

An Away-step Frank-Wolfe Method for Convex Optimization Involving a Log-Homogeneous Barrier

Renbo Zhao

Tippie College of Business
University of Iowa

INFORMS Annual Meeting
Phoenix, AZ
Oct, 2023

Motivating Example: D-Optimal Design

$$\begin{aligned} \min \quad & f(x) := -\ln \det \left(\sum_{i=1}^m x_i a_i a_i^\top \right) \\ \text{s. t.} \quad & x \in \Delta_m := \left\{ \sum_{i=1}^m x_i = 1, x_i \geq 0, \forall i \in [m] \right\}. \end{aligned} \tag{D-OPT}$$

Motivating Example: D-Optimal Design

$$\begin{aligned} \min \quad & f(x) := -\ln \det \left(\sum_{i=1}^m x_i a_i a_i^\top \right) \\ \text{s. t.} \quad & x \in \Delta_m := \left\{ \sum_{i=1}^m x_i = 1, x_i \geq 0, \forall i \in [m] \right\}. \end{aligned} \tag{D-OPT}$$

▷ Problem data: m points $\{a_i\}_{i=1}^m$ that span \mathbb{R}^n .

Motivating Example: D-Optimal Design

$$\begin{aligned} \min \quad & f(x) := -\ln \det \left(\sum_{i=1}^m x_i a_i a_i^\top \right) \\ \text{s. t.} \quad & x \in \Delta_m := \left\{ \sum_{i=1}^m x_i = 1, x_i \geq 0, \forall i \in [m] \right\}. \end{aligned} \tag{D-OPT}$$

- ▷ Problem data: m points $\{a_i\}_{i=1}^m$ that span \mathbb{R}^n .
- ▷ In statistics, (D-OPT) is the continuous relaxation of the (discrete) D-optimal experimental design problem; in computational geometry, it is the dual problem of the minimum volume enclosing ellipsoid (MVEE) problem.

Motivating Example: D-Optimal Design

$$\begin{aligned} \min \quad & f(x) := -\ln \det \left(\sum_{i=1}^m x_i a_i a_i^\top \right) \\ \text{s. t.} \quad & x \in \Delta_m := \left\{ \sum_{i=1}^m x_i = 1, x_i \geq 0, \forall i \in [m] \right\}. \end{aligned} \tag{D-OPT}$$

- ▷ Problem data: m points $\{a_i\}_{i=1}^m$ that span \mathbb{R}^n .
- ▷ In statistics, (D-OPT) is the continuous relaxation of the (discrete) D-optimal experimental design problem; in computational geometry, it is the dual problem of the minimum volume enclosing ellipsoid (MVVE) problem.
- ▷ Despite its seemingly simple structure, (D-OPT) is not quite amenable to (traditional) first-order methods (since f blows up on part of $\partial\Delta_m$, and has no L -smoothness property on Δ_m).

Motivating Example: D-Optimal Design

$$\begin{aligned} \min \quad & f(x) := -\ln \det \left(\sum_{i=1}^m x_i a_i a_i^\top \right) \\ \text{s. t.} \quad & x \in \Delta_m := \left\{ \sum_{i=1}^m x_i = 1, x_i \geq 0, \forall i \in [m] \right\}. \end{aligned} \tag{D-OPT}$$

- ▷ Problem data: m points $\{a_i\}_{i=1}^m$ that span \mathbb{R}^n .
- ▷ In statistics, (D-OPT) is the continuous relaxation of the (discrete) D-optimal experimental design problem; in computational geometry, it is the dual problem of the minimum volume enclosing ellipsoid (MVEE) problem.
- ▷ Despite its seemingly simple structure, (D-OPT) is not quite amenable to (traditional) first-order methods (since f blows up on part of $\partial\Delta_m$, and has no L -smoothness property on Δ_m).
- ▷ Atwood (1973) proposed the following algorithm for solving (D-OPT):

Motivating Example: D-Optimal Design

$$\begin{aligned} \min \quad & f(x) := -\ln \det \left(\sum_{i=1}^m x_i a_i a_i^\top \right) \\ \text{s. t.} \quad & x \in \Delta_m := \left\{ \sum_{i=1}^m x_i = 1, x_i \geq 0, \forall i \in [m] \right\}. \end{aligned} \tag{D-OPT}$$

- ▷ Problem data: m points $\{a_i\}_{i=1}^m$ that span \mathbb{R}^n .
- ▷ In statistics, (D-OPT) is the continuous relaxation of the (discrete) D-optimal experimental design problem; in computational geometry, it is the dual problem of the minimum volume enclosing ellipsoid (MVEE) problem.
- ▷ Despite its seemingly simple structure, (D-OPT) is not quite amenable to (traditional) first-order methods (since f blows up on part of $\partial\Delta_m$, and has no L -smoothness property on Δ_m).
- ▷ Atwood (1973) proposed the following algorithm for solving (D-OPT):

$$\begin{aligned} i_k &\in \arg \min_{i \in [m]} \nabla_i f(x^k), & G_k &:= -\nabla_{i_k} f(x^k) - n, \\ j_k &\in \arg \max_{j: x_j^k > 0} \nabla_j f(x^k), & \tilde{G}_k &:= \nabla_{j_k} f(x^k) + n, \\ d^k &= \begin{cases} e_{i_k} - x^k & \text{if } G_k > \tilde{G}_k \\ x^k - e_{j_k} & \text{otherwise} \end{cases}, & x^{k+1} &:= x^k + \alpha_k d^k, \end{aligned}$$

where the stepsize $\alpha_k \geq 0$ is given by exact line-search.

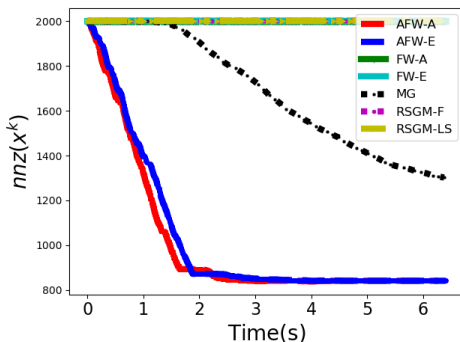
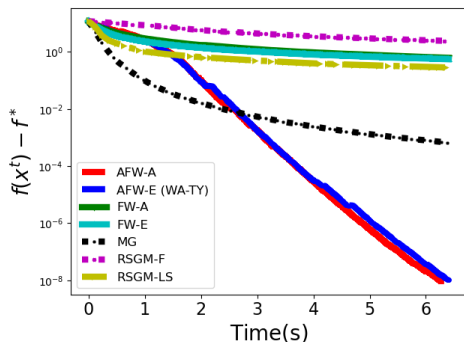
The WA-TY Method

The WA-TY Method

- ▷ Structurally, this method coincides with the Frank-Wolfe method with Wolfe's away-step (1970), and it was rediscovered by Todd and Yildirim (2005) — therefore, it is referred to as the WA-TY method.

The WA-TY Method

- ▷ Structurally, this method coincides with the Frank-Wolfe method with Wolfe's away-step (1970), and it was rediscovered by Todd and Yildirim (2005) — therefore, it is referred to as the WA-TY method.
- ▷ Excellent numerical performance:



ASFW-A & ASFW-E (this work): Away-step FW methods for LHB
FW-A & FW-E [Fed72; Kha96; ZFce]: Generalized FW methods for LHB
RSGM-F & RSGM-LS [BBT17; LFN18]: Relatively smooth gradient method
MG [STT78]: Multiplicative gradient method

Mystery of the WA-TY Method

Mystery of the WA-TY Method

- ▷ The excellent numerical performance of the WA-TY method has attracted some research interests — Ahipasaoglu, Sun and Todd (2008) showed *local* linear convergence of this method, but the *global* linear convergence remains open.

Mystery of the WA-TY Method

- ▷ The excellent numerical performance of the WA-TY method has attracted some research interests — Ahipasaoglu, Sun and Todd (2008) showed *local* linear convergence of this method, but the *global* linear convergence remains open.
- ▷ The authors pointed out two structural difficulties of (D-OPT): i) f is not L -smooth on Δ_m and ii) f is degenerate on the feasible region.

Mystery of the WA-TY Method

- ▷ The excellent numerical performance of the WA-TY method has attracted some research interests — Ahipasaoglu, Sun and Todd (2008) showed *local* linear convergence of this method, but the *global* linear convergence remains open.
- ▷ The authors pointed out two structural difficulties of (D-OPT): i) f is not L -smooth on Δ_m and ii) f is degenerate on the feasible region.
- ▷ This difficulty prevents the recent analyses of the away-step FW (AFW) methods for L -smooth functions [LJJ15; BS17; PR19], as well as for *non-degenerate* generalized self-concordant function [Dvu23] being applied to (D-OPT).

Mystery of the WA-TY Method

- ▷ The excellent numerical performance of the WA-TY method has attracted some research interests — Ahipasaoglu, Sun and Todd (2008) showed *local* linear convergence of this method, but the *global* linear convergence remains open.
- ▷ The authors pointed out two structural difficulties of (D-OPT): i) f is not L -smooth on Δ_m and ii) f is degenerate on the feasible region.
- ▷ This difficulty prevents the recent analyses of the away-step FW (AFW) methods for L -smooth functions [LJJ15; BS17; PR19], as well as for *non-degenerate* generalized self-concordant function [Dvu23] being applied to (D-OPT).
- ▷ Some deeper questions:
 - What is the essential structure of (D-OPT) that drives the linear convergence of the WA-TY method (or the AFW method)?
 - Can it help us develop and analyze a new type of AFW methods for an “unconventional” class of problems?

Mystery of the WA-TY Method

- ▷ The excellent numerical performance of the WA-TY method has attracted some research interests — Ahipasaoglu, Sun and Todd (2008) showed *local* linear convergence of this method, but the *global* linear convergence remains open.
- ▷ The authors pointed out two structural difficulties of (D-OPT): i) f is not L -smooth on Δ_m and ii) f is degenerate on the feasible region.
- ▷ This difficulty prevents the recent analyses of the away-step FW (AFW) methods for L -smooth functions [LJJ15; BS17; PR19], as well as for *non-degenerate* generalized self-concordant function [Dvu23] being applied to (D-OPT).
- ▷ Some deeper questions:
 - What is the essential structure of (D-OPT) that drives the linear convergence of the WA-TY method (or the AFW method)?
 - Can it help us develop and analyze a new type of AFW methods for an “unconventional” class of problems?
- ▷ In this work, we will provide affirmative answers to the questions above.

Problem of Interest

$$F^* := \min_{x \in \mathcal{X}} [F(x) := f(Ax) + cx] \quad (\text{P})$$

Problem of Interest

$$F^* := \min_{x \in \mathcal{X}} [F(x) := f(Ax) + cx] \quad (\text{P})$$

▷ \mathbb{X} and \mathbb{Y} are finite-dimensional vector spaces

Problem of Interest

$$F^* := \min_{x \in \mathcal{X}} [F(x) := f(Ax) + cx] \quad (\text{P})$$

- ▷ \mathbb{X} and \mathbb{Y} are finite-dimensional vector spaces
- ▷ $\mathcal{X} \subseteq \mathbb{X}$ is a polytope such that $\mathcal{X} = \text{conv}(\mathcal{V})$, where \mathcal{V} is a finite set of *atoms*

Problem of Interest

$$F^* := \min_{x \in \mathcal{X}} [F(x) := f(Ax) + cx] \quad (\text{P})$$

- ▷ \mathbb{X} and \mathbb{Y} are finite-dimensional vector spaces
- ▷ $\mathcal{X} \subseteq \mathbb{X}$ is a polytope such that $\mathcal{X} = \text{conv}(\mathcal{V})$, where \mathcal{V} is a finite set of *atoms*
- ▷ $f : \mathbb{Y} \rightarrow \mathbb{R} \cup \{+\infty\}$ is a θ -log-homogeneous self-concordant barrier (θ -LHSCB) for some regular cone $\mathcal{K} \subseteq \mathbb{Y}$

Problem of Interest

$$F^* := \min_{x \in \mathcal{X}} [F(x) := f(Ax) + cx] \quad (\text{P})$$

- ▷ \mathbb{X} and \mathbb{Y} are finite-dimensional vector spaces
- ▷ $\mathcal{X} \subseteq \mathbb{X}$ is a polytope such that $\mathcal{X} = \text{conv}(\mathcal{V})$, where \mathcal{V} is a finite set of *atoms*
- ▷ $f : \mathbb{Y} \rightarrow \mathbb{R} \cup \{+\infty\}$ is a θ -log-homogeneous self-concordant barrier (θ -LHSCB) for some regular cone $\mathcal{K} \subseteq \mathbb{Y}$
- ▷ $A : \mathbb{X} \rightarrow \mathbb{Y}$ is a linear operator such that $A(\mathcal{X}) \subseteq \mathcal{K}$ and $A(\mathcal{X}) \cap \text{int } \mathcal{K} \neq \emptyset$

Problem of Interest

$$F^* := \min_{x \in \mathcal{X}} [F(x) := f(Ax) + cx] \quad (\text{P})$$

- ▷ \mathbb{X} and \mathbb{Y} are finite-dimensional vector spaces
- ▷ $\mathcal{X} \subseteq \mathbb{X}$ is a polytope such that $\mathcal{X} = \text{conv}(\mathcal{V})$, where \mathcal{V} is a finite set of *atoms*
- ▷ $f : \mathbb{Y} \rightarrow \mathbb{R} \cup \{+\infty\}$ is a θ -log-homogeneous self-concordant barrier (θ -LHSCB) for some regular cone $\mathcal{K} \subseteq \mathbb{Y}$
- ▷ $A : \mathbb{X} \rightarrow \mathbb{Y}$ is a linear operator such that $A(\mathcal{X}) \subseteq \mathcal{K}$ and $A(\mathcal{X}) \cap \text{int } \mathcal{K} \neq \emptyset$
- ▷ $c \cdot : \mathbb{X} \rightarrow \mathbb{R}$ is a linear function

Problem of Interest

$$F^* := \min_{x \in \mathcal{X}} [F(x) := f(Ax) + cx] \quad (\text{P})$$

- ▷ \mathbb{X} and \mathbb{Y} are finite-dimensional vector spaces
- ▷ $\mathcal{X} \subseteq \mathbb{X}$ is a polytope such that $\mathcal{X} = \text{conv}(\mathcal{V})$, where \mathcal{V} is a finite set of *atoms*
- ▷ $f : \mathbb{Y} \rightarrow \mathbb{R} \cup \{+\infty\}$ is a θ -log-homogeneous self-concordant barrier (θ -LHSCB) for some regular cone $\mathcal{K} \subseteq \mathbb{Y}$
- ▷ $A : \mathbb{X} \rightarrow \mathbb{Y}$ is a linear operator such that $A(\mathcal{X}) \subseteq \mathcal{K}$ and $A(\mathcal{X}) \cap \text{int } \mathcal{K} \neq \emptyset$
- ▷ $c \cdot : \mathbb{X} \rightarrow \mathbb{R}$ is a linear function
- ▷ Besides D-optimal design, other applications include
 - Budget-constrained D-optimal design
 - Positron emission tomography
 - (Reformulated) Poisson image deblurring with TV-regularization

θ -LHSCB (logarithmically-homogeneous self-concordant barrier)

θ -LHSCB (logarithmically-homogeneous self-concordant barrier)

- ▷ Let $\mathcal{K} \subsetneq \mathbb{Y}$ be a regular cone, i.e., \mathcal{K} is closed, convex, pointed and has nonempty interior.

θ -LHSCB (logarithmically-homogeneous self-concordant barrier)

- ▷ Let $\mathcal{K} \subsetneq \mathbb{Y}$ be a regular cone, i.e., \mathcal{K} is closed, convex, pointed and has nonempty interior.
- ▷ Two prototypical examples:

θ -LHSCB (logarithmically-homogeneous self-concordant barrier)

- ▷ Let $\mathcal{K} \subsetneq \mathbb{Y}$ be a regular cone, i.e., \mathcal{K} is closed, convex, pointed and has nonempty interior.
- ▷ Two prototypical examples:
 - $f(Y) = -\ln \det(Y)$ for $\mathcal{K} := \mathbb{S}_+^n$ and $\theta = n$,

θ -LHSCB (logarithmically-homogeneous self-concordant barrier)

- ▷ Let $\mathcal{K} \subsetneq \mathbb{Y}$ be a regular cone, i.e., \mathcal{K} is closed, convex, pointed and has nonempty interior.
- ▷ Two prototypical examples:
 - $f(Y) = -\ln \det(Y)$ for $\mathcal{K} := \mathbb{S}_+^n$ and $\theta = n$,
 - $f(y) = -\sum_{j=1}^m w_j \ln(y_j)$ for $\mathcal{K} := \mathbb{R}_+^m$ and $\theta = \sum_{j=1}^m w_j$ (where $w_1, \dots, w_n \geq 1$).

θ -LHSCB (logarithmically-homogeneous self-concordant barrier)

- ▷ Let $\mathcal{K} \subsetneq \mathbb{Y}$ be a regular cone, i.e., \mathcal{K} is closed, convex, pointed and has nonempty interior.
- ▷ Two prototypical examples:
 - $f(Y) = -\ln \det(Y)$ for $\mathcal{K} := \mathbb{S}_+^n$ and $\theta = n$,
 - $f(y) = -\sum_{j=1}^m w_j \ln(y_j)$ for $\mathcal{K} := \mathbb{R}_+^m$ and $\theta = \sum_{j=1}^m w_j$ (where $w_1, \dots, w_n \geq 1$).
- ▷ f is a θ -LHSCB on \mathcal{K} with *complexity parameter* $\theta \geq 1$, if f is three-times continuously differentiable and non-degenerate on $\text{int } \mathcal{K}$, and satisfies

θ -LHSCB (logarithmically-homogeneous self-concordant barrier)

- ▷ Let $\mathcal{K} \subsetneq \mathbb{Y}$ be a regular cone, i.e., \mathcal{K} is closed, convex, pointed and has nonempty interior.
- ▷ Two prototypical examples:
 - $f(Y) = -\ln \det(Y)$ for $\mathcal{K} := \mathbb{S}_+^n$ and $\theta = n$,
 - $f(y) = -\sum_{j=1}^m w_j \ln(y_j)$ for $\mathcal{K} := \mathbb{R}_+^m$ and $\theta = \sum_{j=1}^m w_j$ (where $w_1, \dots, w_n \geq 1$).
- ▷ f is a θ -LHSCB on \mathcal{K} with *complexity parameter* $\theta \geq 1$, if f is three-times continuously differentiable and non-degenerate on $\text{int } \mathcal{K}$, and satisfies
 - ① $|D^3 f(y)[w, w, w]| \leq 2\|w\|_y^3 \quad \forall y \in \text{int } \mathcal{K}, \forall w \in \mathbb{Y}$,
 - ② $f(y_k) \rightarrow +\infty$ for any $\{y_k\}_{k \geq 1} \subseteq \text{int } \mathcal{K}$ such that $y_k \rightarrow u \in \text{bd } \mathcal{K}$,
 - ③ $f(ty) = f(y) - \theta \ln(t) \quad \forall y \in \text{int } \mathcal{K}, \forall t > 0$.

where $\|w\|_y := \langle \nabla^2 f(y)w, w \rangle^{1/2}$ denotes the local norm of w at $y \in \text{int } \mathcal{K}$.

Away-step Frank-Wolfe Method for solving (P)

Away-step Frank-Wolfe Method for solving (P)

► **Input:** $x^0 \in \mathcal{X} \cap \text{dom } F$, $\beta^0 \in \Delta_{|\mathcal{V}|}$ such that $x^0 = \sum_{v \in \mathcal{V}} \beta_v^0 v$, $\mathcal{S}_0 := \text{supp}(\beta^0)$.

Away-step Frank-Wolfe Method for solving (P)

- ▶ **Input:** $x^0 \in \mathcal{X} \cap \text{dom } F$, $\beta^0 \in \Delta_{|\mathcal{V}|}$ such that $x^0 = \sum_{v \in \mathcal{V}} \beta_v^0 v$, $\mathcal{S}_0 := \text{supp}(\beta^0)$.
- ▶ **At iteration** $k \geq 0$:

Away-step Frank-Wolfe Method for solving (P)

- ▶ **Input:** $x^0 \in \mathcal{X} \cap \text{dom } F$, $\beta^0 \in \Delta_{|\mathcal{V}|}$ such that $x^0 = \sum_{v \in \mathcal{V}} \beta_v^0 v$, $\mathcal{S}_0 := \text{supp}(\beta^0)$.
- ▶ **At iteration** $k \geq 0$:
 - ▷ (FW direction) Compute $v^k \in \arg \min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$, $d_{\mathbb{F}}^k := v^k - x^k$ and $G_k := \langle -\nabla F(x^k), d_{\mathbb{F}}^k \rangle$. If $G_k = 0$, then STOP.

Away-step Frank-Wolfe Method for solving (P)

- ▶ **Input:** $x^0 \in \mathcal{X} \cap \text{dom } F$, $\beta^0 \in \Delta_{|\mathcal{V}|}$ such that $x^0 = \sum_{v \in \mathcal{V}} \beta_v^0 v$, $\mathcal{S}_0 := \text{supp}(\beta^0)$.
- ▶ **At iteration** $k \geq 0$:
 - ▷ (FW direction) Compute $v^k \in \arg \min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$, $d_{\text{F}}^k := v^k - x^k$ and $G_k := \langle -\nabla F(x^k), d_{\text{F}}^k \rangle$. If $G_k = 0$, then STOP.
 - ▷ (Away direction) If $|\mathcal{S}_k| > 1$, compute $a^k \in \arg \max_{x \in \mathcal{S}_k} \langle \nabla F(x^k), x \rangle$, $d_{\text{A}}^k := x^k - a^k$ and $\tilde{G}_k := \langle -\nabla F(x^k), d_{\text{A}}^k \rangle$.

Away-step Frank-Wolfe Method for solving (P)

- ▶ **Input:** $x^0 \in \mathcal{X} \cap \text{dom } F$, $\beta^0 \in \Delta_{|\mathcal{V}|}$ such that $x^0 = \sum_{v \in \mathcal{V}} \beta_v^0 v$, $\mathcal{S}_0 := \text{supp}(\beta^0)$.
- ▶ **At iteration** $k \geq 0$:
 - ▷ (FW direction) Compute $v^k \in \arg \min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$, $d_{\text{F}}^k := v^k - x^k$ and $G_k := \langle -\nabla F(x^k), d_{\text{F}}^k \rangle$. If $G_k = 0$, then STOP.
 - ▷ (Away direction) If $|\mathcal{S}_k| > 1$, compute $a^k \in \arg \max_{x \in \mathcal{S}_k} \langle \nabla F(x^k), x \rangle$, $d_{\text{A}}^k := x^k - a^k$ and $\tilde{G}_k := \langle -\nabla F(x^k), d_{\text{A}}^k \rangle$.
 - ▷ (Choose direction) If $|\mathcal{S}_k| = 1$ or $G_k > \tilde{G}_k$, let $d^k := d_{\text{F}}^k$ and $\bar{\alpha}_k := 1$; otherwise, let $d^k := d_{\text{A}}^k$ and $\bar{\alpha}_k := \beta_{a^k}^k / (1 - \beta_{a^k}^k)$.

Away-step Frank-Wolfe Method for solving (P)

- ▶ **Input:** $x^0 \in \mathcal{X} \cap \text{dom } F$, $\beta^0 \in \Delta_{|\mathcal{V}|}$ such that $x^0 = \sum_{v \in \mathcal{V}} \beta_v^0 v$, $\mathcal{S}_0 := \text{supp}(\beta^0)$.
- ▶ **At iteration** $k \geq 0$:
 - ▷ (FW direction) Compute $v^k \in \arg \min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$, $d_F^k := v^k - x^k$ and $G_k := \langle -\nabla F(x^k), d_F^k \rangle$. If $G_k = 0$, then STOP.
 - ▷ (Away direction) If $|\mathcal{S}_k| > 1$, compute $a^k \in \arg \max_{x \in \mathcal{S}_k} \langle \nabla F(x^k), x \rangle$, $d_A^k := x^k - a^k$ and $\tilde{G}_k := \langle -\nabla F(x^k), d_A^k \rangle$.
 - ▷ (Choose direction) If $|\mathcal{S}_k| = 1$ or $G_k > \tilde{G}_k$, let $d^k := d_F^k$ and $\bar{\alpha}_k := 1$; otherwise, let $d^k := d_A^k$ and $\bar{\alpha}_k := \beta_{a^k}^k / (1 - \beta_{a^k}^k)$.
 - ▷ (Choose stepsize) Choose $\alpha_k \in (0, \bar{\alpha}_k]$ in one of the following two ways:
 - Adaptive stepsize: Compute $r_k := -\nabla F(x^k) d^k$ and $D_k := \|A d^k\|_{y^k}$. If $D_k = 0$, then $\alpha_k := \bar{\alpha}_k$; otherwise, $\alpha_k := \min\{b_k, \bar{\alpha}_k\}$, where $b_k := r_k / (D_k(r_k + D_k))$.
 - Exact line-search: $\alpha_k \in \arg \min_{\alpha_k \in (0, \bar{\alpha}_k]} F(x^k + \alpha d^k)$.

Away-step Frank-Wolfe Method for solving (P)

- ▶ **Input:** $x^0 \in \mathcal{X} \cap \text{dom } F$, $\beta^0 \in \Delta_{|\mathcal{V}|}$ such that $x^0 = \sum_{v \in \mathcal{V}} \beta_v^0 v$, $\mathcal{S}_0 := \text{supp}(\beta^0)$.
- ▶ **At iteration** $k \geq 0$:
 - ▷ (FW direction) Compute $v^k \in \arg \min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$, $d_F^k := v^k - x^k$ and $G_k := \langle -\nabla F(x^k), d_F^k \rangle$. If $G_k = 0$, then STOP.
 - ▷ (Away direction) If $|\mathcal{S}_k| > 1$, compute $a^k \in \arg \max_{x \in \mathcal{S}_k} \langle \nabla F(x^k), x \rangle$, $d_A^k := x^k - a^k$ and $\tilde{G}_k := \langle -\nabla F(x^k), d_A^k \rangle$.
 - ▷ (Choose direction) If $|\mathcal{S}_k| = 1$ or $G_k > \tilde{G}_k$, let $d^k := d_F^k$ and $\bar{\alpha}_k := 1$; otherwise, let $d^k := d_A^k$ and $\bar{\alpha}_k := \beta_{a^k}^k / (1 - \beta_{a^k}^k)$.
 - ▷ (Choose stepsize) Choose $\alpha_k \in (0, \bar{\alpha}_k]$ in one of the following two ways:
 - Adaptive stepsize: Compute $r_k := -\nabla F(x^k) d^k$ and $D_k := \|A d^k\|_{y^k}$. If $D_k = 0$, then $\alpha_k := \bar{\alpha}_k$; otherwise, $\alpha_k := \min\{b_k, \bar{\alpha}_k\}$, where $b_k := r_k / (D_k(r_k + D_k))$.
 - Exact line-search: $\alpha_k \in \arg \min_{\alpha_k \in (0, \bar{\alpha}_k]} F(x^k + \alpha d^k)$.
 - ▷ (Update iterates) Update $x^{k+1} := x^k + \alpha_k d^k$ and $\beta^{k+1} \in \Delta_{|\mathcal{V}|}$ such that $x^{k+1} = \sum_{v \in \mathcal{V}} \beta_v^{k+1} v$, and let $\mathcal{S}_{k+1} := \text{supp}(\beta^{k+1})$.

Some Remarks

Denote $\dim \mathbb{X} = n$.

Some Remarks

Denote $\dim \mathbb{X} = n$.

- ▷ Depending on \mathcal{X} , we may prefer to solve $\min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$ either by either minimizing over \mathcal{X} (e.g., $\mathcal{X} = \prod_{i=1}^n [a_i, b_i]$) or \mathcal{V} (e.g., $\mathcal{X} = \Delta_n$).

Some Remarks

Denote $\dim \mathbb{X} = n$.

- ▷ Depending on \mathcal{X} , we may prefer to solve $\min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$ either by either minimizing over \mathcal{X} (e.g., $\mathcal{X} = \prod_{i=1}^n [a_i, b_i]$) or \mathcal{V} (e.g., $\mathcal{X} = \Delta_n$).
- ▷ The FW-gap $G_k = \nabla F(x^k)x^k - v^k$ provides an effective stopping criterion:

$$G_k \geq [\delta_k := F(x^k) - F^*] \quad \text{for } k \geq 0.$$

Some Remarks

Denote $\dim \mathbb{X} = n$.

- ▷ Depending on \mathcal{X} , we may prefer to solve $\min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$ either by either minimizing over \mathcal{X} (e.g., $\mathcal{X} = \prod_{i=1}^n [a_i, b_i]$) or \mathcal{V} (e.g., $\mathcal{X} = \Delta_n$).
- ▷ The FW-gap $G_k = \nabla F(x^k)x^k - v^k$ provides an effective stopping criterion:
$$G_k \geq [\delta_k := F(x^k) - F^*] \quad \text{for } k \geq 0.$$
- ▷ If $|\mathcal{V}| = \omega(n)$, we may prefer to maintain a compact representation of \mathcal{S}_k such that $|\mathcal{S}_k| = O(n)$ for $k \geq 0$, at computational cost of $O(n^2)$ per iteration [BS17].

Some Remarks

Denote $\dim \mathbb{X} = n$.

- ▷ Depending on \mathcal{X} , we may prefer to solve $\min_{x \in \mathcal{V}} \langle \nabla F(x^k), x \rangle$ either by either minimizing over \mathcal{X} (e.g., $\mathcal{X} = \prod_{i=1}^n [a_i, b_i]$) or \mathcal{V} (e.g., $\mathcal{X} = \Delta_n$).
- ▷ The FW-gap $G_k = \nabla F(x^k)x^k - v^k$ provides an effective stopping criterion:
$$G_k \geq [\delta_k := F(x^k) - F^*] \quad \text{for } k \geq 0.$$
- ▷ If $|\mathcal{V}| = \omega(n)$, we may prefer to maintain a compact representation of \mathcal{S}_k such that $|\mathcal{S}_k| = O(n)$ for $k \geq 0$, at computational cost of $O(n^2)$ per iteration [BS17].
- ▷ For all applications of interest, computing $D_k = \|\mathbf{A}d^k\|_{y^k} = \nabla^2 F(x^k)d^k d^{k1/2}$ takes $O(n)$ times, instead of $O(n^2)$ time.

Computational Guarantees

$$F^* := \min_{x \in \mathbb{R}^n} [F(x) := f(Ax) + cx]$$

Computational Guarantees

$$F^* := \min_{x \in \mathbb{R}^n} [F(x) := f(Ax) + cx]$$

▷ Define $B := \max_{x, x' \in \mathcal{X}} cx - x'$ (the variation of $c \cdot$ on \mathcal{X}).

Computational Guarantees

$$F^* := \min_{x \in \mathbb{R}^n} [F(x) := f(Ax) + cx]$$

- ▷ Define $B := \max_{x, x' \in \mathcal{X}} cx - x'$ (the variation of $c \cdot$ on \mathcal{X}).
- ▷ Define $q := \min\{|\mathcal{W}| : \mathcal{W} \subseteq \mathcal{V} \text{ such that } \text{conv}\mathcal{W} \cap \text{dom } F \neq \emptyset\}$.

Computational Guarantees

$$F^* := \min_{x \in \mathbb{R}^n} [F(x) := f(Ax) + cx]$$

- ▷ Define $B := \max_{x, x' \in \mathcal{X}} cx - x'$ (the variation of $c \cdot$ on \mathcal{X}).
- ▷ Define $q := \min\{|\mathcal{W}| : \mathcal{W} \subseteq \mathcal{V} \text{ such that } \text{conv}\mathcal{W} \cap \text{dom } F \neq \emptyset\}$.
- ▷ Define $\mathcal{Y} := A(\mathcal{X})$ and $R_{\mathcal{Y}}(y^*) := \sup_{y \in A(\mathcal{X})} \|y - y^*\|_{y^*} < +\infty$.

Computational Guarantees

$$F^* := \min_{x \in \mathbb{R}^n} [F(x) := f(Ax) + cx]$$

- ▷ Define $B := \max_{x, x' \in \mathcal{X}} cx - x'$ (the variation of $c \cdot$ on \mathcal{X}).
- ▷ Define $q := \min\{|\mathcal{W}| : \mathcal{W} \subseteq \mathcal{V} \text{ such that } \text{conv}\mathcal{W} \cap \text{dom } F \neq \emptyset\}$.
- ▷ Define $\mathcal{Y} := A(\mathcal{X})$ and $R_{\mathcal{Y}}(y^*) := \sup_{y \in A(\mathcal{X})} \|y - y^*\|_{y^*} < +\infty$.

Global linear convergence of $\{\delta_k\}_{k \geq 0}$:

Computational Guarantees

$$F^* := \min_{x \in \mathbb{R}^n} [F(x) := f(Ax) + cx]$$

- ▷ Define $B := \max_{x, x' \in \mathcal{X}} cx - x'$ (the variation of $c \cdot$ on \mathcal{X}).
- ▷ Define $q := \min\{|\mathcal{W}| : \mathcal{W} \subseteq \mathcal{V} \text{ such that } \text{conv}\mathcal{W} \cap \text{dom } F \neq \emptyset\}$.
- ▷ Define $\mathcal{Y} := A(\mathcal{X})$ and $R_{\mathcal{Y}}(y^*) := \sup_{y \in A(\mathcal{X})} \|y - y^*\|_{y^*} < +\infty$.

Global linear convergence of $\{\delta_k\}_{k \geq 0}$:

- ▷ $\{\delta_k\}_{k \geq 0}$ is strictly decreasing (until termination).

Computational Guarantees

$$F^* := \min_{x \in \mathbb{R}^n} [F(x) := f(Ax) + cx]$$

- ▷ Define $B := \max_{x, x' \in \mathcal{X}} cx - x'$ (the variation of $c \cdot$ on \mathcal{X}).
- ▷ Define $q := \min\{|\mathcal{W}| : \mathcal{W} \subseteq \mathcal{V} \text{ such that } \text{conv}\mathcal{W} \cap \text{dom } F \neq \emptyset\}$.
- ▷ Define $\mathcal{Y} := A(\mathcal{X})$ and $R_{\mathcal{Y}}(y^*) := \sup_{y \in A(\mathcal{X})} \|y - y^*\|_{y^*} < +\infty$.

Global linear convergence of $\{\delta_k\}_{k \geq 0}$:

- ▷ $\{\delta_k\}_{k \geq 0}$ is strictly decreasing (until termination).
- ▷ For all $k \geq 0$, define $k_{\text{eff}} := \lceil \max\{(k - |\mathcal{S}_0| + q)/2, 0\} \rceil \approx k/2$, and then

$$\delta_k \leq (1 - \rho)^{k_{\text{eff}}} \delta_0, \quad \text{where } \rho := \min \left\{ \frac{1}{5.3(\delta_0 + \theta + B)}, \frac{\mu \Phi(\mathcal{X}, \mathcal{X}^*)^2}{42.4(\theta + B)^2} \right\},$$

where

- μ is the quadratic-growth constant of f on \mathcal{Y} that only depends on $R_{\mathcal{Y}}(y^*)$
- $\Phi(\mathcal{X}, \mathcal{X}^*) > 0$ is a geometric constant about \mathcal{X}^* and \mathcal{X} .

Computational Guarantees

$$F^* := \min_{x \in \mathbb{R}^n} [F(x) := f(Ax) + cx]$$

- ▷ Define $B := \max_{x, x' \in \mathcal{X}} cx - x'$ (the variation of $c \cdot$ on \mathcal{X}).
- ▷ Define $q := \min\{|\mathcal{W}| : \mathcal{W} \subseteq \mathcal{V} \text{ such that } \text{conv}\mathcal{W} \cap \text{dom } F \neq \emptyset\}$.
- ▷ Define $\mathcal{Y} := A(\mathcal{X})$ and $R_{\mathcal{Y}}(y^*) := \sup_{y \in A(\mathcal{X})} \|y - y^*\|_{y^*} < +\infty$.

Global linear convergence of $\{\delta_k\}_{k \geq 0}$:

- ▷ $\{\delta_k\}_{k \geq 0}$ is strictly decreasing (until termination).
- ▷ For all $k \geq 0$, define $k_{\text{eff}} := \lceil \max\{(k - |\mathcal{S}_0| + q)/2, 0\} \rceil \approx k/2$, and then

$$\delta_k \leq (1 - \rho)^{k_{\text{eff}}} \delta_0, \quad \text{where } \rho := \min \left\{ \frac{1}{5.3(\delta_0 + \theta + B)}, \frac{\mu \Phi(\mathcal{X}, \mathcal{X}^*)^2}{42.4(\theta + B)^2} \right\},$$

where

- μ is the quadratic-growth constant of f on \mathcal{Y} that only depends on $R_{\mathcal{Y}}(y^*)$
 - $\Phi(\mathcal{X}, \mathcal{X}^*) > 0$ is a geometric constant about \mathcal{X}^* and \mathcal{X} .
- ▷ All the quantities defining ρ are *affine-invariant* and *norm-independent*.

Computational Guarantees

Global linear convergence of $\{G_k\}_{k \geq 0}$:

For some (affine-invariant) $\bar{D} < +\infty$ and all $k \geq 0$, we have

$$G_k \leq \begin{cases} 4(1 - \rho)^{k_{\text{eff}}} \delta_0 \max\{\bar{D}, 1\}, & \text{if } \delta_k > 1 \\ 4\sqrt{1 - \rho}^{k_{\text{eff}}} \sqrt{\delta_0} \max\{\bar{D}, 1\}, & \text{if } \delta_k \leq 1 \end{cases}.$$

Essentially, this means $\{G_k\}_{k \geq 0}$ converges at the linear rate $\sqrt{1 - \rho}$, which is worse than the rate of $\{\delta_k\}_{k \geq 0}$, namely $(1 - \rho)$.

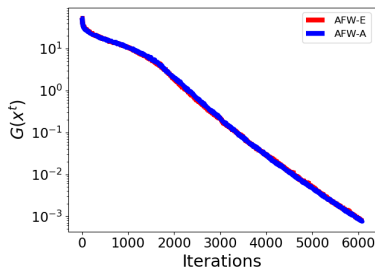
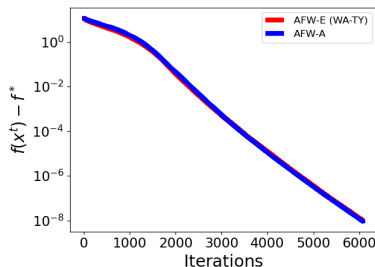
Computational Guarantees

Global linear convergence of $\{G_k\}_{k \geq 0}$:

For some (affine-invariant) $\bar{D} < +\infty$ and all $k \geq 0$, we have

$$G_k \leq \begin{cases} 4(1 - \rho)^{k_{\text{eff}}} \delta_0 \max\{\bar{D}, 1\}, & \text{if } \delta_k > 1 \\ 4\sqrt{1 - \rho}^{k_{\text{eff}}} \sqrt{\delta_0} \max\{\bar{D}, 1\}, & \text{if } \delta_k \leq 1 \end{cases}.$$

Essentially, this means $\{G_k\}_{k \geq 0}$ converges at the linear rate $\sqrt{1 - \rho}$, which is worse than the rate of $\{\delta_k\}_{k \geq 0}$, namely $(1 - \rho)$.



Improved local linear rate

Improved local linear rate

- ▷ Let $\mathcal{X}^* \neq \emptyset$ denote the set of optimal solutions of (P)

Improved local linear rate

- ▷ Let $\mathcal{X}^* \neq \emptyset$ denote the set of optimal solutions of (P)
- ▷ There exists a face of \mathcal{X} , denoted by \mathcal{F} , such that for any $x^* \in \mathcal{X}^*$, if $x \in \mathcal{X}$, then
$$\nabla F(x^*)x - x^* = 0 \iff x \in \mathcal{F}.$$

Improved local linear rate

▷ Let $\mathcal{X}^* \neq \emptyset$ denote the set of optimal solutions of (P)

▷ There exists a face of \mathcal{X} , denoted by \mathcal{F} , such that for any $x^* \in \mathcal{X}^*$, if $x \in \mathcal{X}$, then

$$\nabla F(x^*)x - x^* = 0 \iff x \in \mathcal{F}.$$

▷ Define $\Delta_{\mathcal{F}} := \max_{x^* \in \mathcal{X}^*} \min_{v \in \mathcal{V} \setminus \mathcal{F}} \nabla F(x^*)v - x^* > 0$.

Improved local linear rate

- ▷ Let $\mathcal{X}^* \neq \emptyset$ denote the set of optimal solutions of (P)
- ▷ There exists a face of \mathcal{X} , denoted by \mathcal{F} , such that for any $x^* \in \mathcal{X}^*$, if $x \in \mathcal{X}$, then
$$\nabla F(x^*)x - x^* = 0 \iff x \in \mathcal{F}.$$
- ▷ Define $\Delta_{\mathcal{F}} := \max_{x^* \in \mathcal{X}^*} \min_{v \in \mathcal{V} \setminus \mathcal{F}} \nabla F(x^*)v - x^* > 0$.

Land on \mathcal{F} in finite iterations:

Let $\bar{k} \geq 0$ satisfy that

$$\delta_{\bar{k}} < \min\{V(\Delta_{\mathcal{F}}, R_{\mathcal{Y}}(y^*)), \min_{v \in \mathcal{V} \setminus \mathcal{F}} F(v) - F^*\}.$$

Improved local linear rate

- ▷ Let $\mathcal{X}^* \neq \emptyset$ denote the set of optimal solutions of (P)
- ▷ There exists a face of \mathcal{X} , denoted by \mathcal{F} , such that for any $x^* \in \mathcal{X}^*$, if $x \in \mathcal{X}$, then
$$\nabla F(x^*)x - x^* = 0 \iff x \in \mathcal{F}.$$
- ▷ Define $\Delta_{\mathcal{F}} := \max_{x^* \in \mathcal{X}^*} \min_{v \in \mathcal{V} \setminus \mathcal{F}} \nabla F(x^*)v - x^* > 0$.

Land on \mathcal{F} in finite iterations:

Let $\bar{k} \geq 0$ satisfy that

$$\delta_{\bar{k}} < \min\{V(\Delta_{\mathcal{F}}, R_{\mathcal{Y}}(y^*)), \min_{v \in \mathcal{V} \setminus \mathcal{F}} F(v) - F^*\}.$$

For all $k \geq \bar{k}$, if $x^k \notin \mathcal{F}$, then

- ▷ $\mathcal{S}_{k+1} \subseteq \mathcal{S}_k$, when either exact line-search or adaptive stepsize is used in Step 7,
 - ▷ $\mathcal{S}_{k+1} = \mathcal{S}_k \setminus \{a^k\}$ for some $a^k \in \mathcal{S}_k \cap \bar{\mathcal{V}}_{\mathcal{F}}$, when exact line-search is used in Step 7;
- otherwise, if $x^k \in \mathcal{F}$, then $x^l \in \mathcal{F}$ for all $l \geq k$.

Another Example: Positron Emission Tomography

$$\max_{x \in \Delta_n} \left\{ F(x) := \sum_{j=1}^m p_j \ln(a_j^\top x) \right\} \quad (\text{PET})$$

Another Example: Positron Emission Tomography

$$\max_{x \in \Delta_n} \left\{ F(x) := \sum_{j=1}^m p_j \ln(a_j^\top x) \right\} \quad (\text{PET})$$

- ▷ Known as Positron Emission Tomography (PET) in medical imaging, but has many other applications, e.g., inference of multi-dimensional Hawkes processes [ZZS13] and log-optimal investment [Cov84].

Another Example: Positron Emission Tomography

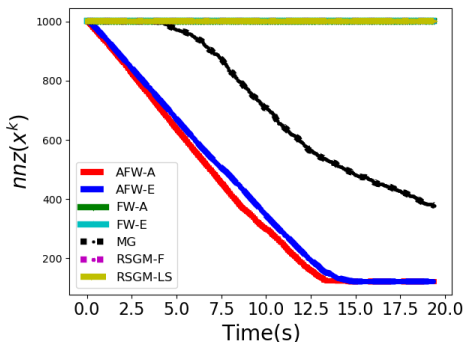
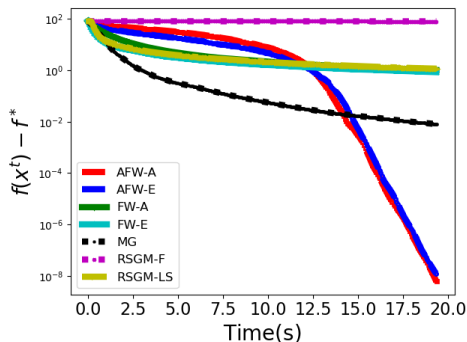
$$\max_{x \in \Delta_n} \left\{ F(x) := \sum_{j=1}^m p_j \ln(a_j^\top x) \right\} \quad (\text{PET})$$

- ▷ Known as Positron Emission Tomography (PET) in medical imaging, but has many other applications, e.g., inference of multi-dimensional Hawkes processes [ZZS13] and log-optimal investment [Cov84].
- ▷ For all $j \in [m]$, let $p_j > 0$, $a_j \in \mathbb{R}_+^n$, $a_j \neq 0$ and $\sum_{j=1}^m p_j = 1$.

Another Example: Positron Emission Tomography

$$\max_{x \in \Delta_n} \left\{ F(x) := \sum_{j=1}^m p_j \ln(a_j^\top x) \right\} \quad (\text{PET})$$

- Known as Positron Emission Tomography (PET) in medical imaging, but has many other applications, e.g., inference of multi-dimensional Hawkes processes [ZZS13] and log-optimal investment [Cov84].
- For all $j \in [m]$, let $p_j > 0$, $a_j \in \mathbb{R}_+^n$, $a_j \neq 0$ and $\sum_{j=1}^m p_j = 1$.



Thank you!

References

- [BBT17] Heinz H. Bauschke, Jérôme Bolte, and Marc Teboulle. “A Descent Lemma Beyond Lipschitz Gradient Continuity: First-Order Methods Revisited and Applications”. In: *Math. Oper. Res.* 42.2 (2017), pp. 330–348.
- [BS17] A. Beck and S. Shtern. “Linearly convergent away-step conditional gradient for non-strongly convex functions”. In: *Math. Program.* 164 (2017), 1–27.
- [Cov84] T. Cover. “An algorithm for maximizing expected log investment return”. In: *IEEE Trans. Inf. Theory* 30.2 (1984), pp. 369–373.
- [Dvu23] P. Dvurechensky et al. “Generalized self-concordant analysis of Frank–Wolfe algorithms”. In: *Math. Program.* 198 (2023), 255–323.
- [Fed72] V. V. Fedorov. *Theory of Optimal Experiments*. Academic Press, 1972.
- [Kha96] Leonid G. Khachiyan. “Rounding of Polytopes in the Real Number Model of Computation”. In: *Math. Oper. Res.* 21.2 (1996), pp. 307–320.
- [LFN18] Haihao. Lu, Robert M. Freund, and Yurii. Nesterov. “Relatively Smooth Convex Optimization by First-Order Methods, and Applications”. In: *SIAM J. Optim.* 28.1 (2018), pp. 333–354.
- [LJJ15] Simon Lacoste-Julien and Martin Jaggi. “On the Global Linear Convergence of Frank-Wolfe Optimization Variants”. In: *Proc. NeurIPS*. Montreal, Canada, 2015, 496–504.
- [PR19] Javier Peña and Daniel Rodríguez. “Polytope Conditioning and Linear Convergence of the Frank–Wolfe Algorithm”. In: *Math. Oper. Res.* 44.1 (2019), pp. 1–18.
- [STT78] S.D. Silvey, D.H. Titterton, and B. Torsney. “An algorithm for optimal designs on a design space”. In: *Commun. Stat. Theory Methods* 7.14 (1978), pp. 1379–1389.

References

- [ZFce] Renbo Zhao and Robert M. Freund. “Analysis of the Frank-Wolfe Method for Convex Composite Optimization involving a Logarithmically-Homogeneous Barrier”. In: *Math. Program.* (accepted, 2022).
- [ZZS13] Ke Zhou, Hongyuan Zha, and Le Song. “Learning Social Infectivity in Sparse Low-rank Networks Using Multi-dimensional Hawkes Processes”. In: *Proc. AISTATS*. 2013, pp. 641–649.