

CS260: Machine Learning Algorithms

Lecture 8: Kernel Methods

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Outline

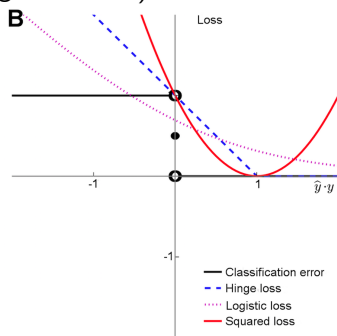
- Linear Support Vector Machines
- Nonlinear SVM, Kernel methods
- Multiclass classification

Support Vector Machines

- Given training examples $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$
Consider binary classification: $y_i \in \{+1, -1\}$
- Linear Support Vector Machine (SVM):

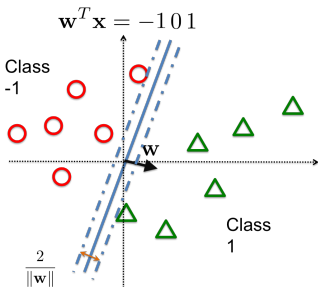
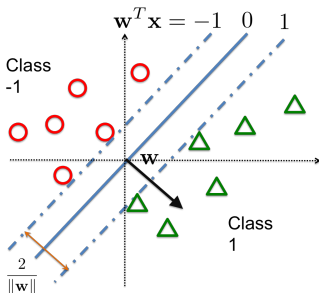
$$\arg \min_{\mathbf{w}} C \sum_{i=1}^n \max(1 - y_i \mathbf{w}^T \mathbf{x}_i, 0) + \frac{1}{2} \mathbf{w}^T \mathbf{w}$$

(hinge loss with L2 regularization)



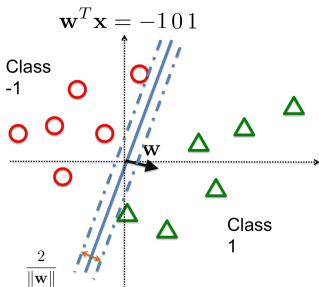
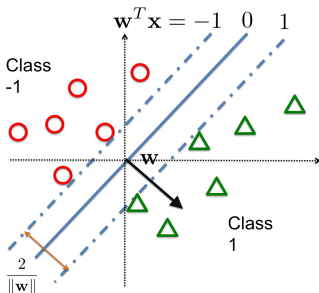
Support Vector Machines

- Goal: Find a hyperplane to separate these two classes of data:
if $y_i = 1$, $\mathbf{w}^T \mathbf{x}_i \geq 1$; if $y_i = -1$, $\mathbf{w}^T \mathbf{x}_i \leq -1$.



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Prefer a hyperplane with **maximum margin**

Size of margin

- minimum of $\|\mathbf{x}\|$ such that $\mathbf{w}^T \mathbf{x} = 1$

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- clearly, $\mathbf{x} = \alpha \frac{\mathbf{w}}{\|\mathbf{w}\|}$ for some α (half margin)
- $\alpha = \frac{1}{\|\mathbf{w}\|}$
- Maximize margin \Rightarrow minimize $\|\mathbf{w}\|$

Support Vector Machines (hard constraints)

- SVM primal problem (with hard constraints):

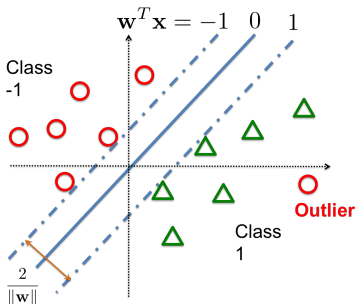
$$\begin{aligned} \min_{\mathbf{w}} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} \\ \text{s.t.} \quad & y_i(\mathbf{w}^T \mathbf{x}_i) \geq 1, i = 1, \dots, n, \end{aligned}$$

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- What if there are outliers?

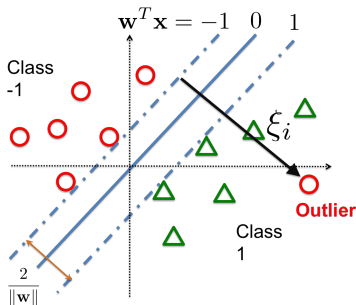


Support Vector Machines

- Given training data $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ with labels $y_i \in \{+1, -1\}$.
- SVM primal problem:

$$\min_{\mathbf{w}, \xi} \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^n \xi_i$$

$$\text{s.t. } y_i(\mathbf{w}^T \mathbf{x}_i) \geq 1 - \xi_i, i = 1, \dots, n,$$
$$\xi_i \geq 0$$



Support Vector Machines

- SVM primal problem:

$$\begin{aligned} \min_{\mathbf{w}, \xi} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^n \xi_i \\ \text{s.t.} \quad & y_i(\mathbf{w}^T \mathbf{x}_i) \geq 1 - \xi_i, i = 1, \dots, n, \\ & \xi_i \geq 0 \end{aligned}$$

- Equivalent to

$$\min_{\mathbf{w}} \quad \underbrace{\frac{1}{2} \mathbf{w}^T \mathbf{w}}_{\text{L2 regularization}} + C \sum_{i=1}^n \underbrace{\max(0, 1 - y_i \mathbf{w}^T \mathbf{x}_i)}_{\text{hinge loss}}$$

- Non-differentiable when $y_i \mathbf{w}^T \mathbf{x}_i = 1$ for some i

Stochastic Subgradient Method for SVM

- A subgradient of $\ell_i(\mathbf{w}) = \max(0, 1 - y_i \mathbf{w}^T \mathbf{x}_i)$:

$$\begin{cases} -y_i \mathbf{x}_i & \text{if } 1 - y_i \mathbf{w}^T \mathbf{x}_i > 0 \\ \mathbf{0} & \text{if } 1 - y_i \mathbf{w}^T \mathbf{x}_i < 0 \\ \mathbf{0} & \text{if } 1 - y_i \mathbf{w}^T \mathbf{x}_i = 0 \end{cases}$$

- Stochastic Subgradient descent for SVM:

For $t = 1, 2, \dots$

Randomly pick an index i

If $y_i \mathbf{w}^T \mathbf{x}_i < 1$, then

$$\mathbf{w} \leftarrow (1 - \eta_t) \mathbf{w} + \eta_t n C y_i \mathbf{x}_i$$

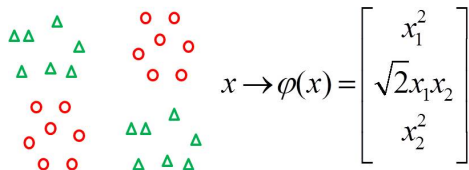
Else (if $y_i \mathbf{w}^T \mathbf{x}_i \geq 1$):

$$\mathbf{w} \leftarrow (1 - \eta_t) \mathbf{w}$$

Kernel SVM

Non-linearly separable problems

- What if the data is not linearly separable?



Solution: map data x_i to higher dimensional(maybe infinite) feature space $\varphi(x_i)$, where they are linearly separable.

SVM with nonlinear mapping

- SVM with nonlinear mapping $\varphi(\cdot)$:

$$\begin{aligned} \min_{\mathbf{w}, \xi} \quad & \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^n \xi_i \\ \text{s.t.} \quad & y_i(\mathbf{w}^T \varphi(\mathbf{x}_i)) \geq 1 - \xi_i, \quad \xi_i \geq 0, \quad i = 1, \dots, n, \end{aligned}$$

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- Hard to solve if $\varphi(\cdot)$ maps to **very high or infinite dimensional space**

Support Vector Machines (dual)

- Primal problem:

$$\begin{aligned} \min_{\mathbf{w}, \xi} \quad & \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i \xi_i \\ \text{s.t.} \quad & y_i \mathbf{w}^T \varphi(\mathbf{x}_i) - 1 + \xi_i \geq 0, \text{ and } \xi_i \geq 0 \quad \forall i = 1, \dots, n \end{aligned}$$

- Equivalent to:

$$\min_{\mathbf{w}, \xi} \max_{\alpha \geq 0, \beta \geq 0} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i \xi_i - \sum_i \alpha_i (y_i \mathbf{w}^T \varphi(\mathbf{x}_i) - 1 + \xi_i) - \sum_i \beta_i \xi_i$$

- Under certain condition (e.g., Slater's condition), exchanging min, max will not change the optimal solution:

$$\max_{\alpha \geq 0, \beta \geq 0} \min_{\mathbf{w}, \xi} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i \xi_i - \sum_i \alpha_i (y_i \mathbf{w}^T \varphi(\mathbf{x}_i) - 1 + \xi_i) - \sum_i \beta_i \xi_i$$

Support Vector Machines (dual)

- Reorganize the equation:

$$\max_{\alpha \geq 0, \beta \geq 0} \min_{\mathbf{w}, \xi} \frac{1}{2} \|\mathbf{w}\|^2 - \sum_i \alpha_i y_i \mathbf{w}^T \varphi(\mathbf{x}_i) + \sum_i \xi_i (C - \alpha_i - \beta_i) + \sum_i \alpha_i$$

- Now, for any given α, β , the minimizer of \mathbf{w} will satisfy

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_i \alpha_i y_i \varphi(\mathbf{x}_i) = 0 \Rightarrow \mathbf{w}^* = \sum_i y_i \alpha_i \varphi(\mathbf{x}_i)$$

Also, we have $C = \alpha_i + \beta_i$, otherwise ξ_i can make the objective function $-\infty$

- Substitue these two equations back we get

$$\max_{\alpha \geq 0, \beta \geq 0, C = \alpha + \beta} -\frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j) + \sum_i \alpha_i$$

Support Vector Machines (dual)

- Therefore, we get the following dual problem

$$\max_{\mathbf{C} \geq \mathbf{\alpha} \geq 0} \left\{ -\frac{1}{2} \mathbf{\alpha}^T Q \mathbf{\alpha} + \mathbf{e}^T \mathbf{\alpha} \right\} := D(\mathbf{\alpha}),$$

where Q is an n by n matrix with $Q_{ij} = y_i y_j \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$

- Based on the derivations, we know
 - ① Primal minimum = dual maximum (under Slater's condition)
 - ② Let $\mathbf{\alpha}^*$ be the dual solution and \mathbf{w}^* be the primal solution, we have

$$\mathbf{w}^* = \sum_i y_i \alpha_i^* \varphi(\mathbf{x}_i)$$

- We can solve the dual problem instead of the primal problem.

Kernel Trick

- Do **not** directly define $\varphi(\cdot)$

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- Instead, define “kernel”

$$K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$$

This is all we need to know for Kernel SVM!

Kernel Trick

- Do **not** directly define $\varphi(\cdot)$
- Instead, define “kernel”

$$K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$$

This is all we need to know for Kernel SVM!

- Examples:
 - Gaussian kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = e^{-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2}$
 - Polynomial kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = (\gamma \mathbf{x}_i^T \mathbf{x}_j + c)^d$
 - Other kernels for specific problems:
 - Graph kernels
(Vishwanathan et al., “Graph Kernels”, JMLR, 2010)
 - Pyramid kernel for image matching
(Grauman and Darrell, “The Pyramid Match Kernel: Discriminative Classification with Sets of Image Features”. In ICCV, 2005)
 - String kernel
(Lodhi et al., “Text classification using string kernels”. JMLR, 2002).

Support Vector Machines (dual)

- Training: compute $\alpha = [\alpha_1, \dots, \alpha_n]$ by solving the **quadratic optimization problem**:

$$\min_{0 \leq \alpha \leq C} \frac{1}{2} \alpha^T Q \alpha - \mathbf{e}^T \alpha$$

where $Q_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$

Support Vector Machines (dual)

- Training: compute $\alpha = [\alpha_1, \dots, \alpha_n]$ by solving the **quadratic optimization problem**:

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where $Q_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$

- Prediction: for a test data \mathbf{x} ,

$$\begin{aligned} \mathbf{w}^T \varphi(\mathbf{x}) &= \sum_{i=1}^n y_i \alpha_i \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}) \\ &= \sum_{i=1}^n y_i \alpha_i K(\mathbf{x}_i, \mathbf{x}) \end{aligned}$$

Kernel Ridge Regression

- Actually, this “kernel method” works for many different losses

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- Actually, this “kernel method” works for many different losses
- Example: ridge regression

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|^2 + \frac{1}{2} \sum_{i=1}^n (\mathbf{w}^T \varphi(\mathbf{x}_i) - y_i)^2$$

- Dual problem:

$$\min_{\alpha} \alpha^T Q \alpha + \|\alpha\|^2 - 2\alpha^T \mathbf{y}$$

Scalability

- Challenge for solving kernel SVMs (for dataset with n samples):
 - **Space:** $O(n^2)$ for storing the n -by- n kernel matrix (can be reduced in some cases);
 - **Time:** $O(n^3)$ for computing the exact solution.

Scalability

- Challenge for solving kernel SVMs (for dataset with n samples):
 - **Space:** $O(n^2)$ for storing the n -by- n kernel matrix (can be reduced in some cases);
 - **Time:** $O(n^3)$ for computing the exact solution.
- Good packages available:
 - LIBSVM (can be called in scikit-learn)

Multiclass classification

Multiclass Learning

- n data points, L labels, d features
- Input: training data $\{\mathbf{x}_i, y_i\}_{i=1}^n$:
 - Each \mathbf{x}_i is a d dimensional feature vector
 - Each $y_i \in \{1, \dots, L\}$ is the corresponding label
 - Each training data belongs to **one category**
- Goal: find a function to predict the correct label

$$f(\mathbf{x}) \approx y$$

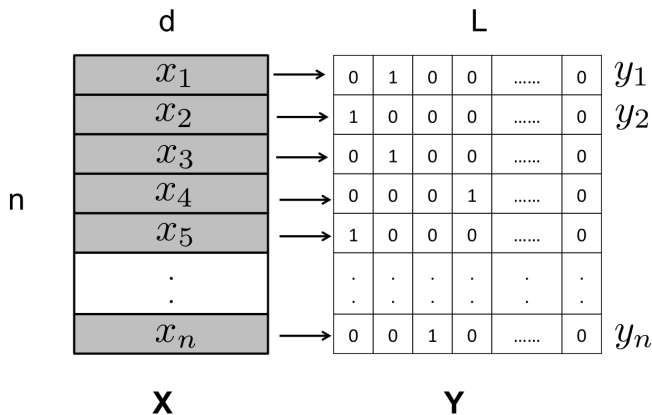


Multi-label Problems

- n data points, L labels, d features
- Input: training data $\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^n$:
 - Each \mathbf{x}_i is a d dimensional feature vector
 - Each $\mathbf{y}_i \in \{0, 1\}^L$ is a label vector (or $Y_i \in \{1, 2, \dots, L\}$)
Example: $\mathbf{y}_i = [0, 0, 1, 0, 0, 1, 1]$ (or $Y_i = \{3, 6, 7\}$)
 - Each training data can belong to **multiple categories**
- Goal: Given a testing sample \mathbf{x} , predict the correct labels

Document 1	{Sports, Politics}
Document 2	{Science, Politics}
⋮	
Document n	{Environment}

Illustration



- Multiclass: each row of L has exact one "1"
- Multilabel: each row of L can have multiple ones

Reduction to binary classification

- Many algorithms for binary classification
- Idea: transform multi-class or multi-label problems to multiple binary classification problems
- Two approaches:
 - One versus All (OVA)
 - One versus One (OVO)

One Versus All (OVA)

- Multi-class/multi-label problems with L categories
- Build L different binary classifiers
- For the t -th classifier:
 - Positive samples: all the points in class t ($\{\mathbf{x}_i : t \in \mathbf{y}_i\}$)
 - Negative samples: all the points not in class t ($\{\mathbf{x}_i : t \notin \mathbf{y}_i\}$)
 - $f_t(\mathbf{x})$: the decision value for the t -th classifier
(larger $f_t \Rightarrow$ higher probability that \mathbf{x} in class t)
- Prediction:
$$f(\mathbf{x}) = \arg \max_t f_t(\mathbf{x})$$
- Example: using SVM to train each binary classifier.

One Versus One (OVO)

- Multi-class/multi-label problems with L categories
- Build $L(L - 1)$ different binary classifiers
- For the (s, t) -th classifier:
 - Positive samples: all the points in class s ($\{\mathbf{x}_i : s \in \mathbf{y}_i\}$)
 - Negative samples: all the points in class t ($\{\mathbf{x}_i : t \in \mathbf{y}_i\}$)
 - $f_{s,t}(\mathbf{x})$: the decision value for this classifier
(larger $f_{s,t}(\mathbf{x}) \Rightarrow$ label s has higher probability than label t)
 - $f_{t,s}(\mathbf{x}) = -f_{s,t}(\mathbf{x})$
- Prediction:

$$f(\mathbf{x}) = \arg \max_s \left(\sum_t f_{s,t}(\mathbf{x}) \right)$$

- Example: using SVM to train each binary classifier.

OVA vs OVO

- Prediction accuracy: depends on datasets
- Computational time:
 - OVA needs to train L classifiers
 - OVO needs to train $L(L - 1)/2$ classifiers
- Is OVA always faster than OVO?

OVA vs OVO

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OVA needs to train L classifiers

OVO needs to train $L(L - 1)/2$ classifiers

- Is OVA always faster than OVO?

NO, depends on the time complexity of the binary classifier

- If the binary classifier requires $O(n)$ time for n samples:
OVA and OVO have similar time complexity
- If the binary classifier requires $O(n^{1.xx})$ time:
OVO is faster than OVA

OVA vs OVO

- Prediction accuracy: depends on datasets
- Computational time:

OVA needs to train L classifiers

OVO needs to train $L(L - 1)/2$ classifiers

- Is OVA always faster than OVO?

NO, depends on the time complexity of the binary classifier

- If the binary classifier requires $O(n)$ time for n samples:
OVA and OVO have similar time complexity
- If the binary classifier requires $O(n^{1.xx})$ time:
OVO is faster than OVA
- LIBSVM (kernel SVM solver): OVO
- LIBLINEAR (linear SVM solver): OVA

Another approach for multi-class classification

- OVA and OVO: decompose the problem by labels
 - But good binary classifiers may not imply good multi-class prediction.

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- OVA and OVO: decompose the problem by labels
But good binary classifiers may not imply good multi-class prediction.
- Design a multi-class loss function and solve a single optimization problem
- Minimize the in-sample error:

$$\min_{\mathbf{w}_1, \dots, \mathbf{w}_L} \sum_{i=1}^n \text{loss}(\mathbf{x}_i, \mathbf{y}_i) + \lambda \sum_{j=1, \dots, L} \mathbf{w}_j^T \mathbf{w}_j$$

Loss functions for multi-class classification

- Ranking based approaches: directly **minimizes the ranking loss**:
 - For multiclass classification, the score of y_i should be larger than other labels

Loss functions for multi-class classification

- Ranking based approaches: directly **minimizes the ranking loss**:
 - For multiclass classification, the score of y_i should be larger than other labels
- Soft-max loss:
measure the **probability** of predicting correct class

Main idea

- For simplicity, we assume a linear model
- Model parameters: $\mathbf{w}_1, \dots, \mathbf{w}_L$
- For each data point \mathbf{x} , compute the decision value for each label:

$$\mathbf{w}_1^T \mathbf{x}, \quad \mathbf{w}_2^T \mathbf{x}, \quad \dots, \quad \mathbf{w}_L^T \mathbf{x}$$

- Prediction:

$$y = \arg \max_t \mathbf{w}_t^T \mathbf{x}$$

- For training data \mathbf{x}_i , y_i is the true label, so we want

$$y_i \approx \arg \max_t \mathbf{w}_t^T \mathbf{x}_i \quad \forall i$$

Softmax

- The **predicted score** for each class:

$$\mathbf{w}_1^T \mathbf{x}_i, \mathbf{w}_2^T \mathbf{x}_i, \dots$$

- Loss for the i -th data is defined by

$$-\log \left(\frac{e^{\mathbf{w}_{y_i}^T \mathbf{x}_i}}{\sum_j e^{\mathbf{w}_j^T \mathbf{x}_i}} \right)$$

(Probability of choosing the **correct label**)

- Solve a single optimization problem

$$\min_{\mathbf{w}_1, \dots, \mathbf{w}_L} \sum_{i=1}^n -\log \left(\frac{e^{\mathbf{w}_{y_i}^T \mathbf{x}_i}}{\sum_j e^{\mathbf{w}_j^T \mathbf{x}_i}} \right) + \lambda \sum_j \mathbf{w}_j^T \mathbf{w}_j$$

Weston-Watkins Formulation

- Proposed in Weston and Watkins, “Multi-class support vector machines”. In ESANN, 1999.

$$\begin{aligned} \min_{\{\mathbf{w}_t\}, \{\xi_i^t\}} \quad & \frac{1}{2} \sum_{t=1}^L \|\mathbf{w}_t\|^2 + C \sum_{i=1}^n \sum_{t=1}^L \xi_i^t \\ \text{s.t.} \quad & \mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_t^T \mathbf{x}_i \geq 1 - \xi_i^t, \quad \xi_i^t \geq 0 \quad \forall t \neq y_i, \quad \forall i = 1, \dots, n \end{aligned}$$

- If point i is in class y_i , for any other labels ($t \neq y_i$), we want

$$\mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_t^T \mathbf{x}_i \geq 1$$

or we pay a penalty ξ_i^t

- Prediction:

$$f(\mathbf{x}) = \arg \max_t \mathbf{w}_t^T \mathbf{x}_i$$

Crammer-Singer Formulation

- Proposed in Crammer and Singer, "On the algorithmic implementation of multiclass kernel-based vector machines". JMLR, 2001.

$$\begin{aligned} \min_{\{\mathbf{w}_t\}, \{\xi_i^t\}} \quad & \frac{1}{2} \sum_{t=1}^L \|\mathbf{w}_t\|^2 + C \sum_{i=1}^n \xi_i \\ \text{s.t.} \quad & \mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_t^T \mathbf{x}_i \geq 1 - \xi_i, \quad \forall t \neq y_i, \quad \forall i = 1, \dots, n \\ & \xi_i \geq 0 \quad \forall i = 1, \dots, n \end{aligned}$$

- If point i is in class y_i , for any other labels ($t \neq y_i$), we want

$$\mathbf{w}_{y_i}^T \mathbf{x}_i - \mathbf{w}_t^T \mathbf{x}_i \geq 1$$

- For each point i , we only pay the largest penalty
- Prediction:

$$f(\mathbf{x}) = \arg \max_t \mathbf{w}_t^T \mathbf{x}_i$$

Conclusions

- SVM, Kernel SVM, Kernel methods

Questions?