Stochastic Optimization of Multiple Objectives and Supervised Machine Learning

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Optimization models in Data Science and Learning

A data set for analysis involving optimization is typically of the form

$$D = \{(a_j, y_j), j = 1, \ldots, N\}$$

where the a_j's vectors are features or attributes

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Often, ϕ is parameterized $\phi(x) = \phi(a; x)$. The parameters are x.

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   The labels may have to be learned while learning ϕ.

5. Data is assumed to be clean for optimization, but still:

   i) (a_j, y_j)'s could be noisy or corrupted.
   ii) Some a_j or y_j's could be missing.
   iii) Data could arrive in streaming fashion (ϕ must be learned online).

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Such data analysis is often referred to as machine learning or data mining.

$$\begin{tikzcd}
 & \text{machine learning} \arrow[dl] \arrow[dr] & \text{data mining} \arrow[d] \\
\text{predictive or supervised learning (when labels exist)} & & \text{unsupervised learning (when labels are null): extract interesting information from data}
\end{tikzcd}$$

The correct/accurate match of the data is typically quantified by a loss function $\ell(a, y; \phi(x))$ and thus learning can be formulated as

$$\min_x \sum_{j=1}^{N} \ell(a_j, y_j; \phi(x))$$

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To avoid overfitting such a model to a sample D, one often adds a regularizer

$$\begin{tikzcd} & \displaystyle\min_x \sum_{j=1}^{N} \ell(a_j, y_j; \phi(x)) + g(x) \arrow[dl] \arrow[dr] & \\ \lambda\|x\|_1 & & \frac{\lambda}{2}\|x\|_2^2 \end{tikzcd}$$

so that ϕ is not so sensitive to changes in D.

The general form of optimization models in DS is

$$\min_{x \in \mathbb{R}^n} \; f(x) + g(x)$$

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where $f : \mathbb{R}^n \to \mathbb{R}$ is smooth.

∇f is at least Lipschitz continuous.

$g : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is convex, proper and closed.

g is typically non-smooth.

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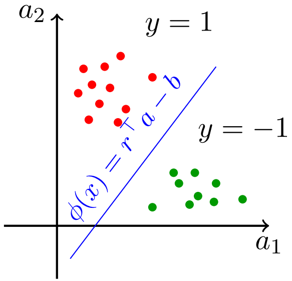
Consider a data set with $y \in \{-1, 1\}$



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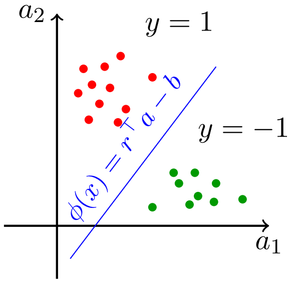


$\phi(x) = \phi(a; r, b) = r^\top a - b$ is a linear classifier. One aims to seek for a optimal parameter $x = (r, b)$ such that

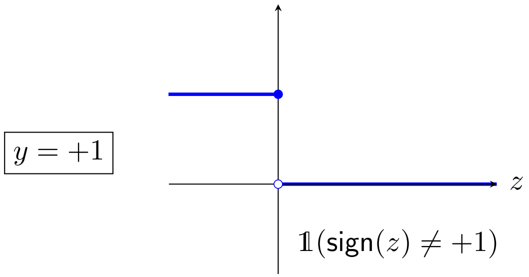
$$\begin{cases} r^\top a_j - b \ \geq \ 0 & \text{when } y_j = 1 \\ r^\top a_j - b \ < \ 0 & \text{when } y_j = -1 \end{cases} \qquad \forall j = 1, \dots, N \quad (*)$$

Logistic regression can be motivated by two arguments.

1. Smoothing/convexifying the true loss.

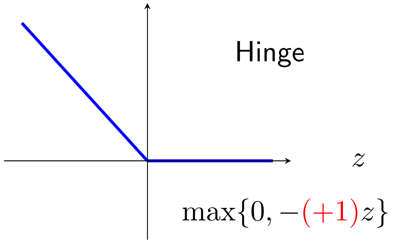
   What we want to do is

$$\min \ \mathbb{1}(\mathsf{sign}(z) \neq y) \qquad \text{where } z = \phi(x).$$



Smoothing/convexifying to Hinge loss (SVM)

$\boxed{y = +1}$



Smoothing to Logistic loss

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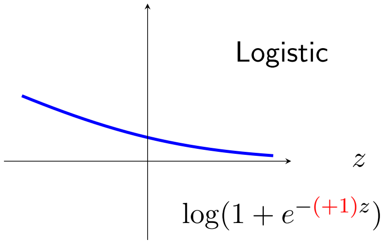

2. Probabilistic argument: $(*)$ is equivalent to

$$\sigma(\phi(x)) \;=\; \frac{1}{1+e^{-\phi(x)}} \begin{cases} \geq 0.5 & \text{when } y = 1 \\ < 0.5 & \text{when } y = -1 \end{cases}$$

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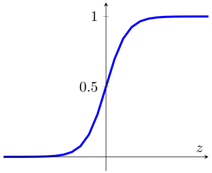

$\frac{1}{1+e^{-z}}$

Think of it as the probability

$$P(y=1|a) = \sigma(\phi(x)) = \frac{1}{1+e^{-(+1)\phi(x)}}$$

$$P(y=-1|a) = 1-\sigma(\phi(x)) = \frac{1}{1+e^{-(-1)\phi(x)}}$$

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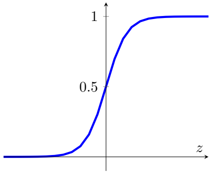

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Assuming data points are i.i.d., the maximum likelihood problem is

$$\max \prod_{j=1}^{N} \underbrace{P(y_j|a_j)}_{\text{prob. of correct prediction}} = \prod_{j=1}^{N} \frac{1}{1+e^{-y_j\phi(x)}}$$

Then, the negative log likelihood leads to the loss minimization problem

$$\min_{r,b} \; \frac{1}{N} \sum_{j=1}^{N} \ell_L(a_j, y_j; \phi(x))$$

with the smooth convex logistic loss function

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Binary classification is formulated as the optimization problem

$$\min_{r,b} \frac{1}{N} \sum_{j=1}^{N} \ell_L(a_j, y_j; \phi(x)) + \frac{\lambda}{2}\|r\|_2^2$$

Presentation outline

Stochastic gradient descent for Stochastic Optimization

Assume a point $(a, y) \in D$ arises with a certain (joint) probability P_Ω.

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When P_Ω is unknown, only having a sample D leads to minimizing the empirical risk of misclassification

$$R_N(x) \; = \; \frac{1}{N} \sum_{j=1}^{N} \ell(a_j, y_j; \phi(x))$$

as an estimation of $R(x)$.

For simplicity, let $f(x) = \ell(a, y; \phi(x))$.

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The general objective could be written as

$$R(x) = \begin{cases} R(x) = \mathbb{E}[f(x; w)] & \text{Online setting (expected risk)} \\ R_N(x) = \frac{1}{N} \sum_{j=1}^{N} f_j(x) & \text{Finite sum setting (empirical risk)} \end{cases}$$

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Both can be minimized by the stochastic gradient method.

The stochastic gradient method

Algorithm 1 Stochastic Gradient (SG) method (Robbins and Monro 1951)

```
1: Choose an initial point $x_0 \in \mathbb{R}^n$.
2: for $k = 0, 1, \dots$ do
3:     Compute a stochastic gradient $g(x_k; w_k)$.
4:     Choose a step-size $\alpha_k > 0$.
5:     Set the new iterate $x_{k+1} = x_k - \alpha_k g(x_k; w_k)$.
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Sutton Monro
Lehigh ISE

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$$\frac{1}{|B_k|} \sum_{j \in B_k} \nabla f(x_k; w_{k,j})$$ mini-batch SG ($|B_k|$ is the mini-batch size)

Classical assumptions for SG method

1. The sequence of realizations $\{w_k\}$ are i.i.d. sample of w.
2. Function R has Lipschitz continuous gradient.
3. The stochastic gradient is an unbiased estimate

$$\mathbb{E}_{w_k}[g(x_k; w_k)] \;=\; \nabla R(x_k)$$

4. The stochastic gradient has bounded variance

$$\mathbb{V}_{w_k}[g(x_k; w_k)] \;\leq\; M + \mathcal{O}(\|\nabla R(x_k)\|^2)$$

5. Function R is bounded below: $R(x) \geq R_*, \forall x$. $R_* = R(x_*)$ where x_* is a minimizer of R.

$\mathbb{E}[\cdot]$ denotes the expected value taken w.r.t. the joint distribution of $\{w_k\}$.

Convergence rates for SG method

The strongly convex case (Sacks 1958)

Consider a diminishing step-size sequence (e.g., $\alpha_k \simeq \mathcal{O}(1/k)$), one has

$$\mathbb{E}[R(x_k)] - R_* \leq \mathcal{O}(1/k)$$

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The convex case (Nemirovski and Yudin 1978)

Consider a diminishing step-size sequence (e.g., $\alpha_k \simeq \mathcal{O}(1/\sqrt{k})$), one has

$$\mathbb{E}[R^k_{\text{best}}] - R_* \;\leq\; \mathcal{O}(1/\sqrt{k})$$

where $R^k_{\text{best}} = \min_{1\leq i\leq k} R(x_i)$.

Presentation outline

Multi-Objective Optimization

Multi-Objective Optimization (MOO) deals with multiple potentially conflicting objectives simultaneously.

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We consider smooth MOO problems of the general form

$$\begin{aligned} \min \;\; & H(x) \; = \; (h_1(x), \ldots, h_m(x)) \\ \text{s.t.} \;\; & x \; \in \; \mathcal{X} \end{aligned}$$

where $h_i : \mathbb{R}^n \to \mathbb{R}$ are smooth functions and $\mathcal{X}$ is a feasible region.

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Definition of optimality for MOO

- x dominates y if $H(x) < H(y)$ componentwise, $\forall x, y \in \mathcal{X}$.
- x is a Pareto minimizer if it is not dominated by any other point in $\mathcal{X}$.

  Also called a non-dominated or efficient point.

Pareto front

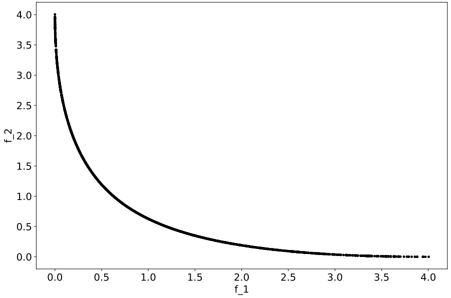

Figure: Pareto front of problem SP1

Denote $\mathcal{P}$ as the set of Pareto minimizers.

Pareto front is a mapping from $\mathcal{P}$ to function value space $\mathbb{R}^m$, i.e.,

$$H(\mathcal{P}) = \{H(x) : x \in \mathcal{P}\}$$

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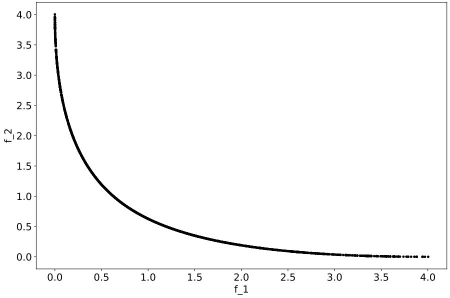

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The goal of MOO: find the set of Pareto minimizers and hence Pareto front to define the best trade-off among several competing criteria.

Necessary condition for Pareto minimizers

Pareto first-order stationary condition: x is a Pareto stationary point if

$$\nexists\, d \in \mathbb{R}^n \text{ such that } \begin{bmatrix} \nabla h_1(x)^\top \\ \vdots \\ \nabla h_m(x)^\top \end{bmatrix} d < 0$$

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Or equivalently, if the convex hull of $\nabla h_i(x)$'s contains the origin

$$\exists \lambda \in \Delta^m \text{ such that } \sum_{i=1}^{m} \lambda_i \nabla h_i(x) = 0$$

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Note: when all the functions are convex, $x \in \mathcal{P}$ iff x is Pareto first-order stationary.

Overview of methods for MOO

Methods with a priori preferences (Ehrgott 2005; Miettinen 2012)

- Weighted-sum method

$$\min\ S(x;a) = \sum_{i=1}^{m} a_i f_i(x), \text{ where } a \in \Delta^m$$

  Limitations: hard to preselect weights for different magnitudes; cannot find Pareto minimizers in non-convex regions.

- ϵ-constraint method

$$\min\ f_i(x) \text{ s.t. } f_j(x) \le \epsilon_j,\ \forall j \neq i$$

  where $\epsilon_j \ge \min_{x\in\mathcal{X}} f_j(x)$ are upper bounds.
  Limitations: inappropriate upper bounds lead to infeasibility.

Common issues: output single nondominated point at one run, produce poorly distributed Pareto front with multiple runs.

Overview of methods for MOO

Methods with a posteriori preferences

Population-based heuristic methods: no convergence proofs, e.g.,

- NSGA-II (genetic algorithms) (Deb et al. 2002).
- AMOSA (simulated annealing) (Bandyopadhyay et al. 2008).

Convergent methods: proved convergence to Pareto stationary points

- multi-gradient method (Fliege and Svaiter 2000).
- Newton's method for MOO (Fliege et al. 2009).
- direct multi-search algorithm (Custódio et al. 2011), etc.

Superiority: able to construct the whole well-spread Pareto front.

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Subproblem 1 (Fliege and Svaiter 2000):

$$d_k \in \operatorname*{argmin}_{d \in \mathbb{R}^n} \max_{1 \leq i \leq m} \{-\nabla h_i(x_k)^\top d\} + \frac{1}{2}\|d\|^2$$

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Subproblem 2: dual problem of Subproblem 1

$$\lambda_k \in \operatorname*{argmin}_{\lambda \in \mathbb{R}^m} \left\| \sum_{i=1}^{m} \lambda_i \nabla h_i(x_k) \right\|^2 \quad \text{s.t.} \quad \lambda \in \Delta^m$$

Then, $d_k = -\sum_{i=1}^{m} (\lambda_k)_i \nabla h_i(x_k)$ is a common descent direction.

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Note: when $m = 1$, one recovers $d_k = -\nabla h_1(x_k)$.

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where $w \in \mathbb{R}^{m\times p}$ are random parameters obeying a certain distribution.

Subproblem 3: replace $\nabla f_i(x_k)$ by an estimate $g_i(x_k;w_k)$ in Subproblem 2

$$\begin{array}{c} \lambda^g(x_k;w_k) \;\in\; \underset{\lambda\in\mathbb{R}^m}{\operatorname{argmin}} \left\| \sum_{i=1}^m \lambda_i g_i(x_k;w_k) \right\|^2 \\ \text{s.t.} \;\; \lambda \in \Delta^m \end{array}$$

$g(x_k;w_k) = \sum_{i=1}^m (\lambda_k^g)_i g_i(x_k;w_k)$ denotes the stochastic multi-gradient.

Stochastic Multi-Objective Optimization

Consider a stochastic multi-objective problem

$$\begin{array}{ll} \min & F(x) \; = \; (f_1(x), \ldots, f_m(x)) \; = \; (\mathbb{E}[f_1(x; w)], \ldots, \mathbb{E}[f_m(x; w)]) \\ \text{s.t.} & x \in \mathcal{X} \end{array}$$

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$g(x_k; w_k) = \sum_{i=1}^{m} (\lambda_k^g)_i g_i(x_k; w_k)$ denotes the stochastic multi-gradient.

The stochastic multi-gradient (SMG) algorithm: $x_{k+1} = x_k - \alpha_k g(x_k; w_k)$

The stochastic multi-gradient method

Consider using an orthogonal projection P when minimize over a closed and convex set $\mathcal{X} \subseteq \mathbb{R}^n$.

The stochastic multi-gradient method

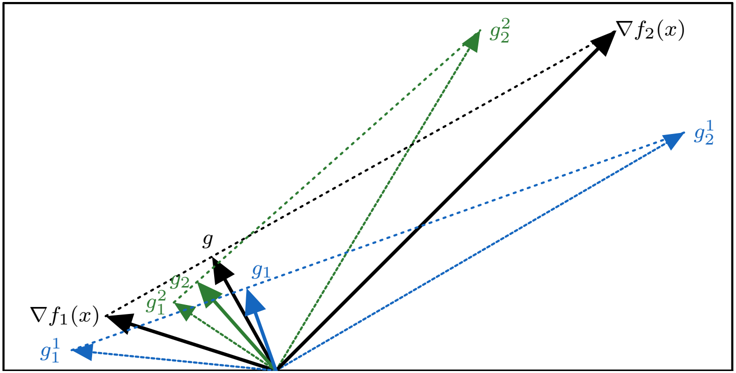
Consider using an orthogonal projection P when minimize over a closed and convex set $\mathcal{X} \subseteq \mathbb{R}^n$.

Algorithm 1 Stochastic Multi-Gradient (SMG) Algorithm

```
1: Choose an initial point $x_0 \in \mathbb{R}^n$ and a step-size sequence $\{\alpha_k\}_{k \in \mathbb{N}} > 0$.
2: for $k = 0, 1, \ldots$ do
3:     Compute the stochastic gradients $g_i(x_k; w_k)$ for $i = 1, \ldots, m$.
4:     Solve Subproblem 3 to obtain the stochastic multi-gradient
           $$g(x_k; w_k) = \sum_{i=1}^{m} (\lambda_k^g)_i g_i(x_k; w_k), \text{ with } \lambda_k^g \in \Delta^m.$$
5:     Update the next iterate $x_{k+1} = P_{\mathcal{X}}(x_k - \alpha_k g(x_k; w_k))$.
6: end for
```

Subproblem 3 illustration

Consider the case $m = 2, n = 2$.



g_1 and g_2 are two stochastic multi-gradients by solving Subproblem 3.

They are estimates of the true multi-gradient g (Subproblem 1 or 2).

Biasedness of the stochastic multi-gradient

Denote

$$\begin{aligned} S(x;\lambda) &= \sum_{i=1}^m \lambda_i f_i(x) \\ \nabla_x S(x;\lambda) &= \sum_{i=1}^m \lambda_i \nabla f_i(x) \end{aligned}$$

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Even under the classical assumption in SG

$$\mathbb{E}_w[g_i(x;w)] = \nabla f_i(x),\ \forall i = 1, \ldots, m$$

it turns out that $g(x;w)$ is a biased estimate, i.e.,

$$\mathbb{E}_w[g(x;w)] \neq \nabla_x S(x;\lambda)$$

where λ are the true coefficients from Subproblem 2.

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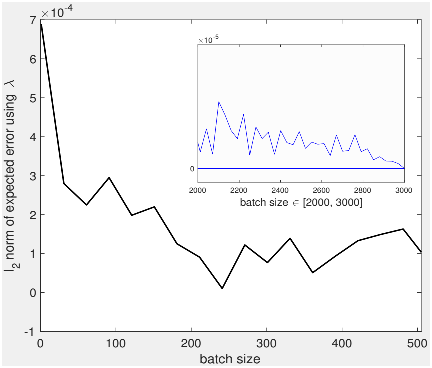
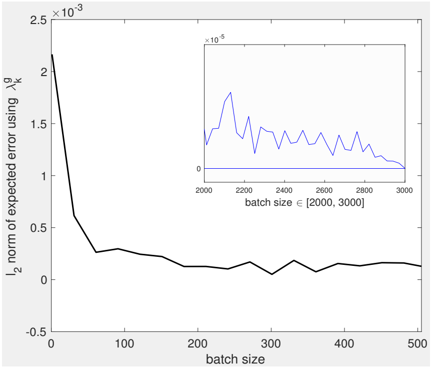
where λ are the true coefficients from Subproblem 2. We also have

$$\mathbb{E}_w[g(x;w)] \neq \mathbb{E}_w[\nabla_x S(x;\lambda^g)]$$

Biasedness illustration

The biasedness using either the true coefficients λ or λ^g decreases as batch size increases and eventually vanishes in the full batch setting.





Assumptions for convergence

1. All objective functions $f_i : \mathbb{R}^n \to \mathbb{R}$ are continuously differentiable with Lipschitz continuous gradients ∇f_i.

2. The feasible region $\mathcal{X} \subseteq \mathbb{R}^n$ is bounded.

3. (Unbiasedness) $\mathbb{E}_w[g_i(x;w)] \; = \; \nabla f_i(x)$.

4. (Bound on the biasedness) There exist $M_1, M_F > 0$ such that

$$\|\mathbb{E}_w[g(x;w) - \nabla_x S(x;\lambda^g)]\| \;\leq\; \alpha\,(M_1 + M_F\|\mathbb{E}_w[\nabla_x S(x;\lambda^g)]\|)$$

   (can be guaranteed by dynamic sampling)

5. (Bound on the second moment) There exist $G, G_V > 0$ such that

$$\mathbb{E}_w[\|g(x;w)\|^2] \;\leq\; G^2 + G_V^2\|\mathbb{E}_w[\nabla_x S(x;\lambda^g)]\|^2$$

Sublinear rate in the strongly convex case

Theorem (Individual f_i are strongly convex (c is max of constants))

Assume $\lambda_t \to \lambda_*$. Let $x_* \in \mathcal{P}$ be associated with λ_*.

Considering a diminishing step-size sequence $\alpha_t = \frac{2}{c(t+1)}$, we have

$$\min_{t=1,\ldots,k} \mathbb{E}[S(x_t;\lambda_t)] - \mathbb{E}[S(x_*;\bar{\lambda}_k)] \;\leq\; \mathcal{O}(1/k)$$

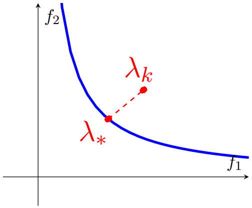
where $\bar{\lambda}_k = \sum_{t=1}^{k} \frac{t}{\sum_{t=1}^{k} t} \lambda_t \in \Delta^m$.

Then, we have $\min_{1\leq t\leq k} \mathbb{E}[S(x_t;\lambda_t)] \to \mathbb{E}[S(x_*;\lambda_*)]$.

Rate in the strongly convex case: stronger assumption

Assume λ_k being a better approximation to λ_*.

We know $\nabla_x S(x_*; \lambda_*)^\top (x_k - x_*) \geq 0$.



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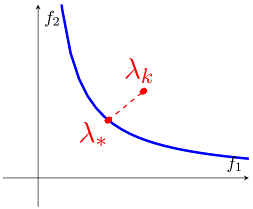


Assumption

For any $x_k \in \mathcal{X}$, one has

$$\nabla_x S(x_*; \lambda_k)^\top (x_k - x_*) \geq 0$$

where λ_k are the true coefficients by solving Subproblem 2.

Rate in the strongly convex case: stronger assumption

Theorem (SL&LNV 2019)

Let x_* be the Pareto minimizer associated with λ_*.

Considering a step-size sequence $\alpha_k = \gamma/k$ with $\gamma > 1/2c$, we have

$$\mathbb{E}[\|x_k - x_*\|^2] \;\leq\; \mathcal{O}(1/k)$$

and

$$\mathbb{E}[S(x_k;\lambda_*)] - \mathbb{E}[S(x_*;\lambda_*)] \;\leq\; \mathcal{O}(1/k)$$

Presentation outline

Pareto-Front stochastic multi-gradient method

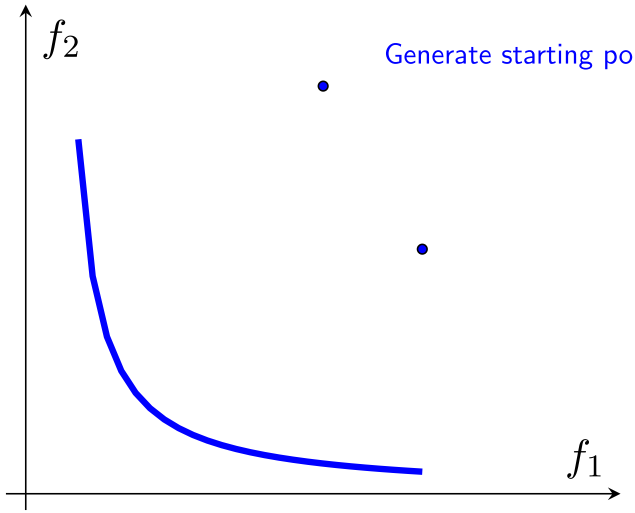
The Pareto-Front version of SMG is designed to obtain a complete Pareto front in a single run.

Algorithm 2 Pareto-Front Stochastic Multi-Gradient (PF-SMG) Algorithm

```
 1: Generate a list of starting points $\mathcal{L}_0$. Select $r, p, q \in \mathbb{N}$.
 2: for $k = 0, 1, \ldots$ do
 3:     Set $\mathcal{L}_{k+1} = \mathcal{L}_k$.
 4:     for each point $x$ in the list $\mathcal{L}_{k+1}$ do
 5:         for $t = 1, \ldots, r$ do
 6:             Add $x + w^t$ to the list $\mathcal{L}_{k+1}$ where $w^t$ is a realization of $w_k$.
 7:     for each point $x$ in the list $\mathcal{L}_{k+1}$ do
 8:         for $t = 1, \ldots, p$ do
 9:             Apply $q$ iterations of the SMG algorithm starting from $x$.
10:             Add the final output point $x_q$ to the list $\mathcal{L}_{k+1}$.
11:     Remove all the dominated points from $\mathcal{L}_{k+1}$.
```

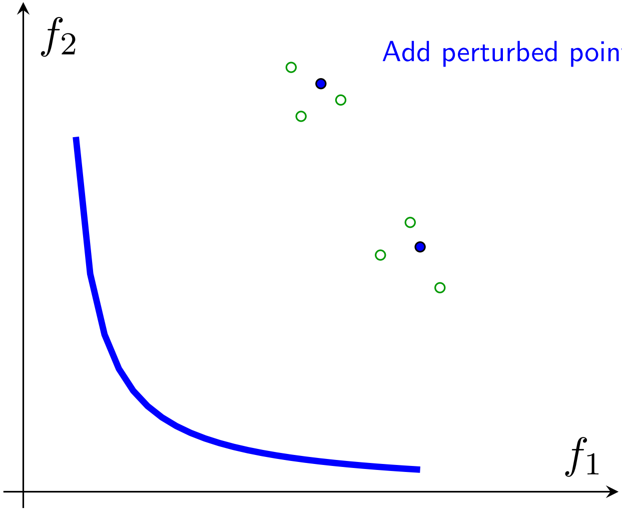
PF-SMG illustration

$r = 3, p = 2$



PF-SMG illustration

$r = 3, p = 2$



PF-SMG illustration

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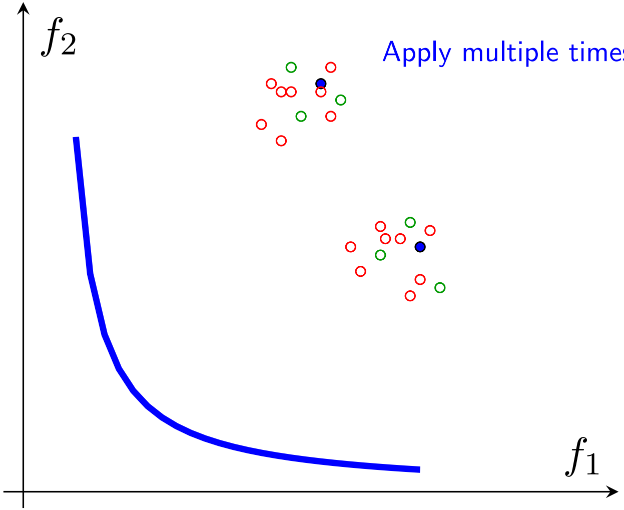

PF-SMG illustration

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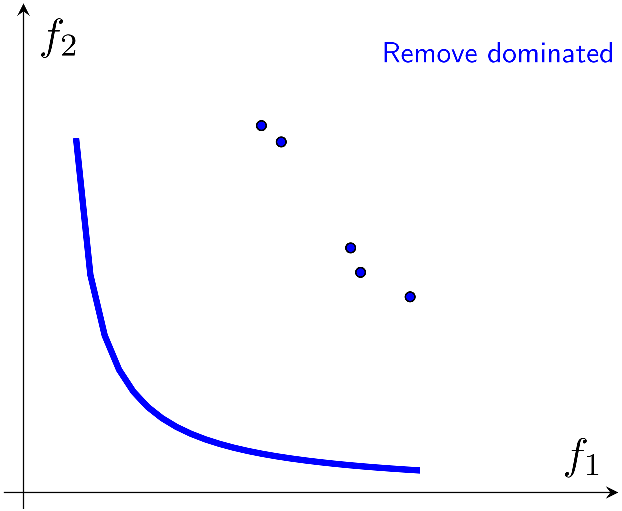
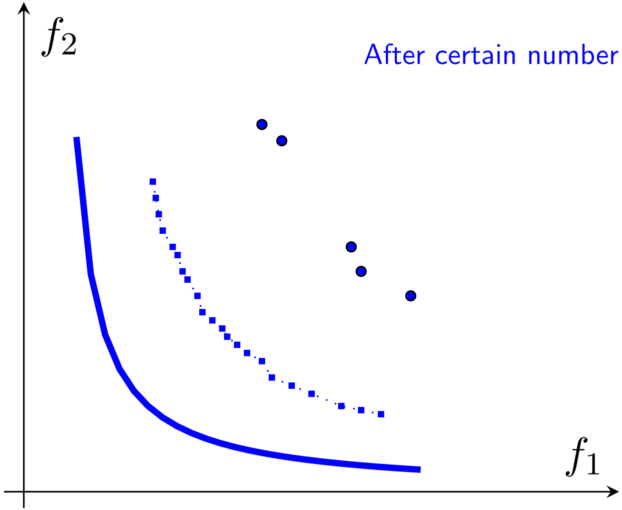


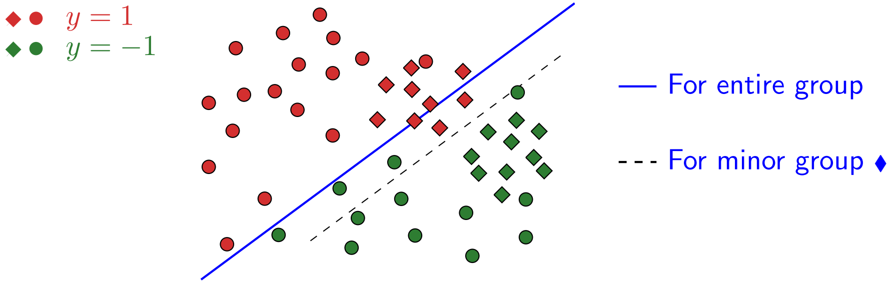
PF-SMG illustration

$r = 3, p = 2$



Numerical results: logistic regression problems

Motivation: consider a set of data points in 2D



Data points labeled by ♦ and ● may be collected from different sources/groups.

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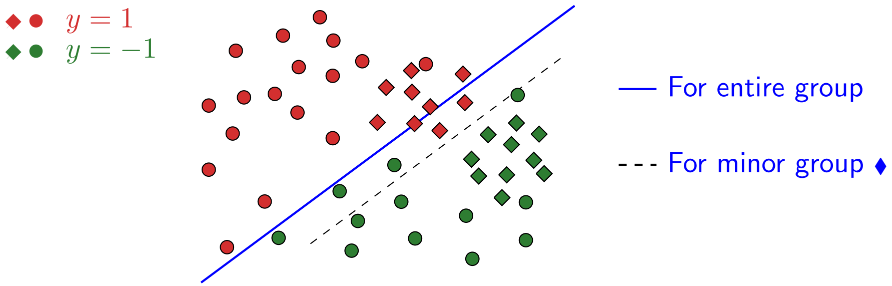


Data points labeled by ♦ and • may be collected from different sources/groups.

Key idea: design a MOO problem to identify the existence of bias in data and define the best trade-off if data bias exists.

- Recall the logistic (prediction) loss function

$$f(r,b) \;=\; \frac{1}{N}\sum_{j=1}^{N}\log(1+e^{-y_j(r^\top a_j-b)})+\frac{\lambda}{2}\|r\|^2$$

where $\{(a_j,y_j)\}_{j=1}^N$ are i.i.d. feature/label pairs sampled from a certain joint probability distribution of (A,Y).

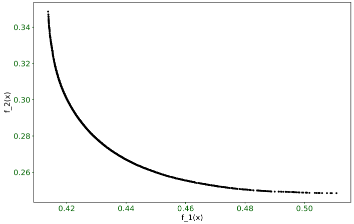
- Testing data sets are selected from LIBSVM (Chang and Lin 2011).
- Split a data set into two groups according to a binary feature. Let J_1 and J_2 be two index sets. A two-objective problem is constructed as

$$\min_{r,b}\,(f_1(r,b),f_2(r,b))$$

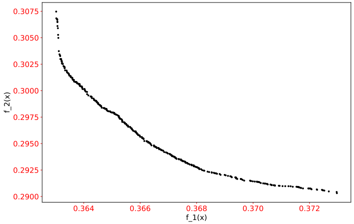
where

$$f_i(r,b) \;=\; \frac{1}{|J_i|}\sum_{j\in J_i}\log(1+e^{-y_j(r^\top a_j-b)})+\frac{\lambda_i}{2}\|r\|^2$$

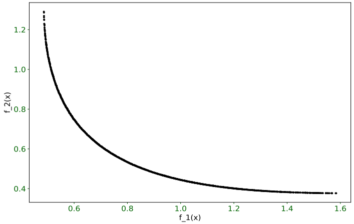
Approximated Pareto fronts for the multi-objective logistic regression problems:



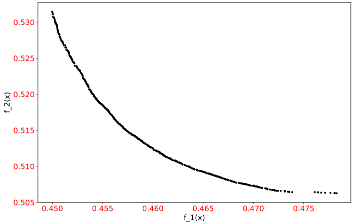
(a) *heart*



(b) *australian*



(c) *svmguide3*



(d) *german.numer*

Consistently, wider Pareto fronts of *heart* and *svmguide3* indicate higher distinction between two groups.

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Two implications:

- Given groups of data instances for the same problem, one can evaluate the bias by observing the range of Pareto fronts.
- New data instance (of unknown group) can be classified more accurately by selecting a set of nondominated points.

Presentation outline

Conclusions

- Established sublinear convergence rates, $\mathcal{O}(1/k)$ for strongly convex and $\mathcal{O}(1/\sqrt{k})$ for convex case in terms of a weighted sum function.
- Designed PF-SMG algorithm that is robust and efficient to generate well-spread and sufficiently accurate Pareto fronts.
- In logistic binary classification, developed a novel tool for identifying bias among potentially different sources of data.

S. Liu and L. N. Vicente, *The stochastic multi-gradient algorithm for multi-objective optimization and its application to supervised machine learning*, ISE Technical Report 19T-011, Lehigh University.

Future directions

- Have a (probabilistic?) result for determining the whole Pareto front.
- Investigate variance reduction techniques.
- Deal with nonconvexity, nonsmoothness, general constraints, . . .
- Expand use of MOO in machine learning:
  - Handling discrimination and unfairness (Calders et al. 2009; Hardt et al. 2016).
  - Conflicting robotic learning.