
- Kriging
- Radial basis functions



- Geometric Modeling, Computer Graphics, and Visualization
- Finite Element/Meshfree Galerkin Methods
- Numerical Estimation and Prediction
- Design and Analysis of Computer Experiments



Motivation: Data Approximation



- Merits of constructing data approximants via a constrained optimization problem
- Introduce the Maximum Entropy Principle, and to present its derivation and implementation for one-dimensional and polygonal approximation
- The promise and potential of **MAXENT** to solve problems with epistemic (ignorance) uncertainty



Meshfree Approximations

- DEM (Nayroles et al, 1992)
- EFG (Belytschko et al, 1994)
- RKPM (Liu et al, 1994)
- PUM (Babuska and Melenk, 1996)
- Hp-Clouds (Duarte and Oden, 1996)
- MLPG (Atluri et al, 1997)
- BNM (Mukherjee et al, 1997)
- Finite Spheres (De and Bathe, 2000)
- NEM (Braun and Sambridge, 1996)
 NEM [Laplace] (Sukumar et al, 2000)



Construction of Basis Functions

- Finite Elements
- MLS/RBFs (L^2 metric)
- Natural Neighbors
- MAXENT





- Defining a good neighborhood: pattern recognition, clustering, learning theory
- EBCs: Interpolants are desirable
- Numerical integration (Galerkin method)



Voronoi Neighbors





Delaunay Circumcircle and Natural Neighbors



Sibson Interpolant



Laplace Interpolant



Properties

- Non-negative and PU: $0 \le \phi_i \le 1$, $\sum \phi_i(\mathbf{x}) = 1$
- Interpolate data: $\phi_i(\mathbf{x}_j) = \delta_{ij}$
- Linear completeness/precision: $\sum \phi_i \mathbf{x}_i = \mathbf{x}$
- Smoothness: $\phi_i^{\text{LAP}} \in C^0(\Omega), \phi_i^{\text{S}} \in C^1(\Omega \setminus \mathbf{X}_j)$
- Linear essential boundary conditions can be exactly imposed



Surface Interpolation (Sibson)

Courtesy of Sung Park, CS@UCD (zoom)

Bathymetry and topography data (~10,000 points) near NW Australia (Courtesy of Malcolm Sambridge)



Volume Reconstruction (Sibson): Human Head





Construction of Polygonal Interpolants

 Wachspress basis functions (Wachspress, 1975; Warren, ACM, 1996; Meyer et al, JGT, 2002; Dasgupta, JAE, 2003; Malsch, Ph.D. thesis, 2003)

 Mean value coordinates (Floater, CAGD, 2003)



 Laplace shape functions (Sukumar and Tabarraei, IJNME, 2004)



Construction of Polygonal Interpolants (Cont'd)

- Maximum entropy (MAXENT) shape functions (Sukumar, IJNME, 2004)
 - ✓ Imposing linear reproducibility leads to an underdetermined system of linear equations for $\{\phi_i\}$
 - ✓ Use Shannon entropy (Shannon, 1948) and max entropy principle (Jaynes, 1957) to find $\{\phi_i\}$
 - Constrained optimization problem is solved



Wachspress Basis Functions



Mean Value Coordinates



(Floater, CAGD, 2003)



Laplace Shape Functions





Polygonal (Laplace) Basis Function





Principle of Maximum Uncertainty/Entropy

(Shannon,1948; Jaynes,1957)

- Provides the least-biased solution when incomplete/ insufficient information is available
- For a discrete probability distribution $\{p_i\}, i = 1, 2, \dots, n$, with $\sum p_i = 1$, let the average (expected) value of property E^r be known: $\sum p_i E_i^r = \langle E^r \rangle$
- Maximizing the information-entropy $H(p_i) = -\sum_{i=1}^{n} p_i \log p_i$ subject to the constraints leads to the most probable solution (Gibbs-Boltzmann distribution in statistical mechanics)

Principle of Minimum Relative Entropy

(Kullback, 1959)

• Given a prior distribution q, the Kullback-Leibler distance (mutual information) between p and q is

$$D(\mathbf{p} | \mathbf{q}) = \sum_{i=1}^{n} p_i \log \frac{p_i}{q_i}, \quad I(X;Y) = \sum_{x,y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)}$$

- Minimizing the relative-entropy with a uniform prior, $q_i = 1/n$, is equivalent to maximizing Shannon entropy
- Other measures: Renyi and Tsallis entropies



MAXENT at Work!

- Coin toss: $p_1 + p_2 = 1$ and **MAXENT** gives $p_1 = p_2 = 1/2$ \equiv Principle of indifference or insufficient reason
- Wallis provided a combinatorial justification for the choice of the specific form of H(p)
- Suppose a die has been tossed N times and we are told that the <u>average</u> number of spots is 4.5 and not 3.5 (*honest die*). Then, MAXENT gives

$$\{p_1, p_2, \dots, p_6\} = \{0.054, 0.079, 0.114, 0.165, 0.240, 0.347\}$$



MAXENT Applications

- Statistical mechanics and physics
- Communication and natural language modeling
- Image reconstruction and biology (protein folding)
- Economics and urban planning
- Materials science (crystallography/microstructure)
- ... and many more where uncertainty resides



MAXENT in Computational Mechanics

- Elegant and least-biased solution for scattered data approximation by associating shape functions with discrete probability measures
- Broader implications in computational mechanics:
 - o Numerical estimation/prediction
 - o Tailored approximants for meshfree methods
 - o Microstructural design and optimization
 - o III-posed (non-unique) inverse problems
 - o Multiscale modeling



Problem Statement: MAXENT Shape Functions

$$\begin{array}{l}
\operatorname{Max} & H(\phi_i) = -\sum_{i=1}^n \phi_i \log \phi_i \quad \text{s.t.} \\
& \sum_{i=1}^n \phi_i = 1 \\
& \sum_{i=1}^n \phi_i x_i = x \\
& \sum_{i=1}^n \phi_i y_i = y
\end{array}$$

$$\begin{array}{l}
\operatorname{P} & \mathbf{\phi} = \mathbf{p} \\
& (3 \times n) \quad (n \times 1) \quad (3 \times 1) \\
& \text{Constraints}
\end{array}$$

 ϕ_i : `Probability of influence' of node *i* at **x**

i=1



General Solution of $\mathbf{P}\boldsymbol{\varphi} = \mathbf{p}$:

$$\varphi = \mathbf{P}^+ \mathbf{p} + (\mathbf{I} - \mathbf{P}^+ \mathbf{P})\mathbf{c}$$

and if **c** = **0** we obtain the min-norm solution:

$$\phi = \mathbf{P}^+ \mathbf{p}, \quad \mathbf{P}^+ \equiv \text{ Generalized Inverse}$$

which is the solution of $Min(H(\varphi) = ||\varphi||_2)$ *s.t.* $P\varphi = p$ Since $\phi_i < 0$ is possible, $H(\bullet)$ is not suitable

as an uncertainty measure



MLS and Weighted Minimum-Norm Solution

MLS: Min
$$|| \mathbf{W}^{1/2} (\mathbf{P}^T \mathbf{a} - \mathbf{u}) ||_2^2 \Rightarrow \mathbf{A}\mathbf{a} = \mathbf{B}\mathbf{u}$$

 $\mathbf{A} = \mathbf{P}\mathbf{W}\mathbf{P}^T, \ \mathbf{B} = \mathbf{P}\mathbf{W} \quad \mathbf{\phi} = \mathbf{B}^T \mathbf{A}^{-1}\mathbf{p} = \mathbf{W}\mathbf{P}^T \boldsymbol{\gamma}$
dual variables
Primal Problem: Min $(\mathbf{\phi}^T \mathbf{W}^{-1}\mathbf{\phi})$ s.t. $\mathbf{P}\mathbf{\phi} = \mathbf{p}$
Let $\mathbf{\psi} = \mathbf{W}^{-1/2}\mathbf{\phi}, \ \mathbf{Q} = \mathbf{P}\mathbf{W}^{1/2}$, then
 $\min || \mathbf{\psi} ||_2^2$ s.t. $\mathbf{Q}\mathbf{\psi} = \mathbf{p}$
 $\mathbf{\phi} = \mathbf{W}^{1/2}\mathbf{Q}^+\mathbf{p} \ (\mathbf{Q}^+: Matlab \ function \ \mathbf{pinv})$



MAXENT Solution Using Lagrange Multipliers

• First variation of augmented Lagrangian is zero ($\delta L = 0$)

$$\begin{split} L &= -\sum_{i=1}^{n} \phi_{i} \log \phi_{i} + \lambda_{0} \left(1 - \sum_{i} \phi_{i} \right) + \lambda_{1} \left(x - \sum_{i} \phi_{i} x_{i} \right) \\ &+ \lambda_{2} \left(y - \sum_{i} \phi_{i} y_{i} \right) \end{split}$$

$$\delta L = (-1 - \log \phi_i - \lambda_0 - \lambda_1 x_i - \lambda_2 y_i) \delta \phi_i = 0 \quad \forall \, \delta \phi_i$$

and since the variations $\delta \phi_i$ are arbitrary

$$-1 - \log \phi_i - \lambda_0 - \lambda_1 x_i - \lambda_2 y_i = 0$$
 (*i* = 1, 2, ..., *n*)



• Letting $\lambda_0 = \log Z - 1$ (Z is the partition function), we get

$$\log \phi_i + \log Z = -\lambda_1 x_i - \lambda_2 y_i$$

• Since $\sum_i \phi_i = 1$,

$$\phi_i = \frac{e^{-\lambda_1 x_i - \lambda_2 y_i}}{Z}, \quad Z = \sum_{j=1}^n e^{-\lambda_1 x_j - \lambda_2 y_j}$$



• If only one constraint exists ($\lambda_1 = \lambda_2 = 0$), then Z = n

$$\phi_i = \frac{1}{n} \forall i$$
 (nearest-neighbor interpolant)

• In general, λ_1 and λ_2 satisfy two non-linear equations:



Numerical Algorithm for MAXENT Shape Functions

• Let
$$\widetilde{x}_i = x_i - x$$
, $\widetilde{y}_i = y_i - y$. Then,

$$f_1(\lambda_1, \lambda_2) = \frac{\partial(\log \widetilde{Z})}{\partial \lambda_1} = 0 \quad \Leftrightarrow \quad -\frac{\sum_{i=1}^n e^{-\lambda_1 \widetilde{x}_i - \lambda_2 \widetilde{y}_i} \widetilde{x}_i}{\widetilde{Z}} = 0$$

$$f_2(\lambda_1, \lambda_2) = \frac{\partial(\log \widetilde{Z})}{\partial \lambda_2} = 0 \quad \Leftrightarrow \quad -\frac{\sum_{i=1}^n e^{-\lambda_1 \widetilde{x}_i - \lambda_2 \widetilde{y}_i} \widetilde{y}_i}{\widetilde{Z}} = 0$$

• The vector field **f** is the gradient of a scalar potential:

$$F = \log \widetilde{Z}(\lambda_1, \lambda_2), \quad \mathbf{f} = \nabla F$$



Numerical Algorithm (Cont'd)

• Recast the MAXENT formulation as a convex minimizer (dual) problem (Agmon et al., JCP, 1979):

Find
$$(\lambda_1, \lambda_2)$$
 s.t. $F = \log \tilde{Z}(\lambda_1, \lambda_2)$ is minimized

- Initial guess Update $\lambda^0 = \mathbf{0}$ $\lambda_r^{k+1} = \lambda_r^k + \alpha \Delta \lambda_r^k, \quad \Delta \lambda^k = -\nabla F$
- α is determined by the condition that $F(\lambda_1^{k+1}, \lambda_2^{k+1})$ is minimized along the search direction

• Convergence criterion:
$$\left\| \nabla F \right\|^{\{k\}} < 10^{-7}$$



MAXENT Shape Functions in 1D

$$\phi_i = \frac{e^{-\lambda_1 x_i}}{Z}, Z = \sum_{j=1}^3 e^{-\lambda_1 x_j} x_1 = 0, x_2 = 1/2, x_3 = 1$$

$$Z = 1 + e^{-\lambda_1/2} + e^{-\lambda_1}, \ \phi_1 = \frac{1}{Z}, \ \phi_2 = \frac{e^{-\lambda_1/2}}{Z}, \ \phi_3 = \frac{e^{-\lambda_1}}{Z}$$

$$\sum_{i=1}^{3} \phi_i x_i = x: \quad \frac{\eta}{2} + \eta^2 = x(1 + \eta + \eta^2), \quad \eta = e^{-\lambda_1/2}$$

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MAXENT Shape Functions in 1D (Cont'd)



MAXENT Shape Functions in 1D (Cont'd)



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Square: MAXENT Shape Functions



Square (Cont'd)

Since
$$\phi_i = \frac{e^{-\lambda_1 x_i - \lambda_2 y_i}}{Z}$$
, $Z = \sum_{j=1}^n e^{-\lambda_1 x_j - \lambda_2 y_j}$,

we obtain
$$Z^{-1} = (1 - x)(1 - y)$$
 and therefore

$$\phi_1(x, y) = (1 - x)(1 - y), \ \phi_2(x, y) = x(1 - y),$$

$$\phi_3(x, y) = xy, \ \phi_4(x, y) = y(1 - x)$$

which are the same as bilinear finite element shape functions



Square (Cont'd)

MAXENT = Bilinear FE Interpolation



Square: Convergence



 $F = \log \tilde{Z} @ x = (0.56, 0.42)$



Square: Convergence (Cont'd)



 $F = \log Z @ x = (0.9, 0.12)$ $F = \log Z @ x = (0.99, 0.12)$

Use of nonlinear CG leads to faster convergence



Hexagon: Shape Functions



Hexagon: Normalized Entropy



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Mean-value coordinates

Laplace



Bubble (Shape) Function



Contour plot



Mid-Side Node: Shape Function

Mid-Side Node: Maximum Entropy Distribution

Shape Function (MAXENT) Derivatives

$$\frac{\partial \phi_i}{\partial \alpha} = \phi_i \left((x - x_i) \frac{\partial \lambda_1}{\partial \alpha} + (y - y_i) \frac{\partial \lambda_2}{\partial \alpha} \right), \ \alpha = x, y$$

$$\begin{bmatrix} \frac{\partial \lambda_1}{\partial x} & \frac{\partial \lambda_1}{\partial y} \\ \frac{\partial \lambda_2}{\partial x} & \frac{\partial \lambda_2}{\partial y} \end{bmatrix} = -\begin{bmatrix} \langle x^2 \rangle - x^2 & \langle xy \rangle - xy \\ \langle xy \rangle - xy & \langle y^2 \rangle - y^2 \end{bmatrix}^{-1},$$

where

 $\langle f \rangle = \sum_{i=1}^{n} \phi_i f_i$

Galerkin Method (Patch Test)

Shape Function Visualization: JAVA Applet

Mouse-click to insert Right-click to delete

Visualization of Shape Functions

Side Node

Side Node (Cont'd)

Interior Node

Interior Node (Cont'd)

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Related Applications: A. Supervised Learning

(Gupta, Ph.D. thesis, Stanford, 2003)

Objective: Estimation of unknown quantities based on observed samples (numerical estimation), for e.g., pollutants in a city, spam e-mail, speech recognition

Feature Random Vector $X \in \mathbf{R}^d$ relationship Vector $X \in \mathbf{R}^d$ Observation $Y \in \mathbf{R}$ /Classification RV

For $d\uparrow$, the curse of dimensionality!

Given $P_{X,Y}$ and iid data $\{(X_1, Y_1), (X_2, Y_2), \dots, (X_2, Y_2)\}$

A. Supervised Learning (LIME Algorithm)

Distortion function $D : \mathbf{R}^d \times \mathbf{R}^d \to \mathbf{R}^+$ is the mean squared error

$$D(r,s) = \frac{1}{d} \sum_{k=1}^{d} (r_k - s_k)^2$$

Compute weights $w_i(X)$ (partition of unity) by solving

Minimize
$$\left[D\left(\sum_{i=1}^{k} w_{j} X_{j}, X\right) - \alpha H(\mathbf{w}) \right],$$

where α is chosen and k training samples are picked

$$\hat{P}_{Y|X}(g \mid x) = \sum_{i=1}^{k} w_i(x) I_{Y_i(X)=g}$$

B. Local MAXENT Meshfree Method

(Arroyo and Ortiz, 2005)

Minimize
$$\left[\beta U(\mathbf{\phi}) - H(\mathbf{\phi})\right]$$

$$U(\mathbf{\phi}) = \sum_{i=1}^{n} \phi_i || \mathbf{x} - \mathbf{x}_i ||^2 \quad \text{(second-order moment)}$$
$$H(\mathbf{\phi}) = -\sum_{i=1}^{n} \phi_i \log \phi_i \qquad \text{(Shannon entropy)}$$

subject to the three linear reproducing conditions

Presentation by Marino Arroyo forthcoming on Wednesday, July 27, 2005 (USNCCM8)

C. Nodal Refinement

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Concluding Remarks

- Linked the use of the maximum entropy principle to data approximation; use of extremum principles to compute shape functions have well-established roots (Kriging, Delaunay, thin-plate splines, MLS, Laplace)
- Numerical formulation to solve the MAXENT problem in 1D and 2D was described, which readily extends to
 R^d (d ∈ **N**). A JAVA applet to plot meshfree shape functions has been developed
- The use of information-theoretic principles in materials and mechanics computations holds promise

