# Using Taylor-Approximated Gradients to Improve the Frank-Wolfe Method for Empirical Risk Minimization

**Zikai Xiong and Robert Freund**

Workshop on Modern Nonsmooth Optimization

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(paper should be available "real soon")

## Happy 60th birthday to Adrian!

We are grateful to Adrian Lewis for advancing optimization, extending its reach to other branches of applied mathematics, and for inspiring us with his intellectual excitement, passion for research and education, and for nurturing a vibrant and collegial community. (Plus he's fun to hang out with.)

# Empirical Risk Minimization

## Empirical risk minimization with "linear prediction"

$$\text{ERM}_\ell: \quad \min_{x \in \mathcal{C} \subset \mathbb{R}^p} \quad F(x) := \frac{1}{n} \sum_{i=1}^{n} \left[ f_i(x) = l_i(w_i^\top x) \right]$$

- $l_i(\cdot)$ is the univariate loss function of observation/sample $i$ for $i \in [n] := \{1, \ldots, n\}$
- "linear prediction" means the model's losses are a function of $\{w_i^\top x\}_i$, as introduced in [1]
- $n$ is the number of observations/samples
- $p$ is the order (dimension) of the model variable $x$ (the number of features)
- $\mathcal{C} \subset \mathbb{R}^p$ is a compact convex set
- Linear Minimization Oracle (LMO) on $\mathcal{C}$ can be efficiently solved
- We are particularly interested in studying this problem when $n \gg 0$ is huge-scale (for instance, $n > p^2$)

# Applications in Machine and Statistical Learning

Applications: support vector machines (SVMs), LASSO, matrix completion, logistic regression, other convex and non-convex models, etc.

- LASSO:

$$\min_{x\in\mathbb{R}^p} \frac{1}{2n}\sum_{i=1}^{n}\left(y_i - w_i^T x\right)^2 \quad \text{s.t. } \|x\|_1 \le \lambda$$

here $l_i(\cdot) := \frac{1}{2}(y_i - \cdot)^2$, and $\mathcal{C} := \{x : \|x\|_1 \le \lambda\}$

- Matrix completion:

$$\min_{X\in\mathbb{R}^{n\times p}} \frac{1}{2|\Omega|}\sum_{(i,j)\in\Omega}(M_{i,j} - X_{i,j})^2 \quad \text{s.t. } \|X\|_* \le \lambda$$

here $l_{(i,j)}(\cdot) := \frac{1}{2}(\cdot - M_{i,j})^2$, and $\mathcal{C} := \{X : \|X\|_* \le \lambda\}$

# Applications, continued

- Sparse logistic regression:

$$\min_{x \in \mathbb{R}} \ \frac{1}{n} \sum_{i=1}^{n} \ln(1 + \exp(-y_i w_i^\top x)) \quad \text{s.t. } \|x\|_1 \leq \lambda$$

here $l_i(\cdot) := \ln(1 + \exp(-y_i \cdot))$, and $\mathcal{C} := \{x : \|x\|_1 \leq \lambda\}$

- Binary classification with sigmoid threshold function $\sigma(\cdot)$:

$$\min_{x} \ \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \sigma(w_i^\top x)\right)^2 \quad \text{s.t. } \|x\|_1 \leq \lambda$$

where $\sigma(v) := \frac{1}{1+\exp(-v)}$

## Classic Gradient Descent for ERM$_\ell$

At iteration $k$ :

1. Compute gradient $g^k := \nabla F(x^k) = \frac{1}{n}\sum_{i=1}^n l_i'(w_i^\top x^k) w_i$
2. $x^{k+1} \leftarrow \arg\min_{x\in\mathcal{C}} \left\|x - (x^k - \gamma_k g^k)\right\|^2$, where $\gamma_t \in (0, +\infty)$

## Classic Frank-Wolfe for ERM$_\ell$

At iteration $k$:

1. Compute gradient $g^k := \nabla F(x^k) = \frac{1}{n}\sum_{i=1}^n l_i'(w_i^\top x^k) w_i$
2. Compute $s^k \leftarrow \text{LMO}(g^k)$, which is $\arg\min_{s\in\mathcal{C}} \langle g^k, s\rangle$
3. Set $x^{k+1} \leftarrow x^k + \gamma_k(s^k - x^k)$, where $\gamma_t \in [0, 1]$

Computing gradients requires at least $\mathcal{O}(np)$ flops, expensive when $n \gg p$

# What can we do when $n$ is huge?

## Naïve stochastic gradient descent (SGD) methods for ERM$_\ell$

At iteration $k$ :

1. Compute gradient estimate $g^k$
   - Sample $i \sim \mathcal{U}([n])$
   - $g^k \leftarrow l_i'(w_i^\top x^k) w_i$
2. $x^{k+1} \leftarrow \arg\min_{x \in \mathcal{C}} \left\| x - (x^k - \gamma_k g^k) \right\|^2$, where $\gamma_t \in (0, +\infty)$

Reasonable convergence under proper assumptions.

## Naïve stochastic Frank-Wolfe methods for ERM$_\ell$

At iteration $k$:

1. Compute gradient estimate $g^k$
   - Sample $i \sim \mathcal{U}([n])$
   - $g^k \leftarrow l_i'(w_i^\top x^k) w_i$
2. Compute $s^k \leftarrow \mathrm{LMO}(g^k)$
3. Set $x^{k+1} \leftarrow x^k + \gamma_k(s^k - x^k)$, where $\gamma_t \in [0, 1]$

Cannot work without increasing batch-size, which is expensive!

# Other stochastic Frank-Wolfe methods

**When loss functions are convex:**

- Baseline (the classic deterministic Frank-Wolfe method [2]): $\mathcal{O}(n/\varepsilon)$
- Lan and Zhou (2016) [3]: $\mathcal{O}(1/\varepsilon^2)$
- Hazan and Luo (2016) [4]: $\mathcal{O}(n\log(1/\varepsilon) + 1/\varepsilon^{3/2})$
- Yurtsever, Sra and Cevher (2019) [5]: $\mathcal{O}(1/\varepsilon^2)$
- Mokhtari, Hassani and Karbasi (2020) [6]: $\mathcal{O}(1/\varepsilon^3)$
- Lu and F (2021) [1]: $\mathcal{O}(n/\varepsilon + n/\sqrt{\varepsilon})$
- Négiar, Dresdner, Tsai, Ghaoui, Locatello, F, and Pedregosa (2020) [7]: $\mathcal{O}(n/\varepsilon + n^{3/2}/\sqrt{\varepsilon})$

**When loss functions are non-convex:**

- Baseline (the deterministic Frank-Wolfe method [8]): $\mathcal{O}(n/\varepsilon^2)$
- Reddi, Sra, Póczos and Smola (2016) [9]: $\mathcal{O}(n + n^{2/3}/\varepsilon^2)$
- Yurtsever, Sra and Cevher (2019) [5]: $\mathcal{O}(n^{1/2}/\varepsilon^2)$
- Shen, Fang, Zhao, Huang and Qian (2019) [10]: $\mathcal{O}(n^{3/4}p/\varepsilon^{3/2} + p/\varepsilon^2)$
- Zhang, Shen, Mokhtari, Hassani and Karbasi (2020) [11]: $\mathcal{O}(p/\varepsilon^3)$
- Hassani, Karbasi, Mokhtari and Shen (2020) [12]: $\mathcal{O}(p/\varepsilon^3)$

(We omit a factor of $p$ for each method's complexity)

# SGD vs. Stochastic Frank-Wolfe

| | SGD | Stochastic FW |
|---|---|---|
| 1) | Many results on reducing the dependence on $n$ while maintaining reasonable dependence on $1/\varepsilon$ | Linear dependence on $n$ in order to maintain good dependence on $1/\varepsilon$ |
| 2) | Requires projections, which can be expensive | Replaces projections by linear minimization oracle (LMO), which is cheaper for many applications |
| 3) | Does not promote structured solutions (sparsity, low-rank) | Promotes structured solutions |

This begs the following question:

Are there efficient stochastic (or deterministic) Frank-Wolfe methods that reduce or eliminate the dependence on the number of observations $n$, in theory and in practice?

# Sneak preview of answer: "Yes: we can *reduce* the dependence on $n$"

**Theoretical Results**

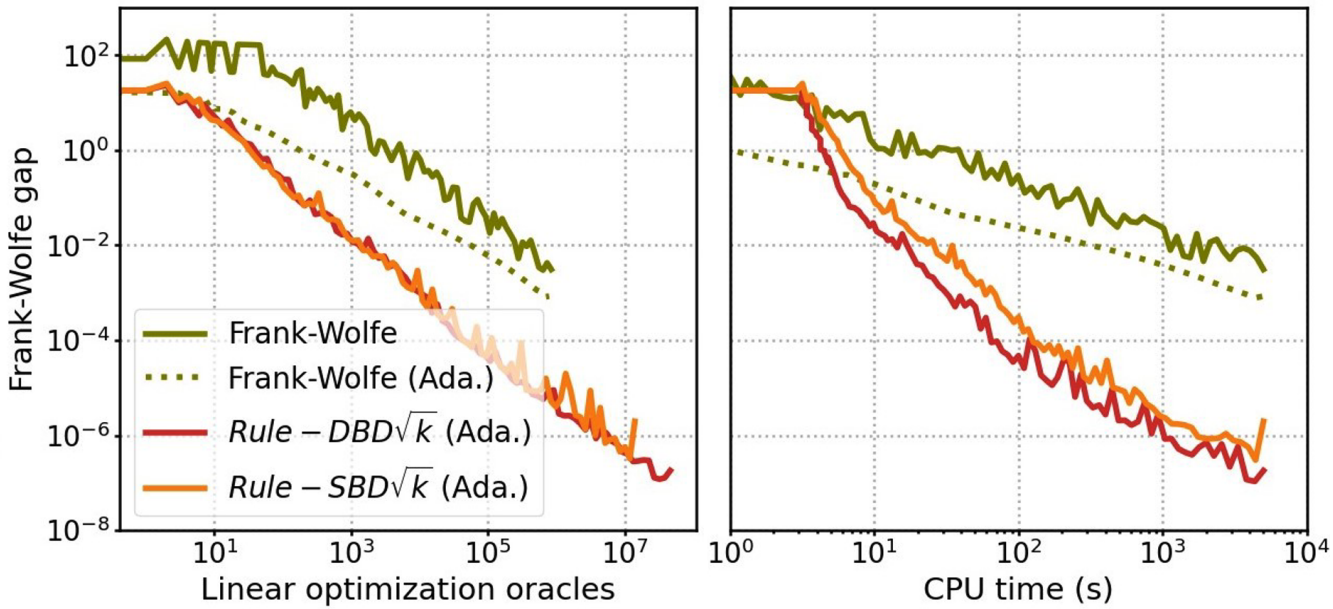
We develop stochastic and deterministic Frank-Wolfe methods, both of which reduce the dependence on $n$

- for convex problems: $\mathcal{O}(n/\varepsilon) \to \mathcal{O}(p/\varepsilon + np/\sqrt{\varepsilon})$
- for non-convex problems: $\mathcal{O}(n/\varepsilon^2) \to \mathcal{O}(p/\varepsilon^2 + np/\varepsilon^{3/2})$

Improvement in the regime of $n \gg p$

**Practical Performance**

All of our FW variants largely outperform the classic Frank-Wolfe method. Results for solving sparse logistic regression on the dataset a9a ($n = 32561,\ p = 123$)



# Smoothness Assumption

## Empirical risk minimization with linear prediction

$$\text{ERM}_\ell: \quad \min_{x \in \mathcal{C} \subset \mathbb{R}^p} \quad F(x) := \frac{1}{n} \sum_{i=1}^{n} \left[ f_i(x) = l_i(w_i^\top x) \right]$$

## Assumption 1

1. $\mathcal{C}$ is compact and convex
2. Linear Minimization Oracle (LMO) on $\mathcal{C}$ can be efficiently solved
3. for any $i$, $l_i(\cdot)$ is twice-differentiable and $l_i'(\cdot)$ is $L$-Lipschitz continuous on the range of $w_i^\top x$ over $x \in \mathcal{C}$, namely

$$|l_i'(\bar{\theta}) - l_i'(\hat{\theta})| \leq L|\bar{\theta} - \hat{\theta}| \quad \text{for any } \bar{\theta}, \hat{\theta} \in w_i(\mathcal{C}), \text{ and}$$

4. for any $i$, $l_i''(\cdot)$ is $\hat{L}$-Lipschitz continuous on the range of $w_i^\top x$ over $x \in \mathcal{C}$, namely

$$|l_i''(\bar{\theta}) - l_i''(\hat{\theta})| \leq \hat{L}|\bar{\theta} - \hat{\theta}| \quad \text{for any } \bar{\theta}, \hat{\theta} \in w_i(\mathcal{C})$$

# Standard smooth loss functions satisfy second-order smoothness

- For LASSO, matrix completion, structured sparse matrix estimation with CUR factorization, and other problems with quadratic losses
  - $L = 1$ and $\hat{L} = 0$
  - see [13, 1] for other models with quadratic losses
- For logistic regression for binary classification

$$\min_{x \in \mathcal{C}} \; F(x) := \frac{1}{n} \sum_{i=1}^{n} \ln(1 + \exp(-y_i w_i^\top x))$$

  - $L \leq 1/4$ and $\hat{L} \leq 1/6\sqrt{3}$
- For binary linear classification with non-convex losses

$$\min_{x \in \mathcal{C}} \; \frac{1}{n} \sum_{i=1}^{n} (y_i - \sigma(w_i^\top x))^2 \;, \text{ such as } \sigma(\cdot) = \frac{1}{1 + \exp(\cdot)}$$

  - For the case when $\sigma$ is the sigmoid function, we have $L \leq .32$ and $\hat{L} \leq .23$
  - More generally let $L_\sigma$ be an upper bound on $|\sigma|$, $|\sigma'|$, and $|\sigma''|$
  - Then $L \leq 2L_\sigma^2 + 2L_\sigma$ and $\hat{L} \leq 6L_\sigma^2 + 2L_\sigma$
  - see [14]

# Taylor-approximated gradients

Classic approach to compute $\nabla F(x^k)$:

1. compute $l_i'(w_i^\top x^k)$ for each $i \in [n]$
2. then $\nabla F(x^k) := \frac{1}{n} \sum_{i=1}^n l_i'(w_i^\top x^k) w_i$

Taylor-approximated gradient estimate $g^k$ of $\nabla F(x^k)$:

1. We have
$$l_i'(w_i^\top x^k) \approx l_i'(w_i^\top b_i) + l_i''(w_i^\top b_i)(w_i^\top x^k - w_i^\top b_i)$$
where $b_i \in \mathcal{C}$ is the "Taylor-point" for the Taylor approximation of $l_i'$
2. Then for each $i \in [n]$ define
$$g_i^k := \left( l_i'(w_i^\top b_i) + l_i''(w_i^\top b_i)(w_i^\top x^k - w_i^\top b_i) \right) w_i$$
and
$$g^k := \frac{1}{n} \sum_{i=1}^n g_i^k$$

# Taylor-point Updating Frank-Wolfe (TUFW)

## Classic Frank-Wolfe method for ERM$_\ell$

At iteration $k$:

1. Compute gradient $g^k := \nabla F(x^k) = \frac{1}{n}\sum_{i=1}^n l_i'(w_i^\top x^k) w_i$
2. Compute $s^k \leftarrow \text{LMO}(g^k)$, which is $\arg\min_{s\in\mathcal{C}} \langle g^k, s\rangle$
3. Set $x^{k+1} \leftarrow x^k + \gamma_k(s^k - x^k)$, where $\gamma_t \in [0,1]$

## Taylor-point Updating Frank-Wolfe (TUFW) for ERM$_\ell$

Initialize Taylor points: $b_i \leftarrow x^0$ for $i \in \{1,\dots,n\}$. Then at iteration $k$:

1. Compute Taylor-approximated gradient estimator $g^k$
   - Update some of the Taylor points:
     use some **Rule** to create a set $\mathcal{B}_k \subset \{1,\dots,n\}$,
     then update $b_i \leftarrow x^k$ for $i \in \mathcal{B}_k$
   - Compute estimates of individual gradients and sum:

$$g^k := \frac{1}{n}\sum_{i=1}^n \left[ g_i^k := \left( l_i'(w_i^\top b_i) + l_i''(w_i^\top b_i)(w_i^\top x^k - w_i^\top b_i) \right) w_i \right]$$

2. Compute $s^k \leftarrow \text{LMO}(g^k)$, which is $\arg\min_{s\in\mathcal{C}} \langle g^k, s\rangle$
3. Set $x^{k+1} \leftarrow x^k + \gamma_k(s^k - x^k)$, where $\gamma_t \in [0,1]$

# Taylor-point Updating Frank-Wolfe (TUFW), continued

## Taylor-point Updating Frank-Wolfe (TUFW) for ERM$_\ell$

Initialize Taylor points: $b_i \leftarrow x^0$ for $i \in \{1, \ldots, n\}$. Then at iteration $k$:

1. Compute Taylor-approximated gradient estimator $g^k$
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     then update $b_i \leftarrow x^k$ for $i \in \mathcal{B}_k$
   - Compute estimates of individual gradients and sum:

$$g^k := \frac{1}{n} \sum_{i=1}^{n} \left[ g_i^k := \left( l_i'(w_i^\top b_i) + l_i''(w_i^\top b_i)(w_i^\top x^k - w_i^\top b_i) \right) w_i \right]$$

2. Compute $s^k \leftarrow \mathrm{LMO}(g^k)$, which is $\arg\min_{s \in \mathcal{C}} \langle g^k, s \rangle$
3. Set $x^{k+1} \leftarrow x^k + \gamma_k(s^k - x^k)$, where $\gamma_t \in [0, 1]$

Many types of **Rules** are possible:

- $\mathcal{B}_k = [n]$ for all $k$ (this corresponds to classic Frank-Wolfe)
- $\mathcal{B}_k$ chosen by random sampling with size $|\mathcal{B}_k| = \bar{\beta}_k$ for some sequence $\{\bar{\beta}_k\}_k$
- $\mathcal{B}_k$ chosen in cyclic fashion with fixed batch-size $B = 50$
- $\mathcal{B}_k = [n]$ for $k = 0$, and $\mathcal{B}_k = \emptyset$ for $k > 0$
- ...

# Efficient computation of gradient estimate $g_k$

The gradient estimator in TUFW can be written as $g^k = q_k + H_k x^k$ where

$$q_k := \frac{1}{n}\sum_{i=1}^{n} l_i'(w_i^\top b_i)w_i - l_i''(w_i^\top b_i)w_i w_i^\top b_i$$

$$H_k := \frac{1}{n}\sum_{j=1}^{n} l_i''(w_i^\top b_i)w_i w_i^\top .$$

By incrementally updating $q_k$ and $H_k$ instead of summing all $n$ components every time, the computation of $g^k$ only requires

$$\mathcal{O}(p^2(|\mathcal{B}_k|+1)) \text{ flops}$$

and the memory needed is

$$\mathcal{O}(n+p^2)$$

# We develop and analyze five Taylor-point Updating **Rules**

**Stochastic Batch-size Decreasing ("SBD")**

*Rule*$-SBD\sqrt{k}$:

$\mathcal{B}_k$ is comprised of $\beta_k$ samples from $\mathcal{U}(\{1,\ldots,n\})$, where $\beta_k := n/\sqrt{k}$

*Rule*$-SBD\sqrt[4]{K}$:

Similar to above, with $\beta_k := n/\sqrt[4]{K}$ for fixed total iteration count $K$

**Deterministic Batch-frequency Decreasing ("DBD")**

*Rule*$-DBD\sqrt{k}$: $\mathcal{B}_k = \begin{cases} [n] & \text{if } \sqrt{k} \in \mathbb{N} \\ \emptyset & \text{if } \sqrt{k} \notin \mathbb{N} \end{cases}$

*Rule*$-DBD\sqrt[4]{K}$: $\mathcal{B}_k = \begin{cases} [n] & \text{if } k/\lfloor\sqrt[4]{K}\rfloor \in \mathbb{N} \\ \emptyset & \text{if } k/\lfloor\sqrt[4]{K}\rfloor \notin \mathbb{N} \end{cases}$

**No updating** (relevant when losses are quadratic, namely $\hat{L} = 0$)

*Rule*$-\emptyset$: $\mathcal{B}_k = \begin{cases} [n] & \text{if } k = 0 \\ \emptyset & \text{if } k \neq 0 \end{cases}$

...

# $\text{ERM}_\ell$ and diameter measures of $\mathcal{C}$

## Empirical risk minimization with linear prediction

$$\text{ERM}_\ell: \quad \min_{x \in \mathcal{C} \subset \mathbb{R}^p} \quad F(x) := \frac{1}{n} \sum_{i=1}^{n} \left[ f_i(x) = l_i(w_i^\top x) \right]$$

- Diameter of $\mathcal{C}$:

$$D := \max_{x,y \in \mathcal{C}} \|x - y\| < \infty$$

- "$q$-Diameter" of $\mathcal{C}$:

$$D_q := \max_{x,y \in \mathcal{C}} \left\| W^\top (x - y) \right\|_q < \infty \text{ for } q \in [1, \infty]$$

  where $W := (w_1, \ldots, w_n) \in \mathbb{R}^{p \times n}$. The $q$-diameter is a common metric used in $\text{ERM}_\ell$, see [1, 7]

- Under the boundedness assumption of feature vectors (there exists $M < \infty$, such that $\|w_i\|_* \leq M$ for any $i$), then

$$D_q \leq n^{1/q} M D$$

  In the worst case, there is an opaque $n^{1/q}$ embedded in the $q$-diameter $D_q$

# Computational Guarantees for Convex Losses

Classic Frank-Wolfe complexity to compute an $\varepsilon$-optimal solution, namely $F(x^k) - F(x^\star) \leq \varepsilon$:

$$\mathcal{O}\left((\mathrm{fLMO} + np)\left[\frac{LM^2D^2}{\varepsilon}\right]\right)$$

Here $\mathrm{fLMO}$ denotes the complexity of an LMO call.

# Computational Guarantees for Convex Losses

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$$\mathcal{O}\left((\mathrm{fLMO} + np)\left[\frac{LM^2D^2}{\varepsilon}\right]\right)$$

Here $\mathrm{fLMO}$ denotes the complexity of an LMO call.

**Theorem** (*Rule*$-SBD\sqrt{k}$)

*Suppose that $F$ is convex and Assumption 1 holds, and TUFW with Rule$-SBD\sqrt{k}$ is applied to ERM$_\ell$ with step-sizes $\gamma_k := 2/(k+2)$. Then:*

$$\mathbb{E}[F(x^k) - F(x^\star)] \leq \frac{2LD_2^2 + 134\hat{L}D_1D_\infty^2}{n(k+1)}$$

Complexity of obtaining $\mathbb{E}[F(x^k) - F(x^\star)] \leq \varepsilon$ is

$$O\left((\mathrm{fLMO} + p^2)\left[\frac{LM^2D^2 + \hat{L}M^3D^3}{\varepsilon}\right] + np^2\left[\frac{\sqrt{LM^2D^2 + \hat{L}M^3D^3}}{\sqrt{\varepsilon}}\right]\right)$$

# Comparison of computational guarantees for convex losses

| Method | Overall Complexity |
|---|---|
| Frank-Wolfe | $\mathcal{O}\left((\mathrm{fLMO} + np) \cdot \frac{c_1}{\varepsilon}\right)$ |
| Négiar et al. [7] | $\mathcal{O}\left((n \cdot \mathrm{fLMO} + np)\left[\frac{c_1}{\varepsilon} + \frac{\sqrt{F(x^0) - F(x^\star)}}{n\sqrt{\varepsilon}} + \frac{\sqrt{nc_1}}{\sqrt{\varepsilon}}\right]\right)$ |
| *Rule−SBD*$\sqrt{k}$ | $\mathcal{O}\left((\mathrm{fLMO} + p^2) \cdot \frac{c_1+c_2}{\varepsilon} + np^2 \cdot \frac{\sqrt{c_1+c_2}}{\sqrt{\varepsilon}}\right)$ |
| *Rule−DBD*$\sqrt{k}$ | $\mathcal{O}\left((\mathrm{fLMO} + p^2) \cdot \frac{c_1+c_2}{\varepsilon} + np^2 \cdot \frac{\sqrt{c_1+c_2}}{\sqrt{\varepsilon}}\right)$ |

- Here $\mathrm{fLMO}$ denotes the cost of the LMO
- $c_1 := LM^2D^2$ and $c_2 := \hat{L}M^3D^3$

# A practical enhancement: adaptive step-sizes

Let $x^{k+1}(\gamma) := x^k + \gamma(s^k - x^k)$, then

$$F(x^{k+1}(\gamma)) = F(x^k) + \gamma(g^k)^\top(s^k - x^k) + \frac{\gamma^2}{2}(s^k - x^k)^\top H_k(s^k - x^k) + \frac{1}{n}\sum_{i=1}^n \int_{t=0}^{\gamma} \Big(\nabla f_i(x^k + t(s^k - x^k)) - \nabla f_i(b_i) - \nabla^2 f_i(b_i)\big(x^k + t(s^k - x^k) - b_i\big)\Big)^\top (s^k - x^k)dt$$

Then $\arg\min_{\gamma\in[0,\gamma_k]} F(x^{k+1}(\gamma))$ is approximated by the following $\tilde{\gamma}_k$:

## Adaptive step-sizes

Let $\gamma_k$ be the traditional step-size ($= \frac{2}{k+2}$). The adaptive step-size defined by

$$\arg\min_{\gamma\in[0,\gamma_k]} F(x^k) + \gamma(g^k)^\top(s^k - x^k) + \frac{\gamma^2}{2}(s^k - x^k)^\top H_k(s^k - x^k)$$

has the closed-form solution:

$$\tilde{\gamma}_k := \begin{cases} \min\left\{\gamma_k, \frac{(g^k)^\top(x^k - s^k)}{(s^k - x^k)^\top H_k(s^k - x^k)}\right\} & \text{when } (s^k - x^k)^\top H_k(s^k - x^k) > 0 \\ \gamma_k & \text{when } (s^k - x^k)^\top H_k(s^k - x^k) \le 0 \end{cases}$$

(Can show that using $\tilde{\gamma}_k$ maintains the same computational guarantees.)

# Computational Experiments on Sparse Logistic Regression Problems

# Experiments on Sparse Logistic Regression Problems

Sparse logistic regression problem:

$$\min_x \; F(x) := \frac{1}{n} \sum_{i=1}^{n} \ln(1 + \exp(-y_i w_i^\top x)) \quad \text{s.t.} \; \|x\|_1 \leq \lambda$$

- We chose 12 large-scale instances (with $n \gg p$) from SVMLIB
- $\lambda$ was chosen by cross-validation (and we also tested $\lambda' := 100\lambda$)
- We tested TUFW with standard step-size $\gamma_k$ and adaptive step-size $\tilde{\gamma}_k$
- We compared our methods with classic Frank-Wolfe (with and without adaptive step-sizes), and two other methods
- For fairness, all methods were implemented without sparse linear algebra
- Implemented in Python, on the MIT Engaging Cluster
- We used the Frank-Wolfe gap $\mathcal{G}(x)$ to (conservatively) bound optimality gaps

# The Frank-Wolfe gap $\mathcal{G}(x)$

## Frank-Wolfe gap

For $x \in \mathcal{C}$, the Frank-Wolfe gap is defined to be:

$$\mathcal{G}(x) := \max_{s \in \mathcal{C}} \langle x - s, \nabla F(x) \rangle$$

- When $F$ is convex, $\mathcal{G}(x)$ is an upper bound on the optimality gap:

$$F(x) - F(x^\star) \leq \mathcal{G}(x)$$

- $\mathcal{G}(x^k)$ is computable (unlike the actual optimality gap $F(x^k) - F(x^\star)$ )

- For non-convex $F$, $\mathcal{G}(x)$ is a measure of stationarity of $x$

# Typical improvement compared to classic Frank-Wolfe

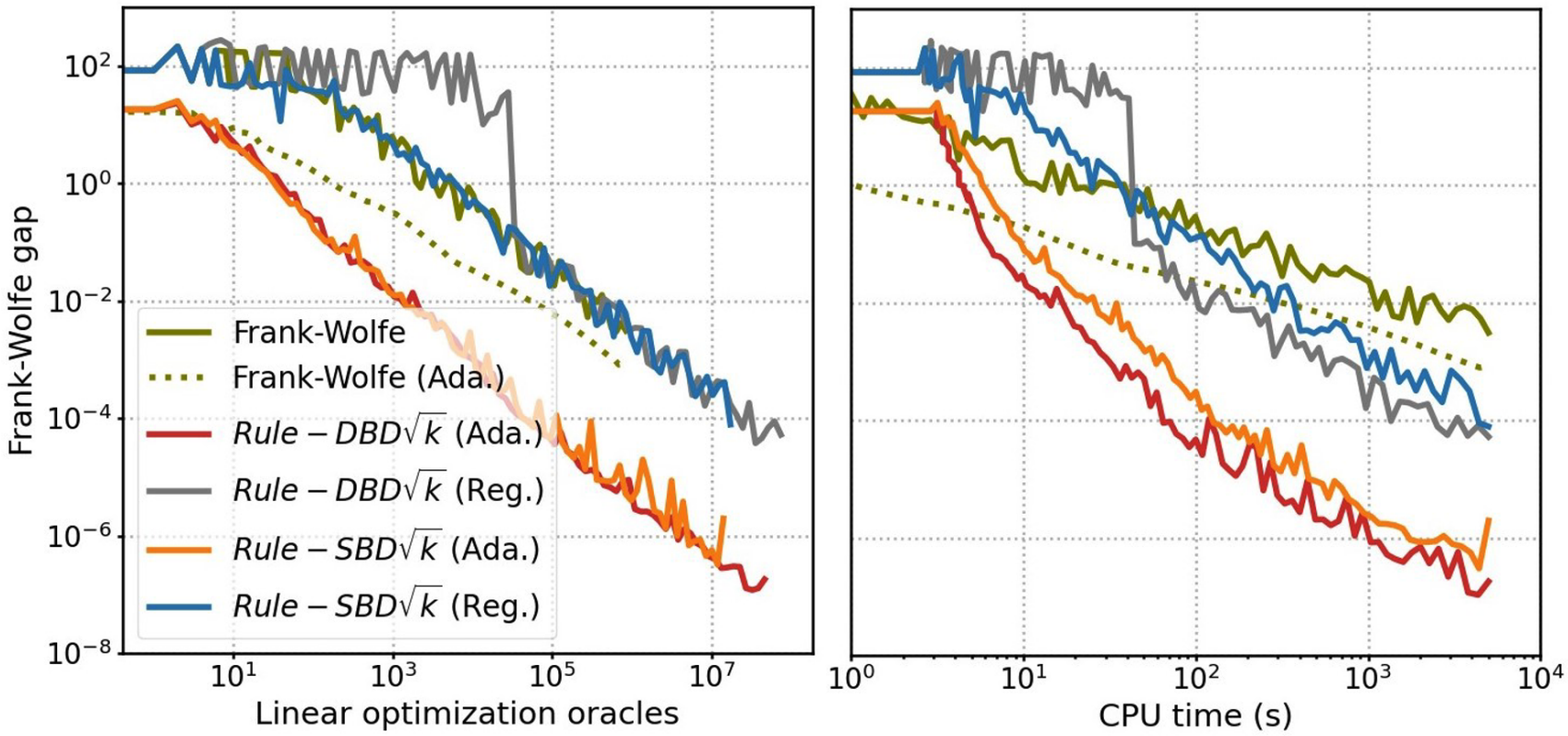


Figure 1: Sparse logistic regression on dataset a9a ($n = 32561,\ p = 123$)

- ▷ TUFW methods significantly outperform classic Frank-Wolfe on most problem instances
- ▷ TUFW LMO complexity outperforms classic Frank-Wolfe in practice (but not in theory)

# Comparison of TUFW with other Frank-Wolfe methods

We compared TUFW (under different Rules) with the following methods:

- (FW): classic Frank-Wolfe
- (FW-ada): classic Frank-Wolfe with adaptive step-sizes $\tilde{\gamma}_k := \min\{1, \mathcal{G}(x^k)/L\|x^k - s^k\|^2\}$
- (SPIDER-FW): Frank-Wolfe with stochastic path-integrated differential estimator technique (Yurtsever, Sra, Cevher [5])
- (CSFW): constant batch-size stochastic Frank-Wolfe (Négiar, Dresdner, Tsai, El-Ghaoui, Locatello, F, Pedregosa [7])

# Runtime comparison of TUFW with other Frank-Wolfe methods ($\lambda$ set by CV)

Runtime required to achieve $\mathcal{G}(x^k) \leq \varepsilon$ (blank indicates $>$ 5000 seconds)

| $\varepsilon$ | dataset | $n$ | $p$ | *Rule−SBD*$\sqrt{k}$ | *Rule−DBD*$\sqrt{k}$ | FW | FW-ada | SPIDER-FW | CSFW | Speed-up |
|---|---|---|---|---|---|---|---|---|---|---|
| 1e-1 | a1a | 1605 | 123 | 0.73 | **0.37** | 2.02 | 1.18 | 348.58 | 5.03 | **3.20** |
| 1e-3 | a1a | 1605 | 123 | 14.40 | **5.14** | 138.87 | 380.10 | | 160.02 | **27.02** |
| 1e-5 | a1a | 1605 | 123 | 3029.61 | **1034.66** | 2956.50 | | | | **2.86** |
| 1e-1 | a2a | 2265 | 123 | 1.02 | **0.52** | 3.03 | 1.55 | 358.72 | 5.47 | **2.97** |
| 1e-3 | a2a | 2265 | 123 | 21.24 | **8.16** | 197.80 | 472.72 | | 167.66 | **20.54** |
| 1e-5 | a2a | 2265 | 123 | 2039.75 | **631.23** | | | | | |
| 1e-1 | a8a | 22696 | 123 | 7.75 | **4.66** | 78.18 | 12.83 | 443.85 | 15.22 | **2.75** |
| 1e-3 | a8a | 22696 | 123 | 51.29 | **23.71** | | 3178.02 | | 1250.12 | **52.72** |
| 1e-5 | a8a | 22696 | 123 | 420.64 | **174.87** | | | | | |
| 1e-1 | a9a | 32561 | 123 | 11.26 | **6.80** | 94.50 | 21.00 | 440.73 | 19.82 | **2.91** |
| 1e-3 | a9a | 32561 | 123 | 65.25 | **31.22** | | 3844.13 | | 1660.13 | **53.17** |
| 1e-5 | a9a | 32561 | 123 | 490.36 | **197.15** | | | | | |
| 1e-1 | w1a | 2477 | 300 | 10.45 | **5.71** | 17.51 | 331.22 | 3566.83 | 44.39 | **3.07** |
| 1e-3 | w1a | 2477 | 300 | 51.51 | **21.93** | 327.38 | | | 1219.03 | **14.93** |
| 1e-5 | w1a | 2477 | 300 | 1743.08 | **541.71** | | | | | |
| 1e-1 | w2a | 3470 | 300 | 13.11 | **6.80** | 37.34 | 574.42 | | 54.06 | **5.50** |
| 1e-3 | w2a | 3470 | 300 | 128.14 | **50.77** | 369.82 | | | 1207.01 | **7.28** |
| 1e-5 | w2a | 3470 | 300 | | **1422.93** | | | | | |
| 1e-1 | w7a | 24692 | 300 | 88.86 | **55.43** | 541.10 | | | 129.19 | **2.33** |
| 1e-3 | w7a | 24692 | 300 | 320.17 | **178.87** | | | | 4413.77 | **24.68** |
| 1e-5 | w7a | 24692 | 300 | 3106.98 | **1516.83** | | | | | |
| 1e-1 | w8a | 49749 | 300 | 174.89 | **114.66** | 1198.35 | | | 212.80 | **1.86** |
| 1e-3 | w8a | 49749 | 300 | 553.94 | **355.23** | | | | | |
| 1e-5 | w8a | 49749 | 300 | | **2707.92** | | | | | |
| 1e-1 | svmguide3 | 1243 | 22 | 0.09 | **0.02** | 1.35 | 0.31 | 21.46 | 2.06 | **13.43** |
| 1e-3 | svmguide3 | 1243 | 22 | 8.01 | **2.64** | 53.64 | 175.49 | | 48.85 | **18.53** |
| 1e-5 | svmguide3 | 1243 | 22 | 1132.50 | **410.63** | 629.39 | | | 1484.23 | **1.53** |
| 1e-7 | svmguide3 | 1243 | 22 | | | | | | | |
| 1e-1 | phishing | 11055 | 68 | 0.47 | 0.38 | 0.01 | 0.71 | 0.01 | **0.01** | 0.02 |
| 1e-3 | phishing | 11055 | 68 | 2.81 | 1.24 | 0.67 | 201.65 | **0.32** | 0.53 | 0.26 |
| 1e-5 | phishing | 11055 | 68 | 45.36 | **16.10** | 47.01 | | 1391.81 | 43.70 | **2.71** |
| 1e-7 | phishing | 11055 | 68 | 2478.92 | **812.38** | 3370.12 | | | | **4.15** |
| 1e-1 | ijcnn1 | 49990 | 22 | 0.85 | 0.24 | 1.21 | 9.02 | **0.22** | 0.92 | 0.91 |
| 1e-3 | ijcnn1 | 49990 | 22 | 4.15 | **0.86** | 54.72 | 565.14 | 193.34 | 71.65 | **63.40** |
| 1e-5 | ijcnn1 | 49990 | 22 | 7.67 | **1.66** | | 2322.76 | | | **1402.31** |
| 1e-7 | ijcnn1 | 49990 | 22 | 10.20 | **2.32** | | 3910.71 | | | **1688.65** |
| 1e-1 | covtype | 581012 | 54 | 54.62 | 29.76 | 143.55 | 123.79 | **5.47** | 18.91 | 0.18 |
| 1e-3 | covtype | 581012 | 54 | 552.47 | **231.70** | 2964.49 | | 843.60 | 690.78 | **2.98** |
| 1e-5 | covtype | 581012 | 54 | | **3777.45** | | | | | |

# Runtime comparison of TUFW on larger feasibility regions ($\lambda' = 100\lambda$)

Runtime required to achieve $\mathcal{G}(x^k) \leq \varepsilon$ (blank indicates $>$ 5000 seconds)

| $\varepsilon$ | dataset | $n$ | $p$ | *Rule−SBD*$\sqrt{k}$ | *Rule−DBD*$\sqrt{k}$ | FW | FW-ada | SPIDER-FW | CSFW | Speed-up |
|---|---|---|---|---|---|---|---|---|---|---|
| 1e0 | a1a | 1605 | 123 | 1.08 | **0.56** | 3322.66 | 21.88 | | | **39.14** |
| 1e-2 | a1a | 1605 | 123 | 61.47 | **22.15** | | 2671.01 | | | **120.59** |
| 1e-4 | a1a | 1605 | 123 | 4561.28 | **1683.57** | | | | | |
| 1e0 | a2a | 2265 | 123 | **2.40** | 4.30 | 3858.43 | 32.69 | | | **13.64** |
| 1e-2 | a2a | 2265 | 123 | 6.70 | **5.68** | | 1959.43 | | | **345.13** |
| 1e-4 | a2a | 2265 | 123 | 28.72 | **13.29** | | | | | |
| 1e0 | a8a | 22696 | 123 | 15.35 | **8.50** | | 268.54 | | | **31.59** |
| 1e-2 | a8a | 22696 | 123 | 34.86 | **17.75** | | | | | |
| 1e-4 | a8a | 22696 | 123 | 60.72 | **30.10** | | | | | |
| 1e0 | a9a | 32561 | 123 | 20.80 | **10.97** | | 326.83 | | | **29.79** |
| 1e-2 | a9a | 32561 | 123 | 52.70 | **24.35** | | | | | |
| 1e-4 | a9a | 32561 | 123 | 97.60 | **45.91** | | | | | |
| 1e0 | w1a | 2477 | 300 | 16.17 | **8.94** | | 4569.30 | | | **511.10** |
| 1e-2 | w1a | 2477 | 300 | 75.05 | **34.01** | | | | | |
| 1e-4 | w1a | 2477 | 300 | 1687.82 | **560.34** | | | | | |
| 1e0 | w2a | 3470 | 300 | 34.13 | **18.39** | | | | | |
| 1e-2 | w2a | 3470 | 300 | 138.82 | **65.27** | | | | | |
| 1e-4 | w2a | 3470 | 300 | 2311.84 | **778.48** | | | | | |
| 1e0 | w7a | 24692 | 300 | 147.81 | **123.91** | | | | | |
| 1e-2 | w7a | 24692 | 300 | 443.15 | **339.27** | | | | | |
| 1e-4 | w7a | 24692 | 300 | 3434.91 | **1740.40** | | | | | |
| 1e0 | w8a | 49749 | 300 | 522.63 | **165.85** | | | | | |
| 1e-2 | w8a | 49749 | 300 | 1053.55 | **515.06** | | | | | |
| 1e-4 | w8a | 49749 | 300 | | **4608.20** | | | | | |
| 1e-1 | svmguide3 | 1243 | 22 | 3.58 | **1.17** | | 127.60 | | | **109.24** |
| 1e-3 | svmguide3 | 1243 | 22 | 11.28 | **3.67** | | 485.90 | | | **132.22** |
| 1e-5 | svmguide3 | 1243 | 22 | 18.83 | **6.08** | | 844.46 | | | **138.80** |
| 1e-7 | svmguide3 | 1243 | 22 | 26.37 | **8.54** | | 1201.28 | | | **140.65** |
| 1e-1 | phishing | 11055 | 68 | 2.26 | **1.20** | 66.23 | 254.91 | 3563.61 | 64.96 | **53.93** |
| 1e-3 | phishing | 11055 | 68 | 5.15 | **2.45** | 3958.88 | 4057.22 | | | **1613.39** |
| 1e-5 | phishing | 11055 | 68 | 19.12 | **8.35** | | | | | |
| 1e-7 | phishing | 11055 | 68 | 592.44 | **207.94** | | | | | |
| 1e-1 | ijcnn1 | 49990 | 22 | 1.52 | **0.47** | | 100.76 | | | **213.41** |
| 1e-3 | ijcnn1 | 49990 | 22 | 2.32 | **0.64** | | 243.63 | | | **378.96** |
| 1e-5 | ijcnn1 | 49990 | 22 | 2.92 | **0.80** | | 425.17 | | | **531.71** |
| 1e-7 | ijcnn1 | 49990 | 22 | 3.45 | **0.92** | | 607.30 | | | **660.82** |
| 1e-1 | covtype | 581012 | 54 | 250.33 | **115.22** | | | | | |
| 1e-3 | covtype | 581012 | 54 | 1163.77 | **484.39** | | | | | |
| 1e-5 | covtype | 581012 | 54 | 2230.09 | **890.50** | | | | | |

# Comments on the experiments

- TUFW methods significantly outperform the other methods on these datasets
- As $1/\varepsilon$ increases, the advantage of TUFW methods grows
- The advantage of TUFW methods over other methods is greater for the larger feasible regions. (Curiously, this is not indicated by the theory.)

# $\text{ERM}_\ell$ with Non-convex Losses

## Empirical risk minimization with linear prediction

$$\text{ERM}_\ell: \quad \min_{x \in \mathcal{C} \subset \mathbb{R}^p} \quad F(x) := \frac{1}{n} \sum_{i=1}^{n} \left[ f_i(x) = l_i(w_i^\top x) \right]$$

For example, consider binary classification with sigmoid threshold function $\sigma(\cdot)$:

$$\min_x \ \frac{1}{n} \sum_{i=1}^{n} \left( y_i - \sigma(w_i^\top x) \right)^2 \quad \text{s.t. } \|x\|_1 \leq \lambda$$

where $\sigma(v) := \frac{1}{1+\exp(-v)}$ .

We will use the Frank-Wolfe gap $\mathcal{G}(x)$ to measure closeness to stationarity:

## Frank-Wolfe gap

For $x \in \mathcal{C}$ :

$$\mathcal{G}(x) := \max_{s \in \mathcal{C}} \langle x - s, \nabla F(x) \rangle$$

# Computational Guarantees for Non-convex Losses

Classic Frank-Wolfe complexity to compute an $\varepsilon$-stationarity point, namely $\mathbb{E}_{\hat{k}\sim U[K]}[\mathcal{G}(x^{\hat{k}})] \leq \varepsilon$ :

$$\mathcal{O}\left((\mathrm{fLMO} + np)\left[\frac{(F(x^0) - F(x^*)) + LM^2D^2}{\varepsilon^2}\right]\right)$$

Here $\mathrm{fLMO}$ denotes the complexity of an LMO call.

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Here $\mathrm{fLMO}$ denotes the complexity of an LMO call.

## Theorem (*Rule−SBD* $\sqrt[4]{K}$)

*Suppose Assumption 1 holds, and TUFW with Rule−SBD* $\sqrt[4]{K}$ *is applied to ERM*$_\ell$ *with step-sizes* $\gamma_k := 1/\sqrt{K+1}$, *where* $K$ *is the fixed number of overall iterations. Then:*

$$\sum_{k=0}^{K} \frac{\mathbb{E}\mathcal{G}(x^k)}{K+1} \leq \frac{\varepsilon_0}{\sqrt{K+1}} + \frac{3\hat{L}D_1D_\infty^2 + LD_2^2}{2n\sqrt{K+1}}$$

Complexity of obtaining $\mathbb{E}_{\hat{k}\sim U[K]}\mathbb{E}[\mathcal{G}(x^{\hat{k}})] \leq \varepsilon$ is

$$\mathcal{O}\left((\mathrm{fLMO} + p^2)\left[\frac{((F(x^0) - F(x^*)) + LM^2D^2 + \hat{L}M^3D^3)^2}{\varepsilon^2}\right]\right.$$
$$\left. + np^2\left[\frac{((F(x^0) - F(x^*)) + LM^2D^2 + \hat{L}M^3D^3)^{3/2}}{\varepsilon^{3/2}}\right]\right)$$

# Comparison of computational guarantees for non-convex losses

| Method | Overall Complexity |
|---|---|
| Frank-Wolfe | $O\left((\mathrm{fLMO} + np) \cdot \frac{(\varepsilon_0 + c_1)^2}{\varepsilon^2}\right)$ |
| *Rule−SBD* $\sqrt[4]{K}$ | $O\left((\mathrm{fLMO} + p^2) \cdot \frac{(\varepsilon_0 + c_1 + c_2)^2}{\varepsilon^2} + np^2 \cdot \frac{(\varepsilon_0 + c_1 + c_2)^{3/2}}{\varepsilon^{3/2}}\right)$ |
| *Rule−DBD* $\sqrt[4]{K}$ | $O\left((\mathrm{fLMO} + p^2) \cdot \frac{(\varepsilon_0 + c_1 + c_2)^2}{\varepsilon^2} + np^2 \cdot \frac{(\varepsilon_0 + c_1 + c_2)^{3/2}}{\varepsilon^{3/2}}\right)$ |

- Here $\mathrm{fLMO}$ denotes the cost of the LMO
- $c_1 := LM^2D^2$, $c_2 := \hat{L}M^3D^3$, and $\varepsilon_0 := F(x^0) - F(x^\star)$

# Computational Experiments on Non-convex Sparse Binary Classification Problems

# Experiments on Sparse Binary Classification Problems with Non-convex Losses

Sparse binary classification problem with non-convex losses:

$$\min_x \ \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \frac{1}{1+\exp(-w_i^\top x)}\right)^2 \quad \text{s.t. } \|x\|_1 \le \lambda \ ,$$

- We used the same 12 large-scale instances from SVMLIB
- Frank-Wolfe gap $\mathcal{G}(x)$ used to measure non-stationarity
- $\lambda$ chosen by cross-validation
- We tested TUFW with standard step-size $\gamma_k$ and adaptive step-size $\tilde{\gamma}_k$
- We performed the same comparisons as done for convex losses, but replaced SPIDER-FW with CASPIDERG from Shen, Fang, Zhao, Huang, and Qian [10]
- All methods were implemented without sparse linear algebra (for fair comparisons)
- Implemented in Python, on the MIT Engaging Cluster

# Typical improvement compared to classic Frank-Wolfe

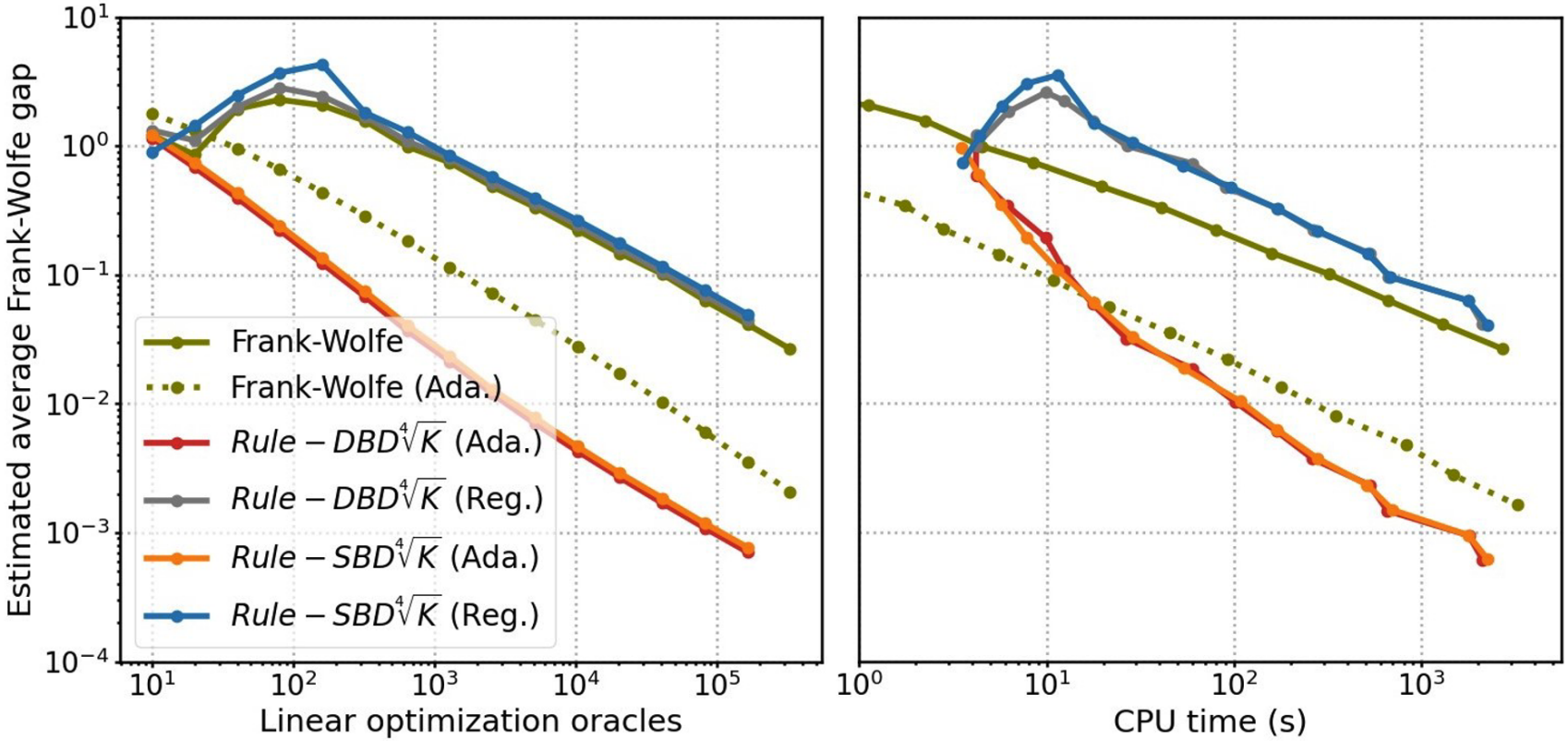


Figure 2: Binary classification on dataset a9a ($n = 32561,\ p = 123$)

For each $K \in 10 \times \{2^0, 2^1 \ldots, 2^{20}\}$ we ran 5 independent trials of each method for at most $K$ iterations

# Runtime comparison of TUFW with other Frank-Wolfe methods ($\lambda$ set by CV)

Least runtime (and the corresponding $K$) to attain $\sum_{i=1}^{k} \mathcal{G}(x^i)/k \leq \varepsilon$

(blank indicates $>$ 5000 seconds or $>$ $10 \times 2^{22}$ *LMO* calls)

| $\mathcal{G}(x^k)$ | dataset | $n$ | $p$ | *Rule−SBD* $\sqrt[4]{K}$ | *Rule−DBD* $\sqrt[4]{K}$ | FW | FW-ada | SPIDER-FW | CASPIDERG | Speed-up |
|---|---|---|---|---|---|---|---|---|---|---|
| 1e-2 | a1a | 1605 | 119 | 6.05(1.8e4) | **4.44(2.3e4)** | 10.46(3.7e6) | 9.01(5.5e6) | 20.13(1.0e7) | | **2.03** |
| 1e-3 | a1a | 1605 | 119 | 90.34(1.6e5) | **65.11(1.6e5)** | | 238.60(7.6e6) | | | **3.66** |
| 1e-4 | a1a | 1605 | 119 | 2225.61(6.3e6) | **1453.87(6.3e6)** | | | | | - |
| 1e-2 | a2a | 2265 | 119 | 6.47(2.3e4) | **4.94(1.6e4)** | 12.62(5.2e6) | 21.92(1.0e1) | 20.21(1.0e7) | | **2.56** |
| 1e-3 | a2a | 2265 | 119 | 93.17(2.0e5) | **70.69(2.0e5)** | | | | | - |
| 1e-4 | a2a | 2265 | 119 | 2168.72(6.3e6) | **1391.30(6.3e6)** | | | | | - |
| 1e-2 | a8a | 22696 | 123 | 46.68(2.5e4) | **41.92(2.5e4)** | 255.85(6.8e6) | 143.41(3.6e5) | | | **3.42** |
| 1e-3 | a8a | 22696 | 123 | 668.35(1.8e5) | **603.88(2.5e5)** | | 3320.78(6.6e5) | | | **5.50** |
| 1e-4 | a8a | 22696 | 123 | | | | | | | - |
| 1e-2 | a9a | 32561 | 123 | 83.24(1.4e4) | **79.91(1.2e4)** | 358.08(6.3e6) | 241.11(6.6e5) | | | **3.02** |
| 1e-3 | a9a | 32561 | 123 | 1165.35(1.3e5) | **1106.16(1.3e5)** | | 5112.72(1.6e6) | | | **4.62** |
| 1e-4 | a9a | 32561 | 123 | | | | | | | - |
| 5e-2 | w1a | 2477 | 300 | 8.99(2.5e4) | 8.82(2.9e4) | **0.44(1.8e4)** | 12.66(1.2e6) | 0.96(6.6e5) | 128.23(9.4e6) | 0.05 |
| 1e-2 | w1a | 2477 | 300 | 74.94(3.3e5) | 102.18(5.2e5) | **4.69(8.2e4)** | 161.72(2.0e6) | 20.15(1.0e7) | | 0.06 |
| 2e-3 | w1a | 2477 | 300 | 1279.97(7.9e6) | | **109.23(1.4e6)** | 1956.39(5.2e6) | | | 0.09 |
| 5e-2 | w2a | 3470 | 300 | 12.64(1.5e4) | 11.90(1.0e4) | **0.50(1.0e4)** | 19.08(1.8e6) | 1.01(7.9e5) | 177.81(8.4e6) | 0.04 |
| 1e-2 | w2a | 3470 | 300 | 93.47(2.8e5) | 122.01(2.9e5) | **7.44(8.2e4)** | 247.44(2.9e6) | 21.83(1.0e7) | | 0.08 |
| 2e-3 | w2a | 3470 | 300 | 900.09(3.1e6) | | **152.15(2.4e6)** | 3538.31(5.2e6) | | | 0.17 |
| 5e-2 | w7a | 24692 | 300 | 95.86(1.4e4) | 90.12(1.6e4) | 7.79(1.2e4) | 272.96(3.7e5) | **2.16(6.6e5)** | 640.45(9.4e6) | 0.02 |
| 1e-2 | w7a | 24692 | 300 | 544.57(1.6e5) | 561.90(4.9e4) | 80.96(4.9e4) | 3805.52(2.5e6) | **29.75(8.4e6)** | | 0.05 |
| 2e-3 | w7a | 24692 | 300 | 4078.15(1.0e6) | 6625.01(2.2e6) | **1631.47(6.6e5)** | | | | 0.40 |
| 5e-2 | w8a | 49749 | 300 | 222.71(2.3e4) | 216.21(1.0e4) | 16.41(1.4e4) | 553.46(2.8e5) | **3.25(5.2e5)** | 1228.59(7.9e6) | 0.02 |
| 1e-2 | w8a | 49749 | 300 | 1292.84(4.1e4) | 1303.19(4.1e4) | 176.70(9.8e4) | | **43.56(8.4e6)** | | 0.03 |
| 2e-3 | w8a | 49749 | 300 | | | **3268.55(7.9e5)** | | | | 0.47 |
| 1e-1 | svmguide3 | 1243 | 22 | 0.47(5.1e4) | **0.15(3.7e4)** | | 1.96(2.2e6) | | | **13.40** |
| 1e-2 | svmguide3 | 1243 | 22 | 7.95(1.4e5) | **2.41(6.6e4)** | | 74.75(4.2e6) | | | **30.99** |
| 1e-3 | svmguide3 | 1243 | 22 | 122.45(1.0e6) | **33.68(1.0e6)** | | | | | - |
| 1e-4 | svmguide3 | 1243 | 22 | 2418.83(1.0e7) | **804.17(2.1e7)** | | | | | - |
| 1e-1 | phishing | 11055 | 68 | 1.59(1.6e4) | 1.17(1.6e4) | 2.36(4.6e5) | 107.09(1.9e6) | **1.17(4.7e6)** | | 0.99 |
| 1e-2 | phishing | 11055 | 68 | 17.53(2.9e4) | **12.18(3.5e4)** | 159.76(1.0e7) | 2814.11(3.1e6) | | | **13.12** |
| 1e-3 | phishing | 11055 | 68 | 216.38(3.9e5) | **154.79(3.9e5)** | | | | | - |
| 1e-4 | phishing | 11055 | 68 | | **3558.37(1.0e7)** | | | | | - |
| 1e-1 | ijcnn1 | 49990 | 22 | 2.32(8.2e3) | **0.96(9.2e3)** | 10.88(6.6e5) | 104.67(5.4e5) | 1.58(3.7e6) | | **1.64** |
| 1e-2 | ijcnn1 | 49990 | 22 | 24.26(2.5e4) | **10.00(1.3e4)** | 804.48(1.0e7) | 2323.78(1.7e6) | | | **80.44** |
| 1e-3 | ijcnn1 | 49990 | 22 | 298.45(1.6e5) | **179.40(1.3e6)** | | | | | - |
| 1e-4 | ijcnn1 | 49990 | 22 | | **2750.09(5.2e6)** | | | | | - |
| 5e-2 | covtype | 581012 | 54 | 156.41(4.5e6) | **110.28(5.8e6)** | | 2916.33(1.3e6) | | | **26.45** |
| 1e-2 | covtype | 581012 | 54 | 785.43(4.7e6) | **572.97(5.8e6)** | | | | | - |
| 2e-3 | covtype | 581012 | 54 | 4292.90(5.8e6) | **3142.24(5.8e6)** | | | | | - |

# Comments on the experiments

- TUFW methods significantly outperform other methods on all datasets except `w1a`, `w2a`, `w7a`, and `w8a`
- As $1/\varepsilon$ increases, the advantage of TUFW methods grows

# Extension to General Empirical Risk Minimization

## General empirical risk minimization with constraints

$$\text{ERM:} \qquad \text{minimize}_{x \in \mathcal{C}} \quad F(x) := \frac{1}{n} \sum_{i=1}^{n} f_i(x)$$

$L$ and $\hat{L}$ are the Lipschitz constants of $\nabla f_i$ and $\nabla^2 f_i$

## Theorem (*Rule*$-SBD\sqrt{k}$ for general ERM)

*Suppose that $F$ is convex and Assumption 1 holds, and TUFW with Rule$-SBD\sqrt{k}$ is applied to ERM with step-sizes $\gamma_k := 2/(k+2)$. Then:*

$$\mathbb{E}[F(x^k) - F(x^\star)] \leq \frac{2LD^2 + 134\hat{L}D^3}{k+1}$$

All other Rules can be extended to general ERM problems

# Summary

- We develop a new family of Frank-Wolfe methods, which we call TUFW, that replaces the exact gradient computation by a sum of (second-order) Taylor-approximated gradients around certain current and previous iterates
- All of our rules for TUFW exhibit a *decreasing* number of gradient calls over the course of iterations, while retaining the optimal LMO complexity, together with a relatively small number of other flops. The joint dependence on $n$ and $\varepsilon$ is $O(n/\sqrt{\varepsilon})$ for convex losses and $O(n/\varepsilon^{3/2})$ for non-convex losses.
- Computational experiments show that TUFW exhibits very significant speed-ups over existing methods on real-world datasets.
- Our TUFW method easily extends to the more general ERM problem, with corresponding versions of our theoretical guarantees
- We also propose a novel adaptive step-size approach with computational experiments that point to its efficiency in practice

*Thank You*

# Brief Proof Idea

Using the same proof techniques as in the classic FW, we have

**Lemma**

*For $ERM_\ell$, suppose that Assumption 1 holds, $F$ is convex, and $\gamma_k = 2/(k+2)$ for all $k \geq 0$. Then*

$$F(x^k) - F(x^\star) \leq \frac{2LD_2^2}{n(k+1)} + \frac{2}{k(k+1)} \sum_{t=1}^{k} t\left(\nabla F(x^{t-1}) - g^{t-1}\right)^\top (s^{t-1} - x^\star)$$

For $Rule{-}SBD\sqrt{k}$, we can further prove that $\mathbb{E}(\cdot) \leq \mathcal{O}(\hat{L}D_1 D_\infty^2/nt)$

Similarly, for non-convex problems we have

$$\sum_{k=0}^{K} \frac{\mathcal{G}(x^k)}{K+1} \leq \frac{\varepsilon_0 + LD_2^2/n}{\sqrt{K+1}} + \frac{1}{K+1} \sum_{k=0}^{K} (\nabla F(x^k) - g^k)^\top (s^k - \bar{s}^k).$$


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