University of California, Davis

Barycentric Finite Element Methods

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UC Davis

Workshop on Generalized Barycentric Coordinates, Columbia University

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Collaborators and Acknowledgements

- **Collaborators**
  - **Alireza Tabarraei** (UNC, Charlotte)
  - **Seyed Mousavi** (University of Texas, Austin)
  - **Kai Hormann** (University of Lugano)

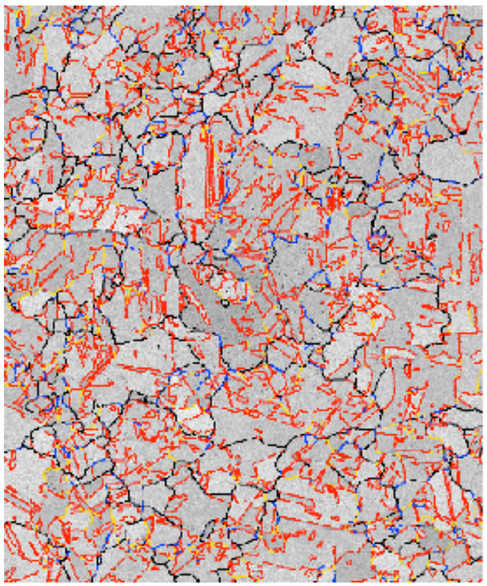
- Research support of the **NSF** is acknowledged

Outline

- Motivation: Why Polygons in Computations?
- Weak and Variational Forms of Boundary-Value Problems
- Conforming Barycentric Finite Elements
- Maximum-Entropy Basis Functions
- Summary and Outlook

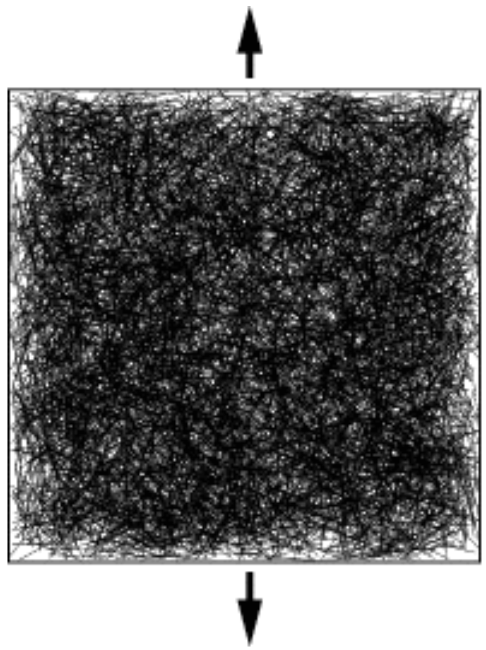
Motivation: Voronoi Tesellations in Mechanics

Polycrystalline alloy



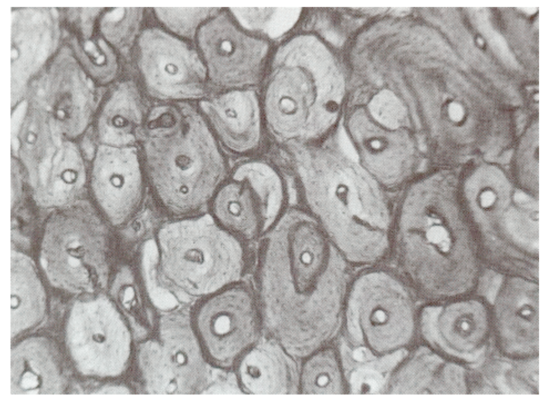
(Courtesy of Kumar, LLNL)

Fiber-matrix composite



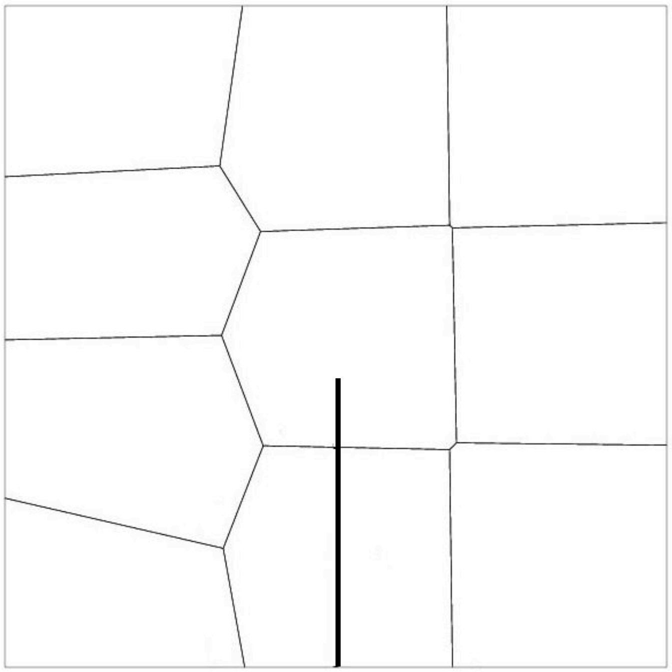
(Bolander and S, PRB, 2004)

Osteonal bone

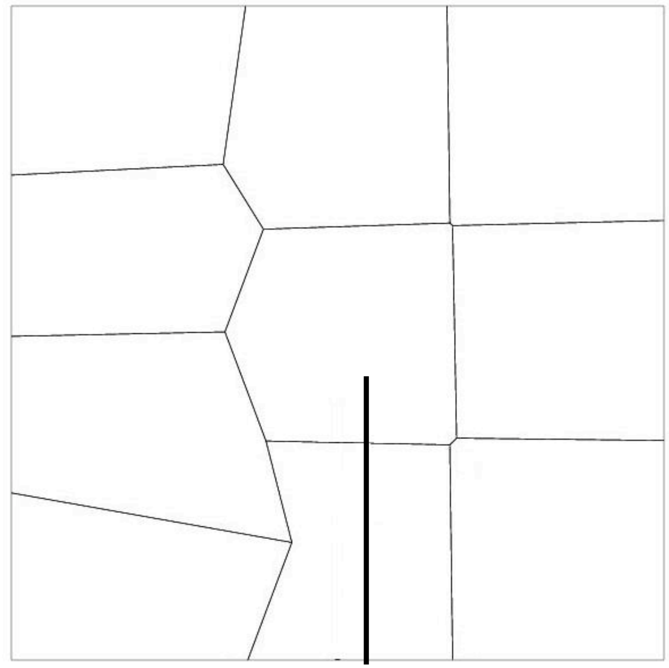


(Martin and Burr, 1989)

Motivation: Flexibility in Meshing & Fracture Modeling

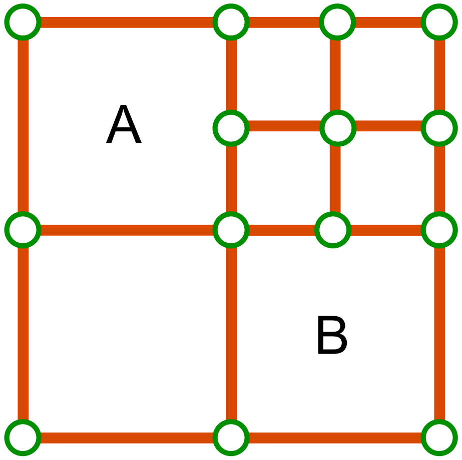


Convex Mesh

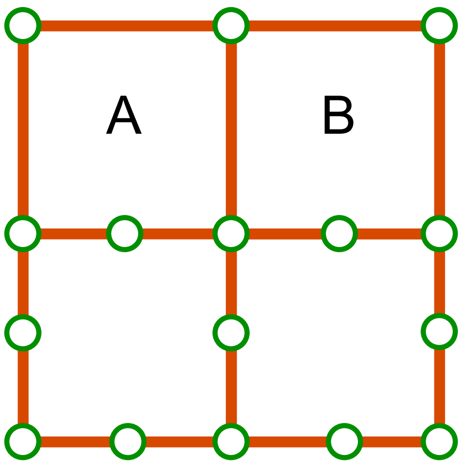


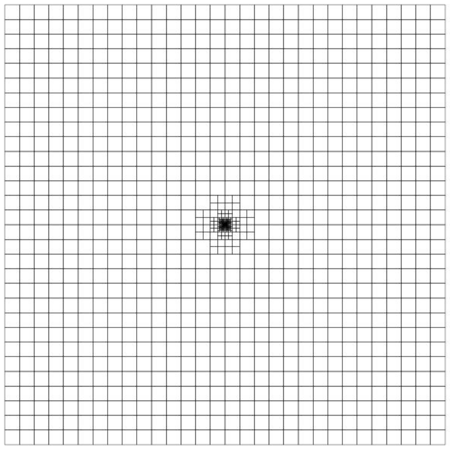
Nonconvex Mesh

Motivation: Transition Elements, Quadtree Meshes

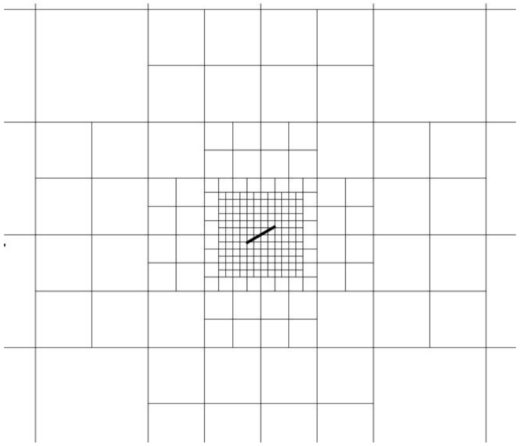


Transition elements





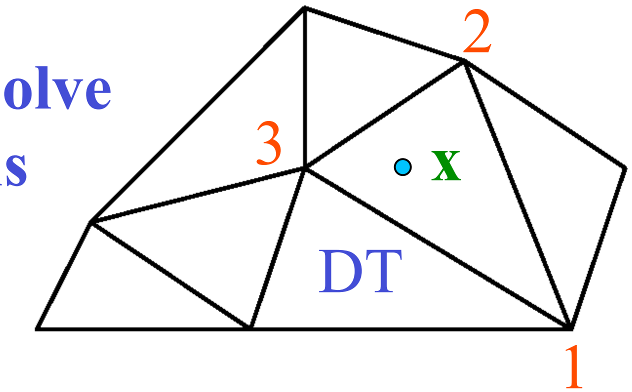
Quadtree



Zoom

Galerkin Finite Element Method (FEM)

FEM: **Function-based method to solve partial differential equations**



steady-state heat conduction, diffusion, or electrostatics

Strong Form: $-\nabla^2 u = f \text{ in } \Omega, \; \underline{u = \bar{u} \text{ on } \partial\Omega}$

Variational Form:

$$u^* = \operatorname*{argmin}_u \left[\pi[u] = \int_\Omega \left(\frac{\nabla u \cdot \nabla u}{2} - f u \right) d\Omega \right]$$

Galerkin FEM (Cont'd)

Variational Form

$$\delta \pi[u] = \delta \int_{\Omega} \left(\frac{\nabla u \cdot \nabla u}{2} - f u \right) d\Omega = 0$$

$$\int_{\Omega} \nabla \delta u \cdot \nabla u \, d\Omega - \int_{\Omega} f \delta u \, d\Omega = 0 \;\; \forall \delta u \in H_0^1(\Omega)$$

δu **must vanish on the boundary**

Finite-dimensional approximations for trial function and admissible variations

$$u^h(\boldsymbol{x}) = \sum_{b=1}^{N} \phi_b(\boldsymbol{x}) u_b, \;\; \delta u^h(\boldsymbol{x}) = \phi_a(\boldsymbol{x})$$

Galerkin FEM (Cont'd)

Discrete Weak Form and Linear System of Equations

$$\int_{\Omega} \nabla \delta u^h \cdot \nabla u^h \, d\Omega = \int_{\Omega} f \delta u^h \, d\Omega$$

$$\sum_{b=1}^{N} \left(\int_{\Omega} \nabla \phi_a \cdot \nabla \phi_b \, d\Omega \right) u_b = \int_{\Omega} f \phi_a \, d\Omega$$

$$\boldsymbol{K}\boldsymbol{d} = \boldsymbol{f}$$

$$K_{ab} = \int_{\Omega} \nabla \phi_a \cdot \nabla \phi_b \, d\Omega, \quad f_a = \int_{\Omega} f \phi_a \, d\Omega$$

Biharmonic Equation

Strong Form

$$\nabla^4 u = u_{,iijj} = f \text{ in } \Omega$$

$$\text{BCs: } u = \bar{u} \text{ and } \partial u / \partial n = 0 \text{ on } \partial\Omega$$

Variational (Weak) Form

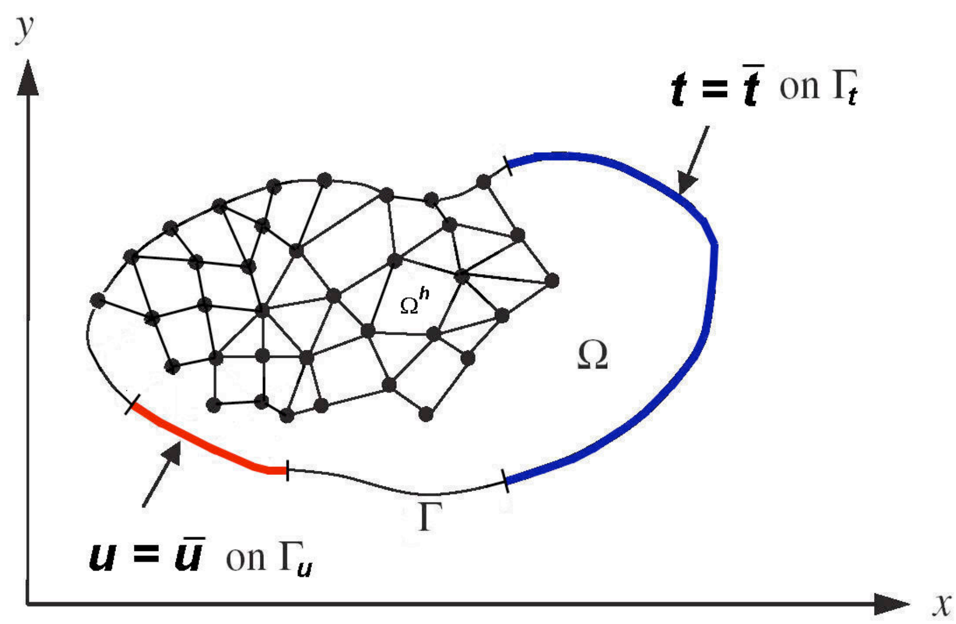
$$\text{Find } u \in S \text{ such that}$$

$$\int_\Omega \nabla^2 u \nabla^2 w \, d\Omega = \int_\Omega f w \, d\Omega \quad \forall w \in V$$

$$S = \{u : u \in H^2(\Omega), \; u = \bar{u} \text{ on } \partial\Omega, \; \partial u/\partial n = 0 \text{ on } \partial\Omega\}$$

$$V = \{w : w \in H^2(\Omega), \; w = 0 \text{ on } \partial\Omega, \; \partial w/\partial n = 0 \text{ on } \partial\Omega\}$$

Elastostatic BVP: Strong Form



$$\nabla \cdot \boldsymbol{\sigma} = 0 \text{ in } \Omega$$
$$\boldsymbol{\sigma} = \mathrm{C}:\boldsymbol{\varepsilon}$$
$$\boldsymbol{\varepsilon} = \nabla_s \mathbf{u}$$

BCs $\begin{cases} \mathbf{u} = \bar{\mathbf{u}} \text{ on } \Gamma_u \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}} \text{ on } \Gamma_t \end{cases}$

Elastostatic BVP: Weak Form/PVW

$$\boxed{\int_\Omega \delta\varepsilon_{ij}\sigma_{ij}\, d\Omega - \int_{\Gamma_t} \delta u_i \bar{t}_i\, d\Gamma = 0 \quad \forall\, \delta u_i \in \mathbb{H}^1_0(\Omega)}$$

Kinematic relation

$$\boldsymbol{\varepsilon} = \boldsymbol{\nabla}_s \mathbf{u}$$

Constitutive relation

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}$$

Approximation for trial function and admissible variations

$$\mathbf{u}^h(\mathbf{x}) = \textstyle\sum_b \phi_b(\mathbf{x})\mathbf{u}_b$$

$$\delta\mathbf{u}^h(\mathbf{x}) = \textstyle\sum_a \phi_a(\mathbf{x})\delta\mathbf{u}_b \quad \longrightarrow \quad \mathbf{Kd} = \mathbf{f}$$

basis function

Elastostatic BVP: Discrete Weak Form

$$\mathbf{K}\mathbf{d} = \mathbf{f}$$

$$\mathbf{K}_{ab} = \int_{\Omega} \mathbf{B}_a^{\mathrm{T}} \mathbf{C} \mathbf{B}_b \, d\Omega \,, \quad \mathbf{f}_a = \int_{\Gamma_t} \phi_a \bar{\mathbf{t}} \, d\Gamma$$

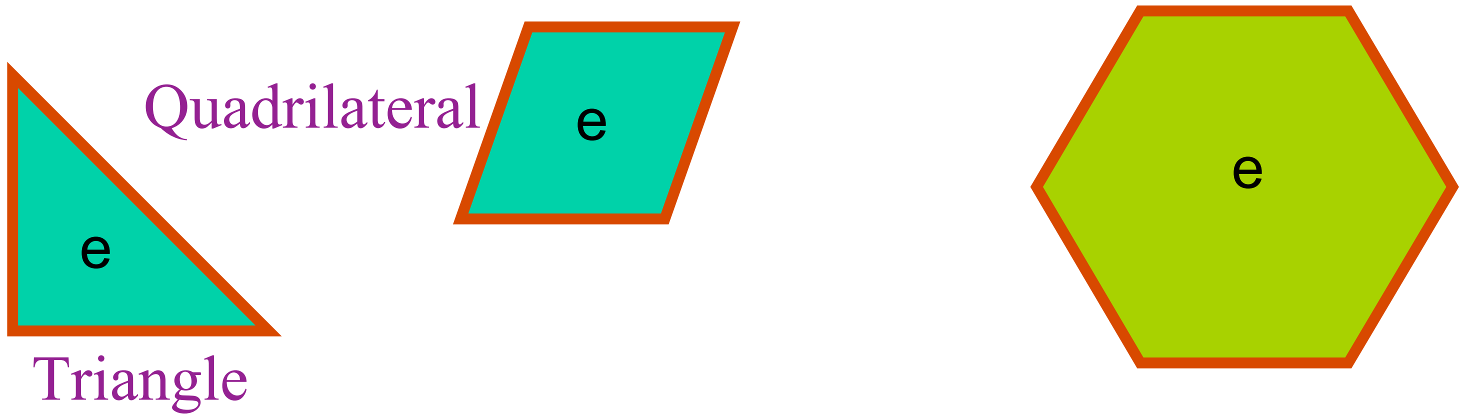
$$\mathbf{B}_a(\mathbf{x}) = \begin{bmatrix} \phi_{a,x} & 0 \\ 0 & \phi_{a,y} \\ \phi_{a,y} & \phi_{a,x} \end{bmatrix}$$

$\mathbf{C} =$ Material moduli matrix

Finite Element versus Polygonal Approximations

Data Approximation

Finite Element　　　　Polygonal Element

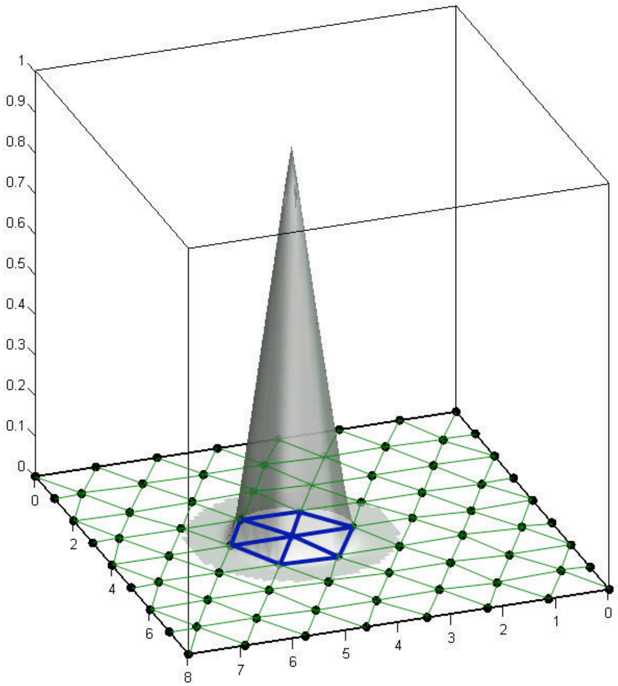


$$\boldsymbol{u}_e^h(\boldsymbol{x}) = \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \boldsymbol{u}_a$$

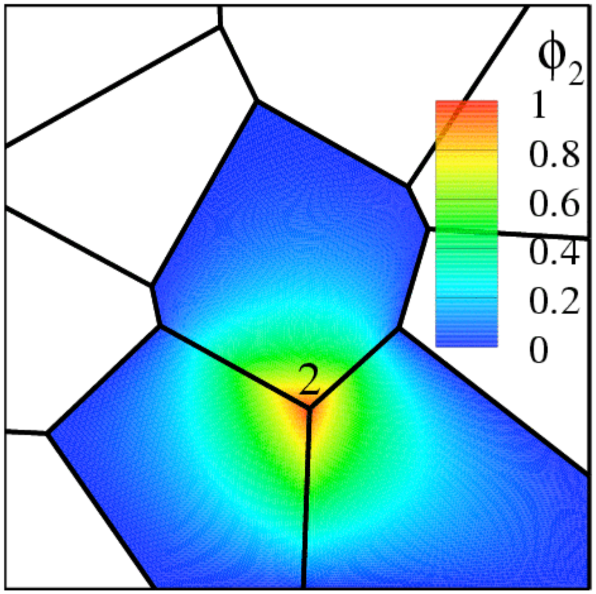
`shape' function

Three-Node FE versus Polygonal FE (Cont'd)

FEM (3-node)



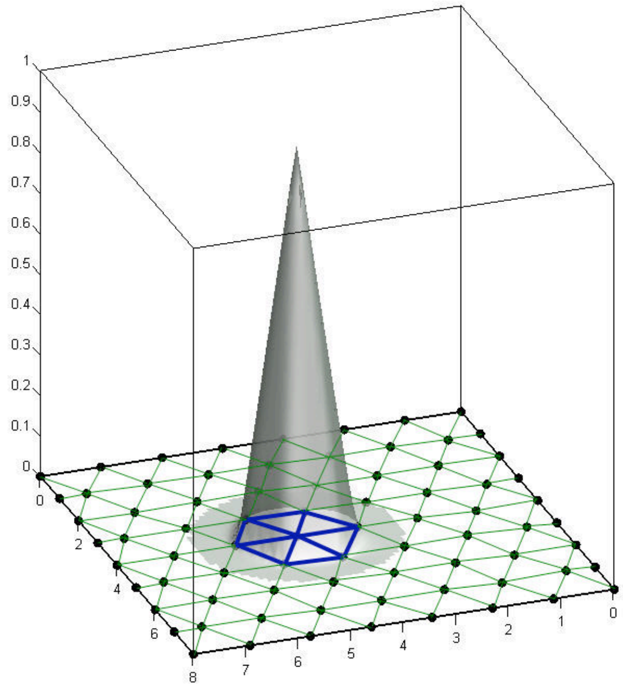
Polygonal



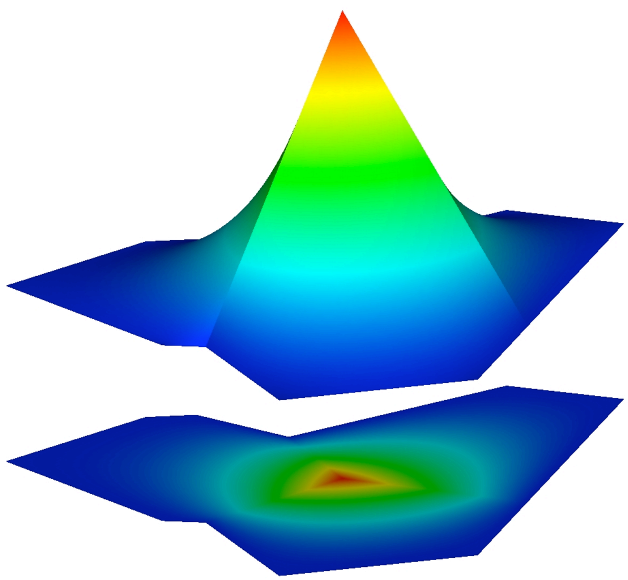
$$\mathbf{K}_{ab} = \int_\Omega \mathbf{B}_a^{\mathrm{T}} \mathbf{C} \mathbf{B}_b \, d\Omega \qquad \mathbf{B}_a = \begin{bmatrix} \phi_{a,x} & 0 \\ 0 & \phi_{a,y} \\ \phi_{a,y} & \phi_{a,x} \end{bmatrix} \qquad a = 1, 2, \ldots, n$$

Three-Node FE versus Polygonal FE (Cont'd)

FEM (3-node)



Polygonal



$$\mathbf{K}_{ab} = \int_\Omega \mathbf{B}_a^{\mathrm{T}} \mathbf{C} \mathbf{B}_b d\Omega \qquad \mathbf{B}_a = \begin{bmatrix} \phi_{a,x} & 0 \\ 0 & \phi_{a,y} \\ \phi_{a,y} & \phi_{a,x} \end{bmatrix} \qquad a = 1, 2, \ldots, n$$

Three-Node FE versus Polygonal FE (Cont'd)

Assembly

FEM

$$\boldsymbol{K}_e = \int_{\Omega_e} \boldsymbol{B}^T \boldsymbol{C} \boldsymbol{B} \, d\Omega$$

$$\mathbf{B} = \begin{bmatrix} N_{1,x} & 0 & N_{2,x} & 0 & N_{3,x} & 0 \\ 0 & N_{1,y} & 0 & N_{2,y} & 0 & N_{3,y} \\ N_{1,y} & N_{1,x} & N_{2,y} & N_{2,x} & N_{3,y} & N_{3,x} \end{bmatrix}$$

$$n = 3$$

Polygonal

$$\boldsymbol{K}_e = \int_{\Omega_e} \boldsymbol{B}^T \boldsymbol{C} \boldsymbol{B} \, d\Omega$$

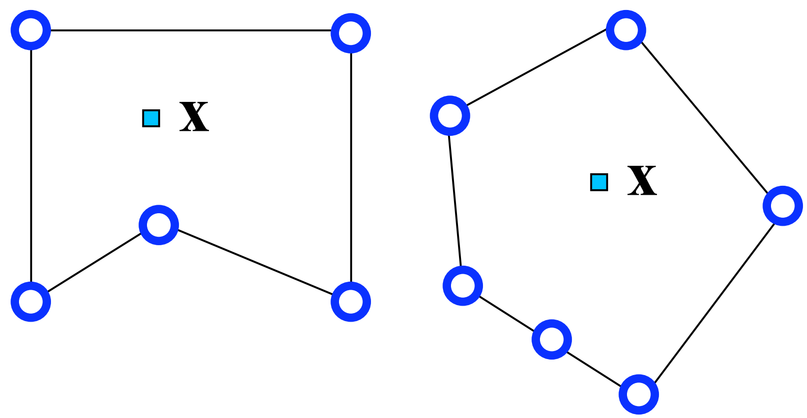
$$\mathbf{B} = \begin{bmatrix} \phi_{1,x} & 0 & \phi_{2,x} & 0 & \cdots & \phi_{n,x} & 0 \\ 0 & \phi_{1,y} & 0 & \phi_{2,y} & \cdots & 0 & \phi_{n,y} \\ \phi_{1,y} & \phi_{1,x} & \phi_{2,y} & \phi_{2,x} & \cdots & \phi_{n,y} & \phi_{n,x} \end{bmatrix}$$

$$n \geq 3$$

Barycentric Coordinates on Polygons

- Wachspress basis functions **(Wachspress, 1975; Meyer et al., 2002; Malsch and Dasgupta, 2004)**

- Mean value coordinates **(Floater, 2003; Floater and Hormann, 2006)**



- Laplace and maximum-entropy basis functions **(S, 2004; S and Tabarraei, 2004)**

Properties of Barycentric Coordinates

- Non-negative

$$\phi_a(\boldsymbol{x}) \geq 0$$

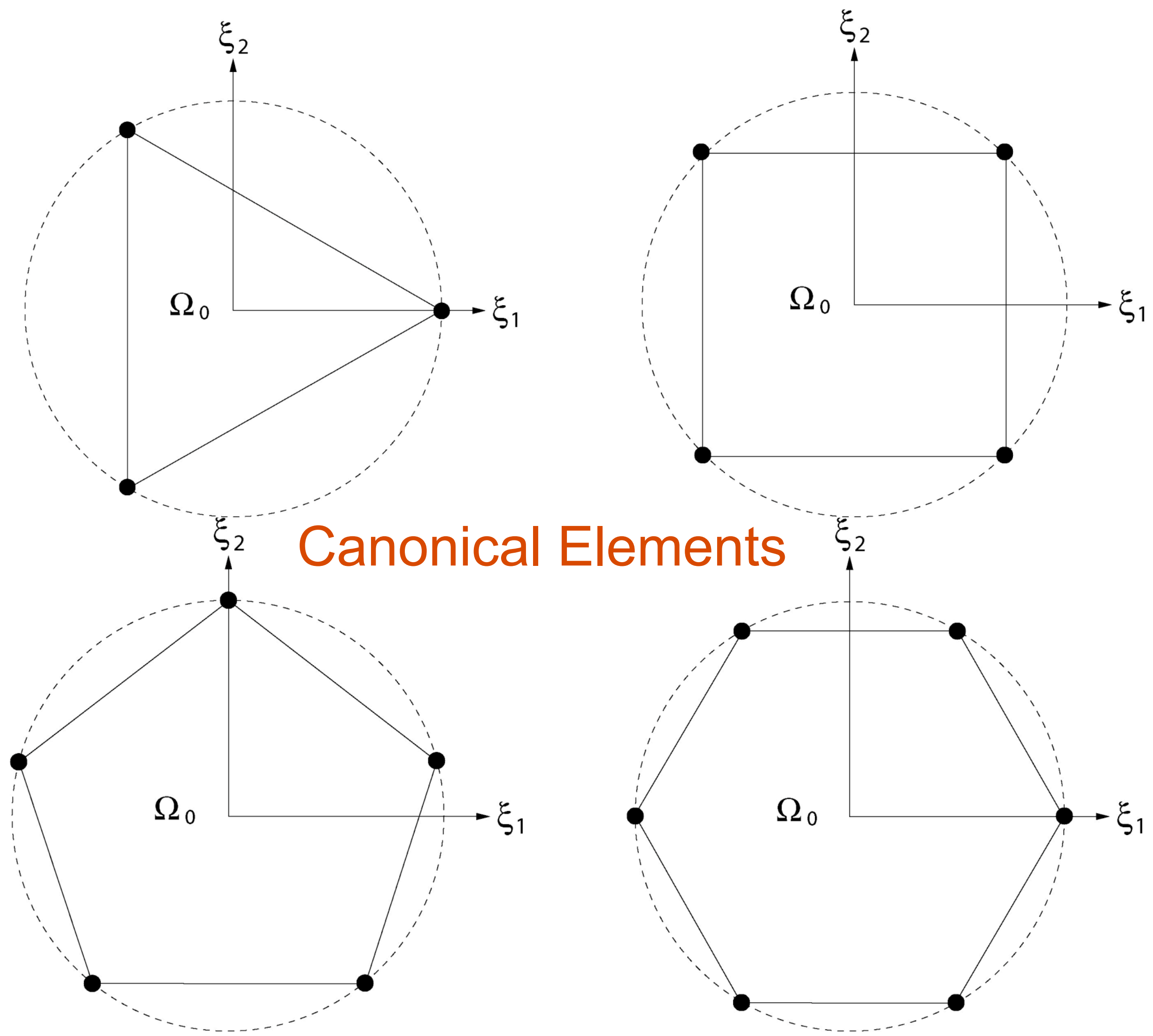
- Partition of unity

$$\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) = 1$$

- Linear reproducing conditions

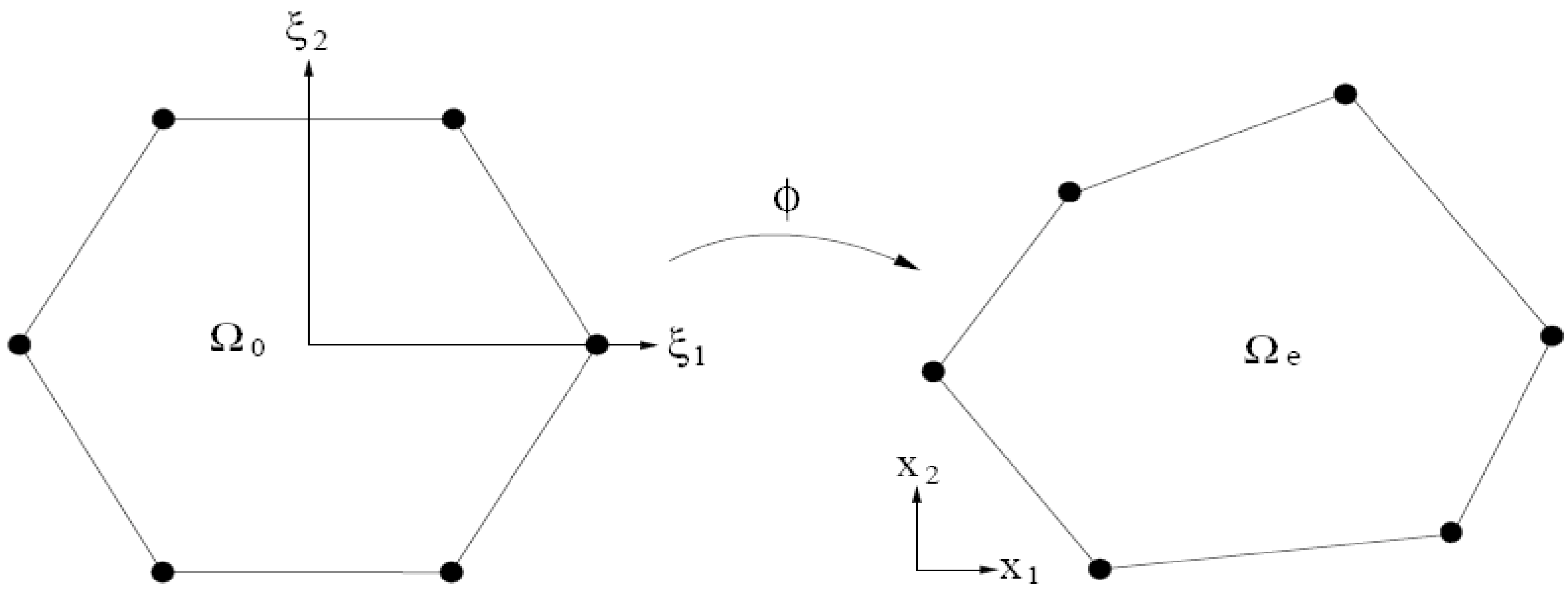
$$\sum_{a=1}^{n} \phi_a(\boldsymbol{x})\boldsymbol{x}_a = \boldsymbol{x}$$

Wachspress Basis Functions: Reference Elements



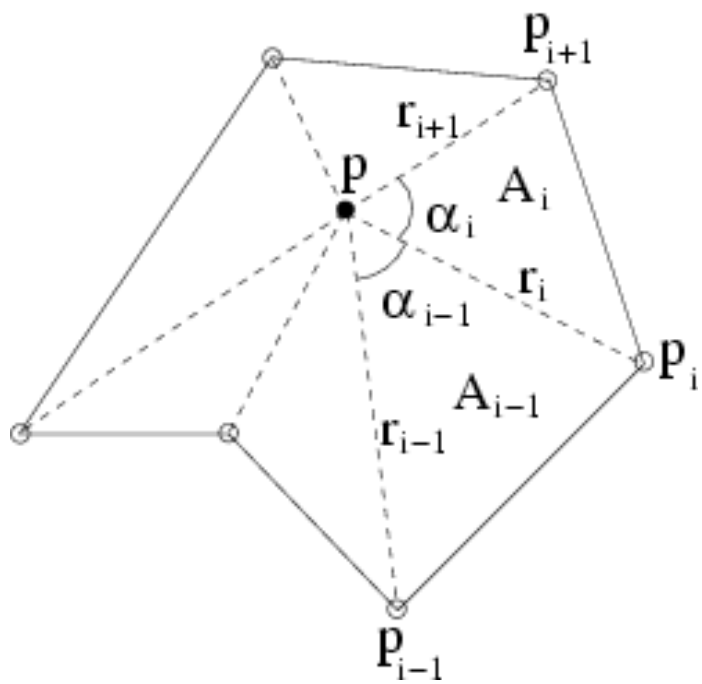
Isoparametric Transformation

(S and Tabarraei, IJNME, 2004)



$$\boxed{\boldsymbol{x}(\boldsymbol{\xi}) = \sum_{a=1}^{n} \phi_a(\boldsymbol{\xi})\boldsymbol{x}_a}$$

Nonconvex Polygons



(Floater, CAGD, 2003; Hormann and Floater, ACM TOG, 2006)

Mean Value Coordinates

$$\phi_i(\boldsymbol{x}) = \frac{w_i(\boldsymbol{x})}{\sum_{j=1}^{n} w_j(\boldsymbol{x})}$$

$$w_i(\mathbf{x}) = \frac{\tan(\alpha_{i-1}/2) + \tan(\alpha_i/2)}{r_i}, \quad \mathbf{r}_i = \mathbf{x}_i - \mathbf{x}$$

$$\tan\left(\frac{\alpha_i}{2}\right) = \frac{\sin\alpha_i}{1+\cos\alpha_i} = \frac{|\mathbf{r}_i \times \mathbf{r}_{i+1}|}{r_i r_{i+1} + \mathbf{r}_i \cdot \mathbf{r}_{i+1}}$$

(Tabarraei and S, CMAME, 2008)

Issues in the Numerical Implementation

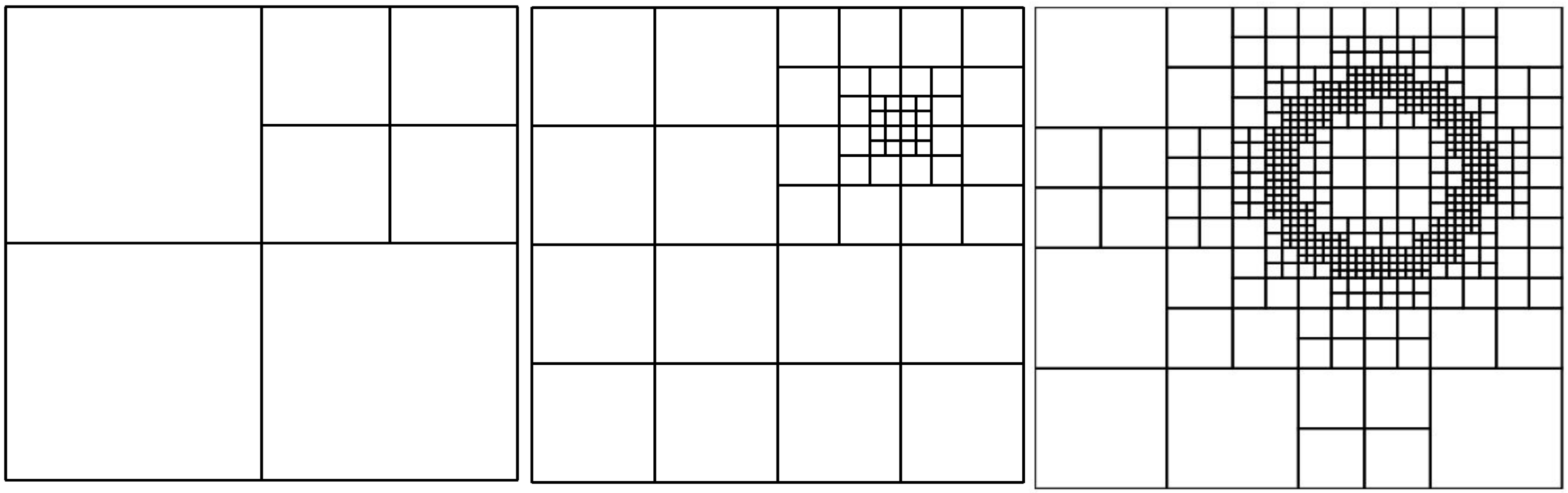
Mesh Generation and Numerical Integration

- Mesh generation with polygonal/polyhedral elements (Lectures to follow by **Julian Rimoli** and **Glaucio Paulino**)

- Numerical integration of bivariate polynomials and generalized barycentric coordinates on polygons (Next lecture by **Seyed Mousavi**)

Patch Test

Quadtree mesh



Mesh a　　Mesh b　　Mesh c

Linear essential (Dirichlet) BCs are imposed on $\partial\Omega$

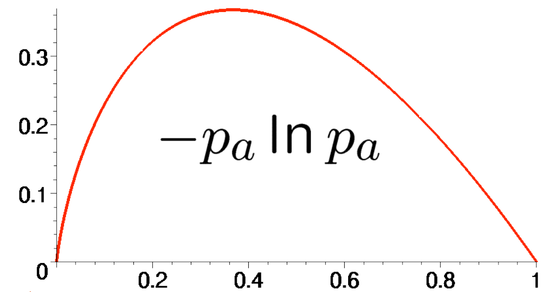
Error in the L^2 norm = $\mathcal{O}(10^{-10})$

Error in the energy norm = $\mathcal{O}(10^{-9})$

Principle of Maximum Entropy

(Shannon, Bell. Sys. Tech. J., 1948; Jaynes, Phy. Rev., 1957)

- *discrete* set of events $\{x_1, \ldots, x_n\}$
- *possibility* of each event $p_a = p(x_a) \in [0, 1]$
- *uncertainty* of each event $-\ln(p_a)$
- *Shannon entropy* $H(p) = -\sum_{a=1}^{n} p_a \ln p_a$
  - average uncertainty
  - concave functional
  - unique maximum

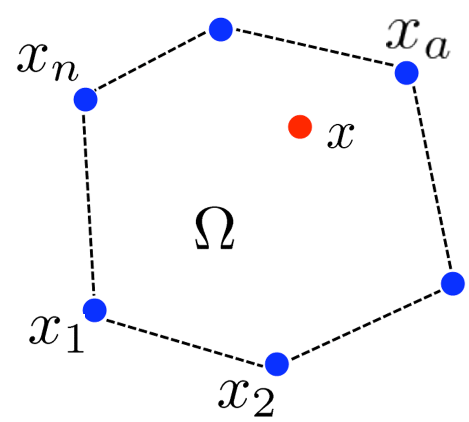


- Jaynes's *principle of maximum entropy*
  - maximizing $H(p)$ s.t. $\sum_{a=1}^{6} p_a = 1$, $\sum_{a=1}^{6} x_a p_a = E[x]$

    gives the *least-biased* probability distribution

Entropy to Generalized Barycentric Coordinates

- convex polygon $\Omega \subset \mathbb{R}^2$ with vertices $\mathbf{x}_1, \ldots, \mathbf{x}_n$



- for any $\mathbf{x} \in \Omega$, maximize

$$- \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \ln \phi_a(\boldsymbol{x})$$

subject to

$$\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) = 1, \; \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \boldsymbol{x}_a = \boldsymbol{x}$$

- maximum entropy basis functions
(S, IJNME, 2004)

Entropy to Generalized Barycentric Coordinates

- convex polygon $\Omega \subset \mathbb{R}^2$ with vertices $\mathbf{x}_1, \ldots, \mathbf{x}_n$

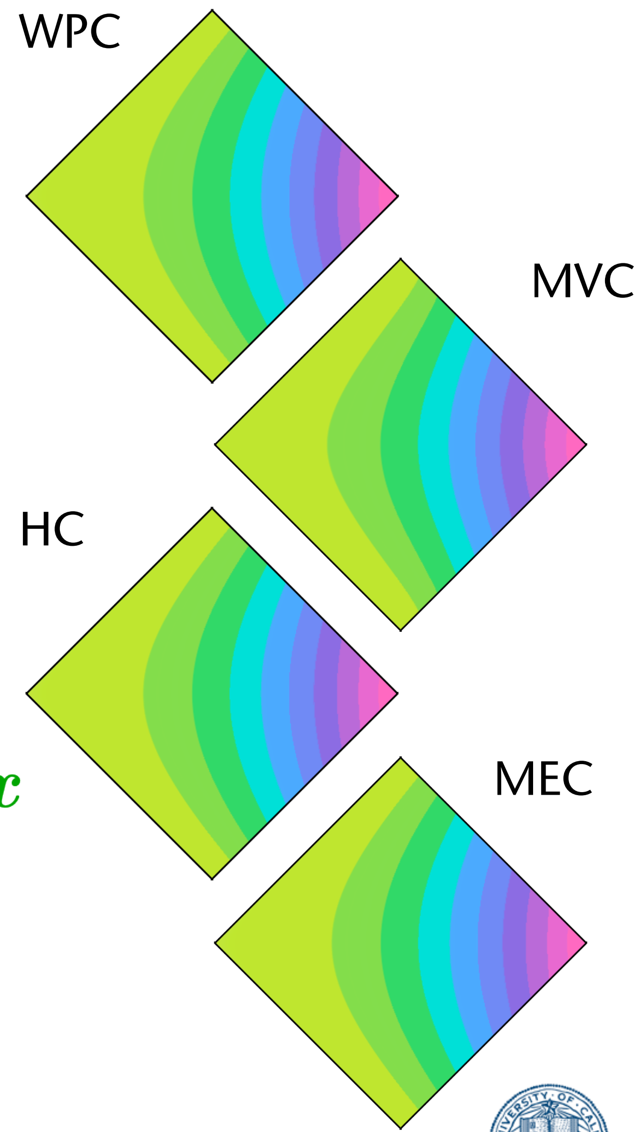
- for any $\mathbf{x} \in \Omega$, maximize

$$- \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \ln \phi_a(\boldsymbol{x})$$

subject to

$$\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) = 1, \; \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \boldsymbol{x}_a = \boldsymbol{x}$$

- maximum entropy basis functions **(S, IJNME, 2004)**



Entropy to Generalized Barycentric Coordinates

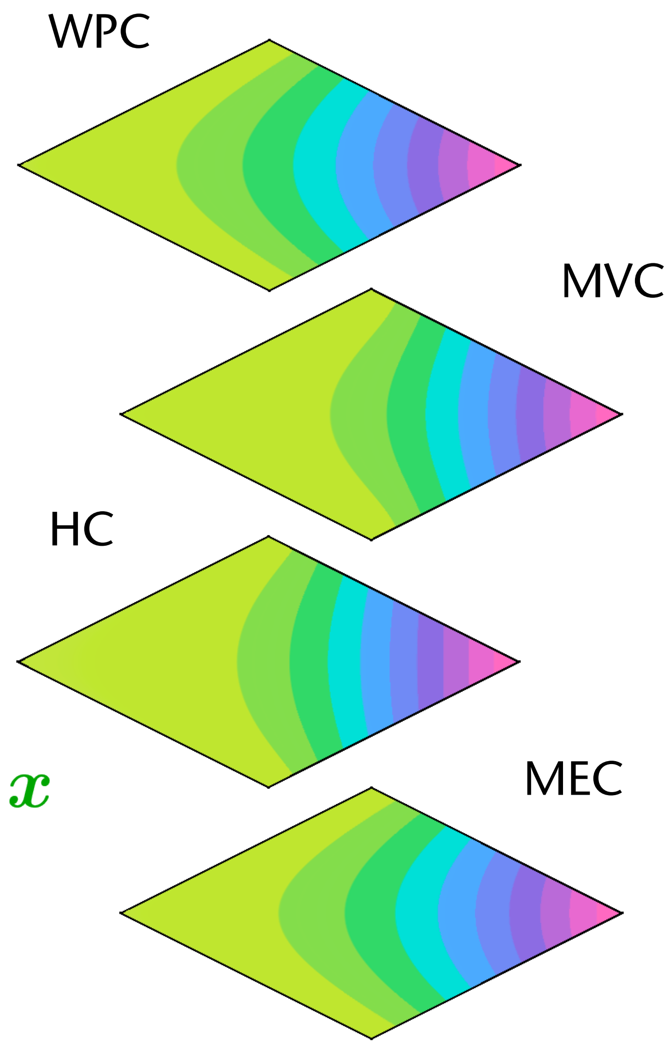
- convex polygon $\Omega \subset \mathbb{R}^2$ with vertices $\mathbf{x}_1, \ldots, \mathbf{x}_n$
- for any $\mathbf{x} \in \Omega$, maximize

$$- \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \ln \phi_a(\boldsymbol{x})$$

subject to

$$\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) = 1, \; \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \boldsymbol{x}_a = \boldsymbol{x}$$

- maximum entropy basis functions **(S, IJNME, 2004)**



Entropy to Generalized Barycentric Coordinates

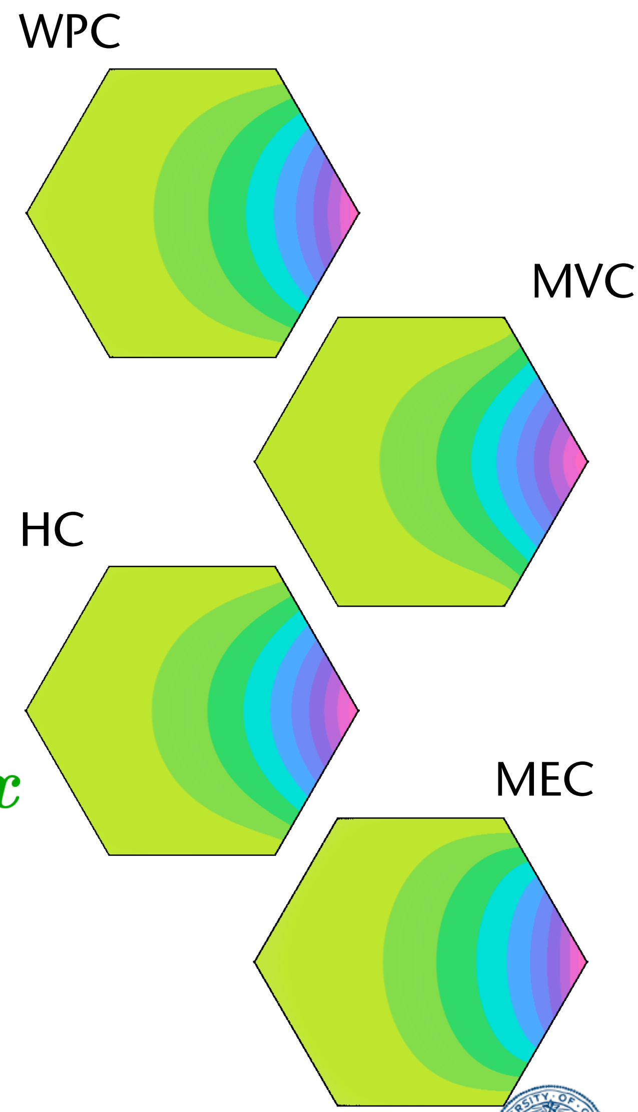
- convex polygon $\Omega \subset \mathbb{R}^2$
  with vertices $\mathbf{x}_1, \ldots, \mathbf{x}_n$
- for any $\mathbf{x} \in \Omega$, maximize

$$-\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \ln \phi_a(\boldsymbol{x})$$

subject to

$$\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) = 1, \ \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \boldsymbol{x}_a = \boldsymbol{x}$$

- maximum entropy basis functions
  (S, IJNME, 2004)



Entropy to Generalized Barycentric Coordinates

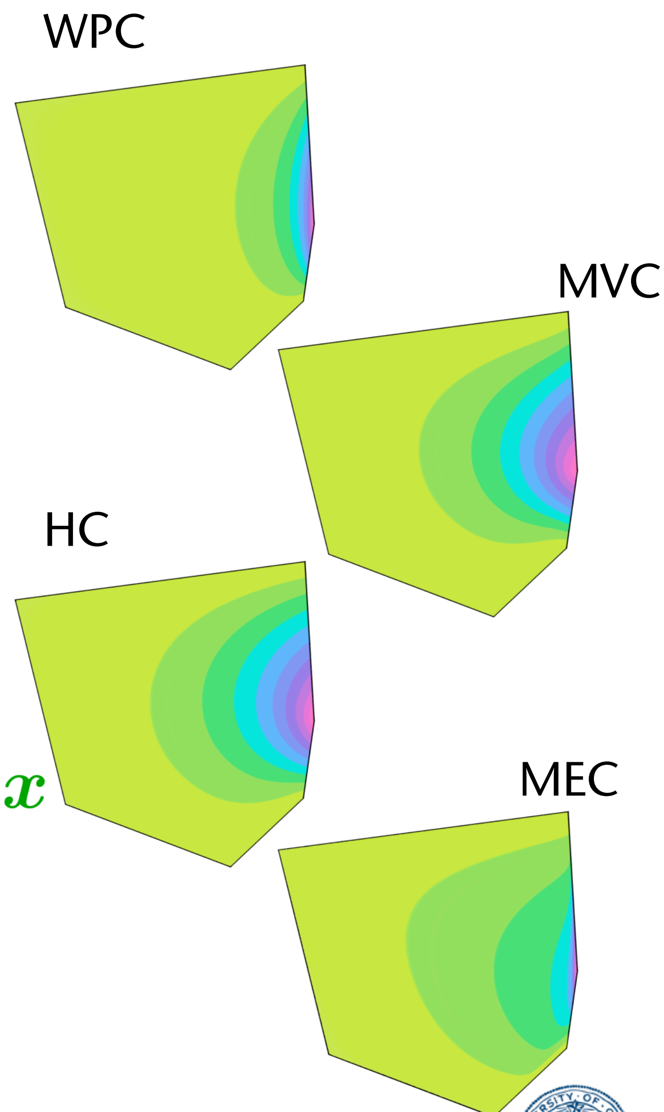
- convex polygon $\Omega \subset \mathbb{R}^2$
  with vertices $\mathbf{x}_1, \ldots, \mathbf{x}_n$

- for any $\mathbf{x} \in \Omega$, maximize

$$-\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \ln \phi_a(\boldsymbol{x})$$

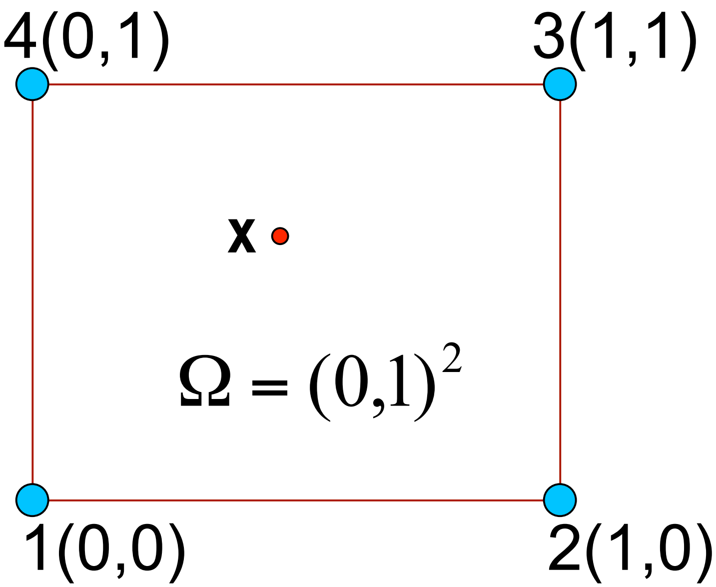
subject to

$$\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) = 1, \ \sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \boldsymbol{x}_a = \boldsymbol{x}$$



- maximum entropy basis functions
  (S, IJNME, 2004)

Max-Ent Basis Functions: Unit Square



$$Z = \sum_{a=1}^{4} e^{-\lambda_1 x_a - \lambda_2 y_b}$$

$$= 1 + e^{-\lambda_1} + e^{-\lambda_2} + e^{-\lambda_1 - \lambda_2}$$

$$\boxed{\begin{aligned} \frac{e^{-\lambda_1} + e^{-\lambda_1 - \lambda_2}}{Z} &= x \\ \frac{e^{-\lambda_2} + e^{-\lambda_1 - \lambda_2}}{Z} &= y \end{aligned}}$$

which simplifies to

$$\frac{e^{-\lambda_1}}{1 + e^{-\lambda_1}} = x, \ \frac{e^{-\lambda_2}}{1 + e^{-\lambda_2}} = y \Rightarrow e^{-\lambda_1} = \frac{x}{1 - x}, e^{-\lambda_2} = \frac{y}{1 - y}$$

Max-Ent Basis Functions: Unit Square (Cont'd)

Since $\phi_a = \dfrac{e^{-\lambda_1 x_a - \lambda_2 y_a}}{Z}, \; Z = \sum_{b=1}^{4} e^{-\lambda_1 x_b - \lambda_2 y_b}$,

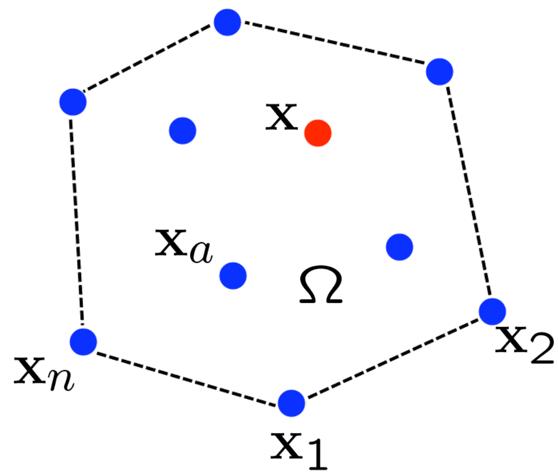
we obtain $Z^{-1} = (1-x)(1-y)$ and therefore

$$\boxed{\begin{gathered} \phi_1(x,y) = (1-x)(1-y), \; \phi_2(x,y) = x(1-y) \\ \phi_3(x,y) = xy, \; \phi_4(x,y) = y(1-x) \end{gathered}}$$

which are the same as bilinear finite element shape functions

Maximum-Entropy Meshfree Basis Functions

- *scattered* nodes in $\Omega \subset \mathbb{R}^2$
  with coordinates $\mathbf{x}_1, \ldots, \mathbf{x}_n$



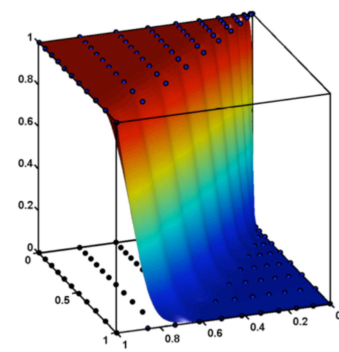
- for any $\mathbf{x} \in \Omega$, maximize

$$H(\phi, w) = -\sum_{a=1}^{n} \phi_a \ln\left(\frac{\phi_a}{w_a}\right)$$

subject to $$\sum_{a=1}^{n} \phi_a(\mathbf{x}) = 1, \qquad \sum_{a=1}^{n} \phi_a(\mathbf{x})\mathbf{x}_a = \mathbf{x}$$

(Arroyo & Ortiz, IJNME, 2006; S & Wright, IJNME, 2007)

convex basis functions
- **pos-def mass matrix**
- **convex hull property**
- **no Runge phenomenon**

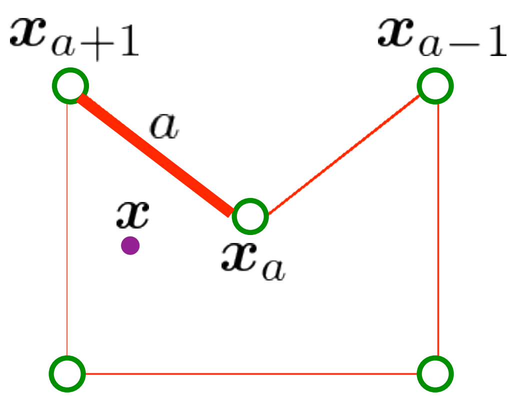


Non-Negative Max-Ent Coordinates

(Hormann and S, Comp. Graph. Forum, 2008)

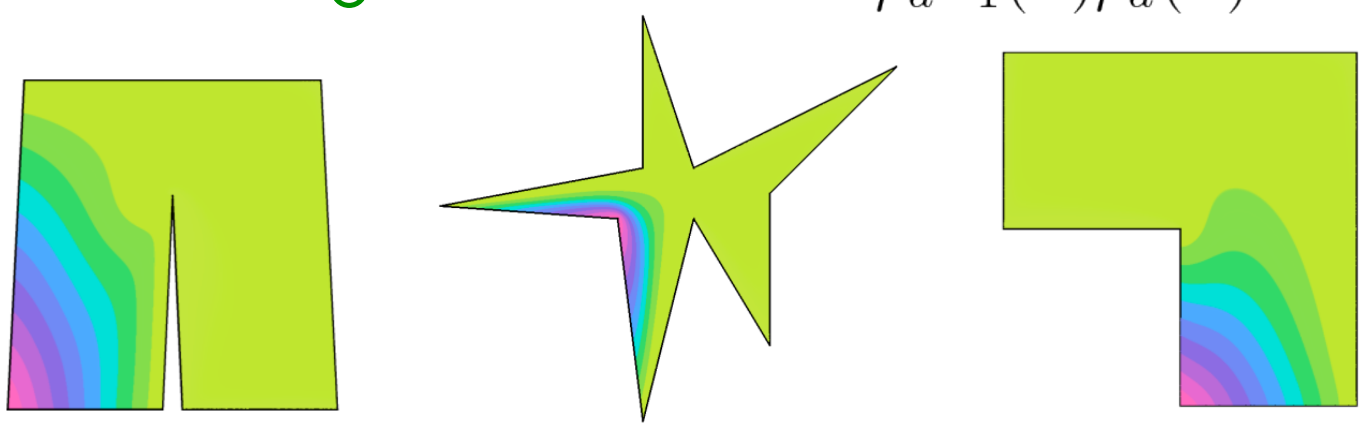
Prior is based on edge weight functions

$$\rho_a(\boldsymbol{x}) = (\boldsymbol{x}_a - \boldsymbol{x}) \cdot (\boldsymbol{x}_{a+1} - \boldsymbol{x}) + |\boldsymbol{x}_a - \boldsymbol{x}||\boldsymbol{x}_{a+1} - \boldsymbol{x}| \geq 0$$



$$w_a(\boldsymbol{x}) = \frac{\Pi_a(\boldsymbol{x})}{\sum_{b=1}^{n} \Pi_b(\boldsymbol{x})}$$

$$\Pi_a(\boldsymbol{x}) = \frac{1}{\rho_{a-1}(\boldsymbol{x})\rho_a(\boldsymbol{x})}$$



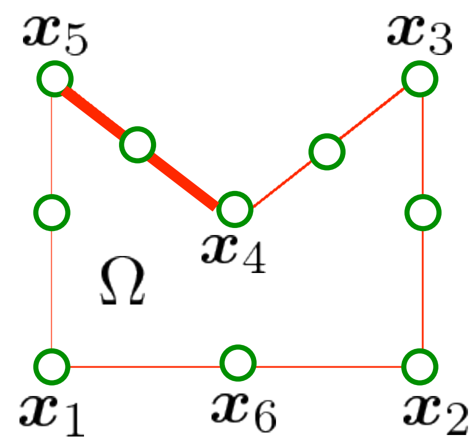
Quadratic Max-Ent Coordinates on Polygons

- ✓ Use notion of a prior in the modified entropy measure (signed basis functions) introduced by **Bompadre et al., CMAME, 2012**
- ✓ Adopt the linear constraints for quadratic precision proposed by **Rand et al., arXiv, 2011**
- ✓ Use nodal priors **(Hormann and S, CGF, 2008)** based on edge weights in the max-ent variational formulation
- ✓ Construction applies to convex and nonconvex planar polygons. On each boundary facet, one-dimensional Bernstein bases **(Farouki, CAGD, 2012)** are obtained

Quadratic Max-Ent Coordinates on Polygons

(S, unpublished, 2012)

- planar polygon $\Omega \subset \mathbb{R}^2$
  with vertices $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$



- for any $\boldsymbol{x} \in \Omega$,

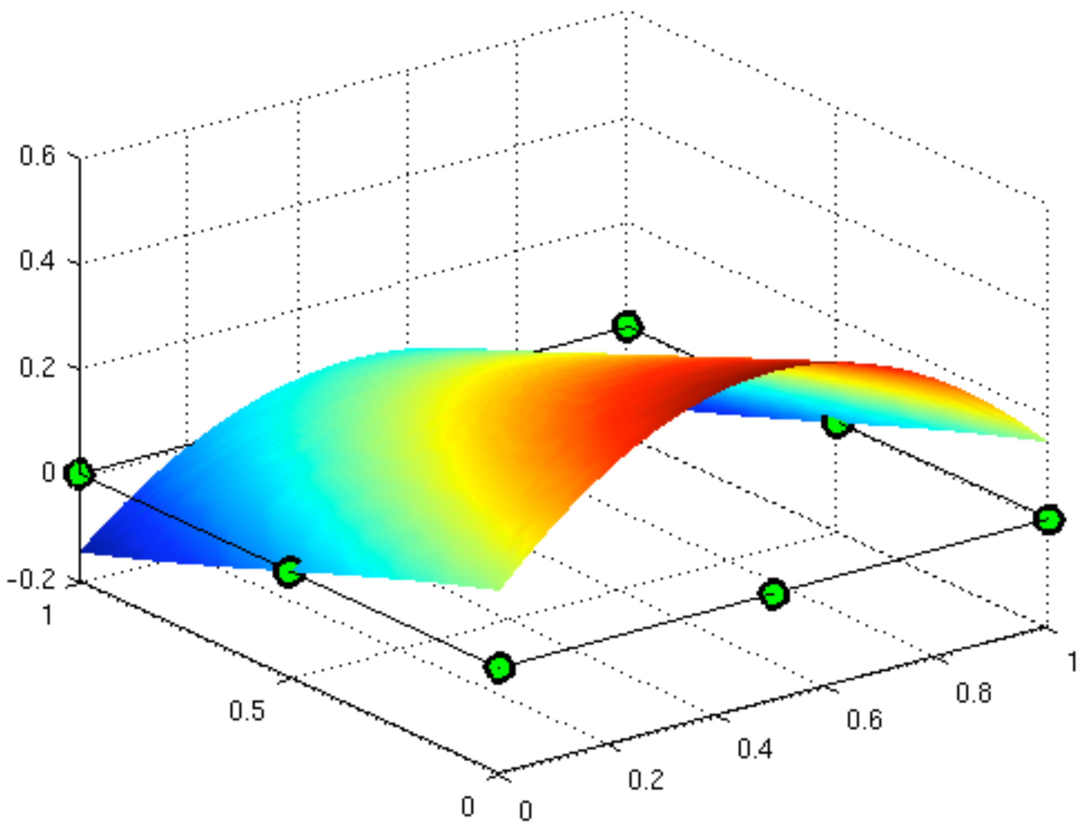
$$\max_{\boldsymbol{p}^+, \boldsymbol{p}^- \in \mathbb{R}^{2n}_+} - \sum_{a=1}^{2n} \left[p_a^+(\boldsymbol{x}) \ln \left(\frac{p_a^+(\boldsymbol{x})}{w_a(\boldsymbol{x})} \right) + p_a^-(\boldsymbol{x}) \ln \left(\frac{p_a^-(\boldsymbol{x})}{w_a(\boldsymbol{x})} \right) \right]$$

subject to 6 linearly independent equality constraints: PU, linear reproducing conditions and

$$\sum_{a=1}^{n} \phi_a(\boldsymbol{x}) \boldsymbol{x}_a \otimes \boldsymbol{x}_a + \sum_{a=1}^{n} \phi_{a+n}(\boldsymbol{x}) \left(\frac{\boldsymbol{x}_a \otimes \boldsymbol{x}_b + \boldsymbol{x}_b \otimes \boldsymbol{x}_a}{2} \right)$$

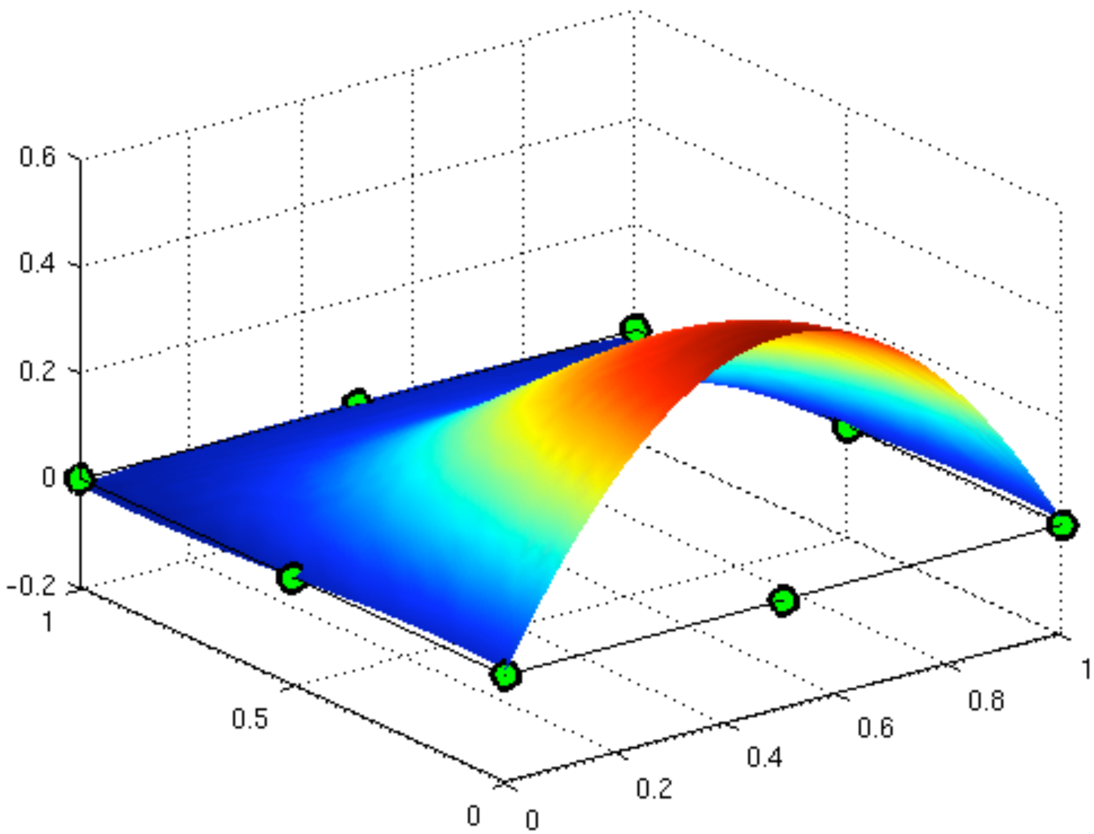
$$= \boldsymbol{x} \otimes \boldsymbol{x}, \ \text{where } \phi_a(\boldsymbol{x}) = p_a^+(\boldsymbol{x}) - p_a^-(\boldsymbol{x}), \ b = \mathrm{mod}(a, n) + 1$$

Quadratic Precision Basis Functions: Square



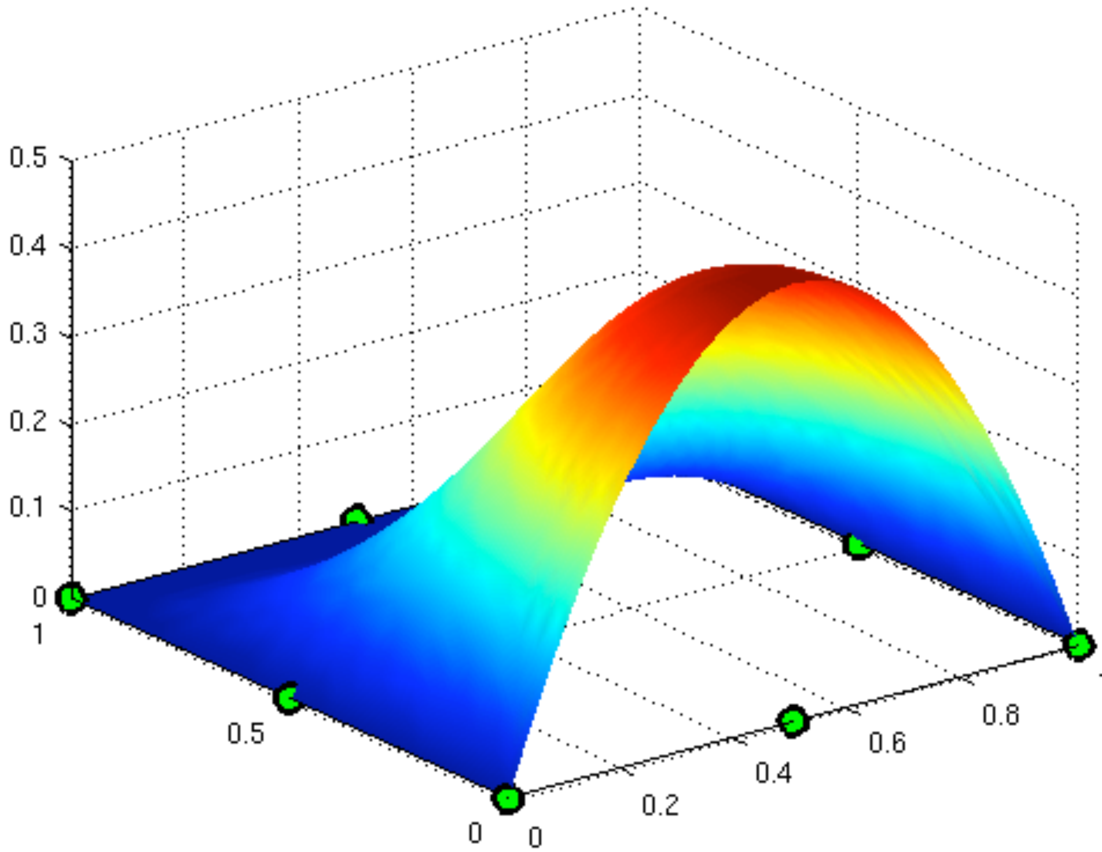
uniform prior

Quadratic Precision Basis Functions: Square



Gaussian prior

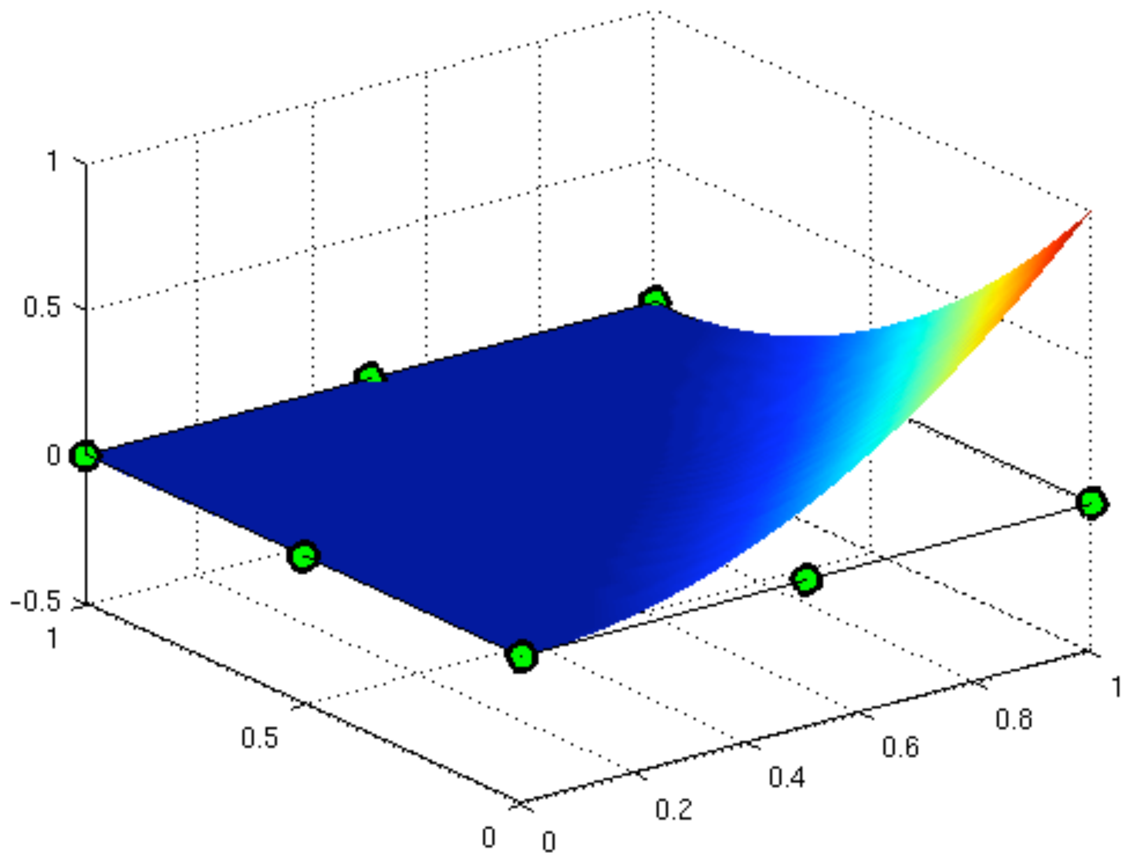
Quadratic Precision Basis Functions: Square



- Convergence tolerance = 10^{-10}
- Average # of iterations = 3.7

edge prior

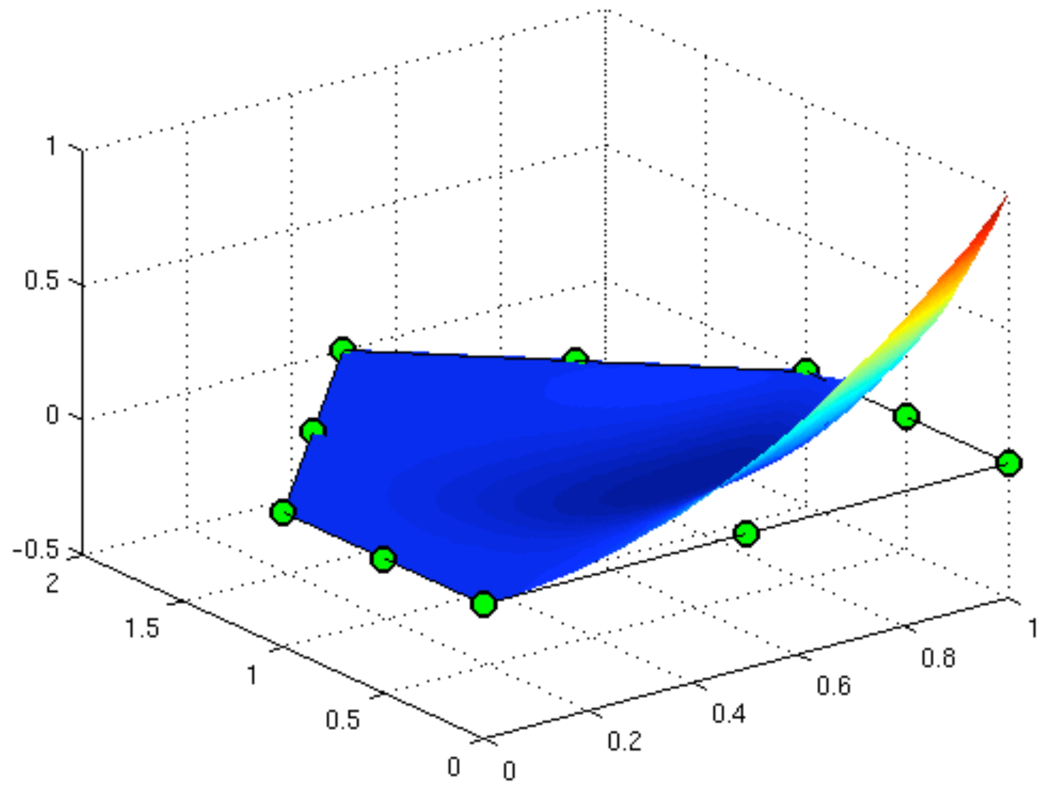
Quadratic Precision Basis Functions: Square



- Convergence tolerance = 10^{-10}
- Average # of iterations = 3.7

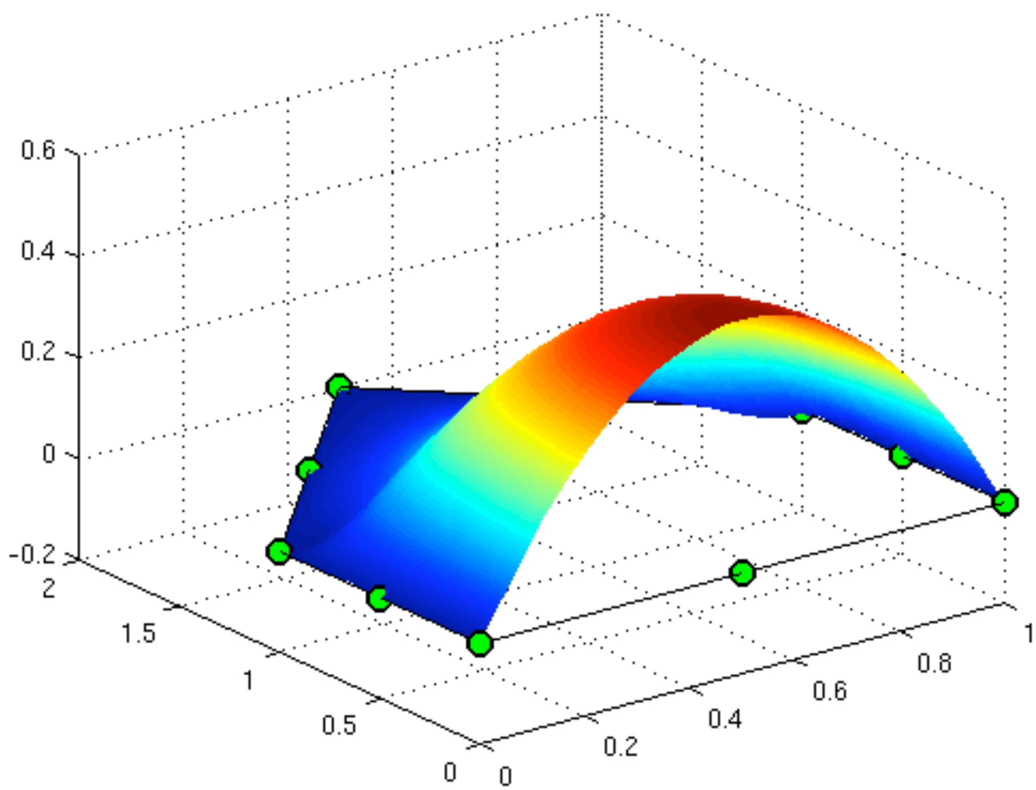
edge prior

Quadratic Precision Basis Functions: Pentagon



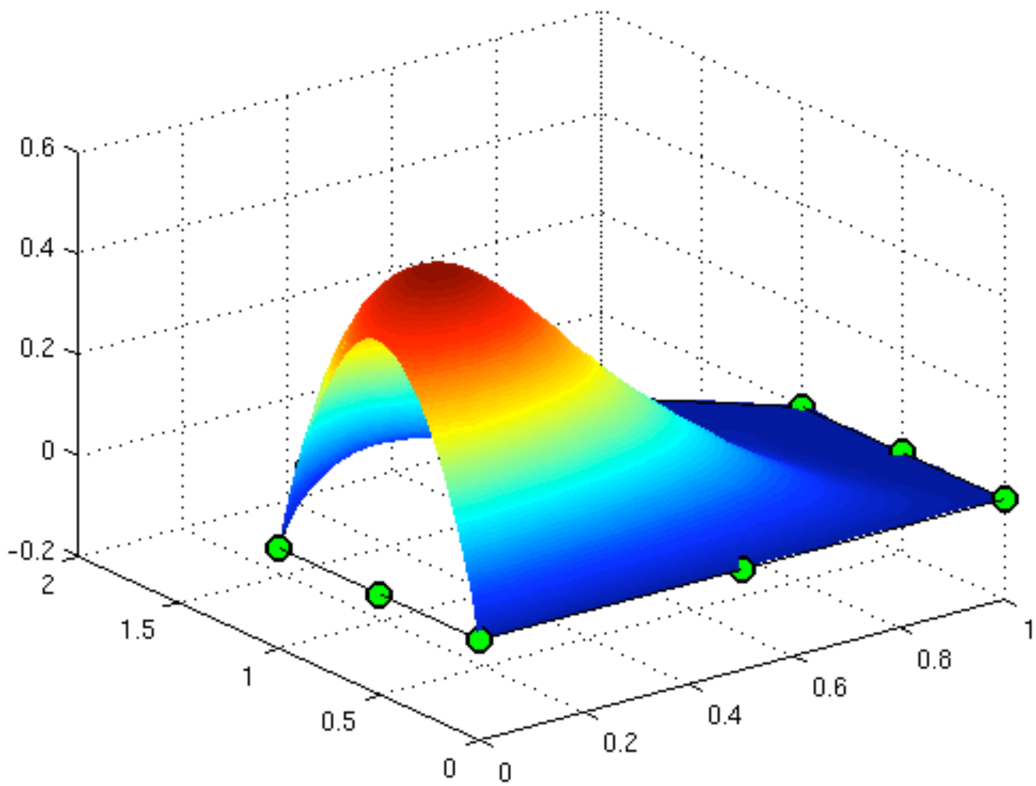
edge prior

Quadratic Precision Basis Functions: Pentagon



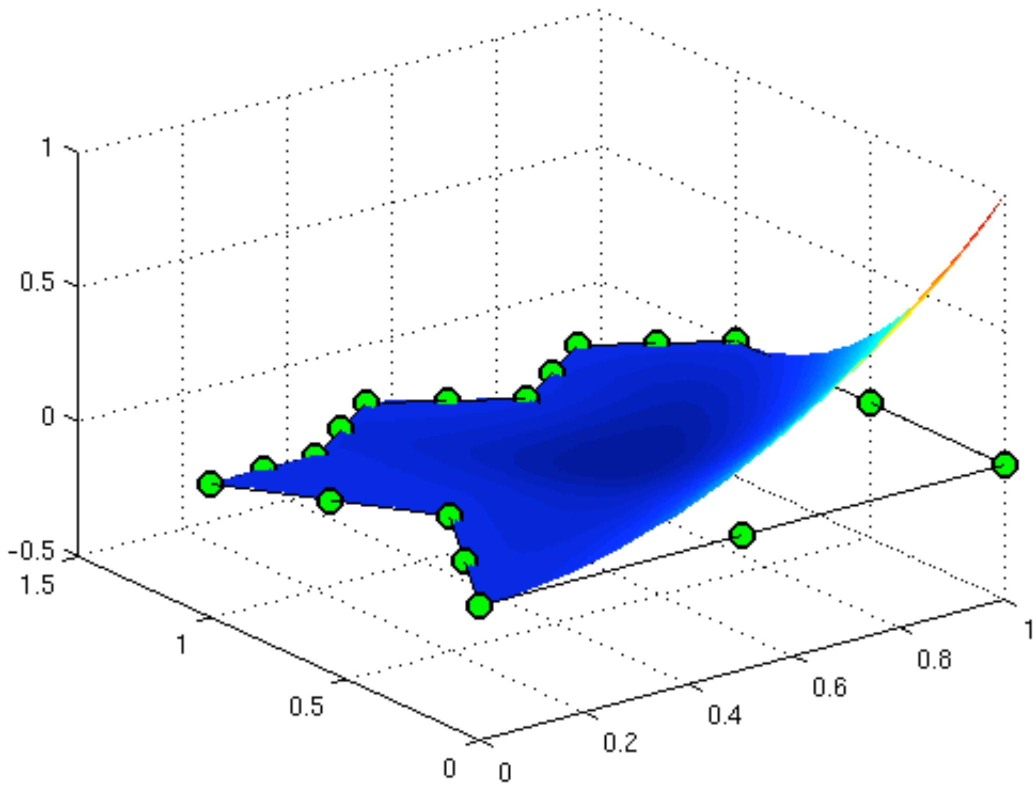
edge prior

Quadratic Precision Basis Functions: Pentagon



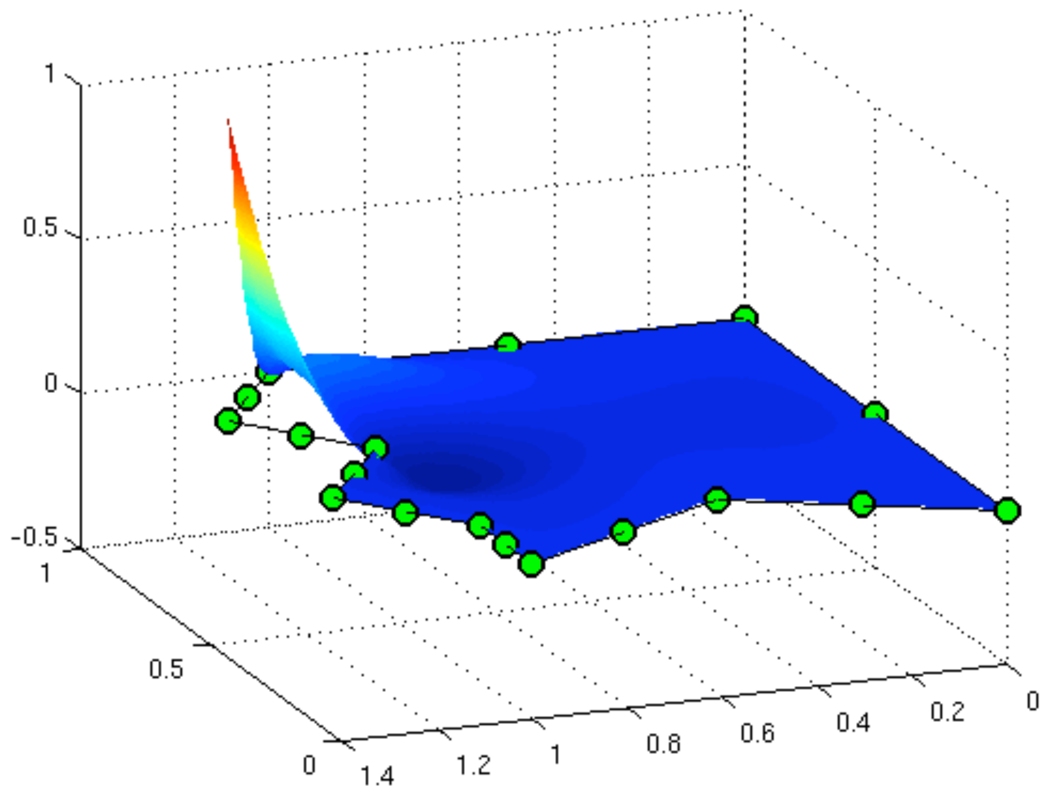
edge prior

Quadratic Precision Basis Functions: Nonconvex



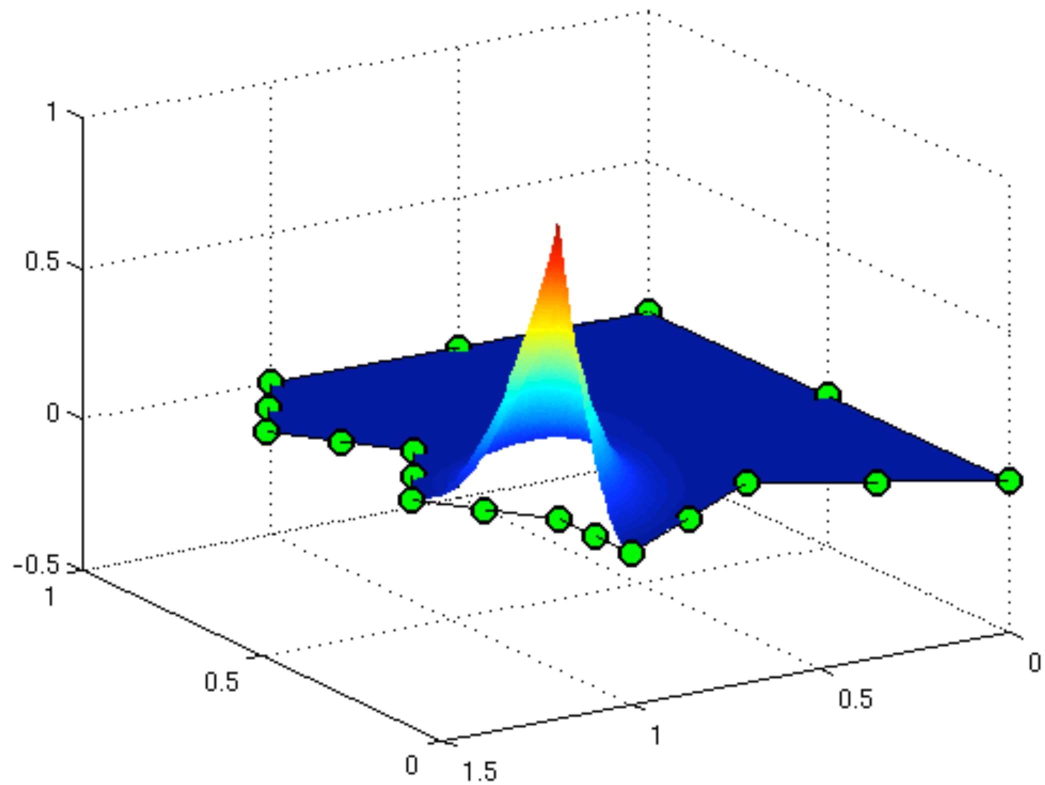
edge prior

Quadratic Precision Basis Functions: Nonconvex



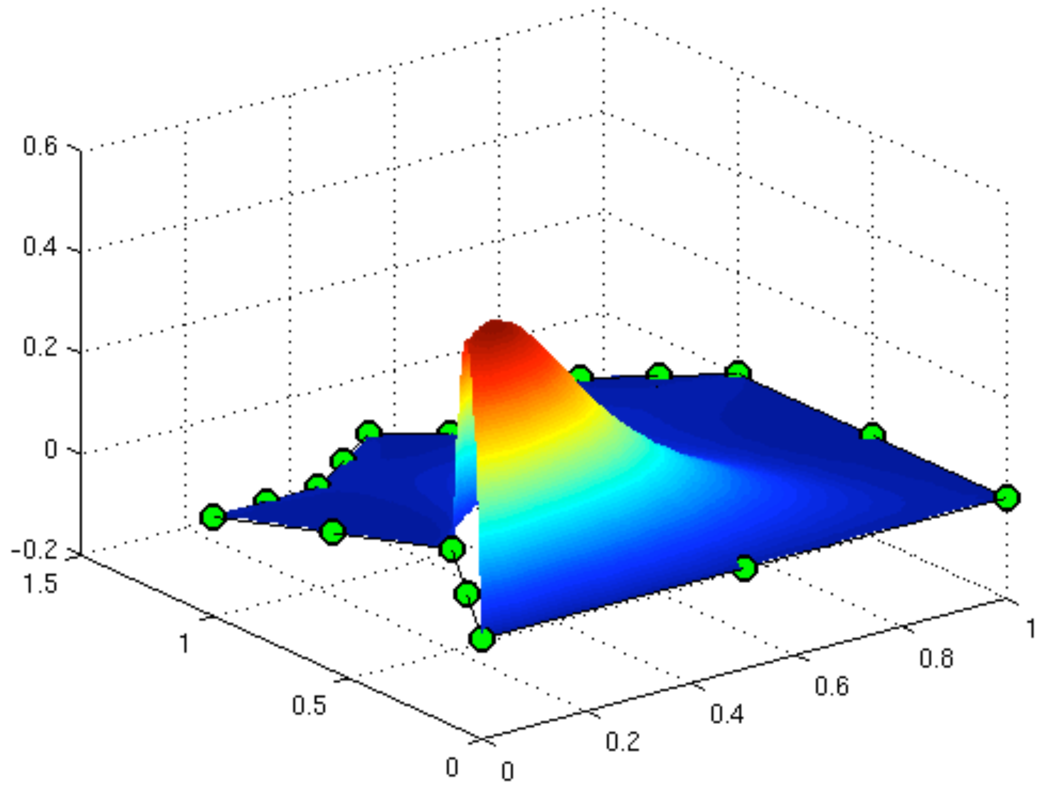
edge prior

Quadratic Precision Basis Functions: Nonconvex



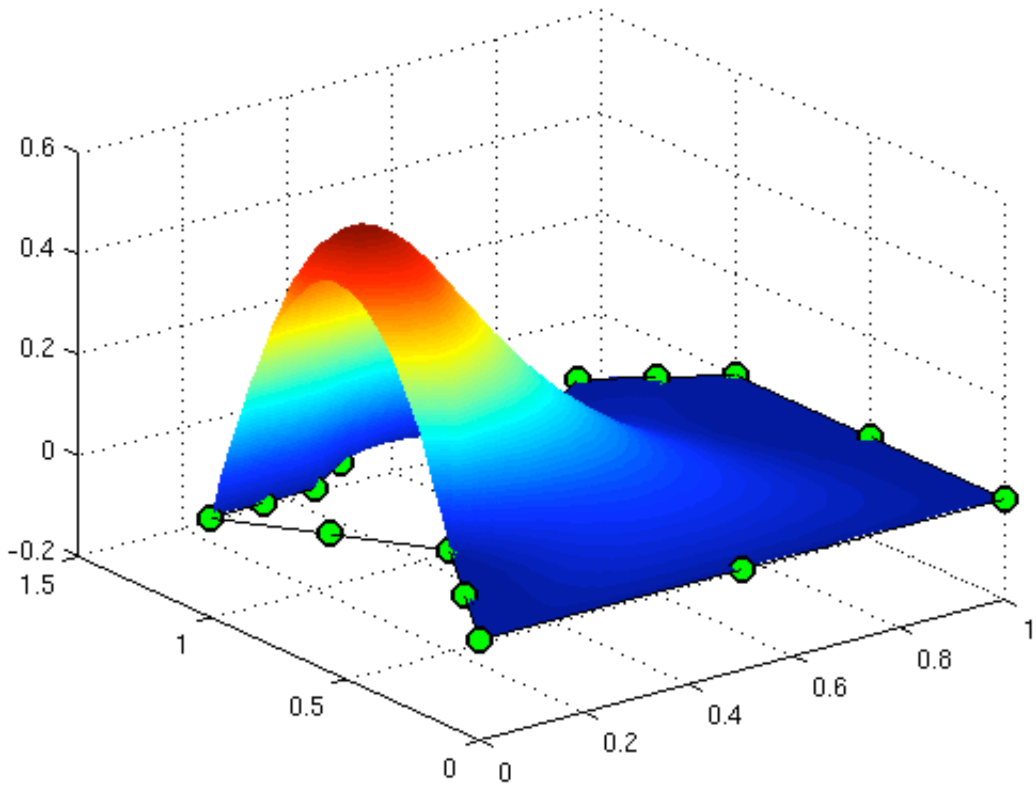
edge prior

Quadratic Precision Basis Functions: Nonconvex



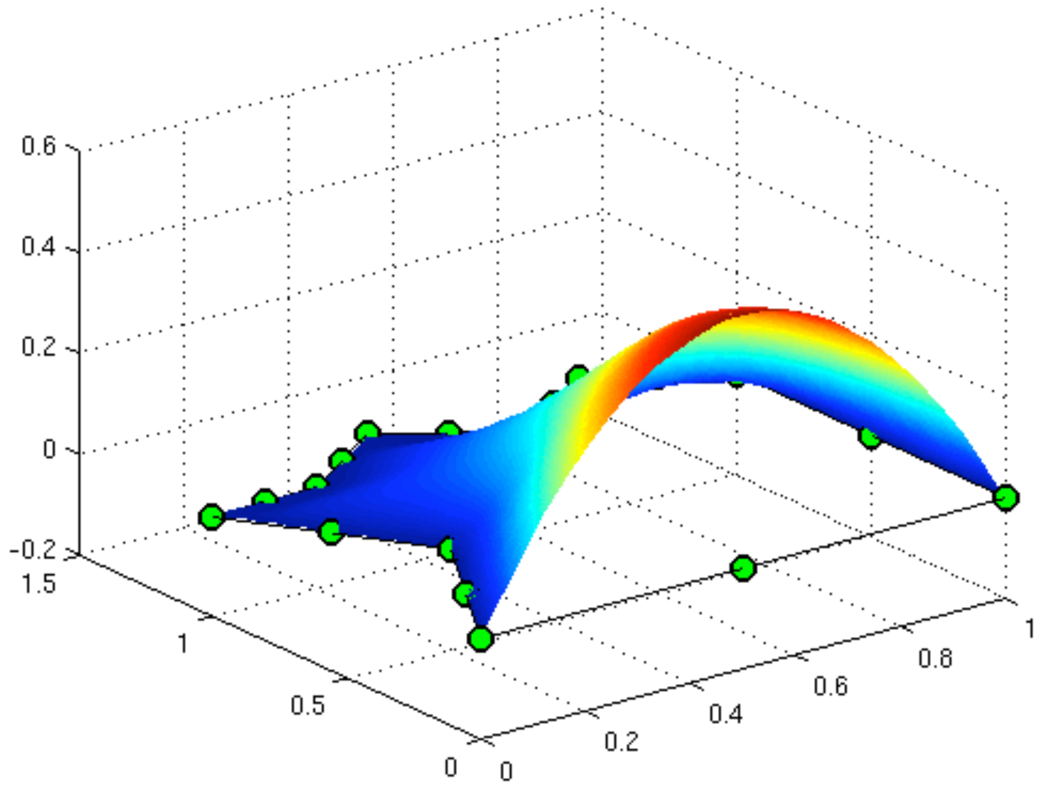
edge prior

Quadratic Precision Basis Functions: Nonconvex



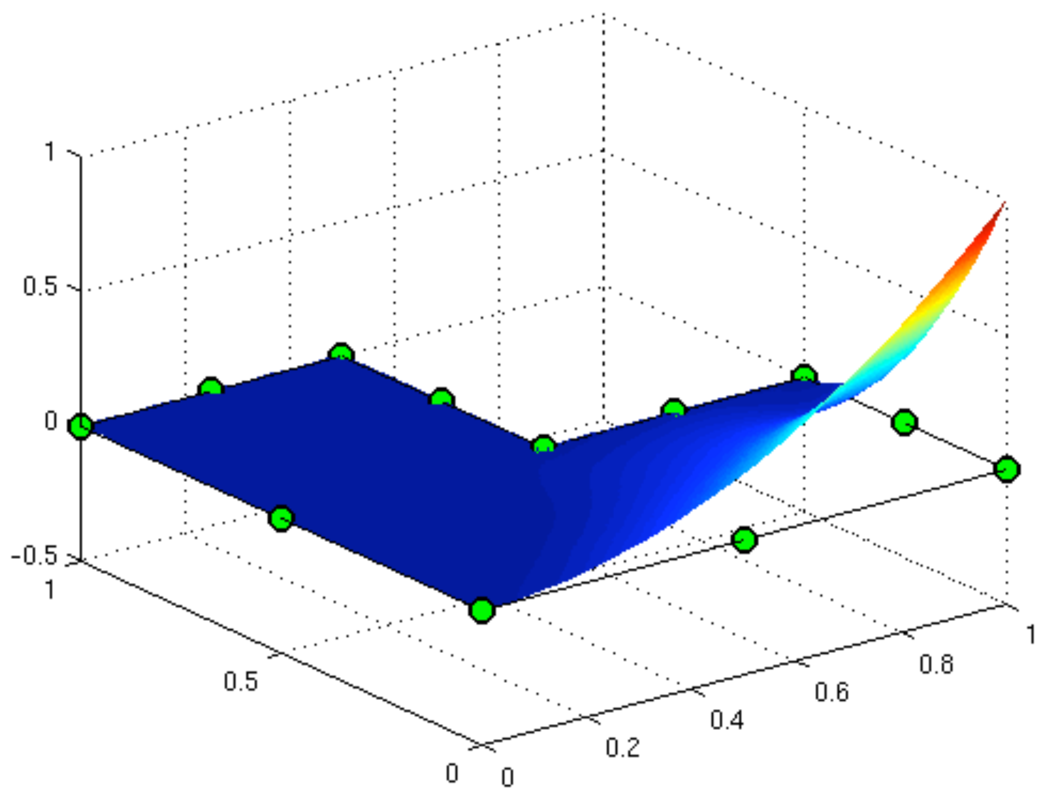
edge prior

Quadratic Precision Basis Functions: Nonconvex



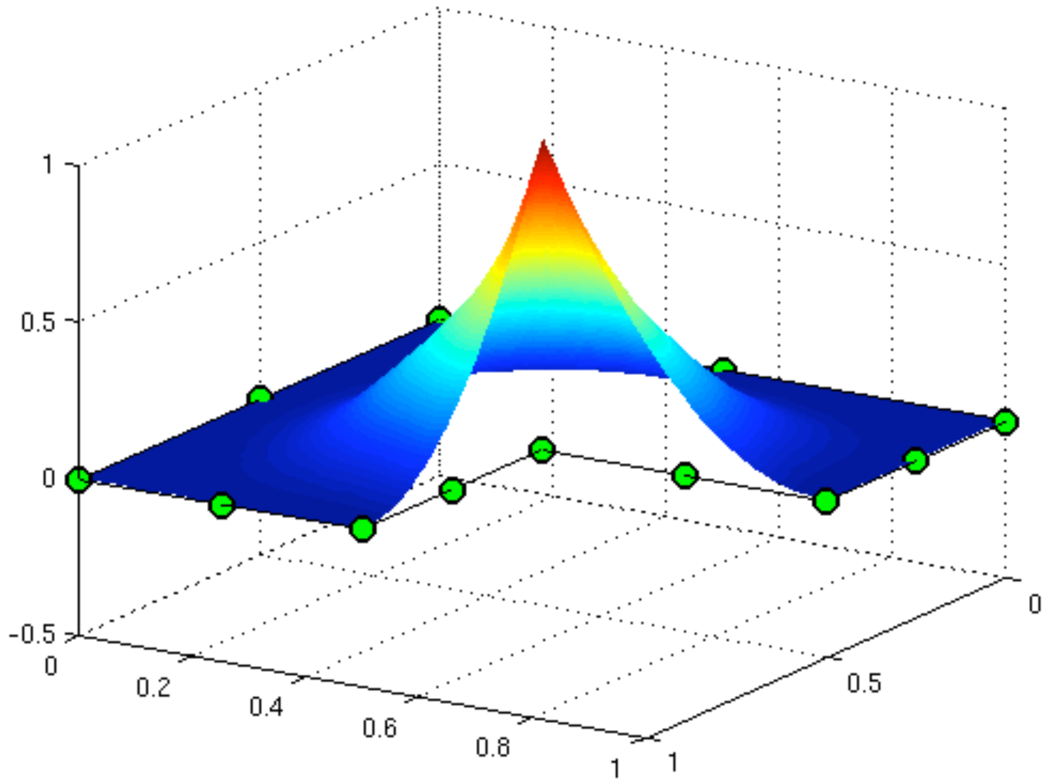
edge prior

Quadratic Precision Basis Functions: L-Shaped



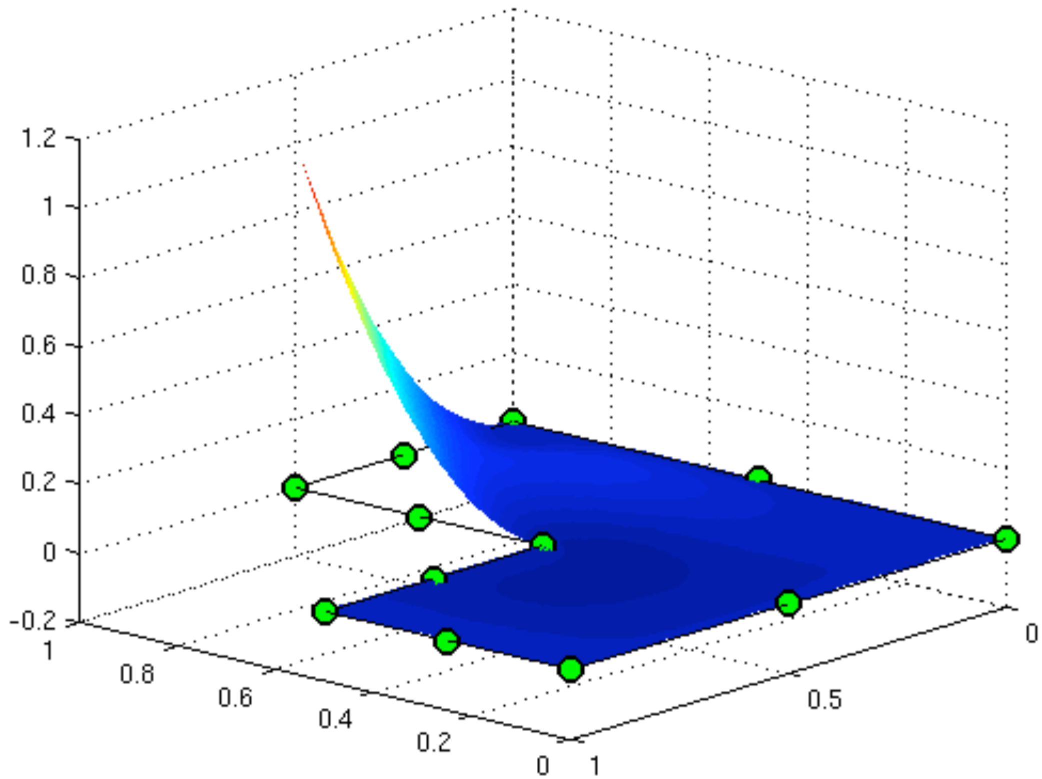
edge prior

Quadratic Precision Basis Functions: L-Shaped



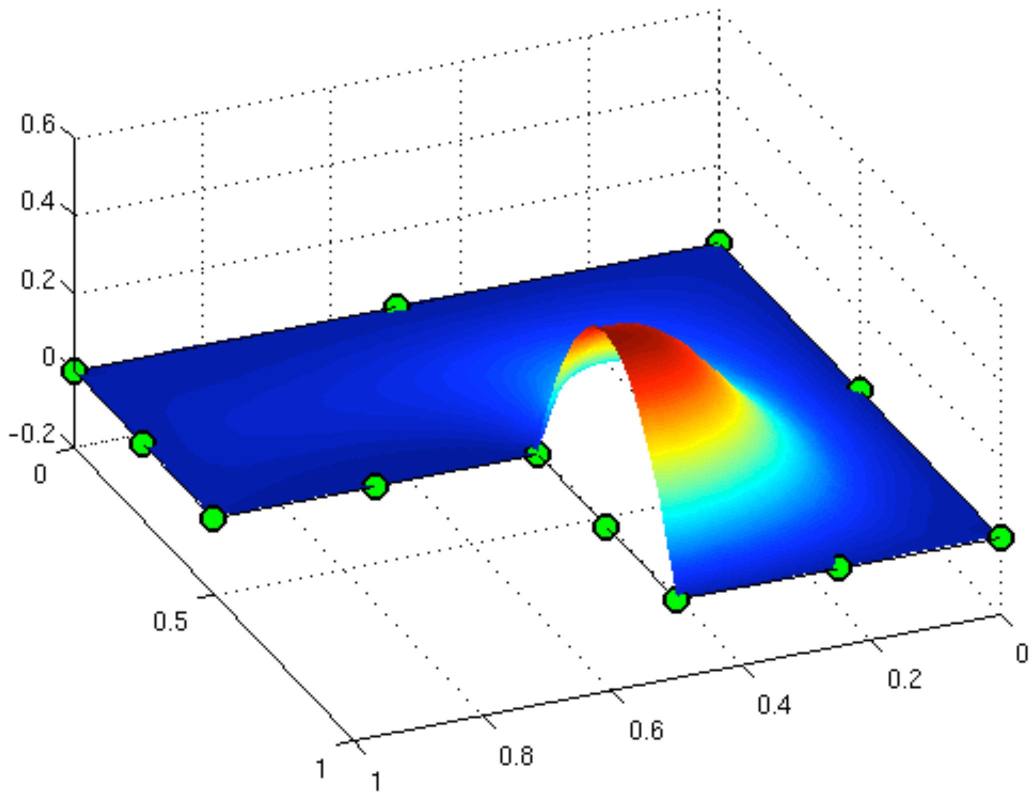
edge prior

Quadratic Precision Basis Functions: L-Shaped



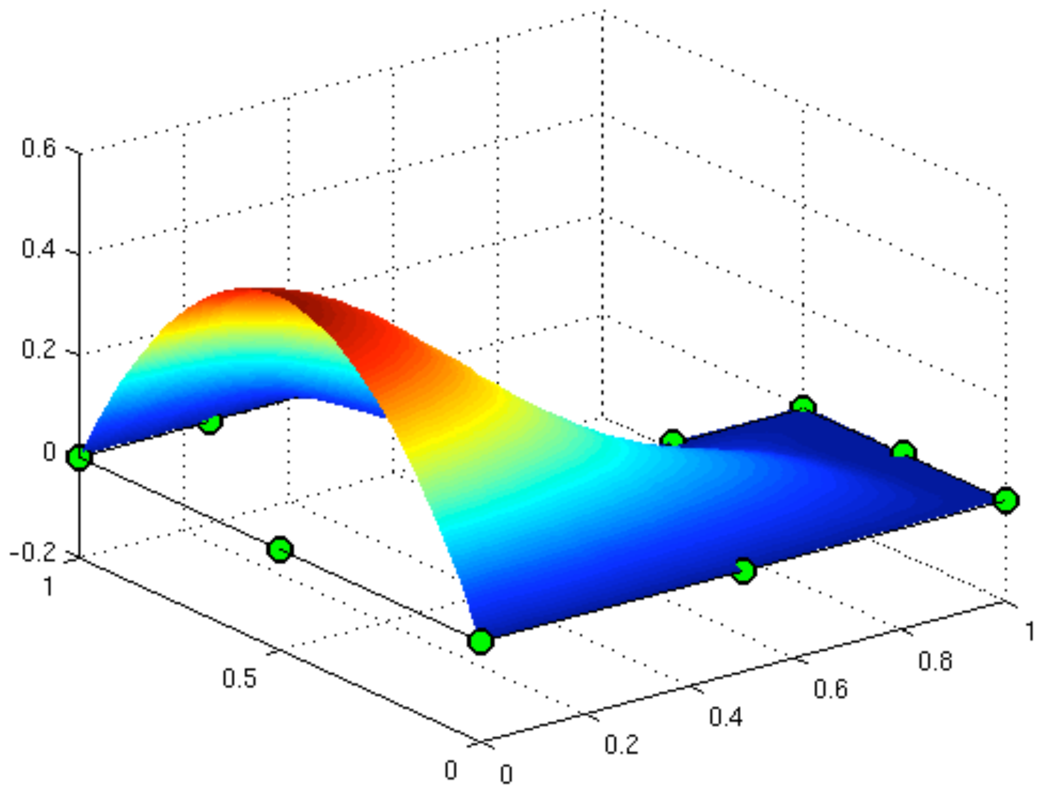
edge prior

Quadratic Precision Basis Functions: L-Shaped



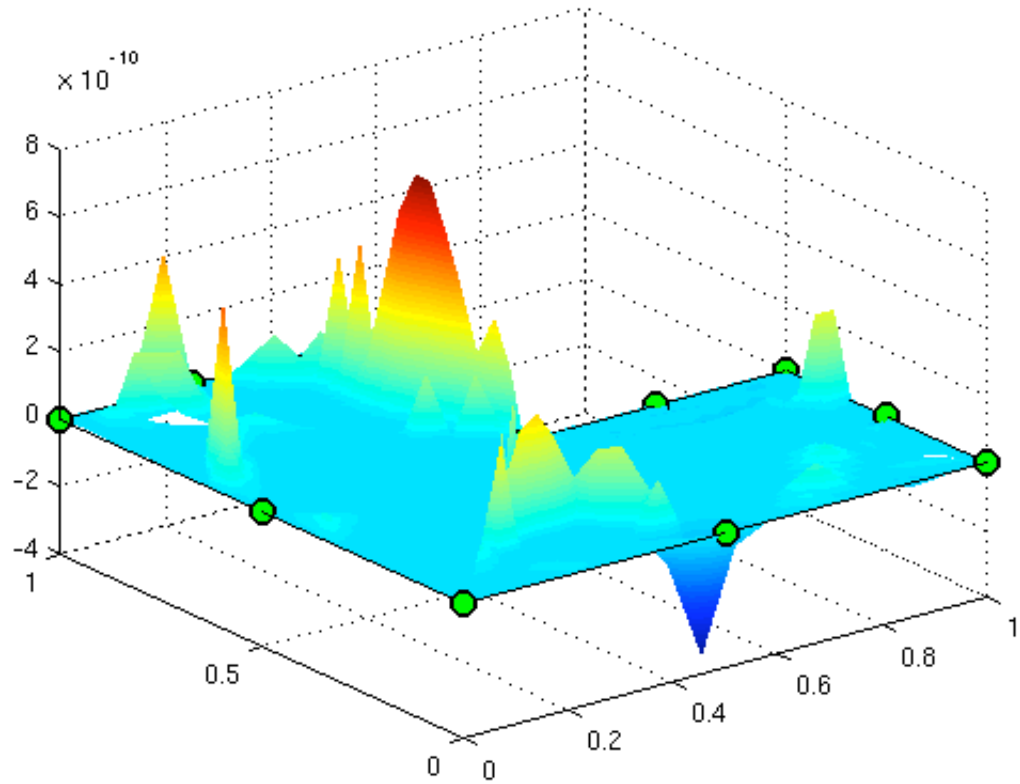
edge prior

Quadratic Precision Basis Functions: L-Shaped



edge prior

Quadratic Precision Basis Functions: L-Shaped



Approximation error for an arbitrary bivariate polynomial

Summary

- Introduced variational/weak forms for boundary-value problems, and presented the discrete equations for standard and polygonal FE
- Discussed construction of basis functions on polygonal meshes and implementation of polygonal finite elements
- Constructed linearly precise basis functions on planar polygons using relative entropy. Initial results for basis functions with quadratic precision on convex and nonconvex polygons were presented