SiMPL Method for Topology Optimization Sigmoidal Mirror descent with Projected Latent variable

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Outline

- Topology Optimization
- Gradient Descent and Mirror Descent
- Backtracking Line Search Algorithm
- Numerical Results

- Compliance Minimization
- Three Field Formulation
- Gradient descent method
- Mirror Descent

- The hello world problem: Compliance minimization
- We use Solid Isotropic Material Penalization (SIMP) and Helmholtz type filter

$$\begin{array}{l} \underset{\rho}{\text{minimize }} & \int_{\Omega} f \cdot u \, \mathrm{d}x \\ \text{subject to } & -\operatorname{div}(r(\tilde{\rho})\mathrm{C}:\varepsilon(u)) = f \text{ in }\Omega, \\ & \mathrm{B.C.s.} \\ & -\nabla(\epsilon^2\nabla\tilde{\rho}) + \tilde{\rho} = \rho \text{ in }\Omega, \\ & \partial_n \tilde{\rho} = 0, \\ & \partial_n \tilde{\rho} = 0, \\ & 0 \leq \rho \leq 1, \\ & \int_{\Omega} \rho \, \mathrm{d}x \leq \theta_M |\Omega|. \end{array}$$

Here, $r(\tilde{\rho}) = \rho_0 + (1 - \rho_0)\tilde{\rho}^p$, $\epsilon = r_{\min}/2\sqrt{3}$

 $\Theta \Phi$



Goal of this Talk

- Introduce a new method, SiMPL, for TO with
 - Point-wise feasible solution at each iteration (even with high-order)
 - Easy to implement
 - No additional memory (variable / large system solve)
 - Fast convergence

 $\Theta \Phi$



13th-order interpolation

1.25

Example 37: Topology Optimization

This example code solves a classical cantilever beam topology optimization problem. The aim is to find an optimal material density field ϱ in $L^1(\Omega)$ to minimize the elastic compliance; i.e.,

minimize
$$\int_{\Omega} \mathbf{f} \cdot \mathbf{u}(\varrho) \, dx$$
 over $\varrho \in L^1(\Omega)$
subject to $0 \le \varrho \le 1$ and $\int_{\Omega} \varrho \, dx = \theta \operatorname{vol}(\Omega)$

Projected Gradient Descent Method

The unconstrained gradient descent method

$$\rho_{k+1} = \rho_k - \alpha_k \nabla F(\rho_k)$$

$$= \underset{\rho}{\operatorname{argmin}} F(\rho_k) + \int_{\Omega} \nabla F(\rho_k) \cdot (\rho - \rho_k) dx + \frac{1}{2\alpha_k} \|\rho - \rho_k\|_{L^2(\Omega)}^2$$

$$= \underset{\rho}{\operatorname{argmin}} \int_{\Omega} \nabla F(\rho_k) \cdot \rho dx + \frac{1}{2\alpha_k} \|\rho - \rho_k\|_{L^2(\Omega)}^2$$

 For constrained minimization problem, we obtain a "Projected" gradient method

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$$\rho_{k+1} = \underset{\rho \in \mathcal{C}}{\operatorname{argmin}} \int_{\Omega} \nabla F(\rho_k) \cdot \rho dx + \frac{1}{2\alpha_k} \|\rho - \rho_k\|_{L^2(\Omega)}^2$$
$$= \mathcal{P}_{\mathcal{C}}(\rho_k - \alpha_k \nabla F(\rho_k))$$

Mirror Descent Method

Mirror descent is a generalized gradient descent method

$$\rho_{k+1,GD} = \underset{\rho \in \mathcal{C}}{\operatorname{argmin}} \int_{\Omega} \nabla F(\rho_k) \cdot \rho dx + \frac{1}{\alpha_k} \frac{1}{2} \|\rho - \rho_k\|_{L^2(\Omega)}^2$$

$$\rho_{k+1,MD} = \underset{\rho \in \mathcal{C}}{\operatorname{argmin}} \int_{\Omega} \nabla F(\rho_k) \cdot \rho dx + \frac{1}{\alpha_k} D_{\varphi}(\rho, \rho_k)$$

$$= \mathcal{P}_{\mathcal{C}}((\nabla \varphi)^{-1} (\nabla \varphi(\rho_k) - \alpha_k \nabla F(\rho_k))) \qquad \mathcal{P}_{\mathcal{C}}(\rho) = \underset{q \in \mathcal{C}}{\operatorname{argmin}} D_{\varphi}(q, \rho)$$

The Bregman divergence is a generalized squared distance

•
$$D_{\varphi}(\rho, q) = \varphi(\rho) - \varphi(q) - \int_{\Omega} \nabla \varphi(q) \cdot (\rho - q) dx$$

- If arphi is strictly (or strongly) convex, then so is $D_{arphi}(\cdot,q)$
- Not symmetric, No triangle inequality

Bregman Divergence and Mapping

Fermi-Dirac entropy
$$\varphi(\rho) = \int_{\Omega} \rho \log(\rho) + (1-\rho) \log(1-\rho) dx$$

$$\nabla \varphi(\rho) = \log\left(\frac{\rho}{1-\rho}\right)$$

$$(\nabla \varphi)^{-1}(\psi) = \frac{1}{1+\exp(-\psi)}$$

$$= \sigma(\psi)$$

Projected Mirror Descent

The projected mirror descent

 $\rho_{k+1} = \mathcal{P}_{\mathcal{C}}((\nabla \varphi)^{-1}(\nabla \varphi(\rho_k) - \alpha_k \nabla F(\rho_k)))$ $= \mathcal{P}_{\mathcal{C}}(\sigma(\sigma^{-1}(\rho_k) - \alpha_k \nabla F(\rho_k)))$ $= \sigma(\sigma^{-1}(\rho_k) - \alpha_k \nabla F(\rho_k) + \mu_{k+1})$

Here, $\mu_{k+1} \in \mathbb{R}$ solves the volume correction equation

$$\int_{\Omega} \sigma(\sigma^{-1}(\rho_k) - \alpha_k \nabla F(\rho_k) + \mu_{k+1}) dx = \theta |\Omega|$$



SiMPL - Latent Variable

Introduce the latent variable $\psi = \sigma^{-1}(
ho)$

 $\rho_{k+1} = \sigma(\sigma^{-1}(\rho_k) - \alpha_k \nabla F(\rho_k) + \mu_{k+1})$ $\sigma^{-1}(\rho_{k+1}) = \phi_k^{-1}(\rho_{k+1}) \nabla F(\rho_k) \nabla F(\rho_k) + \mu_{k+1}$

- We find a discrete approximation $\psi_{k,k}$

 $\rho_{k,h} = \sigma(\psi_{k,h})$

- Major benefits
 - Update step is linear in ψ with a scalar nonlinear equation
 - No logarithmic transform $\sigma^{-1}(x) = \log(x/(1-x))$
 - Bound constraint is satisfied point-wise

$$\sigma^{-1}(\rho) = \log\left(rac{
ho}{1-
ho}
ight)$$

$$\sigma(40) - \sigma(20) \approx 10^{-5}$$



Backtracking Line Search

Step size plays a key role to obtain an efficient and stable algorithm



B. Keith and T. M. Surowiec, Proximal Galerkin: A structure preserving finite element method for pointwise bound constraints, arXiv:2307.12444v5, 2024

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Backtracking Line Search

- Step size plays a key role to obtain an efficient and stable algorithm
- Convergence analysis may be carried out with "relative smoothness"

$$\left| \int_{\Omega} (\nabla F(x) - \nabla F(y))(x - y)dx \right| < L \int_{\Omega} (\nabla \varphi(x) - \nabla \varphi(y))(x - y)dx \quad \forall x, y \in Q$$

$$L_k := \frac{\left| \int_{\Omega} (\nabla F(\rho_k) - \nabla F(\rho_{k-1}))(\rho_k - \rho_{k-1})dx \right|}{\int_{\Omega} (\psi_k - \psi_{k-1})(\rho_k - \rho_{k-1})dx}$$

$$\alpha_k := L_k^{-1}.$$

► We use a generalized Armijo rule (SiMPL-A) or Bregman rule (SiMPL-B) with the above initial step size $F(\rho_{k+1,q}) \leq F(\rho_{k,q})$

$$F(\boldsymbol{\rho}_{k+1,q}) \leq F(\boldsymbol{\rho}_{k,q}) + c_1 \nabla F(\boldsymbol{\rho}_{k,q})^T \boldsymbol{M}_q(\boldsymbol{\rho}_{k+1,q} - \boldsymbol{\rho}_{k,q}) + \frac{1}{\alpha_k} D_{\varphi}(\boldsymbol{\rho}_{k+1,q}, \boldsymbol{\rho}_{k,q})$$

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- Implemented in MFEM C++ Library
- Comparison with MMA and OCM
- Mesh independent behavior
- Beyond compliance minimization
 - Bridge Design

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Compliant mechanism

Numerical Results

Method of Moving Asymptotes #4486

11 Open talinke wants to merge 8 commits into master from MMA_PR

MBB Beam Problem with h=1/256



MBB Beam Problem with h=1/256



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MBB Beam Problem with h=1/256





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Cantilever - 3D





Converged after 44 iterations

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Self-weight Compliance Minimization

Self-weight bridge design





Compliant Mechanism

Force Inverter



Concluding Remarks

- We introduce the SiMPL method for topology optimization
 - The solution at each iteration is point-wise feasible
 - Update rule in the latent space is easy to implement
 - Computational cost at each iteration is equivalent to gradient descent methods
 - Backtracking line search results in fast and stable convergence
 - It outperforms OCM and MMA for all benchmark problems we tested
- A high-order interpolation in the latent space does NOT suffer from the oscillation in the primal space
 - Extend it to high-order scheme Requires bound-preserving high-order filter solver
- Multi-material topology optimization
 - Multi-material constraints can be handled when we employ different entropy
- More general constraints
 - Stress constrained optimization, ...

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SiMPL makes topology optimization SIMPLer!



Proximal Point Method

- Censor and Zenios 1992, Chen and Teboulle 1993

$$\min_{\boldsymbol{x}} \quad F(\boldsymbol{x}) \\ \text{s.t.} \quad \boldsymbol{x} \in K$$

The proximal point method is an iterative method

$$x_{k+1} = \arg \min_{x} \{F(x) + \frac{1}{2\alpha_k} \|x - x_k\|^2\}$$

We replace the Euclidean distance to a Bregman distance

$$x_{k+1} = \arg \min_{x} \{F(x) + \frac{1}{\alpha_k} D_h(x, x_{k+1})\}$$

where the Bregman divergence is defined by

$$D_h(\boldsymbol{x}, \boldsymbol{y}) = h(\boldsymbol{x}) - h(\boldsymbol{y}) - \langle h'(\boldsymbol{y}), \boldsymbol{x} - \boldsymbol{y} \rangle$$

with a strictly convex and differentiable function h

Proximal Minimization Algorithm with D-Functions^{1,2}

Y. CENSOR³ AND S. A. ZENIOS⁴

Communicated by O. L. Mangasarian

Abstract. The original proximal minimization algorithm employs quadratic additive terms in the objectives of the subproblems. In this paper, we replace these quadratic additive terms by more general D-functions which resemble (but are not strictly) distance functions. We characterize the properties of such D-functions which, when used in the proximal minimization algorithm, preserve its overall convergence. The quadratic case as well as an entropy-oriented proximal minimization algorithm are obtained as special cases.

CONVERGENCE ANALYSIS OF A PROXIMAL-LIKE MINIMIZATION ALGORITHM USING BREGMAN FUNCTIONS*

GONG CHEN† AND MARC TEBOULLE†

Abstract. An alternative convergence proof of a proximal-like minimization algorithm using Bregman functions, recently proposed by Censor and Zenios, is presented. The analysis allows the establishment of a global convergence rate of the algorithm expressed in terms of function values.

 ${\bf Key}$ words. Bregman functions, proximal methods, convex programming

AMS subject classification. 90C25

1. Introduction. Consider the convex optimization problem

where $f : \mathbb{R}^n \mapsto (-\infty, +\infty]$ is a proper, lower semicontinuous convex function. One method of solving (P) is to regularize the objective function by using the proximal mapping as introduced by Moreau [12]. Given a real positive number λ , a proximal approximation of f is defined by

2)
$$f_{\lambda}(x) = \inf_{u} \{ f(u) + 1/2\lambda \| x - u \|^2 \}.$$

Proximal Point Method

The proximal iterate

$$\boldsymbol{x}_{k+1} = \arg \min_{\boldsymbol{x}} \{F(\boldsymbol{x}) + \frac{1}{\alpha_k} D_h(\boldsymbol{x}, \boldsymbol{x}_{k+1})\}$$

can be found by solving the first-order optimality condition

$$\alpha \nabla_{\boldsymbol{x}} F(\boldsymbol{x}) + \nabla_{\boldsymbol{x}} h(\boldsymbol{x}) = \nabla_{\boldsymbol{x}} h(\boldsymbol{x}_k)$$

- When we consider a constrained optimization problem, *h* is often selected so that *dom(h) = K* and its gradient has closed form inverse
- Then we always have feasible iterates
- Converges provided with $\sum \alpha_k \to \infty$

Latent Variable Proximal Point Method

- Keith and Surowiec 2023

If we define dual variable, $m{x}^* =
abla_{m{x}} h(m{x})$, then

 $lpha_k
abla_{m{x}} F({m{x}}_{k+1}) + {m{x}}^*_{k+1} = {m{x}}^*_k$ ${m{x}}_{k+1} -
abla_{m{x}} h^{-1}({m{x}}^*_{k+1}) = 0.$

- In a continuous setting, the dual variable has no crucial role
- However, in a discrete setting,

 $egin{aligned} &lpha_k
abla_{m{x}} F_h(m{x}_{h,k+1}) + m{x}^*_{h,k+1} &= m{x}^*_{h,k} \ &m{x}_{h,k+1} -
abla_{m{x}} h^{-1}(m{x}^*_{h,k+1}) &= 0, \end{aligned}$

we have an additional representation of solution, $x \approx \nabla_x h^{-1}(x_h^*)$ This is feasible point-wisely

PROXIMAL GALERKIN: A STRUCTURE-PRESERVING FINITE ELEMENT METHOD FOR POINTWISE BOUND CONSTRAINTS

BRENDAN KEITH* AND THOMAS M. SUROWIEC[†]

Dedicated with respect and admiration to Leszek Demkowicz on the occasion of his 70th birthday anniversary.

Abstract. The proximal Galerkin finite element method is a high-order, low iteration complexity, nonlinear numerical method that preserves the geometric and algebraic structure of pointwise bound constraints in infinite-dimensional function spaces. This paper introduces the proximal Galerkin method and applies it to solve free boundary problems, enforce discrete maximum principles, and develop a scalable, mesh-independent algorithm for optimal design problems with pointwise bound constraints. This paper also provides a derivation of the latent variable proximal point (LVPP) algorithm, an unconditionally stable alternative to the interior point method. LVPP is an infinitedimensional optimization algorithm that may be viewed as having an adaptive barrier function that is updated with a new informative prior at each (outer loop) optimization iteration. One of its main benefits is witnessed when analyzing the classical obstacle problem. Therein, we find that the original variational *inequality* can be replaced by a sequence of second-order partial differential *equations* (PDEs) that are readily discretized and solved with, *e.g.*, high-order finite elements. Throughout this method are elements and an element of the second particle for the second pa

interest. The algebraic/gec infinite-dimer density-based combines ide geometry and and numerica to facilitate r ay be of independent sson equation; (2) an stizations and certain gorithm for two-field, Jalerkin methodology ebra, and differential as within variational utions of our methods

Latent Variable Mirror Descent

The first-order approximation of objective function

$$\begin{aligned} \boldsymbol{x}_{k+1} &= \arg \min_{\boldsymbol{x}} \{F(\boldsymbol{x}_k) + (\nabla_{\boldsymbol{x}} F(\boldsymbol{x}_k), \boldsymbol{x} - \boldsymbol{x}_k) + \frac{1}{\alpha_k} D_h(\boldsymbol{x}, \boldsymbol{x}_{k+1})\} \\ &= \arg \min_{\boldsymbol{x}} \{(\nabla_{\boldsymbol{x}} F(\boldsymbol{x}_k), \boldsymbol{x}) + \frac{1}{\alpha_k} D_h(\boldsymbol{x}, \boldsymbol{x}_{k+1})\} \end{aligned}$$

- This method is called mirror descent, and it has explicit form $\boldsymbol{x}_{k+1} = \nabla h_{\boldsymbol{x}}^{-1} (\nabla_{\boldsymbol{x}} h(\boldsymbol{x}_k) - \alpha_k \nabla_{\boldsymbol{x}} F(\boldsymbol{x}_k))$
- In terms of the latent variable, $m{x}^* =
 abla_{m{x}} h(m{x})$

 $\boldsymbol{x}_{k+1}^* = \boldsymbol{x}_k^* - \alpha_k \nabla_{\boldsymbol{x}} F(\boldsymbol{x}_k)$



- What is Topology Optimization
- Projected Mirror Descent with Latent Variable
- Adaptive Step Size Guided Initial Guess







$$\begin{split} \min_{\boldsymbol{\rho} \in L^{\infty}(\Omega)} & (\boldsymbol{f}, \boldsymbol{u}) \\ \text{s.t.} \quad \nabla \cdot (r(\tilde{\rho})\mathcal{C} : \boldsymbol{\varepsilon}(\boldsymbol{u})) = \boldsymbol{f} \quad \text{in } \Omega + \text{ B.C} \\ -\epsilon^2 \Delta \tilde{\rho} + \tilde{\rho} = \rho \quad \text{in } \Omega, \\ \partial_n \tilde{\rho} = 0 \quad \text{on } \partial\Omega, \\ \partial_n \tilde{\rho} = 0 \quad \text{on } \partial\Omega, \\ \int_{\Omega} \rho = \theta |\Omega|, \\ 0 < \rho < 1. \end{split}$$
where $r(\tilde{\rho}) = \rho_0 + (1 - \rho_0) \tilde{\rho}^{\dagger}$



 $(\mathbf{P} \mathbf{P})$



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Projected Mirror Descent Method

Algorithm 2 Projected Mirror Descent

1: Given dual density $\rho_k^* \in Q_h^*$ and step size α_k .

2: Solve for filtered density $\tilde{\rho}_k \in \tilde{Q}_h$,

$$\epsilon^2(\nabla \tilde{\rho}_k, \nabla \tilde{q}) + (\tilde{\rho}_k, \tilde{q}) = (S(\rho_k^*), q) \quad \forall \tilde{q} \in \tilde{Q}_h.$$

3: Solve for displacement $\boldsymbol{u}_k \in V_h$

 $(r(ilde{
ho}_k)\mathcal{C}:arepsilon(oldsymbol{u}_h),
ablaoldsymbol{v})=(oldsymbol{f},oldsymbol{v})\quadoralloldsymbol{v}\in V_h.$

4: Compute gradient $G_k = \prod_h \tilde{w}_h \in Q_h^*$ where $\tilde{w}_h \in \tilde{Q}_h$ solves

 $\epsilon^2(\nabla \tilde{w}_k, \nabla \tilde{q}) + (\tilde{w}_k, \tilde{q}) = -(r'(\tilde{\rho}_k)(\mathcal{C} : \varepsilon(\boldsymbol{u}_k)) : \varepsilon(\boldsymbol{u}_k), \tilde{q}) \quad \forall \tilde{q} \in \tilde{Q}_h.$

5: Set $\rho_{k+1}^* = \rho_k^* - \alpha_k G_k + \mu$ where $\mu \in \mathbb{R}$ solves $\int_{\Omega} S(\rho_k^* - \alpha_k G_k + \mu) = \theta |\Omega|$

Adaptive Step Size

The convergence of Mirror Descent can be proved

$$\alpha_k^{-1} \ge \gamma^{-1} := \sup_{\boldsymbol{x}, \boldsymbol{y} \in K} \frac{(\nabla F(\boldsymbol{x}) - \nabla F(\boldsymbol{y}), \boldsymbol{x} - \boldsymbol{y})}{(\nabla h(\boldsymbol{x}) - \nabla h(\boldsymbol{y}), \boldsymbol{x} - \boldsymbol{y})}$$
$$= \sup_{\boldsymbol{x}, \boldsymbol{y} \in K} \frac{(\nabla F(\boldsymbol{x}) - \nabla F(\boldsymbol{y}), \boldsymbol{x} - \boldsymbol{y})}{(\boldsymbol{x}^* - \boldsymbol{y}^*, \boldsymbol{x} - \boldsymbol{y})}$$

This motivates the choice of step size

 $\Theta \Phi$

$$\alpha_k := \frac{(\rho_{h,k}^* - \rho_{h,k-1}^*, \rho_{h,k} - \rho_{h,k-1})}{(\nabla F(\rho_{h,k}) - \nabla F(\rho_{h,k-1}), \rho_{h,k} - \rho_{h,k-1})}$$

Armijo condition is used to have monotone decreasing objective

$$F(\rho_{h,k+1}) \le F(\rho_{h,k}) - c_1(\nabla F(\rho_{h,k}), \rho_{h,k+1} - \rho_{h,k})$$

Main Results

1. $h: L^{\infty}_{(0,1)}(\Omega) \to \mathbb{R}$ is strictly convex and differentiable. Also, we can find primal representation, $\nabla h \in L^{\infty}(\Omega)$ by

$$(\nabla_{\rho}h(\rho),q) = (\ln \frac{\rho}{1-\rho},q) \quad \forall q \in L^1(\Omega).$$

2. F is differentiable with respect to ρ . Its gradient $\nabla_{\rho} F(\rho) \in L^{\infty}(\Omega)$ can be represented by

$$(\nabla_{\rho}F(\rho),q) = (\tilde{w},q) \quad \forall q \in L^{1}(\Omega).$$

3. The step size α_k satisfies the Armijo condition in finite iteration with

$$\alpha_k \geq \frac{1-c_1}{L}$$

where L is Lipschitz constant of $\nabla_{\rho} F$.

4. $\{F(\rho_k) = F(S(\rho_k^*))\}$ is a monotone decreasing sequence, and has a convergent subsequence

$$\rho_{\ell_k} \rightharpoonup \rho^*$$

and ρ^* satisfies the KKT condition.



- MBB Beam
- Self-weight Compliance Minimization
- Compliant Mechanism

Numerical Results



Discrete Spaces and Parameters

Discrete Spaces

$$Q_h^* = \{ \rho^* \in L^2(\Omega) : \rho^* |_T \in \mathbb{P}_0(T) \ \forall T \in \mathcal{T}_h \},$$

$$\tilde{Q}_h = \{ \tilde{\rho} \in H^1(\Omega) : \tilde{\rho} |_T \in \mathbb{P}_1(T) \ \forall T \in \mathcal{T}_h \},$$

$$V_h = \{ \boldsymbol{u} \in [H^1(\Omega)]^2 : \boldsymbol{u} |_T \in [\mathbb{P}_1(T)]^2 \ \forall T \in \mathcal{T}_h \},$$

Parameters

 Ψ

$$\epsilon = 0.05/(2\sqrt{3}),$$

$$r(\tilde{\rho}) = \rho_0 + (1 - \rho_0)\tilde{\rho}^3$$

$$\rho_0 = 10^{-6},$$

$$c_1 = 10^{-4}.$$

MFEM: Open source C++ FEM Library @ LLNL

Self-weight Compliance Minimization

$$\min_{\rho \in L^{\infty}(\Omega)} (\boldsymbol{g}\rho, \boldsymbol{u})$$

s.t. $\nabla \cdot (\rho \mathcal{C} : \varepsilon(\boldsymbol{u})) = \boldsymbol{f}$ in Ω + B.Cs
$$\int_{\Omega} \rho = \theta |\Omega|,$$

 $0 < \rho < 1.$

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Compliant Mechanism



Conclusion

- We derived Latent Variable Projected Mirror Descent Method
- The discrete density satisfies the bound constraint point-wisely even when high-order approximation is used
- Adaptive step size with a heuristic initial guess outperform traditional methods
- Efficiency and robustness of the proposed algorithm has been shown numerically
- High-order approximation also can be employed while maintaining bound-preserving property