Czech Technical University in Prague V. Franc

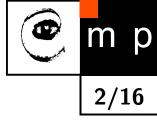
February 24, 2020

- Cutting Plane Algorithm
- Bundle Method for Risk Minimization

• Subgradients

XEP33SML – Structured Model Learning, Summer 2020

Structured Output SVM



• Learning $h(x; w) = \operatorname{Argmax}_{y \in \mathcal{Y}} \langle w, \phi(x, y) \rangle$ from examples $\mathcal{T}^m = \{(x^i, y^i) \in (\mathcal{X} \times \mathcal{Y}) \mid i = 1, \dots, m\}$ by ERM leads to

$$\boldsymbol{w}^* \in \operatorname{Argmin}_{\boldsymbol{w} \in \mathbb{R}^n} R_{\mathcal{T}^m}(\boldsymbol{w}) \quad \text{where} \quad R_{\mathcal{T}^m}(\boldsymbol{w}) = \frac{1}{m} \sum_{i=1}^m \ell(y^i, h(x^i; \boldsymbol{w}))$$

The SO-SVM approximates the ERM by a convex problem

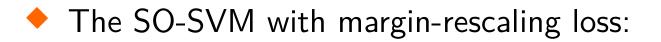
$$oldsymbol{w}^* \in \mathop{\mathrm{Argmin}}_{oldsymbol{w} \in \mathbb{R}^n} \left(rac{\lambda}{2} \|oldsymbol{w}\|^2 + R^\psi(oldsymbol{w})
ight) \quad ext{where} \quad R^\psi(oldsymbol{w}) = rac{1}{m} \sum_{i=1}^m \psi(x^i, y^i, oldsymbol{w})$$

• The surrograte loss $\psi \colon \mathcal{X} \times \mathcal{Y} \times \mathbb{R}^n \to \mathbb{R}$ is an upper bound:

 $\ell(y, h(x; \boldsymbol{w})) \leq \psi(x, y, \boldsymbol{w}), \quad \forall (x, y, \boldsymbol{w}) \in (\mathcal{X} \times \mathcal{Y} \times \mathbb{R}^n)$

which is convex in \boldsymbol{w} for any (x, y).

SO-SVM leads to a convex **QP**



$$\boldsymbol{w}^{*} \in \operatorname{Argmin}_{\boldsymbol{w} \in \mathbb{R}^{n}} \left(\frac{\lambda}{2} \|\boldsymbol{w}\|^{2} + \frac{1}{m} \sum_{i=1}^{m} \max_{y \in \mathcal{Y}} \{\ell_{i}(y) + \langle \boldsymbol{w}, \boldsymbol{\phi}_{i}(y) \rangle \} \right)_{R^{\psi}(\boldsymbol{w})}$$

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By using slack variables it can be rewritten as a Quadratic Program:

$$oldsymbol{w}^* = rgmin_{oldsymbol{w}\in\mathbb{R}^n,oldsymbol{\xi}\in\mathbb{R}^m} \left(rac{\lambda}{2} \|oldsymbol{w}\|^2 + rac{1}{m}\sum_{i=1}^m \xi_i
ight)$$

subject to

$$\xi_i \ge \ell_i(y) + \langle \boldsymbol{w}, \boldsymbol{\phi}_i(y) \rangle, \quad \forall i \in \{1, \dots, m\}, \forall y \in \mathcal{Y}$$

• Note that the QP has $m|\mathcal{Y}|$ linear constaints !



The SO-SVM with margin-rescaling loss:

$$oldsymbol{w}^* \in \operatorname*{Argmin}_{oldsymbol{w} \in \mathbb{R}^n} \left(rac{\lambda}{2} \|oldsymbol{w}\|^2 + R^{\psi}(oldsymbol{w})
ight)$$

Equivalent formulation: for any $\lambda > 0$ there exists r > 0 such that

$$oldsymbol{w}^* \in \operatorname{Argmin}_{oldsymbol{w} \in \mathcal{W}} R^{\psi}(oldsymbol{w})$$
 (1)

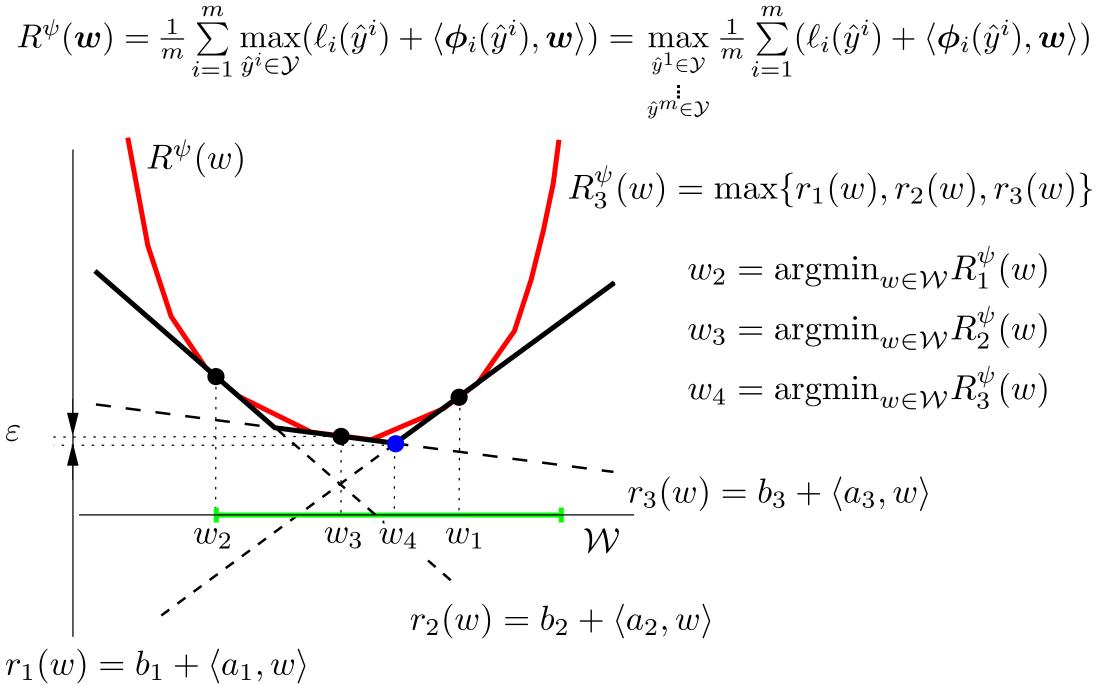
where $\mathcal{W} = \{ \boldsymbol{w} \in \mathbb{R}^n \mid \|\boldsymbol{w}\| \leq r \}$ is a ball of radius r.

• CP algorithm: approximate (1) by a series of simpler problems

$$\boldsymbol{w}_{t+1} \in \operatorname{Argmin}_{\boldsymbol{w} \in \mathcal{W}} R_t^{\psi}(\boldsymbol{w}), \qquad t = 1, 2, \dots$$

where $R_t^{\psi}(oldsymbol{w})$ is a successively tighter lower bound of $R^{\psi}(oldsymbol{w})$.







1. $oldsymbol{w}_1 \in \mathcal{W} = \{oldsymbol{w} \in \mathbb{R}^n \mid \|oldsymbol{w}\| \leq r\}$, $t \leftarrow 1$

2. Compute a new cutting plane and the objective value:

$$\boldsymbol{a}_t = \frac{1}{m} \sum_{i=1}^m \boldsymbol{\phi}_i(\hat{y}^i), \quad b_t = \frac{1}{m} \sum_{i=1}^m \ell_i(\hat{y}^i), \quad R^{\psi}(\boldsymbol{w}_t) = b_t + \langle \boldsymbol{w}_t, \boldsymbol{a}_t \rangle$$

where \hat{y}^i is a solutions of loss augmented prediction problem:

$$\hat{y}^{i} = \operatorname*{argmax}_{y \in \mathcal{Y}} \left(\ell_{i}(y) + \langle \boldsymbol{w}, \boldsymbol{\phi}_{i}(y) \rangle \right) = \operatorname*{argmax}_{y \in \mathcal{Y}} \left(\ell(y^{i}, y) + \langle \boldsymbol{w}, \boldsymbol{\phi}(x^{i}, y) \rangle \right)$$

3. Solve a reduced problem

$$oldsymbol{w}_{t+1} = \operatorname*{argmin}_{oldsymbol{w} \in \mathcal{W}} R_t^\psi(oldsymbol{w}) \quad ext{where} \quad R_t^\psi(oldsymbol{w}) = \operatorname*{max}_{i=1,...,t} (b_i + \langle oldsymbol{w}, oldsymbol{a}_i
angle)$$

4. If $\min_{i=1,...,t} R^{\psi}(\boldsymbol{w}_t) - R_t^{\psi}(\boldsymbol{w}_{t+1}) \leq \varepsilon$ exit else $t \leftarrow t+1$ and go to 2.

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- 1. $\boldsymbol{w}_1 \in \mathbb{R}^n$, $t \leftarrow 1$
- 2. Compute a new cutting plane and the objective value:

$$\boldsymbol{a}_t = \frac{1}{m} \sum_{i=1}^m \boldsymbol{\phi}_i(\hat{y}^i), \quad b_t = \frac{1}{m} \sum_{i=1}^m \ell_i(\hat{y}^i), \quad R^{\psi}(\boldsymbol{w}_t) = b_t + \langle \boldsymbol{w}_t, \boldsymbol{a}_t \rangle$$

where \hat{y}^i is a solutions of loss augmented prediction problem:

Bundle Method for Risk Minimization

$$\hat{y}^{i} = \operatorname*{argmax}_{y \in \mathcal{Y}} \left(\ell_{i}(y) + \langle \boldsymbol{w}, \boldsymbol{\phi}_{i}(y) \rangle \right) = \operatorname*{argmax}_{y \in \mathcal{Y}} \left(\ell(y^{i}, y) + \langle \boldsymbol{w}, \boldsymbol{\phi}(x^{i}, y) \rangle \right)$$

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$$oldsymbol{w}_{t+1} = \operatorname*{argmin}_{oldsymbol{w} \in \mathbb{R}^n} \left(rac{\lambda}{2} \|oldsymbol{w}\|^2 + R_t^\psi(oldsymbol{w})
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 where $R_t^\psi(oldsymbol{w}) = \max_{i=1,...,t} (b_i + \langle oldsymbol{w}, oldsymbol{a}_i
angle)$

4. If $\min_{i=1,...,t} \left(\frac{\lambda}{2} \|\boldsymbol{w}_i\|^2 + R^{\psi}(\boldsymbol{w}_i)\right) - \left(\frac{\lambda}{2} \|\boldsymbol{w}_{t+1}\|^2 + R_t^{\psi}(\boldsymbol{w}_{t+1})\right) \leq \varepsilon$ exit else $t \leftarrow t+1$ and go to 2.

Bundle Method for Risk Minimization

The original convex problem

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^n} F(\boldsymbol{w}) := \left(\frac{\lambda}{2} \|\boldsymbol{w}\|^2 + R(\boldsymbol{w})\right)$$

is reduced to a sequence of reduced convex problems

$$\boldsymbol{w}_{t+1} = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^n} F_t(\boldsymbol{w}) := \left(\frac{\lambda}{2} \|\boldsymbol{w}\|^2 + R_t(\boldsymbol{w})\right)$$

where $R_t(\boldsymbol{w})$ is the "cutting plane model"

$$R_t(\boldsymbol{w}) = \max_{i=0,\dots,t} \left[R(\boldsymbol{w}_i) + \langle \boldsymbol{g}_i, \boldsymbol{w} - \boldsymbol{w}_i \rangle \right]$$

and $\boldsymbol{g}_i = \partial R(\boldsymbol{w}_i)$ is a subgradient of $R(\boldsymbol{w})$ at \boldsymbol{w}_i .

By construction it holds that $R_t(\boldsymbol{w}) \leq R(\boldsymbol{w})$, $\forall \in \mathbb{R}^n$.



Subgradient

• Let $f: \mathcal{X} \to \mathbb{R}$ be a convex function where $\mathcal{X} \subseteq \mathbb{R}^n$ is a convex set.

• For differentiable f the gradient $\nabla f(x') \in \mathbb{R}^n$ at point $x' \in \mathcal{X}$ determines a global under-estimator of f

$$f(\boldsymbol{x}) \geq f(\boldsymbol{x}') + \nabla f(\boldsymbol{x}')^T (\boldsymbol{x} - \boldsymbol{x}'), \quad \forall \boldsymbol{x} \in \mathcal{X}.$$

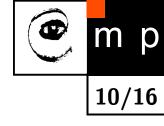
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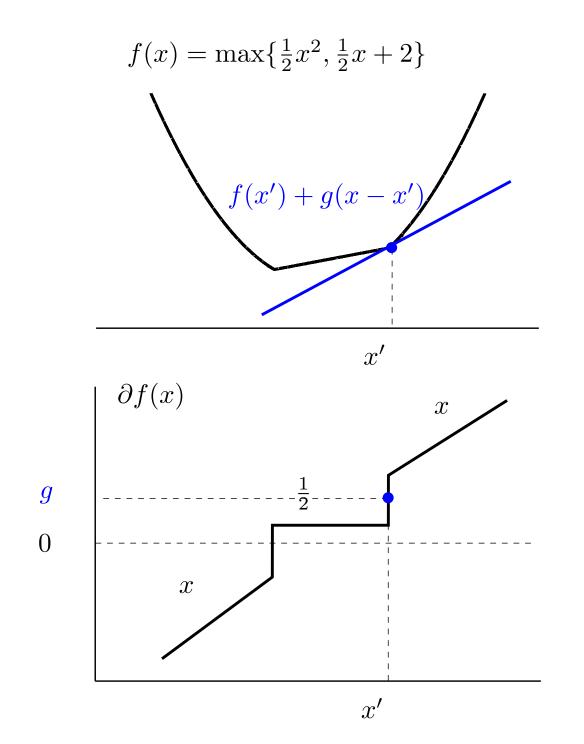
• For non-differentiable f we can still construct a global under-estimator: the vector $g \in \mathbb{R}^n$ is a subgradient of f at point $x' \in \mathcal{X}$ if

$$f(\boldsymbol{x}) \geq f(\boldsymbol{x}') + \boldsymbol{g}^T(\boldsymbol{x} - \boldsymbol{x}'), \quad \forall \boldsymbol{x} \in \mathcal{X}.$$

• There can be more then one subgradient at given point: the collection of subgradients of f at point $x \in \mathcal{X}$ is the subdifferential $\partial f(x)$.

An example: non-differentiable function and its subgradients





Basic subgradient calculus

- $\partial f(\boldsymbol{x})$ is a closed convex set.
- $\partial f(\boldsymbol{x}) = \{\boldsymbol{g}\} \iff f \text{ is differentiable and } \boldsymbol{g} = \nabla f(\boldsymbol{x}).$
- scaling: $\partial(\alpha f(\boldsymbol{x})) = \alpha \partial f(\boldsymbol{x})$ if $\alpha > 0$.
- addition: $\partial(f_1(\boldsymbol{x}) + f_2(\boldsymbol{x})) = \partial f_1(\boldsymbol{x}) + \partial f_2(\boldsymbol{x}).$
- point-wise maximum: $f(x) = \max_{i=1,...,m} f_i(x)$ when $f_i(x)$ are differentiable then

$$\partial f(\boldsymbol{x}) = \mathbf{Co} \{ \nabla f_i(\boldsymbol{x}) \mid f_i(\boldsymbol{x}) = f(\boldsymbol{x}) \},\$$

i.e., convex hull of gradients of active functions at x.

• Optimality condition for a convex f:

$$f(\boldsymbol{x}^*) = \inf_{\boldsymbol{x}} f(\boldsymbol{x}) \iff \boldsymbol{0} \in \partial f(\boldsymbol{x}^*)$$



Example: cutting plane model for SVM

The convex problem to solver

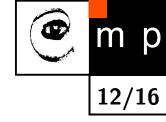
$$\boldsymbol{w}^* \in \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^n} \left(\frac{\lambda}{2} \|\boldsymbol{w}\|^2 + \underbrace{\frac{1}{m} \sum_{i=1}^m \max\left\{ 0, 1 - y^i \langle \boldsymbol{w}, \boldsymbol{x}^i \rangle \right\}}_{R(\boldsymbol{w})} \right)$$

• The cutting plane model of $R(\boldsymbol{w})$ reads

$$R_t(\boldsymbol{w}) = \max_{i=0,\dots,t-1} \left[R(\boldsymbol{w}_i) + \langle \boldsymbol{g}_i, \boldsymbol{w} - \boldsymbol{w}_i \rangle \right]$$

• The subgradient of $R(\boldsymbol{w})$ at \boldsymbol{w}

$$oldsymbol{g}_i = -rac{1}{m}\sum_{i=1}^m y^i \, oldsymbol{x}^i \, [\![\langle oldsymbol{w}, oldsymbol{x}^i
angle \leq 1]\!]$$





$$\boldsymbol{w}^{*} \in \underset{\boldsymbol{w} \in \mathbb{R}^{n}}{\operatorname{argmin}} \left(\frac{\lambda}{2} \|\boldsymbol{w}\|^{2} + \underbrace{\frac{1}{m} \sum_{i=1}^{m} \max_{y \in \mathcal{Y}} \{\ell_{i}(y) + \langle \boldsymbol{w}, \boldsymbol{\phi}_{i}(y) \rangle \}}_{R(\boldsymbol{w})} \right)$$

• The cutting plane model of $R(\boldsymbol{w})$ reads

$$R_t(\boldsymbol{w}) = \max_{i=0,\dots,t-1} \left[R(\boldsymbol{w}_i) + \langle \boldsymbol{g}_i, \boldsymbol{w} - \boldsymbol{w}_i \rangle \right]$$

• The subgradient of $R(\boldsymbol{w})$ at \boldsymbol{w}

$$\boldsymbol{g}_i = \frac{1}{m} \sum_{i=1}^m \boldsymbol{\phi}_i(\hat{y}^i)$$
 where $\hat{y}^i = \operatorname*{argmax}_{y \in \mathcal{Y}} \{\ell_i(y) + \langle \boldsymbol{w}_i, \boldsymbol{\phi}_i(y) \rangle \}$

Bundle Method for Risk Minimization

1. Init: $t \leftarrow 0$, $oldsymbol{w}_0 \in \mathbb{R}^n$

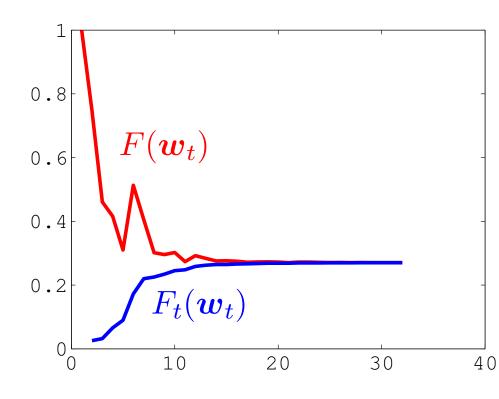
2. Compute $R(\boldsymbol{w}_t)$ and $\boldsymbol{g}_t \in \partial R(\boldsymbol{w}_t)$

3.
$$\boldsymbol{w}_{t+1} = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^n} \left(\frac{\lambda}{2} \| \boldsymbol{w} \|^2 + R_t(\boldsymbol{w}) \right)$$

where

$$R_t(\boldsymbol{w}) = \max_{i=0,\dots,t} \left[R(\boldsymbol{w}_i) + \langle \boldsymbol{g}_i, \boldsymbol{w} - \boldsymbol{w}_i \rangle \right]$$

4. if $\min_{i=1,...,t} F(\boldsymbol{w}_i) - F_t(\boldsymbol{w}_{t+1}) \leq \varepsilon$ stop else $t \leftarrow t+1$ go to 2.





How to solve the reduced problem

- Let us define a matrix $\mathbf{A} = [\mathbf{g}_0, \dots, \mathbf{g}_t] \in \mathbb{R}^{n \times t}$ and a vector $b = [b_0, \dots, b_{t-1}]$ with components $b_i = R(\mathbf{w}_i) \langle \mathbf{g}_i, \mathbf{w}_i \rangle$.
- The reduced problem can be expressed as

$$\boldsymbol{w}_{t+1} = \operatorname*{argmin}_{\boldsymbol{w} \in \mathbb{R}^n, \xi \in \mathbb{R}} \left[\frac{\lambda}{2} \| \boldsymbol{w} \|^2 + \xi \right]$$
 s.t. $\xi \ge \langle \boldsymbol{w}, \boldsymbol{g}_i \rangle + b_i, i \in \{0, \dots, t\}$

The Lagrange dual of the reduced problem reads

$$\boldsymbol{\alpha}_{t+1} = \operatorname*{argmax}_{\boldsymbol{\alpha} \in \mathbb{R}^t} \left[\langle \boldsymbol{\alpha}, \boldsymbol{b} \rangle - \frac{1}{2\lambda} \langle \boldsymbol{\alpha}, \mathbf{A}^T \mathbf{A} \boldsymbol{\alpha} \rangle \right] \quad \text{s.t.} \quad \|\boldsymbol{\alpha}\|_1 = 1, \boldsymbol{\alpha} \ge \mathbf{0}$$

• The primal solution is $oldsymbol{w}_{t+1} = -\lambda^{-1} \mathbf{A} oldsymbol{lpha}_{t+1}$



Bundle Method for Risk Minimization

(+) Provides a certificate of optimility:

$$F(\boldsymbol{w}_t) \leq F(\boldsymbol{w}^*) + \varepsilon$$

(+) Converges for arbitrary $\varepsilon > 0$ in

$$\log_2 \frac{\lambda F(\mathbf{0})}{G^2} + \frac{4G^2}{\lambda \varepsilon} - 1$$

iteration at most where $G \geq \|\boldsymbol{g}\|_2$, $\forall \boldsymbol{g} \in \partial R(\boldsymbol{w})$, $\boldsymbol{w} \in \mathbb{R}^n$.

(+) Requires only the first order oracle computing R(w) and $g \in \partial R(w)$. (-) Slow convergence for $\lambda \to 0$.

