Notice

- Homework assignments Week 13:
 - 1 programming work (6%).
 - Due date: 21 p.m. on December 25, 2021.

Outline

- Lecture 6: Primal and dual problems
 - Lagrangian dual problems
- Lecture 7: Alternating Direction Method of Multipliers
 - The basic form
 - Application I: Sparse group lasso estimation
 - Application II: Support vector machines
 - Application III: Splitting across examples
- Lecture 8: More on convex analysis
 - Subdifferentials and subgradients
- Solutions to quizzes in Week 12 and homework assignments in Week 11

Computation in Data Science: Week 13 Lecture 6

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Constrained optimization problems:

Consider the following constrained optimization problem:

$$\begin{aligned} & \min_{\mathbf{X}} & & l(\mathbf{x}) \\ \text{subject to} & & \mathbf{x} \in \mathcal{C}, \end{aligned} \tag{1}$$

where $l:\mathbb{R}^p\mapsto\mathbb{R}$ is the objective function of the problem (1), and $\mathcal C$ is defined as

$$C = \left\{ \mathbf{x} : \mathbf{x} \in \mathbb{R}^p, f_i(\mathbf{x}) \le 0 \text{ for } i = 1, 2, \dots, m, \right.$$

$$\text{and } h_j(\mathbf{x}) = 0 \text{ for } j = 1, 2, \dots, n \right\}. \tag{2}$$

ullet C is assumed to be nonempty.

- The basic idea:
 - Introduce a set of variables $\mathbf{u}=(u_1,u_2,\cdots,u_m)$ and $\mathbf{v}=(v_1,v_2,\cdots,v_n)$ to formulate the following function:

$$L(\mathbf{x}, \mathbf{u}, \mathbf{v}) = l(\mathbf{x}) + \sum_{i=1}^{m} u_i f_i(\mathbf{x}) + \sum_{j=1}^{n} v_j h_j(\mathbf{x}).$$
(3)

Here (3) is called the **Lagrangian** corresponding to the primal problem (1), and the quantities u_i 's and v_j 's are called the **Lagrange multipliers**.

With (3) we formulate another optimization problem as

$$\max_{\mathbf{U},\mathbf{V}} \qquad \left\{ \min_{\mathbf{X}} \left[l(\mathbf{x}) + \sum_{i=1}^{m} u_i f_i(\mathbf{x}) + \sum_{j=1}^{n} v_j h_j(\mathbf{x}) \right] \right\}$$
 subject to
$$u_i \geq 0 \text{ for } i = 1, 2, \cdots, m. \tag{4}$$

The optimization problem (4) is called the Lagrangian dual of (1).

- Duality gap:
 - Define

$$L(\mathbf{u}, \mathbf{v}) = \min_{\mathbf{X}} \left[l(\mathbf{x}) + \sum_{i=1}^{m} u_i f_i(\mathbf{x}) + \sum_{j=1}^{n} v_j h_j(\mathbf{x}) \right].$$

 Assume x** is a solution to the primal problem (1) and (u**, v**) is a solution to the Lagrangian dual problem (4). We have

$$\mathsf{opt}^{\mathsf{dual}} = L(\mathbf{u}^{**}, \mathbf{v}^{**}) \le L(\mathbf{x}^{**}, \mathbf{u}^{**}, \mathbf{v}^{**}) \le l(\mathbf{x}^{**}) = \mathsf{opt}^{\mathsf{primal}},$$

which implies the duality gap $opt^{primal} - opt^{dual} \ge 0$.

 Remark: If opt^{primal} = opt^{dual}, then we say strong duality holds for the primal problem (1) and dual problem (4).

- The Karush-Kuhn-Tucker conditions:
 - Now assume l(x), f_i(x)'s and h_j(x)'s are differentiable. Consider the following conditions for point (x*, u*, v*):

$$\begin{split} &f_i(\mathbf{x}^*) \leq 0 \text{ for } i=1,2,\cdots,m \text{ (Primal feasibility)}, \\ &h_j(\mathbf{x}^*) = 0 \text{ for } j=1,2,\cdots,n \text{ (Primal feasibility)}, \\ &u_i^* \geq 0 \text{ for } i=1,2,\cdots,m \text{ (Dual feasibility)}, \\ &u_i^* f_i(\mathbf{x}^*) = 0 \text{ for } i=1,2,\cdots,m \text{ (Complementary slackness)}, \\ &\nabla l(\mathbf{x}^*) + \sum_{i=1}^m u_i^* \nabla f_i(\mathbf{x}^*) + \sum_{j=1}^n v_j^* \nabla h_j(\mathbf{x}^*) = \mathbf{0} \text{ (Stationarity)}. \end{split}$$

These conditions are called the Karush-Kuhn-Tucker conditions or KKT conditions.

- Implications of the Karush-Kuhn-Tucker conditions:
 - The KKT conditions are necessary conditions for checking whether a point is a solution to an optimization problem.
 - The KKT conditions further turn out to be sufficient conditions when
 - i). l, f_i 's and h_j 's are differentiable;
 - ii). l is convex;
 - iii). C is a convex set;
 - iv). h_j 's are affine maps on x.
 - If i), ii), iii) and iv) are satisfied and the point (x^*, u^*, v^*) satisfies the KKT conditions, then x^* is a solution to the primal problem (1), and (u^*, v^*) is a solution to the dual problem (4).

In this situation, \mathbf{x}^* is called the **primal optimal point** and $(\mathbf{u}^*, \mathbf{v}^*)$ is called the **dual optimal point**.

- An example of the Lagrangian dual problem:
 - Now consider the following optimization problem:

$$\label{eq:local_problem} \begin{aligned} & & & \text{minimize} & & & & & l(\mathbf{x}) \\ & & & & & & \mathbf{A}\mathbf{x} \leq \mathbf{b} \\ & & & & & & \mathbf{C}\mathbf{x} = \mathbf{d}. \end{aligned}$$

By definition, the dual objective is

$$\begin{split} L(\mathbf{u}, \mathbf{v}) &= & \min_{\mathbf{X}} \{l(\mathbf{x}) + \mathbf{u}^T (\mathbf{A} \mathbf{x} - \mathbf{b}) + \mathbf{v}^T (\mathbf{C} \mathbf{x} - \mathbf{d}) \} \\ &= & -\mathbf{b}^T \mathbf{u} - \mathbf{d}^T \mathbf{v} + \min_{\mathbf{X}} \{l(\mathbf{x}) + \mathbf{x}^T (\mathbf{A}^T \mathbf{u} + \mathbf{C}^T \mathbf{v}) \} \\ &= & -\mathbf{b}^T \mathbf{u} - \mathbf{d}^T \mathbf{v} - \max_{\mathbf{X}} \{\mathbf{x}^T (-\mathbf{A}^T \mathbf{u} - \mathbf{C}^T \mathbf{v}) - l(\mathbf{x}) \} \\ &= & -\mathbf{b}^T \mathbf{u} - \mathbf{d}^T \mathbf{v} - l^* (-\mathbf{A}^T \mathbf{u} - \mathbf{C}^T \mathbf{v}). \end{split}$$

• Therefore the Lagrangian dual problem is

• Why derives the Lagrangian dual problem?

- The Lagrangian dual problem provides a lower bound for the primal problem.
- When strong duality holds, solving the Lagrangian dual problem is equivalent to solving the primal problem.
- In some cases it may be easier to solve the dual problem than to solve the primal problem.

• Why derives the KKT conditions?

 The KKT conditions provide a guide for how the possible primal and dual optimal points should behave, which is key to formulate stopping criteria for relevant optimization algorithms.

Computation in Data Science: Week 13 Lecture 7

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• Now consider the following optimization problem:

$$\begin{aligned} & \text{minimize}_{\pmb{\beta},\pmb{\gamma}} & & & l(\pmb{\beta}) + g(\pmb{\gamma}) \\ & \text{subject to} & & & \mathbf{U}\pmb{\beta} + \mathbf{V}\pmb{\gamma} = \mathbf{b}, \end{aligned} \tag{5}$$

where ${\bf U}$ is an $m\times p$ matrix, ${\bf V}$ is an $m\times q$ matrix, ${\boldsymbol \beta}\in\mathbb{R}^p$, ${\boldsymbol \gamma}\in\mathbb{R}^q$ and ${\bf b}\in\mathbb{R}^m.$

• The augmented Lagrangian: For (5) it is

$$\begin{split} \tilde{L}_{\rho}(\boldsymbol{\beta}, \boldsymbol{\gamma}, \mathbf{a}) &= l(\boldsymbol{\beta}) + g(\boldsymbol{\gamma}) + \mathbf{a}^{T}(\mathbf{U}\boldsymbol{\beta} + \mathbf{V}\boldsymbol{\gamma} - \mathbf{b}) \\ &+ \frac{\rho}{2} ||\mathbf{U}\boldsymbol{\beta} + \mathbf{V}\boldsymbol{\gamma} - \mathbf{b}||_{2}^{2}, \end{split} \tag{6}$$

where ${\bf a}$ is an m-dimensional vector of Lagrange multipliers.

• Remark: The last term of (6) is a coupling quadratic term that connects the linear transform of $U\beta$ and $V\gamma$.

• Now let $\mathbf{v} = \mathbf{U}\boldsymbol{\beta} + \mathbf{V}\boldsymbol{\gamma} - \mathbf{b}$. Putting \mathbf{v} into the last two terms of (6) yields

$$\mathbf{a}^{T}\mathbf{v} + \frac{\rho}{2}||\mathbf{v}||_{2}^{2} = \frac{\rho}{2}\left(\mathbf{v}^{T}\mathbf{v} + \frac{2}{\rho}\mathbf{a}^{T}\mathbf{v} + \frac{1}{\rho^{2}}\mathbf{a}^{T}\mathbf{a}\right) - \frac{1}{2\rho}\mathbf{a}^{T}\mathbf{a}$$

$$= \frac{\rho}{2}||\mathbf{v} + (1/\rho)\mathbf{a}||_{2}^{2} - \frac{1}{2\rho}||\mathbf{a}||_{2}^{2}. \tag{7}$$

Putting $\alpha = (1/\rho)a$ into (7) and replacing the last two terms of (6) with the scaled form (7), we obtain

$$\begin{split} &\tilde{L}_{\rho}(\boldsymbol{\beta},\boldsymbol{\gamma},\mathbf{a})\\ &= L_{\rho}(\boldsymbol{\beta},\boldsymbol{\gamma},\boldsymbol{\alpha})\\ &= l(\boldsymbol{\beta}) + g(\boldsymbol{\gamma}) + \frac{\rho}{2}||\mathbf{U}\boldsymbol{\beta} + \mathbf{V}\boldsymbol{\gamma} - \mathbf{b} + \boldsymbol{\alpha}||_{2}^{2} - \frac{\rho}{2}||\boldsymbol{\alpha}||_{2}^{2}. \end{split} \tag{8}$$

• Here we call β the primal variables, γ the auxiliary variables and α the dual variables.

An iterative scheme:

 The scaled augmented Lagrangian (8) can be minimized by using the following iterative scheme to find a minimizer:

$$\begin{split} \boldsymbol{\beta}^{r+1} &= & \arg\min_{\boldsymbol{\beta}} \left\{ l(\boldsymbol{\beta}) + \frac{\rho}{2} || \mathbf{U}\boldsymbol{\beta} + \mathbf{V}\boldsymbol{\gamma}^r - \mathbf{b} + \boldsymbol{\alpha}^r ||_2^2 \right\} \\ \boldsymbol{\gamma}^{r+1} &= & \arg\min_{\boldsymbol{\gamma}} \left\{ g(\boldsymbol{\gamma}) + \frac{\rho}{2} || \mathbf{U}\boldsymbol{\beta}^{r+1} + \mathbf{V}\boldsymbol{\gamma} - \mathbf{b} + \boldsymbol{\alpha}^r ||_2^2 \right\} \\ \boldsymbol{\alpha}^{r+1} &= & \boldsymbol{\alpha}^r + \mathbf{U}\boldsymbol{\beta}^{r+1} + \mathbf{V}\boldsymbol{\gamma}^{r+1} - \mathbf{b}. \end{split} \tag{9}$$

- The iterative scheme (9) is an example of the alternating direction method of multipliers.
- Remark: Each line in (9) updates a set of parameters given that all other parameters are fixed.

- Stopping criteria:
 - KKT conditions: If (β^*, γ^*) is a solution to the primal problem of (5) and α^* is a solution to the Lagrangian dual problem associated with (5), then the following conditions must be satisfied:
 - The primal feasibility condition:

$$\mathbf{U}\boldsymbol{\beta}^* + \mathbf{V}\boldsymbol{\gamma}^* = \mathbf{b}.$$

• The stationarity condition:

$$\mathbf{0} \in \begin{bmatrix} \partial l(\boldsymbol{\beta}^*) + \rho \mathbf{U}^T \boldsymbol{\alpha}^* \\ \partial g(\boldsymbol{\gamma}^*) + \rho \mathbf{V}^T \boldsymbol{\alpha}^* \end{bmatrix}.$$

Stopping criteria (contd):

• One can show that β^{r+1} should satisfy the following relationship:

$$\begin{aligned} \mathbf{0} &\in & \partial l(\boldsymbol{\beta}^{r+1}) + \rho \mathbf{U}^T (\mathbf{U} \boldsymbol{\beta}^{r+1} + \mathbf{V} \boldsymbol{\gamma}^r - \mathbf{b} + \boldsymbol{\alpha}^r) \\ &= & \partial l(\boldsymbol{\beta}^{r+1}) + \rho \mathbf{U}^T \boldsymbol{\alpha}^r + \rho \mathbf{U}^T \mathbf{U} \boldsymbol{\beta}^{r+1} - \rho \mathbf{U}^T \mathbf{b} + \rho \mathbf{U}^T \mathbf{V} \boldsymbol{\gamma}^r. \end{aligned}$$
 (10)

This is the **stationarity condition** for the first line of the iterative scheme (9).

• On the other hand, from the third line of (9) we have

$$\mathbf{U}^T \boldsymbol{\alpha}^{r+1} = \mathbf{U}^T \boldsymbol{\alpha}^r + \mathbf{U}^T \mathbf{U} \boldsymbol{\beta}^{r+1} + \mathbf{U}^T \mathbf{V} \boldsymbol{\gamma}^{r+1} - \mathbf{U}^T \mathbf{b}.$$
 (11)

Plugging in (11) into (10) and rearranging it yields

$$\rho \mathbf{U}^T \mathbf{V} (\boldsymbol{\gamma}^{r+1} - \boldsymbol{\gamma}^r) \in \partial l(\boldsymbol{\beta}^{r+1}) + \rho \mathbf{U}^T \boldsymbol{\alpha}^{r+1}.$$

- Stopping criteria (contd):
 - Now define

$$\begin{aligned} \mathbf{t}^{r+1} &= & \mathbf{U}\boldsymbol{\beta}^{r+1} + \mathbf{V}\boldsymbol{\gamma}^{r+1} - \mathbf{b}, \\ \mathbf{s}^{r+1} &= & \rho \mathbf{U}^T \mathbf{V} (\boldsymbol{\gamma}^{r+1} - \boldsymbol{\gamma}^r). \end{aligned}$$

• As suggested by Boyd et al. (2010), one may use the following criteria:

$$\begin{split} &\frac{||\mathbf{t}^r||_2}{\sqrt{m}} & \leq & \epsilon^{\mathsf{abs}} + \frac{10^{-4}}{\sqrt{m}} \max\{||\mathbf{U}\boldsymbol{\beta}^r||_2, ||\mathbf{V}\boldsymbol{\beta}^r||_2, ||\mathbf{b}||_2\}, \\ &\frac{||\mathbf{s}^r||_2}{\sqrt{p}} & \leq & \epsilon^{\mathsf{abs}} + \frac{10^{-4}}{\sqrt{p}} ||\rho \mathbf{U}^T \boldsymbol{\alpha}^r||_2 \end{split}$$

to stop the iterative scheme (9).

- Here t^r and s^r are called the primal residual and the dual residual at the rth iteration, respectively.
- As shown by Boyd et al. (2010), when both l and q are convex,

$$l(\boldsymbol{\beta}^r) + g(\boldsymbol{\gamma}^r) - \text{ opt}^{\mathsf{primal}} \leq ||\rho \boldsymbol{\alpha}^r||_2 ||\mathbf{t}^r||_2 + ||\boldsymbol{\beta}^r - \boldsymbol{\beta}^*||_2 ||\mathbf{s}^r||_2.$$

• Choices of ρ :

- The scale parameter ρ measures the penalty to which the constraints or the **primal feasibility** (The constraints $U\beta + V\gamma = b$) are violated.
- We can either fix ρ during the iteration or vary it to adjust the ratio between the primal and dual residuals.
- Boyd et al. (2010) provided an adaptive method for computing ρ .

Sparse group lasso estimation:

• Suppose $\mathbf{X}=(\mathbf{X}_{[1]},\mathbf{X}_{[2]},\cdots,\mathbf{X}_{[m]})$, where $\mathbf{X}_{[j]}$ is an $n\times p_j$ matrix, and \mathbf{X} is an $n\times p$ matrix, where $p=\sum_{j=1}^m p_j$. We model response \mathbf{y} as

$$\mathbf{y} = \mathbf{X}\boldsymbol{eta} + \boldsymbol{\epsilon} = \sum_{j=1}^{m} \mathbf{X}_{[j]} \boldsymbol{eta}_j + \boldsymbol{\epsilon},$$

where $\beta = (\beta_1, \beta_2, \cdots, \beta_m)$, and ϵ is an n-dimensional vector of residuals.

- We want to do "variable selection" that can simultaneously select X_[j] and columns of X_[j], i.e. both between-group and within-group sparsity are considered.
- The sparse group lasso estimation aims to simultaneously do between-group and within-group variable selection:

$$\widehat{\boldsymbol{\beta}}^{\mathsf{SGL}} = \arg\min_{\boldsymbol{\beta}_{j}'s} \left\{ \frac{1}{2} \left\| \mathbf{y} - \sum_{i=1}^{m} \mathbf{X}_{[j]} \boldsymbol{\beta}_{j} \right\|_{2}^{2} + \sum_{i=1}^{m} \left(\lambda_{j} || \boldsymbol{\beta}_{j} ||_{2} + \lambda_{0} || \boldsymbol{\beta}_{j} ||_{1} \right) \right\}. \tag{12}$$

- Sparse group lasso estimation (contd):
 - We reformulate the optimization problem (12) by introducing a set of auxiliary vectors $\boldsymbol{\gamma}_j$'s and a set of equality constraints $\boldsymbol{\gamma}_j = \boldsymbol{\beta}_j$:

$$\begin{aligned} & \text{minimize}_{\boldsymbol{\beta}_{j}'s} & & \left\{ \frac{1}{2} \left| \left| \mathbf{y} - \sum_{j=1}^{m} \mathbf{X}_{[j]} \boldsymbol{\beta}_{j} \right| \right|_{2}^{2} + \sum_{j=1}^{m} \left(\lambda_{j} || \boldsymbol{\gamma}_{j} ||_{2} + \lambda_{0} || \boldsymbol{\gamma}_{j} ||_{1} \right) \right\} \\ & \text{subject to} & & \boldsymbol{\gamma}_{j} = \boldsymbol{\beta}_{j} \text{ for } j = 1, 2, \cdots, m. \end{aligned} \tag{13}$$

• The augmented Lagrangian corresponding to (13) is

$$L_{\rho}(\boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{\alpha}) = \frac{1}{2} \left\| \mathbf{y} - \sum_{j=1}^{m} \mathbf{X}_{[j]} \boldsymbol{\beta}_{j} \right\|_{2}^{2} + \sum_{j=1}^{m} \left(\lambda_{j} || \boldsymbol{\gamma}_{j} ||_{2} + \lambda_{0} || \boldsymbol{\gamma}_{j} ||_{1} \right) + \frac{\rho}{2} \sum_{j=1}^{m} \left(|| \boldsymbol{\beta}_{j} - \boldsymbol{\gamma}_{j} + \boldsymbol{\alpha}_{j} ||_{2}^{2} - || \boldsymbol{\alpha}_{j} ||_{2}^{2} \right),$$
(14)

where α_j 's are newly introduced scaled dual variables.

- Sparse group lasso estimation (contd):
 - We use the following iterative scheme to find a solution to the problem of minimizing (14):

$$\beta^{r+1} = \arg \min_{\beta} \left\{ \frac{1}{2} \left\| \mathbf{y} - \sum_{j=1}^{m} \mathbf{X}_{[j]} \beta_{j} \right\|_{2}^{2} + \frac{\rho}{2} \sum_{j=1}^{m} \left(||\beta_{j} - \gamma_{j}^{r} + \alpha_{j}^{r}||_{2}^{2} \right) \right\}$$

$$\gamma_{j}^{r+1} = \arg \min_{\gamma_{j}} \left(\frac{\lambda_{j}}{\rho} ||\gamma_{j}||_{2} + \frac{\lambda_{0}}{\rho} ||\gamma_{j}||_{1} + \frac{1}{2} ||\gamma_{j} - \beta_{j}^{r+1} - \alpha_{j}^{r}||_{2}^{2} \right)$$
for $j = 1, 2, \dots, m$

$$\alpha_{j}^{r+1} = \alpha_{j}^{r} + \beta_{j}^{r+1} - \gamma_{j}^{r+1} \text{ for } j, 1, 2, \dots, m.$$
(15)

• The first line of (15) has a closed form representation:

$$\boldsymbol{\beta}^{r+1} = (\mathbf{X}^T \mathbf{X} + \rho \mathbf{I}_{p \times p})^{-1} [\mathbf{X}^T \mathbf{y} + \rho (\boldsymbol{\gamma}^r - \boldsymbol{\alpha}^r)], \tag{16}$$

where $\gamma=(\gamma_1,\gamma_2,\cdots,\gamma_m)$ and $\alpha=(\alpha_1,\alpha_2,\cdots,\alpha_m)$.

- Sparse group lasso estimation (contd):
 - The second line of (15) also has a heuristic representation:

$$\gamma_{j}^{r+1} = \left(||S_{\lambda_{0}/\rho} \circ (\beta_{j}^{r+1} + \alpha_{j}^{r})||_{2} - \frac{\lambda_{j}}{\rho} \right)_{+} \frac{S_{\lambda_{0}/\rho} \circ (\beta_{j}^{r+1} + \alpha_{j}^{r})}{||S_{\lambda_{0}/\rho} \circ (\beta_{j}^{r+1} + \alpha_{j}^{r})||_{2}},$$
(17)

where $S_{\lambda_0/\rho}(a)$ is the soft thresholding operator, i.e.

$$S_{\lambda_0/\rho}(a) = \operatorname{sign}(a) \left(|a| - \frac{\lambda_0}{\rho} \right)_+$$

and o is the elementarywise operator.

- Remark 1: Computation of (16) can be done by first computing the Cholesky decomposition of X^TX + \rho I_{p \times p}, and then storing the lower triangular matrix of the Cholesky decomposition for reuse during the iteration.
- Remark 2: Computation of (17) is straightforward and usually can be done in O(p) flops.

- Sparse group lasso estimation (contd):
 - Remark 3: When $\lambda_j=0$ for all j's, the problem (12) becomes the lasso estimation problem, and (17) becomes

$$\boldsymbol{\gamma}_j^{r+1} = S_{\lambda_0/\rho} \circ (\boldsymbol{\beta}_j^{r+1} + \boldsymbol{\alpha}_j^r), \tag{18}$$

which is the soft thresholding operator or the proximal operator of l_1 -norm on the vector $\beta_j^{r+1} + \alpha_j^r$.

When $\lambda_0=0$, the problem (12) becomes the group lasso estimation problem, and (17) becomes

$$\gamma_{j}^{r+1} = \left(||\beta_{j}^{r+1} + \alpha_{j}^{r}||_{2} - \frac{\lambda_{j}}{\rho} \right)_{+} \frac{\beta_{j}^{r+1} + \alpha_{j}^{r}}{||\beta_{j}^{r+1} + \alpha_{j}^{r}||_{2}}, \tag{19}$$

which is the proximal operator of the l_2 -norm on the vector $oldsymbol{eta}_j^{r+1} + oldsymbol{lpha}_j^r$

- Quiz:
 - 1. Consider soft thresholding operator:

$$S_{\lambda}(a) = \operatorname{sign}(a) \bigg(|a| - \lambda \bigg)_{+}.$$

Which of the following statements are true?

a. $S_{\lambda}(a)$ is the solution to the following problem:

$$\min_{x} \frac{1}{2}(x-a)^2 + \lambda x.$$

b. $S_{\lambda}(a)$ is the solution to the following problem:

$$\min_{x} \frac{\lambda}{2} (x - a)^2 + |x|.$$

c. $S_{\lambda}(a)$ is the solution to the following problem:

$$\min_{x} \frac{1}{2}(x-a)^2 + \lambda |x|.$$

- Support vector machines:
 - Remember the support vector machine problem:

$$\begin{aligned} & \min_{\pmb{\theta},\alpha} & & \frac{1}{2}||\pmb{\theta}||_2^2 \\ \text{subject to} & & -y_i(\mathbf{x}_i^T\pmb{\theta}+\alpha) \leq -1 \text{ for } i=1,2,\cdots,n. \end{aligned} \tag{20}$$

• Regularized estimation form for (20): To do that, we first introduce a set of slack variables $\xi_i \geq 0$ for $i = 1, 2, \dots, n$ to the inequality constraints to *relax* the problem (20) as

$$\begin{split} \min_{\pmb{\theta},\alpha} & & \frac{1}{2}||\pmb{\theta}||_2^2 + \frac{1}{\lambda}\sum_{i=1}^n \xi_i \\ \text{subject to} & & -y_i(\mathbf{x}_i^T\pmb{\theta} + \alpha) - \xi_i \leq -1, \xi_i \geq 0 \text{ for } i = 1, 2, \cdots, n \text{(21)} \end{split}$$

where $\lambda>0$ is a tuning parameter adjusting the impact of the penalty function $\sum_{i=1}^n \xi_i$.

- The problem (21) approximates to (20) when $\xi_i \to 0$ for all i's. This makes sense since we add a penalty term $(1/\lambda)\sum_{i=1}^n \xi_i$ to indicate that we want ξ_i 's as small as possible.
- ξ_i can be approximated as

$$\xi_i \approx \max\{0, 1 - y_i(\mathbf{x}_i^T \boldsymbol{\theta} + \alpha)\}. \tag{22}$$

- Support vector machines (contd):
 - With (22) we can trun the problem (21) as a regularized estimation problem:

$$(\widehat{\boldsymbol{\theta}}, \widehat{\alpha}) = \arg\min_{\boldsymbol{\theta}, \alpha} \left\{ \sum_{i=1}^{n} \max\{0, 1 - y_i(\mathbf{x}_i^T \boldsymbol{\theta} + \alpha)\} + \frac{\lambda}{2} ||\boldsymbol{\theta}||_2^2 \right\}.$$
 (23)

- (23) is a regularized estimation form for the SVM problem (20).
- The function

$$l(f) = \max\{0, 1 - f\}$$

is called the **hinge loss** of f.

• We can write (23) in ADMM form as

$$\label{eq:linear_equation} \begin{split} \min_{\pmb{\theta},\alpha} & \quad (l \circ [\mathbf{y} \circ (\mathbf{X} \pmb{\theta} + \alpha \mathbf{1})])^T \mathbf{1} + \frac{\lambda}{2} ||\gamma||_2^2 \\ \text{subject to} & \quad \pmb{\theta} = \pmb{\gamma}. \end{split} \tag{24}$$

- Support vector machines (contd):
 - The augmented Lagrangian corresponding to (24) is

$$L(\boldsymbol{\theta}, \alpha, \boldsymbol{\gamma}, \boldsymbol{\tau}) = (l \circ [\mathbf{y} \circ (\mathbf{X}\boldsymbol{\theta} + \alpha \mathbf{1})])^T \mathbf{1} + \frac{\lambda}{2} ||\boldsymbol{\gamma}||_2^2$$

$$+ \frac{\rho}{2} ||\boldsymbol{\theta} - \boldsymbol{\gamma} + \boldsymbol{\tau}||_2^2 - \frac{\rho}{2} ||\boldsymbol{\tau}||_2^2.$$
 (25)

The iterative scheme for solving the problem of minimizing (25) is:

$$\begin{split} (\boldsymbol{\theta}^{r+1}, \boldsymbol{\alpha}^{r+1}) &=& \arg\min_{\boldsymbol{\theta}} \left\{ (l \circ [\mathbf{y} \circ (\mathbf{X}\boldsymbol{\theta} + \boldsymbol{\alpha} \mathbf{1})])^T \mathbf{1} + \frac{\rho}{2} || \boldsymbol{\theta} - \boldsymbol{\gamma}^r + \boldsymbol{\tau}^r ||_2^2 \right\} \\ \boldsymbol{\gamma}^{r+1} &=& \arg\min_{\boldsymbol{\gamma}} \left\{ \frac{\lambda}{2\rho} || \boldsymbol{\gamma} ||_2^2 + \frac{1}{2} || \boldsymbol{\gamma} - \boldsymbol{\theta}^{r+1} - \boldsymbol{\tau}^r ||_2^2 \right\} \\ &=& \frac{\boldsymbol{\theta}^{r+1} + \boldsymbol{\tau}^r}{\lambda/\rho + 1} \\ \boldsymbol{\tau}^{r+1} &=& \boldsymbol{\tau}^r + \boldsymbol{\theta}^{r+1} - \boldsymbol{\gamma}^{r+1}. \end{split}$$

Splitting across examples:

- The Splitting across Examples is a distributed optimization technique useful in situations when there are large amounts of examples (samples) but relatively small number of features in model fitting tasks.
- Consider the following optimization problem:

minimize
$$\sum_{i=1}^{m} l_i(\mathbf{X}_i \boldsymbol{\beta}) + g(\boldsymbol{\beta}), \tag{26}$$

where \mathbf{X}_i is an $n_i \times p$ matrix, and $\boldsymbol{\beta}$ is a p-dimensional vector.

• Example 1: We have

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \\ \vdots \\ \mathbf{X}_m \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y} \end{bmatrix} \Rightarrow \frac{1}{2}||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 = \frac{1}{2}\sum_{i=1}^m ||\mathbf{y}_i - \mathbf{X}_i\boldsymbol{\beta}||_2^2.$$

- Splitting across examples (contd):
 - To use the idea of ADMM, we introduce the following equality constraints:

$$\boldsymbol{\theta}_i - \boldsymbol{\beta} = 0 \text{ for } i = 1, 2, \cdots, m.$$

 With the above constraints, we can reformulate the optimization problem (26) as

$$\begin{array}{ll} \text{minimize} & \sum_{i=1}^m l_i(\mathbf{X}_i\boldsymbol{\theta}_i) + g(\boldsymbol{\beta}) \\ \\ \text{subject to} & \boldsymbol{\theta}_i = \boldsymbol{\beta} \text{ for } i=1,2,\cdots,m. \end{array} \tag{27}$$

The augmented Lagrangian for (27) is

$$L_{\rho}(\boldsymbol{\theta}_{i}'s, \boldsymbol{\beta}, \boldsymbol{\alpha}) = \sum_{i=1}^{m} l_{i}(\mathbf{X}_{i}\boldsymbol{\theta}_{i}) + g(\boldsymbol{\beta})$$
$$+ \frac{\rho}{2} \sum_{i=1}^{m} ||\boldsymbol{\theta}_{i} - \boldsymbol{\beta} + \boldsymbol{\alpha}_{i}||_{2}^{2} - \frac{\rho}{2} \sum_{i=1}^{m} ||\boldsymbol{\alpha}_{i}||_{2}^{2}. \quad (28)$$

- Splitting across examples (contd):
 - We can minimize (28) using the following iterative scheme:

$$\begin{aligned} \boldsymbol{\theta}_{i}^{r+1} &= & \arg\min_{\boldsymbol{\theta}_{i}} \left\{ l_{i}(\mathbf{X}_{i}\boldsymbol{\theta}_{i}) + \frac{\rho}{2} ||\boldsymbol{\theta}_{i} - \boldsymbol{\beta}^{r} + \boldsymbol{\alpha}_{i}^{r}||_{2}^{2} \right\} \text{ for } i = 1, 2, \cdots, m \\ \boldsymbol{\beta}^{r+1} &= & \arg\min_{\boldsymbol{\beta}} \left\{ g(\boldsymbol{\beta}) + \frac{m\rho}{2} \left| \left| \boldsymbol{\beta} - \frac{1}{m} \sum_{i=1}^{m} \boldsymbol{\theta}_{i}^{r+1} - \frac{1}{m} \sum_{i=1}^{m} \boldsymbol{\alpha}_{i}^{r} \right| \right|_{2}^{2} \right\} \\ \boldsymbol{\alpha}_{i}^{r+1} &= & \boldsymbol{\alpha}_{i}^{r} + \boldsymbol{\theta}_{i}^{r+1} - \boldsymbol{\beta}^{r+1} \text{ for } i = 1, 2, \cdots, m. \end{aligned} \tag{29}$$

 Derivation of the second line of (29): Note that to solve the second line of (29), the following first-order condition must be satisfied:

$$\begin{split} \mathbf{0} &\in \partial g(\boldsymbol{\beta}^{r+1}) - \rho \bigg(\sum_{i=1}^m \boldsymbol{\theta}_i^{r+1} - m \boldsymbol{\beta}^{r+1} + \sum_{i=1}^m \boldsymbol{\alpha}_i^r \bigg) \\ \Rightarrow &\quad \mathbf{0} \in \partial g(\boldsymbol{\beta}^{r+1}) + m \rho \bigg(\boldsymbol{\beta}^{r+1} - \frac{1}{m} \sum_{i=1}^m \boldsymbol{\theta}_i^{r+1} - \frac{1}{m} \sum_{i=1}^m \boldsymbol{\alpha}_i^r \bigg), \end{split}$$

which is equivalent to solving the following optimization problem:

$$\boldsymbol{\beta}^{r+1} = \arg\min_{\boldsymbol{\beta}} \left\{ g(\boldsymbol{\beta}) + \frac{m\rho}{2} \left| \left| \boldsymbol{\beta} - \frac{1}{m} \sum_{i=1}^{m} \boldsymbol{\theta}_{i}^{r+1} - \frac{1}{m} \sum_{i=1}^{m} \boldsymbol{\alpha}_{i}^{r} \right| \right|_{2}^{2} \right\}. \quad (30)$$

Computation in Data Science: Week 13 Lecture 8

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• Motivation: For a function $f:\mathbb{R}^p\mapsto\mathbb{R}$ that is convex and differentiable, one has

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x})$$

for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^p$, i.e. the first-order characterization of convex functions.

• What if f is convex but is *not* differentiable at some points in \mathbb{R}^p ?

• **Definition:** Assume $\mathcal{C} \in \mathbb{R}^p$ is a non-empty set. For a function $f: \mathcal{C} \mapsto \mathbb{R}$, the subdifferential of f at $\mathbf{x} \in \mathcal{C}$ is defined by

$$\partial f(\mathbf{x}) = \{\mathbf{u} : f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{u}^T(\mathbf{y} - \mathbf{x}) \text{ for all } \mathbf{y} \in \mathcal{C}\}$$

$$= \bigcap_{\mathbf{y} \in \mathcal{C}} \{\mathbf{u} : f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{u}^T(\mathbf{y} - \mathbf{x})\}, \tag{31}$$

that is, the subdifferential $\partial f(\mathbf{x})$ evaluated at \mathbf{x} is a set of all p-dimensional vectors \mathbf{u} such that the inequality

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \mathbf{u}^T(\mathbf{y} - \mathbf{x})$$

holds for any $\mathbf{y} \in \mathcal{C}$.

- Theorem (existence of subdifferentials): Assume $\mathcal C$ is a convex set. A function $f:\mathcal C\mapsto\mathbb R$ is a convex function if and only if the corresponding subdifferentials are non-empty at any $\mathbf x\in\mathcal C$, i.e. $\partial f(\mathbf x)\neq\emptyset$ for all $\mathbf x\in\mathcal C$.
- Remark: We will call any vector $\mathbf{u} \in \partial f(\mathbf{x})$ the subgradient of f evaluated at \mathbf{x} . A subgradient is an element in the subdifferential.

• First-order characterization: If $f:\mathcal{C}\mapsto\mathbb{R}$ is convex and differentiable, then we have

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x})$$

for all $\mathbf{x}, \mathbf{y} \in \mathcal{C}$. This implies $\partial f(\mathbf{x}) = \nabla f(\mathbf{x})$.

• Solutions to a convex optimization problem: If $l: \mathcal{C} \mapsto \mathbb{R}$ is convex and $\mathbf{x}^* \in \mathcal{C}$ minimizes l, then we must have

$$l(\mathbf{y}) \geq l(\mathbf{x}^*) = l(\mathbf{x}^*) + \mathbf{0}^T(\mathbf{y} - \mathbf{x}^*) \text{ for all } \mathbf{y} \in \mathcal{C},$$

which implies

$$\mathbf{0} \in \partial l(\mathbf{x}^*).$$

• Composition with an affine mapping: Assume $l:\mathcal{C}\mapsto\mathbb{R}$ is convex. Define $\mathbf{f}=\mathbf{X}\boldsymbol{\beta}\in\mathcal{C}$ with $\boldsymbol{\beta}\in\mathbb{R}^p$, and $g(\boldsymbol{\beta})=l(\mathbf{X}\boldsymbol{\beta}).$ Then we have $g(\boldsymbol{\beta})$ is a convex function of $\boldsymbol{\beta}$ and

$$\partial g(\boldsymbol{\beta}) = \Big\{ \mathbf{u} : \mathbf{u} = \mathbf{X}^T \mathbf{v}, \mathbf{v} \in \partial l(\mathbf{f}), \mathbf{f} = \mathbf{X} \boldsymbol{\beta} \Big\}.$$

- Example 1 (The l₁-norm):
 - Consider the l_1 -norm $||\mathbf{x}||_1$ with $\mathbf{x} \in \mathbb{R}^p$. Since $||.||_1$ is convex on \mathbb{R}^p , if \mathbf{u} is a subgradient of $||\mathbf{x}||_1$, we must have

$$(\mathbf{y} - \mathbf{x})^T \mathbf{u} + ||\mathbf{x}||_1 \leq ||\mathbf{y}||_1$$

for any $\mathbf{y} \in \mathbb{R}^p$.

Case 1: Obviously for $x_i \neq 0$ we have

$$\frac{\partial ||\mathbf{x}||_1}{\partial x_j} = \frac{\partial}{\partial x_j} \bigg(\sum_{j=1}^p |x_j| \bigg) = \ \mathrm{sign}(x_j).$$

Case 2: For $x_j = 0$, if u_j is a subgradient of $|x_j|$, we must have

$$(y-0)u_j + 0 \le |y| \Rightarrow yu_j \le |y| \Rightarrow u_j \in [-1,1],$$

i.e. u_i is any point in [-1,1].

Case 3: For $\mathbf{x}=\mathbf{0},$ if \mathbf{u} is a subgradient of $||\mathbf{x}||_1$, then for any $\mathbf{y}\in\mathbb{R}^p$ we must have

$$\mathbf{y}^T\mathbf{u} \leq ||\mathbf{y}||_1 \Rightarrow \max_{\mathbf{u}} \mathbf{y}^T\mathbf{u} \leq ||\mathbf{y}||_1 \Rightarrow ||\mathbf{y}||_1 ||\mathbf{u}||_\infty \leq ||\mathbf{y}||_1 \Rightarrow ||\mathbf{u}||_\infty \leq 1.$$

• From the above results we conclude for $\mathbf{x} \in \mathbb{R}^p$,

$$\partial ||\mathbf{x}||_1 = \{\mathbf{u}: ||\mathbf{u}||_\infty \leq 1 \text{ and } \mathbf{u}^T\mathbf{x} = ||\mathbf{x}||_1\}.$$

- Example 2 (The l_2 -norm):
 - Consider the l_2 -norm $||\mathbf{x}||_2$ with $\mathbf{x} \in \mathbb{R}^p$.

Case 1: Obviously for $x \neq 0$ we have

$$\frac{\partial ||\mathbf{x}||_2}{\partial \mathbf{x}} = \frac{\mathbf{x}}{||\mathbf{x}||_2}.$$

Case 2: For ${\bf x}={\bf 0},$ if ${\bf u}$ is a subgradient of $||{\bf x}||_2$, then for any ${\bf y}\in\mathbb{R}^p$ we must have

$$\mathbf{y}^T\mathbf{u} \leq ||\mathbf{y}||_2 \Rightarrow \max_{\mathbf{u}} \mathbf{y}^T\mathbf{u} \leq ||\mathbf{y}||_2 \Rightarrow ||\mathbf{y}||_2 ||\mathbf{u}||_2 \leq ||\mathbf{y}||_2 \Rightarrow ||\mathbf{u}||_2 \leq 1.$$

From the above results we conclude for $\mathbf{x} \in \mathbb{R}^p$,

$$\partial ||\mathbf{x}||_2 = {\mathbf{u} : ||\mathbf{u}||_2 \le 1 \text{ and } \mathbf{u}^T \mathbf{x} = ||\mathbf{x}||_2}.$$

- Example 3 (The rectified linear unit (ReLU)):
 - Consider the rectified linear unit $f(x) = \max\{0, x\}$ with $x \in \mathbb{R}$. The function is a convex function of $x \in \mathbb{R}$ but is not differentiable at x = 0.

Case 1: Obviously for x > 0 we have

$$\frac{d \max\{0, x\}}{dx} = \frac{dx}{dx} = 1.$$

Case 2: For x < 0, we have

$$\frac{d\max\{0,x\}}{dx} = \frac{d0}{dx} = 0.$$

Case 3: For x=0, if u is a subgradient of $\max\{0,x\}$, then for all $y\in\mathbb{R}$, we must have

$$(y-0)u + \max\{0,0\} \le \max\{0,y\} \Rightarrow yu \le \max\{0,y\} \Rightarrow u \in [0,1].$$

- Computation of subdifferentials (contd):
 - Example 4 (The hinge loss): The hinge loss of f is defined as $l(f) = \max\{0, 1 f\}$ with $f \in \mathbb{R}$.
 - l(f) is convex since for any $f,h\in\mathbb{R}$ and $\alpha\in[0,1]$,

$$\begin{split} \max\{0, 1 - [\alpha f + (1 - \alpha)h]\} &= \max\{0, \alpha (1 - f) + (1 - \alpha)(1 - h)\} \\ &\leq \max\{0, \alpha (1 - f)\} + \max\{0, (1 - \alpha)(1 - h)\} \\ &= \alpha \max\{0, 1 - f\} + (1 - \alpha) \max\{0, 1 - h\}. \end{split}$$

• If u is a subgradient of l(f), then for any $h \in \mathbb{R}$, the following inequality must be satisfied:

$$(h-f)u + \max\{0, 1-f\} \le \max\{0, 1-h\}.$$

Case 1: Obviously for f > 1 we have

$$\frac{d\max\{0,1-f\}}{df} = \frac{d0}{df} = 0.$$

Case 2: For f < 1, we have

$$\frac{d \max\{0, 1 - f\}}{dx} = \frac{d(1 - f)}{df} = -1.$$

- Computation of subdifferentials (contd):
 - Example 4 (contd):

Case 3: For f=1, if u is a subgradient of l(f), then for all $h\in\mathbb{R}$, we must have

$$(h-0)u + \max\{0,0\} \leq \max\{0,1-h\} \Rightarrow hu \leq \max\{0,1-h\} \Rightarrow u \in [-1,0].$$

• Now let $\mathbf{f} = \mathbf{X}\boldsymbol{\beta}$, where \mathbf{X} is an $n \times p$ matrix, and $\boldsymbol{\beta}$ is a p-dimensional vector. Consider the loss function with $l(f) = \max\{0, 1-f\}$:

$$\sum_{i=1}^{n} l(f_i) = (l \circ \mathbf{X}\boldsymbol{\beta})^T \mathbf{1} = g(\boldsymbol{\beta}),$$

where $\mathbf{1} = (1, 1, \dots, 1)$.

We have

$$\partial g(\boldsymbol{\beta}) = \bigg\{ \mathbf{u} : \mathbf{u} = \mathbf{X}^T \mathbf{v}, \mathbf{v} \in \partial \{ (l \circ \mathbf{f})^T \mathbf{1} \}, \mathbf{f} = \mathbf{X} \boldsymbol{\beta} \bigg\}.$$

Here ${\bf u}$ is a p-dimensional vector, and ${\bf v}$ is an n-dimensional vector and can be expressed as

$$(\mathbf{v})_i = \begin{cases} -1 \text{ if } \mathbf{x}_i^T \boldsymbol{\beta} < 1 \\ 0 \text{ if } \mathbf{x}_i^T \boldsymbol{\beta} > 1 \\ \text{any point } \in [-1,0] \text{ otherwise} \end{cases}$$

for $i = 1, 2, \dots, n$.

About non-convex functions:

• For a non-convex function, subdifferentials may not exist for some points. For example, for $x \in \mathbb{R}$ consider the following function:

$$f(x) = \begin{cases} 1 & \text{if } x \neq 0 \\ 0 & \text{otherwise} \end{cases}.$$

- f(x) is non-convex in x.
- Assume the subdifferential of f(x) evaluated at x=0 is non-empty. Then for any y>0 there exists a u in the subdifferential such that

$$(y-0)u + f(0) \le f(y)$$
 \Rightarrow $u \le \frac{f(y)}{y} = \frac{1}{y}$
 \Rightarrow $u \in (-\infty, 1/y],$

i.e. u is dependent on y and therefore is contradict to the definition of the subdifferential of f(x) evaluated at x=0.

• Quiz:

- 1. Consider the l_{∞} -norm $||\mathbf{x}||_{\infty}$ with $\mathbf{x} \in \mathbb{R}^p$. Which of the following statements are true?
 - **a.** For $x_j = (\mathbf{x})_j$ with $x_j \neq 0$, we have

$$\frac{\partial ||\mathbf{x}||_{\infty}}{\partial x_j} = \begin{cases} 1 \text{ if } |x_j| = \max_{j'} |x_{j'}| \\ 0 \text{ otherwise} \end{cases}$$

b. For $\mathbf{x}=\mathbf{0}$, if \mathbf{u} is a subgradient of $||\mathbf{x}||_{\infty}$, we must have

$$(\mathbf{y} - \mathbf{0})^T \mathbf{u} + ||\mathbf{0}||_{\infty} \le ||\mathbf{y}||_{\infty} \Rightarrow ||\mathbf{u}||_1 \le 1$$

for any $\mathbf{y} \in \mathbb{R}^p$.

c. In general we have

$$\partial ||\mathbf{x}||_{\infty} = {\mathbf{u} \in \mathbb{R}^p : 1 \le ||\mathbf{u}||_1 < \infty \text{ and } \mathbf{u}^T \mathbf{x} = ||\mathbf{x}||_{\infty}}.$$

Week 13

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