Conditional Gradients: a tour d'horizon

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MATH+

What is this talk about?

Introduction

A very versatile and simple optimization method for projection-free optimization that promotes sparsity.

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Outline

- The basics: Conditional Gradients a.k.a. the Frank-Wolfe algorithm
- Several examples:
  - Deep Learning
  - Rate-Distortion Explanation
  - Sparse Regression
  - Matrix Completion
- High-performance Julia Package: FrankWolfe.jl

(Hyperlinked) References are not exhaustive; check references contained therein.

Conditional Gradients
a.k.a. the Frank-Wolfe algorithm

—The Basics—

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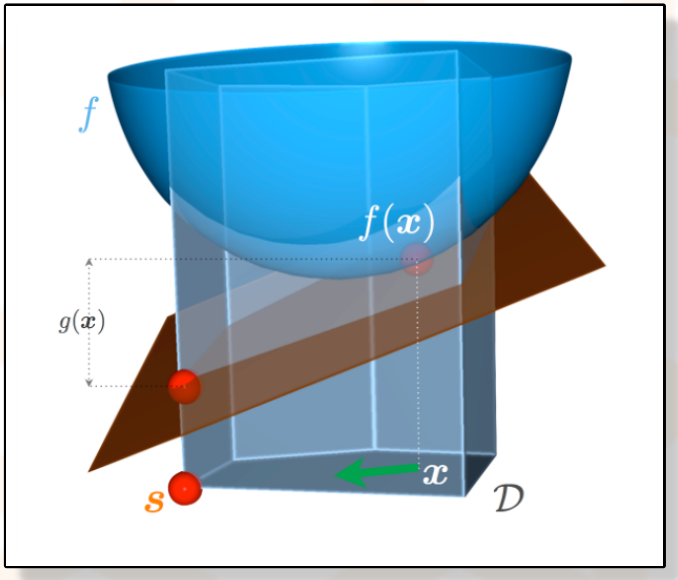
$$\min_{x \in P} f(x) \qquad \text{(baseProblem)}$$



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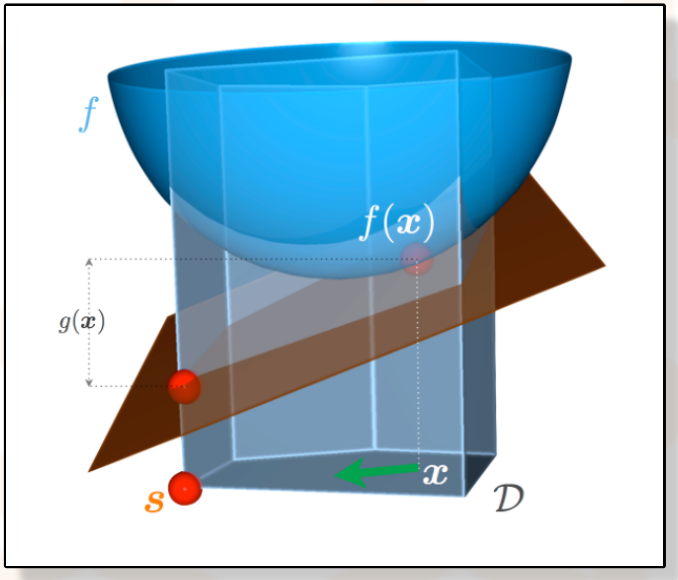

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1. Very versatile model
2. Can use various types of information about both f and P
3. Works very well in (continuous) real-world applications
4. At the core of many (all?) learning algorithms (albeit mostly non-convex case)

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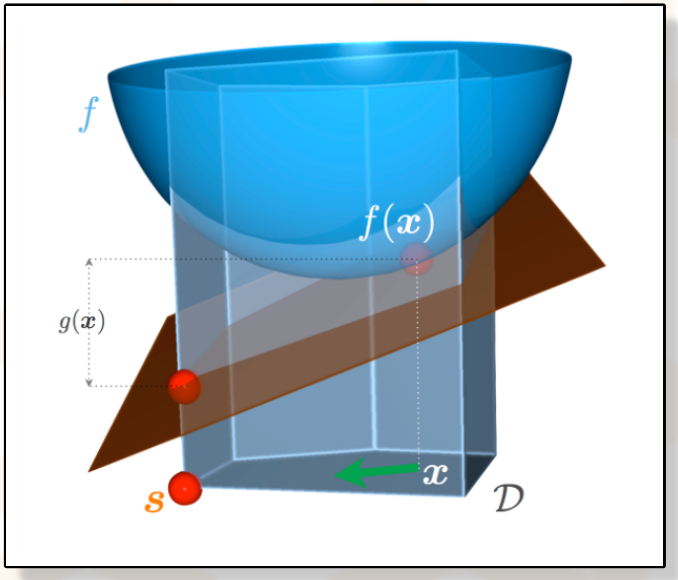

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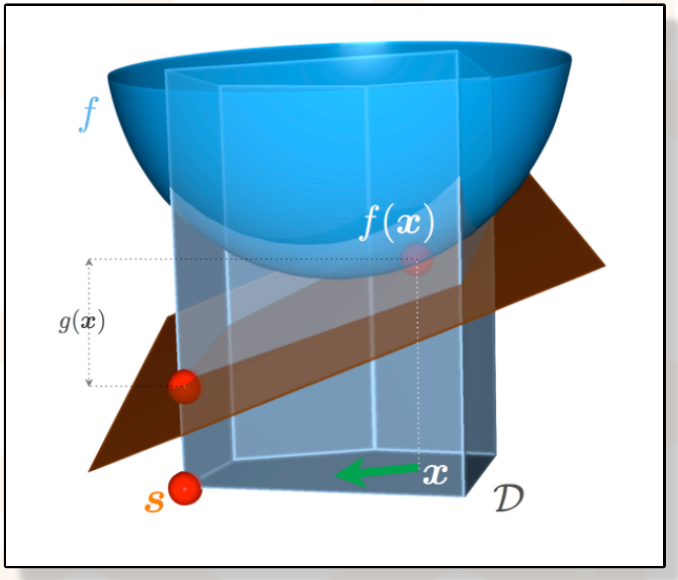

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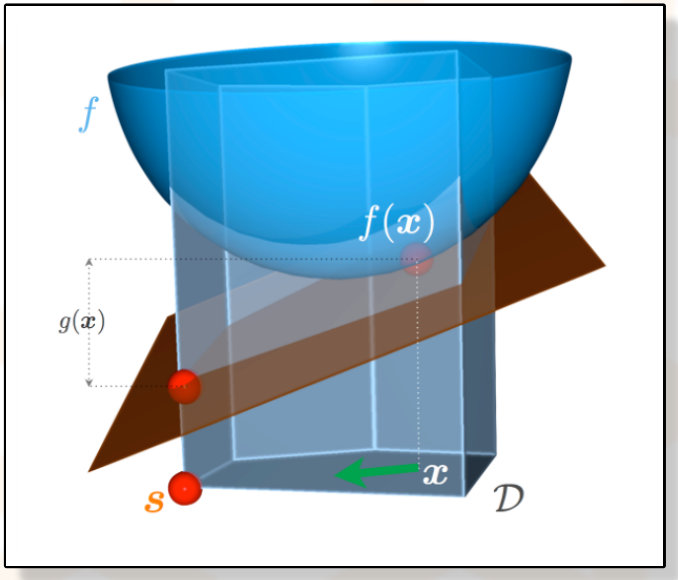

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$\Rightarrow$ *Complexity of convex optimization relative to LO/FO oracle*

Interlude: why LMOs?

Conditional Gradients a.k.a. the Frank-Wolfe algorithm

LMO model has many advantages.

1. Includes explicit formulation via constraints
2. Some problems do not posess 'small' formulations but have efficient LMOs.
   Example: Matching Polytope [Rothvoss, 2014, Braun and Pokutta, 2015a,b, Braun et al., 2015, 2017b]
3. Allows modeling of compact convex constraints as long as we have an LMO.
   Example: SDP cone
4. Often much faster than projection.
   Example: nuclear norm. Largest singular vector (Lanczos method) vs. full SVD
5. LMO is a black box for the algorithms
6. For many LMOs of interest close form solutions available.
   Example: ℓ_1-ball for LASSO regression.

For an overview see: [Combettes and Pokutta, 2021+]

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For all x, y it holds:

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In particular, all local minima are global minima.

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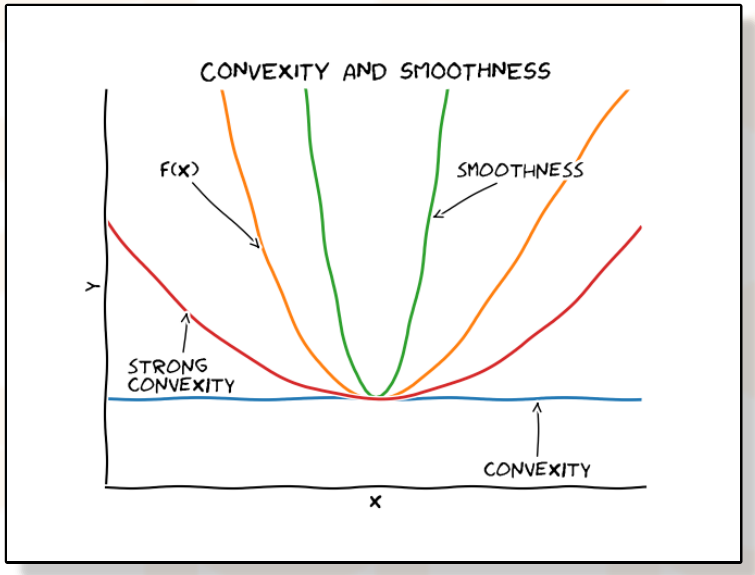

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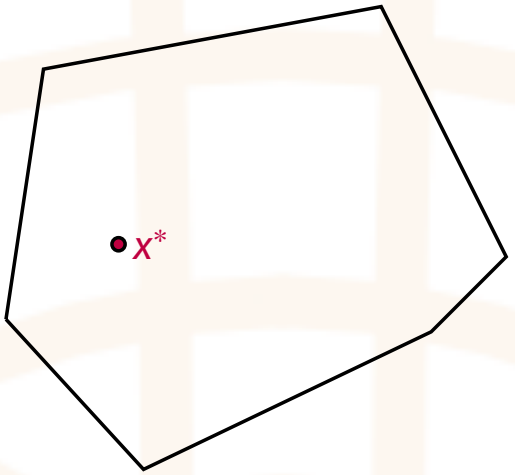

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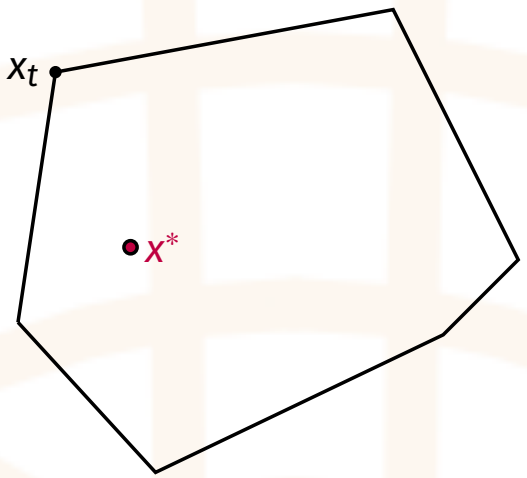

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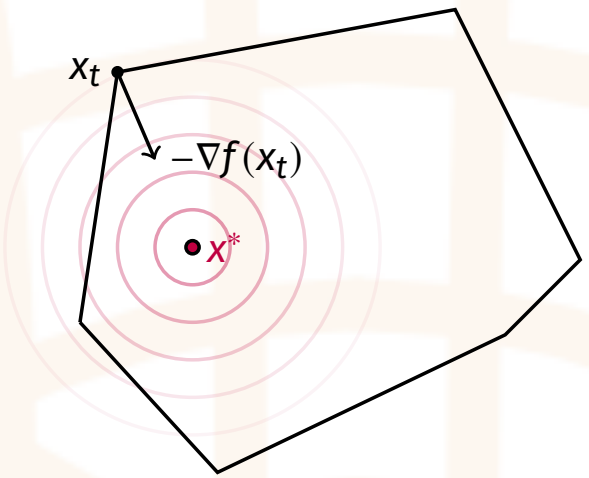

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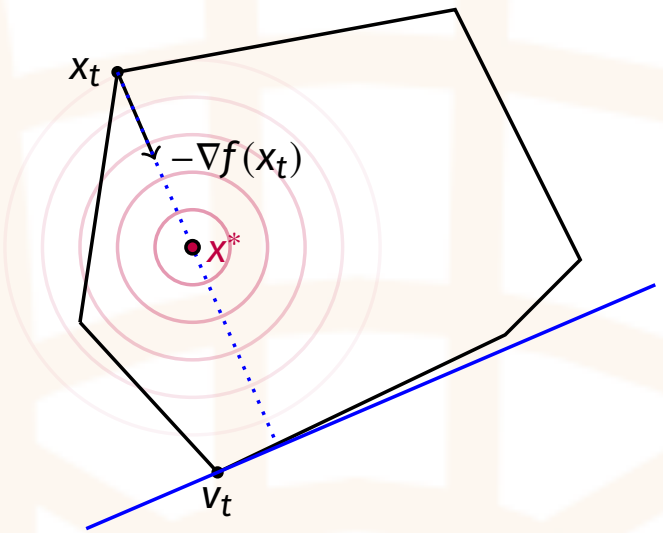

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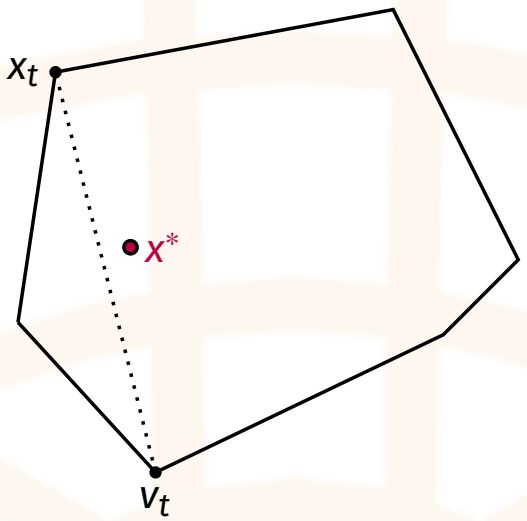

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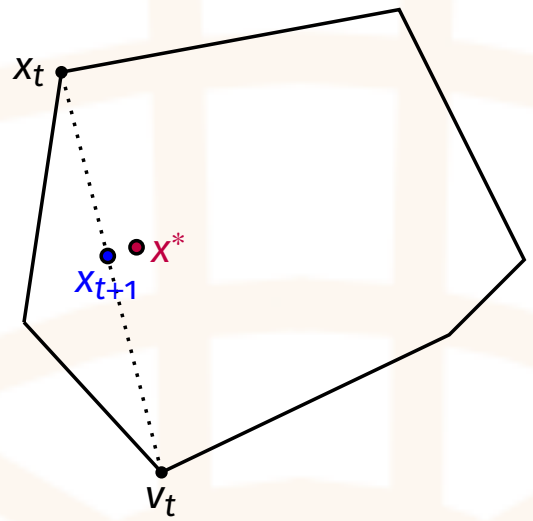

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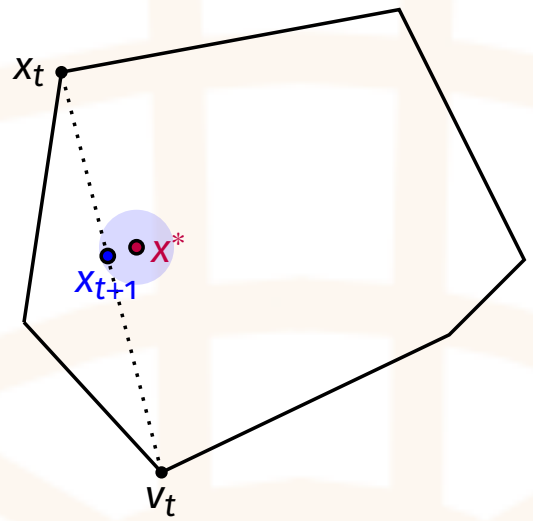

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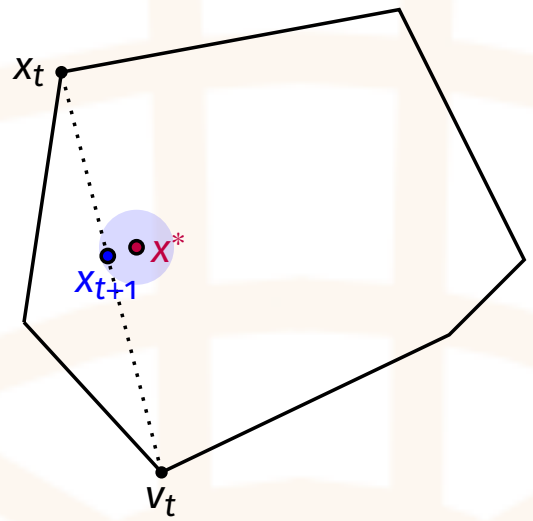

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- Extremely simple and robust: no complicated data structures to maintain
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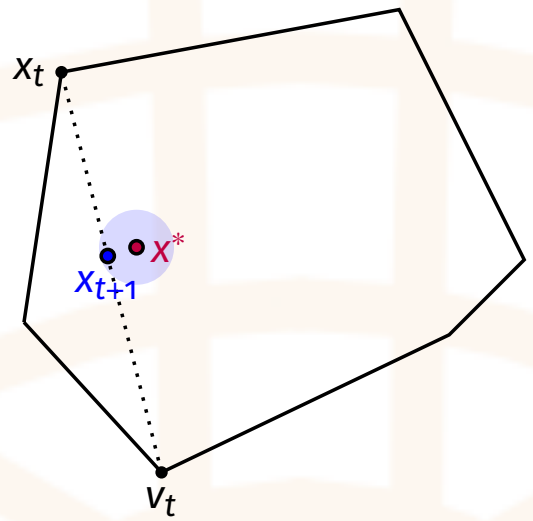

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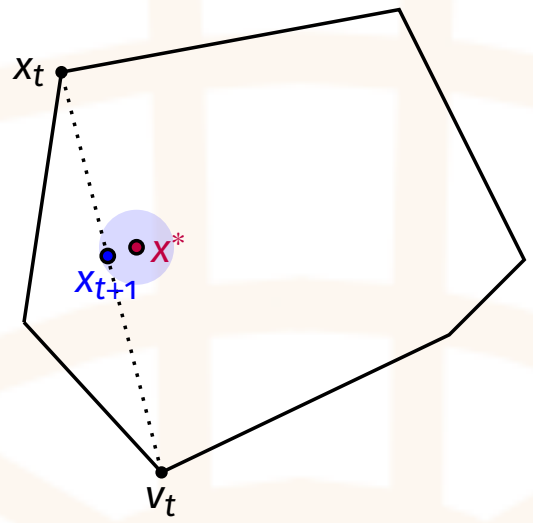

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$\Rightarrow$ *Despite (theoretically) suboptimal rate heavily used in applications due to simplicity.*

Simple Convergence Proof

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Theorem (Convergence rate of the vanilla Frank-Wolfe Algorithm)

Let f be L-smooth convex, P be polytope with diameter D. With choice $\gamma_t \doteq \frac{2}{t+3}$:

$$f(x_t) - f(x^*) \leq \frac{2LD^2}{t+3}.$$

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LP maximality and convexity: $\langle \nabla f(x_t), v_t - x_t \rangle \leq \langle \nabla f(x_t), x^* - x_t \rangle \leq f(x^*) - f(x_t)$. Moreover, $\|v_t - x_t\| \leq D$.

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Thus:

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By Induction (plugging in the guarantee + definition of γ_t):

$$f(x_{t+1}) - f(x^*) \leq \left(1 - \frac{2}{t+3}\right) \frac{2LD^2}{t+3} + \frac{4}{(t+3)^2} \cdot \frac{LD^2}{2} = \frac{2LD^2(t+2)}{(t+3)^2} \leq \frac{2LD^2}{t+4},$$

by $(t+2)(t+4) \leq (t+3)^2$.

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A matching lower bound

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Thus lower bound. $f(x_t) - f(x^*) \geq \frac{1}{t} - \frac{1}{n}$

$\Rightarrow$ *Any LP method converges no faster than $O(1/t)$.*

Note: Strong consequences for strongly convex case and also provides a sparsity vs. optimality trade-off.

see also for non-smooth variants: [Braun et al., 2017a]

A matching lower bound

Conditional Gradients a.k.a. the Frank-Wolfe algorithm

Consider $P = \operatorname{conv}(\{e_1, \dots, e_n\})$ the probability simplex and $f = \|x\|^2$.

Clearly. $\arg\min_{x \in P} f(x) = x^* \doteq \frac{1}{n} e$ with $f(x^*) = \frac{1}{n}$.

Observe. Starting from any vertex e_i after $t < n$ iterations we picked up at most t vertices of P.

Easy to see. For any iterate x_t:

$$f(x_t) \geq \min_{\substack{x \in \operatorname{conv}(\mathcal{S}) \\ \mathcal{S} \subseteq \{e_1, \dots, e_n\} \\ |\mathcal{S}| \leq t}} f(x) = 1/t,$$

Thus lower bound. $f(x_t) - f(x^*) \geq \frac{1}{t} - \frac{1}{n}$

$\Rightarrow$ *Any LP method converges no faster than $O(1/t)$.*

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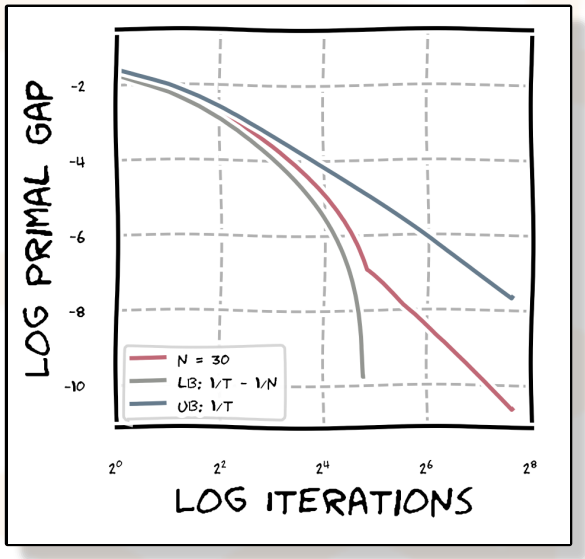

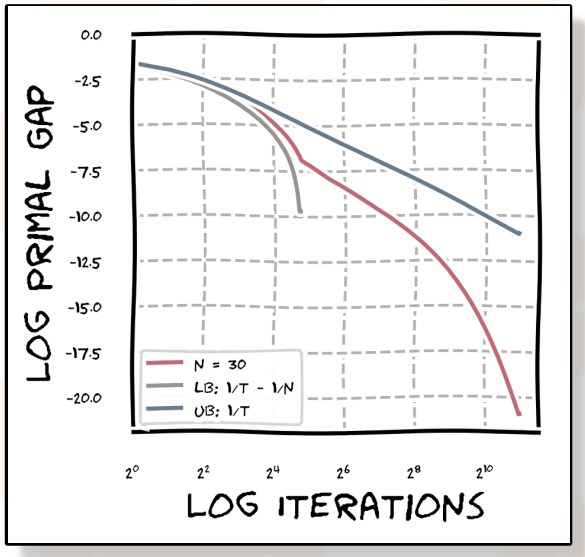

Significant progress over the recent years (incomplete list)

Conditional Gradients a.k.a. the Frank-Wolfe algorithm

1. Strongly convex case [Garber and Hazan, 2013, Lacoste-Julien and Jaggi, 2015, Lan and Zhou, 2016, Garber and Meshi, 2016]
2. Non-convex case [Lacoste-Julien, 2016]
3. Online case [Hazan and Kale, 2012]
4. Stochastic variants and adaptive gradients [Hazan and Luo, 2016, Reddi et al., 2016, Combettes et al., 2020]
5. Sharp functions and sharp regions [Kerdreux et al., 2019, 2021a,b]
6. Acceleration [Diakonikolas et al., 2020, Bach, 2020, Carderera et al., 2021]
7. Specialized variants [Freund et al., 2017, Braun et al., 2017c, 2019b,a]

Conditional Gradients very competitive: simple, robust, real-world performance.

For more background etc see upcoming survey!

Stochastic Conditional Gradients

—Training Neural Networks with Frank-Wolfe—

joint work with Christoph Spiegel and Max Zimmer

[Pokutta et al., 2020]

The Stochastic Frank-Wolfe Algorithm (with Momentum)

Training Neural Networks with Conditional Gradients

Algorithm Stochastic FW Algorithm (SFW)

$m_0 \leftarrow 0$
for $t = 0$ **to** $T - 1$ **do**
  uniformly sample i.i.d. $i_1, \ldots, i_{b_t} \sim [\![1, m]\!]$
  $\tilde{\nabla} L(\theta_t) \leftarrow \frac{1}{b_t} \sum_{j=1}^{b_t} \nabla \ell_{i_j}(\theta_t)$
  $m_t \leftarrow (1 - \rho_t)\, m_{t-1} + \rho_t\, \tilde{\nabla} L(\theta_t)$
  $v_t \leftarrow \arg\min_{v \in P} \langle m_t, v \rangle$
  $\theta_{t+1} \leftarrow \theta_t + \alpha_t (v_t - \theta_t)$
end for

e.g., [Reddi et al., 2016]

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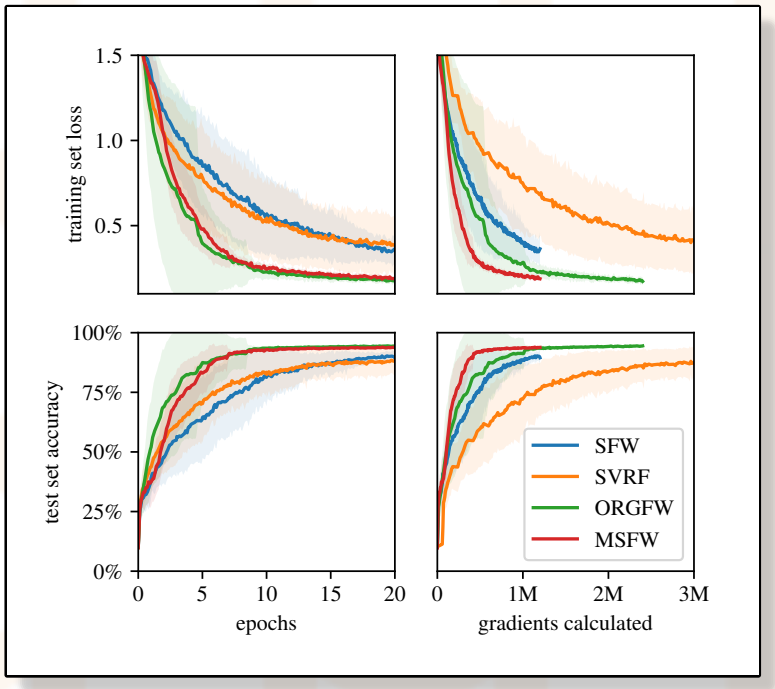

SFW variants

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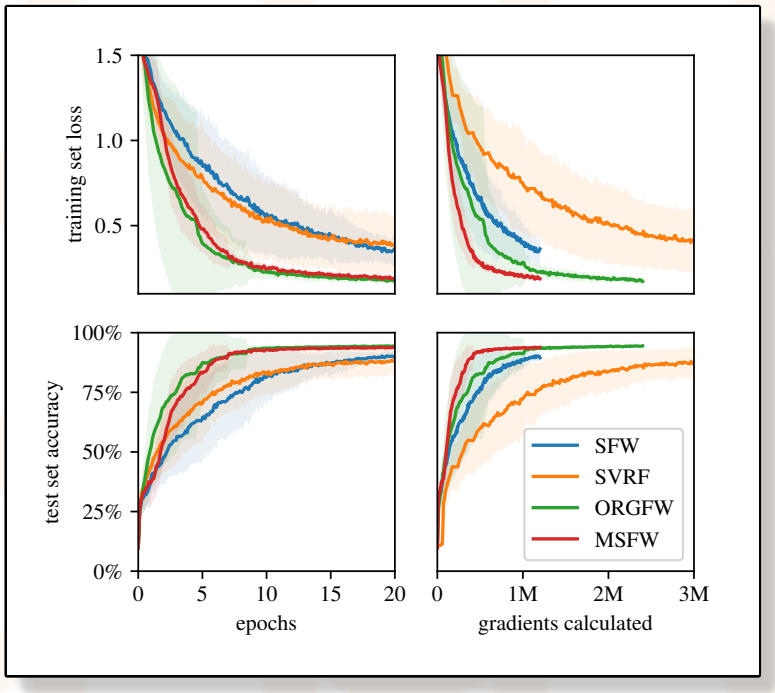
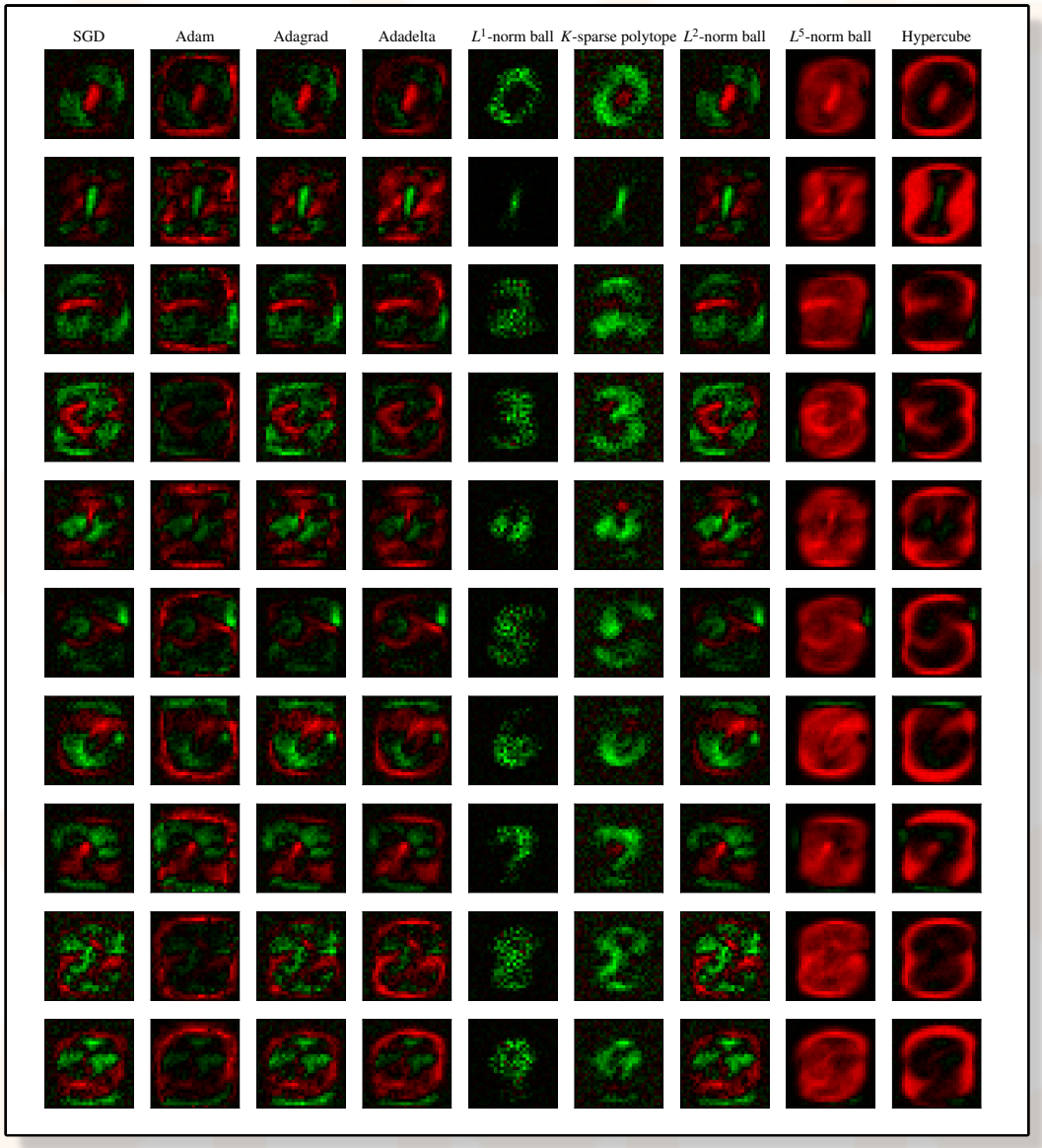


SFW variants

- Convergence rate: In the non-convex stochastic smooth case $O(1/\sqrt{T})$-rate
- Speed: Works well for very large data sets due to mini-batched gradients
- Projection-free: Remains projection-free and allows for constraints

Relevance maps under different optimizers / feasible regions

Training Neural Networks with Conditional Gradients



Robust Rate-Distortion Explanations via Conditional Gradients

joint work with Mathieu Besançon and Jan Macdonald

The problem formulation

Rate-Distortion Explanation

[Macdonald et al., 2019]

Expected Distortion of S.

$$D(S) \coloneqq D(S, \Phi, x, V) \coloneqq \underbrace{\mathbb{E}_{y \sim V}\left[\frac{1}{2}(\Phi(x) - \Phi(y))^2\right]}_{\text{Stability of } \Phi \text{ when varying outside of } S}$$

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$$R(\varepsilon) \coloneqq \underbrace{\min\{\operatorname{card}(S) : D(S) \leq \varepsilon\}}_{\text{smallest set of fixings } S}$$

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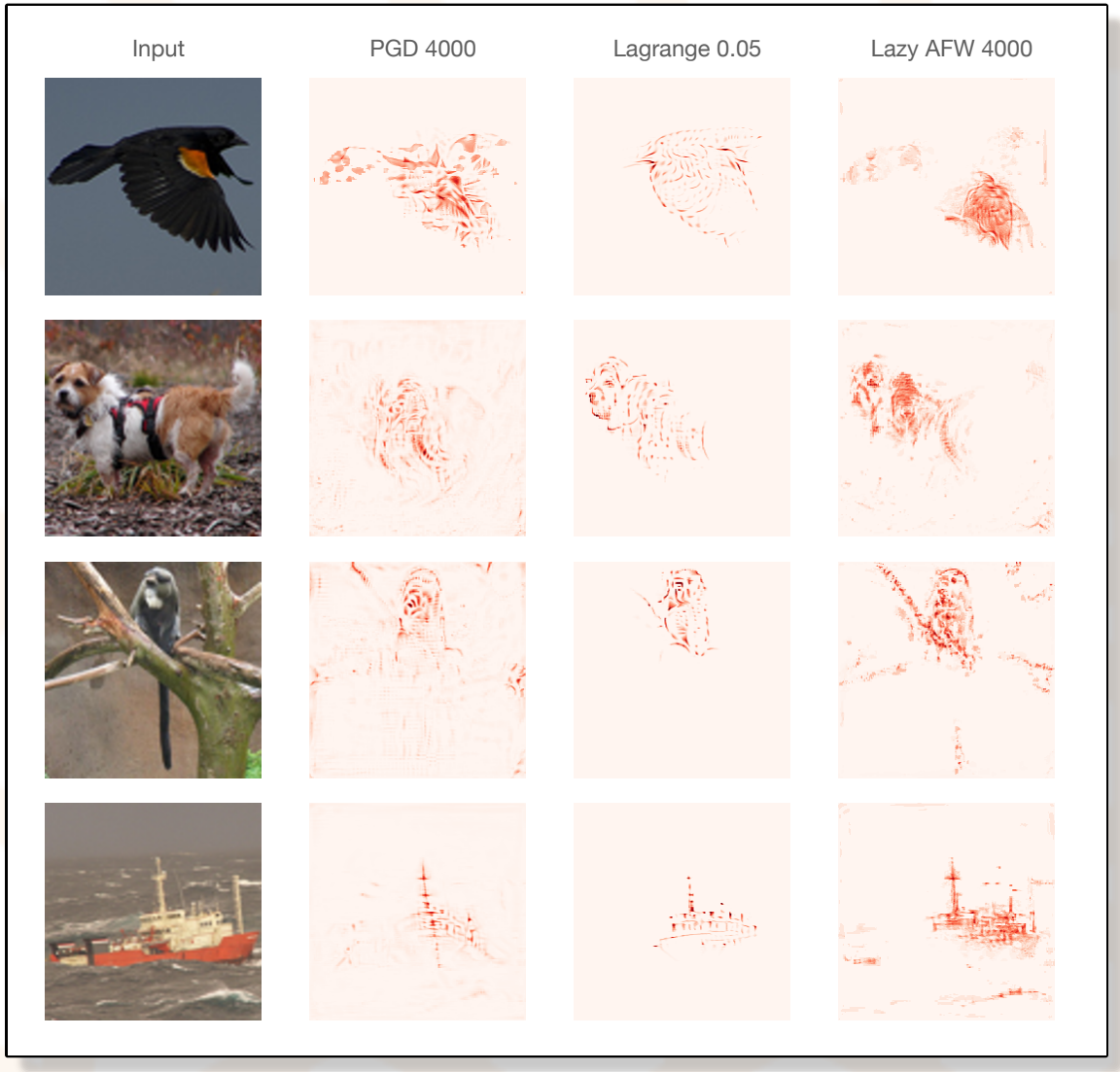
$\Rightarrow$ Typical sparse regression problem or LASSO problem.

Examples

Rate-Distortion Explanation



All methods had the same budget for picking relevant pixels. However, sparser solutions of Conditonal Gradients focus weight on most relevant pixels rather than spreading out.

Matrix Completion and Recommender Systems

The problem formulation

Matrix Completion and Recommender Systems

Task. Find matrix of low rank that coincides with given entries (observations).

Matrix Completion is a the core of many recommender systems, e.g., MovieLens.

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Matrix Completion. Common relaxation via nuclear norm.

$$\min_{\|X\|_* \leq \tau} \sum_{(i,j) \in \mathcal{I}} \left(X_{i,j} - Y_{i,j} \right)^2$$

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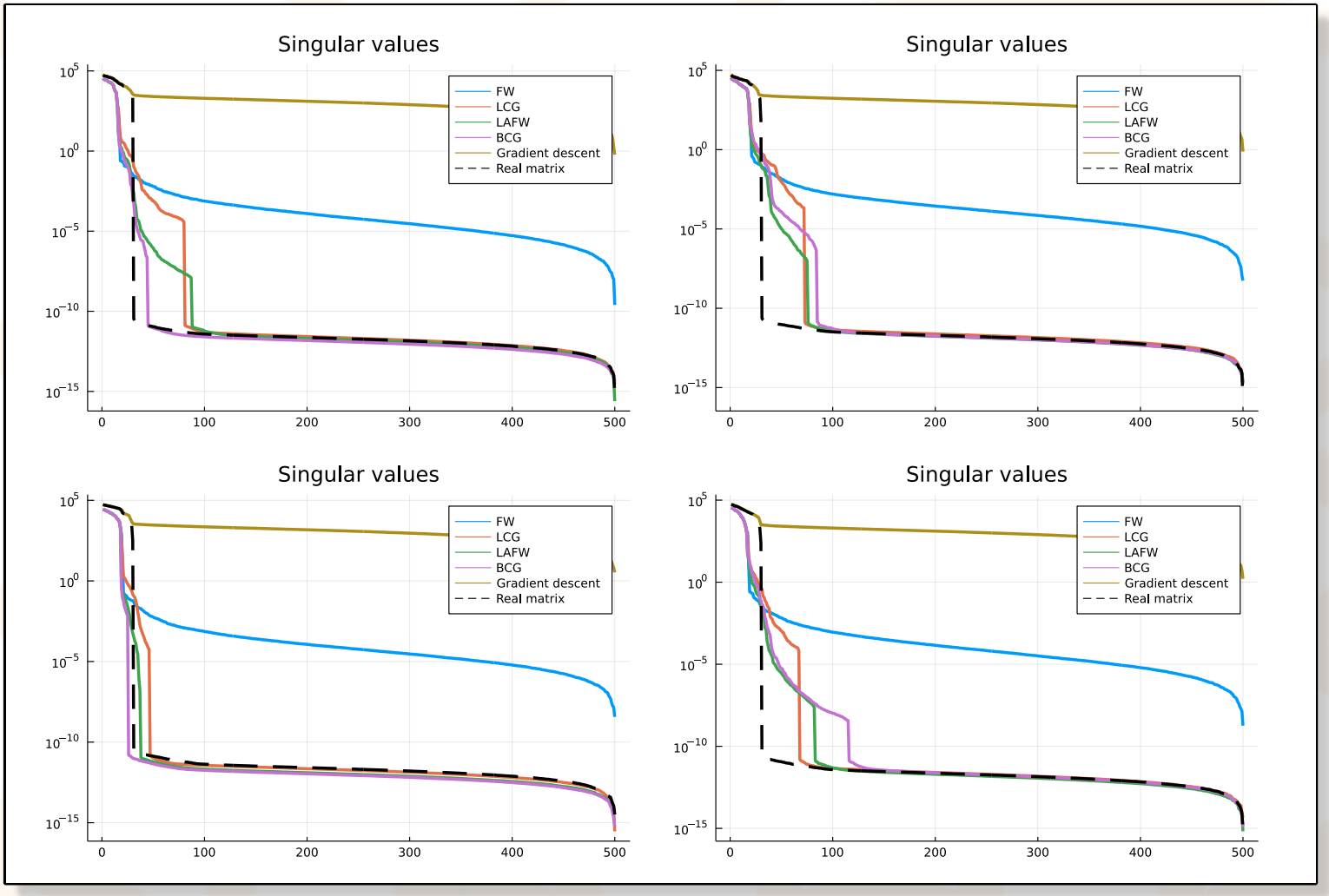
Note. While nuclear norm is a convex surrogate for rank, solving the problem with, e.g., projected gradient descent does not provide low rank solutions.

Examples

Matrix Completion and Recommender Systems



Characteristics. Reconstruction of matrix from 500 observations. True rank is 30.

FrankWolfe.jl

a high-performance Julia package for Conditional Gradients

joint work with Mathieu Besançon and Alejandro Carderera

[Besançon et al., 2021]

Overview and Features

FrankWolfe.jl

In a nutshell.

- Implemented in Julia
- Open source under MIT License
- Generic numeric types: reduced (16, 32, 64 bits) and extended (128, GNU MP) precision, rationals
- Memory-saving mode, in-place gradient computations
- Scales well (solved some problems with 1B variables)
- Switch components - bring your own LMO / ∇f / step size.

Give it a try.

```
using Pkg
Pkg.add("FrankWolfe")
```

Example

FrankWolfe.jl

```
using LinearAlgebra
using FrankWolfe

n = 1000
xp = rand(n)

f(x) = norm(x - xp)^2

function grad!(storage, x)
    @. storage = 2 * (x - xp)
    return nothing
end


# create a L_1-norm ball of radius 2.5
lmo_radius = 2.5
lmo = FrankWolfe.LpNormLMO{Float64,1}(lmo_radius)

x0 = FrankWolfe.compute_extreme_point(lmo, zeros(n))

x_sol, _ = frank_wolfe(f, grad!, lmo, x0)
```

Thank you!

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