The reduced basis method and its application to inverse problems

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The reduced basis method[1]

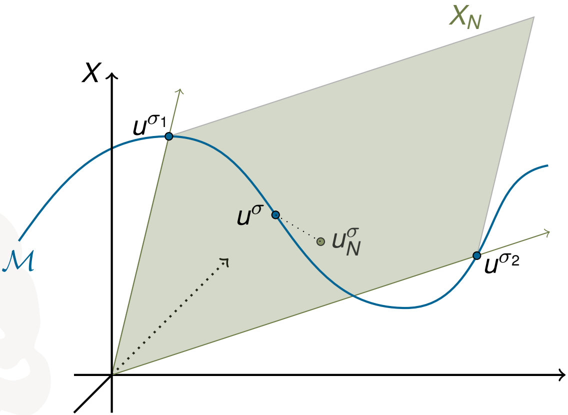
[1] Haasdonk, Chapter to appear in P. Benner, A. Cohen, M. Ohlberger and K. Willcox: ”Model Reduction and Approximation for Complex Systems”, SIAM.

Motivation

- Desired simulation result $\rightsquigarrow$ parametrized PDE with parametric solution $u^\sigma \in X$ and parameter domain $\mathcal{P}$
- **Different szenarios**
  - Many-query: u^σ required for many different $\sigma \in \mathcal{P}$ (optimization, inverse problems, design)
  - Real-time: u^σ required very fast (control, others)
  - Slim-computing: computational capabilities are limited - still simulation results are required (tablet/smartphone apps, techincal controllers)

$\rightsquigarrow$ **model order reduction**

Idea



- Solution manifold $\mathcal{M} := \{u^\sigma \mid \sigma \in \mathcal{P}\}$
- Construction of X_N via *carefully* chosen *snapshots* u^{σ_i}

The detailed problem

Consider

$$\nabla \cdot (\sigma(x)\nabla u(x)) = 1,\ x \in \Omega := (0,1)^2,\ u(x) = 0,\ x \in \partial\Omega.$$

Assume: σ is piecewise constant $\rightsquigarrow \sigma(x) = \sum_{q=1}^{p} \boldsymbol{\sigma}_q \chi_{\Omega_q}(x)$.

Detailed problem (e.g. fine grid FEM)

For $\sigma \in \mathcal{P} \subset \mathbb{R}^p$, find $u^\sigma \in X \subset H_0^1(\Omega)$, the detailed solution, of

$$b(u^\sigma, v; \sigma) = f(v), \text{ for all } v \in X, \text{ with}$$

$$b(u, w; \sigma) := \int_\Omega \sigma \nabla u \cdot \nabla w \, dx, \quad f(v) := -\int_\Omega v \, dx.$$

The reduced problem

Assume

Reduced basis (RB) space $X_N := \mathrm{span}\{\Phi_N\} = \mathrm{span}\{\phi_1, \dots, \phi_N\}$, e.g. with $\phi_i = u^{\sigma_i}$ *carefully* selected *snapshots*, is given.

Reduced problem (Galerkin projection)

For $\sigma \in \mathcal{P}$, find $u_N^\sigma \in X_N \subset X \subset H_0^1(\Omega)$, the reduced solution, of

$$b(u_N^\sigma, v; \sigma) = f(v), \quad \forall v \in X_N.$$

Properties

- Existence, Uniqueness & stability: via Lax-Milgram
- Reproduction of solutions: $u^\sigma \in X_N \;\Rightarrow\; u_N^\sigma = u^\sigma$

Certification - rigorous a-posteriori error estimator

$$\|u^\sigma - u_N^\sigma\|_X \leq \Delta_N(\sigma) := \frac{\|v_r\|_X}{\alpha(\sigma)}, \text{ with}$$

$$\langle v_r, v \rangle_X := r(v;\sigma) := f(v) - b(u_N^\sigma, v; \sigma), \forall v \in X$$

Constructing X_N - the Greedy-Algorithm

Algorithm 1 Greedy-Algorithm(M_{train}, ε_{tol}, $\Delta_N(\cdot)$)

$X_N := \{0\}$, $\Phi_N := \emptyset$
repeat
  $\sigma^\star := \arg\max_{\sigma \in M_{train}} \Delta_N(\sigma)$
  $\phi := u^{\sigma^\star}$, $\Phi_N := \Phi_N \cup \phi$, $X_N := X_N + \mathrm{span}(\phi)$
  $\varepsilon := \max_{\sigma \in M_{train}} \Delta_N(\sigma)$
until $\varepsilon \leq \varepsilon_{tol}$
return Φ_N, X_N

- Convergence: Binev, Cohen, Dahmen, DeVore, Petrova, Wojtaszczyk, 2011; Buffa, Maday, Patera, Prud'homme, Turinici, 2012
- Relies on finite M_{train} covering $\mathcal{P} \subset \mathbb{R}^p$
  $\rightsquigarrow$ only viable for small p (say ≤ 10)

Computational efficiency - Offline/Online decomposition I

Recall $\sigma(x) = \sum_{q=1}^{p} \boldsymbol{\sigma}_q \chi_{\Omega_q}(x)$ piecewise constant

$\rightsquigarrow$ b, f are *parameter-separable*

$$b(u, v; \sigma) = \int_\Omega \sigma \nabla u \cdot \nabla w \, dx = \sum_{q=1}^{p} \boldsymbol{\sigma}_q \int_{\Omega_q} \nabla u \cdot \nabla w \, dx := \sum_{q=1}^{p} \Theta_b^q(\sigma) b^q(u, v),$$

$$f(v) = -\int_\Omega v \, dx = 1 \cdot f(v) := \sum_{q=1}^{1} \Theta_f^q(\sigma) f^q(v),$$

for all $u, \; v \in X$, with coefficients and components.

$\rightsquigarrow$ σ-independant components can be precomputed!

Computational efficiency - Offline/Online decomposition II

Offline-phase (once)

- Compute RB $\Phi_N = \{\phi_1, \dots, \phi_N\}$ and RB-space X_N
- Galerkin projection of components onto X_N:
  $\mathbf{B}_N^q := (b^q(\phi_i, \phi_j))_{i,j=1}^N \in \mathbb{R}^{N \times N}$ and $\mathbf{f}_N^1 := \left(f^1(\phi_i)\right)_{i=1}^N \in \mathbb{R}^N$

Online-phase (for each new σ)

- Evaluate parameter-dependant coefficients $\Theta_b^q(\sigma)$, $\Theta_f^1(\sigma)$
- Assemble $\mathbf{B}_N(\sigma)$, $\mathbf{f}_N(\sigma)$, solve $\mathbf{B}(\sigma)\mathbf{u}_N^\sigma = \mathbf{f}(\sigma)$ and obtain u_N^σ

Note: Offline/Online decomposition of error estimator possible

Extensions - problem variety

- General coercive, elliptic problem[2]:
  - b non-symmetric, f parameter dependant
  - Add output $s(\sigma) := l(u^\sigma)$ with functional l to detailed problem
  - primal/dual approach $\rightsquigarrow$ sharper output error bound
- Instationary Problems[2]
- Inf-sup stability: Veroy, Prud'homme, Rovas, Patera, 2003
- Missing parameter-separability/nonlinear problems: Barrault, Maday, Nguyen, Patera 2004 (EIM)
- Nonlinear problems: Veroy, Prud'homme, Patera, 2003 (Burgers); Veroy, Patera, 2005 (steady incomp. NS)

[2] Haasdonk, Chapter to appear in P. Benner, A. Cohen, M. Ohlberger and K. Willcox: "Model Reduction and Approximation for Complex Systems", SIAM.

Extensions - constructing X_N

- Efficient Greedy: Hesthaven, Stamm, Zhang, 2013
- Optimization Greedy: Urban, Volkwein, Zeeb, 2014
- Partitioning methods: Eftang, Patera, Rønquist, 2010; Eftang, Knezevic, Patera, 2011; Haasdonk, Dihlmann, Ohlberger, 2012
- Domain decomposition: Huynh, Knezevic, Patera, 2013

RBM and Inverse problems

G./Haasdonk/Harrach, A Reduced Basis Landweber method for nonlinear inverse problems, 2016 Inverse Problems 32 (3) (doi).

Forward problem

Consider: $\nabla \cdot (\sigma(x) \nabla u(x)) = 1,\ x \in \Omega := (0,1)^2,\ u(x) = 0,\ x \in \partial\Omega.$

Forward operator

$F : \mathcal{P} \longrightarrow X,\ \sigma \longmapsto u^\sigma$ with u^σ, the detailed solution, solving

$$b(u^\sigma, v; \sigma) = f(v), \text{ for all } v \in X. \tag{1}$$

Reduced forward operator ($X_N \subset X$ given)

$F_N : \mathcal{P} \longrightarrow X_N,\ \sigma \longmapsto u_N^\sigma$ with u_N^σ, the reduced solution, solving

$$b(u_N^\sigma, v; \sigma) = f(v), \text{ for all } v \in X_N.$$

Inverse problem and its difficulties

Inverse Problem

For given solution $u \in X$ of (1), find corresponding parameter $\sigma^+ \in \mathcal{P}$ with $F(\sigma^+) = u$ („a-example“).

- Naive inversion (solving $\sigma^+ = F^{-1}(u)$) fails due to ill-posedness of the problem (in general F^{-1} discontinuous!)

  $\rightsquigarrow$ Small errors get amplified!

- Typically only noisy data u^δ ($\|u - u^\delta\|_X < \delta$) given

  $$\rightsquigarrow F^{-1}(u^\delta) \nrightarrow F^{-1}(u) \text{ as } \delta \to 0!$$

Goal: $R_{n(u^\delta,\delta)}(u^\delta) \to F^{-1}(u)$ as $\delta \to 0$.

Landweber method - a Fixed-point iteration

Idea (linear F)

- solve $F\sigma = u$ for $\sigma \rightsquigarrow$ Gaussian normal equation
- Fixed-point formulation

$$\sigma = \sigma - \omega(F^* F\sigma - F^* u) = \sigma + \omega F^*(u - F\sigma)$$

- Iteration (for $u^\delta \in X$): $\sigma^\delta_{n+1} := \sigma^\delta_n + \omega F^*(u^\delta - F\sigma^\delta_n)$

Landweber iteration (nonlinear[3] - $F(\sigma) = u$)

- $\sigma^\delta_{n+1} := \sigma^\delta_n + \omega F'(\sigma^\delta_n)^*(u^\delta - F(\sigma^\delta_n))$
- Terminate as $\|F(\sigma^\delta_n) - u^\delta\|_X \leq \tau\delta$ (discrepancy principle)

$\rightsquigarrow$ **Many-query setting**

[3]Hanke, Neubauer, Scherzer 1995

RBM & Landweber method - Various approaches

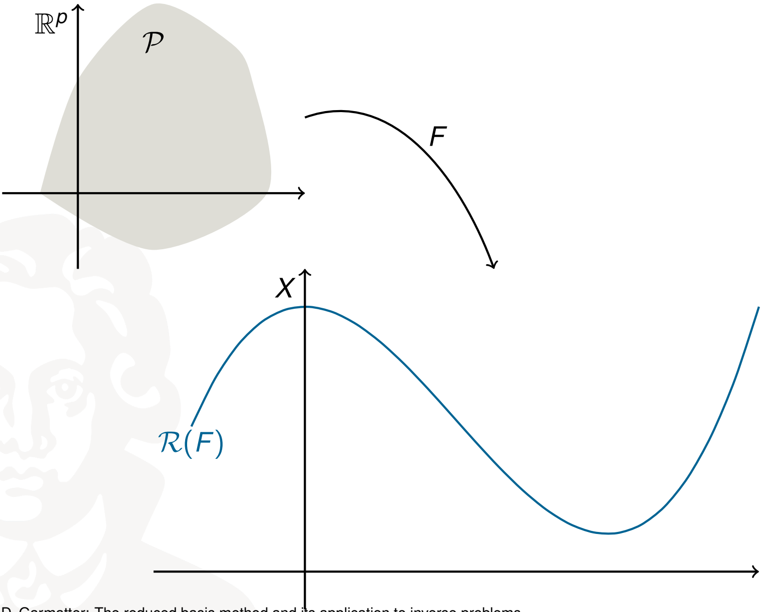
Naive approach

- Construct global X_N approximating whole $\mathcal{R}(F)$ ($\equiv \mathcal{M}$) $\rightsquigarrow$ offline-phase
- Rapidly compute $F_N(\sigma)$ and substitute $F(\sigma)$ for $F_N(\sigma)$ in the Landweber iteration $\rightsquigarrow$ „online-phase“

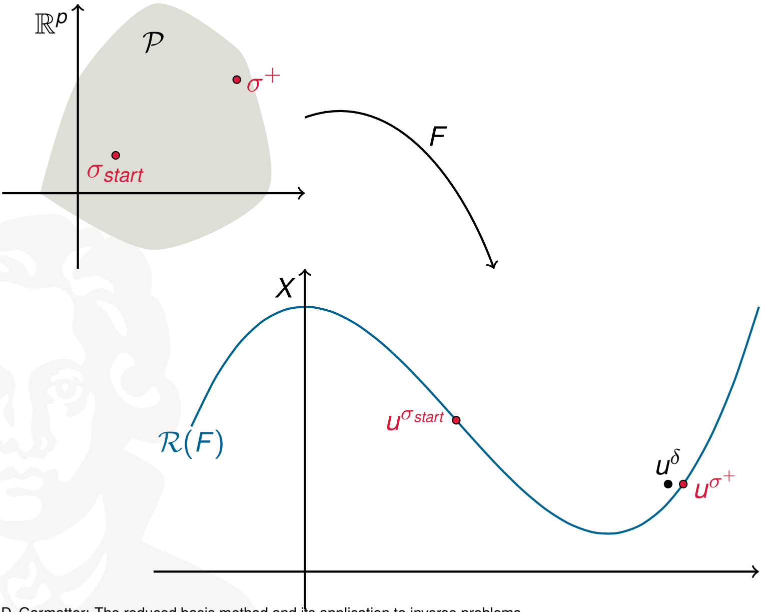
Limitation: Only feasible for low-dimensional parameter spaces ($\leq$ 30), not feasible for imaging.

Our approach: Create problem-adapted RB-space by iterative enrichment (inspired by Druskin & Zaslavski 2007, Zahr & Fahrhat 2015 and Lass 2014).

Combining RBM & LW - Idea



Combining RBM & LW - Idea



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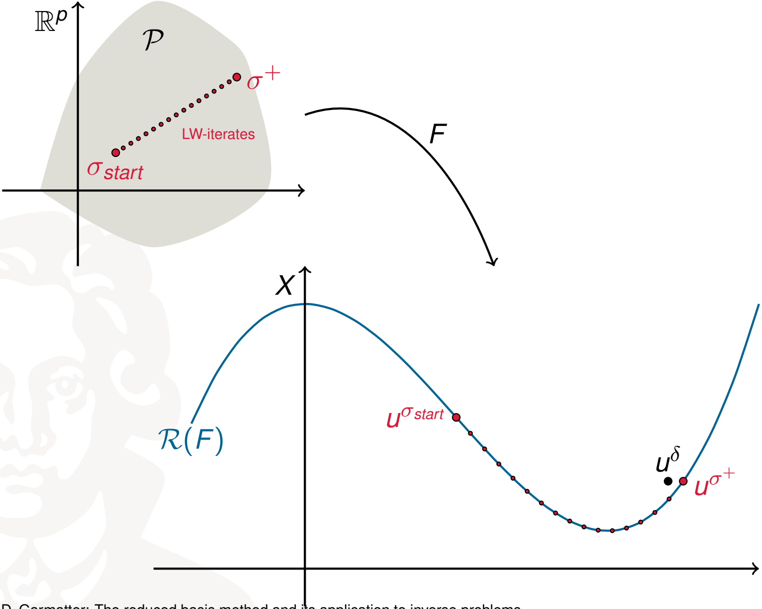

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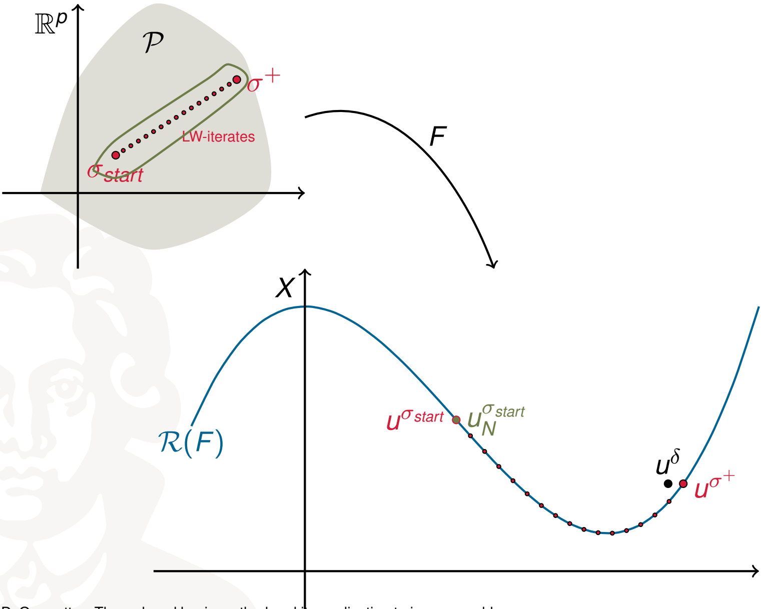

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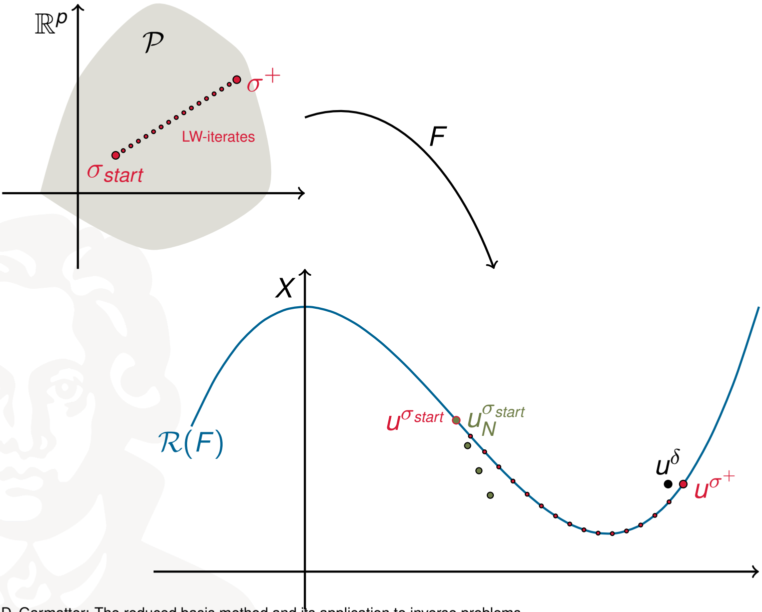
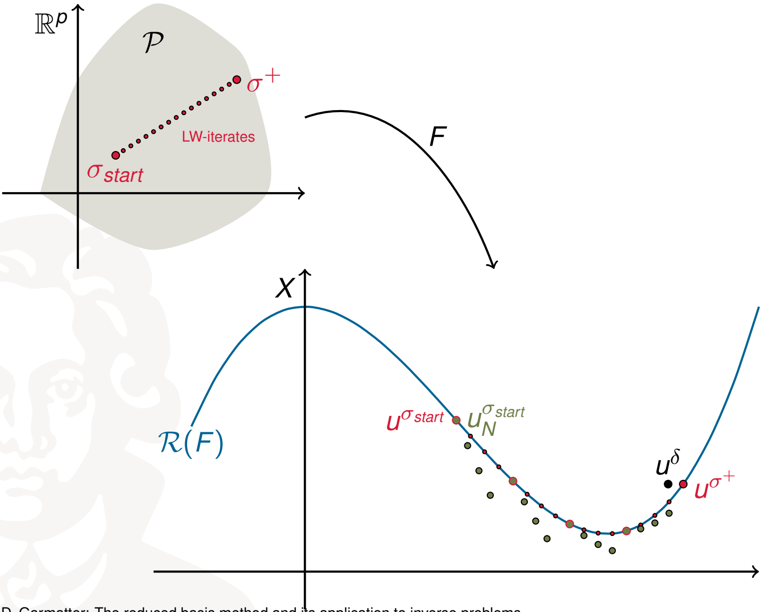
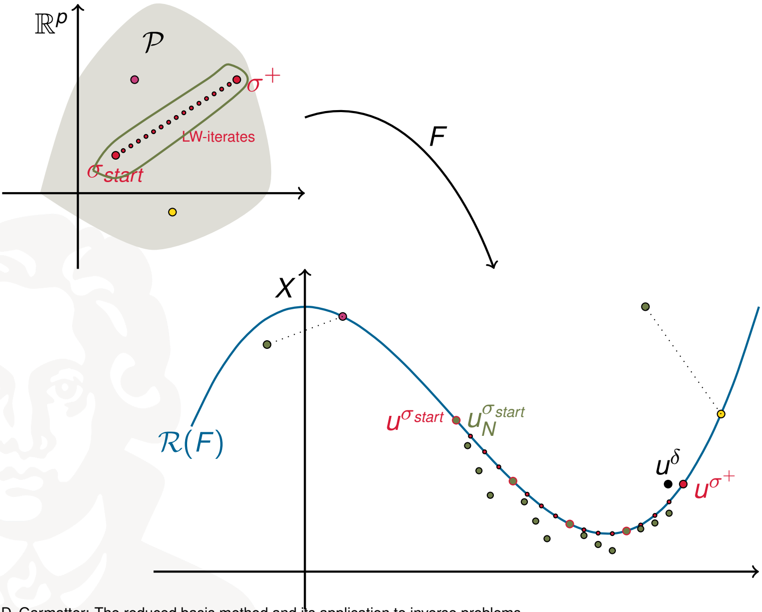


Combining RBM & LW - Idea



Combining RBM & LW - Idea



Reduced Basis Landweber (RBL) method

Algorithm 2 RBL($\sigma_{start}, \tau, \Phi_N$)

$n := 0,\ \sigma_0^\delta := \sigma_{start}$
while $\|F(\sigma_n^\delta) - u^\delta\|_X > \tau\delta$ **do**
  enrich RB Φ_N using σ_n^δ
  $i := 1,\ \sigma_i^\delta := \sigma_n^\delta$
  repeat
    calculate reduced Landweber update $s_{n,i}$
    $\sigma_{i+1}^\delta := \sigma_i^\delta + \omega s_{n,i}$
    $i := i + 1$
  until $\|F_N(\sigma_i^\delta) - u^\delta\|_X \leq \tau\delta$ **or** $\Delta_N(\sigma_i^\delta) > (\tau - 2)\delta$
  $\sigma_{n+1}^\delta := \sigma_i^\delta$
  $n := n + 1$
end while
return $\sigma_{RBL} := \sigma_n^\delta$

The dual problem

Recall $\sigma_{n+1}^\delta := \sigma_n^\delta + \omega F'(\sigma_n^\delta)^*(u^\delta - F(\sigma_n^\delta))$

For $\sigma, \kappa \in \mathcal{P}$ and $l \in X$, one can show

$$\langle \kappa, F'(\sigma)^* \, l \rangle_{\mathcal{P}} = \int_\Omega \kappa \nabla u^\sigma \cdot \nabla u_l^\sigma \, dx, \tag{2}$$

with $u_l^\sigma \in X$ the unique solution of the dual problem

$$b(u, v; \sigma) = m(v; l), \text{ for all } v \in X, \quad m(v; l) := -\int_\Omega l \, v \, dx.$$

In Algorithm 2 ⇝ two RB spaces $X_{N,1}$, $X_{N,2}$

- enrich $X_{N,1}$ via $F(\sigma_n^\delta)$ and $X_{N,2}$ via $u_l^{\sigma_n^\delta}$ with $l := u^\delta - F(\sigma_n^\delta)$
- calculate $s_{n,i}$ using (2) and associated reduced solutions

Numerics - compare reconstructions

Setting: $p = 900$, $\tau = 2.5$, $\delta = 1\%$ and $\omega = \frac{1}{2}(\|F'(\sigma_{start})\|)^{-1}$.

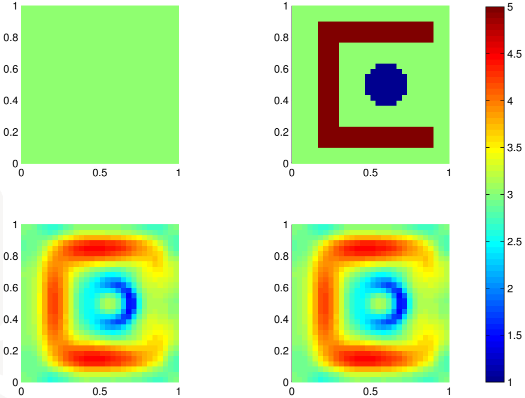


Figure: σ_{start} (top left), exact solution σ^+ (top right). Reconstruction via RBL method (bottom left) and Landweber method (bottom right).

Numerics - time comparison

- **Outer iteration:** space enrichment, projection („offline“)
- **Inner iteration:** one iteration of repeat loop („online“)

Algorithm	Landweber	RBL	
time (s)	187189	14661	
# Iterations	608067	outer	20
		inner	608083
time per Iteration (s)	0.308	outer	3.705
		inner	0.024
# forward solves	1216134	40	

$$\|\sigma_{RBL} - \sigma_{LW}\|_{\mathcal{P}} \approx 1.118 \cdot 10^{-5}$$

Numerics - algorithmic behaviour

Update error - $\|s_{n,RBL} - s_{n,LW}\|_{\mathcal{P}}$

$$s_{n,RBL} := \sigma_{n+1,RBL} - \sigma_{n,RBL}, \quad s_{n,LW} := \sigma_{n+1,LW} - \sigma_{n,LW}$$

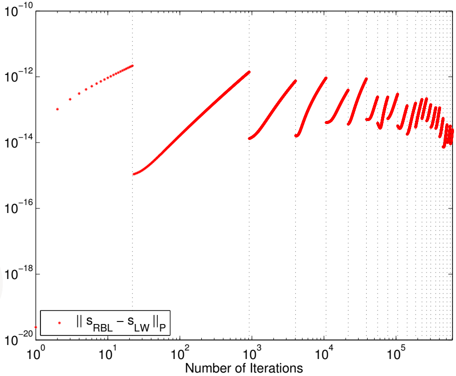


Figure: Update error $\|s_{n,RBL} - s_{n,LW}\|_{\mathcal{P}}$ over the course of the iteration.

Numerics - convergence

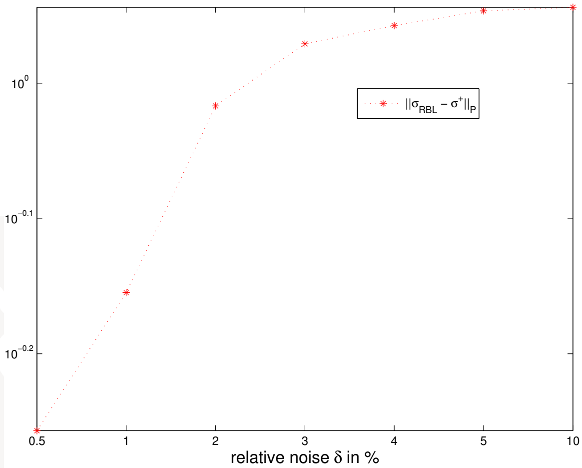


Figure: Error $\|\sigma_{RBL} - \sigma^{+}\|_{\mathcal{P}}$ over the decreasing relative noise level δ.

Conclusion

- Solving inverse coefficient problem requires many PDE solves
- Reduced basis (RB) approach can speed up PDE solution
- But standard RB approach is only applicable for low dimensional parameter spaces
- Using adaptive problem-specific RB enrichment, we can handle high-dimensional parameter spaces, e.g. for imaging problems

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$\rightsquigarrow$ RBL method outperforms standard Landweber (exp.: 13 times faster without loss of accuracy)

Future work

- Theoretical investigation of RBL method (convergence)
- Apply methodology to other inverse problems and more sophisticated regularization algorithms

Thank you for your attention!