

A Posteriori Existence in Numerical Computations

Christoph Ortner

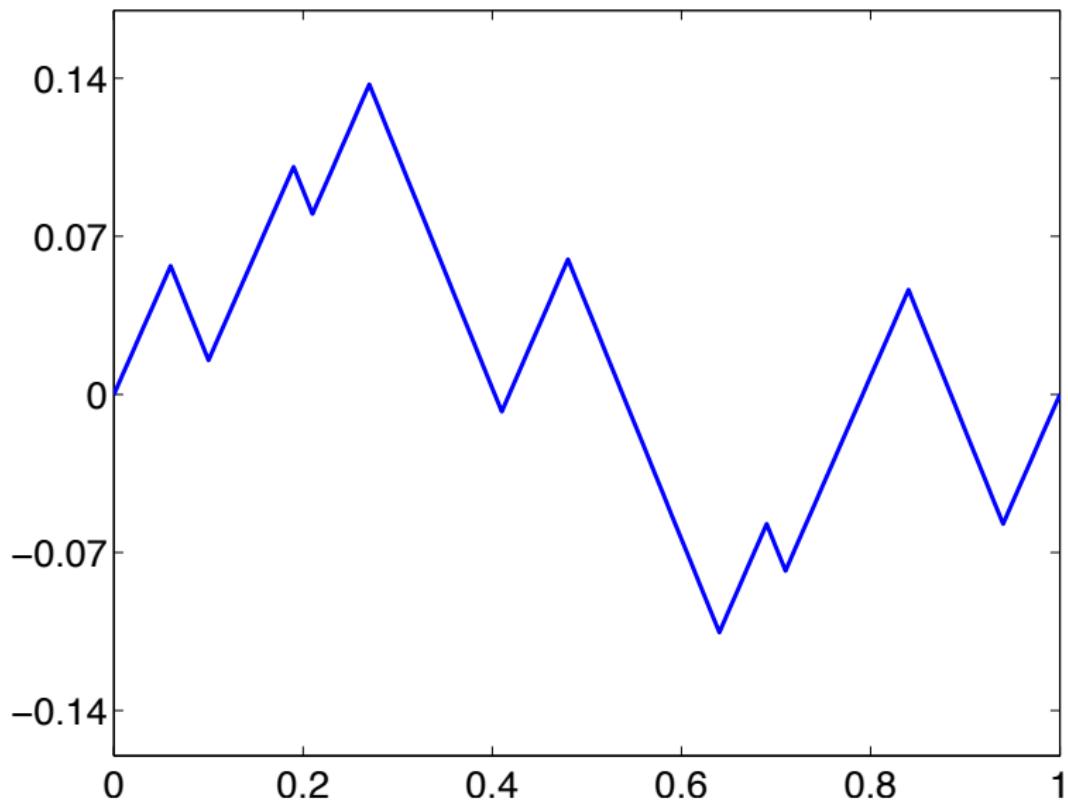
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OXPDE: Oxford Centre for Nonlinear PDE

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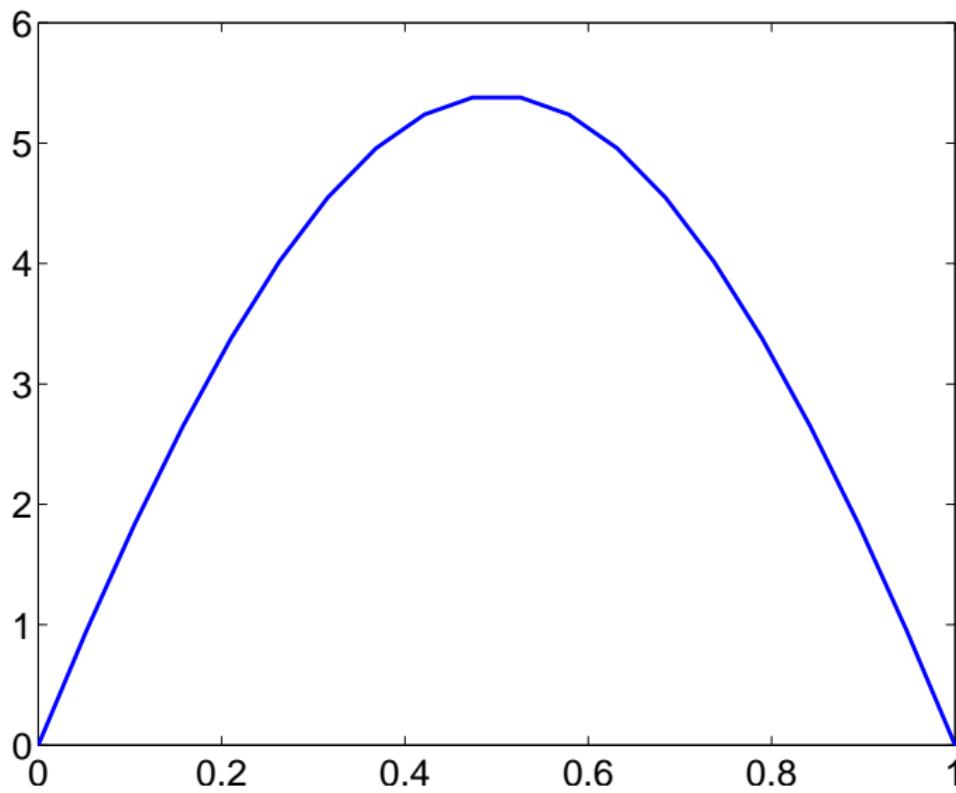
Introduction

- Non-linear problems are handled via the implicit function theorem.

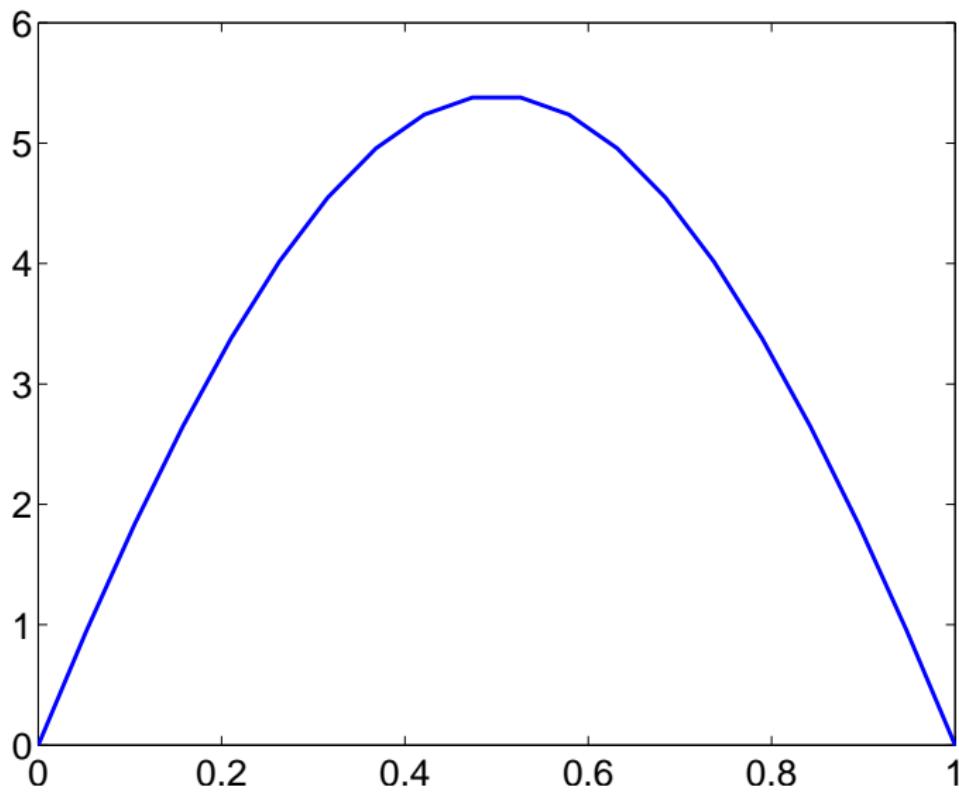
Example: $-(u_x^3 - u_x)_x + u = 0, \quad u(0) = u(1) = 0$



Example: $-u_{xx} = u^2 + 22.60$, $u(0) = u(1) = 0$



Example: $-u_{xx} = u^2 + 22.61$, $u(0) = u(1) = 0$



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Abstract Setting: For, \mathcal{X}, \mathcal{Y} Banach spaces, $\mathcal{F} : \mathcal{X} \rightarrow \mathcal{Y}$, solve

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- non-existence of solutions
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- non-existence of solutions
- spurious solutions in numerical approximations

Given a computed “approximate solution” U , does an exact solution u exist which is “near” U ?

Introduction

Basic Idea for an *A Posteriori Existence Proof*:

- Let $U \in \mathcal{X}$ be a computed “approximation”. U solves

$$v \mapsto \mathcal{F}(v) - \mathcal{F}(U) = 0$$

- $u \in \mathcal{X}$ satisfies $\mathcal{F}(u) = 0$ if it solves

$$v \mapsto \mathcal{F}(v) - \mathcal{F}(U) = -\mathcal{F}(U)$$

(this perturbs the above problem)

- Estimate $\|\mathcal{F}(U)\|_{\mathcal{Y}}$ and $\|\mathcal{F}'(U)^{-1}\|_{\mathcal{L}(\mathcal{Y}, \mathcal{X})}$ and apply the Inverse Function Theorem.

History

- **Monotonicity Methods:** inclusion in an function interval
 $u(x) \in [u_0(x), u_1(x)]$; [Collatz, ArchMath, 1952]
- Methods based on interval arithmetic [Nakao et al., from about 1988]
- **Fixed point methods:** applications mostly to nonlinear Poisson problems, rigorous computational proofs; [Plum et al., from about 1990]
- Shadowing: for dynamical systems; [Hammel et al., Complexity, 1987]

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- Bibliography on **Enclosure Methods** by G. Bohlender

A Posteriori Existence : Abstract Result

Suppose that \mathcal{F} is Fréchet differentiable and that

$$\|\mathcal{F}'(v) - \mathcal{F}'(w)\|_{\mathcal{L}(\mathcal{X}, \mathcal{Y})} \leq g(\|w\|_{\mathcal{X}}; \|v - w\|_{\mathcal{X}}),$$

where $g(s; \cdot)$ is continuous and increasing.

Proposition

Suppose that $U \in \mathcal{X}$ and $R > 0$ satisfy

$$(i) \quad \|\mathcal{F}(U)\|_{\mathcal{Y}} \leq \eta$$

$$(ii) \quad \|\mathcal{F}'(U)^{-1}\|_{\mathcal{L}(\mathcal{Y}, \mathcal{X})} \leq 1/\sigma$$

$$(iii) \quad \eta + \int_0^R g(\|U\|_{\mathcal{X}}; r) dr \leq \sigma R$$

$$(iv) \quad g(\|U\|_{\mathcal{X}}; R) < \sigma$$

Then there exists a unique $u \in B(U, R)$ such that $\mathcal{F}(u) = 0$.

Proof: Track constants in proof of Inverse Function Theorem.

A Posteriori Existence : Proof

1. Define Fixed-Point Map: $\mathcal{N} : \mathcal{X} \rightarrow \mathcal{X}$

$$\mathcal{F}'(U)(\mathcal{N}(v) - U) = -\mathcal{F}(U) - [\mathcal{F}(v) - \mathcal{F}(U) - \mathcal{F}'(U)(v - U)]$$

$\rightarrow \mathcal{F}(u) = 0$ if, and only if, $\mathcal{N}(u) = u$.

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2. $\mathcal{N}(B(U, R)) \subset B(U, R)$:

$$\begin{aligned} \|\mathcal{N}(v) - U\|_{\mathcal{X}} &\leq \|\mathcal{F}'(U)^{-1}\|_{\mathcal{L}(\mathcal{Y}, \mathcal{X})} \times \left(\|\mathcal{F}(U)\|_{\mathcal{Y}} + \right. \\ &\quad \left. + \|\mathcal{F}(v) - \mathcal{F}(U) - \mathcal{F}'(U)(v - U)\|_{\mathcal{Y}} \right) \stackrel{!}{\leq} R \end{aligned}$$

\rightarrow reduces to $\sigma^{-1}(\eta + \int_0^R g(r)dr) \leq R$

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3. \mathcal{N} is a contraction: reduces to the condition to $\sigma^{-1}g(R) < 1$

Example: Semi-linear Poisson Problem

Strong form: Ω convex domain in \mathbb{R}^2

$$\begin{aligned}-\Delta u &= f(u), && \text{in } \Omega; \\ u &= 0, && \text{on } \partial\Omega.\end{aligned}$$

Example: Semi-linear Poisson Problem

Strong form: Ω convex domain in \mathbb{R}^2

$$\begin{aligned}-\Delta u &= f(u), && \text{in } \Omega; \\ u &= 0, && \text{on } \partial\Omega.\end{aligned}$$

Weak form: Find $u \in H_0^1(\Omega)$ such that

$$\int_{\Omega} [\nabla u \cdot \nabla w - f(u)w] dx = 0 \quad \forall w \in H_0^1(\Omega)$$

- $\mathcal{X} = H_0^1(\Omega)$, $\mathcal{Y} = H^{-1}(\Omega)$
- $\langle \mathcal{F}(u), w \rangle = \int_{\Omega} [\nabla u \cdot \nabla w - f(u)w] dx$
- $\langle \mathcal{F}'(u)v, w \rangle = \int_{\Omega} [\nabla v \cdot \nabla w - f'(u)vw] dx$

Discretization

- \mathcal{T} : regular subdivision of Ω .
- $S_0(\mathcal{T}) \subset H_0^1(\Omega)$: conforming finite element space.
- Galerkin Projection:

$$\langle \mathcal{F}(U), W \rangle = \int_{\Omega} [\nabla U \cdot \nabla W + f(U)W] dx = 0 \quad \forall W \in S_0(\mathcal{T}).$$

(solved using Newton's method)

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We need:

- I. Residual Estimate: $\|\mathcal{F}(U)\|_{\mathcal{Y}} \leq \eta$
- II. Stability Estimate: $\|\mathcal{F}'(U)^{-1}\|_{\mathcal{L}(\mathcal{Y}, \mathcal{X})} \leq 1/\sigma$
- III. Bound the Modulus of Continuity of \mathcal{F}'

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Example: $-\Delta u = u^2 + \lambda$ on $\Omega = (0, 1)^2 \Rightarrow \mathcal{F}'(u)v = -\Delta v - 2uv$

$$\begin{aligned} \|(-\Delta v - 2u_1 v) - (-\Delta v - 2u_2 v)\|_{H^{-1}} &\leq \|2(u_1 - u_2)v\|_{H^{-1}} \\ \implies g(R) &= 2C_s^3 R \end{aligned}$$

where $C_s \leq 0.55$ is the constant for $\|u\|_{L^3} \leq C_s \|\nabla u\|_{L^2}$.

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More general: $-\Delta u = f(u)$

If f'' has p -growth (in 2D) then

$$g(s; R) = C(1 + s + R)^p R$$

where C depends on embedding constants which can be computed explicitly and on f''

I. Residual Estimate – version 1

Standard Residual Estimate: If U is an *exact* solution of the finite element discretization then

$$\begin{aligned}\|\mathcal{F}(U)\|_{H^{-1}} \leq C(\mathcal{T}) & \left[\sum_{T \in \mathcal{T}} h_T^2 \|\Delta U + f(U)\|_{L^2(T)}^2 \right. \\ & \left. + \sum_{e \in \mathcal{E}} h_e \|[\nabla U]\|_{L^2(e)}^2 \right]^{1/2}\end{aligned}$$

Advantages:

- efficient to compute
- analytically well-understood (lower bounds, optimality, etc.)

Problems:

- Difficult to obtain a sharp constant $C(\mathcal{T})$
- U is in general not an *exact* discrete solution, so also need to estimate the *discrete residual*

I. Residual Estimate – version 2

Alternative Idea: Let $G \in H(\text{div})$

$$\begin{aligned}\int [\nabla U \cdot \nabla w - fw] dx &= \int [(\nabla U - G) \cdot \nabla w + G \nabla w - fw] dx \\&= \int (\nabla U - G) \cdot \nabla w dx - \int (\text{div} G + f) w dx \\&\leq \|\nabla U - G\|_{L^2} \|\nabla w\|_{L^2} + C_p \|\text{div} G + f\|_{L^2} \|\nabla w\|_{L^2}\end{aligned}$$

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Residual Estimate: [Repin], [Plum, LinearAlgebraApp, 2001]

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$$\|\Delta u + f(u)\|_{H^{-1}} \leq \|\nabla U - G\|_{L^2} + C_p \|\text{div} G + f\|_{L^2}$$

- Compute G by solving a quadratic optimization problem:

$$\|\nabla U - G\|_{L^2}^2 + C_p^2 \|\text{div} G + f\|_{L^2}^2 \longrightarrow \min$$

- In my examples: G minimizes this quadratic in $S_0(\mathcal{T})^n$

II. Stability Estimate – version 2

Residual Estimate:

$$\|\Delta u + f(u)\|_{H^{-1}} \leq \|\nabla U - G\|_{L^2} + C_p \|\operatorname{div} G + f\|_{L^2} =: \eta$$

Advantages of this Estimate:

- Requires only the computation of the Poincaré constant
- Seems quite sharp for many problems
- Requires no information on U or G , so can be made **rigorous** in exact arithmetic (Mathematica or Maple) or interval arithmetic

Disadvantage:

- G may be more expensive to compute than the solution

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Optimal Constant:

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Challenges:

- In general, $\Sigma > \sigma_{\text{opt}}$, so we require an error estimate
- H^1 -eigenvalue problem is ill-posed since eigenvalues cluster at 1.
- ? Can Σ be computed reliably?

II. Stability Estimate

Some Possibilities:

- Weinstein bounds [Chatelin, Academic Press, 1983]
- Kato bounds [Kato, JPhysSocJapan, 1949]
- A posteriori error estimate for eigenvalue problem
e.g. [Larsen, SINUM, 2000], ...

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Here: direct **a priori error estimate** for Σ !

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Fix $\rho < 1$!

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Suppose that Ω is **convex**, then

$$\|\nabla^2 v\|_{L^2} \leq \frac{\|f'\|_{L^\infty} \|v\|_{L^2}}{1 - \lambda} \leq \frac{C_p \|f'\|_{L^\infty}}{1 - \rho}$$

II. Stability Estimate – step 2

Let $V \in S_0(\mathcal{T})$ be the Ritz projection of v , then

$$\|\nabla V\|_{\Sigma} \leq \sup_{\|\nabla W\|=1} \int [\nabla V \cdot \nabla W - f' V W] \, dx$$

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Standard H^1 and L^2 error estimates:

$$\begin{aligned}\|\nabla(v - V)\|_{L^2} &\leq C_i h_{\mathcal{T}} \|\nabla^2 v\|_{L^2} \leq \frac{C_i C_p \|f'\|_{L^\infty}}{1 - \rho} \times h_{\mathcal{T}} \\ \|v - V\|_{L^2} &\leq C_i^2 h_{\mathcal{T}}^2 \|\nabla^2 v\|_{L^2} \leq \frac{C_i^2 C_p \|f'\|_{L^\infty}}{1 - \rho} \times h_{\mathcal{T}}^2\end{aligned}$$

(Note: $C_i = 1/(4\sqrt{2})$ in my computations)

II. Stability Estimate

Choose $\rho < 1$ and find $0 < \sigma \leq \sigma_{\text{opt}}$:

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Proposition

$$\sigma_{\text{opt}} \geq \min \left[\rho, \Sigma \left(1 - \epsilon / (1 - \rho) \right) - \epsilon^2 / (1 - \rho) \right] =: \sigma,$$

where

$$\epsilon = \|f'\|_{L^\infty} C_i C_\rho h_T,$$

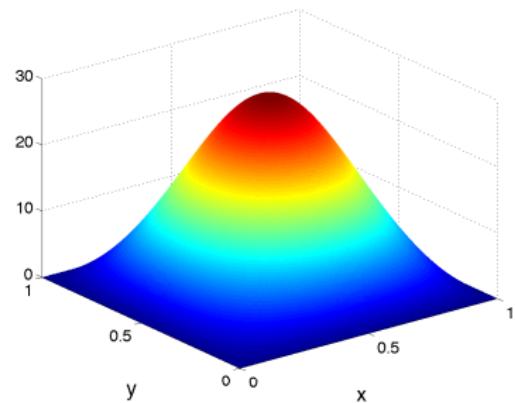
and the optimal ρ is given by

$$\rho = \frac{1 + \Sigma - \sqrt{(1 - \Sigma)^2 + \epsilon + \epsilon^2}}{2}$$

Example: $-\Delta u = u^2$, $\Omega = (0, 1)^2$

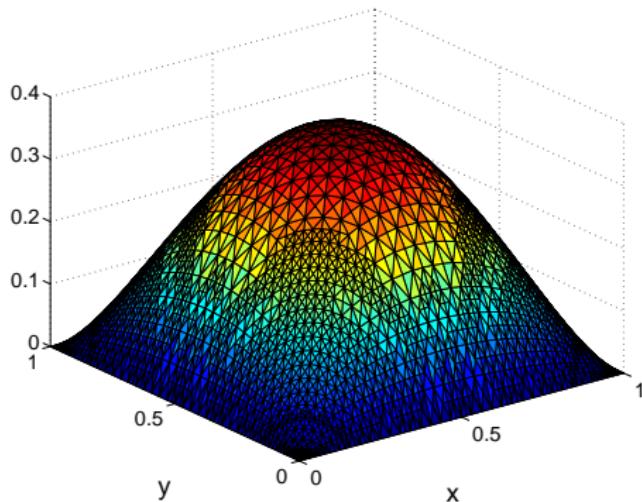
Example: $-\Delta u = u^2$, $\Omega = (0, 1)^2$

η	σ	R	a.p.e.c.	$\#\mathcal{T}$
6.3	0.3	21	23	512
4.4	0.3	15	16	1189
2.8	0.33	8.6	8.4	2574
1.9	0.34	5.5	5.2	5665
1.3	0.35	3.7	3.4	12166
0.85	0.35	2.4	2.2	25758
0.63	0.36	1.8	1.8	54268
0.41	0.36	1.1	1.5	113942
0.3	0.36	1.2	1.2	248098
0.19	0.36	0.94	0.99	511838



Example: $-\Delta u = u^2 + 20$, $\Omega = (0, 1)^2$

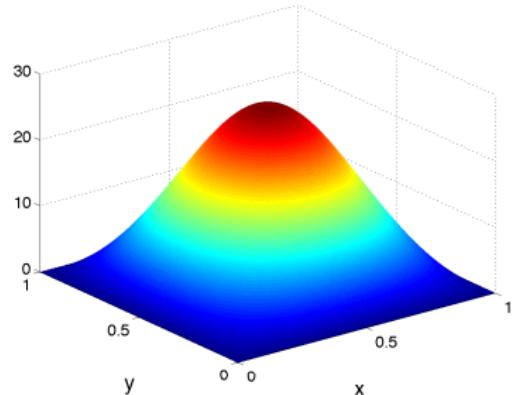
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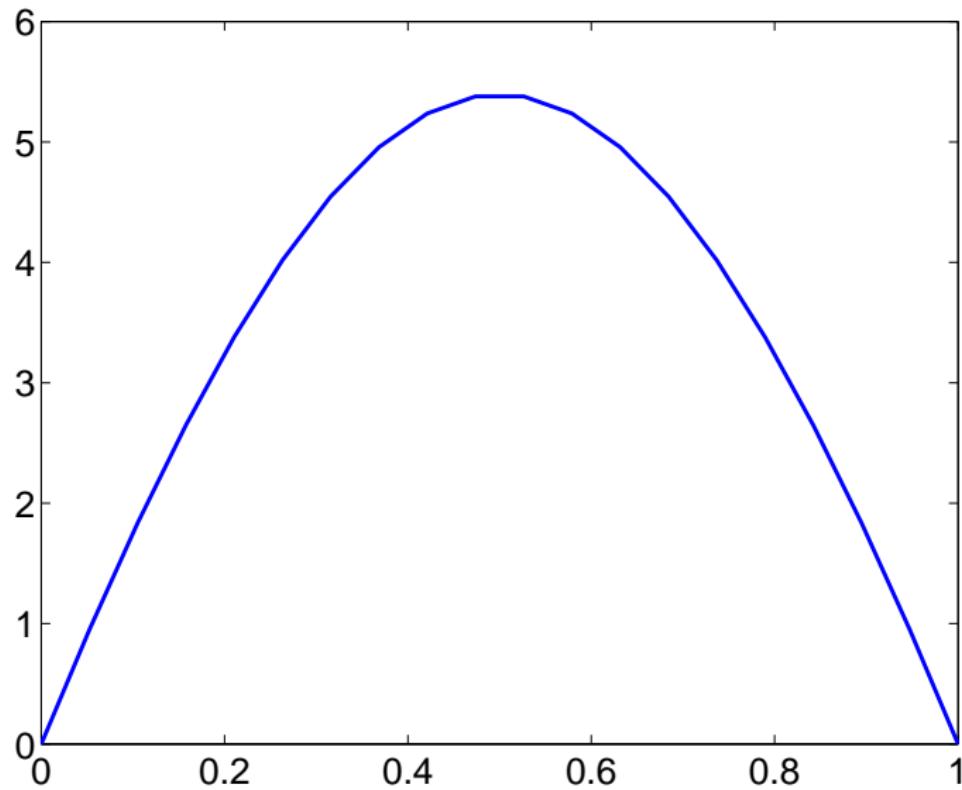
η	σ	R	a.p.e.c.	$\#\mathcal{T}$
0.099	0.94	0.12	0.91	512
0.065	0.94	0.078	0.91	1174
0.043	0.95	0.05	0.91	2544

Example: $-\Delta u = u^2 + 20$, $\Omega = (0, 1)^2$

η	σ	R	a.p.e.c.	$\#\mathcal{T}$
5.8	0.33	18	17	512
4	0.33	12	12	1198
2.6	0.37	7	6.2	2618
1.7	0.38	4.4	3.8	5872
1.2	0.39	3	2.6	12786
0.76	0.39	2	1.8	27330
0.55	0.39	1.4	1.6	60262
0.35	0.39	1.4	1.2	128094
0.25	0.4	1.3	1.1	285168
0.17	0.4	0.54	1	596156



1D Example: $-u_{xx} = u^2 + \lambda$



Computation in 1D: $-u_{xx} = u^2 + \lambda$

■ $\lambda = 22.6$

it.	$\#\mathcal{T}$	η	Σ	σ	a.p.e.c.	err.est.
1	20	0.65	0.070	0.043	71.05	—
3	77	0.17	0.027	0.025	55.28	—
5	305	0.042	0.021	0.021	19.36	—
6	609	0.021	0.021	0.021	9.90	—
7	1217	0.011	0.021	0.021	4.98	—
8	2433	0.0053	0.021	0.021	2.49	—
9	4865	0.0026	0.021	0.021	1.25	—
10	8135	0.0016	0.021	0.021	0.74	0.099

Computation in 1D: $-u_{xx} = u^2 + \lambda$

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6	609	0.021	0.021	0.021	9.90	—
7	1217	0.011	0.021	0.021	4.98	—
8	2433	0.0053	0.021	0.021	2.49	—
9	4865	0.0026	0.021	0.021	1.25	—
10	8135	0.0016	0.021	0.021	0.74	0.099

■ $\lambda = 22.61$

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1	20	0.65	0.067	0.040	83.95	—
2	39	0.33	0.033	0.026	99.56	—
3	77	0.17	0.016	0.014	163.97	—
4	153	0.085	0.0075	0.0070	350.19	—
5	305	0.043	0.0019	0.0018	2650.28	—

Quasilinear BVPs in 1D

Model Problem:

$$-(a(u_x))_x = f(u), \quad u(0) = u(1) = 0.$$

If solutions are expected to be Lipschitz then take

$$\mathcal{X} = W_0^{1,\infty}(0,1) \quad \text{and} \quad \mathcal{Y} = W^{-1,\infty}(0,1)$$

Quasilinear BVPs in 1D

Model Problem:

$$-(a(u_x))_x = f(u), \quad u(0) = u(1) = 0.$$

If solutions are expected to be Lipschitz then take

$$\mathcal{X} = W_0^{1,\infty}(0,1) \quad \text{and} \quad \mathcal{Y} = W^{-1,\infty}(0,1)$$

1. Residual Estimate:

$$\|(a(u_x))_x + f(u)\|_{W^{-1,\infty}} \leq \eta := \frac{1}{2} \max_k h_k \|(a(u_x))_x + f(u)\|_{L^\infty(x_{k-1}, x_k)}$$

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2. Stability Estimate:

$$\|F'(u)^{-1}\|_{\mathcal{L}(W^{-1,\infty}, W_0^{1,\infty})}^{-1} \geq \sigma := (2 + \frac{1}{\pi} \|f'\|_{L^2}/\sigma_2)/a_0,$$

where $a_0 = \text{ess.inf. } a'(u_x)$ and σ_2 is the smallest H^1 -singular value.

Quasilinear BVPs in 1D: The Stability Constant

1. inf-sup condition

$$\frac{a_0}{2} \leq \inf_{\|v_x\|_{L^\infty}=1} \sup_{\|w_x\|_{L^1}=1} \int_0^1 a'(u_x) v_x w_x \, dx$$

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2. This implies

$$\begin{aligned} \frac{1}{2} a_0 \|v_x\|_{L^\infty} &\leq \sup_{\|w_x\|_{L^1}=1} \left[\int_0^1 \left(a'(u_x) v_x w_x - f'(u) v w \right) \, dx \right. \\ &\quad \left. + \|f'(u)\|_{L^2} \|v\|_{L^2} \|w\|_{L^\infty} \right] \\ &\leq \|(a'(u_x) v_x)_x + f'(u) v\|_{W^{-1,\infty}} + \frac{1}{2\pi} \|f'(u)\|_{L^2} \|v_x\|_{L^2} \end{aligned}$$

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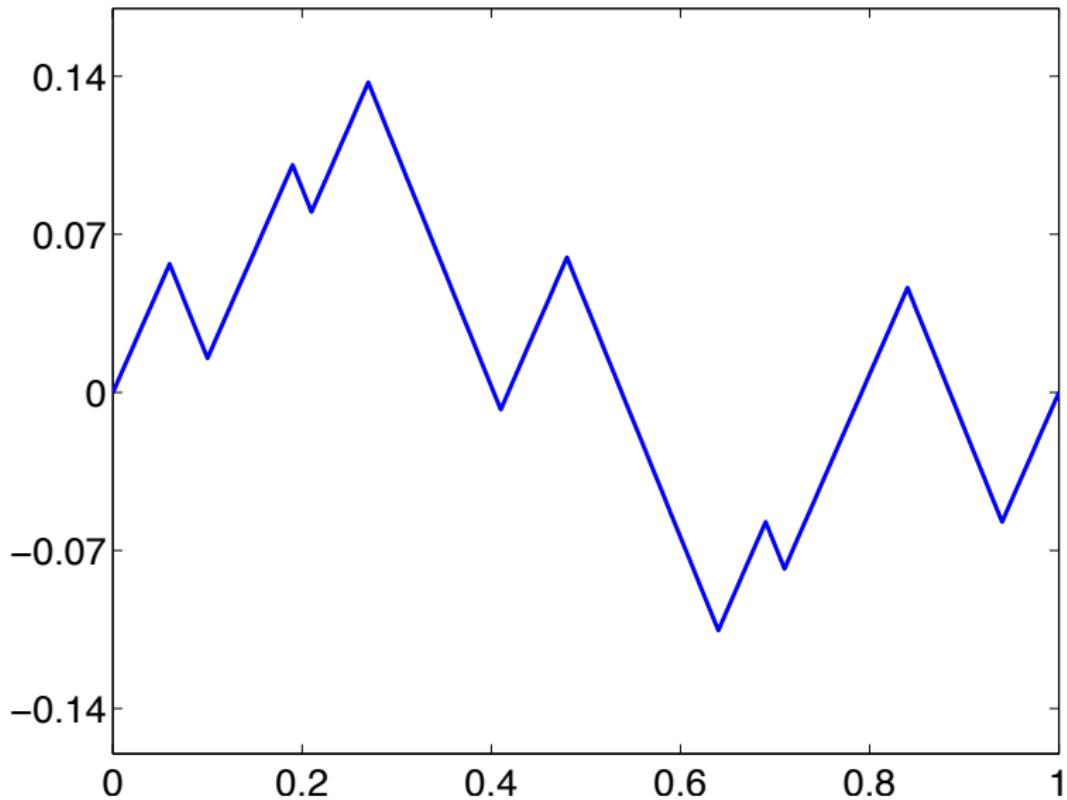
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3. Use singular value estimate

$$\sigma_2 \|v_x\|_{L^2} \leq \|(a'(u_x)v_x)_x + f'(u)v\|_{H^{-1}} \quad (\leq \|(a'(u_x)v_x)_x + f'(u)v\|_{W^{-1,\infty}})$$

Example: $-(u_x^3 - u_x)_x + u = 0$



Conclusion

- Examples of *A Posteriori Existence*:
 - ✓ Nonlinear Poisson Problem: $-\Delta u = f(x, u)$
 - ✓ Quasilinear BVPs in 1D
- **Idea:** Residual Estimate + Local Stability Estimate (regularity theory for the PDE) + Inverse Function Theorem implies existence of exact solution.
- Crucial additional step on top of existing methodology:
estimating the local stability constant
- **Some Possible Extensions:**
 - ✓ Rigorous computation of solution branches: [Plum, JComputApplMath, 1995]
 - ✓ Time-dependent problems (“shadowing”): e.g. [Coomes *et al.*, NumerMath, 1995]
 - ? Singular solutions (corner singularities, vortices, dislocations, ...)
 - ? Quasilinear BVPs in 2D and 3D

Bibliography

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