

Introduction to Machine Learning - CS725

Instructor: Prof. Ganesh Ramakrishnan

Lecture 10 - Optimization Foundations Applied to Regression  
Formulations

# Building on questions on Least Squares Linear Regression

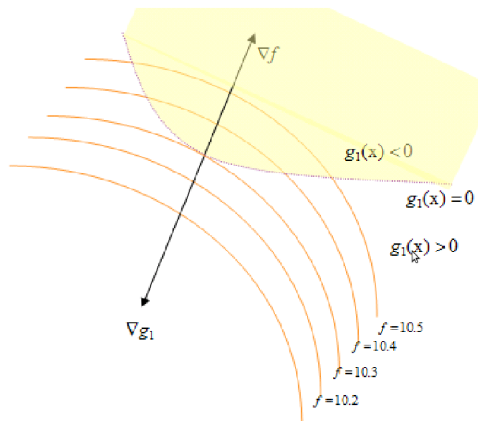
- ① Is there a probabilistic interpretation?
  - Gaussian Error, Maximum Likelihood Estimate
- ② Addressing overfitting
  - Bayesian and Maximum A posteriori Estimates, Regularization, Support Vector Regression
- ③ How to minimize the resultant and more complex error functions?
  - Level Curves and Surfaces, Gradient Vector, Directional Derivative, Gradient Descent Algorithm, Convexity, Necessary and Sufficient Conditions for Optimality

# Constrained convex problems

**Q.** *How to solve such constrained problems?*

**A.** Canonical example:

$$\text{Minimize } f(\mathbf{w}) \text{ s.t. } g_1(\mathbf{w}) \leq 0 \quad (1)$$



# Constrained Convex Problems

- If  $\mathbf{w}^*$  is on the boundary of  $g_1$ , i.e., if  $g_1(\mathbf{w}^*) = 0$ ,

$$\nabla f(\mathbf{w}^*) = -\lambda \nabla g_1(\mathbf{w}^*) \text{ for some } \lambda \geq 0$$


- **Intuition:** If the above didn't hold, then we would have  $\nabla f(\mathbf{w}^*) = \lambda_1 \nabla g_1(\mathbf{w}^*) + \lambda_2 \nabla_{\perp} g_1(\mathbf{w}^*)$ , where, by moving in direction<sup>1</sup>  $\pm \nabla_{\perp} g_1(\mathbf{w}^*)$  ( or  $-\nabla g_1(\mathbf{w}^*)$ ), we remain on boundary  $g_1(\mathbf{w}^*) = 0$ , ( or within  $g_1(\mathbf{w}^*) \leq 0$ ) while decreasing the value of  $f$ , which is not possible at the point of optimality.
- Thus, at the point of optimality<sup>2</sup>, for some  $\lambda \geq 0$ ,

$$\text{Either } g_1(\mathbf{w}^*) < 0 \quad \& \quad \nabla f(\mathbf{w}^*) = 0 \tag{2}$$

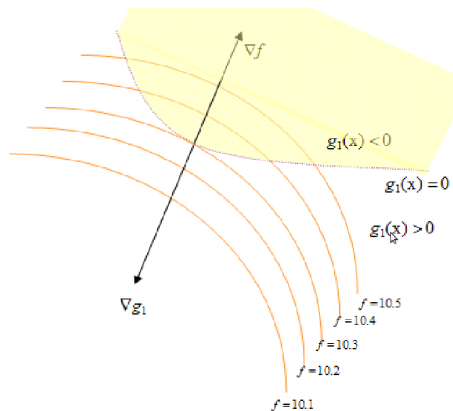
$$\text{Or } g_1(\mathbf{w}^*) = 0 \quad \& \quad \nabla f(\mathbf{w}^*) = -\lambda \nabla g_1(\mathbf{w}^*) \tag{3}$$

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<sup>1</sup> $\nabla_{\perp} g_1(\mathbf{w}^*)$  is the direction orthogonal to  $\nabla g_1(\mathbf{w}^*)$

<sup>2</sup>Section 4.4, pg-72: [cs725/notes/BasicsOfConvexOptimization.pdf](https://www.cs.cmu.edu/~725/notes/BasicsOfConvexOptimization.pdf) 

# Explaining the Figure



**Figure 2:** Two conditions under which a minimum can occur: a) When the minimum is on the constraint function boundary, in which case the gradients are in opposite directions; b) When point of minimum is inside the constraint space (shown in yellow shade), in which case  $\nabla f(\mathbf{w}^*) = \mathbf{0}$ .

# More Explanation and Lagrange Function

- The first condition occurs when minima lies on the boundary of function  $g$ . In this case, gradient vectors corresponding to the functions  $f$  and  $g$ , at  $\mathbf{w}^*$ , point in opposite directions barring multiplication by a real constant.
- Second condition represents the case that point of minimum lies inside the constraint space. This space is shown shaded in Figure 1. Clearly, for this case,  $\nabla f(\mathbf{w}) = \mathbf{0}$ .
- An Alternative Representation:  $\nabla L(\mathbf{w}, \lambda) = 0$  for some  $\lambda \geq 0$  where

$$L(\mathbf{w}, \lambda) = f(\mathbf{w}) + \lambda \mathbf{g}(\mathbf{w}); \lambda \in \mathbb{R}$$

is called the lagrange function which has objective function augmented by weighted sum of constraint functions

# Duality and KKT conditions

For a convex objective and constraint function, the minima,  $\mathbf{w}^*$ , can satisfy one of the following two conditions:

- ①  $g(\mathbf{w}^*) = \mathbf{0}$  and  $\nabla f(\mathbf{w}^*) = -\lambda \nabla g(\mathbf{w}^*)$
- ②  $g(\mathbf{w}^*) < \mathbf{0}$  and  $\nabla f(\mathbf{w}^*) = \mathbf{0}$

# Duality and KKT conditions

- Here, we wish to penalize higher magnitude coefficients, hence, we wish  $g(\mathbf{w})$  to be negative while minimizing the lagrangian. In order to maintain such direction, we must have  $\lambda \geq 0$ . Also, for solution  $\mathbf{w}$  to be feasible,  $\nabla g(\mathbf{w}) \leq \mathbf{0}$ .
- Due to complementary slackness condition, we further have  $\lambda g(\mathbf{w}) = \mathbf{0}$ , which roughly suggests that the lagrange multiplier is zero unless constraint is active at the minimum point. As  $\mathbf{w}$  minimizes the lagrangian  $L(\mathbf{w}, \lambda)$ , gradient must vanish at this point and hence we have  $\nabla f(\mathbf{w}) + \lambda \nabla g(\mathbf{w}) = \mathbf{0}$



# 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:

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

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

# 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:
  - $\nabla f(\hat{\mathbf{w}}) + \sum_{i=1}^m \hat{\lambda}_i \nabla g_i(\hat{\mathbf{w}}) + \sum_{j=1}^p \hat{\mu}_j \nabla h_j(\hat{\mathbf{w}}) = 0$
  - $g_i(\hat{\mathbf{w}}) \leq 0; 1 \leq i \leq m$
  - $\hat{\lambda}_i \geq 0; 1 \leq i \leq m$
  - $\hat{\lambda}_i g_i(\hat{\mathbf{w}}) = 0; 1 \leq i \leq m$
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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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$$\operatorname{argmax}_{\lambda, \mu} L^*(\lambda, \mu) = \operatorname{argmax}_{\lambda, \mu} \min_{\mathbf{w}} L(\mathbf{w}, \lambda, \mu)$$

## 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  $\lambda$  and  $\mu$

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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  $\lambda$  and  $\mu$
- 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

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# KKT and Dual for SVR

- $$\min_{\mathbf{w}, b, \xi_i, \xi_i^*} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i (\xi_i + \xi_i^*)$$
$$\text{s.t. } \forall i,$$
$$y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon + \xi_i,$$
$$b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i \leq \epsilon + \xi_i^*,$$
$$\xi_i, \xi_i^* \geq 0$$

- Let's consider the lagrange multipliers  $\alpha_i$ ,  $\alpha_i^*$ ,  $\mu_i$  and  $\mu_i^*$  corresponding to the above-mentioned constraints.
- The Lagrange Function is

# KKT and Dual for SVR

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s.t.  $\forall i,$

$$y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon + \xi_i,$$

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

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- Let's consider the lagrange multipliers  $\alpha_i$ ,  $\alpha_i^*$ ,  $\mu_i$  and  $\mu_i^*$  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

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

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



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- Differentiating the Lagrangian w.r.t.  $\mathbf{w}$ ,  
 $\mathbf{w} - \alpha_i \phi(\mathbf{x}_i) + \alpha_i^* \phi(\mathbf{x}_i) = 0$  i.e.,  $\mathbf{w} = \sum_{i=1}^m (\alpha_i - \alpha_i^*) \phi(\mathbf{x}_i)$
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$$L(\mathbf{w}, \alpha, \alpha^*, \mu, \mu^*) = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i (\xi_i + \xi_i^*) + \sum_{i=1}^m \alpha_i (y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i) + \sum_{i=1}^m \alpha_i^* (b + \mathbf{w}^\top \phi(\mathbf{x}_i) - y_i - \epsilon - \xi_i^*) - \sum_{i=1}^m \mu_i \xi_i - \sum_{i=1}^m \mu_i^* \xi_i^*$$

- Differentiating the Lagrangian w.r.t.  $\mathbf{w}$ ,  
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- Differentiating the Lagrangian w.r.t.  $\xi_i$ ,  
 $C - \alpha_i - \mu_i = 0$  i.e.,  $\alpha_i + \mu_i = C$
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- Differentiating the Lagrangian w.r.t.  $\xi_i$ ,  
 $C - \alpha_i - \mu_i = 0$  i.e.,  $\alpha_i + \mu_i = C$
- Differentiating the Lagrangian w.r.t  $\xi_i^*$ ,  
 $\alpha_i^* + \mu_i^* = C$
- Differentiating the Lagrangian w.r.t  $b$ ,

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- Differentiating the Lagrangian w.r.t.  $\mathbf{w}$ ,  
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- Differentiating the Lagrangian w.r.t  $b$ ,  
 $\sum_i (\alpha_i^* - \alpha_i) = 0$
- Complimentary slackness:

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

# 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  $\epsilon$  band
- Using any point  $\mathbf{x}_j$  (that is with  $\alpha_j \in (0, C)$ ) on margin, we can recover  $b$  as:  
$$b = y_j - \mathbf{w}^\top \phi(\mathbf{x}_j) - \epsilon$$

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# KKT conditions for SVR

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 $C - \alpha_i - \mu_i = 0$  i.e.,  $\alpha_i + \mu_i = C$
- Differentiating the Lagrangian w.r.t  $\xi_i^*$ ,  
 $\alpha_i^* + \mu_i^* = C$
- 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  $\mu_i^* \xi_i^* = 0$

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  $\epsilon$  band
- Using any point  $\mathbf{x}_j$  (that is with  $\alpha_j \in (0, C)$ ) on margin, we can recover  $b$  as:  
$$b = y_j - \mathbf{w}^\top \phi(\mathbf{x}_j) - \epsilon$$

# Support Vector Regression

## Dual Objective



# Weak Duality

- $L^*(\alpha, \alpha^*, \mu, \mu^*) = \min_{\mathbf{w}, b, \xi, \xi^*} L(\mathbf{w}, b, \xi, \xi^*, \alpha, \alpha^*, \mu, \mu^*)$
- By weak duality theorem, we have:  
$$\min_{\mathbf{w}, b, \xi, \xi^*} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^m (\xi_i + \xi_i^*) \geq L^*(\alpha, \alpha^*, \mu, \mu^*)$$

s.t.  $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon - \xi_i$ , and  
 $\mathbf{w}^\top \phi(\mathbf{x}_i) + b - y_i \leq \epsilon - \xi_i^*$ , and  
 $\xi_i, \xi_i^* \geq 0, \forall i = 1, \dots, n$
- The above is true for any  $\alpha_i, \alpha_i^* \geq 0$  and  $\mu_i, \mu_i^* \geq 0$
- Thus,

# Weak Duality

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$$\text{s.t. } y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon - \xi_i, \text{ and}$$

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$$\xi_i, \xi_i^* \geq 0, \forall i = 1, \dots, n$$

- The above is true for any  $\alpha_i, \alpha_i^* \geq 0$  and  $\mu_i, \mu_i^* \geq 0$

- Thus,

$$\min_{\mathbf{w}, b, \xi, \xi^*} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^m (\xi_i + \xi_i^*) \geq \max_{\alpha, \alpha^*, \mu, \mu^*} L^*(\alpha, \alpha^*, \mu, \mu^*)$$

$$\text{s.t. } y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon - \xi_i, \text{ and}$$

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# Dual objective

- $L^*(\alpha, \alpha^*, \mu, \mu^*) = \min_{\mathbf{w}, b, \xi, \xi^*} L(\mathbf{w}, b, \xi, \xi^*, \alpha, \alpha^*, \mu, \mu^*)$
- Assume: In case of SVR, we have a strictly convex objective and linear constraints  
 $\Rightarrow$  KKT conditions are necessary and sufficient and strong duality holds:

$$\min_{\mathbf{w}, b, \xi, \xi^*} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^m (\xi_i + \xi_i^*) = \max_{\alpha, \alpha^*, \mu, \mu^*} L^*(\alpha, \alpha^*, \mu, \mu^*)$$

s.t.  $y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b \leq \epsilon - \xi_i$ , and

$\mathbf{w}^\top \phi(\mathbf{x}_i) + b - y_i \leq \epsilon - \xi_i^*$ , and

$\xi_i, \xi_i^* \geq 0, \forall i = 1, \dots, n$

- This value is precisely obtained at the  $(\mathbf{w}, b, \xi, \xi^*, \alpha, \alpha^*, \mu, \mu^*)$  that satisfies the necessary (and sufficient) KKT optimality conditions
- Given strong duality, we can equivalently solve

$$\max_{\alpha, \alpha^*, \mu, \mu^*} L^*(\alpha, \alpha^*, \mu, \mu^*)$$

- $$L(\alpha, \alpha^*, \mu, \mu^*) = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^m (\xi_i + \xi_i^*) + \sum_{i=1}^m (\alpha_i (y_i - \mathbf{w}^\top \phi(\mathbf{x}_i) - b - \epsilon - \xi_i) + \alpha_i^* (\mathbf{w}^\top \phi(\mathbf{x}_i) + b - y_i - \epsilon - \xi_i^*)) - \sum_{i=1}^m (\mu_i \xi_i + \mu_i^* \xi_i^*)$$
- We obtain  $\mathbf{w}$ ,  $b$ ,  $\xi_i$ ,  $\xi_i^*$  in terms of  $\alpha$ ,  $\alpha^*$ ,  $\mu$  and  $\mu^*$  by using the KKT conditions derived earlier as  $\mathbf{w} = \sum_{i=1}^m (\alpha_i - \alpha_i^*) \phi(\mathbf{x}_i)$  and  $\sum_{i=1}^m (\alpha_i - \alpha_i^*) = 0$  and  $\alpha_i + \mu_i = C$  and  $\alpha_i^* + \mu_i^* = C$
- Thus, we get:

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

$$\begin{aligned} &L(\mathbf{w}, b, \xi, \xi^*, \alpha, \alpha^*, \mu, \mu^*) \\ &= \frac{1}{2} \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \phi^\top(\mathbf{x}_i) \phi(\mathbf{x}_j) + \\ &\sum_i (\xi_i (C - \alpha_i - \mu_i) + \xi_i^* (C - \alpha_i^* - \mu_i^*)) - b \sum_i (\alpha_i - \alpha_i^*) - \epsilon \sum_i (\alpha_i + \alpha_i^*) + \\ &\sum_i y_i (\alpha_i - \alpha_i^*) - \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \phi^\top(\mathbf{x}_i) \phi(\mathbf{x}_j) \end{aligned}$$

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

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Kernel function:  $K(\mathbf{x}_i, \mathbf{x}_j) = \phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j)$

- $\mathbf{w} = \sum_{i=1}^m (\alpha_i - \alpha_i^*) \phi(\mathbf{x}_i) \Rightarrow$  the final decision function  
 $f(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b = \sum_{i=1}^m (\alpha_i - \alpha_i^*) \phi^T(\mathbf{x}_i) \phi(\mathbf{x}) + y_j - \sum_{i=1}^m (\alpha_i - \alpha_i^*) \phi^T(\mathbf{x}_i) \phi(\mathbf{x}_j) - \epsilon$   
 $\mathbf{x}_j$  is any point with  $\alpha_j \in (0, C)$ . Recall similarity with

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- The dual optimization problem to compute the  $\alpha$ 's for SVR is:



## Kernel function: $K(\mathbf{x}_i, \mathbf{x}_j) = \phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j)$

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$$\begin{aligned} \max_{\alpha_i, \alpha_i^*} & -\frac{1}{2} \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \phi^T(\mathbf{x}_i) \phi(\mathbf{x}_j) \\ & - \epsilon \sum_i (\alpha_i + \alpha_i^*) + \sum_i y_i (\alpha_i - \alpha_i^*) \end{aligned}$$

s.t.

- $\sum_i (\alpha_i - \alpha_i^*) = 0$
- $\alpha_i, \alpha_i^* \in [0, C]$
- **We notice that the only way these three expressions involve  $\phi$  is through  $\phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j) = K(\mathbf{x}_i, \mathbf{x}_j)$ , for some  $i, j$**

# Recap from Quiz 1: Kernelizing Ridge Regression

- Given  $w = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T y$  and using the identity  $(P^{-1} + B^T R^{-1} B)^{-1} B^T R^{-1} = P B^T (B P B^T + R)^{-1}$ 
  - $\Rightarrow w = \Phi^T (\Phi \Phi^T + \lambda I)^{-1} y = \sum_{i=1}^m \alpha_i \phi(x_i)$  where  $\alpha_i = ((\Phi \Phi^T + \lambda I)^{-1} y)_i$
  - $\Rightarrow$  the final decision function  $f(\mathbf{x}) = \phi^T(\mathbf{x}) \mathbf{w} = \sum_{i=1}^m \alpha_i \phi^T(\mathbf{x}) \phi(\mathbf{x}_i)$
- Again, **We notice that the only way the decision function  $f(\mathbf{x})$  involves  $\phi$  is through  $\phi^T(\mathbf{x}_i) \phi(\mathbf{x}_j)$ , for some  $i, j$**

# The Kernel function

- We call  $\phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$  a **kernel function**:  
 $K(\mathbf{x}_i, \mathbf{x}_j) = \phi^\top(\mathbf{x}_i)\phi(\mathbf{x}_j)$
- The Kernel Trick: For some important choices of  $\phi$ , compute  $K(\mathbf{x}_i, \mathbf{x}_j)$  directly and more efficiently than having to explicitly compute/enumerate  $\phi(\mathbf{x}_i)$  and  $\phi(\mathbf{x}_j)$
- The expression for decision function becomes  $f(x) = \sum_{i=1}^m \alpha_i K(\mathbf{x}, \mathbf{x}_i)$
- Computation of  $\alpha_i$  is specific to the objective function being minimized: Closed form exists for Ridge regression but NOT for SVR

# Back to the Kernelized version of SVR

- The kernelized dual problem:

$$\begin{aligned} \max_{\alpha_i, \alpha_i^*} & -\frac{1}{2} \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) K(\mathbf{x}_i, \mathbf{x}_j) \\ & -\epsilon \sum_i (\alpha_i + \alpha_i^*) + \sum_i y_i (\alpha_i - \alpha_i^*) \end{aligned}$$

s.t.

- $\sum_i (\alpha_i - \alpha_i^*) = 0$
- $\alpha_i, \alpha_i^* \in [0, C]$
- The kernelized decision function:  
 $f(\mathbf{x}) = \sum_i (\alpha_i - \alpha_i^*) K(\mathbf{x}_i, \mathbf{x}) + b$
- Using any point  $\mathbf{x}_j$  with  $\alpha_j \in (0, C)$ :  
 $b = y_j - \sum_i (\alpha_i - \alpha_i^*) K(\mathbf{x}_i, \mathbf{x}_j)$
- Computing  $K(\mathbf{x}_1, \mathbf{x}_2)$  often does not even require computing  $\phi(\mathbf{x}_1)$  or  $\phi(\mathbf{x}_2)$  explicitly

# Basis function expansion and the Kernel trick

- We started off with the functional form<sup>3</sup>

$$f(\mathbf{x}) = \sum_{j=1}^p w_j \phi_j(\mathbf{x})$$

Each  $\phi_j$  is called a *basis function* and this representation is called *basis function expansion*<sup>4</sup>

- And we landed up with an equivalent

$$f(\mathbf{x}) = \sum_{i=1}^m \alpha_i K(\mathbf{x}, \mathbf{x}_i)$$

for Ridge regression and Support Vector Regression

- Aside: For  $p \in [0, \infty)$ , with what  $K$ , kind of regularizers, loss functions, etc., will these dual representations hold?<sup>5</sup>

<sup>3</sup>The additional  $b$  term can be either absorbed in  $\phi$  or kept separate as discussed on several occasions.

<sup>4</sup>Section 2.8.3 of Tibshi

<sup>5</sup>Section 5.9.1 of Tibshi

# An Example Kernel

- Let  $K(\mathbf{x}_1, \mathbf{x}_2) = (1 + \mathbf{x}_1^\top \mathbf{x}_2)^2$
- What  $\phi(\mathbf{x})$  will give  $\phi^\top(\mathbf{x}_1)\phi(\mathbf{x}_2) = K(\mathbf{x}_1, \mathbf{x}_2) = (1 + \mathbf{x}_1^\top \mathbf{x}_2)^2$
- Is such a  $\phi$  guaranteed to exist?
- Is there a unique  $\phi$  for given  $K$ ?

# An Example Kernel

- We can prove that such a  $\phi$  exists
- For example, for a 2-dimensional  $\mathbf{x}_i$ :

$$\phi(\mathbf{x}_i) = \begin{bmatrix} 1 \\ x_{i1}\sqrt{2} \\ x_{i2}\sqrt{2} \\ x_{i1}x_{i2}\sqrt{2} \\ x_{i1}^2 \\ x_{i2}^2 \end{bmatrix}$$

- $\phi(\mathbf{x}_i)$  exists in a 5-dimensional space
- But, to compute  $K(\mathbf{x}_1, \mathbf{x}_2)$ , all we need is  $\mathbf{x}_1^\top \mathbf{x}_2$  without having to enumerate  $\phi(\mathbf{x}_i)$





# More on the Kernel Trick

- **Kernels** operate in a *high-dimensional, implicit* feature space without necessarily computing the coordinates of the data in that space, but rather by simply computing the Kernel function
- This approach is called the "*kernel trick*" and will subsequently talk about *valid kernels*
- This operation is often computationally cheaper than the explicit computation of the coordinates
- Claim: If  $\mathcal{K}_{ij} = K(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$  are entries of an  $n \times n$  **Gram Matrix**  $\mathcal{K}$  then

- $\mathcal{K}$  must be positive semi-definite

- Proof:  $\mathbf{b}^T \mathcal{K} \mathbf{b} = \sum_{i,j} b_i \mathcal{K}_{ij} b_j = \sum_{i,j} b_i b_j \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$

$$= \langle \sum_i b_i \phi(\mathbf{x}_i), \sum_j b_j \phi(\mathbf{x}_j) \rangle = \left\| \sum_i b_i \phi(\mathbf{x}_i) \right\|_2^2 \geq 0$$

# Existence of basis expansion $\phi$ for symmetric $K$ ?

- *Positive-definite kernel*: For any dataset  $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m\}$  and for any  $m$ , the Gram matrix  $\mathcal{K}$  must be positive definite

$$\mathcal{K} = \begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & \dots & K(\mathbf{x}_1, \mathbf{x}_n) \\ \dots & K(\mathbf{x}_i, \mathbf{x}_j) & \dots \\ K(\mathbf{x}_m, \mathbf{x}_1) & \dots & K(\mathbf{x}_m, \mathbf{x}_m) \end{bmatrix}$$

so that  $\mathcal{K} = U\Sigma U^T = (U\Sigma^{\frac{1}{2}})(U\Sigma^{\frac{1}{2}})^T = RR^T$  where rows of  $U$  are linearly independent and  $\Sigma$  is a positive diagonal matrix

---

<sup>6</sup>Eigen-decomposition wrt linear operators. See

[https://en.wikipedia.org/wiki/Mercer%27s\\_theorem](https://en.wikipedia.org/wiki/Mercer%27s_theorem)

<sup>7</sup>That is, if every Cauchy sequence is convergent.

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$$\mathcal{K} = \begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & \dots & K(\mathbf{x}_1, \mathbf{x}_n) \\ \dots & K(\mathbf{x}_i, \mathbf{x}_j) & \dots \\ K(\mathbf{x}_m, \mathbf{x}_1) & \dots & K(\mathbf{x}_m, \mathbf{x}_m) \end{bmatrix}$$

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- *Mercer kernel*: Extending to eigenfunction decomposition<sup>6</sup>:

$$K(\mathbf{x}_1, \mathbf{x}_2) = \sum_{j=1}^{\infty} \alpha_j \phi_j(\mathbf{x}_1) \phi_j(\mathbf{x}_2) \text{ where } \alpha_j \geq 0 \text{ and } \sum_{j=1}^{\infty} \alpha_j^2 < \infty$$

- *Mercer kernel* and *Positive-definite kernel* turn out to be equivalent if the input space  $\{x\}$  is *compact*<sup>7</sup>

---

<sup>6</sup>Eigen-decomposition wrt linear operators. See

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- **Mercer kernel:**  $K(\mathbf{x}_1, \mathbf{x}_2)$  is a Mercer kernel if
$$\int \int K(\mathbf{x}_1, \mathbf{x}_2) g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 \geq 0$$
for all square integrable functions  $g(\mathbf{x})$   
( $g(\mathbf{x})$  is square integrable iff  $\int (g(\mathbf{x}))^2 d\mathbf{x}$  is finite)
- **Mercer's theorem:**  
An implication of the theorem:  
for any Mercer kernel  $K(\mathbf{x}_1, \mathbf{x}_2)$ ,  $\exists \phi(\mathbf{x}) : \mathbb{R}^n \mapsto H$ ,  
s.t.  $K(\mathbf{x}_1, \mathbf{x}_2) = \phi^\top(\mathbf{x}_1) \phi(\mathbf{x}_2)$ 
  - where  $H$  is a Hilbert space<sup>8</sup>, the infinite dimensional version of the Euclidean space.
  - Euclidean space:  $(\mathbb{R}^n, \langle \cdot, \cdot \rangle)$  where  $\langle \cdot, \cdot \rangle$  is the standard dot product in  $\mathbb{R}^n$
  - Advanced: Formally, Hilbert Space is an inner product space with associated norms, where every Cauchy sequence is convergent

---

<sup>8</sup>Do you know Hilbert? No? Then what are you doing in his space? :)

# Prove that $(\mathbf{x}_1^\top \mathbf{x}_2)^d$ is a Mercer kernel ( $d \in \mathbb{Z}^+, d \geq 1$ )

- We want to prove that

$$\int_{\mathbf{x}_1} \int_{\mathbf{x}_2} (\mathbf{x}_1^\top \mathbf{x}_2)^d g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 \geq 0,$$

for all square integrable functions  $g(\mathbf{x})$

- Here,  $\mathbf{x}_1$  and  $\mathbf{x}_2$  are vectors s.t  $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^t$
- Thus,  $\int_{\mathbf{x}_1} \int_{\mathbf{x}_2} (\mathbf{x}_1^\top \mathbf{x}_2)^d g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2$

$$= \int_{x_{11}} \dots \int_{x_{1t}} \int_{x_{21}} \dots \int_{x_{2t}} \left[ \sum_{n_1 \dots n_t} \frac{d!}{n_1! \dots n_t!} \prod_{j=1}^t (x_{1j} x_{2j})^{n_j} \right] g(x_1) g(x_2) dx_{11} \dots dx_{1t} dx_{21} \dots dx_{2t}$$

s.t.  $\sum_{i=1}^t n_i = d$   
(taking a leap)

Prove that  $(\mathbf{x}_1^\top \mathbf{x}_2)^d$  is a Mercer kernel ( $d \in \mathbb{Z}^+, d \geq 1$ )

$$\begin{aligned} &= \sum_{n_1 \dots n_t} \frac{d!}{n_1! \dots n_t!} \int_{\mathbf{x}_1} \int_{\mathbf{x}_2} \prod_{j=1}^t (x_{1j} x_{2j})^{n_j} g(x_1) g(x_2) dx_1 dx_2 \\ &= \sum_{n_1 \dots n_t} \frac{d!}{n_1! \dots n_t!} \int_{\mathbf{x}_1} \int_{\mathbf{x}_2} (x_{11}^{n_1} x_{12}^{n_2} \dots x_{1t}^{n_t}) g(x_1) (x_{21}^{n_1} x_{22}^{n_2} \dots x_{2t}^{n_t}) g(x_2) dx_1 dx_2 \end{aligned}$$

Prove that  $(\mathbf{x}_1^\top \mathbf{x}_2)^d$  is a Mercer kernel ( $d \in \mathbb{Z}^+, d \geq 1$ )

$$\begin{aligned} &= \sum_{n_1 \dots n_t} \frac{d!}{n_1! \dots n_t!} \int_{\mathbf{x}_1} \int_{\mathbf{x}_2} \prod_{j=1}^t (x_{1j} x_{2j})^{n_j} g(x_1) g(x_2) dx_1 dx_2 \\ &= \sum_{n_1 \dots n_t} \frac{d!}{n_1! \dots n_t!} \int_{\mathbf{x}_1} \int_{\mathbf{x}_2} (x_{11}^{n_1} x_{12}^{n_2} \dots x_{1t}^{n_t}) g(x_1) (x_{21}^{n_1} x_{22}^{n_2} \dots x_{2t}^{n_t}) g(x_2) dx_1 dx_2 \\ &= \sum_{n_1 \dots n_t} \frac{d!}{n_1! \dots n_t!} \left( \int_{\mathbf{x}_1} (x_{11}^{n_1} \dots x_{1t}^{n_t}) g(x_1) dx_1 \right) \left( \int_{\mathbf{x}_2} (x_{21}^{n_1} \dots x_{2t}^{n_t}) g(x_2) dx_2 \right) \\ &\quad \text{(integral of decomposable product as product of integrals)} \\ &\quad \text{s.t. } \sum_i^t n_i = d \end{aligned}$$

Prove that  $(\mathbf{x}_1^\top \mathbf{x}_2)^d$  is a Mercer kernel ( $d \in \mathbb{Z}^+$ ,  $d \geq 1$ )

- Realize that both the integrals are basically the same, with different variable names
- Thus, the equation becomes:

$$\sum_{n_1 \dots n_t} \frac{d!}{n_1! \dots n_t!} \left( \int_{\mathbf{x}_1} (x_{11}^{n_1} \dots x_{1t}^{n_t}) g(\mathbf{x}_1) d\mathbf{x}_1 \right)^2 \geq 0$$

*(the square is non-negative for reals)*

- Thus, we have shown that  $(\mathbf{x}_1^\top \mathbf{x}_2)^d$  is a Mercer kernel.



What about  $\sum_{d=1}^r \alpha_d (\mathbf{x}_1^\top \mathbf{x}_2)^d$  s.t.  $\alpha_d \geq 0$ ?

- $K(\mathbf{x}_1, \mathbf{x}_2) = \sum_{d=1}^r \alpha_d (\mathbf{x}_1^\top \mathbf{x}_2)^d$
- Is  $\int_{\mathbf{x}_1} \int_{\mathbf{x}_2} \left( \sum_{d=1}^r \alpha_d (\mathbf{x}_1^\top \mathbf{x}_2)^d \right) g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 \geq 0$ ?
- We have

$$\int_{\mathbf{x}_1} \int_{\mathbf{x}_2} \left( \sum_{d=1}^r \alpha_d (\mathbf{x}_1^\top \mathbf{x}_2)^d \right) g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 =$$

What about  $\sum_{d=1}^r \alpha_d (\mathbf{x}_1^\top \mathbf{x}_2)^d$  s.t.  $\alpha_d \geq 0$ ?

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- We have

$$\int_{\mathbf{x}_1} \int_{\mathbf{x}_2} \left( \sum_{d=1}^r \alpha_d (\mathbf{x}_1^\top \mathbf{x}_2)^d \right) g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 =$$
$$\sum_{d=1}^r \alpha_d \int_{\mathbf{x}_1} \int_{\mathbf{x}_2} (\mathbf{x}_1^\top \mathbf{x}_2)^d g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2$$

What about  $\sum_{d=1}^r \alpha_d (\mathbf{x}_1^\top \mathbf{x}_2)^d$  s.t.  $\alpha_d \geq 0$ ?

- We have already proved that  $\int_{\mathbf{x}_1} \int_{\mathbf{x}_2} (\mathbf{x}_1^\top \mathbf{x}_2)^d g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 \geq 0$
- Also,  $\alpha_d \geq 0, \forall d$
- Thus,

$$\sum_{d=1}^r \alpha_d \int_{\mathbf{x}_1} \int_{\mathbf{x}_2} (\mathbf{x}_1^\top \mathbf{x}_2)^d g(\mathbf{x}_1) g(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 \geq 0$$

- By which,  $K(\mathbf{x}_1, \mathbf{x}_2) = \sum_{d=1}^r \alpha_d (\mathbf{x}_1^\top \mathbf{x}_2)^d$  is a Mercer kernel.
- Examples of Mercer Kernels: Linear Kernel, Polynomial Kernel, Radial Basis Function Kernel

- Recall:

$$\max_{\alpha_i, \alpha_i^*} - \frac{1}{2} \sum_i \sum_j (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) K(\mathbf{x}_i, \mathbf{x}_j) - \epsilon \sum_i (\alpha_i + \alpha_i^*) + \sum_i y_i (\alpha_i - \alpha_i^*)$$

and the decision function:

$$f(\mathbf{x}) = \sum_i (\alpha_i - \alpha_i^*) K(\mathbf{x}_i, \mathbf{x}) + b$$

are all in terms of the kernel  $K(\mathbf{x}_i, \mathbf{x}_j)$  only

- One can now employ any mercer kernel in SVR or Ridge Regression to implicitly perform linear regression in higher dimensional spaces*



# Equivalent Forms of Ridge Regression

- Consider the formulation in which we limit the weights of the coefficients by putting a constraint on size of the L2 norm of the weight vector:

$$\operatorname{argmin}_{\mathbf{w}} (\Phi \mathbf{w} - \mathbf{y})^T (\Phi \mathbf{w} - \mathbf{y})$$

$$\|\mathbf{w}\|_2^2 \leq \xi$$

- The objective function, namely  $f(\mathbf{w}) = (\Phi \mathbf{w} - \mathbf{y})^T (\Phi \mathbf{w} - \mathbf{y})$  is strictly convex. The constraint function,  $g(\mathbf{w}) = \|\mathbf{w}\|_2^2 - \xi$ , is also convex.
- For convex  $g(\mathbf{w})$ , the set  $\{\mathbf{w} | g(\mathbf{w}) \leq 0\}$ , is also convex. (Why?)

# Equivalent Forms of Ridge Regression

- To minimize the error function subject to constraint  $\|\mathbf{w}\| \leq \xi$ , we apply KKT conditions at the point of optimality  $\mathbf{w}^*$

$$\nabla_{\mathbf{w}^*}(f(\mathbf{w}) + \lambda g(\mathbf{w})) = \mathbf{0}$$

(the first KKT condition). Here,  $f(\mathbf{w}) = (\Phi\mathbf{w} - \mathbf{y})^T(\Phi\mathbf{w} - \mathbf{y})$  and,  $g(\mathbf{w}) = \|\mathbf{w}\|^2 - \xi$ .

- Solving we get,

$$\mathbf{w}^* = (\Phi^T\Phi + \lambda I)^{-1}\Phi^T\mathbf{y}$$

From the second KKT condition we get,

$$\|\mathbf{w}^*\|^2 \leq \xi$$

From the third KKT condition,

$$\lambda \geq 0$$

From the fourth condition

$$\lambda\|\mathbf{w}^*\|^2 = \lambda\xi$$

# Equivalent Forms of Ridge Regression

- Values of  $\mathbf{w}$  and  $\lambda$  that satisfy all these equations would yield an optimal solution. That is, if

$$\|\mathbf{w}^*\| = \|(\Phi^T \Phi)^{-1} \Phi^T \mathbf{y}\| \leq \xi$$

then  $\lambda = 0$  is the solution. Else, for some sufficiently large value,  $\lambda$  will be the solution to

$$\|\mathbf{w}^*\| = \|(\Phi^T \Phi + \lambda I)^{-1} \Phi^T \mathbf{y}\| = \xi$$



# Bound on $\lambda$ in the regularized least square solution

- Consider,

$$(\Phi^T \Phi + \lambda I)^{-1} \Phi^T \mathbf{y} = \mathbf{w}^*$$

We multiply  $(\Phi^T \Phi + \lambda I)$  on both sides and obtain,

$$\|(\Phi^T \Phi) \mathbf{w}^* + (\lambda I) \mathbf{w}^*\| = \|\Phi^T \mathbf{y}\|$$

Using the triangle inequality we obtain,

$$\|(\Phi^T \Phi) \mathbf{w}^*\| + (\lambda) \|\mathbf{w}^*\| \geq \|(\Phi^T \Phi) \mathbf{w}^* + (\lambda I) \mathbf{w}^*\| = \|\Phi^T \mathbf{y}\|$$

- By the Cauchy Schwarz inequality,  $\|(\Phi^T \Phi) \mathbf{w}^*\| \leq \alpha \|\mathbf{w}^*\|$  for some  $\alpha = \|(\Phi^T \Phi)\|$ . Substituting in the previous equation,

$$(\alpha + \lambda) \|\mathbf{w}^*\| \geq \|\Phi^T \mathbf{y}\|$$

i.e.

$$\lambda \geq \frac{\|\Phi^T \mathbf{y}\|}{\|\mathbf{w}^*\|} - \alpha$$

Note that when  $\|\mathbf{w}^*\| \rightarrow \mathbf{0}$ ,  $\lambda \rightarrow \infty$ . (Any intuition?) Using  $\|\mathbf{w}^*\|^2 \leq \xi$  we get,

# Bound on $\lambda$ in the regularized least square solution

$\|(\Phi^T \Phi) \mathbf{w}^*\| \leq \alpha \|\mathbf{w}^*\|$  for some  $\alpha$  for finite  $\|(\Phi^T \Phi) \mathbf{w}^*\|$ . Substituting in the previous equation,

$$(\alpha + \lambda) \|\mathbf{w}^*\| \geq \|\Phi^T \mathbf{y}\|$$

i.e.

$$\lambda \geq \frac{\|\Phi^T \mathbf{y}\|}{\|\mathbf{w}^*\|} - \alpha$$

Note that when  $\|\mathbf{w}^*\| \rightarrow 0, \lambda \rightarrow \infty$ . (Any intuition?) Using  $\|\mathbf{w}^*\|^2 \leq \xi$  we get,

$$\lambda \geq \frac{\|\Phi^T \mathbf{y}\|}{\sqrt{\xi}} - \alpha$$

This is not the exact solution of  $\lambda$  but the bound proves the existence of  $\lambda$  for some  $\xi$  and  $\Phi$ .

# The Resultant alternative objective function

Substituting  $g(\mathbf{w}) = \|\mathbf{w}\|^2 - \xi$ , in the first KKT equation considered earlier:

$$\nabla_{\mathbf{w}^*}(f(\mathbf{w}) + \lambda \cdot (\|\mathbf{w}\|^2 - \xi)) = \mathbf{0}$$

This is equivalent to solving

$$\min(\|\Phi\mathbf{w} - \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|^2)$$

for the same choice of  $\lambda$ . This form of **regularized** ridge regression is the **penalized ridge regression**.