## University of California, Davis

## 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


## Motivation



Seek $u^{h}$ s.t. $\int \begin{aligned} & \text { Polynomial interpolants }\end{aligned}$

- Splines

$$
u^{h}\left(\mathbf{x}_{i}\right)=y_{i}
$$

- Radial basis functions


## Motivation: Applications

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


## Motivation: Data Approximation



## Objectives

- 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


## ISSUES



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


## Voronoi Neighbors



## Delaunay Circumcircle and Natural Neighbors


p lies outside the circumcircles in green

## Sibson Interpolant



## Laplace Interpolant


(Christ et al, 1982; Belikov et al, 1997; Hiyoshi and Sugihara, 1999)

## Properties

- Non-negative and PU: $0 \leq \phi_{i} \leq 1, \sum_{i} \phi_{i}(\mathbf{x})=1$
- Interpolate data: $\quad \phi_{i}\left(\mathbf{x}_{j}\right)=\delta_{i j}$
- Linear completeness/precision: $\sum_{i} \phi_{i} \mathbf{x}_{i}=\mathbf{x}$
- Smoothness: $\phi_{i}^{\mathrm{LAP}} \in C^{0}(\Omega), \phi_{i}^{\mathrm{S}} \in C^{1}\left(\Omega \backslash \mathbf{x}_{j}\right)$
- Linear essential boundary conditions can be exactly imposed


## Surface Interpolation (Sibson)



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

## Volume Reconstruction (Sibson): Human Head


$256^{3}$

$10^{4} \quad / 5 \times 10^{5}$
(CT scan courtesy of
NC Memorial Hospital)
Courtesy of Sung Park, CS@UCD

## 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)
$\checkmark$ Imposing linear reproducibility leads to an underdetermined system of linear equations for $\left\{\phi_{i}\right\}$
$\checkmark$ Use Shannon entropy (Shannon, 1948) and max entropy principle (Jaynes, 1957) to find $\left\{\phi_{i}\right\}$
$\checkmark$ Constrained optimization problem is solved


## Wachspress Basis Functions


(Meyer et al., JGT, 2002)

$$
\phi_{i}(\mathbf{x})=\frac{w_{i}(\mathbf{x})}{\sum_{j=1}^{n} w_{j}(\mathbf{x})}, \quad w_{i}(\mathbf{x})=\frac{\cot \gamma_{i}+\cot \delta_{i}}{\left\|\mathbf{x}-\mathbf{x}_{i}\right\|^{2}}
$$

## Mean Value Coordinates


(Floater, CAGD, 2003)

$$
\phi_{i}(\mathbf{x})=\frac{w_{i}(\mathbf{x})}{\sum_{j=1}^{n} w_{j}(\mathbf{x})}, w_{i}(\mathbf{x})=\frac{\tan \left(\alpha_{i-1} / 2\right)+\tan \left(\alpha_{i} / 2\right)}{\left\|\mathbf{x}-\mathbf{x}_{i}\right\|}
$$

## Laplace Shape Functions



## Polygon Interpolant Using Affine Mapping

Laplace Shape Function


## 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 $\left\{p_{i}\right\}, i=1,2, \cdots, n$, with $\sum p_{i}=1$, let the average (expected) value of property $E^{r}$ be known: $\sum_{i} p_{i} E_{i}^{r}=<E^{r}>$
- Maximizing the information-entropy $H\left(p_{i}\right)=-\sum_{i=1}^{n} p_{i} \log p_{i}$ 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 $\mathbf{q}$, the Kullback-Leibler distance (mutual information) between $\mathbf{p}$ and $\mathbf{q}$ is

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

- 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 $\mathrm{H}(\mathbf{p})$
- Suppose a die has been tossed $N$ times and we are told that the average number of spots is 4.5 and not 3.5 (honest die). Then, MAXENT gives

$$
\begin{aligned}
\left\{p_{1}, p_{2}, \ldots, p_{6}\right\}= & \{0.054,0.079,0.114, \\
& 0.165,0.240,0.347\}
\end{aligned}
$$

## 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 Ill-posed (non-unique) inverse problems
o Multiscale modeling


## Problem Statement: MAXENT Shape Functions

$$
\left.\begin{array}{c}
\underset{\boldsymbol{\varphi}}{\operatorname{Max}} H\left(\phi_{i}\right)=-\sum_{i=1}^{n} \phi_{i} \log \phi_{i} \quad \text { s.t. } \\
\sum_{i=1}^{n} \phi_{i}=1 \\
\sum_{i=1}^{n} \phi_{i} x_{i}=x \\
\sum_{i=1}^{n} \phi_{i} y_{i}=y
\end{array}\right\} \underset{(3 \times n)}{\mathbf{P}} \underset{(n \times 1)}{\boldsymbol{\varphi}}=\underset{(3 \times 1)}{\mathbf{p}}
$$

$\phi_{i}$ : 'Probability of influence' of node $i$ at $\mathbf{x}$

## Minimum Norm Solution

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

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

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

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

which is the solution of $\operatorname{Min}\left(H(\boldsymbol{\varphi})=\|\boldsymbol{\varphi}\|_{2}\right)$
s.t. $\mathbf{P} \varphi=\mathbf{p}$

Since $\phi_{i}<0$ is possible, $H(\bullet)$ is not suitable as an uncertainty measure

## MLS and Weighted Minimum-Norm Solution

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

$$
\mathbf{A}=\mathbf{P W P}^{\mathrm{T}}, \mathbf{B}=\mathbf{P W} \underset{\text { dual variables }}{\underset{\boldsymbol{q}}{ }} \underset{\mathbf{B}^{T}}{\boldsymbol{\varphi}=\mathbf{B}^{T} \mathbf{A}^{-1} \mathbf{p}=\mathbf{W} \mathbf{P}^{T} \boldsymbol{\gamma}}
$$

Primal Problem: $\operatorname{Min}\left(\boldsymbol{\varphi}^{T} \mathbf{W}^{-1} \boldsymbol{\varphi}\right)$ s.t. $\mathbf{P} \boldsymbol{\varphi}=\mathbf{p}$

$$
\begin{array}{ll}
\text { Let } & \boldsymbol{\psi}=\mathbf{W}^{-1 / 2} \boldsymbol{\varphi}, \mathbf{Q}=\mathbf{P} \mathbf{W}^{1 / 2} \text {, then } \\
& \operatorname{Min}\|\boldsymbol{\psi}\|_{2}^{2} \text { s.t. } \mathbf{Q} \boldsymbol{\psi}=\mathbf{p}
\end{array}
$$

$$
\boldsymbol{\varphi}=\mathbf{W}^{1 / 2} \mathbf{Q}^{+} \mathbf{p}\left(\mathbf{Q}^{+}: \text {Matlab function pinv }\right)
$$

## MAXENT Solution Using Lagrange Multipliers

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

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

$$
\delta L=\left(-1-\log \phi_{i}-\lambda_{0}-\lambda_{1} x_{i}-\lambda_{2} y_{i}\right) \delta \phi_{i}=0 \quad \forall \delta \phi_{i}
$$

and since the variations $\delta \phi_{i}$ are arbitrary

$$
-1-\log \phi_{i}-\lambda_{0}-\lambda_{1} x_{i}-\lambda_{2} y_{i}=0(i=1,2, \ldots, n)
$$

## MAXENT Solution (Cont'd)

- 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 $\sum_{i} \phi_{i}=1$,

$$
\phi_{i}=\frac{e^{-\lambda_{1} x_{i}-\lambda_{2} y_{i}}}{Z}, Z=\sum_{j=1}^{n} e^{-\lambda_{1} x_{j}-\lambda_{2} y_{j}}
$$

## MAXENT Solution (Cont'd)

- If only one constraint exists ( $\lambda_{1}=\lambda_{2}=0$ ), then $Z=n$

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

- In general, $\lambda_{1}$ and $\lambda_{2}$ satisfy two non-linear equations:

$$
\begin{array}{r}
-\frac{\partial(\log Z)}{\partial \lambda_{1}}=x \Leftrightarrow \frac{\sum_{i=1} e^{-\lambda_{1} x_{i}-\lambda_{2} y_{i}} x_{i}}{Z}-x=0 \\
-\frac{\partial(\log Z)}{\partial \lambda_{2}}=y \Leftrightarrow \frac{\sum_{i=1}^{n} e^{-\lambda_{1} x_{i}-\lambda_{2} y_{i}} y_{i}}{Z}-y=0
\end{array}
$$

## Numerical Algorithm for MAXENT Shape Functions

- Let $\tilde{x}_{i}=x_{i}-x, \tilde{y}_{i}=y_{i}-y$. Then,

$$
\begin{aligned}
& f_{1}\left(\lambda_{1}, \lambda_{2}\right)=\frac{\partial(\log \tilde{Z})}{\partial \lambda_{1}}=0 \Leftrightarrow-\frac{\sum_{i=1}^{n} e^{-\lambda_{1} \tilde{x}_{i}-\lambda_{2} \tilde{y}_{i} \tilde{x}_{i}}}{\tilde{Z}}=0 \\
& f_{2}\left(\lambda_{1}, \lambda_{2}\right)=\frac{\partial(\log \tilde{Z})}{\partial \lambda_{2}}=0 \Leftrightarrow-\frac{\sum_{i=1}^{n} e^{-\lambda_{1} \tilde{x}_{i}-\lambda_{2} \tilde{y}_{i} \tilde{y}_{i}}}{\tilde{Z}}=0
\end{aligned}
$$

- The vector field $\mathbf{f}$ is the gradient of a scalar potential:

$$
F=\log \tilde{Z}\left(\lambda_{1}, \lambda_{2}\right), \quad \mathbf{f}=\nabla F
$$

## Numerical Algorithm (Cont'd)

- Recast the MAXENT formulation as a convex minimizer (dual) problem (Agmon et al., JCP, 1979):
Find $\left(\lambda_{1}, \lambda_{2}\right)$ s.t. $F=\log \tilde{Z}\left(\lambda_{1}, \lambda_{2}\right)$ is minimized
- Initial guess

$$
\lambda^{0}=\mathbf{0}
$$

$$
\lambda_{r}^{k+1}=\lambda_{r}^{k}+\alpha \Delta \lambda_{r}^{k}, \quad \Delta \lambda^{k}=-\nabla F
$$

- $\alpha$ is determined by the condition that $F\left(\lambda_{1}^{k+1}, \lambda_{2}^{k+1}\right)$ is minimized along the search direction
- Convergence criterion: $\|\nabla F\|^{\{k\}}<10^{-7}$


## MAXENT Shape Functions in 1D

$$
\begin{aligned}
& 1(0,0) \\
& \phi_{i}=\frac{e^{-\lambda_{1} x_{i}}}{Z}, Z=\sum_{j=1}^{3} e^{-\lambda_{1} x_{j}} x_{1 / 2,0)}^{3(1,0)}, 0, x_{2}=1 / 2, x_{3}=1 \\
& Z=1+e^{-\lambda_{1} / 2}+e^{-\lambda_{1}}, \phi_{1}=\frac{1}{Z}, \phi_{2}=\frac{e^{-\lambda_{1} / 2}}{Z}, \phi_{3}=\frac{e^{-\lambda_{1}}}{Z} \\
& \sum_{i=1}^{3} \phi_{i} x_{i}=x: \frac{\eta}{2}+\eta^{2}=x\left(1+\eta+\eta^{2}\right), \eta=e^{-\lambda_{1} / 2}
\end{aligned}
$$

## MAXENT Shape Functions in 1D (Cont'd)



## MAXENT Shape Functions in 1D (Cont'd)




$$
\mathrm{n}=11
$$

$$
\mathrm{n}=6
$$

## Square: MAXENT Shape Functions

$$
\begin{aligned}
& Z=\sum_{j=1}^{4} e^{-\lambda_{1} x_{j}-\lambda_{2} y_{j}} \\
&=1+e^{-\lambda_{1}}+e^{-\lambda_{2}}+e^{-\lambda_{1}-\lambda_{2}} \\
& \frac{e^{-\lambda_{1}}+e^{-\lambda_{1}-\lambda_{2}}}{Z}=x \\
& \\
& \frac{e^{-\lambda_{2}}+e^{-\lambda_{1}-\lambda_{2}}}{Z}=y
\end{aligned}
$$

which simplifies to

$$
\frac{e^{-\lambda_{1}}}{1+e^{-\lambda_{1}}}=x, \frac{e^{-\lambda_{2}}}{1+e^{-\lambda_{2}}}=y \Rightarrow e^{-\lambda_{1}}=\frac{x}{1-x}, e^{-\lambda_{2}}=\frac{y}{1-y}
$$

## 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

$$
\begin{gathered}
\phi_{1}(x, y)=(1-x)(1-y), \phi_{2}(x, y)=x(1-y), \\
\phi_{3}(x, y)=x y, \phi_{4}(x, y)=y(1-x)
\end{gathered}
$$

which are the same as bilinear finite element shape functions

## Square (Cont'd)

## MAXENT $\equiv$ Bilinear FE Interpolation



Shape Function


## Square: Convergence



## Square: Convergence (Cont'd)



## Hexagon: Shape Functions



Mean-Value Coordinates


## Hexagon: Normalized Entropy



## Bubble (Shape) Function



Contour plot


3D

## Mid-Side Node: Shape Function



Five-node element


Shape function of node a

## Mid-Side Node: Maximum Entropy Distribution



## Shape Function (MAXENT) Derivatives

$$
\frac{\partial \phi_{i}}{\partial \alpha}=\phi_{i}\left(\left(x-x_{i}\right) \frac{\partial \lambda_{1}}{\partial \alpha}+\left(y-y_{i}\right) \frac{\partial \lambda_{2}}{\partial \alpha}\right), \alpha=x, y
$$

$$
\left[\begin{array}{cc}
\frac{\partial \lambda_{1}}{\partial x} & \frac{\partial \lambda_{1}}{\partial y} \\
\frac{\partial \lambda_{2}}{\partial x} & \frac{\partial \lambda_{2}}{\partial y}
\end{array}\right]=-\left[\begin{array}{cc}
<x^{2}>-x^{2} & <x y>-x y \\
<x y>-x y & <y^{2}>-y^{2}
\end{array}\right]^{-1},
$$

where $\quad\langle f\rangle=\sum_{i=1}^{n} \phi_{i} f_{i}$

## Galerkin Method (Patch Test)



Error norms: $\frac{\left\|u-u^{h}\right\|_{2}}{\|u\|_{2}} \approx 10^{-8}, \frac{\left\|u-u^{h}\right\|_{E}}{\|u\|_{E}} \approx 10^{-7}$

## Shape Function Visualization: JAVA Applet


Shape Function / Plot
Set a node:




## JAVA Applet (Cont'd)



Auto nodes:

| E) Poly | Rand |
| :--- | :--- | :--- |
| Dromomen $=$ moula. |  |

## JAVA Applet (Cont'd)



## JAVA Applet (Cont'd)



## JAVA Applet (Cont'd)



Mouse-click to insert
Right-click to delete
Set a node:

| $2:(0.5,0.8)$ |  |  |
| :---: | :---: | :---: |

Set a node:
乡 2: (D, 5, D, 时)

## JAVA Applet (Cont'd)



## Visualization of Shape Functions



## Side Node



## Side Node (Cont'd)



3D Plot

## Interior Node



## Interior Node (Cont'd)



## 3D Plot

## 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 $\xrightarrow{\text { relationship }}$ Observation $Y \in \mathbf{R}$ Vector $X \in \mathbf{R}^{d} \longleftrightarrow$ /Classification RV

For $d \uparrow$, the curse of dimensionality!
Given $P_{X, Y}$ and iid data $\left\{\left(X_{1}, Y_{1}\right),\left(X_{2}, Y_{2}\right), \ldots,\left(X_{2}, Y_{2}\right)\right\}$

$$
\text { ESTIMATE } P_{Y \mid X}
$$

## A. Supervised Learning (LIME Algorithm)

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

$$
D(r, s)=\frac{1}{d} \sum_{k=1}^{d}\left(r_{k}-s_{k}\right)^{2}
$$

Compute weights $w_{i}(X)$ (partition of unity) by solving

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

where $\alpha$ is chosen and $k$ training samples are picked

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

## B. Local MAXENT Meshfree Method

## (Arroyo and Ortiz, 2005)

## Minimize $[\beta \mathrm{U}(\boldsymbol{\varphi})-H(\boldsymbol{\varphi})]$

$\mathrm{U}(\boldsymbol{\varphi})=\sum_{i=1}^{n} \phi_{i}\left\|\mathbf{x}-\mathbf{x}_{i}\right\|^{2} \quad$ (second-order moment)
$H(\varphi)=-\sum_{i=1}^{n} \phi_{i} \log \phi_{i} \quad$ (Shannon entropy)
subject to the three linear reproducing conditions
Presentation by Marino Arroyo forthcoming on Wednesday, July 27, 2005 (USNCCM8)

## C. Nodal Refinement



## 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 $\mathbf{R}^{d}(d \in \mathbf{N})$. A JAVA applet to plot meshfree shape functions has been developed
- The use of information-theoretic principles in materials and mechanics computations holds promise

