Meshfree Approximation with MATLAB

Lecture VI: Nonlinear Problems: Nash Iteration and Implicit Smoothing

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Outline

Generic nonlinear elliptic PDE

$$\mathcal{L}u = f \qquad \text{on } \Omega \subset \mathbb{R}^s$$

Approximate Newton Iteration

$$u_k = u_{k-1} - T_{h_k}(u_{k-1})F(u_{k-1}), \qquad k \geq 1$$

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Nash-Moser Iteration [Nash (1956), Moser (1966), Hörmander (1976), Jerome (1985), F. & Jerome (1999)]

$$u_k = u_{k-1} - S_{\theta_k} T_{h_k}(u_{k-1})F(u_{k-1}), \qquad k \geq 1$$

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Matérn Radial Basic Functions

Definition

$$\Phi_{s,\beta}(\boldsymbol{x}) = \frac{K_{\beta-\frac{s}{2}}(\|\boldsymbol{x}\|)\|\boldsymbol{x}\|^{\beta-\frac{s}{2}}}{2^{\beta-1}\Gamma(\beta)}, \qquad \beta > \frac{s}{2}$$

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Properties:

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$$\widehat{\Phi}_{s,\beta}(\omega) = \left(1 + \|\omega\|^2\right)^{-\beta} > 0$$

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[Wu & Schaback (1993)]

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  [Narcowich, Ward & Wendland (2005)]

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- $K_\nu > 0 \Longrightarrow \Phi_{s,\beta} > 0$

Examples

Let $r = \varepsilon\|\boldsymbol{x}\|$, $t = \frac{\|\boldsymbol{\omega}\|}{\varepsilon}$

β	$\Phi_{3,\beta}(r)/\sqrt{2\pi}$	$\varepsilon^3\widehat{\Phi}_{3,\beta}(t)$
3	$(1+r)\,\frac{e^{-r}}{16}$	$\left(1+t^2\right)^{-3}$
4	$\left(3+3r+r^2\right)\,\frac{e^{-r}}{96}$	$\left(1+t^2\right)^{-4}$
5	$\left(15+15r+6r^2+r^3\right)\,\frac{e^{-r}}{768}$	$\left(1+t^2\right)^{-5}$
6	$\left(105+105r+45r^2+10r^3+r^4\right)\,\frac{e^{-r}}{7680}$	$\left(1+t^2\right)^{-6}$

Table: Matérn functions and their Fourier transforms for $s = 3$ and various choices of β.

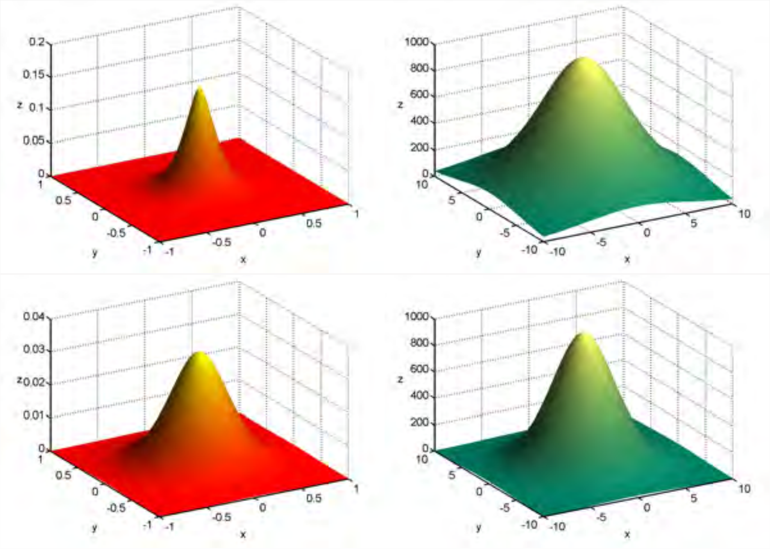

Figure: Matérn functions and Fourier transforms for $\Phi_{3,3}$ (top) and $\Phi_{3,6}$ (bottom) centered at the origin in $\mathbb{R}^2$ ($\varepsilon = 10$ scaling used).

Implicit Smoothing [F. (1999), Beatson & Bui (2007)]

Crucial property of Matérn RBFs

$$\Phi_{s,\beta} * \Phi_{s,\alpha} = \Phi_{s,\alpha+\beta}, \qquad \alpha, \beta > 0$$

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Therefore with

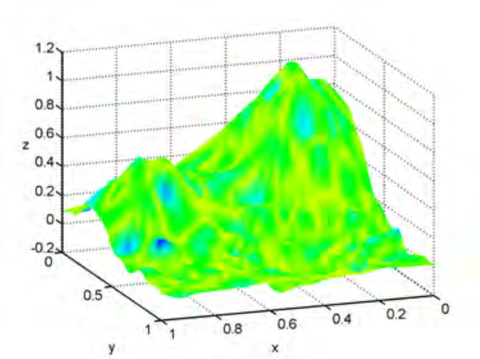
$$u(\boldsymbol{x}) = \sum_{j=1}^{N} c_j \Phi_{s,\beta}(\boldsymbol{x} - \boldsymbol{x}_j)$$

we get

$$\begin{aligned} u * \Phi_{s,\alpha} &= \left[\sum_{j=1}^{N} c_j \Phi_{s,\beta}(\cdot - \boldsymbol{x}_j)\right] * \Phi_{s,\alpha} \\ &= \sum_{j=1}^{N} c_j \Phi_{s,\alpha+\beta}(\cdot - \boldsymbol{x}_j) \\ &=: S_\alpha u \end{aligned}$$

Return

Noisy and smoothed interpolants



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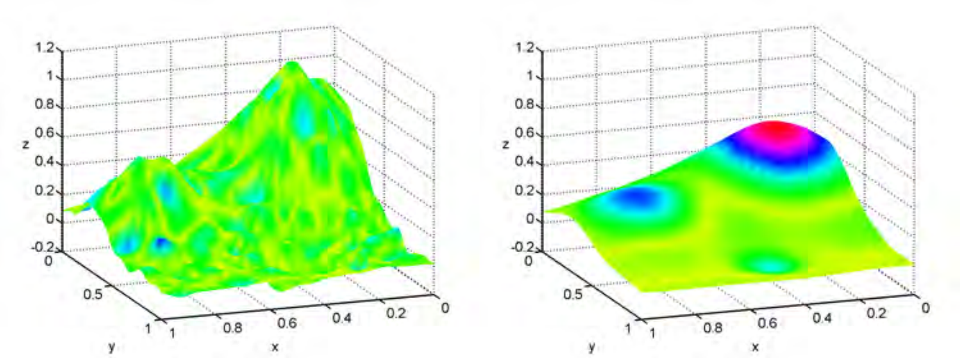

Figure: Solved and evaluated with $\Phi_{3,3}$ (left), evaluated with $\Phi_{3,4}$ (right).

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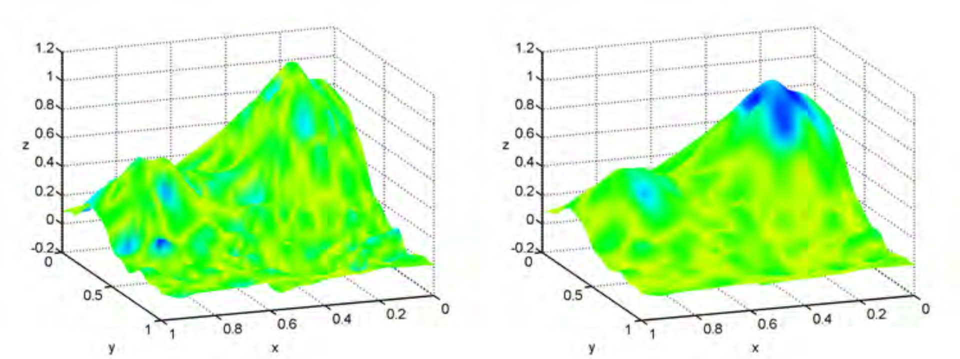

Figure: Solved and evaluated with $\Phi_{3,3}$ (left), evaluated with $\Phi_{3,3.2}$ (right).

Algorithm (Approximate Newton Iteration)

[F. & Jerome (1999), F., Gartland & Jerome (2000), F. (2002), Bernal & Kindelan (2007)]

- Create computational “grids” $\mathcal{X}_1 \subseteq \cdots \subseteq \mathcal{X}_K \subset \Omega$, and choose initial guess u_0
- For $k = 1, 2, \ldots, K$
  1. Solve the linearized problem

$$L_{u_{k-1}} v = f - \mathcal{L}u_{k-1} \quad \text{on } \mathcal{X}_k$$

  3. Perform Newton update of k-th iterate

$$u_k = u_{k-1} + v$$

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  2. Perform optional smoothing of Newton correction
  $$v \leftarrow S_{\theta_k} v$$
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Why Do We Need Smoothing?

- Approximate Newton method based on approximation of $(F')^{-1}$ by numerical inversion T_h, i.e., for u, v in appropriate Banach spaces

$$\| \left[F'(u) T_h(u) - I \right] v \| \leq \tau(h) \|v\|$$

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- [Jerome (1985)] used Newton-Kantorovich theory to show an appropriate smoothing of the Newton update will yield global superlinear convergence for approximate Newton iteration

Hörmander's Smoothing

Theorem ([Hörmander (1976), F. & Jerome (1999)])

Let $0 \le \ell \le k$ *and* p *be integers. In Sobolev spaces* $W_p^k(\Omega)$ *there exist smoothings* S_θ *satisfying*

1. *Semigroup property:* $\|S_\theta u - u\|_{L_p} \to 0$ *as* $\theta \to \infty$
2. *Bernstein inequality:* $\|S_\theta u\|_{W_p^k} \le C\theta^{k-\ell}\|u\|_{W_p^\ell}$
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Note: Jackson and Bernstein theorems known for interpolation with Matérn functions, but not for smoothing [Beatson & Bui (2007)]

Non-symmetric RBF Collocation

Linear(ized) BVP

$$\begin{aligned} Lu(\boldsymbol{x}) &= f(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega \subset \mathbb{R}^s \\ Bu(\boldsymbol{x}) &= g(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial\Omega \end{aligned}$$

Use *Ansatz* $\quad u(\boldsymbol{x}) = \sum_{j=1}^{N} c_j \varphi(\|\boldsymbol{x} - \boldsymbol{x}_j\|) \quad$ [Kansa (1990)]

Collocation at $\{\underbrace{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_I}_{\in\Omega}, \underbrace{\boldsymbol{x}_{I+1}, \ldots, \boldsymbol{x}_N}_{\in\partial\Omega}\}$ leads to linear system

$$\mathsf{A}\boldsymbol{c} = \boldsymbol{y}$$

with

$$\mathsf{A} = \begin{bmatrix} \mathsf{A}_L \\ \mathsf{A}_B \end{bmatrix}, \qquad \boldsymbol{y} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{bmatrix}$$

Computational Grids for $N = 289$

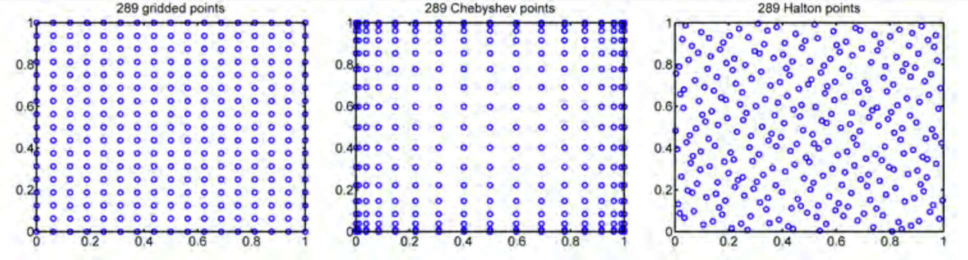

Figure: Uniform (left), Chebyshev (center), and Halton (right) collocation points.

Numerical Illustration

- Nonlinear PDE: $\mathcal{L}u = f$

$$\begin{aligned} -\mu^2\nabla^2 u - u + u^3 &= f, \qquad \text{in } \Omega = (0,1)\times(0,1) \\ u &= 0, \qquad \text{on } \partial\Omega \end{aligned}$$

- Linearized equation: $L_u v = f - \mathcal{L}u$

$$-\mu^2\nabla^2 v + (3u^2 - 1)v = f + \mu^2\nabla^2 u + u - u^3$$

- Computational grids: uniformly spaced, Chebyshev, or Halton points in $[0,1]\times[0,1]$
- Use $\mu = 0.1$ for all examples

Numerical Illustration (cont.)

- RBFs used: Matérn functions

$$\Phi_{s,\beta}(\boldsymbol{x}) = \frac{K_{\beta-\frac{s}{2}}(\|\varepsilon\boldsymbol{x}\|)\|\varepsilon\boldsymbol{x}\|^{\beta-\frac{s}{2}}}{2^{\beta-1}\Gamma(\beta)}, \qquad \beta > \frac{s}{2}$$

$$\Phi_{s,\beta}(\mathbf{0}) = \frac{\Gamma(\beta-\frac{s}{2})}{\sqrt{2^s}\Gamma(\beta)}$$

with

$$\begin{aligned}\nabla^2\Phi_{s,\beta}(\boldsymbol{x}) &= \Big[\Big(\|\varepsilon\boldsymbol{x}\|^2 + 4(\beta-\frac{s}{2})^2\Big)K_{\beta-\frac{s}{2}}(\|\varepsilon\boldsymbol{x}\|) \\ &\quad -2(\beta-\frac{s}{2})\|\varepsilon\boldsymbol{x}\|K_{\beta-\frac{s}{2}+1}(\|\varepsilon\boldsymbol{x}\|)\Big]\frac{\varepsilon^2\|\varepsilon\boldsymbol{x}\|^{\beta-\frac{s}{2}-2}}{2^{\beta-1}\Gamma(\beta)}\end{aligned}$$

$$\nabla^2\Phi_{s,\beta}(\mathbf{0}) = \frac{\varepsilon^2\Gamma(\beta-\frac{s}{2}-1)}{\sqrt{2^s}\Gamma(\beta)}$$

- Fixed shape parameter $\varepsilon = \sqrt{N}/2$

```
function rbf_definitionMatern
global rbf Lrbf
rbf = @(ep,r,s,b) matern(ep,r,s,b);  % Matern functions
Lrbf = @(ep,r,s,b) Lmatern(ep,r,s,b); % Laplacian

function rbf = matern(ep,r,s,b)
scale = gamma(b-s/2)*2^(-s/2)/gamma(b);
rbf = scale*ones(size(r));
nz = find(r~=0);
rbf(nz) = 1/(2^(b-1)*gamma(b))*besselk(b-s/2,ep*r(nz))...
          .*(ep*r(nz)).^(b-s/2);

function Lrbf = Lmatern(ep,r,s,b)
scale = -ep^2*gamma(b-s/2-1) / (2^(s/2)*gamma(b));
Lrbf = scale*ones(size(r));
nz = find(r~=0);
Lrbf(nz) = ep^2/(2^(b-1)*gamma(b))*(ep*r(nz)).^(b-s/2-2).*...
           (((ep*r(nz)).^2+4*(b-s/2)^2).* besselk(b-s/2,ep*r(nz)).
             -2*(b-s/2)*(ep*r(nz)).*besselk(b-s/2+1,ep*r(nz)));
```

Exact solution and initial guess

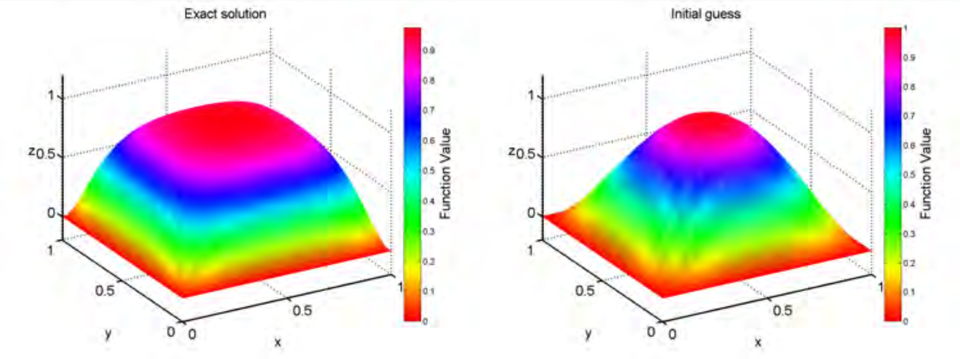

Figure: Solution u (left), initial guess $u(x, y) = 16x(1 - x)y(1 - y)$ (right).

Newton and Nash Iteration on Single Uniform Grid

	Newton		Nash		
N	RMS-error	K	RMS-error	K	ρ
25(41)	$1.356070\,10^{-1}$	7	$1.064151\,10^{-1}$	5	0.328
81(113)	$2.404571\,10^{-2}$	9	$2.183223\,10^{-2}$	10	0.527
289(353)	$4.237178\,10^{-3}$	9	$2.276646\,10^{-3}$	20	0.953
1089(1217)	$8.982388\,10^{-4}$	9	$3.450676\,10^{-4}$	37	0.999
4225(4481)	$1.855711\,10^{-4}$	10	$7.780351\,10^{-5}$	32	0.999

Matérn parameters: $s = 3$, $\beta = 4$, uniform points

Nash smoothing: $\alpha = \rho^{\theta b^k}$ with $\theta = 1.1435$, $b = 1.2446$
Sample MATLAB calls: `Newton_NLPDE(289,'u',3,4,0)`, `Newton_NLPDE(289,'u',3,4,0.953)`

Newton approximations and updates for $N = 289$

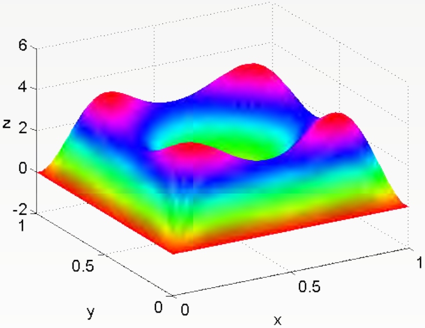

Figure: Approximate solution (left), and updates (right).

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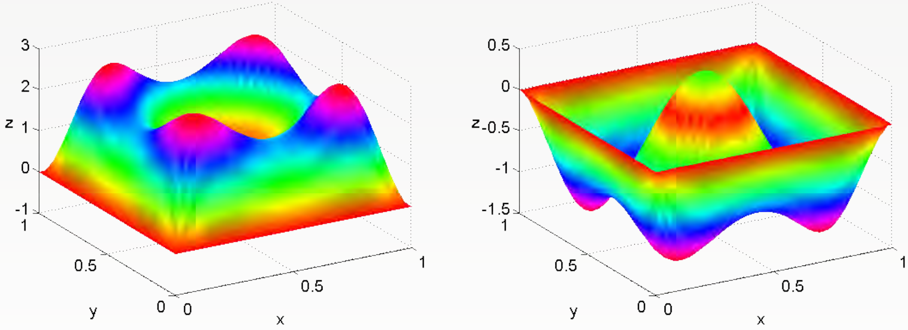

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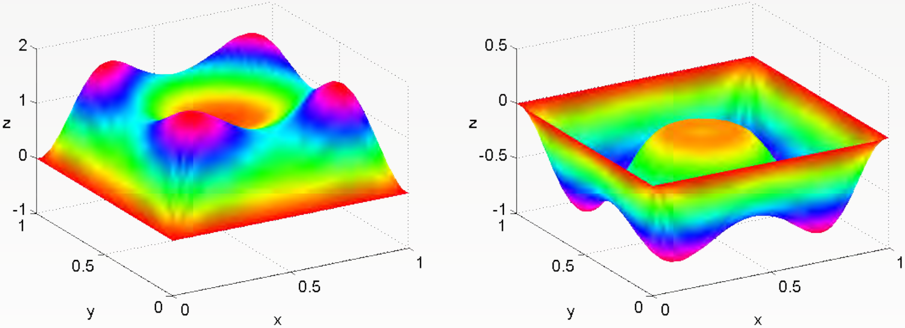

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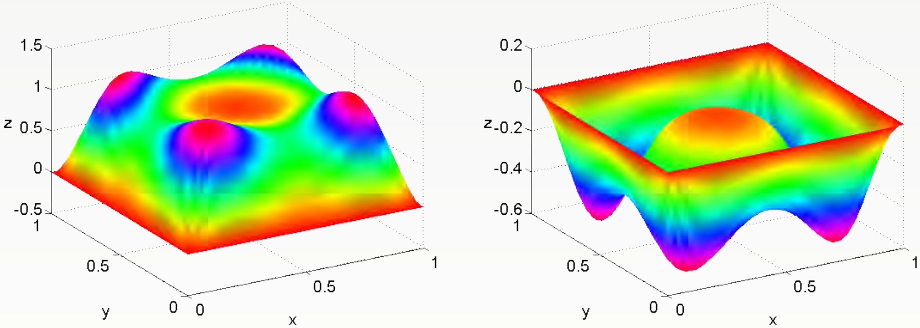

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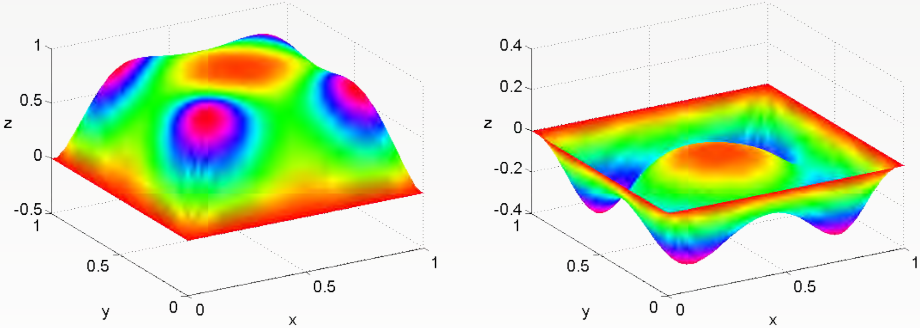

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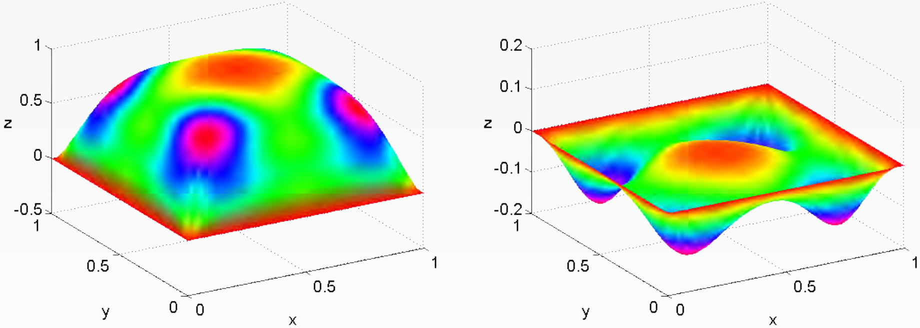

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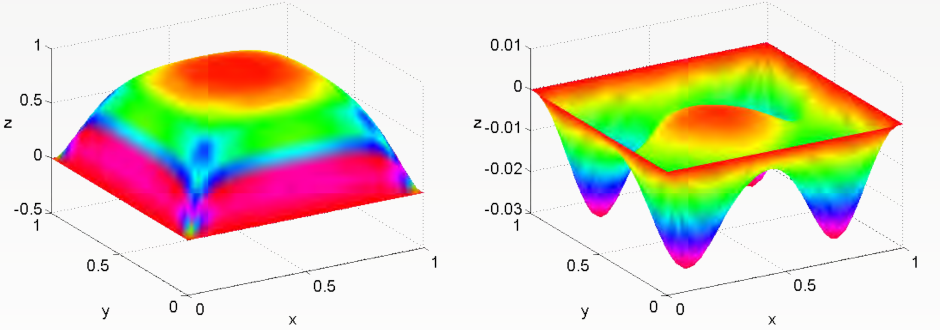

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Newton approximations and updates for $N = 289$

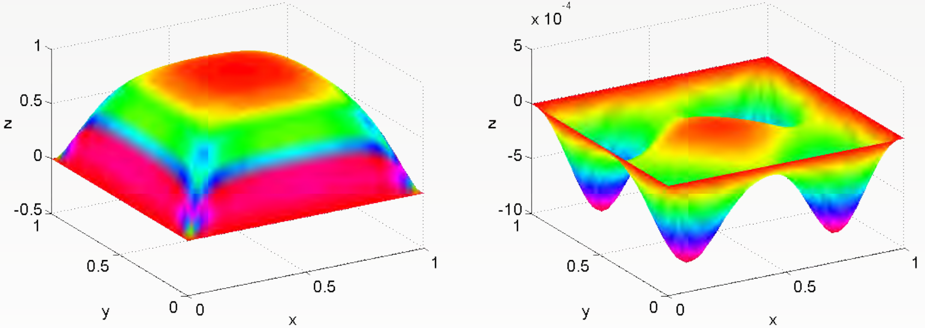
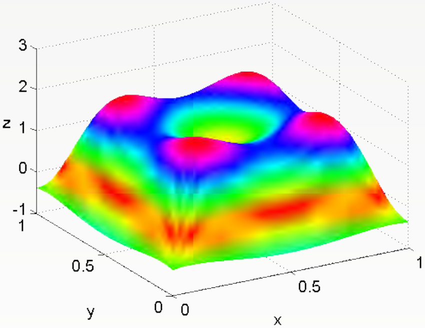


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$



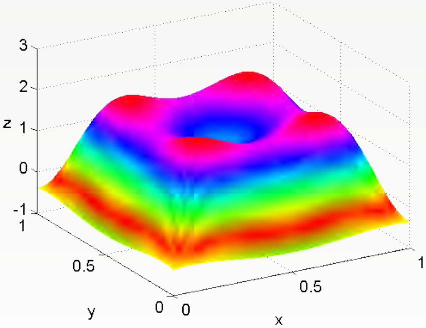
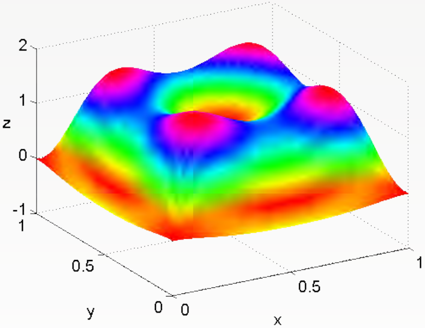


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$



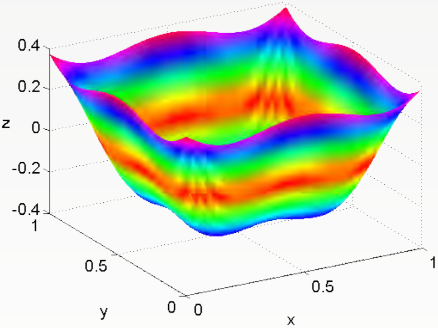


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

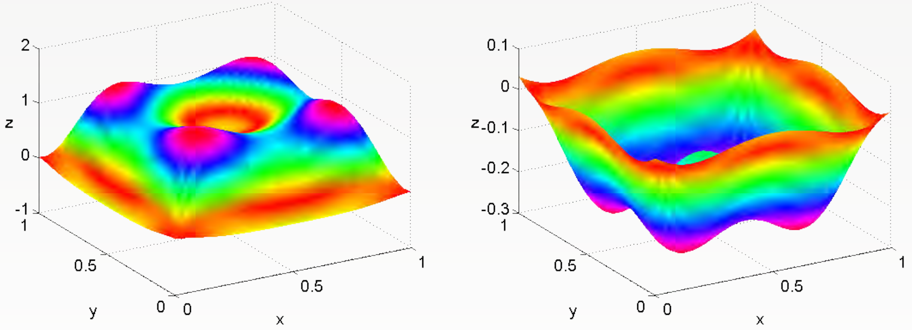
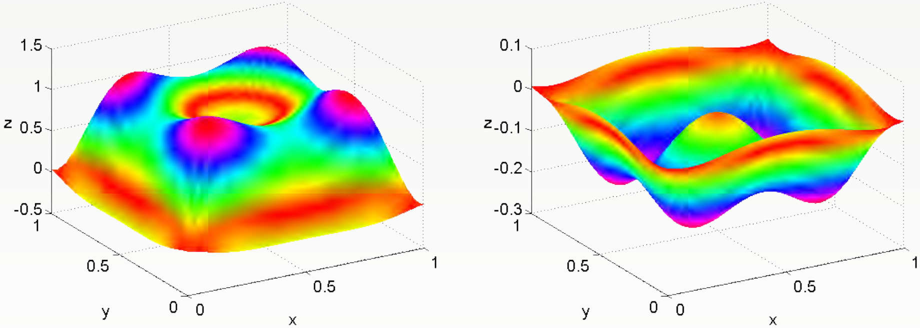


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$



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Nash approximations and updates for $N = 289$

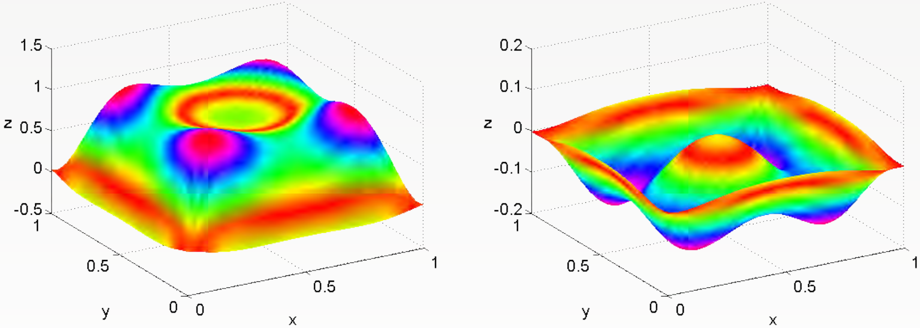
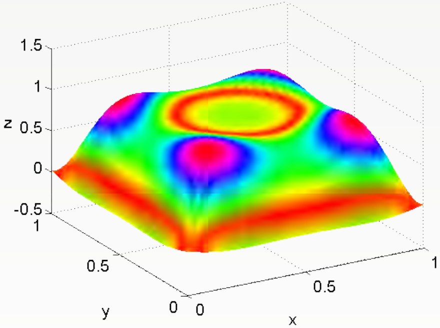


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$



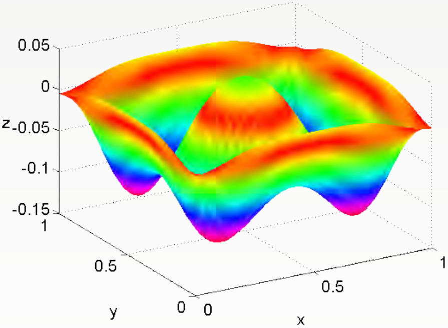


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

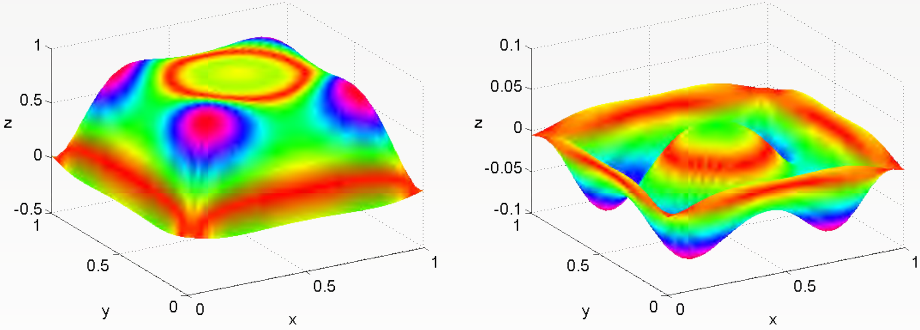


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

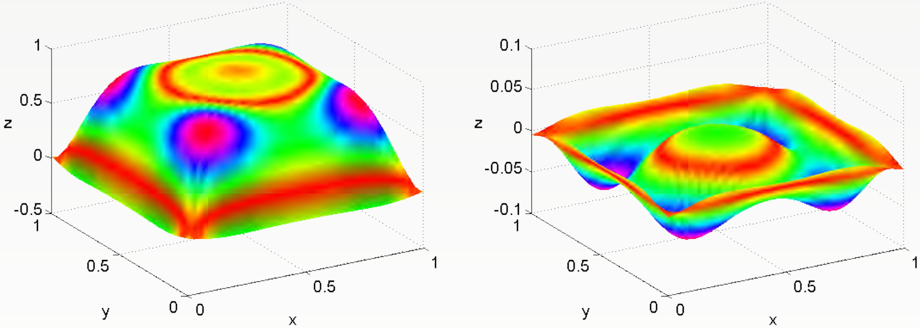
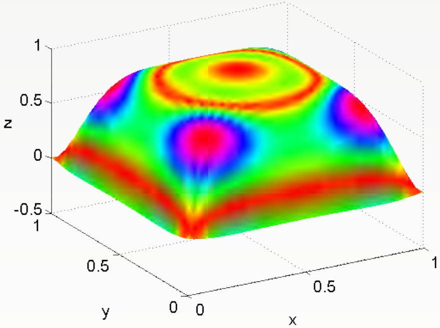


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$



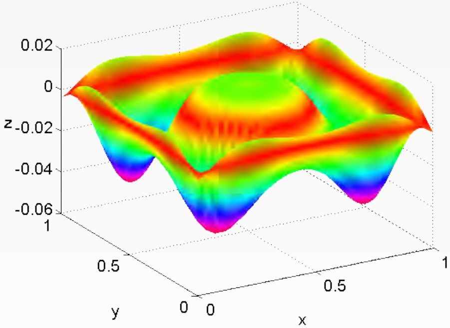


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

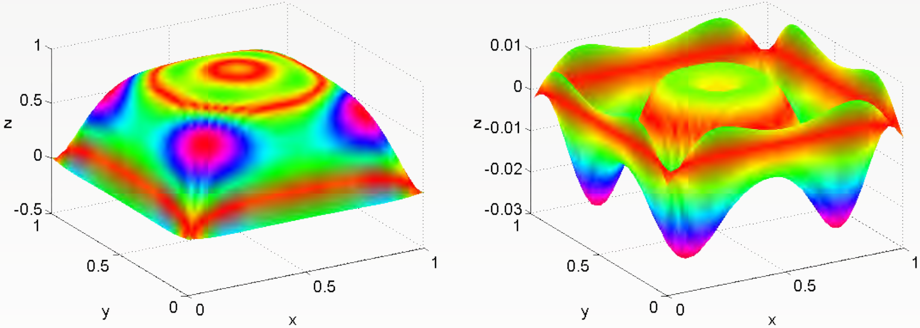


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

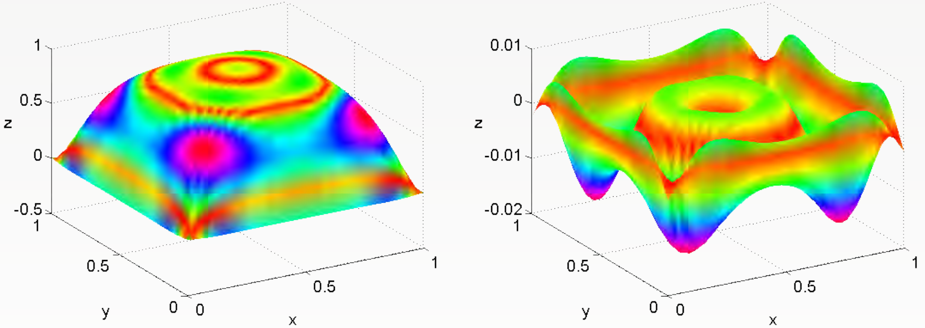


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

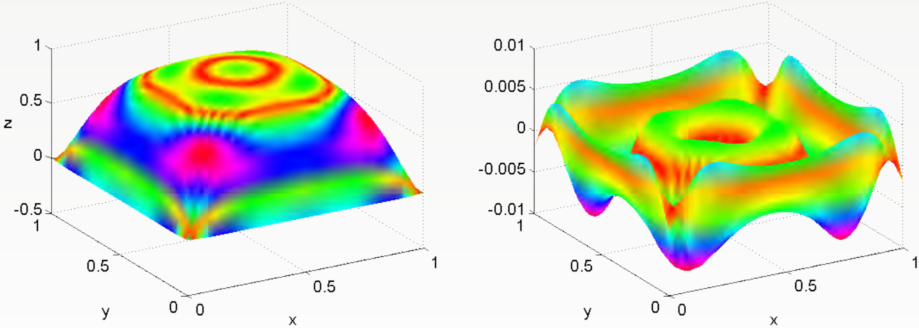


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

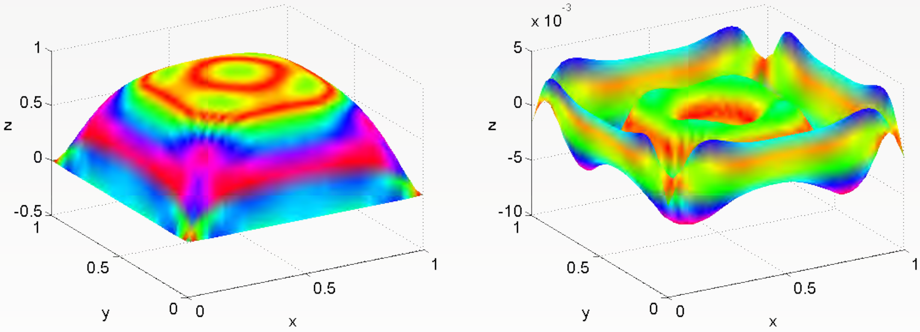


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

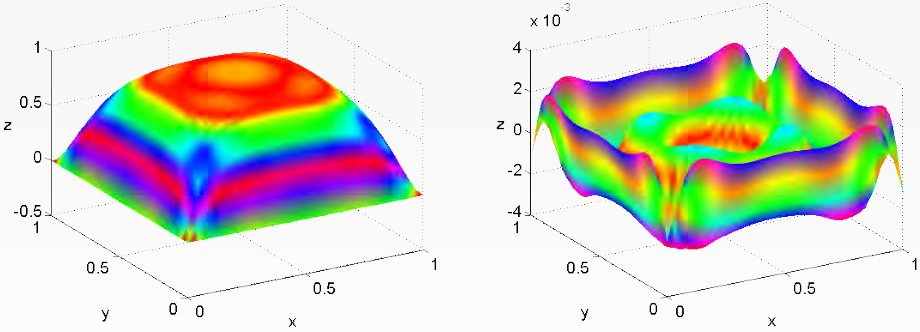
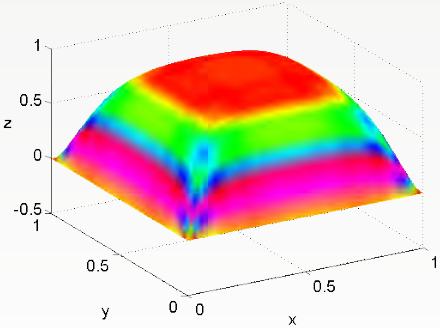


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$



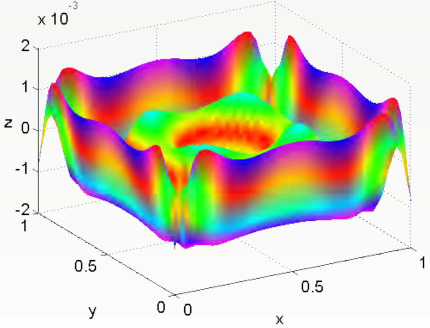
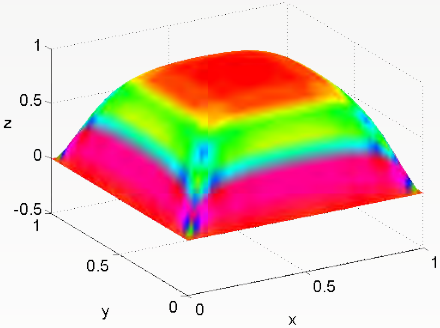


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$



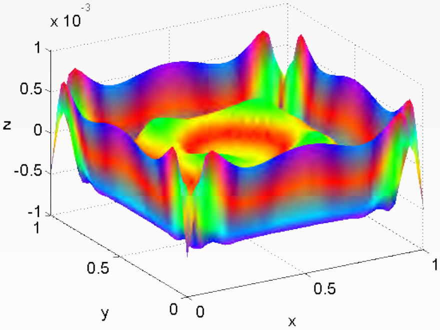


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

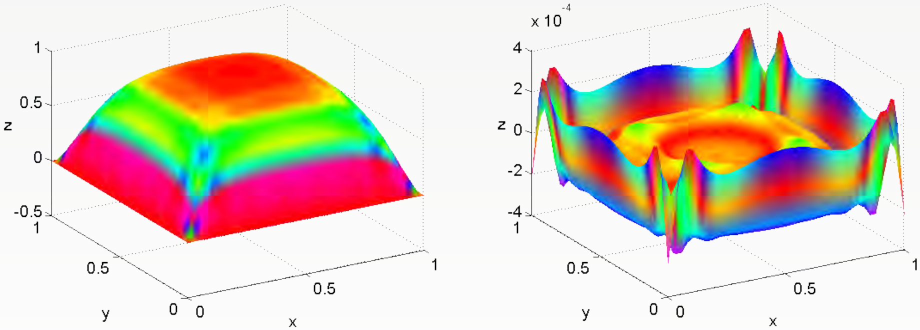


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$

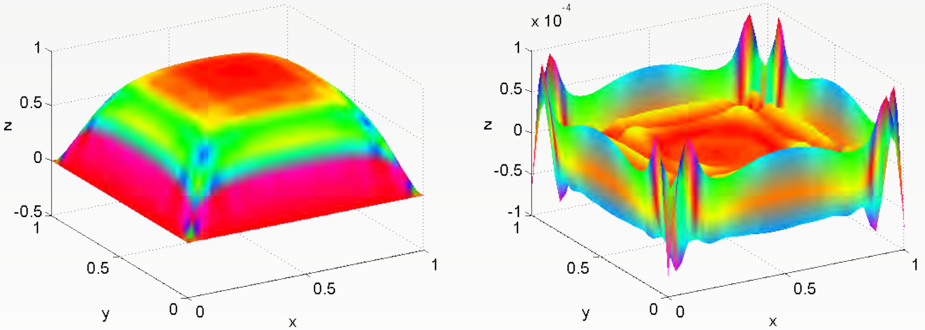
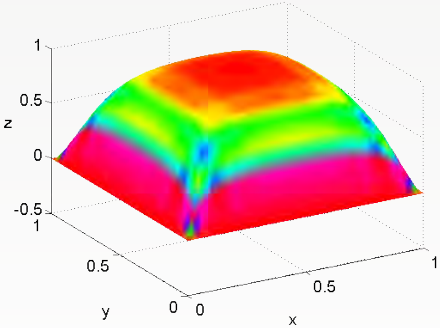


Figure: Approximate solution (left), and updates (right).

Nash approximations and updates for $N = 289$



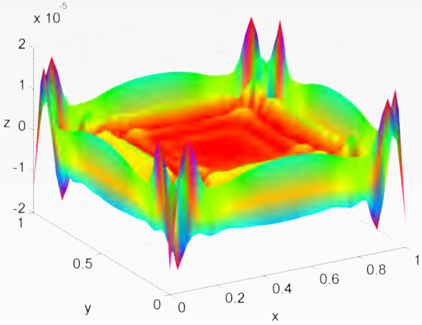


Figure: Approximate solution (left), and updates (right).

Error drops and smoothing parameters for $N = 289$

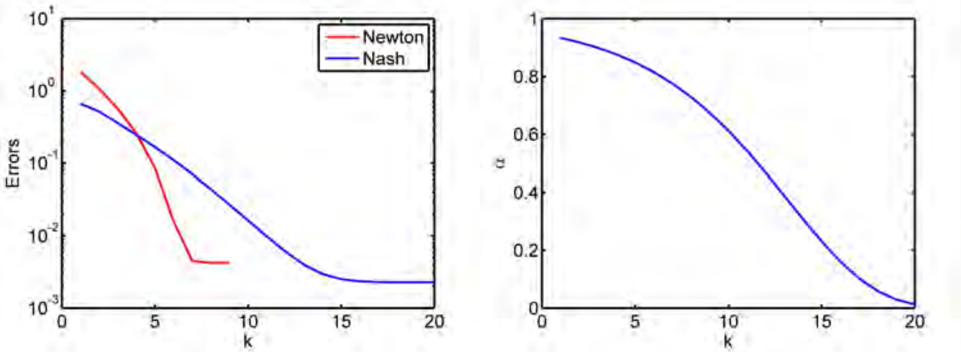


Figure: Drop of RMS error (left), and smoothing parameter α (right).

Newton and Nash Iteration on Single Chebyshev Grid

	Newton		Nash		
N	RMS-error	K	RMS-error	K	ρ
25(41)	$8.809920\,10^{-2}$	8	$7.825548\,10^{-2}$	8	0.299
81(113)	$3.546179\,10^{-3}$	9	$3.277817\,10^{-3}$	8	0.541
289(353)	$6.198255\,10^{-4}$	9	$8.420461\,10^{-5}$	35	0.999
1089(1217)	$1.495895\,10^{-4}$	8	$5.470357\,10^{-6}$	37	0.999
4225(4481)	$3.734340\,10^{-4}$	7	$7.790757\,10^{-6}$	35	0.999

Matérn parameters: $s = 3$, $\beta = 4$, Chebyshev points

Nash smoothing: $\alpha = \rho^{\theta b^k}$ with $\theta = 1.1435$, $b = 1.2446$

Newton and Nash Iteration on Single Halton Grid

	Newton		Nash		
N	RMS-error	K	RMS-error	K	ρ
25(41)	$3.160062\,10^{-2}$	7	$2.597881\,10^{-2}$	7	0.389
81(113)	$9.828342\,10^{-3}$	9	$8.125240\,10^{-3}$	13	0.791
289(353)	$2.896087\,10^{-3}$	9	$1.981563\,10^{-3}$	15	0.953
1089(1217)	$9.480208\,10^{-4}$	9	$3.305680\,10^{-4}$	36	0.999
4225(4481)	$3.563199\,10^{-4}$	8	$1.330167\,10^{-4}$	37	0.999

Matérn parameters: $s = 3$, $\beta = 4$, Halton points

Nash smoothing: $\alpha = \rho^{\theta b^k}$ with $\theta = 1.1435$, $b = 1.2446$

Convergence for Different Collocation Point Sets

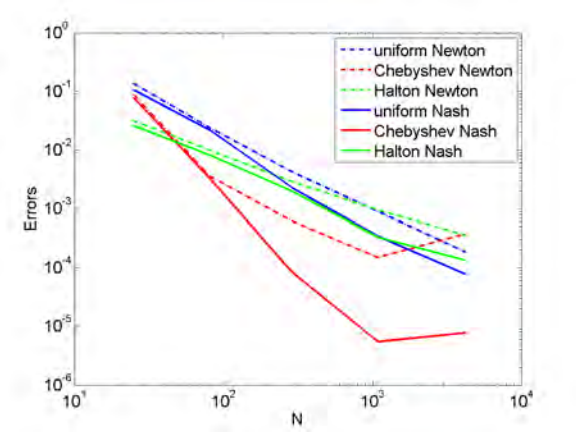


Figure: Convergence of Newton and Nash iteration for different choices of collocation points.

Newton and Nash Iteration on Single Chebyshev Grid

	Newton		Nash		
β	RMS-error	K	RMS-error	K	ρ
3	$4.022065\,10^{-3}$	7	$9.757401\,10^{-4}$	38	0.999
4	$6.198255\,10^{-4}$	9	$8.420461\,10^{-5}$	35	0.999
5	$1.803903\,10^{-4}$	9	$9.620937\,10^{-5}$	8	0.447
6	$2.715679\,10^{-4}$	8	$1.259029\,10^{-4}$	8	0.376
7	$2.279834\,10^{-4}$	8	$1.237608\,10^{-4}$	9	0.320

Matérn parameters: $N = 289$, $s = 3$, Chebyshev points

Nash smoothing: $\alpha = \rho^{\theta b^k}$ with $\theta = 1.1435$, $b = 1.2446$

Convergence for Different Matérn Functions

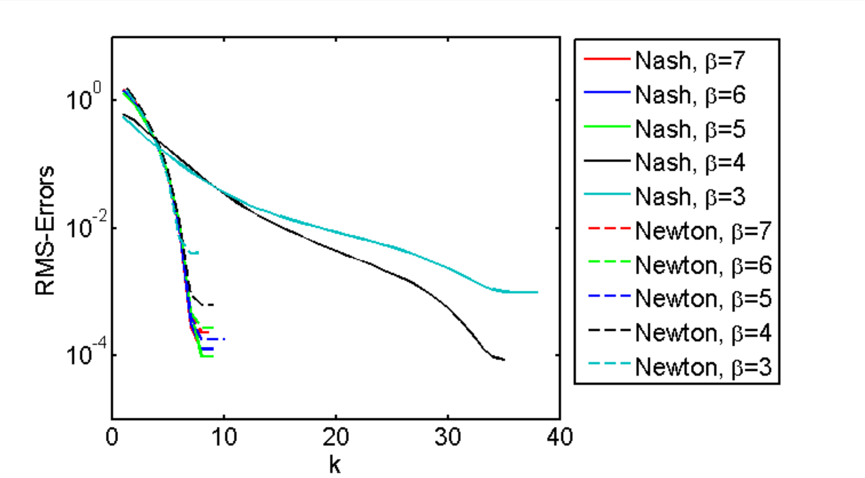


Figure: Convergence of Newton and Nash iteration for different Matérn functions (β).

Conclusions and Future Work

- Conclusions
  - Implicit smoothing improves convergence of non-symmetric RBF collocation for nonlinear test case
  - Implicit smoothing easy and cheap to implement for RBF collocation
  - Smoothing with Matérn kernels recovers some of the “loss of derivative” of numerical inversion. Can’t really work since saturated.
  - More accurate results than earlier with MQ-RBFs
  - Required more than 2000^2 points with earlier FD experiments [F., Gartland & Jerome (2000)] (without smoothing) for same accuracy as 1089 points here

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  - More accurate results than earlier with MQ-RBFs
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- Future Work
  - Try mesh refinement within Newton algorithm via adaptive collocation
  - Further investigate use of different Matérn parameters
  - Couple smoothing parameter to current residuals
  - Do smoothing with an approximate smoothing kernel
  - Apply similar ideas in RBF-PS framework

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