# MULTIVARIATE OPTIMIZATION FOR NON-DECOMPOSABLE PERFORMANCE MEASURES

Debojyoti Dey (15511264) Nimisha Agarwal (15511267) (Group 15)

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#### Overview

- Proposed Work
- Existing Stochastic Algorithm
- Basic Ideas
- Formulation of Optimization Problem
- Gradient Ascent
- Opening Problems
- References

#### Problem Statement

Finding general optimization technique to maximize performance which are non-decomposable in nature. Our work will primarily consider some concave measures of performance.

- Examples: Min, G-mean, H-mean etc.
- Expressed as f(TPR, TNR).
- TPR = True Positive Rate, TNR = True Negative Rate

## Stochastic Primal Dual Method [NarasimhanK015]

The existing online method has following shortcomings:

- Requires performance measure function to be L-Lipschitz.
- Works with non-Lipschitz functions with some restriction.
- Example: G-mean

## Decomposable vs Non-decomposable

• Misclassification rate is decomposable. Loss function:

$$\Delta(\overline{y}, \overline{y}^*) = \frac{1}{n} \sum_{i=1}^n \frac{1 - y_i y_i^*}{2}$$

•  $F_{\beta}$  score is non-decomposable. Performance measure:

$$\phi(\overline{y}, \overline{y}^*) = \frac{(1+\beta^2)TP}{(1+\beta^2)TP + \beta^2FN + FP}$$

- Problem with misclassification rate?
  - class imbalanced setting

## Multivariate Optimization Setting

• Hypothesis function  $\overline{h}$  maps  $\overline{x} \in \overline{\mathcal{X}}$  and  $\overline{x} = \{x_1, x_2, \cdots, x_n\}$  to  $\overline{y} \in \overline{\mathcal{Y}}$  and  $\overline{y} = \{y_1, y_2, \cdots, y_n\}$  where  $y_i \in \{+1, -1\}$ 

$$\overline{h}: \overline{\mathcal{X}} \to \overline{\mathcal{Y}}$$

We define score for a particular input-output combination as follows:

$$f_w(\overline{x},\overline{y}) = w^T \psi(\overline{x},\overline{y})$$

• Hypothesis function gives  $\overline{y}$  with highest score for an input  $\overline{x}$ .

$$\overline{h}_{w}(\overline{x}) = \arg\max_{\overline{y} \in \mathcal{Y}} (w^{T} \psi(\overline{x}, \overline{y}))$$

ullet We use the following form of  $\psi$ 

$$\psi(\overline{x},\overline{y}) = \sum_{i=1}^{n} y_i^* x_i$$

#### Structural SVM

• Struct SVM by [Joachims:2005] used for multi-class classification.

$$\min_{\substack{w,\xi \geq 0}} \frac{1}{2} ||w||^2 + C\xi$$

$$s.t \quad \forall \overline{y} \in \overline{\mathcal{Y}} \setminus \overline{y}^* : w^T [\psi(\overline{x}, \overline{y}^*) - \psi(\overline{x}, \overline{y})] \geq \Delta(\overline{y}^*, \overline{y}) - \xi$$

$$\Rightarrow \Delta(\overline{y}^*, \overline{y}) + \Sigma(y_i - y_i^*) w^T x_i \leq \xi$$

where  $\Delta(\overline{y}^*, \overline{y})$  is loss function.

- $\xi$  is the upper bound of loss function.
- ullet We substitute margin violation  $\xi$  in objective function by

$$\mathcal{L}_{w}(\overline{x}, \overline{y}^{*}) = \max_{\overline{y} \in \{1, -1\}^{n}} \{ \Delta(\overline{y}^{*}, \overline{y}) + \sum_{i=1}^{n} (y_{i} - y_{i}^{*}) w^{T} x_{i} \}$$
 (1)

#### Performance measure in Fenchel Dual

Performance measure G-mean is given by

$$\phi(P, N) = \sqrt{PN}$$

$$= \min_{\alpha, \beta} \{\alpha P + \beta N - \phi^*(\alpha, \beta)\}$$

as  $\phi$  is a concave function. P,N stands for TPR and TNR respectively.

We define our loss function as

$$\Delta(\overline{y}^*, \overline{y}) = -\phi(P, N)$$

$$= \max_{\alpha, \beta} \{-\alpha P - \beta N + \phi^*(\alpha, \beta)\}$$

## Optimization Problem

We can re-write equation 1 as,

$$\mathcal{L}_{w}(\overline{x}, \overline{y}^{*})$$

$$= \max_{\overline{y} \in \{1, -1\}^{n}} \{ \max_{\alpha, \beta} \{ -\alpha P - \beta N + \phi^{*}(\alpha, \beta) \} + \frac{1}{n} \sum_{i=1}^{n} (y_{i} - y_{i}^{*}) w^{T} x_{i} \}$$

$$= \max_{\alpha, \beta} \{ \max_{\overline{y}} \{ -\alpha P - \beta N + \frac{1}{n} \sum_{i=1}^{n} (y_{i} - y_{i}^{*}) w^{T} x_{i} \} + \phi^{*}(\alpha, \beta) \}$$
 (2)

Express P and N as following:

$$P = \sum_{i=1}^{n} P_i(y_i, y_i^*) = \frac{1}{n_+} \sum_{i=1}^{n} \frac{(1+y_i)(1+y_i^*)}{4}$$

#### Continued...

$$N = \sum_{i=1}^{n} N_i(y_i, y_i^*) = \frac{1}{n_-} \sum_{i=1}^{n} \frac{(1 - y_i)(1 - y_i^*)}{4}$$

Substituting, inner maximization becomes,

$$\sum_{i=1}^{n} \max_{y_{i} \in \{-1,+1\}} -\frac{\alpha}{n_{+}} \frac{(1+y_{i})(1+y_{i}^{*})}{4} - \frac{\beta}{n_{-}} \frac{(1-y_{i})(1-y_{i}^{*})}{4} + \frac{1}{n} (y_{i} - y_{i}^{*}) w^{T} x_{i}$$

using independence among the data points.

Now we can perform maximization for each point separately.

#### Continued...

Solving the above maximization, we get the following weighted hinge loss like function with some additional constants,

$$\sum_{i=1}^{n} \left(\frac{\alpha}{n_{+}} \max\{0, 1 - y_{i}^{*} \frac{2n_{+}}{\alpha n} w^{T} x_{i}\} - \frac{\alpha}{n_{+}}\right) \mathbb{I}(y_{i}^{*} = 1) + \left(\frac{\beta}{n_{-}} \max\{0, 1 - y_{i}^{*} \frac{2n_{-}}{\beta n} w^{T} x_{i}\} - \frac{\beta}{n_{-}}\right) \mathbb{I}(y_{i}^{*} = -1)$$

Now we can re-write equation 2 as following

$$\mathcal{L}_{w}(\overline{x}, \overline{y}^{*}) = \max_{\alpha, \beta} \left\{ \frac{\alpha}{n_{+}} \sum_{y_{i}^{*}=1} \max\{0, 1 - y_{i}^{*} \frac{2n_{+}}{\alpha n} w^{T} x_{i}\} \right.$$
$$\left. + \frac{\beta}{n_{-}} \sum_{y_{i}^{*}=-1} \max\{0, 1 - y_{i}^{*} \frac{2n_{-}}{\beta n} w^{T} x_{i}\} \right.$$
$$\left. - (\alpha + \beta) + \phi^{*}(\alpha, \beta) \right\}$$

## Objective function

We can substitute the loss in struct SVM:

$$\begin{aligned} \min_{w} \frac{||w||^{2}}{2} + C\mathcal{L}_{w}(\overline{x}, \overline{y}^{*}) \\ &\equiv \min_{w} \frac{||w||^{2}}{2} + C \max_{\alpha, \beta} \{ \frac{\alpha}{n_{+}} \sum_{y_{i}^{*}=1} \max\{0, 1 - y_{i}^{*} \frac{2n_{+}}{\alpha n} w^{T} x_{i} \} \\ &+ \frac{\beta}{n_{-}} \sum_{y_{i}^{*}=-1} \max\{0, 1 - y_{i}^{*} \frac{2n_{-}}{\beta n} w^{T} x_{i} \} \\ &- (\alpha + \beta) + \phi^{*}(\alpha, \beta) \} \end{aligned}$$

## Solution Steps

We perform the following steps in each iterative cycle:

- Fix w
- ② Gradient ascent on  $\mathcal{L}_w(\overline{x}, \overline{y}^*)$  wrt  $\alpha, \beta$
- $\bullet$  Fix  $\alpha, \beta$
- SVM wrt w
- Go to step 1

We can use Liblinear solver to perform SVM.

## Conjugate function of $\phi(P, N)$

For any concave  $\phi$ 

$$\phi(P, N) = \min_{\alpha, \beta} \{\alpha P + \beta N - \phi^*(\alpha, \beta)\}$$

For G-mean as  $\phi$ 

$$\phi(P, N) = \sqrt{PN}$$
$$\phi^*(\alpha, \beta) = \min_{P, N} \{\alpha P + \beta N - \sqrt{PN}\}$$

Solving for 
$$g'(P, N) = 0$$
 where  $g = \alpha P + \beta N - \sqrt{PN}$ , we get  $\alpha = \frac{1}{2}\sqrt{\frac{N}{P}}$  and  $\beta = \frac{1}{2}\sqrt{\frac{P}{N}}$  giving

$$\phi^*(\alpha,\beta) = 0 \tag{3}$$

## Dual feasible region

Trivial:  $\alpha > 0, \beta > 0$  as  $P, N \ge 0$ 

$$g = \alpha P + \beta N - \sqrt{PN}$$
$$= (\sqrt{\alpha P} - \sqrt{\beta N})^2 + \sqrt{PN}(2\sqrt{\alpha\beta} - 1)$$

By ensuring  $P=\frac{\beta N}{\alpha}$  we can show the first part to be zero. For large P,N,  $g\to -\infty$  if  $2\sqrt{\alpha\beta}<1$ . Hence the feasible dual region is defined by,

$$dom(\alpha,\beta) = \{\alpha,\beta | \alpha\beta \ge \frac{1}{4}, \alpha > 0, \beta > 0\}$$

 $\mathbb{Q}$ . P, N has to be the number of true positives/negatives, not rate?

## Gradient computation

•  $h(\alpha) = \frac{\alpha}{n_+} \max\{0, 1 - y_i^* \frac{2n_+}{\alpha n} w^T x_i\}$ . By Danskin's theorem it can be shown that,

$$h'(\alpha) = \begin{cases} 0, & \text{if } y_i^* \frac{2n_+}{\alpha n} w^T x_i \ge 1\\ \frac{1}{n_+}, & \text{otherwise} \end{cases}$$

• Similarly for  $h(\beta) = \frac{\beta}{n_-} \max\{0, 1 - y_i^* \frac{2n_-}{\alpha n} w^T x_i\}$ . By Danskin's theorem it can be shown that,

$$h'(\beta) = \begin{cases} 0, & \text{if } y_i^* \frac{2n_-}{\beta n} w^T x_i \ge 1\\ \frac{1}{n_-}, & \text{otherwise} \end{cases}$$

• We have proved  $\phi^*(a,b) = 0$  for G-mean, hence its derivative gives 0.

#### Problem with Gradient Ascent

ullet Unbounded increase in dual variables in  $\mathbb{R}^2_+$ 

#### References



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## Thank You!