SVM (Contd), Multiclass and One-Class SVM

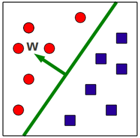
Piyush Rai

Introduction to Machine Learning (CS771A)

September 4, 2018

Recap: Hyperplane-based Classification

- Basic idea: Learn to separate by a hyperplane $\boldsymbol{w}^\top \boldsymbol{x} + b = 0$



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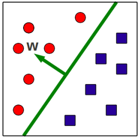

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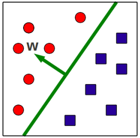

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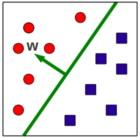

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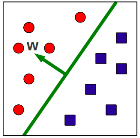

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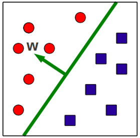

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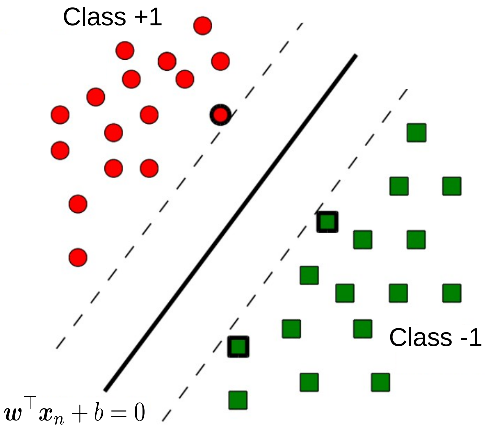
- The hyperplane need not be linear (e.g., can be made nonlinear using kernel methods - next class)

Recap: Hyperplanes and Margin



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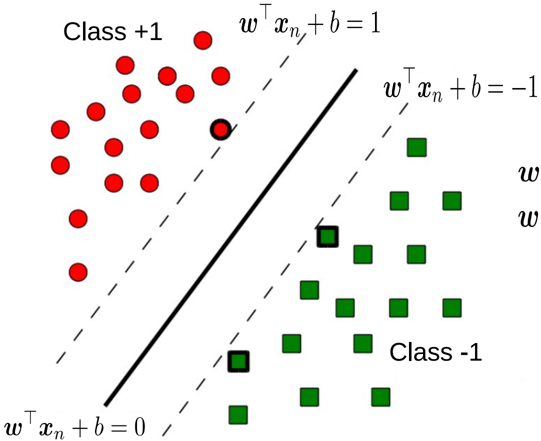

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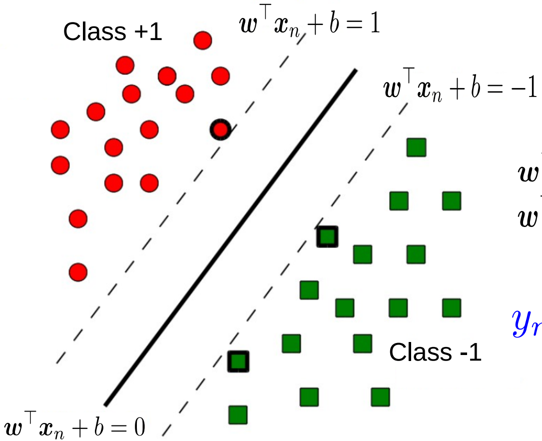

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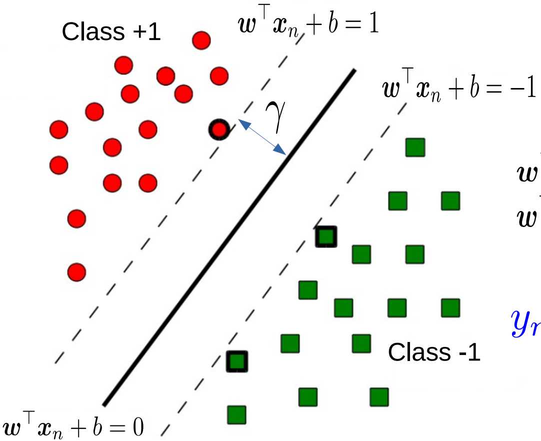

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$$\gamma = \min_{1 \leq n \leq N} \frac{|\boldsymbol{w}^\top \boldsymbol{x}_n + b|}{||\boldsymbol{w}||} = \frac{1}{||\boldsymbol{w}||}$$

(Margin on each side)

Recap: Maximum-Margin Hyperplane

Total margin

$$(\hat{\boldsymbol{w}}, \hat{b}) = \arg\max_{\boldsymbol{w},b} \overset{(2\gamma)}{\boxed{\frac{2}{||\boldsymbol{w}||}}}, \quad \text{s.t.} \quad y_n(\boldsymbol{w}^\top \boldsymbol{x}_n + b) \geq 1$$

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↓ (equivalent to)

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Hard-margin SVM

(“hard” = want all points to satisfy the margin constraint)

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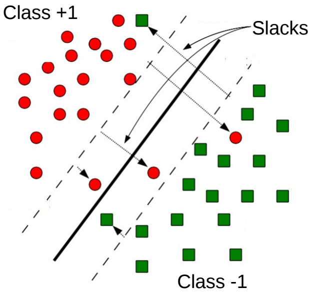

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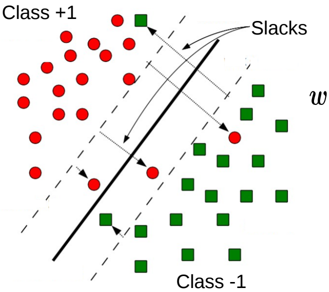

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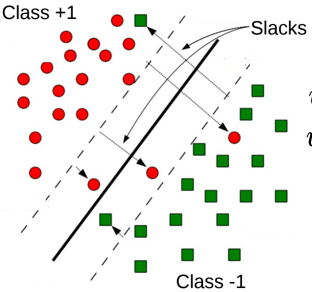

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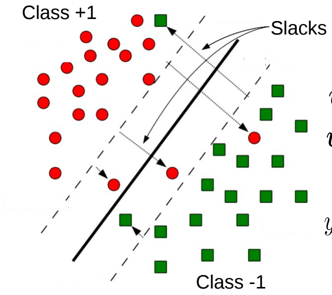

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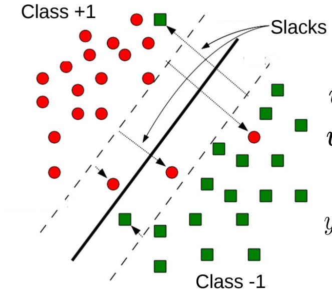

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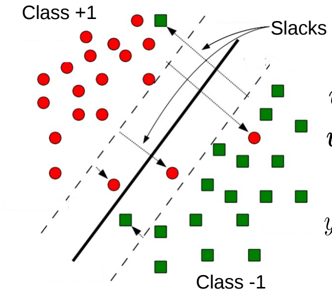

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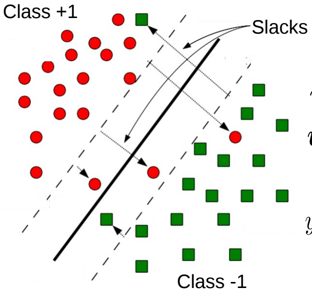

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- **Note:** Can also think of the sum of slacks as the total training error

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Maximize the margin

Hyperparmeter to balance the two

Minimize the sum of slacks (don't have too many violations)

$$(\hat{\boldsymbol{w}}, \hat{b}, \boldsymbol{\xi}) = \arg\min_{\boldsymbol{w}, b} \frac{||\boldsymbol{w}||^2}{2} + C \sum_{n=1}^{N} \xi_n$$

$$\text{s.t.} \quad y_n(\boldsymbol{w}^\top \boldsymbol{x}_n + b) \geq 1 - \xi_n$$

Slack-relaxed constraints

$$\xi_n \geq 0$$

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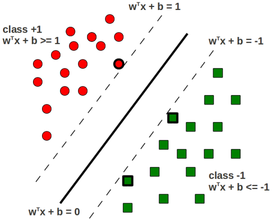
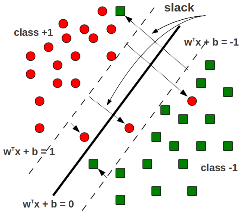
- Very small C: Large margin but also large training error. :-(
- Very large C: Small training error but also small margin. :-(
- C controls the trade-off between large margin and small training error

Summary: Hard-Margin SVM vs Soft-Margin SVM





- Objective for the hard-margin SVM (unknowns are $\boldsymbol{w}$ and b)

$$\begin{aligned} &\arg\min_{\boldsymbol{w},b} \frac{||\boldsymbol{w}||^2}{2} \\ &\text{subject to} \quad y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \geq 1, \qquad n = 1,\ldots,N \end{aligned}$$

- Objective for the soft-margin SVM (unknowns are $\boldsymbol{w}$, b, and $\{\xi_n\}_{n=1}^N$)

$$\begin{aligned} &\arg\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \frac{||\boldsymbol{w}||^2}{2} + C\sum_{n=1}^{N}\xi_n \\ &\text{subject to} \quad y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \geq 1 - \xi_n, \quad \xi_n \geq 0 \qquad n = 1,\ldots,N \end{aligned}$$

- In either case, we have to solve a constrained, convex optimization problem

Solving SVM Objectives

Solving Hard-Margin SVM

- The hard-margin SVM optimization problem is:

$$\boxed{\begin{aligned} &\arg\min_{\boldsymbol{w},b} \frac{||\boldsymbol{w}||^2}{2} \\ &\text{subject to} \quad 1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \leq 0, \qquad n = 1, \ldots, N \end{aligned}}$$

- A constrained optimization problem. Can solve using Lagrange's method

Solving Hard-Margin SVM

- The hard-margin SVM optimization problem is:

$$\boxed{\begin{array}{l} \underset{\boldsymbol{w},b}{\arg\min} \dfrac{||\boldsymbol{w}||^2}{2} \\ \text{subject to} \quad 1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \leq 0, \qquad n = 1, \ldots, N \end{array}}$$

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- Introduce Lagrange Multipliers α_n $(n = \{1, \ldots, N\})$, one for each constraint, and solve

$$\boxed{\min_{\boldsymbol{w},b} \max_{\boldsymbol{\alpha}\geq 0} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{||\boldsymbol{w}||^2}{2} + \sum_{n=1}^{N} \alpha_n\{1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b)\}}$$

- Note: $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_N]$ is the vector of Lagrange multipliers

Solving Hard-Margin SVM

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- Note: $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_N]$ is the vector of Lagrange multipliers
- Note: It is easier (and helpful; we will soon see why) to solve the dual problem: min and then max

Solving Hard-Margin SVM

- The dual problem (min then max) is

$$\boxed{\max_{\boldsymbol{\alpha} \geq 0} \min_{\boldsymbol{w}, b} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{\boldsymbol{w}^\top \boldsymbol{w}}{2} + \sum_{n=1}^{N} \alpha_n \{1 - y_n(\boldsymbol{w}^T \boldsymbol{x}_n + b)\}}$$

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- Take (partial) derivatives of $\mathcal{L}$ w.r.t. $\boldsymbol{w}$, b and set them to zero

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = 0 \Rightarrow \boxed{\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n} \qquad \frac{\partial \mathcal{L}}{\partial b} = 0 \Rightarrow \sum_{n=1}^{N} \alpha_n y_n = 0$$

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- Important: Note the form of the solution $\boldsymbol{w}$ - it is simply a weighted sum of all the training inputs $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ (and α_n is like the "importance" of $\boldsymbol{x}_n$)

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- Important: Note the form of the solution $\boldsymbol{w}$ - it is simply a weighted sum of all the training inputs $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ (and α_n is like the "importance" of $\boldsymbol{x}_n$)
- Substituting $\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n$ in Lagrangian, we get the dual problem as (verify)

$$\boxed{\max_{\boldsymbol{\alpha} \geq 0} \quad \mathcal{L}_D(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\boldsymbol{x}_m^T \boldsymbol{x}_n)}$$

Solving Hard-Margin SVM

- Can write the objective more compactly in vector/matrix form as

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  - Using co-ordinate ascent methods (optimize for one α_n at a time); often very fast

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Hard-Margin SVM: The Solution

- Once we have the α_n's, $\boldsymbol{w}$ and b can be computed as:

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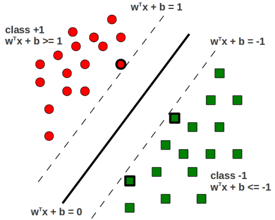

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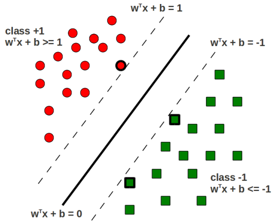

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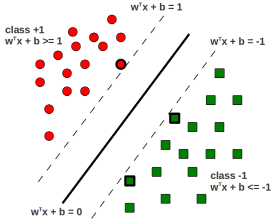

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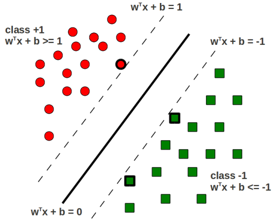

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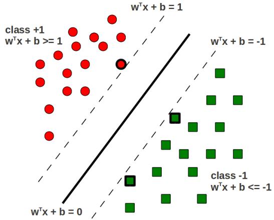

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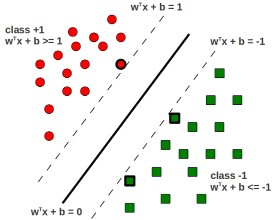

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  - Recall the support vectors "support" the margin boundaries

Solving Soft-Margin SVM

Solving Soft-Margin SVM

- Recall the soft-margin SVM optimization problem:

$$\boxed{\begin{array}{l} \underset{\boldsymbol{w},b,\boldsymbol{\xi}}{\min} \quad f(\boldsymbol{w},b,\boldsymbol{\xi}) = \frac{||\boldsymbol{w}||^2}{2} + C\sum_{n=1}^{N}\xi_n \\ \text{subject to} \quad 1 \leq y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) + \xi_n, \quad -\xi_n \leq 0 \qquad n = 1,\ldots,N \end{array}}$$

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$$\boxed{\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \max_{\boldsymbol{\alpha}\geq 0,\boldsymbol{\beta}\geq 0} \mathcal{L}(\boldsymbol{w},b,\xi,\alpha,\beta) = \frac{||\boldsymbol{w}||^2}{2} + +C\sum_{n=1}^{N}\xi_n + \sum_{n=1}^{N}\alpha_n\{1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) - \xi_n\} - \sum_{n=1}^{N}\beta_n\xi_n}$$

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- Two sets of dual variables $\boldsymbol{\alpha} = [\alpha_1, \dots, \alpha_N]$ and $\boldsymbol{\beta} = [\beta_1, \dots, \beta_N]$. We'll eliminate the primal variables $\boldsymbol{w}, b, \boldsymbol{\xi}$ to get dual problem containing the dual variables (just like in the hard margin case)

Solving Soft-Margin SVM

- The Lagrangian problem to solve

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- Substituting these in the Lagrangian $\mathcal{L}$ gives the Dual problem

$$\boxed{\max_{\boldsymbol{\alpha}\leq C,\boldsymbol{\beta}\geq 0} \mathcal{L}_D(\boldsymbol{\alpha},\boldsymbol{\beta}) = \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{m,n=1}^{N}\alpha_m\alpha_n y_m y_n(\boldsymbol{x}_m^T\boldsymbol{x}_n)}$$

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Support Vectors in Soft-Margin SVM

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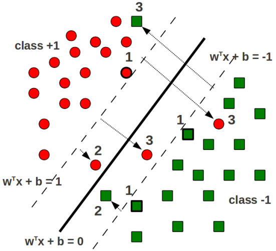

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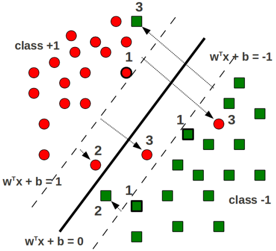

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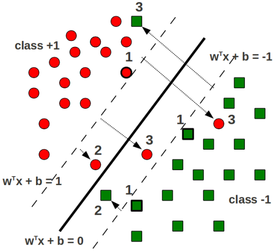

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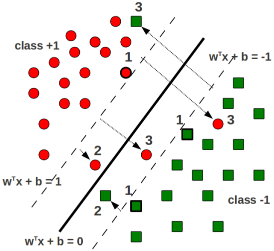

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SVMs via Dual Formulation: Some Comments

- Recall the final dual objectives for hard-margin and soft-margin SVM

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- A lot of work[†] on speeding up SVM in these settings (e.g., can use co-ord. descent for $\boldsymbol{\alpha}$)

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SVM: The Regularized Loss Function View

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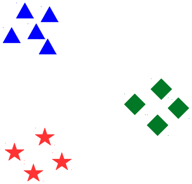

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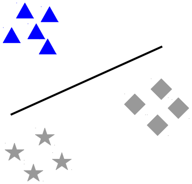
- Note: These approaches can be used with other binary classifiers too (e.g., logistic regression)
- One-vs-All (also called One-vs-Rest): Construct K binary classification problems



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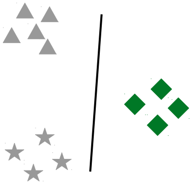

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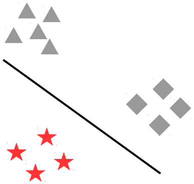

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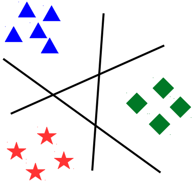

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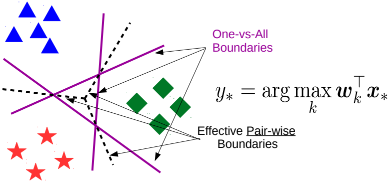

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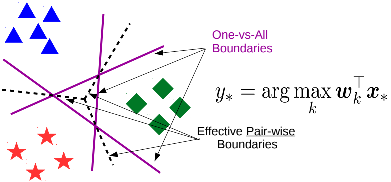

- All-Pairs: Learn K-choose-2 binary classifiers, one for each pair of classes (j, k)

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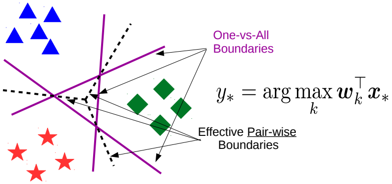

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- All-Pairs approach can be expensive at training and test time (but ways to speed up)

One-Class Classification

- Can we learn from examples of just one class, say positive examples?
- May be desirable if there are many types of negative examples

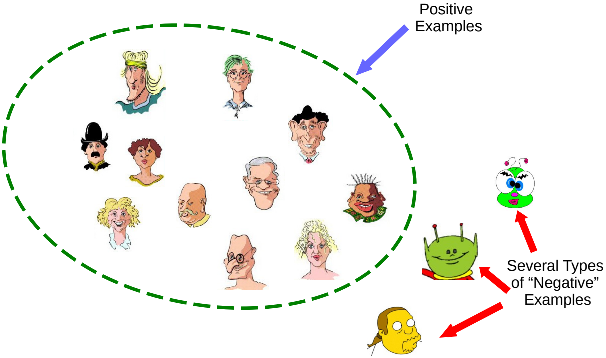

Figure credit: Refael Chickvashvili

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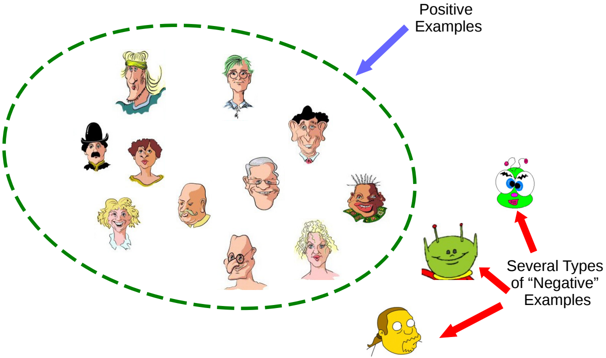

- “Outlier/Novelty Detection” problems can also be formulated like this

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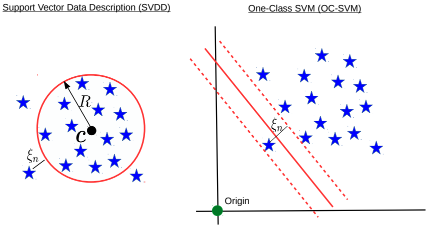
One-Class Classification via SVM-like methods

- There are two popular SVM-type approaches to solve one-class problems



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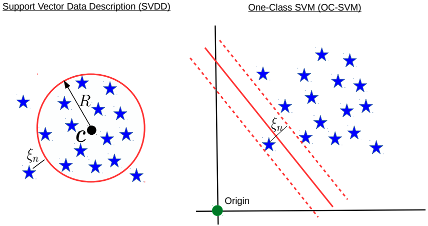

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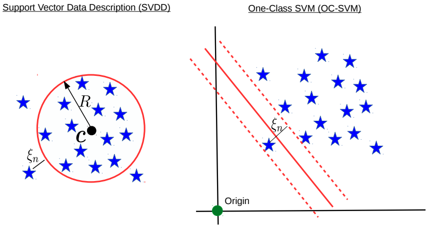

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Support Vector Data Description (SVDD)

$$\arg\min_{R,\boldsymbol{c},\xi} R^2 + \frac{1}{\nu N}\sum_{n=1}^{N}\xi_n$$

$$\text{s.t. } ||\boldsymbol{x}_n - \boldsymbol{c}||^2 \leq R^2 + \xi_n \quad \forall n$$

$$\xi_n \geq 0$$

Prediction Rule: $y_* = +1 \quad \text{if } ||\boldsymbol{x}_* - \boldsymbol{c}||^2 - R^2 < 0$

One-Class SVM (OC-SVM)

$$\arg\min_{\boldsymbol{w},\rho,\xi} ||\boldsymbol{w}||^2 + \frac{1}{\nu N}\sum_{n=1}^{N}\xi_n - \rho$$

$$\text{s.t. } \boldsymbol{w}^\top \boldsymbol{x}_n \geq \rho - \xi_n \quad \forall n$$

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- Optimization problems for both cases can be solved similary as in binary SVM (e.g., via Lagrangian)

Nonlinear SVM ?

- A nice property of SVM (and many other models) is that inputs only appear as inner products
- For example, recall the dual problem for soft-margin SVM had the form

$$\underset{\boldsymbol{\alpha} \leq C}{\arg\max} \ \mathcal{L}_D(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{G}\boldsymbol{\alpha}$$

where $\mathbf{G}$ is an $N \times N$ matrix with $G_{mn} = y_m y_n \boldsymbol{x}_m^\top \boldsymbol{x}_n$, and $\mathbf{1}$ is a vector of 1s

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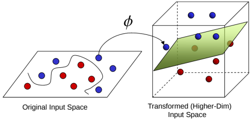

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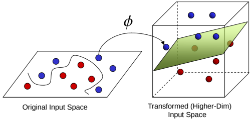

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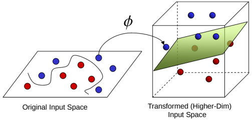

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- Can still learn a linear model in the new space but be nonlinear in the original space (wondeful!)

SVM: Some Notes

- A hugely (perhaps the most!) popular classification algorithm
- Reasonably mature, highly optimized SVM softwares freely available (perhaps the reason why it is more popular than various other competing algorithms)
  - Some popular ones: libSVM, LIBLINEAR, scikit-learn also provides SVM

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- Nonlinear extensions possible via kernels (next class)

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