Homeomorphism Methods for Efficient Decision-Making with Hard Constraints

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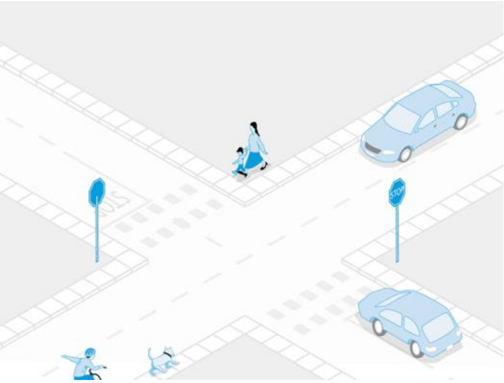
Decision-Making with Hard Constraints



Autonomous driving with
mixed traffic flow **constraints**

Power grid with physical
and operational **constraints**

4G/5G parameter optimization
with load balance **constraints**

Constrained Optimization

$$\min_x f(x,\theta)$$
$$\text{s.t.. } h(x,\theta) = 0$$
$$g(x,\theta) \le 0$$

Parameter	|	θ
Decision	|	x
Objective	|	f
Constraints	|	h, g

Goals: safe, economic, rea-time decisions

A Concrete Example in Power Grid Operation

- Minimizing generation cost to serve the load, with an accurate AC model

$$
\begin{aligned}
\min \quad & \textstyle\sum_{i\in\mathcal{N}_g} \left(\lambda_{i,2}P_{gi}^2 + \lambda_{i,1}P_{gi} + \lambda_{i,0}\right) \\
\text{s.t.} \quad & P_{gi} - P_{di} = \sum_{j:(i,j)\in\mathcal{E}} V_iV_j(g_{ij}\cos\theta_{ij} + b_{ij}\sin\theta_{ij}), \ \ \forall i \in \mathcal{N}, \\
& Q_{gi} - Q_{di} = \sum_{j:(i,j)\in\mathcal{E}} V_iV_j(g_{ij}\sin\theta_{ij} - b_{ij}\cos\theta_{ij}), \ \ \forall i \in \mathcal{N}, \\
& P_{gi}^{\min} \le P_{gi} \le P_{gi}^{\max}, \ \ \forall i \in \mathcal{N}_g, \\
& Q_{gi}^{\min} \le Q_{gi} \le Q_{gi}^{\max}, \ \ \forall i \in \mathcal{N}_g, \\
& V_i^{\min} \le V_i \le V_i^{\max}, \ \ \forall i \in \mathcal{N}_g, \\
& \theta_{ij}^{\min} \le \theta_{ij} \le \theta_{ij}^{\max}, \ \ \forall (i,j) \in \mathcal{E}, \\
& 0 \le P_{ij}^2 + Q_{ij}^2 \le \left(S_{ij}^{\max}\right)^2, \ \ \forall (i,j) \in \mathcal{E}, \\
& P_{ij} = g_{ij}\left(V_i^2 - V_iV_j\cos\theta_{ij}\right) - b_{ij}V_iV_j\sin\theta_{ij}, \ \ \forall (i,j) \in \mathcal{E}, \\
& Q_{ij} = b_{ij}\left(-V_i^2 + V_iV_j\cos\theta_{ij}\right) - g_{ij}V_iV_j\sin\theta_{ij}, \ \ \forall (i,j) \in \mathcal{E}, \\
\text{var.} \quad & P_{gi}, Q_{gi}, \forall i \in \mathcal{N}_g; V_i, \theta_i, \forall i \in \mathcal{N}.
\end{aligned}
$$

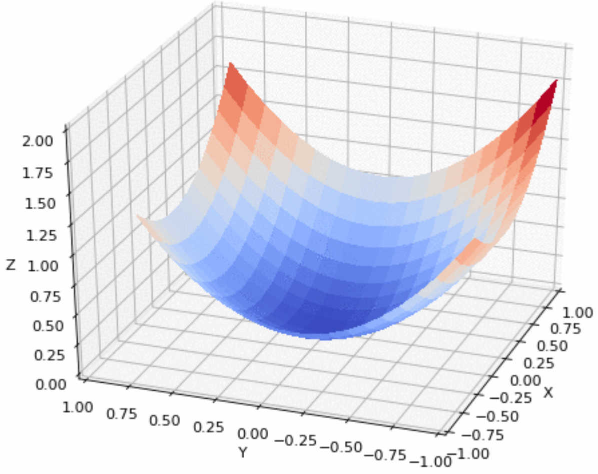
generation cost

AC power flow equations

Generation and voltage limit constraints

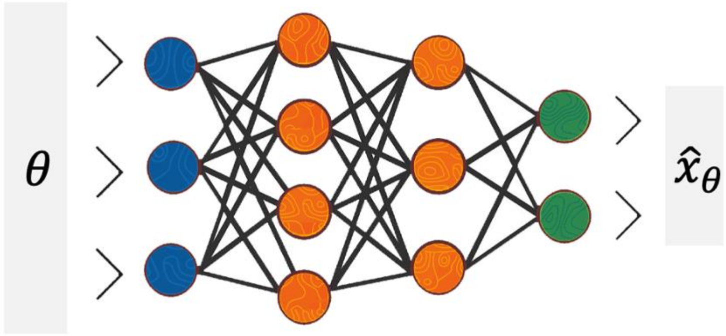
Branch flow limit constraints

Iterative Algorithm *vs* Machine Learning



$$\min_{x} \; f(x,\theta)$$
$$\text{s.t.. } h(x,\theta) = 0$$
$$g(x,\theta) \leq 0$$

θ: parameter | x: decisions



Given θ, update iteratively to pursue optimal solution x_θ^*

- $x_\theta^{n+1} = x_\theta^n - g(x_\theta^n)$
- E.g., interior point methods, Gurobi, …

Feasible, optimal, but **slow**

Training neural network to predict solutions end-to-end

- $\hat{x}_\theta = F_{nn}(\theta)$
- E.g., supervised training $\min_{F_{nn}} \sum_i ||F_{nn}(\theta_i) - x_i^*||$

Fast, near-optimal, but **non-feasible**

Homeomorphism Methods

Motivation: transform complex constrained problem into simple constraint domain (e.g., ball)

Homeomorphism

- *Bijective* & *Bi-continuous* mapping
- Preserve topological structures

Our contributions

Accelerate iterative algorithms [1]

- The ***first*** work achieving optimal convergence rates without expensive oracles over general convex sets

+

Ensure neural network feasibility [2,3]

- The ***first*** work ensuring NN solution feasibility with bounded opt. gap and low-complexity over a class of non-convex sets

Goals: safe, economic, rea-time decisions

[1] C. Liu, E. Liang*, M. Chen*, "*Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set*". **NeurIPS 2025. Spotlight.**
[2] E. Liang, M. Chen, S. Low, "*Low Complexity Homeomorphic Projection to Ensure NN Solution Feasibility for Optimization over (Non-)Convex Set*", **ICML. 2023.**
[3] E. Liang, M. Chen, S. Low, "*Homeomorphic Projection to Ensure NN Solution Feasibility for Constrained Optimization*". **JMLR. 2024.**

Homeomorphism Methods: Part I

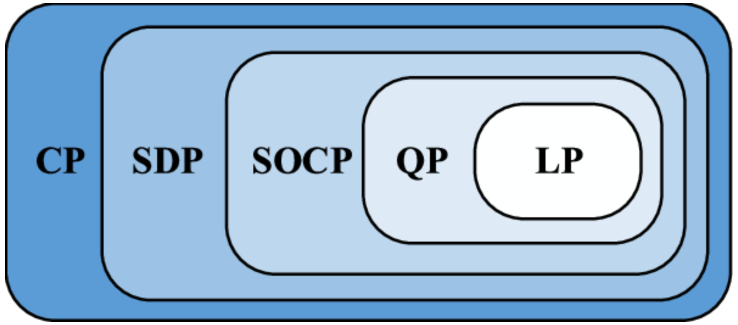
Hom-PGD to Accelerate Iterative Algorithms

[1] C. Liu, E. Liang*, M. Chen*, "*Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set*". **NeurIPS 2025. Spotlight.**

Key Metrics for Iterative Algorithms

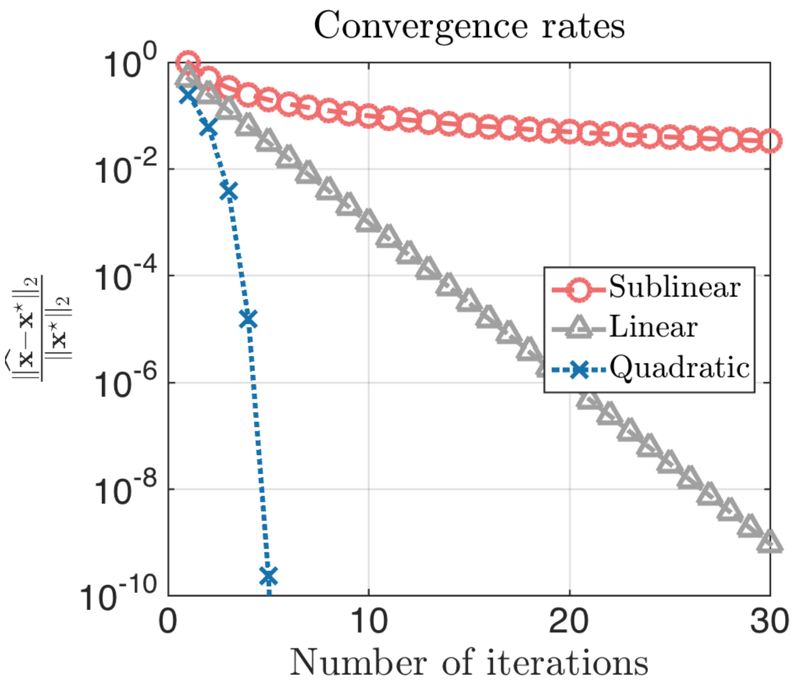
Applicable Scenarios:

- Objective: linear, quadratic, convex,…
- Constraints: polytope, convex cones,…



Convergence rate: num. of steps to optimum

- Sublinear: $N = O(1/\varepsilon)$
- Linear: $N = O(\log 1/\varepsilon)$



Per-step cost: $x_\theta^{n+1} = x_\theta^n - g(x_\theta^n)$

- Memory cost: store medium variables.
- Computational cost: $O(n^2), O(n^3)$

[1] Boyd S., Vandenberghe L. Convex optimization. Cambridge university press; 2004.

Existing Iterative Algorithms

Second-order methods (*Hessian*)

- Primal-Dual Interior Points (in MOSEK)

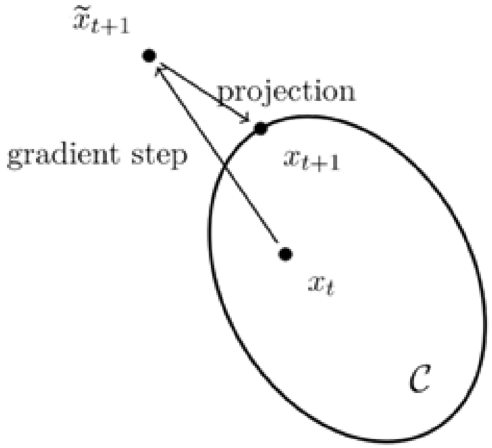
High memory & per-step cost

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix} \quad \text{and} \quad \nabla^2 f = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

First-order methods (*Gradient*)

- Projection Gradient Descent (PGD)
- Projection-free Frank-Wolfe (FW)
- Augmented Lagrangian (e.g., ADMM)

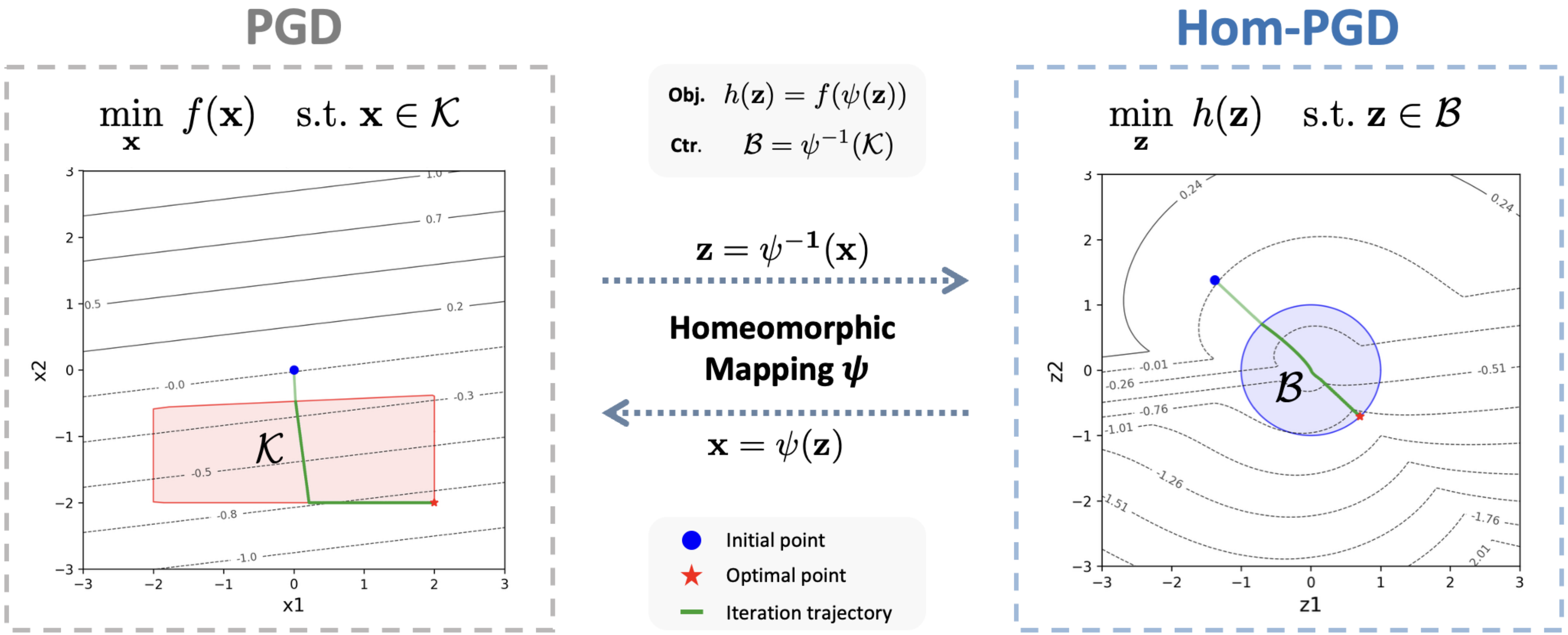
Non-trivial sub-problems



$$x_{t+1} = \Pi_{\mathcal{C}}(\tilde{x}_{t+1}) := \arg\min_{x \in \mathcal{C}} \frac{1}{2} \|x - \tilde{x}_{t+1}\|_2^2$$

Research Gap: design an algorithm that with **low per-iter costs**, matching **optimal convergence**, working for **general convex set**

Hom-PGD to Accelerate Iterative Algorithms



1. Construct homeomorphism for general convex set
2. Transform the problem into ball-constrained space
3. Projection gradient descent over ball is easy

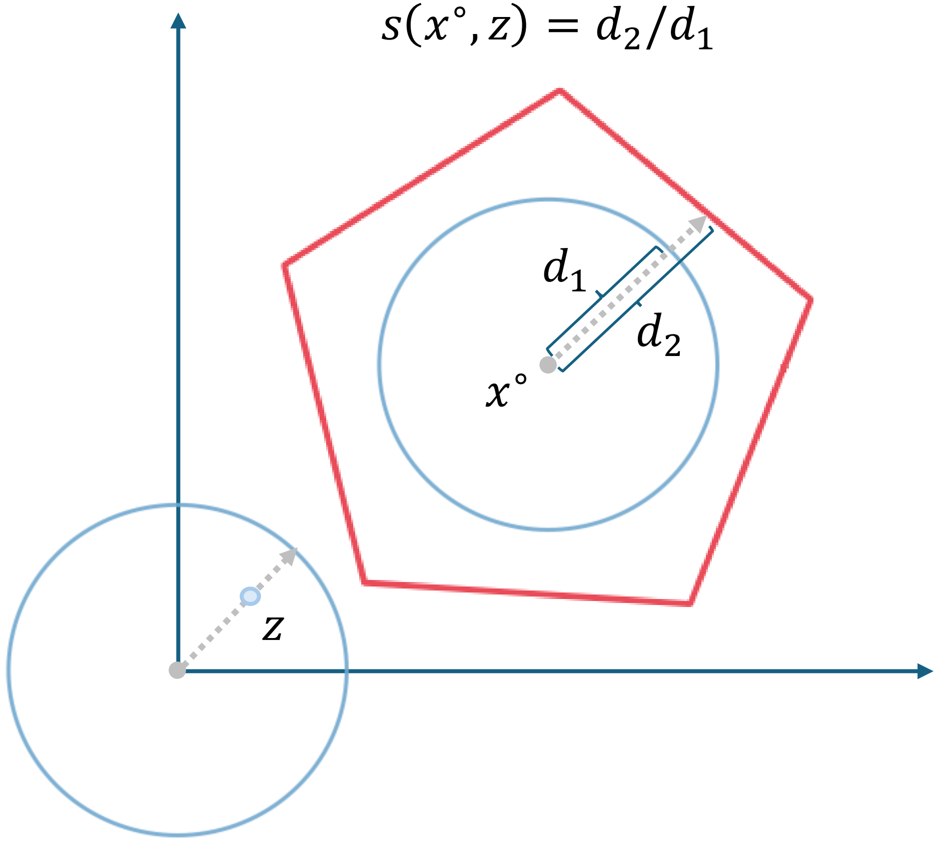
[1] C. Liu, E. Liang*, M. Chen*, *"Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set"*. **NeurIPS 2025. Spotlight.**

Gauge Mapping: Homeomorphism for Convex Set

$$\Phi(z) = x^\circ + s(x^\circ, z) \cdot z$$

- Translating by $x^\circ \in \mathrm{int}(\mathcal{C})$
- Scaling by $s(x^\circ, z) \in \mathbb{R}_+$

- Properties of Φ:
  - Continuous + Invertible → Homeomorphism
  - Bi-Lipschitz → Beneficial for algorithm [4]
- Computation of Φ:
  - Closed-form for common convex sets [1-2]
    - ✓ Linear, quadratic, SOC, LMI.
  - Bisection for general compact convex set [3]



[1] Tabas, D., & Zhang, B. Computationally efficient safe reinforcement learning for power systems. IEEE ACC 2022.
[2] Tordesillas, J., How, J. P., & Hutter, M. Rayen: Imposition of hard convex constraints on neural networks. arXiv 2023.
[3] Mhammedi, Z. Efficient projection-free online convex optimization with membership oracle. COLT 2022.
[4] C. Liu, E. Liang* , M. Chen*, "Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set". NeurIPS 2025. Spotlight.

Computation of Gauge Mapping

Constraints	Formulation	Inverse Distance Function
Intersections	$\{g_1(x) \leq 0, \cdots, g_m(x) \leq 0\}$	$\kappa_g(x^\circ, v) = \max_{1 \leq i \leq m} \{\kappa_{g_i}(x^\circ, v)\}$
Linear	$g_L(x) = a^\top x - b \leq 0$	$\kappa_{g_L}(x^\circ, v) = \{\frac{a^\top v}{b - a^\top x^\circ}\}^+$
Quadratic	$g_Q(x) = x^\top Q x + a^\top x - b \leq 0$	$\kappa_{g_Q}(x^\circ, v) = \{1/\mathrm{root}(A_Q, B_Q, C_Q)\}^+$
Second Order Cone	$g_S(x) = \lVert A^\top x + p \rVert_2 - (a^\top x + b) \leq 0$	$\kappa_{g_S}(x^\circ, v) = \{1/\mathrm{root}(A_S, B_S, C_S)\}^+$
Linear Matrix Inequality	$g_M(x) = \sum_{i=1}^n x_i \cdot F_i + F_0 \succeq 0$	$\kappa_{g_M}(x^\circ, v) = \{\mathrm{eig}(L^\top(-S)L)\}^+$

[1] Notation: $x, a \in \mathbb{R}^n$, $b \in \mathbb{R}$, $Q \in \mathbb{S}^n_+$, $A \in \mathbb{R}^{n \times m}$, $p \in \mathbb{R}^m$, $F_0, \cdots, F_n \in \mathbb{R}^{m \times m}$, $X \in \mathbb{R}^{n \times n}$

[2] $(\cdot)^+ = \max(\cdot, 0)$

[3] $\mathrm{root}(x_1, x_2, x_3) = \frac{-x_2 \pm \sqrt{x_2^2 - 4x_1x_3}}{2x_1}$ denotes the quadratic equation solution

[4] $\mathrm{eig}(X) = \lambda_1, \cdots, \lambda_n$ denotes the eigenvalues satisfying $\det(X - \lambda I) = 0$

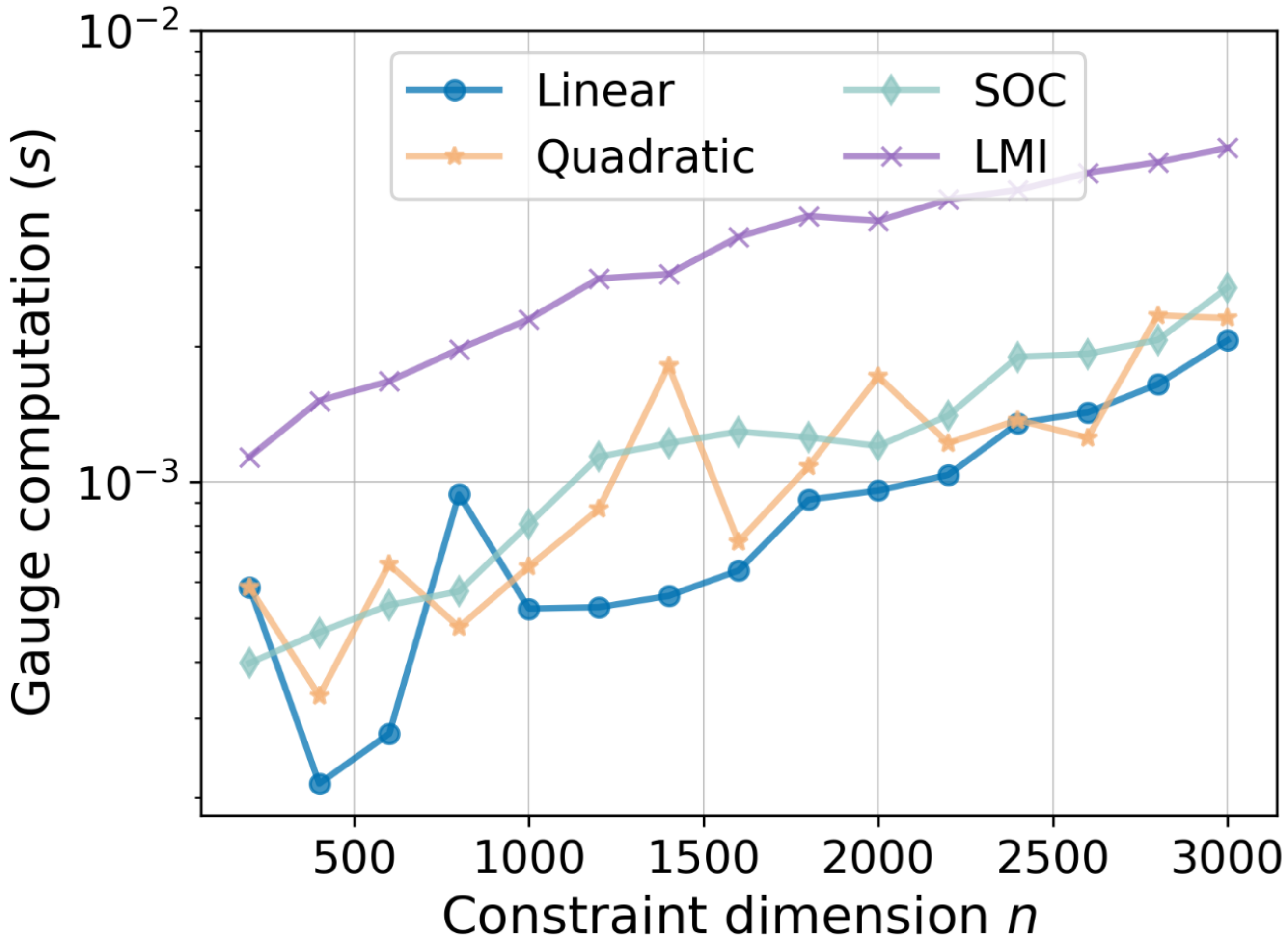
[5] $A_Q = v^\top Q v,\ B_Q = 2x^{\circ\top} Q v + a^\top v,\ C_Q = x^{\circ\top} Q x^\circ + a^\top x^\circ - b$

[6] $A_S = (A^\top v)^\top (A^\top v) - (a^\top v)^2,\ B_S = 2(A^\top x^\circ + p)^\top (A^\top v) - 2(a^\top x^\circ + b)(a^\top v),\ C_S = (A^\top x^\circ + p)^\top (A^\top x^\circ + p) - (a^\top x^\circ + b)^2$

[7] $H = F_0 + \sum_{i=1}^n x_i^\circ F_i$, $H^{-1} = L^\top L$, $S = \sum_{i=1}^n v_i F_i$

[1] C. Liu, E. Liang* , M. Chen*, "Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set". **NeurIPS 2025. Spotlight.**

Computation of Gauge Mapping



[1] C. Liu, E. Liang* , M. Chen*, "Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set". **NeurIPS 2025. Spotlight.**

Landscape Analysis and Algorithm Design

- Original Problem: **(P)**

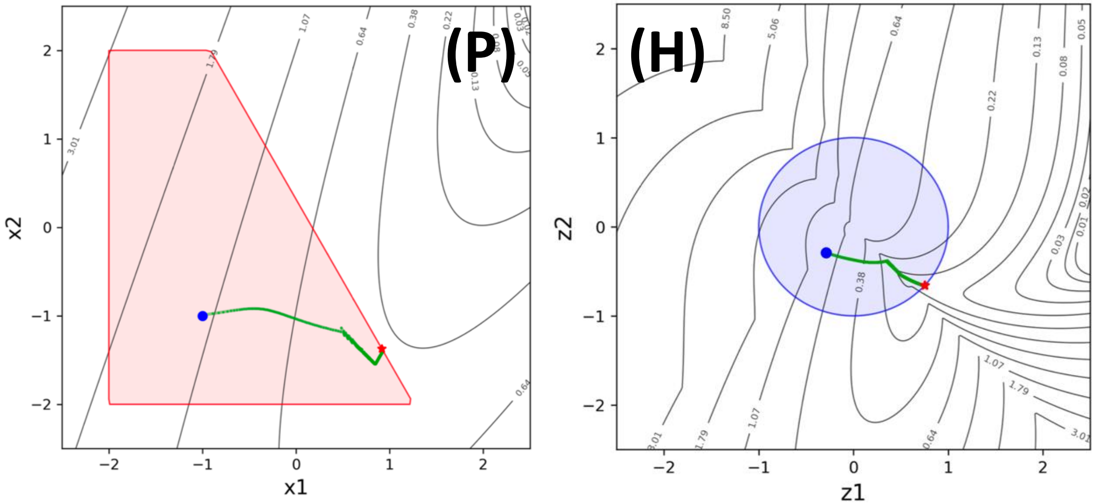
$$\min_{\mathbf{x}} \ f(\mathbf{x}) \quad \text{s.t. } \mathbf{x} \in \mathcal{K}$$

$\mathcal{B} = \psi^{-1}(\mathcal{K})$

- Transformed Problem: **(H)**

$$\min_{\mathbf{z}} \ h(\mathbf{z}) \quad \text{s.t. } \mathbf{z} \in \mathcal{B}$$

$h(\mathbf{z}) = f(\psi(\mathbf{z}))$



Equivalence between **(P)** and **(H)**

Theorem 1: For convex $(\mathbf{P})$ with global optimum x^*, under mild constraint qualification conditions, any stationary point $\boldsymbol{z}^*$ for $(\mathbf{H})$ is
- a global optimum of $(\mathbf{H})$: $h(z^*) \leq h(z)$
- a global optimum of $(\mathbf{P})$: $x^* = \psi(z^*)$

Algorithm 1 Hom-PGD

Input: initial point $\mathbf{z}_0$, problem $\mathbf{H}$ with ψ and maximum iteration number K
for $k = 0$ **to** K **do**
  Compute stepsize α_k
  Update: $\mathbf{z}_{k+1} = \Pi_{\mathcal{B}}\left(\mathbf{z}_k - \alpha_k \nabla h(\mathbf{z}_k)\right)$
end for
Output: $\mathbf{x}_K = \psi(\mathbf{z}_K)$

[1] C. Liu, E. Liang*, M. Chen*, *"Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set"*. **NeurIPS 2025. Spotlight.**

Convergence Rates Analysis : Part I

- Convergence rates [1]:

Theorem 2: Under mild regularity conditions, for compact convex constraint, **Hom-PGD** over ($\mathbf{H}$) match the same convergence rates of **PGD** over **(P)**:

Objective of (**P**)	Strongly Convex	Convex	Non-Convex
Convergence Rate	$\mathcal{O}(\log \epsilon^{-1})$	$\mathcal{O}(\epsilon^{-1})$	$\mathcal{O}(\epsilon^{-2})$

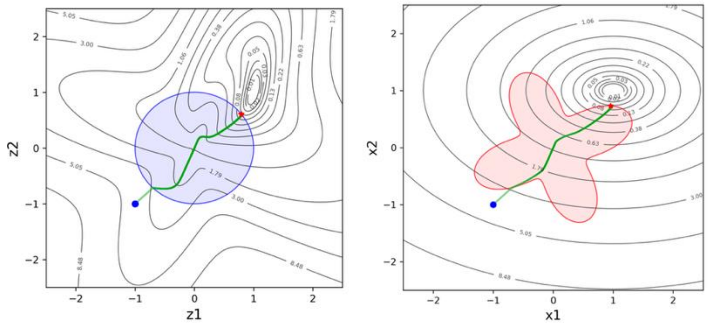
➢Reach the optimal convergence rates under unaccelerated settings [2]

➢Per-iteration cost of $\mathcal{O}(n^2)$, without expensive inner optimization

- **Extension** to structured non-convex settings

➢Proximal-PL objective [3]: $\mathcal{O}(\log \epsilon^{-1})$ rate (match PGD)

➢Star-convex constraints [4]: $\mathcal{O}(\epsilon^{-2})$ rate (beyond PGD)



[1] C. Liu, E. Liang* , M. Chen*, "*Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set*". **NeurIPS 2025. Spotlight.**

[2] Altschuler JM, Parrilo PA. Acceleration by stepsize hedging: Multi-step descent and the silver stepsize schedule. Journal of the ACM. 2025.

[3] Karimi H, Nutini J, Schmidt M. Linear convergence of gradient and proximal-gradient methods under the polyak-łojasiewicz condition. Springer. 2016.

[4] Lee JM. Introduction to topological manifolds. New York, NY: Springer New York; 2000 May 25.

Convergence Rates Analysis: Part II

- Remarks on convergence rates [1]:
  - Under mild conditions, Hom-PGD with **any homeomorphism** can reach the **same order** of convergence rates
  - The **Bi-Lipschitz constants** of homeomorphism impact the **hidden constants** in the convergence rates
- Bi-Lipschitz constants of Gauge Mapping

Proposition 3.3 (Bi-Lipschitz Constants of the Gauge Mapping). *Let $\mathcal{K} \subset \mathbb{R}^n$ be a compact convex set and let $\mathbf{x}^\circ \in \mathrm{int}(\mathcal{K})$ be an interior point. Define the inner and outer radii with respect to $\mathbf{x}^\circ$ as*

$$r_{\mathrm{i}} := \sup\{r \geq 0 : \mathcal{B}(\mathbf{x}^\circ, r) \subseteq \mathcal{K}\}, \quad r_{\mathrm{o}} := \inf\{r \geq 0 : \mathcal{K} \subseteq \mathcal{B}(\mathbf{x}^\circ, r)\},$$

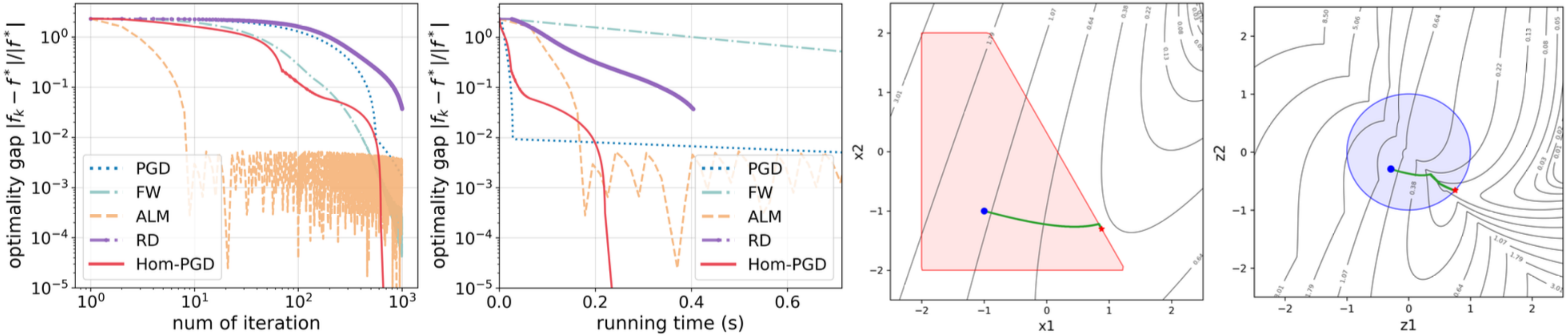
such that $\mathcal{B}(\mathbf{x}^\circ, r_{\mathrm{i}}) \subseteq \mathcal{K} \subseteq \mathcal{B}(\mathbf{x}^\circ, r_{\mathrm{o}})$. Then the Lipschitz constant (denoted as $\mathrm{L}(\cdot)$) of gauge mapping ψ associated with $\mathcal{K}$ satisfies the following bounds:

$$\textit{Forward Lipschitz:} \quad \kappa_2 := \mathrm{L}(\psi) \leq 2\, r_{\mathrm{o}} + r_{\mathrm{o}}^2 / r_{\mathrm{i}}, \quad \textit{Inverse Lipschitz:} \quad \frac{1}{\kappa_1} := \mathrm{L}(\psi^{-1}) \leq 2 / r_{\mathrm{i}}.$$

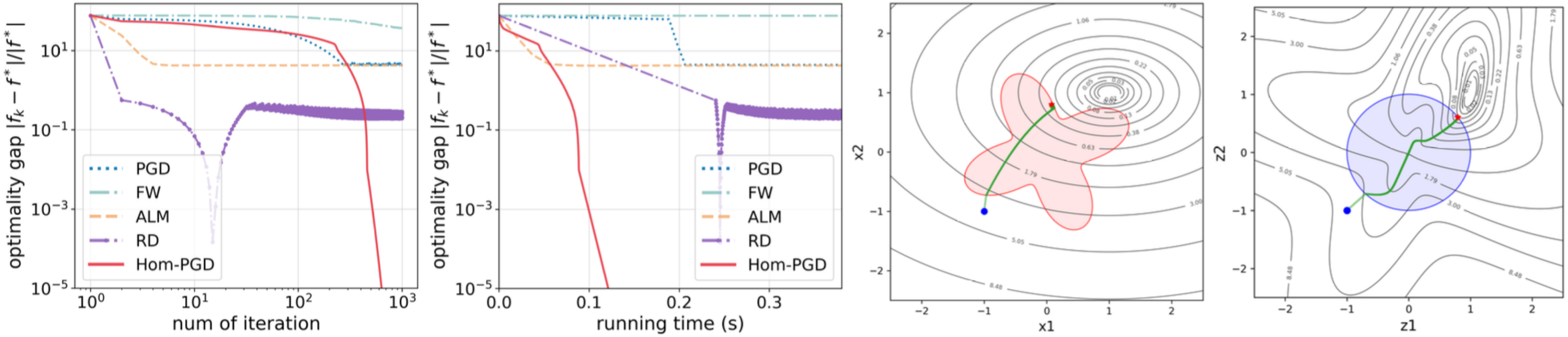
Central interior point → **Smaller** Lipschitz → **Faster** Convergence

[1] C. Liu, E. Liang*, M. Chen*, *"Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set"*. **NeurIPS 2025. Spotlight.**

Illustrative Examples: Convex & Star-convex Cases



(a) convergence rate (b) running time (s) (c) PGD iteration (d) Hom-PGD iteration

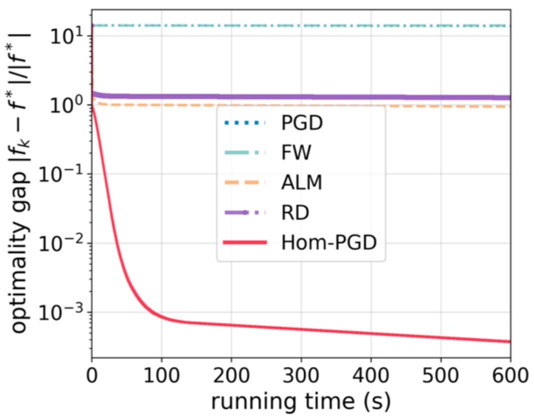


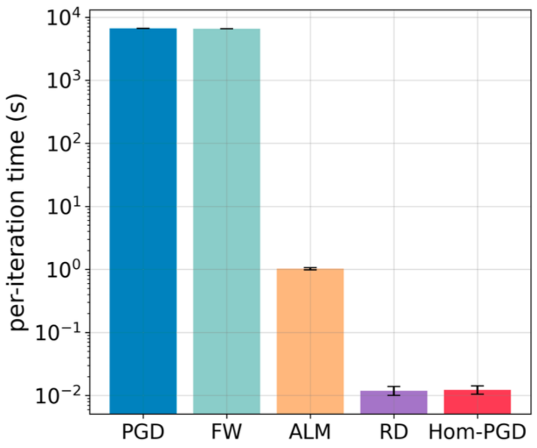
(e) convergence rate (f) running time (s) (g) PGD iteration (h) Hom-PGD iteration

1000+ Dim. Convex Programs: SOCP & SDP

SOCP

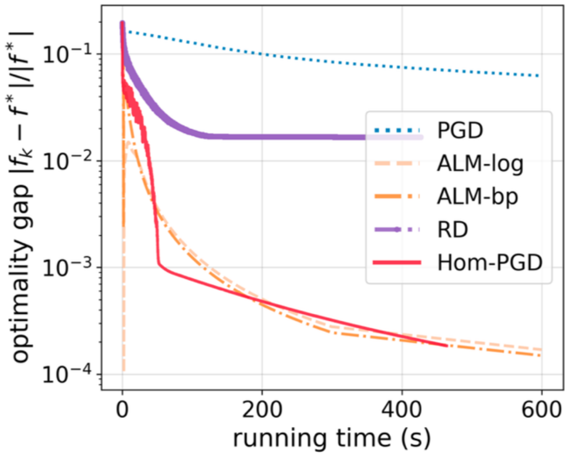
$$\min_{\mathbf{L}\leq\mathbf{x}\leq\mathbf{U}} \frac{1}{2}\mathbf{x}^\top\mathbf{Q}\mathbf{x}+\mathbf{p}^\top\mathbf{x}$$
$$\text{s.t. } \|\mathbf{G}_i\mathbf{x}+\mathbf{h}_i\|_2 \leq \mathbf{c}_i^\top\mathbf{x}+d_i,\ i\in[n_{\text{soc}}]$$

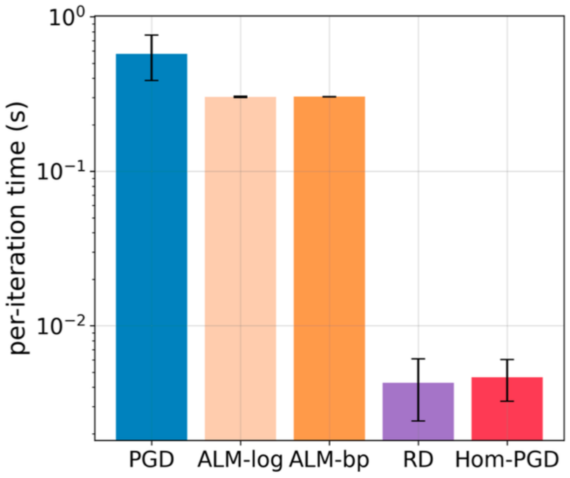




Max-Cut SDP

$$\max_{-1\preceq\mathbf{X}\preceq 1} \sum_{(i,j)\in\mathcal{E}} (1-x_{ij})/2$$
$$\text{s.t. } x_{ii}=1,\quad i\in[n]$$
$$\mathbf{X}\succeq\mathbf{0}$$

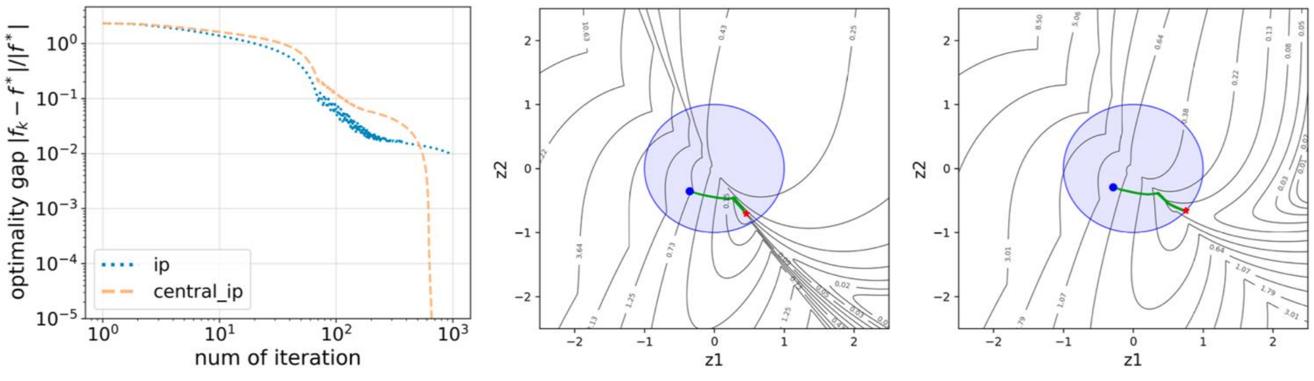




2-4 order reduction on per-iter. cost, **faster** convergence to optimum, per-step **feasibility** guarantees

Ablation Study

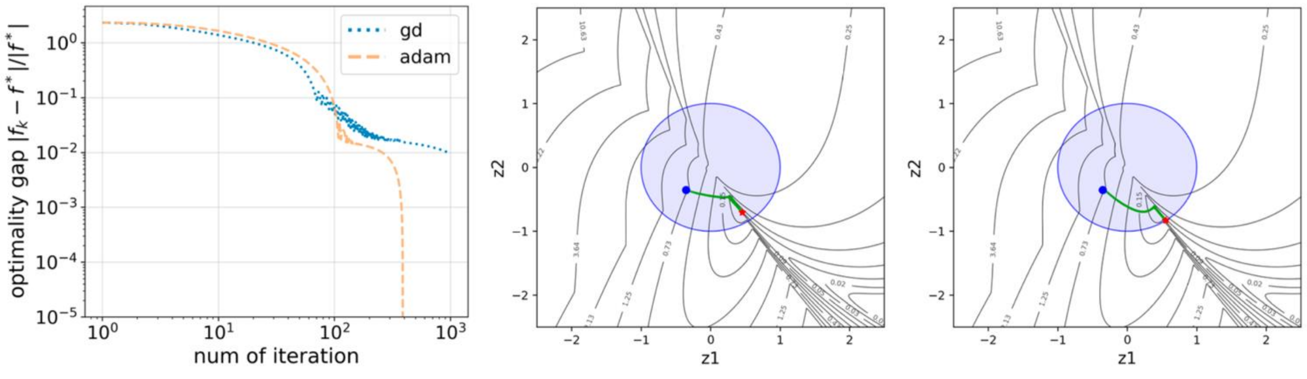
- Impacts of gauge mapping: $\Phi(z) = x^{\circ} + s(x^{\circ}, z) \cdot z$



(a) Convergence comparison. (b) Near-Boundary IP (c) "Central" IP

Central interior point →
Smaller Lipschitz →
Faster Convergence

- Impacts of gradient methods: GD *vs* Adam



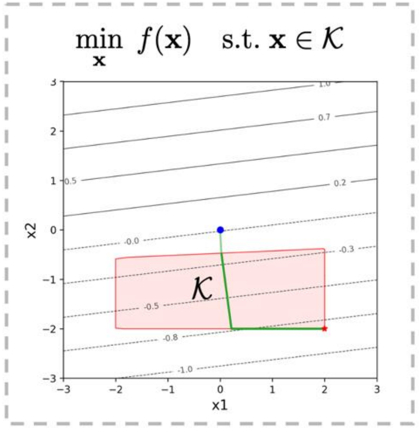
(a) Convergence comparison. (b) Gradient descent (c) Adam [KB14]

Adaptive/Accelerated methods **excel in** non-convex landscapes

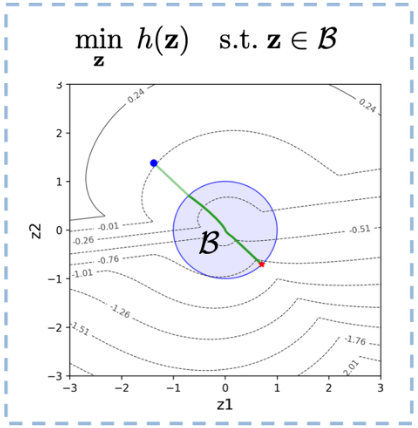
Takeaways: Hom-PGD

- **Idea:**
  - ➢Transform complex constrained problems into simple ones via homeomorphism.
- **Contributions:**
  - ➢Construct **explicit-form homeomorphism** for any compact convex set via **gauge mapping**
  - ➢Hom-PGD as an algorithm that with **low per-iter costs**, matching **optimal convergence**
- **Future works:**
  - ➢Advanced gradient methods (Nesterov, momentum, Adam)
  - ➢Extend to more general non-convex constraints [2]

PGD



Hom-PGD



[1] C. Liu, E. Liang*, M. Chen*, "*Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set*". **NeurIPS 2025. Spotlight.**

[2] C. Liu, E. Liang*, M. Chen*, "*Hom-PGD+: Homeomorphic Reformulation for Efficient Optimization over Non-convex Sets*". Under review

Homeomorphism Methods: Part II

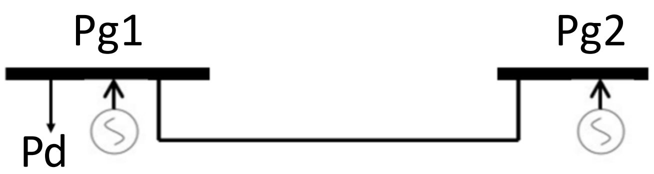
Hom-Proj. to Ensure Neural Network Feasibility

[1] E. Liang, M. Chen, S. Low, "*Low Complexity Homeomorphic Projection to Ensure NN Solution Feasibility for Optimization over (Non-)Convex Set*", **ICML, 2023.**
[2] E. Liang, M. Chen, S. Low, "*Homeomorphic Projection to Ensure NN Solution Feasibility for Constrained Optimization*". **JMLR 2024**.

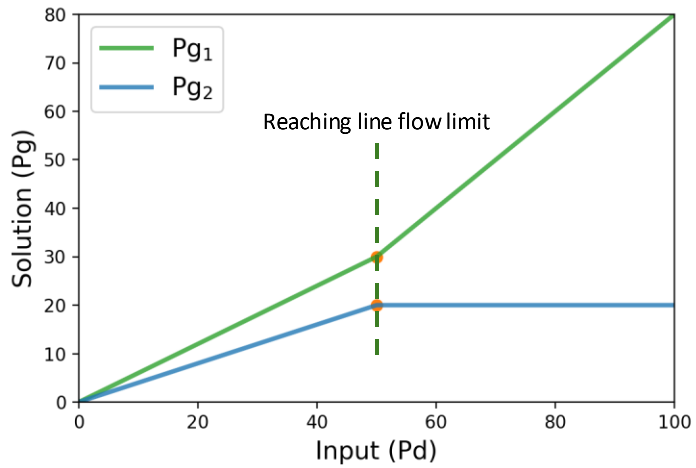
Input-Solution Mapping for Optimization Problems

Input		Solution
$\theta_1,$ $\theta_2,$ …	→ **Iterative Solver** →	$x_1^*,$ $x_2^*,$ …

Optimal power flow problem



Pd: demand; **Pg**: generation



- Learn the mapping between input and solution
  - ➢ **Continuous** (a.e.) mapping for optimization with continuous objective and constraints [1-4]

[1] Dontchev, A. L., & Rockafellar, R. T. *Implicit functions and solution mappings* (Vol. 543). New York: Springer. 2009
[2] P. Tøndel, T. A., Johansen and A. Bemporad. *An algorithm for multi-parametric quadratic programming and explicit MPC solutions*. Automatica, 2003
[3] X. Pan, T. Zhao, M. Chen, and S. Zhang. *DeepOPF: A deep neural network approach for security-constrained dc optimal power flow*. IEEE Trans. Pow. Sys. 2019
[4] X. Pan, M. Chen, T. Zhao, S. H. Low. *DeepOPF: A feasibility-optimized deep neural network approach for AC optimal power flow problems*. IEEE Sys. J. 2022

Machine Learning Approach

- Use NN to learn the input-to-solution mapping
  - **Why**: Universal Approximation Theorem [1-5]

> *NNs (e.g., FCNN, CNN, ResNet, Transformer, …) can approximate "any" continuous mapping arbitrarily well with sufficient parameters.*

  - **How**: e.g., supervised learning

Problem

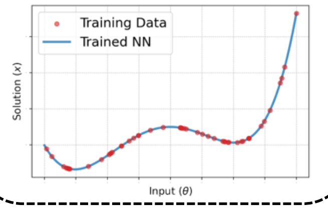
$$\min_x f(x,\theta) \quad \text{s.t.. } h(x,\theta)=0, \quad g(x,\theta)\le 0$$

Dataset

θ_1, θ_2, … → Iterative solver → x_1^*, x_2^*, …

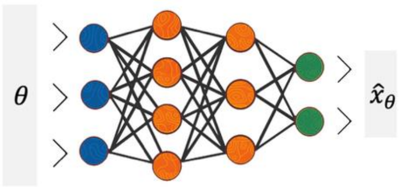
Training

$$\min_{F_{nn}} \sum_i ||F_{nn}(\theta_i) - x_i^*||$$



Applying

$$\hat{x}_\theta = F_{nn}(\theta)$$



- NN can predict near-optimal solutions in real-time

[1] K. Hornik, "Approximation capabilities of multilayer feed forward networks," Neural networks, vol.4, no.2, pp. 251–257,1991.
[2] G. Cybenko, "Approximation by superpositions of a sigmoidal function", Math. Control Signals Systems, 2(4):303–314, 1989.
[3] Pinkus, Allan. "Approximation theory of the MLP model in neural networks." Acta numerica, 8 :143-195, 1999.
[4] Zhou, D. X. Universality of deep convolutional neural networks. *Applied and computational harmonic analysis*, *48*(2), 787-794. 2020.
[5] Lin, H., & Jegelka, S. Resnet with one-neuron hidden layers is a universal approximator. NeurIPS 2018.

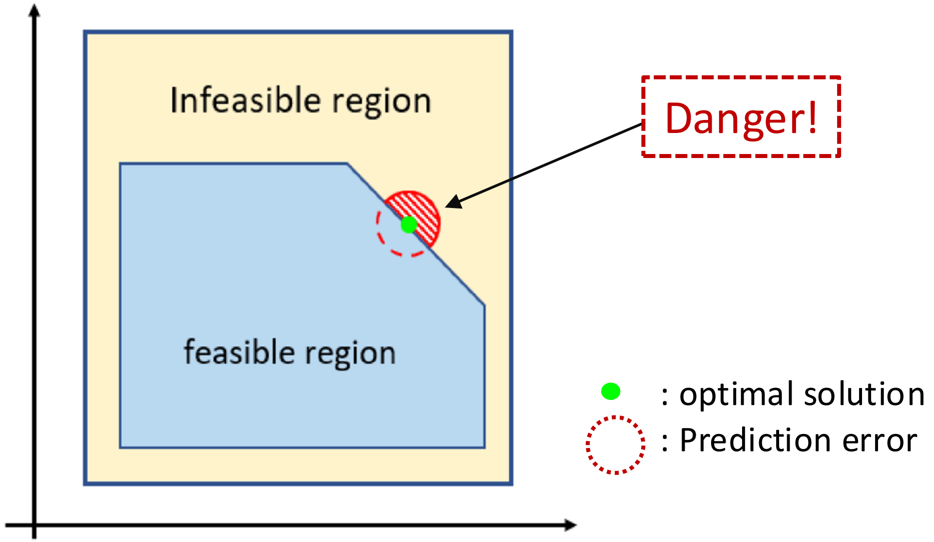
Progress and Significant Results

- Algorithmic design
  - ➢Unsupervised, self-supervised, GNN[1-3]
- Theoretical advance
  - ➢Approximation capability of deep NN & ResNet [4-6]
  - ➢Universal approximation of GNN [7]
- Real-world applications
  - ➢Power grid [8-9], wireless network [10], PDE solvers [11],…

[1] Park, S., & Van Hentenryck, P. Self-supervised primal-dual learning for constrained optimization. AAAI. 2023
[2] Huang, W., Chen, M., & Low, S. H. Unsupervised Learning for Solving AC Optimal Power Flows: Design, Analysis, and Experiment. IEEE Trans. Power Syst. 2024
[3] Owerko, D., Gama, F., & Ribeiro, A. Optimal power flow using graph neural networks. IEEE ICASSP. 2020.
[4] Yarotsky, D. Error bounds for approximations with deep ReLU networks. Neural networks, 94, 103-114. 2017
[5] Liang, S., & Srikant, R. Why deep neural networks for function approximation. ICLR. 2017
[6] Liu, C, Liang, E., & Chen, M. Characterizing ResNet's Universal Approximation Capability. ICML. 2024
[7] Chen Z, Liu J, Wang X, Lu J, Yin W. On representing linear programs by graph neural networks. ICLR 2023.
[8] X. Pan, T. Zhao, M. Chen, and S. Zhang. DeepOPF: A deep neural network approach for security-constrained dc optimal power flow. IEEE Trans. Pow. Sys. 2019
[9] Pan, X., Chen, M., Zhao, T., & Low, S. H. DeepOPF: A feasibility-optimized deep neural network approach for AC optimal power flow problems. IEEE Syst. J. 2022
[10] Shen, Y., Zhang, J., Song, S. H., & Letaief, K. B. Graph neural networks for wireless communications: From theory to practice. IEEE Trans. Wireless Commun. 2022
[11] Greenfeld D, Galun M, Basri R, Yavneh I, Kimmel R. Learning to optimize multigrid PDE solvers. ICML 2019.

Challenge: Ensuring Neural Network Feasibility

- Feasible solution is crucial for safety-critical systems
  - E.g., in power grid operation, violating line capacity limits can cause grid failure

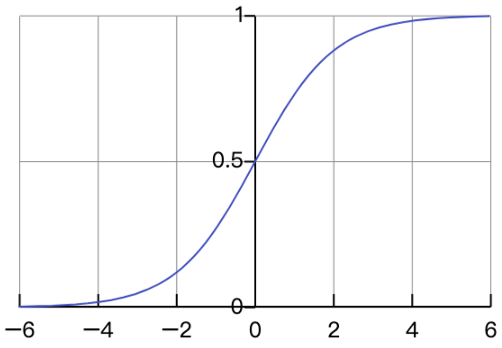


- Hard to guarantee NN feasibility due to prediction errors

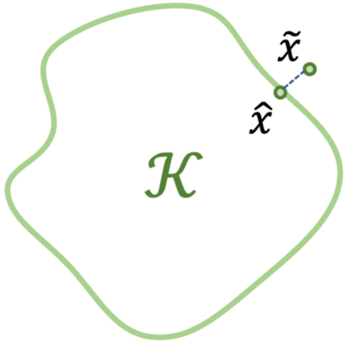
Existing Works on Neural Network Feasibility

Existing Work	Constraint Setting	Feasibility Ensuring	Optimality Bound	Low Run-time
Activation layer	Simplex/Box	✓	✓	✓
Penalty/Lagrangian	General	✗	✗	✓
Orthogonal projection	General	✓	✓	✗
Sampling approach	General	✓	✓	✗
Preventive learning	Linear	✓	✗	✓
Gauge/RAYEN	Convex	✓	✓	✓

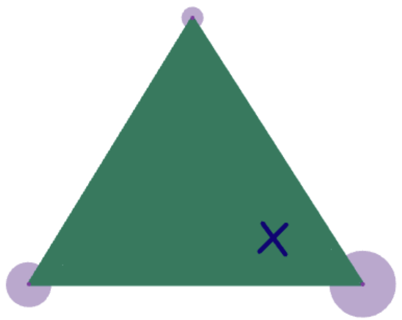
Sigmoid activation



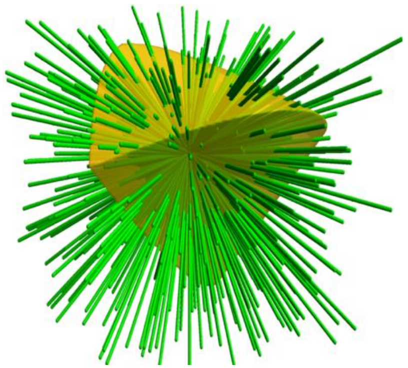
l_2 projection



Sampling-based



RAYEN



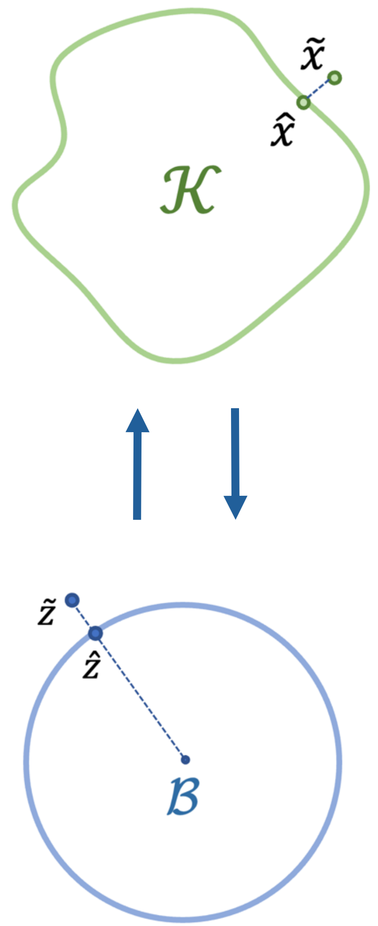
Previous works either **lack** performance guarantees, or applicable to **limited** constraint sets, or **slow** in run-time

Motivation and Ball-Homeomorphism

- NN predicts near-optimal but infeasible solutions
- Solve projection for feasibility
  - ➢ over a non-convex set: **hard**
  - ➢ over a ball: **easy**

$$x_{t+1} = \Pi_{\mathcal{K}}\left(\tilde{x}_{t+1}\right) := \arg\min_{x\in\mathcal{K}} \frac{1}{2}\|x-\tilde{x}_{t+1}\|_2^2$$

Transform the hard projection to easy projection over ball



- Homeomorphism:
  - ➢ *Bijective* & *Bi-continuous* mapping
  - ➢ Preserve topological structures
- **Ball-homeomorphic** constraint set ?

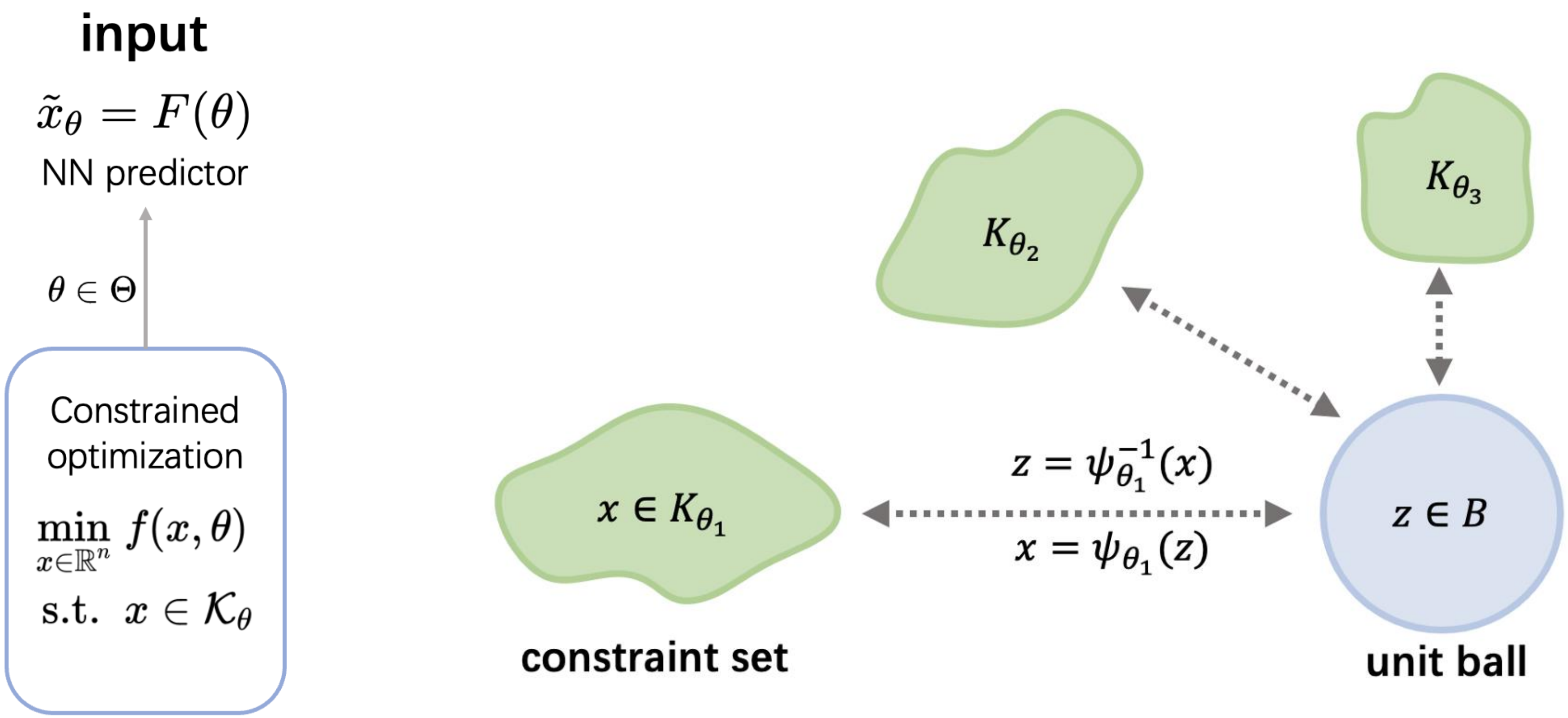
Ball-Homeomorphic Constraint Set

- All compact (star-)convex sets [1]
- For compact and contractible manifold [2]
  - in 6 (or higher)-dim space and its boundary is **simply connected**
  - in 5-dim space and its boundary is **diffeomorphic** to a **4-dim sphere**
- All open simply-connected sets in 2-dimension space [3]

Ball-Homeomorphic set a **general** class of **non-convex** set beyond convex and star-convex set

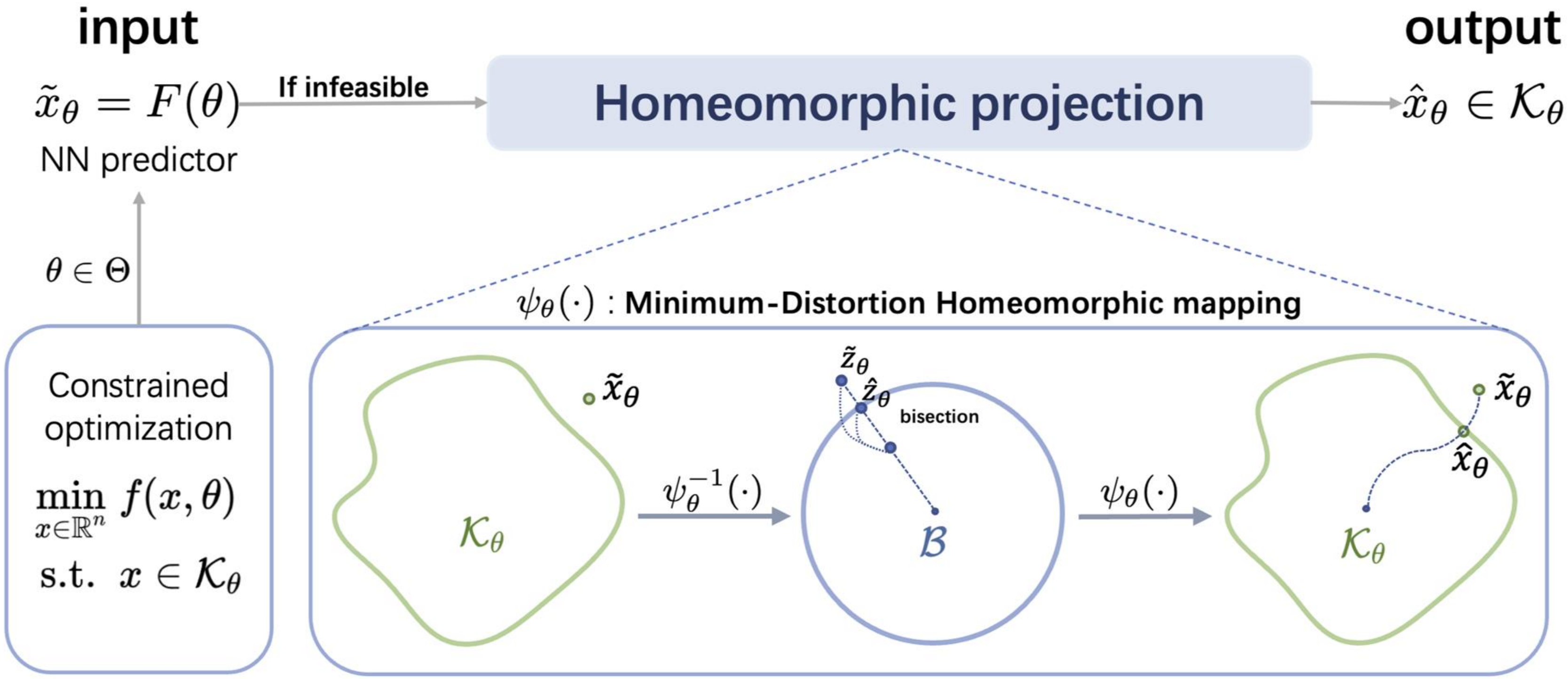
[1] Geschke, S. (2012). Convex open subsets of Rn are homeomorphic to n-dimensional open balls. Hausdorff Center for Mathematic.
[2] Smale, S. (1962). On the structure of manifolds. American Journal of Mathematics, 84(3), 387-399 (**Theorem 5.1**)
[3] **Riemann Mapping Theorem**

Homeomorphic Projection



Setting: recover NN solution feasibility over ball-homeomorphic sets

Homeomorphic Projection



1. Learn homeomorphism for a class of non-convex set
2. Transform the hard projection problem into ball space
3. Perform bisection over the ball for feasible solution

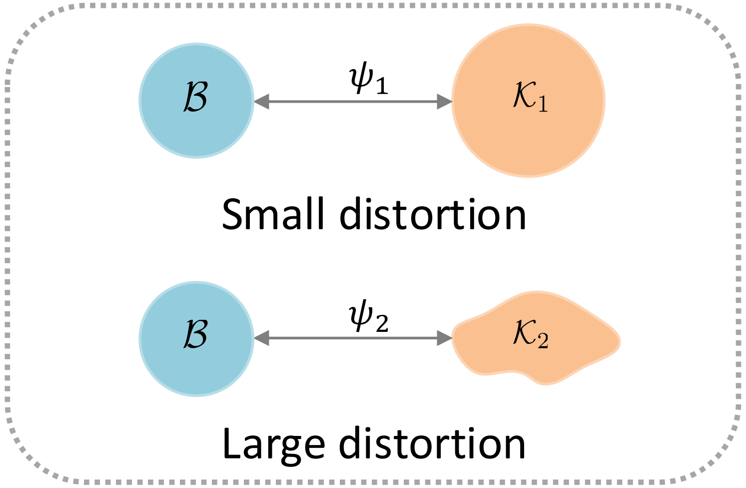
[1] E. Liang, M. Chen, S. Low, "*Low Complexity Homeomorphic Projection to Ensure NN Solution Feasibility for Optimization over (Non-)Convex Set*", **ICML, 2023.**
[2] E. Liang, M. Chen, S. Low, "*Homeomorphic Projection to Ensure NN Solution Feasibility for Constrained Optimization*". **JMLR 2024**.

Distortion and Homeomorphism

Distortion: $\mathrm{D}(\psi) = k_2/k_1 \geq 1$

$$k_2 = \sup_{z_1,z_2}\left\{\frac{||\psi(z_1)-\psi(z_2)||}{||z_1-z_2||}\right\}, \quad k_1 = \inf_{z_1,z_2}\left\{\frac{||\psi(z_1)-\psi(z_2)||}{||z_1-z_2||}\right\}$$

- Ratio of max & min distance **variations** by ψ
- **Multiple** homeomorphic mappings between two sets



Prop. 1. Let ψ be a homeomorphic mapping between $\mathcal{B}$ and $\mathcal{K}$, the homeomorphic projection as:

$$\mathrm{HP}_{\mathcal{K}}(x) = \psi(\Pi_{\mathcal{B}}(\psi^{-1}(x)))$$

Then the projection distance is bounded as:

$$||\Pi_{\mathcal{K}}(x) - x|| \leq ||\mathrm{HP}_{\mathcal{K}}(x) - x|| \leq \mathrm{D}(\psi) \cdot ||\Pi_{\mathcal{K}}(x) - x||$$

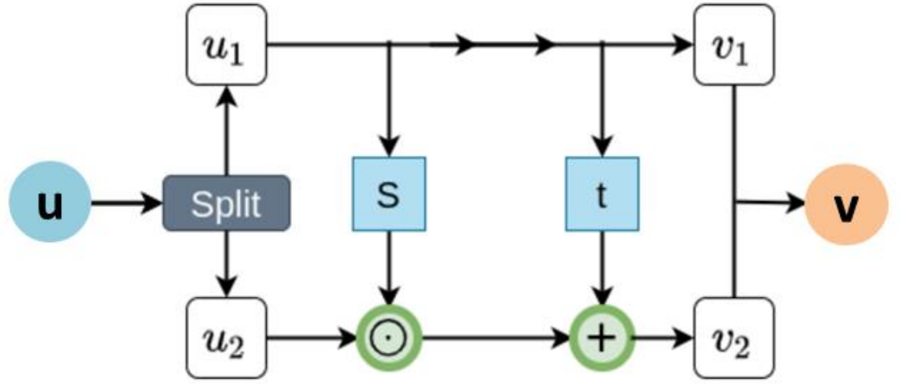
Orthogonal projection distance	Homeomorphic projection distance	Distortion of Homeomorphism

Minimum Distortion Homeomorphism (MDH)

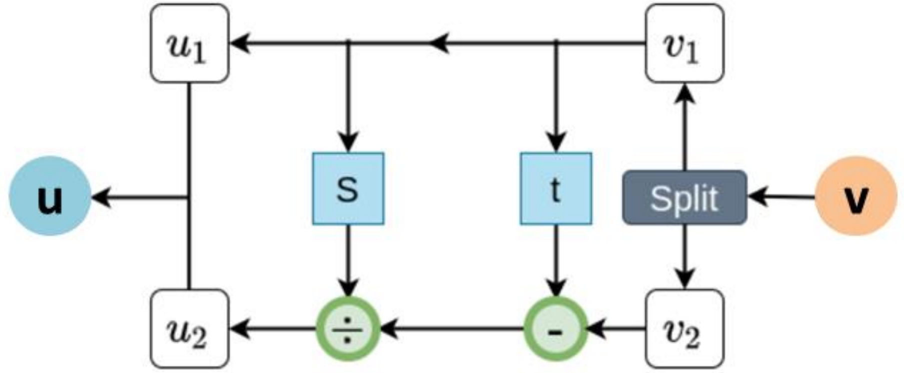
$$\min_{\psi_\theta \in \mathcal{H}^n} \quad \log \mathrm{D}\left(\psi_\theta\right)$$
$$\text{s.t.} \quad \mathcal{K}_\theta = \psi_\theta(\mathcal{B})$$

Invertible NN Can Approximate MDH

- Invertible Neural Network Φ :
  - NN with invertibility
  - E.g., coupling layers [1]
- Properties of Φ:
  - Continuous + Invertible → Homeomorphism
- Universal approximation of INN
  - INN can approximate "any" homeomorphic mapping arbitrarily well with sufficient layers [2]



coupling layer: **forward**



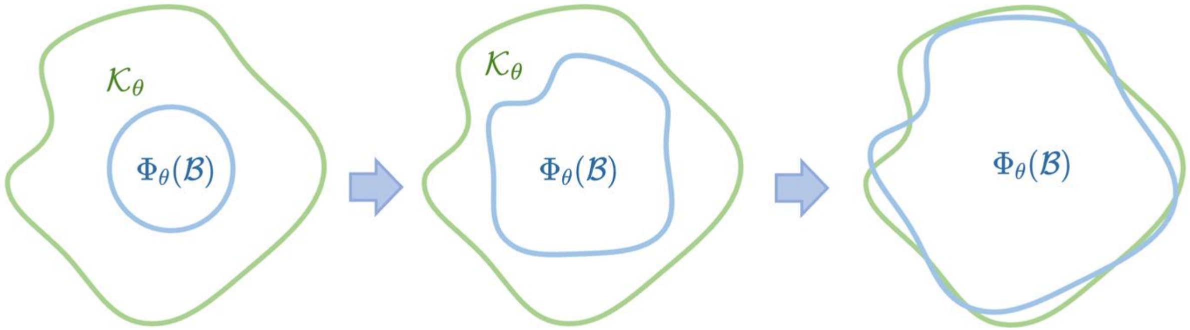
coupling layer: **inverse**

Challenge: How to design the loss function?

[1] L. Dinh, D. Krueger, and Y. Bengio. Nice: Non-linear independent components estimation. ICLR 2015.
[2] T. Teshima, I. Ishikawa, K. Tojo, K. Oono, M. Ikeda, and M. Sugiyama. Coupling-based invertible neural networks are universal diffeomorphism approximators. NeurIPS 2020

Training INN to Approximate MDH

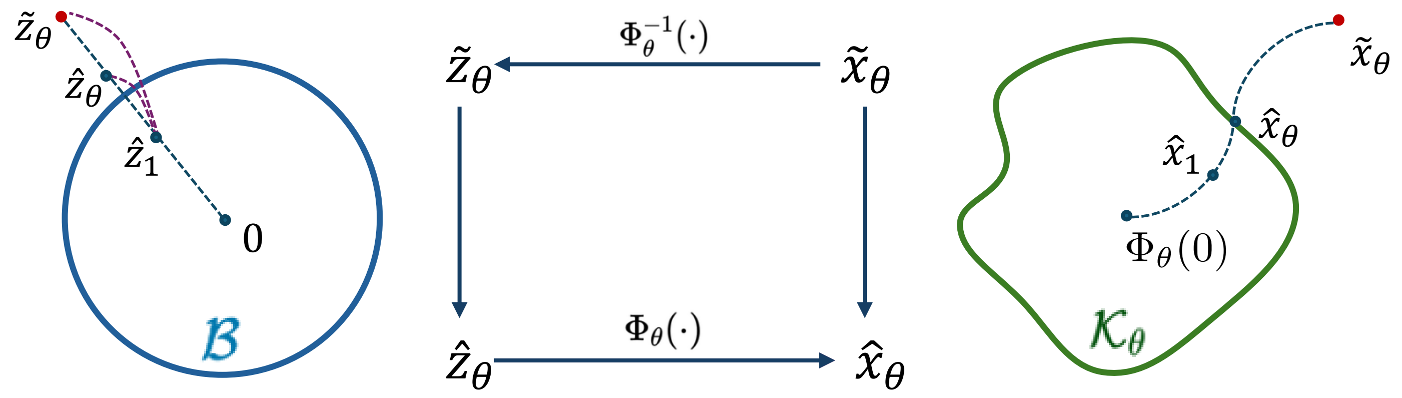
- Training INN for homeomorphism between $\mathcal{B}$ and $\mathcal{K}$
  - Loss design: $\mathcal{L}(\Phi_\theta) = \underbrace{\widehat{\mathrm{V}}(\Phi_\theta(\mathcal{B}))}_{\text{Volume maximization}} - \lambda_1 \underbrace{\mathrm{P}(\Phi_\theta(\mathcal{B}))}_{\text{Penalty for } \Phi_\theta(\mathcal{B}) \subseteq \mathcal{K}_\theta} - \lambda_2 \underbrace{\widehat{\mathrm{D}}(\Phi_\theta)}_{\text{Distortion regularization}}$
  - Training dynamics:



  - θ-dependent constraint $\mathcal{K}_\theta \implies$ optimize total loss $\mathbb{E}_\theta[L(\Phi_\theta)]$

- Training requirement: a **valid** trained INN, i.e., $\Phi_\theta(0) \in \mathcal{K}_\theta$
  - Mapping the center of ball to a feasible point

Bisection Algorithm



- Given a **valid** INN and an infeasible solution
  - **Step 1:** map it to ball space:

$$\tilde{z}_\theta = \Phi_\theta^{-1}(\tilde{x}_\theta)$$

  - **Step 2**: bisection for α

$$\alpha^* = \sup_{\alpha\in[0,1]} \{\Phi_\theta(\alpha \cdot \tilde{z}_\theta) \in \mathcal{K}_\theta\}$$

  - **Step 3**: map it back

$$\hat{x}_\theta = \Phi_\theta(\alpha^* \cdot \tilde{z}_\theta)$$

Feasibility, Optimality, and Run-time

Theorem 1. For a ball-homeomorphic set, given a valid m-layer INN and an infeasible n-dim solution, the k-step bisection will return a solution with

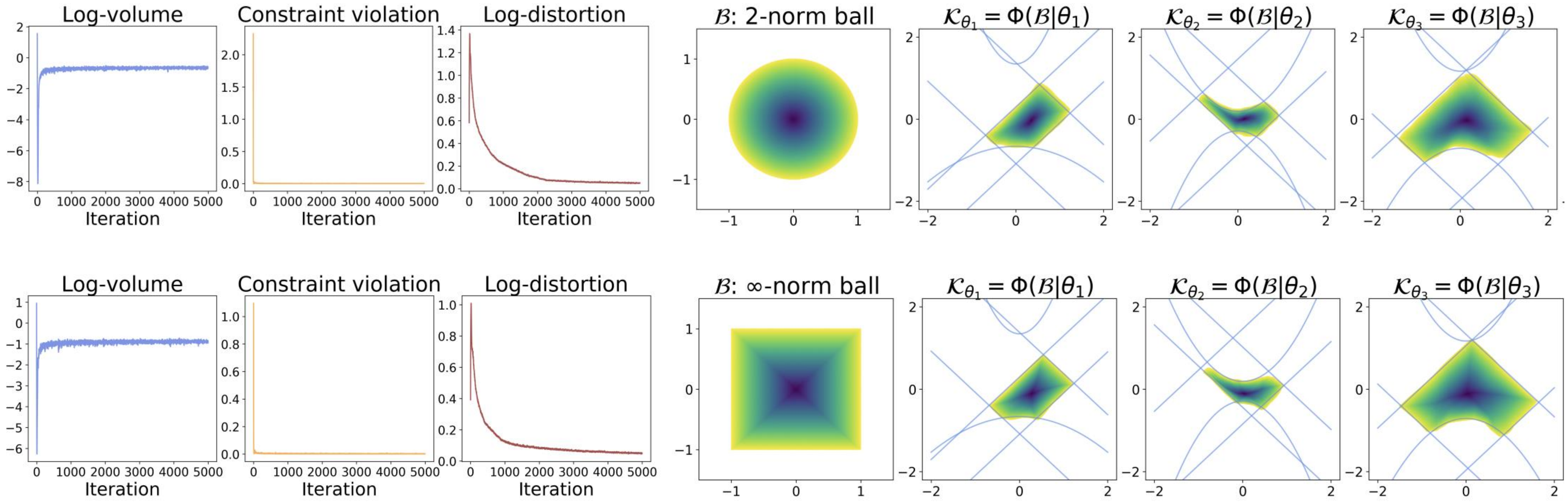
- **Feasibility guarantee**
- **Bounded optimality loss**: $\epsilon_{\text{pre}} + \epsilon_{\text{bis}} + \ \epsilon_{\text{hom}}$
  - ϵ_{pre}: NN prediction error
  - $\epsilon_{\text{bis}} = O(2^{-k})$: bisection-induced optimal loss
  - $\epsilon_{\text{hom}} \leq \mathrm{D}(\Phi_\theta)(2\epsilon_{\text{inn}} + \epsilon_{\text{pre}})$: homeomorphism-induced optimality loss
- **Run-time complexity**: $O(kmn^2)$

Performance guarantees over ball-homeomorphic constrains beyond convex ones

INN Learns Homeomorphism

- Learning the MDH mapping between a unit ball and a non-convex quadratic constraint set (with different input θ)

$$\mathcal{K}_\theta = \{x \in \mathbb{R}^2 \mid x^\top Q x + q^\top x + b \leq 0, \quad \theta = [Q, q, b]\}\}$$



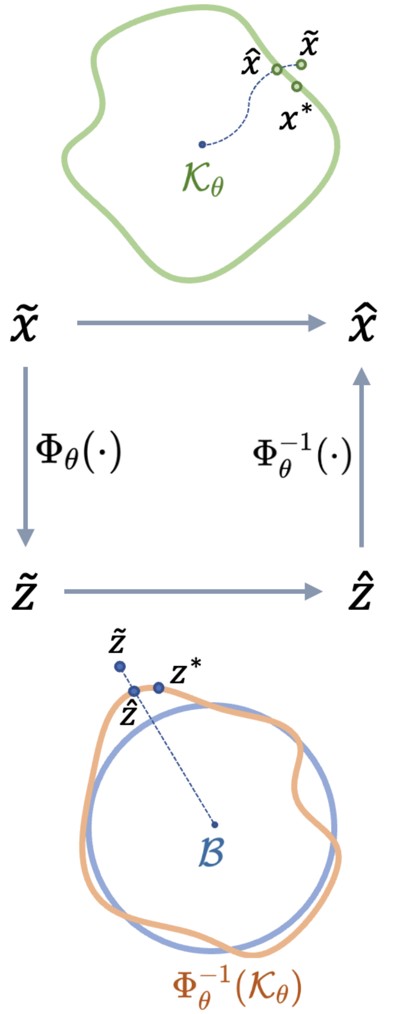
Recovering Feasibility for Constrained Problems

- NN solutions for QCQP, SOCP, and non-convex AC-OPF
  - **100%** feasibility, **0.2%** extra optimality loss, **2-4 order** speedup

Method		Feasibility			Optimality				Speedup	
NN Predictor	Post Processing	feas. rate % (↑)	ineq. vio. 1-norm (↓)	eq. vio. 1-norm (↓)	solution error ave. % (↓)	solution error cor. % (↓)	objective error ave. % (↓)	objective error cor. % (↓)	ave. × (↑)	cor. × (↑)
		Convex QCQP: $n = 200,\ d = 100,\ n_{\text{eq}} = 100,\ n_{\text{ineq}} = 100$								
NN	–	93.95	0.047	0	4.16	4.36	1.45	1.42	10^6	–
NN	WS	100	0	0	3.9	0	1.37	0	12.8	0.8
NN	Proj	100	0	0	4.16	4.36	1.45	1.43	21.3	1.3
NN	D-Proj	94.14	0.015	0	4.16	4.36	1.45	1.42	805	48.8
NN	H-Proj	100	0	0	4.17	4.52	1.47	1.69	8353	511
		SOCP: $n = 200,\ d = 100,\ n_{\text{eq}} = 100,\ n_{\text{ineq}} = 100$								
NN	–	88.96	0.192	0	4.8	5.27	1.35	0.99	10^6	–
NN	WS	100	0	0	4.22	0	1.24	0	12.9	1.4
NN	Proj	100	0	0	4.8	5.26	1.37	1.14	13.6	1.5
NN	D-Proj	93.85	0.007	0	4.84	5.56	1.38	1.22	308	34
NN	H-Proj	100	0	0	4.83	5.47	1.41	1.56	6724	749
		118-node AC-OPF: $n = 344,\ d = 236,\ n_{\text{eq}} = 236,\ n_{\text{ineq}} = 452$								
NN	–	94.92	0.002	0	9.05	9.08	0.69	0.59	10^4	–
NN	WS	100	0	0	8.59	0	0.66	0	29	1.5
NN	Proj	100	0	0	9.13	10.75	0.69	0.59	33.1	1.7
NN	D-Proj	95.41	0.002	0	9.05	9.08	0.69	0.59	24.6	1.3
NN	H-Proj	100	0	0	9.36	15.3	0.78	2.44	370	22.9

Takeaways: **Hom-Proj.**

- **Idea**:
  - ➢Transform complex projection problems into easy ones via homeomorphism.
- **Contributions:**
  - ➢Learn **homeomorphism** for non-convex set via invertible neural network (with universal approximation)
  - ➢Hom-Proj to ensure NN output **feasibility** with **bounded optimality gaps** and **low complexity**
- **Future works:**
  - ➢More general non-convex constraint set [1]
  - ➢Extend to stochastic constraints [2-3]



[1] E. Liang, M. Chen, "*Efficient Bisection Projection to Ensure NN Solution Feasibility over General Set*", **ICML 2025.**

[2] M. Zhou, E. Liang*, M. Chen*, S. Low. "*Partially Permutation-Invariant Neural Network for Solving Two-Stage Stochastic AC-OPF Problem.*", **IEEE Trans. on Power System. 2025.**

[3] E. Liang*, M. Zhou, J. Zhao, M. Chen* "Solving Chance-Constrained AC-OPF Problem by Neural Network with Bisection-based Projection", **ACM E-energy. 2025.**

Conclusion

- **Homeomorphism** methods for decision-making with hard constraints
  - **Idea**: transform complex problem into simple domains
    - — **Hom-PGD** to accelerate iterative algorithms [1,2]
    - — **Hom-Proj.** to ensure neural network feasibility [3,4]
  - **Goals**: safe, economic, rea-time decisions

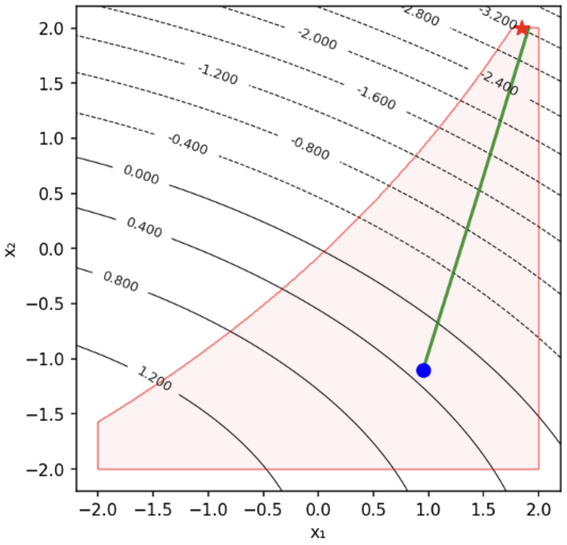
- Leverage ML, optimization, and topology for smarter decision making
  - Leverage symmetry/low-dim. to further reduce complexity [5-6]
  - Generative models with hard constraints [7-8]
  - Combinatorial & Discrete Problems

[1] C. Liu, E. Liang* , M. Chen*, "*Fast Projection-Free Algorithm (without Optimization Oracles) for Optimization over General Convex Set*". **NeurIPS 2025. Spotlight.**
[2] C. Liu, E. Liang*, M. Chen*, "*Hom-PGD+: Homeomorphic Reformulation for Efficient Optimization over Non-convex Sets*". Under review
[3] E. Liang, M. Chen, S. Low, "*Low Complexity Homeomorphic Projection to Ensure NN Solution Feasibility for Optimization over (Non-)Convex Set*", **ICML, 2023.**
[4] E. Liang, M. Chen, S. Low, "*Homeomorphic Projection to Ensure NN Solution Feasibility for Constrained Optimization*". **JMLR 2024**.
[5] E. Liang, M. Chen, "*Efficient Bisection Projection to Ensure NN Solution Feasibility over General Set*", **ICML 2025.**
[6] M. Zhou, E. Liang*, M. Chen*, S. Low. "*Partially Permutation-Invariant NN for Solving Two-Stage Stochastic AC-OPF Problem.*", **IEEE Trans. on Power System.**
[7] X. Li*, E. Liang*, M. Chen, "*Gauge Flow Matching for Efficient Constrained Generative Modelling over General Convex Set.*", **ICLR 2025 Delta Workshop. Outstanding Short Paper Award**
[8] E. Liang, M. Chen, "*Generative Learning for Solving Non-Convex Problem with Multi-Valued Input-Solution Mapping*", **ICLR 2024.**

Extension I: Hom-PGD for Non-convex Constraints

Original Space

$$\min_{\mathbf{x}} \; f_\theta(\mathbf{x}) \quad \text{s.t. } \mathbf{x} \in \mathcal{K}_\theta$$

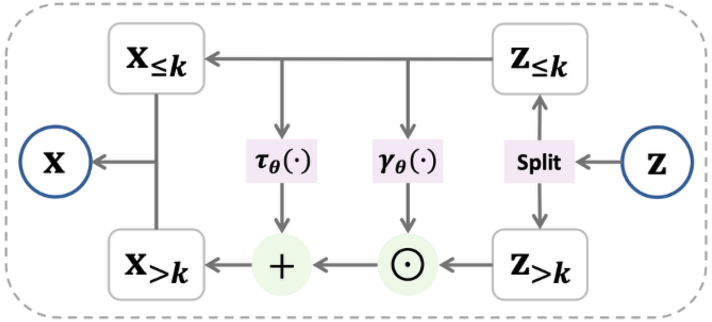


Invertible Neural Network Φ_θ

Objective: $H_\theta(\mathbf{z}) = f_\theta(\Phi_\theta(\mathbf{z}))$ **Constraint:** $\widetilde{\mathcal{B}} = \Phi_\theta^{-1}(\mathcal{K})$

$\mathbf{x} = \Phi_\theta(\mathbf{z})$

$\times l$

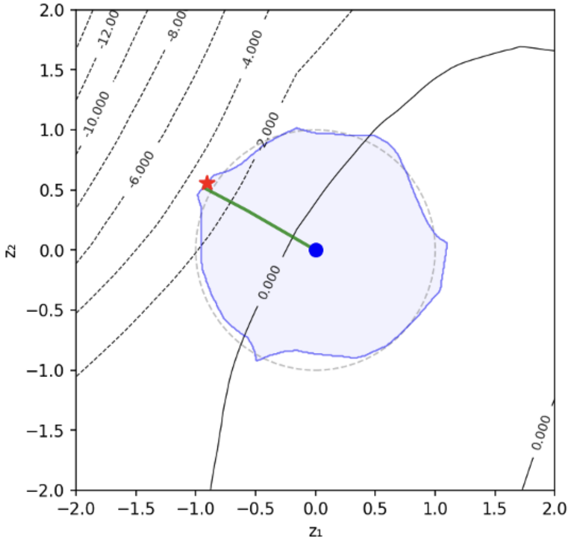


$\mathbf{z} = \Phi_\theta^{-1}(\mathbf{x})$

Initial point — Iteration trajectory — Optimal point

Hom. Space

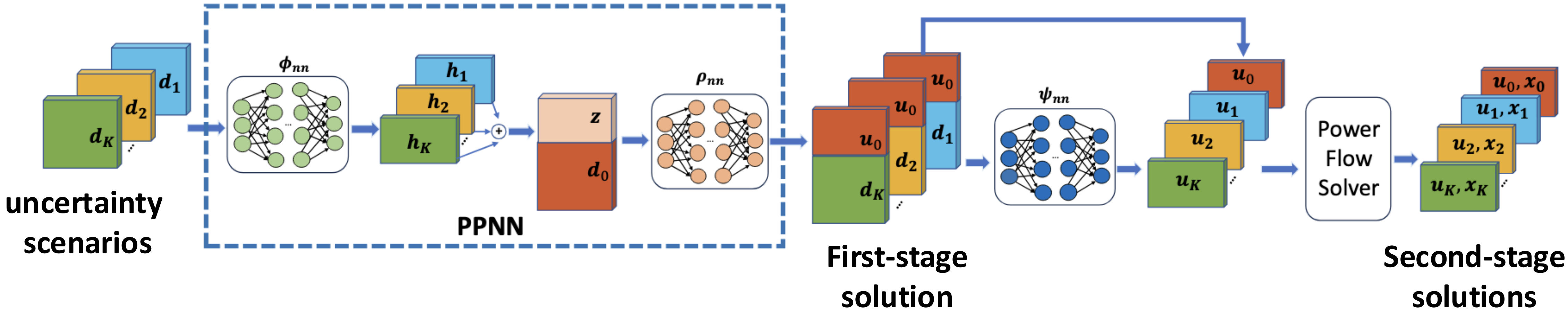
$$\min_{\mathbf{z}} \; H_\theta(\mathbf{z}) \quad \text{s.t. } \mathbf{z} \in \widetilde{\mathcal{B}}$$



[1] C. Liu, E. Liang*, M. Chen*, "*Hom-PGD+: Homeomorphic Reformulation for Efficient Optimization over Non-convex Sets*". Under review

Extension II: Extension to Stochastic Problems

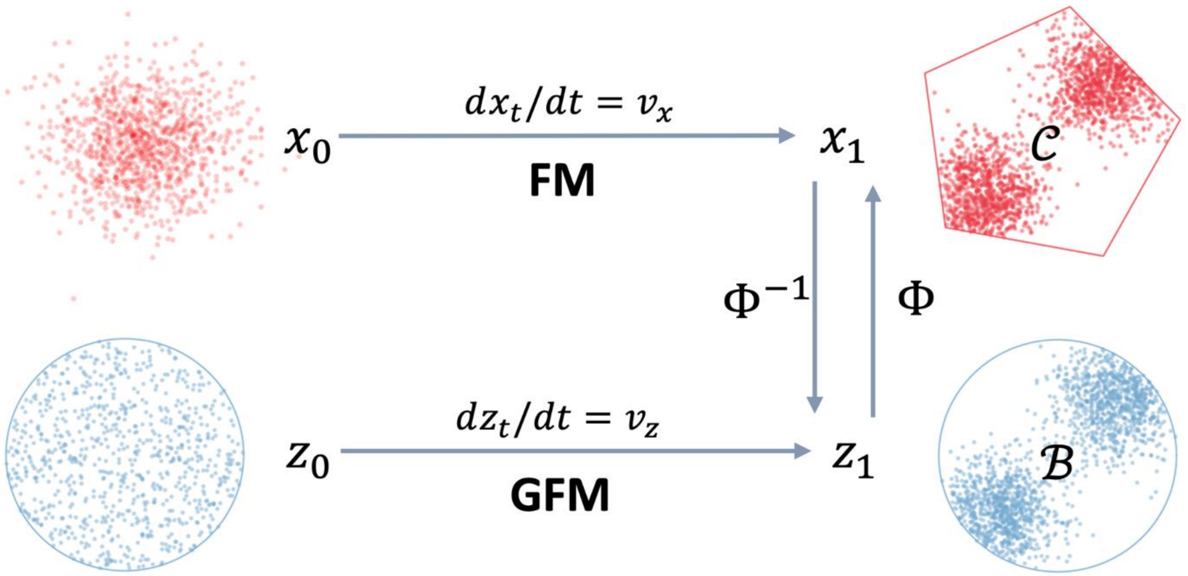
- Two-stage Stochastic Programs
  - *Curse of dimensionality* with increasing number of scenarios
  - Partially permutation-invariant NN to predicting solutions [1]

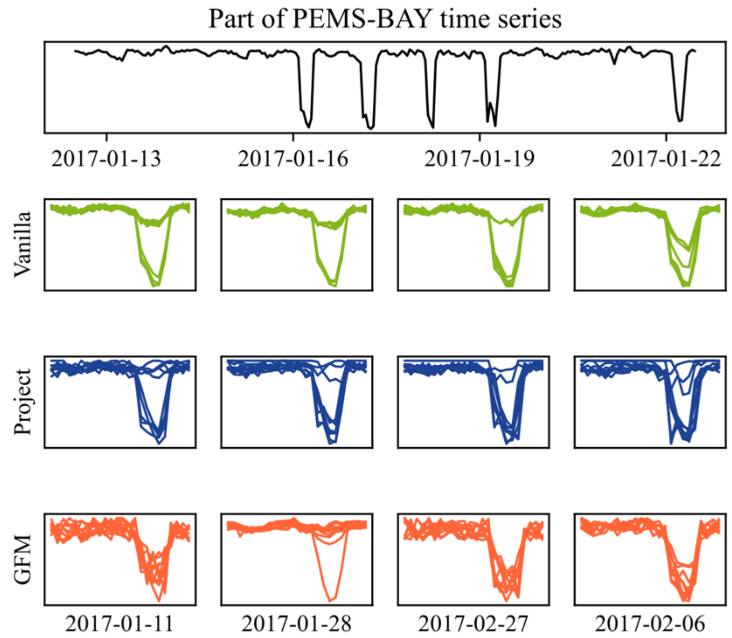


- Apply Hom-Proj. or Bis-Proj. to ensure solution feasibility [2]
- **2-order** speedup, **0.95%** optimality gap over 793-bus grid

[1] M. Zhou, E. Liang*, M. Chen*, S. Low. "*Partially Permutation-Invariant Neural Network for Solving Two-Stage Stochastic AC-OPF Problem.*", **IEEE Trans. on Power System. 2025.**
[2] E. Liang, M. Chen, "*Efficient Bisection Projection to Ensure NN Solution Feasibility over General Set*", **ICML 2025.**

Extension III: Hard-Constrained Generative Models





(a) FM (b) Projection (c) Reflection (d) GFM

[1] X. Li*, E. Liang*, M. Chen, *"Gauge Flow Matching for Efficient Constrained Generative Modelling over General Convex Set."*, **ICLR 2025 Delta Workshop. Outstanding Short Paper Award**

[2] X. Li, E. Liang*, M. Chen*, *"Gauge Flow Matching: Efficient Constrained Generative Modelling over General Convex Set and Beyond."*, **ICLR 2026**

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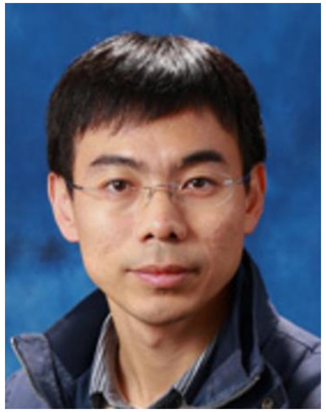
(Linnan U)

Prof. Wanjun Huang
(Beihang U)



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Prof. Minghua Chen
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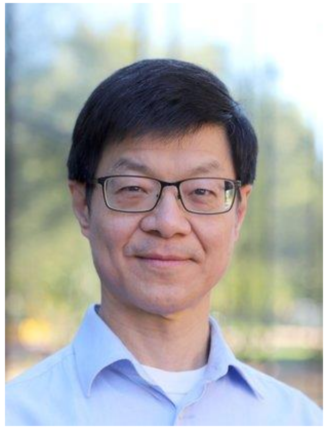


Prof. Steven Low
(Caltech)

Thanks!
Q&A

Personal webpage

Homeomorphism Methods: Part III

Gauge Flow Matching for Efficient Constrained Generative Modelling

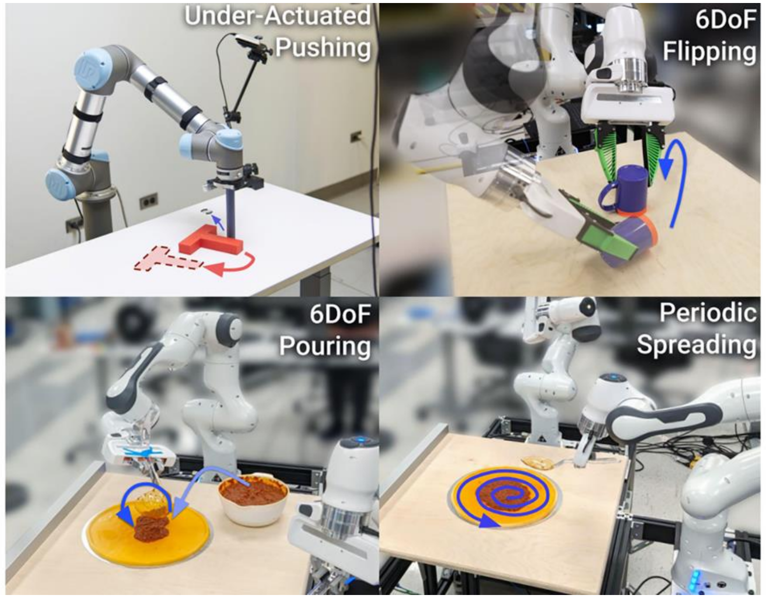
[1] E. Liang, M. Chen, S. Low, "*Low Complexity Homeomorphic Projection to Ensure NN Solution Feasibility for Optimization over (Non-)Convex Set*", **ICML, 2023.**
[2] E. Liang, M. Chen, S. Low, "*Homeomorphic Projection to Ensure NN Solution Feasibility for Constrained Optimization*". **JMLR 2024**.

Success of DM/FM-based Generative Models

Picture/Video

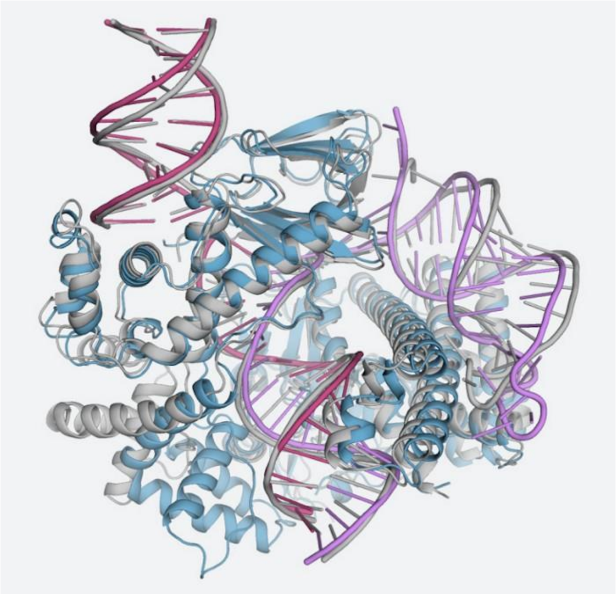
[1,2]

Robotic planning



[3]

Protein/Material

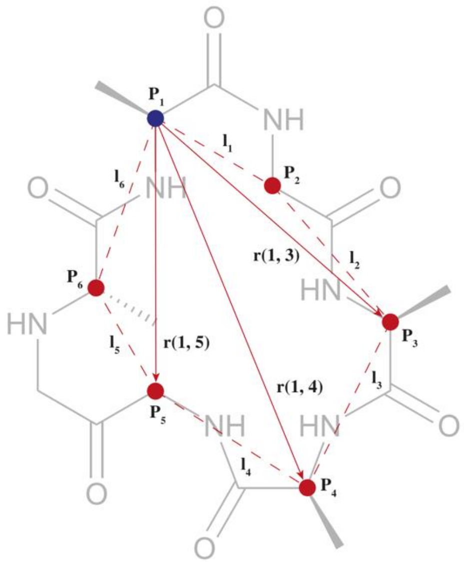


[4,5]

[1] Ramesh, A., Dhariwal, P., Nichol, A., Chu, C., & Chen, M. Hierarchical text-conditional image generation with clip latents. arXiv preprint arXiv . 2022
[2] Betker, J., Goh, G., Jing, L., Brooks, T., Wang, J., Li, L., ... & Ramesh, A. Improving image generation with better captions. OpenAI. 2023
[3] Chi, C., Xu, Z., Feng, S., Cousineau, E., Du, Y., Burchfiel, B., ... & Song, S. Diffusion policy: Visuomotor policy learning via action diffusion. ICRR 2023.
[4] Abramson, J., Adler, J., Dunger, J., Evans, R., Green, T., Pritzel, A., ... & Jumper, J. M. Accurate structure prediction of biomolecular interactions with AlphaFold 3. Nature. 2024
[5] Zeni, C., Pinsler, R., Zügner, D., Fowler, A., Horton, M., Fu, X., ... & Xie, T. A generative model for inorganic materials design. Nature, 2025.

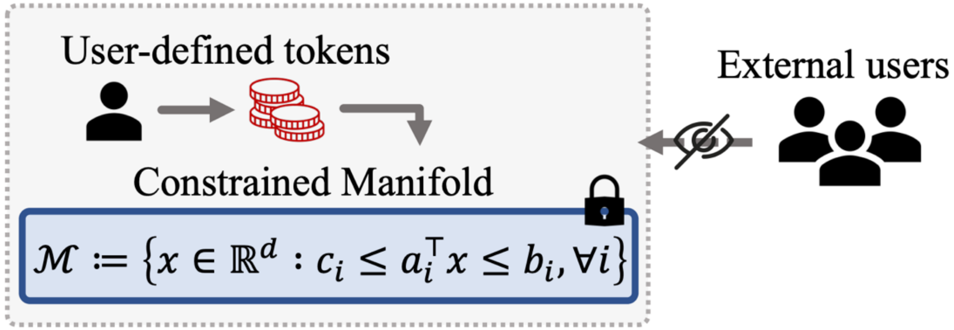
Constraint Matters in Many Applications

Physical Constraints



- Safety-critical constraints for robotics [1]
- Structure constraints in protein/material [2]

Watermarked Generation



- Embed invisible information by constraining user-defined tokens [3]

[1] Chi, C., Xu, Z., Feng, S., Cousineau, E., Du, Y., Burchfiel, B., ... & Song, S. Diffusion policy: Visuomotor policy learning via action diffusion. ICRR 2023.
[2] Fishman, N., Klarner, L., De Bortoli, V., Mathieu, E., & Hutchinson, M. J. Diffusion Models for Constrained Domains. TMLR 2023.
[3] Liu, G. H., Chen, T., Theodorou, E., & Tao, M. Mirror diffusion models for constrained and watermarked generation. NeurIPS. 2023.

DM/FM Suffers from Feasibility Issues

DM/FM Generation

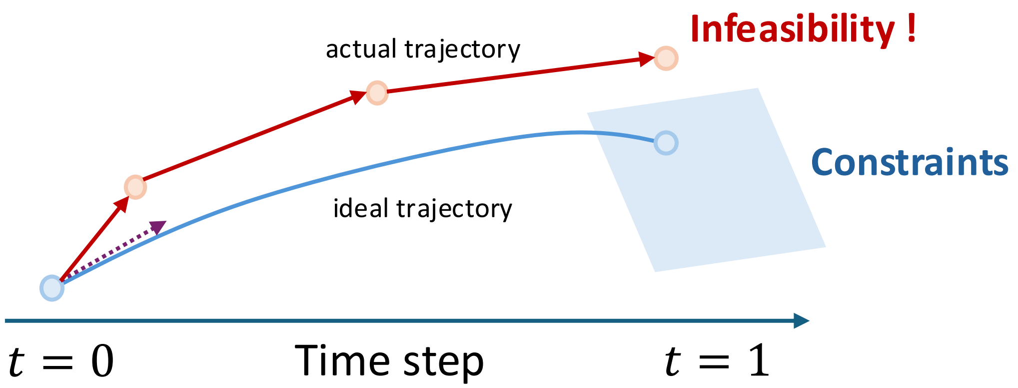
$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{f}(\mathbf{x}, t) + \sigma(\mathbf{x}, t)\omega_t$$

Drift Diffusion

Error sources:

- NN approximation error (score function / vector field)
- Discretized SDE/ODE integration error

Error Propagation [1]



- The error bound "typically" has exponential dependency on the Lipschitz constants of the score functions [2,3] / vector fields [4].

[1] Li, Y., & van der Schaar, M. On Error Propagation of Diffusion Models. ICLR. 2024.
[2] Kwon, D., Fan, Y., & Lee, K. Score-based generative modeling secretly minimizes the wasserstein distance. NeurIPS 2022.
[3] Chen, S., Daras, G., & Dimakis, A. Restoration-degradation beyond linear diffusions: A non-asymptotic analysis for ddim-type samplers. ICML 2023
[4] Benton, J., Deligiannidis, G., & Doucet, A. Error bounds for flow matching methods. TMLR. 2024.

Existing Studies on Constrained DM/FM

Limited constraint sets / lack guarantees / high complexity

Methods	Constraint setting	Feasibility guarantee	Approximation bound	Training complexity	Inference complexity	
RDM[a] [FKDB+23]	Convex	✓	✗	+++	+++	Reflection
RDM[b] [LE23]	Cube/Simplex	✓	✗	++	+	
RSB [DCY+24]	Smooth + Bounded	✓	✓	+++	+++	
RFM [XZY+24]	Convex	✓	✓	+	+++	
Metropolis sampling [FKM+24]	Manifold	✗	✓	+	++	
MDM [LCTT24]	Ball/Simplex	✓	✗	+	+	Mirror Map
NAMM [FBB24]	(Non)-Convex	✗	✗	+++	+	
Projection-based [SKZ+23, CBF24]	Convex	✓	✓	+	+++	Guidance
Barrier methods [FKDB+23]	Convex	✓	✗	+	+	
Penalty-based [LDDB24, KDR24]	General	✗	✗	+	+	Training
Gauge Flow Matching	Convex	✓	✓	+	+	Ours

[1] Training/inference complexity is compared with the unconstrained versions of those generative models.

Gauge Flow Matching

Dataset:

- $x_1 \sim p_{\text{data}}$ over a compact convex set $\mathcal{C}$

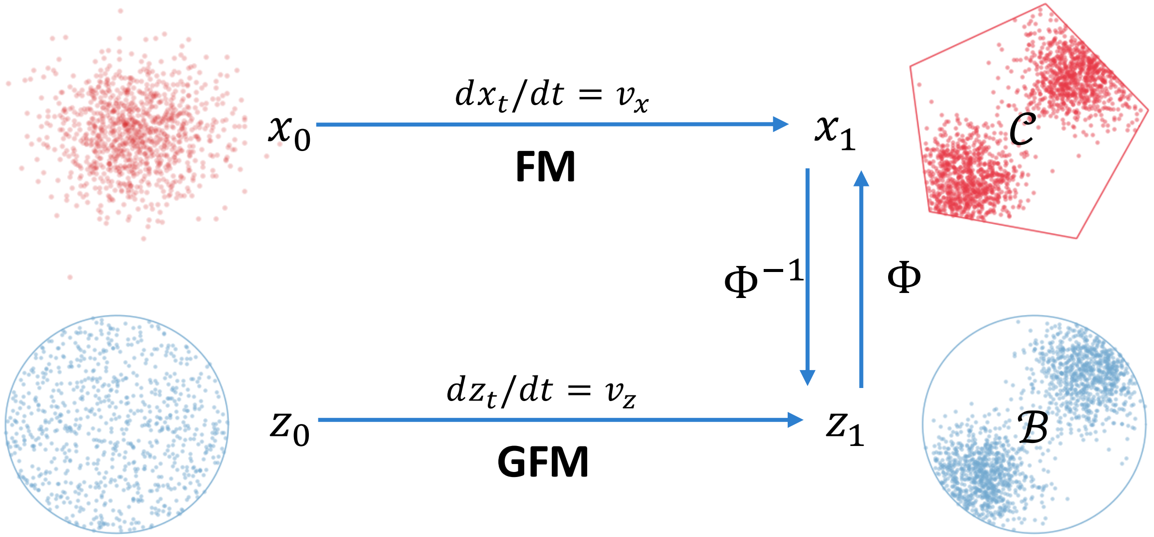
Training:

- Invers mapping: $z_1 = \Phi^{-1}(x_1)$
- Regular flow matching over ball [1]

Inference:

- Reflected generation over ball [2]
- Forward mapping: $x_1 = \Phi(z_1)$

Framework



How to find invertible Φ for general convex set with low-complexity ?

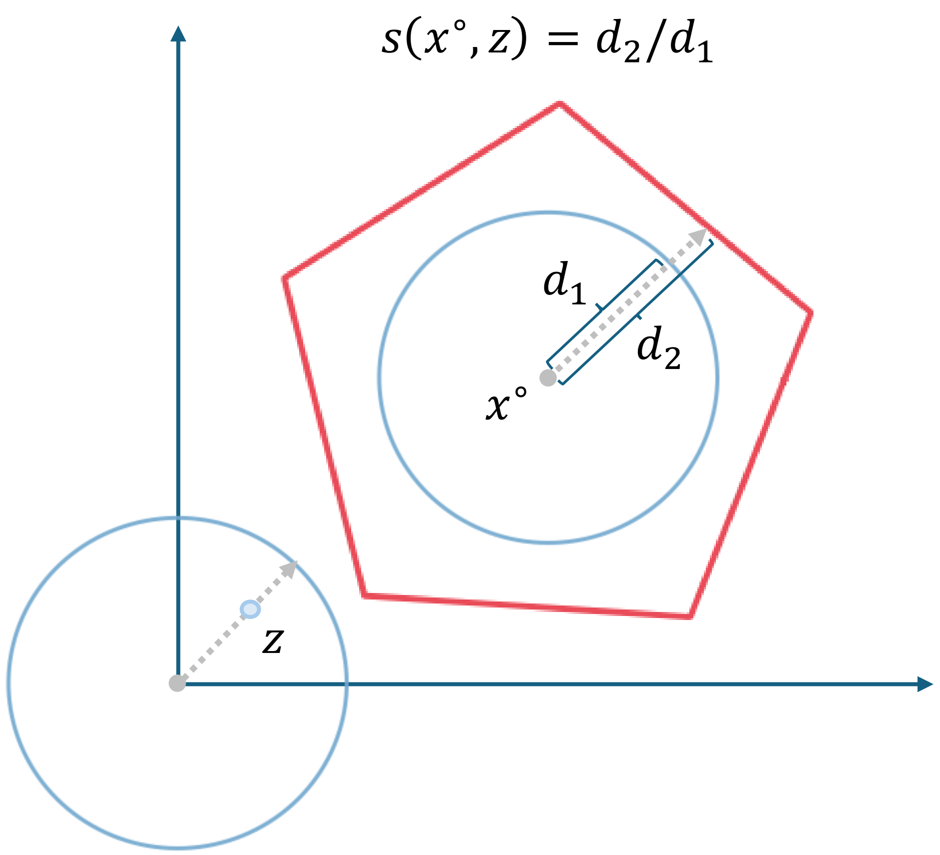
[1] X. Li*, E. Liang*, M. Chen, "*Gauge Flow Matching for Efficient Constrained Generative Modelling over General Convex Set*.", **ICLR 2025 Delta Workshop. Outstanding Short Paper Award**
[2] X. Li, E. Liang*, M. Chen*, "*Gauge Flow Matching: Efficient Constrained Generative Modelling over General Convex Set and Beyond*.", **ICLR 2026**

Gauge Mapping: Homeomorphism for Convex Set

$$\Phi(z) = x^\circ + s(x^\circ, z) \cdot z$$

- **Translating** by $x^\circ \in \mathrm{int}(\mathcal{C})$
- **Scaling** by $s(x^\circ, z) \in \mathbb{R}_+$

- Properties of Φ:
  - Continuous + Invertible → Homeomorphism
  - Bi-Lipschitz → Beneficial for algorithm [4]
- Computation of Φ:
  - Closed-form for common convex sets [1-2]
    - ✓ Linear, quadratic, SOC, LMI.
  - Bisection for general compact convex set [3]



[1] Tabas, D., & Zhang, B. Computationally efficient safe reinforcement learning for power systems. IEEE ACC 2022.
[2] Tordesillas, J., How, J. P., & Hutter, M. Rayen: Imposition of hard convex constraints on neural networks. arXiv 2023.
[3] Mhammedi, Z. Efficient projection-free online convex optimization with membership oracle. COLT 2022.
[4] X. Li*, E. Liang*, M. Chen, "*Gauge Flow Matching for Efficient Constrained Generative Modelling over General Convex Set*.", **ICLR 2025 Delta Workshop. Outstanding Short Paper Award**

Theorical Analysis of GFM

Approximation Error

$$\mathcal{W}_2(p_{\text{data}}, p_\theta) \leq L_\Phi \cdot \underbrace{e^{0.5+L_\theta} \cdot \epsilon_\theta}_{\textbf{RFM error [1]}}$$

- L_θ: Lipschitz of NN-based vector field
- ϵ_θ: l_2 flow matching loss over ball
- L_Φ: Lipschitz of gauge mapping
  - Reduced by selecting a "central" interior point $x^\circ \in \text{int}(\mathcal{C})$

Inference Complexity

$$\mathcal{O}(\underbrace{\text{NFE} \cdot n^2}_{\textbf{Regular FM complexity}} + m \cdot C)$$

- NFE: num of function evaluation
- n: dimension of data
- $m \cdot C$: gauge mapping calculation
  - m: num of constraints $\{g_i(x) \leq 0\}_{i=1}^m$
  - C: same order of complexity to calculate $g_i(x)$

Bounded approximation error + minor additional complexity

[1] Xie, T., Zhu, Y., Yu, L., Yang, T., Cheng, Z., Zhang, S., ... & Zhang, C. Reflected Flow Matching. ICML. 2024.

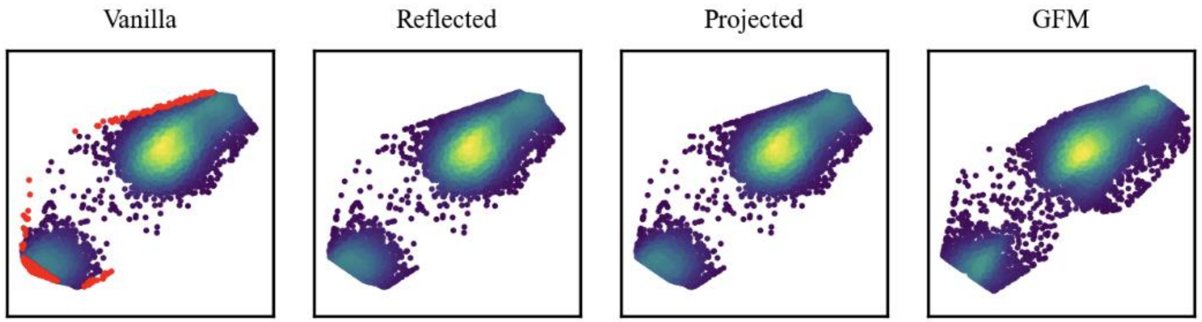
Empirical Study

Low-dim Toy Example

Simple constraints

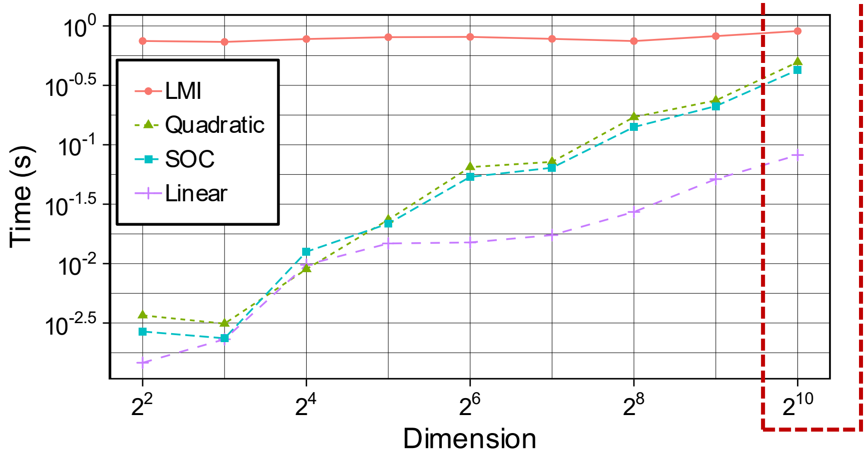
Constraint	Metrics	Vanilla FM	Reflected FM	Projected FM	GFM
Polytope ($n = 2$)	MMD (↓)	0.06209	0.06155	0.06165	0.04154
	Feasibility Rate (%)	95.69	100	100	100
	Inference Time (s)	3.412	5.616	4.776	3.746
Quadratic set ($n = 3$)	MMD (↓)	0.06311	0.06313	-	0.05866
	Feasibility Rate (%)	89.98	100	-	100
	Inference Time (s)	3.679	10.22	>3600	3.675

Joint linear + quadratic constraints

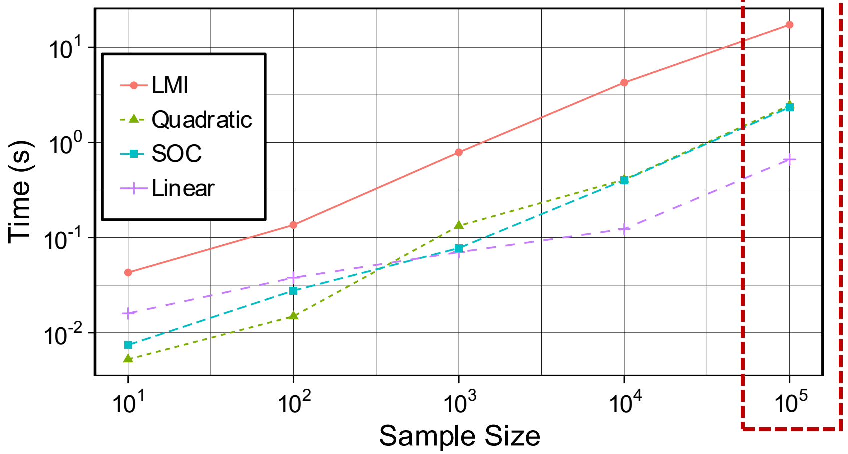


Scalability of Gauge Mapping

Constraints dimension

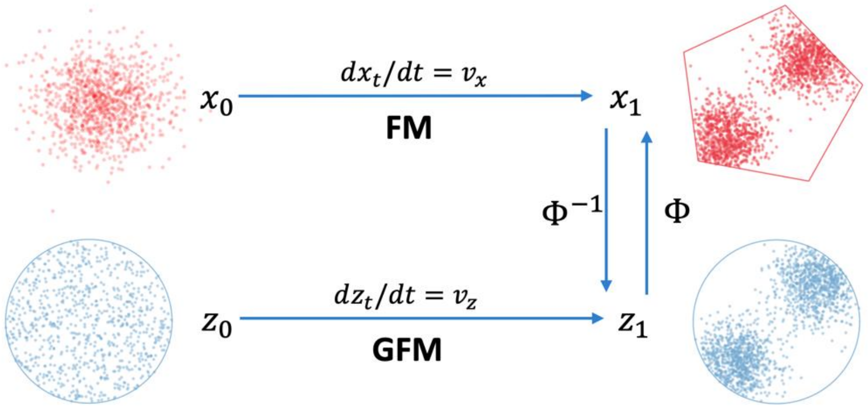


Input sample size



Summary

Takeaway messages



- Bijective gauge mapping for general compact convex set
- Enable low-complexity constrained generation

Future works

- Extend to non-convex set
  - Star/geodesic-convex set [1]
  - Ball-homeomorphic set [2]

- One-step generation
  - Constrained distillation/consistency
- More real-world applications

[1] X. Li*, <u>E. Liang</u>*, M. Chen, "*Gauge Flow Matching for Efficient Constrained Generative Modelling over General Convex Set*.", **ICLR 2025 Delta Workshop. Outstanding Short Paper Award**
[2] X. Li, <u>E. Liang</u>*, M. Chen*, "*Gauge Flow Matching: Efficient Constrained Generative Modelling over General Convex Set and Beyond*.", **ICLR 2026**

Supplementary Slides

Supplementary Slides

Property of Input-Solution Mapping

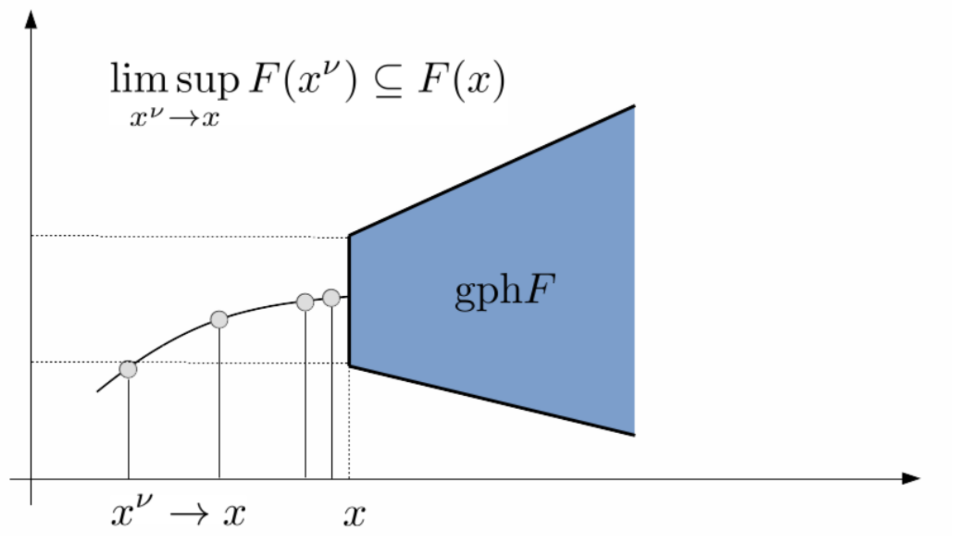
- **Convex optimization**
  - Strongly convex (e.g., QP)
    - Continuous solution mapping
  - General convex (e.g., LP)
    - Continuous (a.e.) solution mapping
- **Continuous optimization**
  - Unique solution
    - Continuous solution mapping
  - General continuous
    - "Continuous" solution mapping
      - Set-valued mapping

Theorem 3B.5 (basic continuity properties of solution mappings in optimization). *In the preceding notation, let $\bar{p} \in P$ be fixed with the feasible set $S_{\text{feas}}(\bar{p})$ nonempty and bounded, and suppose that:*

(a) *the mapping S_{feas} is Pompeiu–Hausdorff continuous at $\bar{p}$ relative to P, or equivalently, S_{feas} is continuous at $\bar{p}$ relative to P with $S_{\text{feas}}(Q \cap P)$ bounded for some neighborhood Q of $\bar{p}$,*

(b) *the function f_0 is continuous relative to $P \times \mathbb{R}^n$ at $(\bar{p}, \bar{x})$ for every $\bar{x} \in S_{\text{feas}}(\bar{p})$.*

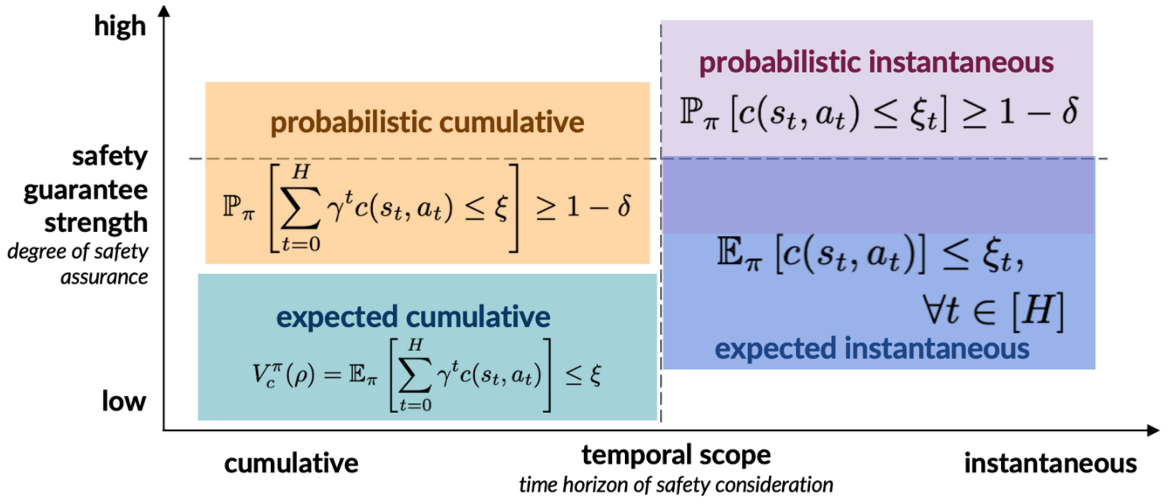
Then the optimal value mapping S_{val} is continuous at $\bar{p}$ relative to P, whereas the optimal set mapping S_{opt} is osc at $\bar{p}$ relative to P.



[1] Dontchev, A. L., & Rockafellar, R. T. (2009). Implicit functions and solution mappings (Vol. 543). New York: Springer.

Feasibility of Sequential Problems

- Explicit-form constraints
  - Deterministic sequential problems (e.g., MPC)
    - Unroll it as a large CO / utilize problem structure
  - Stochastic sequential problems (e.g., MSP)
    - Sampling $\Longrightarrow$ det. problem $\Longrightarrow$ feasibility with prob.
  - Infinite horizon problem (e.g., Stability)
    - Construct explicit safe state/policy set



- Unknown, but can sampling
  - Constrained MDP
    - Zero-duality gap
    - Primal-dual algorithm
    - Feasibility with prob.

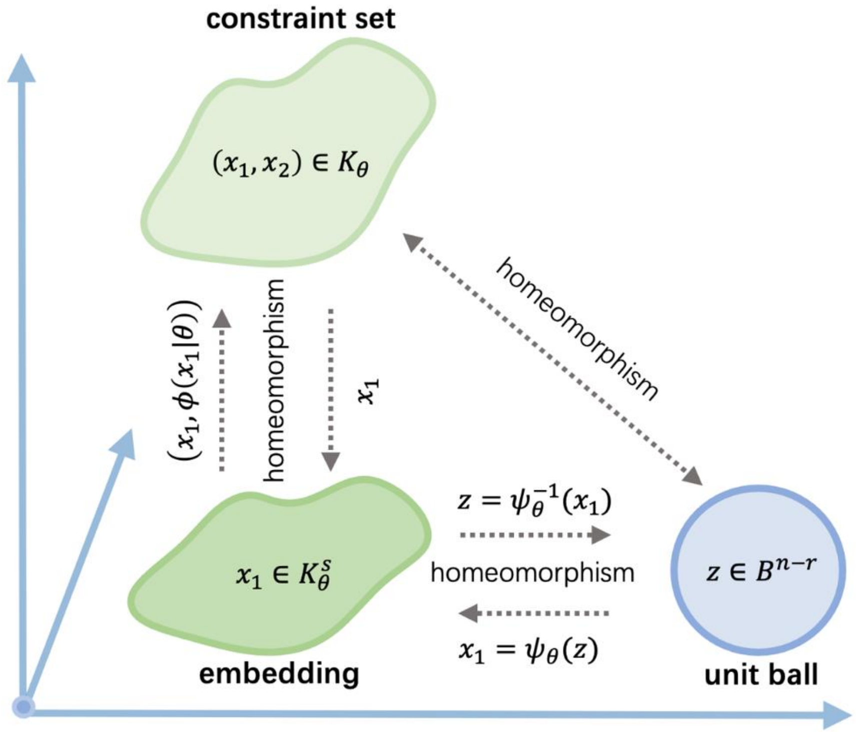
Discrete & Combinatorial Problems

- Solving continuous sub-problems
  - Continuous relaxation + B&B/cutting-plane
    - ML to predict continuous problems [3]
    - ML to accelerate B&B/cutting-plane [4-5]
- Equivalent continuous formulation
  - Motzkin-Straus formulation of Max-Clique problem
    - Constrained indefinite quadratic program [1]
- Relaxation + Recovering
  - SDP relaxation + randomized rounding for Max-Cut problem
    - 0.879 approximation ratio [2]

[1] Gibbons, L. E., Hearn, D. W., Pardalos, P. M., & Ramana, M. V. Continuous characterizations of the maximum clique problem. MATH OPER 1997.
[2] M. X. Goemans and D. P. Williamson. .879-approximation algorithms for max cut and max 2sat. STOC 1994.
[3] Kool, W., van Hoof, H., & Welling, M. Attention, Learn to Solve Routing Problems!. ICLR 2019
[4] Khalil, E., Le Bodic, P., Song, L., Nemhauser, G., & Dilkina, B. Learning to branch in mixed integer programming. AAAI 2016
[5] Balcan, M. F., Dick, T., Sandholm, T., & Vitercik, E. Learning to branch. ICML 2018.

Equality and Inequality Constraint

- Constraint set: $\mathcal{K}_\theta = \{x | g(x,\theta) \leq 0, h(x,\theta) = 0\}$
  - **Algorithmic view:**
    - **predict-then-reconstruct** [1-2]
    - $x = [x_1, x_2]$
    - $h(x_1, \phi(x_1)) = 0$
      - Linear $\Longrightarrow$ linear mapping ϕ
      - Non-linear $\Longrightarrow$ implicit mapping ϕ
    - $\mathcal{K}_\theta^s = \{x | g(x_1, \phi(x_1)) \leq 0\}$
  - **Topological view:**
    - **Constant-Level-Set Theorem** [3]
    - $\mathcal{K}_\theta \cong \mathcal{K}_\theta^s \cong \mathcal{B}$



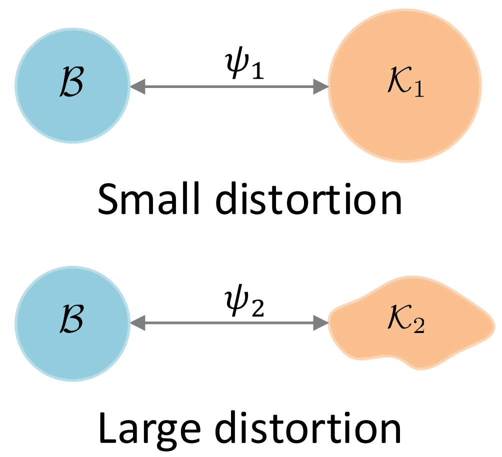
[1] Pan, X., Chen, M., Zhao, T., & Low, S. H. DeepOPF: A feasibility-optimized deep neural network approach for AC optimal power flow problems. IEEE SJ
[2] Donti, P. L., Rolnick, D., & Kolter, J. Z. DC3: A learning method for optimization with hard constraints. ICLR 2021
[3] Lee, J. M., & Lee, J. M. (2012). Smooth manifolds (pp. 1-31). Springer New York.

Distortion and Homeomorphic Mapping

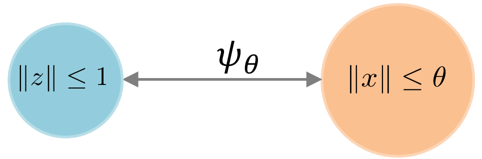
- Distortion: $\mathrm{D}(\psi) = k_2/k_1 \geq 1$

$$k_2 = \sup_{z_1,z_2}\left\{\frac{||\psi(z_1)-\psi(z_2)||}{||z_1-z_2||}\right\},\quad k_1 = \inf_{z_1,z_2}\left\{\frac{||\psi(z_1)-\psi(z_2)||}{||z_1-z_2||}\right\}$$

  - Ratio of max & min distance **variations** by ψ
  - Exist **multiple** homeomorphic mappings between two sets
  - **Bi-Lipschitz** Constants: $\mathrm{D}(\psi) = Lip(\psi) \cdot Lip(\psi^{-1})$



- Minimum Distortion Homeomorphism (MDH)
  - In Hom-PGD:
    - Small distortion $\Longrightarrow$ faster convergence speed
  - In Hom-Proj:
    - Small distortion $\Longrightarrow$ small opt. loss by HP



Small distortion ψ_θ^1: $x = \theta z$
- $\mathrm{D}(\psi_\theta^1) = 1$

Large distortion ψ_θ^2: $x = \theta\mathrm{R}(||z||)z$
- $\mathrm{D}(\psi_\theta^2) \approx 2.5$

Calculation of Gauge Mapping II

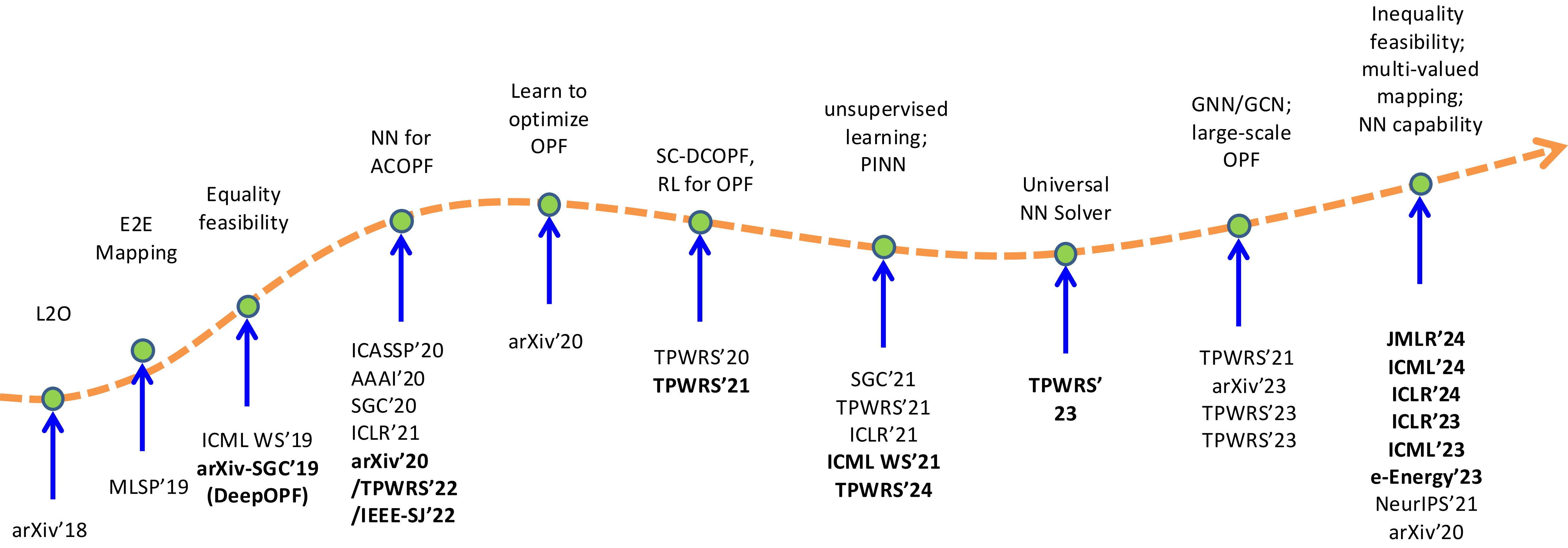
Algorithm 1 Bisection Algorithm for Point-to-Boundary Distance

Input: A compact convex set $\mathcal{C}$, an interior point $x^\circ \in \text{int}(\mathcal{C})$, and a unit vector v.

Initialize: $\alpha_l = 0$ and $\alpha_u = 1$
while $|\alpha_l - \alpha_u| \geq \epsilon$ **do**
    if $x^\circ + \alpha_u \cdot v \in \mathcal{C}$ **then**
        increase lower bound: $\alpha_l \leftarrow \alpha_u$
        double upper bound: $\alpha_u \leftarrow 2 \cdot \alpha_m$
    else
        bisection: $\alpha_m = (\alpha_l + \alpha_u)/2$
        if $x^\circ + \alpha_m \cdot v \in \mathcal{C}$ **then**
            increase lower bound: $\alpha_l \leftarrow \alpha_m$
        else
            decrease upper bound: $\alpha_u \leftarrow \alpha_m$
        end if
    end if
end while

Output: $d_{\mathcal{C}}(x^\circ, v) \approx \alpha_m$

Research Landscape



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