

10-701: Introduction to Machine Learning

# Lecture 24 –SVMs and Kernels

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\* Slides adopted from F24 offering of 10701 by Henry Chai.

# Summary Thus Far

- The margin of a linear separator is the distance between it and the nearest training data point
- Questions:
  1. How can we efficiently find a maximal-margin linear separator? **By solving a constrained quadratic optimization problem using quadratic programming**
  2. Why are linear separators with larger margins better? **They're simpler \*waves hands\***
  3. What can we do if the data is not linearly separable? **Next!**

# Hard-margin SVMs

$$\begin{aligned} & \text{minimize} \quad \frac{1}{2} \mathbf{w}^T \mathbf{w} \\ & \text{subject to} \quad y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + b) \geq 1 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \end{aligned}$$

- When  $\mathcal{D}$  is not linearly separable, there are no feasible solutions to this optimization problem

# Soft-margin SVMs

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi^{(i)} \\ & \text{subject to} && y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + b) \geq 1 - \xi^{(i)} \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ & && \xi^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

# Primal-Dual Optimization

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \mathbf{w}^T \mathbf{w} \\ & \text{subject to} && y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \geq 1 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \end{aligned}$$

↔

$$\begin{aligned} & \text{maximize} && -\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)T} \mathbf{x}^{(j)} + \sum_{i=1}^N \alpha^{(i)} \\ & \text{subject to} && \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0 \\ & && \alpha^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

# Note: Primal-Dual Optimization

- **Lagrange Method** handles constraints by incorporating them into the objective using multipliers.
- Provides *necessary* optimality conditions for equality-constrained problems. No dual problem.
- **Primal–Dual Optimization** considers the primal problem and its dual—tracking both primal variables and Lagrange multipliers—to find optimality.

# SVM

$$\begin{array}{ll} \text{minimize}_{\mathbf{w}, w_0} & \frac{1}{2} \mathbf{w}^T \mathbf{w} + \max_{\alpha^{(i)} \geq 0} \sum_{i=1}^N \alpha^{(i)} \left( 1 - y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \right) \\ \Updownarrow & \\ \text{minimize}_{\mathbf{w}, w_0} & \max_{\alpha^{(i)} \geq 0} \frac{1}{2} \mathbf{w}^T \mathbf{w} + \sum_{i=1}^N \alpha^{(i)} \left( 1 - y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \right) \\ \Updownarrow & \\ \max_{\alpha^{(i)} \geq 0} & \text{minimize}_{\mathbf{w}, w_0} \frac{1}{2} \mathbf{w}^T \mathbf{w} + \sum_{i=1}^N \alpha^{(i)} \left( 1 - y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \right) \\ \Updownarrow & \\ \max_{\boldsymbol{\alpha} \geq 0} & \text{minimize}_{\mathbf{w}, w_0} L(\boldsymbol{\alpha}, \mathbf{w}, w_0) \end{array}$$

# Karush-Kuhn-Tucker (KKT) Conditions

$$\underset{\boldsymbol{w}, w_0}{\text{minimize}} \quad L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0)$$

$$L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0) = \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + \sum_{i=1}^N \alpha^{(i)} \left( 1 - y^{(i)} (\boldsymbol{w}^T \boldsymbol{x}^{(i)} + w_0) \right)$$

$$\frac{\partial L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0)}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_{i=1}^N \alpha^{(i)} y^{(i)} \boldsymbol{x}^{(i)} \rightarrow \hat{\boldsymbol{w}} = \sum_{i=1}^N \alpha^{(i)} y^{(i)} \boldsymbol{x}^{(i)}$$

$$\frac{\partial L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0)}{\partial w_0} = - \sum_{i=1}^N \alpha^{(i)} y^{(i)} \rightarrow \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

# Minimizing the Lagrangian

$$\hat{\mathbf{w}} = \sum_{i=1}^N \alpha^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

$$\sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$L(\boldsymbol{\alpha}, \hat{\mathbf{w}}, \hat{w}_0) = \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + \sum_{i=1}^N \alpha^{(i)} \left( 1 - y^{(i)} (\hat{\mathbf{w}}^T \mathbf{x}^{(i)} + \hat{w}_0) \right)$$

## Minimizing the Lagrangian

$$\hat{\mathbf{w}} = \sum_{i=1}^N \alpha^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

$$\sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$\begin{aligned} L(\boldsymbol{\alpha}, \hat{\mathbf{w}}, \hat{w}_0) &= \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + \sum_{i=1}^N \alpha^{(i)} \left( 1 - y^{(i)} (\hat{\mathbf{w}}^T \mathbf{x}^{(i)} + \hat{w}_0) \right) \\ &= \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} \\ &\quad + \sum_{i=1}^N \alpha^{(i)} - \sum_{i=1}^N \alpha^{(i)} y^{(i)} \hat{\mathbf{w}}^T \mathbf{x}^{(i)} - \hat{w}_0 \sum_{i=1}^N \alpha^{(i)} y^{(i)} \\ &= \frac{1}{2} \left( \sum_{i=1}^N \alpha^{(i)} y^{(i)} \mathbf{x}^{(i)} \right) \left( \sum_{j=1}^N \alpha^{(j)} y^{(j)} \mathbf{x}^{(j)} \right) \\ &\quad + \sum_{i=1}^N \alpha^{(i)} - \sum_{i=1}^N \alpha^{(i)} y^{(i)} \left( \sum_{j=1}^N \alpha^{(j)} y^{(j)} \mathbf{x}^{(j)} \right)^T \mathbf{x}^{(i)} \end{aligned}$$

# Minimizing the Lagrangian

$$\hat{\mathbf{w}} = \sum_{i=1}^N \alpha^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

$$\sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$\begin{aligned} L(\boldsymbol{\alpha}, \hat{\mathbf{w}}, \hat{w}_0) &= \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + \sum_{i=1}^N \alpha^{(i)} \left( 1 - y^{(i)} (\hat{\mathbf{w}}^T \mathbf{x}^{(i)} + \hat{w}_0) \right) \\ &= \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} \\ &\quad + \sum_{i=1}^N \alpha^{(i)} - \sum_{i=1}^N \alpha^{(i)} y^{(i)} \hat{\mathbf{w}}^T \mathbf{x}^{(i)} \\ &= -\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)T} \mathbf{x}^{(j)} + \sum_{i=1}^N \alpha^{(i)} \end{aligned}$$

# Maximizing the Minimum

$$\begin{array}{ll} \text{maximize}_{\alpha \geq 0} & \text{minimize}_{\mathbf{w}, w_0} L(\alpha, \mathbf{w}, w_0) \end{array}$$

⇓

$$\begin{array}{l} \text{maximize} \quad -\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)T} \mathbf{x}^{(j)} + \sum_{i=1}^N \alpha^{(i)} \\ \text{subject to} \quad \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0 \\ \quad \alpha^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \end{array}$$

# Primal-Dual Optimization

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \mathbf{w}^T \mathbf{w} \\ & \text{subject to} && y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \geq 1 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \end{aligned}$$

Primal

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)}^T \mathbf{x}^{(j)} - \sum_{i=1}^N \alpha^{(i)} \\ & \text{subject to} && \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0 \\ & && \alpha^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

Dual

# Primal-Dual Optimization

- Primal
  - Directly returns the weights,  $[\hat{w}_0, \hat{\mathbf{w}}]$
  - Support vectors are all  $(\mathbf{x}^{(s)}, y^{(s)}) \in \mathcal{D}$  s.t.

$$y^{(s)}(\hat{\mathbf{w}}^T \mathbf{x}^{(s)} + \hat{w}_0) = 1$$

- Dual
  - Returns the vector,  $\hat{\boldsymbol{\alpha}}$

$$\hat{\mathbf{w}} = \sum_{i=1}^N \hat{\alpha}^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

$$\hat{w}_0 = ???$$

# Complementary Slackness

$$\begin{aligned} & \text{minimize } \frac{1}{2} \mathbf{w}^T \mathbf{w} \\ \text{subject to } & 1 - y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \leq 0 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ & \Updownarrow \\ & \text{minimize}_{\mathbf{w}, w_0} \frac{1}{2} \mathbf{w}^T \mathbf{w} + \max_{\alpha^{(i)} \geq 0} \sum_{i=1}^N \alpha^{(i)} (1 - y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0)) \end{aligned}$$

- Theorem:  $\hat{\alpha}^{(i)} (1 - y^{(i)} (\hat{\mathbf{w}}^T \mathbf{x}^{(i)} + \hat{w}_0)) = 0 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}$
- If  $\hat{\alpha}^{(s)} > 0$ , then  $1 - y^{(s)} (\hat{\mathbf{w}}^T \mathbf{x}^{(s)} + \hat{w}_0) = 0$

# Computing $\widehat{w}_0$

$$\widehat{\alpha}^{(i)} \left( 1 - y^{(i)} (\widehat{\mathbf{w}}^T \mathbf{x}^{(i)} + \widehat{w}_0) \right) = 0 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}$$

$$\text{If } \widehat{\alpha}^{(s)} > 0 \rightarrow 1 - y^{(s)} (\widehat{\mathbf{w}}^T \mathbf{x}^{(s)} + \widehat{w}_0) = 0$$

$$\rightarrow y^{(s)} (\widehat{\mathbf{w}}^T \mathbf{x}^{(s)} + \widehat{w}_0) = 1$$

$$\rightarrow y^{(s)^2} (\widehat{\mathbf{w}}^T \mathbf{x}^{(s)} + \widehat{w}_0) = y^{(s)}$$

$$\rightarrow \widehat{\mathbf{w}}^T \mathbf{x}^{(s)} + \widehat{w}_0 = y^{(s)}$$

$$\rightarrow \widehat{w}_0 = y^{(s)} - \widehat{\mathbf{w}}^T \mathbf{x}^{(s)}$$

# Primal-Dual Optimization

- Primal
  - Directly returns the weights,  $[\hat{w}_0, \hat{\mathbf{w}}]$
  - Support vectors are all  $(\mathbf{x}^{(s)}, y^{(s)}) \in \mathcal{D}$  s.t.  
$$y^{(s)}(\hat{\mathbf{w}}^T \mathbf{x}^{(s)} + \hat{w}_0) = 1$$
- Dual
  - Returns the vector,  $\hat{\alpha}$   
$$\hat{\mathbf{w}} = \sum_{i=1}^N \hat{\alpha}^{(i)} y^{(i)} \mathbf{x}^{(i)}$$
  
$$\hat{w}_0 = y^{(s)} - \hat{\mathbf{w}}^T \mathbf{x}^{(s)}$$
 for any  $s$  s.t.  $\hat{\alpha}^{(s)} > 0$
  - Support vectors are all  $(\mathbf{x}^{(s)}, y^{(s)}) \in \mathcal{D}$  s.t.  $\hat{\alpha}^{(s)} > 0$

# Primal-Dual Optimization

- Primal

- $\hat{y} = \text{sign}(\hat{\mathbf{w}}^T \vec{x} + \hat{w}_0)$

- Dual

- $\hat{y} = \text{sign}(\hat{\mathbf{w}}^T \vec{x} + \hat{w}_0)$

$$= \text{sign} \left( \left( \sum_{i=1}^N \hat{\alpha}^{(i)} y^{(i)} \mathbf{x}^{(i)} \right)^T \mathbf{x} + \hat{w}_0 \right)$$

$$= \text{sign} \left( \sum_{i : \hat{\alpha}^{(i)} > 0} \hat{\alpha}^{(i)} y^{(i)} \mathbf{x}^{(i)T} \mathbf{x} + \hat{w}_0 \right)$$

# Primal-Dual Soft-Margin SVMs

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi^{(i)} \\ & \text{subject to} && y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \geq 1 - \xi^{(i)} \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ & && \xi^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

Primal

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)}^T \mathbf{x}^{(j)} - \sum_{i=1}^N \alpha^{(i)} \\ & \text{subject to} && \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0 \\ & && 0 \leq \alpha^{(i)} \leq C \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

Dual

# Primal-Dual Soft-Margin SVMs

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi^{(i)} \\ & \text{subject to} && y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \geq 1 - \xi^{(i)} \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ & && \xi^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

Primal

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)}^T \mathbf{x}^{(j)} - \sum_{i=1}^N \alpha^{(i)} \\ & \text{subject to} && \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0 \\ & && 0 \leq \alpha^{(i)} \leq C \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

Dual

# Recall: Nonlinear Transforms

- Decide on some transformation  $\Phi: \mathcal{X} \rightarrow \mathcal{Z}$
- Given  $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ , learn a hypothesis,  $\tilde{h}(\mathbf{z})$ ,  
using  $\tilde{\mathcal{D}} = \{(\mathbf{z}^{(i)} = \Phi(\mathbf{x}^{(i)}), y^{(i)})\}_{i=1}^N$
- Return the corresponding predictor in the original space:  
$$h(\mathbf{x}) = \tilde{h}(\Phi(\mathbf{x}))$$

# Nonlinear SVMs

- Decide on some transformation  $\Phi: \mathcal{X} \rightarrow \mathcal{Z}$
- Find a maximal-margin separating hyperplane in the transformed space,  $[\tilde{\mathbf{w}}, \tilde{w}_0]$ , by solving the QP:

$$\text{minimize } \frac{1}{2} \tilde{\mathbf{w}}^T \tilde{\mathbf{w}}$$

$$\text{subject to } y^{(i)} (\tilde{\mathbf{w}}^T \Phi(\mathbf{x}^{(i)}) + \tilde{w}_0) \geq 1 \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}$$

- Return the corresponding predictor in the original space:

$$h(\mathbf{x}) = \text{sign}(\tilde{\mathbf{w}}^T \Phi(\mathbf{x}) + \tilde{w}_0)$$

# Nonlinear Dual SVMs

- Decide on some transformation  $\Phi: \mathcal{X} \rightarrow \mathcal{Z}$
- Find a maximal-margin separating hyperplane in the transformed space by solving the QP:

$$\text{minimize} \quad \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x}^{(j)}) - \sum_{i=1}^N \alpha^{(i)}$$

$$\text{subject to} \quad \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$0 \leq \alpha^{(i)} \leq C \quad \forall i \in \{1, \dots, N\}$$

- Return the corresponding predictor in the original space:

$$h(\mathbf{x}) = \text{sign} \left( \sum_{i: \hat{\alpha}^{(i)} > 0} \hat{\alpha}^{(i)} y^{(i)} \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x}) + \tilde{\mathbf{w}}_0 \right)$$

# Efficiency

- Depending on the transformation  $\Phi$  and the dimensionality of the original input space  $\mathcal{X}$ , computing  $\Phi(\mathbf{x})$  can be prohibitively computationally expensive
  - Computing  $\Phi_2(\mathbf{x}) = [x_1, x_2, \dots, x_D, x_1^2, x_1 x_2, \dots, x_D^2]$  requires  $D + \binom{D}{2} + D = \frac{D^2+3D}{2} = O(D^2)$  time
  - Computing  $\Phi_{10}(\mathbf{x})$  requires  $O(D^{10})$  time
- Tradeoff:
  - High-dimensional transformations can result in good hypotheses (as long as they don't overfit)
  - High-dimensional transformations are expensive

# Nonlinear Dual SVMs

- Insight:  $\Phi$  only appears in **inner products**!
- Find a maximal-margin separating hyperplane in the transformed space by solving the QP:

$$\text{minimize} \quad \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x}^{(j)}) - \sum_{i=1}^N \alpha^{(i)}$$

$$\text{subject to} \quad \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$0 \leq \alpha^{(i)} \leq C \quad \forall i \in \{1, \dots, N\}$$

- Return the corresponding predictor in the original space:

$$h(\mathbf{x}) = \text{sign} \left( \sum_{i: \hat{\alpha}^{(i)} > 0} \hat{\alpha}^{(i)} y^{(i)} \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x}) + \tilde{\mathbf{w}}_0 \right)$$

# Nonlinear Dual SVMs

- Insight:  $\Phi$  only appears in **inner products**!
- Find a maximal-margin separating hyperplane in the transformed space by solving the QP:

$$\text{minimize} \quad \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x}^{(j)}) - \sum_{i=1}^N \alpha^{(i)}$$

$$\text{subject to} \quad \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$0 \leq \alpha^{(i)} \leq C \quad \forall i \in \{1, \dots, N\}$$

- Return the corresponding predictor in the original space:

$$h(\mathbf{x}) = \text{sign} \left( \sum_{i: \hat{\alpha}^{(i)} > 0} \hat{\alpha}^{(i)} y^{(i)} \Phi(\mathbf{x}^{(i)})^T \Phi(\mathbf{x}) + \tilde{\mathbf{w}}_0 \right)$$

# The Kernel Trick

- Approach: instead of computing  $\Phi(\mathbf{x})$ , find some function  $K_\Phi$  s.t.  $K_\Phi(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x})^T \Phi(\mathbf{x}') \forall \mathbf{x}, \mathbf{x}' \in \mathcal{X}$ 
  - $K_\Phi(\mathbf{x}, \mathbf{x}')$  should be cheaper to compute than  $\Phi(\mathbf{x})$

## Example

- Approach: instead of computing  $\Phi(\mathbf{x})$ , find some function  $K_\Phi$  s.t.  $K_\Phi(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x})^T \Phi(\mathbf{x}') \forall \mathbf{x}, \mathbf{x}' \in \mathcal{X}$ 
  - $K_\Phi(\mathbf{x}, \mathbf{x}')$  should be cheaper to compute than  $\Phi(\mathbf{x})$
- Example:  $\Phi'_2(\mathbf{x}) = [x_1, \dots, x_D, x_1^2, \sqrt{2}x_1x_2, \dots, \sqrt{2}x_{D-1}x_D, x_D^2]$

$$K_{\Phi'_2}(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}' + (\mathbf{x}^T \mathbf{x}')^2$$

- Computing  $\Phi'_2(\mathbf{x})^T \Phi'_2(\mathbf{x}')$  requires  $O(D^2)$  time whereas computing  $K_{\Phi'_2}(\mathbf{x}, \mathbf{x}')$  only takes  $O(D)$ !

## Example

- Approach: instead of computing  $\Phi(\mathbf{x})$ , find some function  $K_\Phi$  s.t.  $K_\Phi(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x})^T \Phi(\mathbf{x}') \forall \mathbf{x}, \mathbf{x}' \in \mathcal{X}$ 
  - $K_\Phi(\mathbf{x}, \mathbf{x}')$  should be cheaper to compute than  $\Phi(\mathbf{x})$
- Example:  $\Phi'_2(\mathbf{x}) = [x_1, \dots, x_D, x_1^2, \sqrt{2}x_1x_2, \dots, \sqrt{2}x_{D-1}x_D, x_D^2]$ 
$$\begin{aligned}\Phi'_2(\mathbf{x})^T \Phi'_2(\mathbf{x}') &= \sum_{i=1}^D x_i x'_i + \sum_{i=1}^D x_i^2 x'^{2i} + \sum_{i=1}^D \sum_{j>i} 2x_i x'_i x_j x'_j \\ &= \sum_{i=1}^D x_i x'_i + \left( \sum_{i=1}^D x_i x'_i \right)^2 = \mathbf{x}^T \mathbf{x}' + (\mathbf{x}^T \mathbf{x}')^2\end{aligned}$$
$$K_{\Phi'_2}(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}' + (\mathbf{x}^T \mathbf{x}')^2$$
  - Computing  $\Phi'_2(\mathbf{x})^T \Phi'_2(\mathbf{x}')$  requires  $O(D^2)$  time whereas computing  $K_{\Phi'_2}(\mathbf{x}, \mathbf{x}')$  only takes  $O(D)$ !

# Common Kernels

- $K_{\Phi'_2}(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}' + (\mathbf{x}^T \mathbf{x}')^2$ 
  - Implied feature transformation:
$$\Phi'_2(\mathbf{x}) = [x_1, \dots, x_D, x_1^2, \sqrt{2}x_1x_2, \dots, \sqrt{2}x_{D-1}x_D, x_D^2]$$
  - Implied dimensionality:  $\frac{D^2+3D}{2}$
- $K_{\Phi_2^{(\gamma)}}(\mathbf{x}, \mathbf{x}') = (1 + \gamma \mathbf{x}^T \mathbf{x}')^2 - 1$ 
  - Implied feature transformation:
$$\Phi_2^{(\gamma)}(\mathbf{x}) = [\sqrt{2\gamma}x_1, \dots, \sqrt{2\gamma}x_D, \gamma x_1^2, \gamma x_1 x_2, \dots, \gamma x_D^2]$$
  - $\gamma$  affects the geometry of the transform
  - Implied dimensionality:  $\frac{D^2+3D}{2}$

# Common Kernels

- Polynomial Kernel:  $K_{\Phi_Q^{(\gamma)}}(\mathbf{x}, \mathbf{x}') = (1 + \gamma \mathbf{x}^T \mathbf{x}')^Q - 1$ 
  - Implied dimensionality:  $O(D^Q)$
  - $\gamma$  affects the geometry of the transform
- Gaussian-RBF Kernel:  $K_{\Phi_r}(\mathbf{x}, \mathbf{x}') = e^{-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2r}}$ 
  - Implied feature transformation:  $\Phi_r(\mathbf{x}) = \left[ e^{-\frac{x_1^2}{2r}}, \dots, e^{-\frac{x_D^2}{2r}}, e^{-\frac{x_1^2}{2r}\sqrt{\frac{(x_1)^2}{1!r^1}}}, \dots, e^{-\frac{x_D^2}{2r}\sqrt{\frac{(x_D)^2}{1!r^1}}}, e^{-\frac{x_1^2}{2r}\sqrt{\frac{(x_1^2)^2}{2!r^2}}}, \dots, e^{-\frac{x_D^2}{2r}\sqrt{\frac{(x_D^2)^2}{2!r^2}}}, \dots \right]$

# Common Kernels

- Polynomial Kernel:  $K_{\Phi_Q^{(\gamma)}}(\mathbf{x}, \mathbf{x}') = (1 + \gamma \mathbf{x}^T \mathbf{x}')^Q - 1$ 
  - Implied dimensionality:  $O(D^Q)$
  - $\gamma$  affects the geometry of the transform
- Gaussian-RBF Kernel:  $K_{\Phi_r}(\mathbf{x}, \mathbf{x}') = e^{-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2r}}$ 
  - Implied feature transformation:  $\Phi_r(\mathbf{x}) = \left[ \left[ e^{-\frac{x_1^2}{2r}} \sqrt{\frac{(x_1^d)^2}{d!r^d}}, \dots, e^{-\frac{x_D^2}{2r}} \sqrt{\frac{(x_1^d)^2}{d!r^d}} \right] : d \in \mathbb{N} \right]$
  - Implied dimensionality:  $\infty!$

# Nonlinear Dual SVMs

- Decide on a (valid) kernel function  $K_\Phi$
- Find a maximal-margin separating hyperplane in the transformed space by solving the QP:

$$\text{minimize} \quad \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} K_\Phi(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) - \sum_{i=1}^N \alpha^{(i)}$$

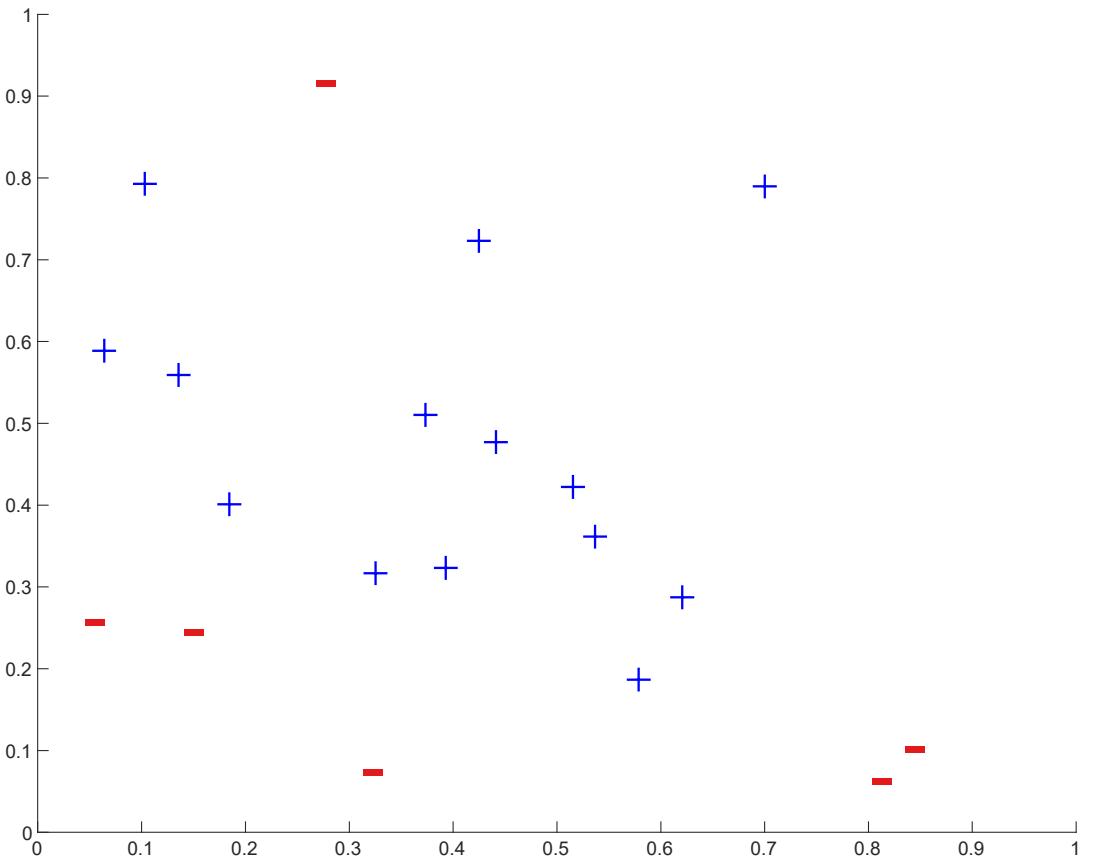
$$\text{subject to} \quad \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$0 \leq \alpha^{(i)} \quad \forall i \in \{1, \dots, N\}$$

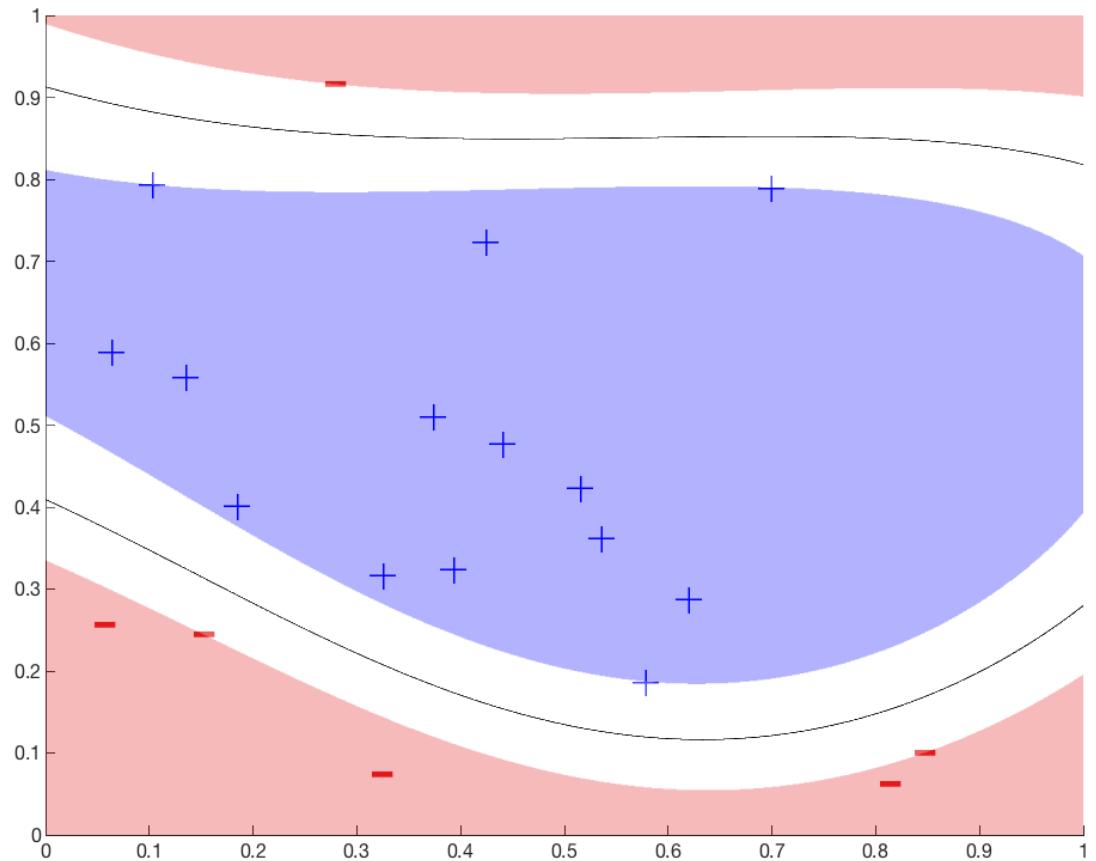
- Return the corresponding predictor in the original space:

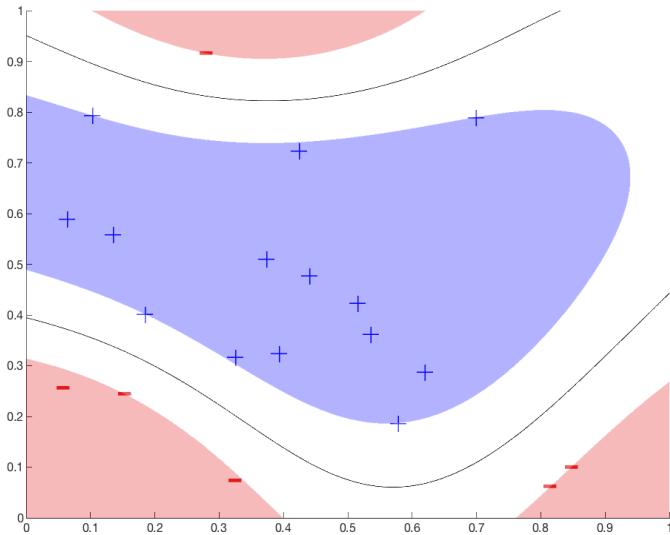
$$h(\mathbf{x}) = \text{sign} \left( \sum_{i: \hat{\alpha}^{(i)} > 0} \hat{\alpha}^{(i)} y^{(i)} K_\Phi(\mathbf{x}^{(i)}, \mathbf{x}) + \tilde{w}_0 \right)$$

# Gaussian-RBF Kernel

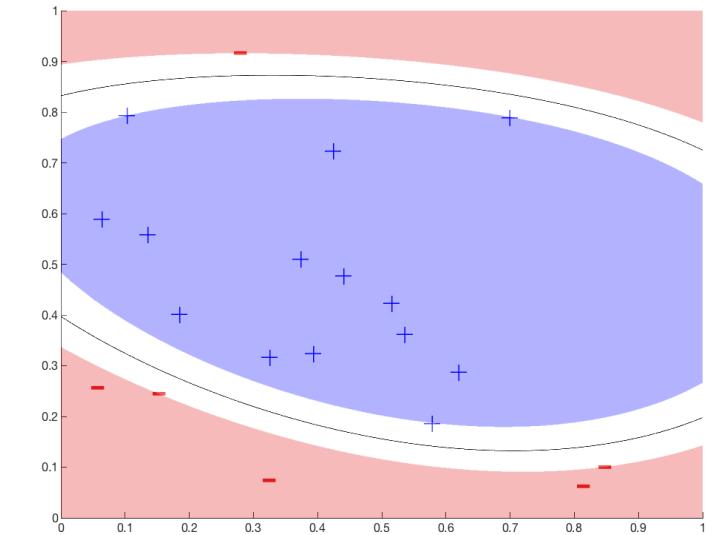
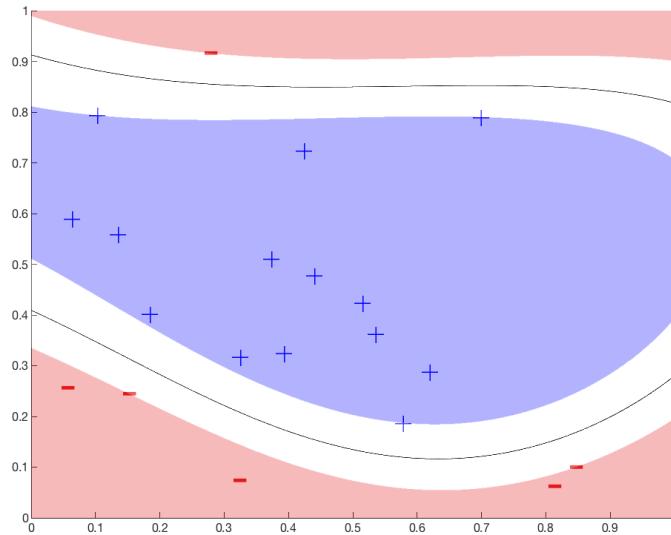


# Gaussian-RBF Kernel





Smaller  $r$



Larger  $r$

# Gaussian-RBF Kernel

# Valid Kernels

- Any function  $K$  is a valid kernel if and only if:

- $\exists$  a transformation  $\Phi$  s.t.

$$K(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x})^T \Phi(\mathbf{x}') \quad \forall \mathbf{x}, \mathbf{x}'$$

$\Updownarrow$

- the Gram matrix

$$\mathbf{K} = \begin{bmatrix} K(\mathbf{x}^{(1)}, \mathbf{x}^{(1)}) & K(\mathbf{x}^{(1)}, \mathbf{x}^{(2)}) & \dots & K(\mathbf{x}^{(1)}, \mathbf{x}^{(N)}) \\ K(\mathbf{x}^{(2)}, \mathbf{x}^{(1)}) & K(\mathbf{x}^{(2)}, \mathbf{x}^{(2)}) & \dots & K(\mathbf{x}^{(2)}, \mathbf{x}^{(N)}) \\ \vdots & \vdots & \ddots & \vdots \\ K(\mathbf{x}^{(N)}, \mathbf{x}^{(1)}) & K(\mathbf{x}^{(N)}, \mathbf{x}^{(2)}) & \dots & K(\mathbf{x}^{(N)}, \mathbf{x}^{(N)}) \end{bmatrix}$$

is symmetric and positive semi-definite  $\forall$  sets

$$\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N)}\}$$

# Building New Kernels

- For any valid kernels  $K_1, K_2$  with implied feature transformations  $\Phi_1, \Phi_2$  and non-negative coefficients  $c_1, c_2$ , the following are all valid kernels:

$$1. \quad K(\mathbf{x}, \mathbf{x}') = c_1 K_1(\mathbf{x}, \mathbf{x}') + c_2 K_2(\mathbf{x}, \mathbf{x}')$$

$$\Phi(\mathbf{x}) = [\sqrt{c_1} \Phi_1(\mathbf{x}), \sqrt{c_2} \Phi_2(\mathbf{x})]$$

$$2. \quad K(\mathbf{x}, \mathbf{x}') = c_1 K_1(\mathbf{x}, \mathbf{x}') K_2(\mathbf{x}, \mathbf{x}')$$

$$\Phi(\mathbf{x}) = \left[ \{\sqrt{c_1} \phi_i(\mathbf{x}) \phi_j(\mathbf{x})\}_{\phi_i(\mathbf{x}) \in \Phi_1(\mathbf{x}), \phi_j(\mathbf{x}) \in \Phi_2(\mathbf{x})} \right]$$

$$3. \quad K(\mathbf{x}, \mathbf{x}') = e^{K_1(\mathbf{x}, \mathbf{x}')}$$

$$\text{Taylor series: } e^{K_1(\mathbf{x}, \mathbf{x}')} = 1 + K_1(\mathbf{x}, \mathbf{x}') + \frac{K_1(\mathbf{x}, \mathbf{x}')^2}{2!} + \frac{K_1(\mathbf{x}, \mathbf{x}')^3}{3!} + \dots$$

# Kernels Everywhere!

- Any method that only depends on the Euclidean distance between data points is an inner product method:

$$\|\mathbf{x} - \mathbf{x}'\|_2 = \sqrt{(\mathbf{x} - \mathbf{x}')^T (\mathbf{x} - \mathbf{x}')} = \sqrt{\mathbf{x}^T \mathbf{x} - 2\mathbf{x}^T \mathbf{x}' + \mathbf{x}'^T \mathbf{x}'}$$

- We can kernelize  $k$ NN!
- We can also kernelize linear/ridge regression!
- See Murphy, Chapter 14.4

# Key Takeaways

- SVMs provide a principled way of finding linear decision boundaries with maximal margins
  - Larger margins can lead to better generalization
  - Defined as a constrained optimization problem
  - Interpretation of solution and definition of support vectors
  - Soft margins for linearly inseparable data
- Dual formulations
  - Interpretation of solution and definition of support vectors
- Kernels and the “kernel trick” allow for efficient use of feature transformations for inner product methods
  - Definition of valid kernels
  - Common kernels and combining kernels

# Primal-Dual Soft-Margin SVMs

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi^{(i)} \\ & \text{subject to} && y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \geq 1 - \xi^{(i)} \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ & && \xi^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

Primal

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)}^T \mathbf{x}^{(j)} - \sum_{i=1}^N \alpha^{(i)} \\ & \text{subject to} && \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0 \\ & && 0 \leq \alpha^{(i)} \leq C \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

Dual

# Soft-Margin SVMs

$$\begin{aligned} & \text{minimize} \quad \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi^{(i)} \\ & \text{subject to} \quad y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \geq 1 - \xi^{(i)} \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ & \quad \xi^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

↔

$$\begin{aligned} & \text{maximize}_{\alpha, \beta \geq 0} \quad \text{minimize}_{\mathbf{w}, w_0, \xi} \quad L(\alpha, \mathbf{w}, w_0, \beta, \xi) \end{aligned}$$

$$\begin{aligned} L(\alpha, \mathbf{w}, w_0, \beta, \xi) = & \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi^{(i)} \\ & + \sum_{i=1}^N \alpha^{(i)} \left( 1 - \xi^{(i)} - y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \right) - \sum_{i=1}^N \beta^{(i)} \xi^{(i)} \end{aligned}$$

# Karush-Kuhn-Tucker (KKT) Conditions

$$\underset{\boldsymbol{w}, w_0, \xi}{\text{minimize}} \quad L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0, \boldsymbol{\beta}, \xi)$$

$$L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0, \boldsymbol{\beta}, \xi) = \frac{1}{2} \boldsymbol{w}^T \boldsymbol{w} + C \sum_{i=1}^N \xi^{(i)}$$

$$+ \sum_{i=1}^N \alpha^{(i)} \left( 1 - \xi^{(i)} - y^{(i)} (\boldsymbol{w}^T \boldsymbol{x}^{(i)} + w_0) \right) - \sum_{i=1}^N \beta^{(i)} \xi^{(i)}$$

$$\frac{\partial L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0, \boldsymbol{\beta}, \xi)}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_{i=1}^N \alpha^{(i)} y^{(i)} \boldsymbol{x}^{(i)} \rightarrow \hat{\boldsymbol{w}} = \sum_{i=1}^N \alpha^{(i)} y^{(i)} \boldsymbol{x}^{(i)}$$

$$\frac{\partial L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0, \boldsymbol{\beta}, \xi)}{\partial w_0} = - \sum_{i=1}^N \alpha^{(i)} y^{(i)} \rightarrow \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$\frac{\partial L(\boldsymbol{\alpha}, \boldsymbol{w}, w_0, \boldsymbol{\beta}, \xi)}{\partial \xi^{(i)}} = C - \alpha^{(i)} - \beta^{(i)} \rightarrow \beta^{(i)} = C - \alpha^{(i)} \quad \forall i \in \{1, \dots, N\}$$

## Minimizing the Lagrangian

$$\hat{\mathbf{w}} = \sum_{i=1}^N \alpha^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

$$\sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0$$

$$\beta^{(i)} = C - \alpha^{(i)} \quad \forall i$$

$$\begin{aligned} L(\alpha, \hat{\mathbf{w}}, \hat{w}_0, \beta, \hat{\xi}) &= \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + C \sum_{i=1}^N \hat{\xi}^{(i)} \\ &\quad + \sum_{i=1}^N \alpha^{(i)} \left( 1 - \hat{\xi}^{(i)} - y^{(i)} (\hat{\mathbf{w}}^T \mathbf{x}^{(i)} + \hat{w}_0) \right) - \sum_{i=1}^N \beta^{(i)} \hat{\xi}^{(i)} \\ &= \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + C \sum_{i=1}^N \hat{\xi}^{(i)} - \sum_{i=1}^n (C - \alpha^{(i)}) \hat{\xi}^{(i)} \\ &\quad + \sum_{i=1}^N \alpha^{(i)} \left( 1 - \hat{\xi}^{(i)} - y^{(i)} (\hat{\mathbf{w}}^T \mathbf{x}^{(i)} + \hat{w}_0) \right) \\ &= \frac{1}{2} \hat{\mathbf{w}}^T \hat{\mathbf{w}} + \sum_{i=1}^N \alpha^{(i)} \left( 1 - y^{(i)} (\hat{\mathbf{w}}^T \mathbf{x}^{(i)} + \hat{w}_0) \right) \end{aligned}$$

# Maximizing the Minimum

$$\begin{aligned} & \text{minimize} && \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)T} \mathbf{x}^{(j)} - \sum_{i=1}^N \alpha^{(i)} \\ & \text{subject to} && \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0 \\ & && \alpha^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \\ & && \beta^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \\ & && \beta^{(i)} = C - \alpha^{(i)} \quad \forall i \in \{1, \dots, N\} \\ & \Updownarrow && \\ & \text{minimize} && \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha^{(i)} \alpha^{(j)} y^{(i)} y^{(j)} \mathbf{x}^{(i)T} \mathbf{x}^{(j)} - \sum_{i=1}^N \alpha^{(i)} \\ & \text{subject to} && \sum_{i=1}^N \alpha^{(i)} y^{(i)} = 0 \\ & && 0 \leq \alpha^{(i)} \leq C \quad \forall i \in \{1, \dots, N\} \end{aligned}$$

# Primal-Dual Soft-Margin SVMs

- Primal
  - Directly returns the weights,  $[\hat{w}_0, \hat{\mathbf{w}}]$
  - Support vectors are all  $(\mathbf{x}^{(s)}, y^{(s)}) \in \mathcal{D}$  s.t.

$$y^{(s)}(\hat{\mathbf{w}}^T \mathbf{x}^{(s)} + \hat{w}_0) = 1$$

- Dual
  - Returns the vector,  $\hat{\boldsymbol{\alpha}}$

$$\hat{\mathbf{w}} = \sum_{i=1}^N \hat{\alpha}^{(i)} y^{(i)} \mathbf{x}^{(i)}$$

$$\hat{w}_0 = ???$$

# Complementary Slackness

$$\begin{aligned} & \text{minimize} \quad \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi^{(i)} \\ & \text{subject to} \quad y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \geq 1 - \xi^{(i)} \quad \forall (\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ & \quad \xi^{(i)} \geq 0 \quad \forall i \in \{1, \dots, N\} \\ & \Updownarrow \\ & \text{maximize}_{\boldsymbol{\alpha}, \boldsymbol{\beta} \geq 0} \quad \text{minimize}_{\mathbf{w}, w_0, \boldsymbol{\xi}} \quad L(\boldsymbol{\alpha}, \mathbf{w}, w_0, \boldsymbol{\beta}, \boldsymbol{\xi}) \\ & L(\boldsymbol{\alpha}, \mathbf{w}, w_0, \boldsymbol{\beta}, \boldsymbol{\xi}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^N \xi^{(i)} \\ & \quad + \sum_{i=1}^N \alpha^{(i)} \left( 1 - \xi^{(i)} - y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + w_0) \right) - \sum_{i=1}^N \beta^{(i)} \xi^{(i)} \end{aligned}$$

# Complementary Slackness

$$\begin{aligned} & \text{maximize}_{\alpha, \beta \geq 0} \quad \text{minimize}_{w, w_0, \xi} \quad L(\alpha, w, w_0, \beta, \xi) \\ & L(\alpha, w, w_0, \beta, \xi) = \frac{1}{2} w^T w + C \sum_{i=1}^N \xi^{(i)} \\ & \quad + \sum_{i=1}^N \alpha^{(i)} \left( 1 - \xi^{(i)} - y^{(i)}(w^T x^{(i)} + w_0) \right) - \sum_{i=1}^N \beta^{(i)} \xi^{(i)} \\ & \bullet \text{ Theorem: } \hat{\beta}^{(i)} \hat{\xi}^{(i)} = (C - \hat{\alpha}^{(i)}) \hat{\xi}^{(i)} = 0 \quad \forall (x^{(i)}, y^{(i)}) \in \mathcal{D} \text{ and} \\ & \hat{\alpha}^{(i)} \left( 1 - \hat{\xi}^{(i)} - y^{(i)}(\hat{w}^T x^{(i)} + \hat{w}_0) \right) = 0 \quad \forall (x^{(i)}, y^{(i)}) \in \mathcal{D} \\ & \bullet \text{ If } 0 < \hat{\alpha}^{(s)}, \text{ then } 1 - \hat{\xi}^{(i)} - y^{(i)}(\hat{w}^T x^{(i)} + \hat{w}_0) = 0 \\ & \bullet \text{ If } \hat{\alpha}^{(s)} < C, \text{ then } \hat{\xi}^{(i)} = 0 \\ & \bullet \text{ If } 0 < \hat{\alpha}^{(s)} < C, \text{ then } 1 - y^{(i)}(\hat{w}^T x^{(i)} + \hat{w}_0) = 0 \end{aligned}$$

# Primal-Dual Soft-Margin SVMs

- Dual
  - Returns the vector,  $\hat{\alpha}$
  - Support vectors are all  $(\mathbf{x}^{(s)}, y^{(s)}) \in \mathcal{D}$  s.t.  $0 < \hat{\alpha}^{(s)} < C$
  - If  $0 < \hat{\alpha}^{(s)} < C$ , then  $y^{(s)}(\hat{\mathbf{w}}^T \mathbf{x}^{(s)} + \hat{w}_0) = 1 \Rightarrow (\mathbf{x}^{(s)}, y^{(s)})$  defines the margin
  - If  $\hat{\alpha}^{(s)} = C$ , then  $\hat{\xi}^{(s)} > 0 \Rightarrow (\mathbf{x}^{(s)}, y^{(s)})$  is inside the margin or misclassified.