Introduction to Machine Learning - CS725
Instructor: Prof. Ganesh Ramakrishnan
Lecture 12 - KKT Conditions, Duality, SVR Dual

KKT conditions for the Constrained (Convex) Problem

- The general optimization problem we consider with (convex) inequality and (linear) equality constraints is:

$$\min_{\mathbf{w}} f(\mathbf{w})$$

$$\text{subject to } g_i(\mathbf{w}) \leq 0; 1 \leq i \leq m$$

$$h_j(\mathbf{w}) = 0; 1 \leq j \leq p$$

KKT conditions for the Constrained (Convex) Problem

- Here, $\mathbf{w} \in \mathbb{R}^n$ and the domain is the intersection of all functions. Lagrangian is:

$$L(\mathbf{w}, \lambda, \mu) = f(\mathbf{w}) + \sum_{i=1}^{m} \lambda_i g_i(\mathbf{w}) + \sum_{j=1}^{p} \mu_j h_j(\mathbf{w})$$

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- KKT **necessary** conditions for all differentiable functions (i.e. f, g_i, h_j) with optimality points $\hat{\mathbf{w}}$ and $(\hat{\lambda}, \hat{\mu})$ are:
  - $\nabla f(\hat{\mathbf{w}}) + \sum_{i=1}^{m} \hat{\lambda}_i \nabla g_i(\hat{\mathbf{w}}) + \sum_{j=1}^{p} \hat{\mu}_j \nabla h_j(\hat{\mathbf{w}}) = 0$
  - $g_i(\hat{\mathbf{w}}) \leq 0; 1 \leq i \leq m$
  - $\hat{\lambda}_i \geq 0; 1 \leq i \leq m$
  - $\hat{\lambda}_i g_i(\hat{\mathbf{w}}) = 0; 1 \leq i \leq m$
  - $h_j(\hat{\mathbf{w}}) = 0; 1 \leq j \leq p$

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  - $g_i(\hat{\mathbf{w}}) \leq 0; 1 \leq i \leq m$
  - $\hat{\lambda}_i \geq 0; 1 \leq i \leq m$
  - $\hat{\lambda}_i g_i(\hat{\mathbf{w}}) = 0; 1 \leq i \leq m$
  - $h_j(\hat{\mathbf{w}}) = 0; 1 \leq j \leq p$
- When f and $g_i, \forall i \in [1, m]$ are convex and $h_j, \forall j \in [1, p]$ are affine, KKT conditions are also **sufficient** for optimality at $\hat{\mathbf{w}}$ and $(\hat{\lambda}, \hat{\mu})$

Lagrangian Duality and KKT conditions

- With $\mathbf{w} \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}^m, \mu \in \mathbb{R}^p$, Lagrangian is:

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$$L^*(\lambda, \mu) = \min_{\mathbf{w}} L(\mathbf{w}, \lambda, \mu)$$

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$$\operatorname*{argmax}_{\lambda,\mu} L^*(\lambda, \mu) = \operatorname*{argmax}_{\lambda,\mu} \min_{\mathbf{w}} L(\mathbf{w}, \lambda, \mu)$$

Extra: Lagrangian Duality and KKT conditions

- The dual function yields lower bound for minimizer of the primal formulation.
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$$\max_{\lambda,\mu} L^*(\lambda, \mu) = \max_{\lambda,\mu} \min_{\mathbf{w}} L(\mathbf{w}, \lambda, \mu) \leq L(\mathbf{w}, \lambda, \mu)$$

- **Duality Gap:** The gap between primal and dual solutions. In the KKT conditions, $\hat{\mathbf{w}}$ correspond to primal optimal and $(\hat{\lambda}, \hat{\mu})$ to dual optimal points $\Rightarrow$ Duality gap is $f(\hat{\mathbf{w}}) - L^*(\hat{\lambda}, \hat{\mu})$
- Duality gap characterizes suboptimality of the solution and can be approximated by $f(\mathbf{w}) - L^*(\lambda, \mu)$ for any feasible $\mathbf{w}$ and corresponding λ and μ

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- Duality gap characterizes suboptimality of the solution and can be approximated by $f(\mathbf{w}) - L^*(\lambda, \mu)$ for any feasible $\mathbf{w}$ and corresponding λ and μ
- When functions f and $g_i, \forall i \in [1, m]$ are convex and $h_j, \forall j \in [1, p]$ are affine, Karush-Kuhn-Tucker (KKT) conditions are both necessary and sufficient for points to be both primal and dual optimal with zero duality gap.

Support Vector Regression and its Dual

Instructor: Prof. Ganesh Ramakrishnan

KKT and Dual for SVR

- $\min_{\mathbf{w},b,\xi_i,\xi_i^*} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i + \xi_i^*)$
  s.t. $\forall i$,
  $y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b \leq \epsilon + \xi_i$,
  $b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i \leq \epsilon + \xi_i^*$,
  $\xi_i, \xi_i^* \geq 0$
- Let's consider the lagrange multipliers α_i, α_i^*, μ_i and μ_i^* corresponding to the above-mentioned constraints.
- The Lagrange Function is

KKT and Dual for SVR

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  $\xi_i, \xi_i^* \geq 0$
- Let's consider the lagrange multipliers α_i, α_i^*, μ_i and μ_i^* corresponding to the above-mentioned constraints.
- The Lagrange Function is $L(\mathbf{w}, \alpha, \alpha^*, \mu, \mu^*) =$
  $$\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i + \xi_i^*) + \sum_{i=1}^m \alpha_i\left(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i\right) +$$
  $$\sum_{i=1}^m \alpha_i^*\left(b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*\right) - \sum_{i=1}^m \mu_i\xi_i - \sum_{i=1}^m \mu_i^*\xi_i^*$$

KKT conditions for SVR

$$L(\mathbf{w}, \alpha, \alpha^*, \mu, \mu^*) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i + \xi_i^*) + \sum_{i=1}^{m}\alpha_i\left(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i\right) +$$
$$\sum_{i=1}^{m}\alpha_i^*\left(b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*\right) - \sum_{i=1}^{m}\mu_i\xi_i - \sum_{i=1}^{m}\mu_i^*\xi_i^*$$

- Differentiating the Lagrangian w.r.t. $\mathbf{w}$,

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- Differentiating the Lagrangian w.r.t. $\mathbf{w}$,

$$\mathbf{w} - \alpha_i \phi(\mathbf{x}_i) + \alpha_i^* \phi(\mathbf{x}_i) = 0 \text{ } i.e., \text{ } \mathbf{w} = \sum_{i=1}^m (\alpha_i - \alpha_i^*)\phi(\mathbf{x}_i)$$

- Differentiating the Lagrangian w.r.t. ξ_i,

KKT conditions for SVR

$$L(\mathbf{w}, \alpha, \alpha^*, \mu, \mu^*) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i + \xi_i^*) + \sum_{i=1}^{m}\alpha_i\left(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i\right) + \sum_{i=1}^{m}\alpha_i^*\left(b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*\right) - \sum_{i=1}^{m}\mu_i\xi_i - \sum_{i=1}^{m}\mu_i^*\xi_i^*$$

- Differentiating the Lagrangian w.r.t. $\mathbf{w}$,

  $$\mathbf{w} - \alpha_i\phi(\mathbf{x}_i) + \alpha_i^*\phi(\mathbf{x}_i) = 0 \text{ } i.e., \text{ } \mathbf{w} = \sum_{i=1}^{m}(\alpha_i - \alpha_i^*)\phi(\mathbf{x}_i)$$

- Differentiating the Lagrangian w.r.t. ξ_i,

  $C - \alpha_i - \mu_i = 0$ *i.e.*, $\alpha_i + \mu_i = C$

- Differentiating the Lagrangian w.r.t ξ_i^*,

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$$L(\mathbf{w}, \alpha, \alpha^*, \mu, \mu^*) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i + \xi_i^*) + \sum_{i=1}^{m}\alpha_i\left(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i\right) + \sum_{i=1}^{m}\alpha_i^*\left(b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*\right) - \sum_{i=1}^{m}\mu_i\xi_i - \sum_{i=1}^{m}\mu_i^*\xi_i^*$$

- Differentiating the Lagrangian w.r.t. $\mathbf{w}$,

  $$\mathbf{w} - \alpha_i\phi(\mathbf{x}_i) + \alpha_i^*\phi(\mathbf{x}_i) = 0 \text{ } i.e., \text{ } \mathbf{w} = \sum_{i=1}^{m}(\alpha_i - \alpha_i^*)\phi(\mathbf{x}_i)$$

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- Differentiating the Lagrangian w.r.t ξ_i^*,

  $\alpha_i^* + \mu_i^* = C$

- Differentiating the Lagrangian w.r.t b,

KKT conditions for SVR

$$L(\mathbf{w}, \alpha, \alpha^*, \mu, \mu^*) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i(\xi_i + \xi_i^*) + \sum_{i=1}^m \alpha_i \left(y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i\right) + \sum_{i=1}^m \alpha_i^* \left(b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*\right) - \sum_{i=1}^m \mu_i \xi_i - \sum_{i=1}^m \mu_i^* \xi_i^*$$

- Differentiating the Lagrangian w.r.t. $\mathbf{w}$,
  $\mathbf{w} - \alpha_i \phi(\mathbf{x}_i) + \alpha_i^* \phi(\mathbf{x}_i) = 0$ *i.e.*, $\mathbf{w} = \sum_{i=1}^m (\alpha_i - \alpha_i^*)\phi(\mathbf{x}_i)$
- Differentiating the Lagrangian w.r.t. ξ_i,
  $C - \alpha_i - \mu_i = 0$ *i.e.*, $\alpha_i + \mu_i = C$
- Differentiating the Lagrangian w.r.t ξ_i^*,
  $\alpha_i^* + \mu_i^* = C$
- Differentiating the Lagrangian w.r.t b,
  $\sum_i (\alpha_i^* - \alpha_i) = 0$
- Complimentary slackness:

KKT conditions for SVR

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- Differentiating the Lagrangian w.r.t. $\mathbf{w}$,
  $\mathbf{w} - \alpha_i\phi(\mathbf{x}_i) + \alpha_i^*\phi(\mathbf{x}_i) = 0$ *i.e.*, $\mathbf{w} = \sum_{i=1}^{m}(\alpha_i - \alpha_i^*)\phi(\mathbf{x}_i)$
- Differentiating the Lagrangian w.r.t. ξ_i,
  $C - \alpha_i - \mu_i = 0$ *i.e.*, $\alpha_i + \mu_i = C$
- Differentiating the Lagrangian w.r.t ξ_i^*,
  $\alpha_i^* + \mu_i^* = C$
- Differentiating the Lagrangian w.r.t b,
  $\sum_i(\alpha_i^* - \alpha_i) = 0$
- Complimentary slackness:
  $\alpha_i(y_i - \mathbf{w}^\top\phi(\mathbf{x}_i) - b - \epsilon - \xi_i) = 0$ AND $\mu_i\xi_i = 0$ AND
  $\alpha_i^*(b + \mathbf{w}^\top\phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*) = 0$ AND $\mu_i^*\xi_i^* = 0$

Conclusions from the KKT conditions:

$$\alpha_i \in (0, C) \Rightarrow ?$$

$$\alpha_i^* \in (0, C) \Rightarrow ?$$

KKT conditions

- Differentiating the Lagrangian w.r.t. $\mathbf{w}$,
  $w - \alpha_i \phi(\mathbf{x}_i) + \alpha_i^* \phi(\mathbf{x}_i) = 0$
  i.e. $\mathbf{w} = \sum_{i=1}^{m} (\alpha_i - \alpha_i^*) \phi(\mathbf{x}_i)$
- Differentiating the Lagrangian w.r.t. ξ_i,
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  $\sum_i^m (\alpha_i^* - \alpha_i) = 0$
- Complimentary slackness:
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  $\mu_i \xi_i = 0$
  $\alpha_i^* (b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*) = 0$
  $\mu_i^* \xi_i^* = 0$

Conclusions from the KKT conditions:

$$\alpha_i(y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i) = 0$$

and

$$\alpha_i^*(b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*) = 0$$

$\Rightarrow$?

Conclusions from the KKT conditions:

$$\alpha_i \in (0, C) \Rightarrow ?$$

$$(C - \alpha_i)\xi_i = 0 \Rightarrow ?$$

$$\alpha_i^* \in (0, C) \Rightarrow ?$$

$$(C - \alpha_i^*)\xi_i^* = 0 \Rightarrow ?$$

For Support Vector Regression, since the original objective and the constraints are convex, any $(\mathbf{w}, b, \alpha, \alpha^*, \mu, \mu^*, \xi, \xi^*)$ that satisfy the necessary KKT conditions gives optimality (conditions are also sufficient)

Some observations

- $\alpha_i, \alpha_i^* \geq 0$, $\mu_i, \mu_i^* \geq 0$, $\alpha_i + \mu_i = C$ and $\alpha_i^* + \mu_i^* = C$
  Thus, $\alpha_i, \mu_i, \alpha_i^*, \mu_i^* \in [0, C]$, $\forall i$
- If $0 < \alpha_i < C$, then $0 < \mu_i < C$
  (as $\alpha_i + \mu_i = C$)
- $\mu_i \xi_i = 0$ and $\alpha_i(y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i) = 0$ are complementary slackness conditions
  So $0 < \alpha_i < C \Rightarrow \xi_i = 0$ and $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b = \epsilon + \xi_i = \epsilon$
  - All such points lie on the boundary of the ϵ band
  - Using any point $\mathbf{x}_j$ (that is with $\alpha_j \in (0, C)$) on margin, we can recover b as:
    $b = y_j - \mathbf{w}^\top \phi(\mathbf{x}_j) - \epsilon$