Learning Maximum-Margin Hyperplanes: Support Vector Machines

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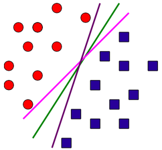
Machine Learning (CS771A)

Aug 24, 2016

Perceptron and (Lack of) Margins

- Perceptron learns a hyperplane (of many possible) that separates the classes



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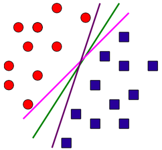

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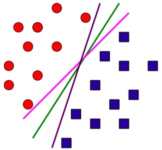

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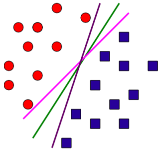

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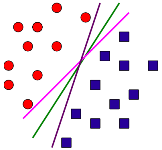

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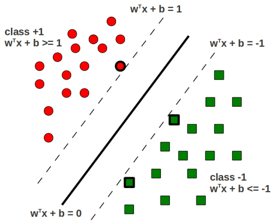
  - **Support Vector Machine (SVM)** offers a more principled way of doing this by learning the maximum margin hyperplane

Support Vector Machine (SVM)

- Learns a hyperplane such that the positive and negative class training examples are as far away as possible from it (ensures good generalization)



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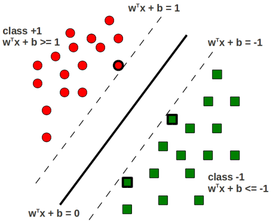

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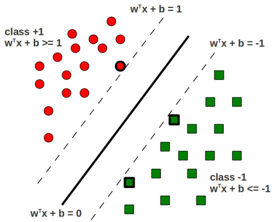

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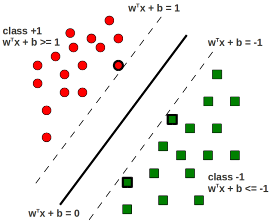

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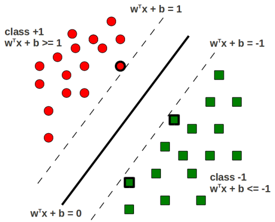

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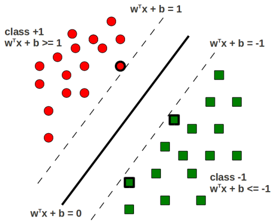

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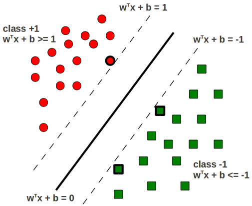
- Reason behind the name "Support Vector Machine"? SVM finds the most important examples (called "support vectors") in the training data
  - These examples also "balance" the margin boundaries (hence called "support"). Also, even if we throw away the remaining training data and re-learn the SVM classifier, we'll get the same hyperplane

Learning a Maximum Margin Hyperplane



- *Suppose* there exists a hyperplane $\boldsymbol{w}^\top \boldsymbol{x} + b = 0$ such that
  - $\boldsymbol{w}^T \boldsymbol{x}_n + b \geq 1$ for $y_n = +1$
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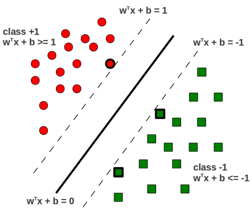

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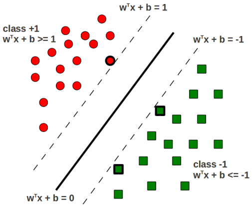

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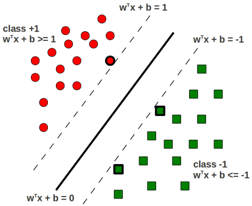

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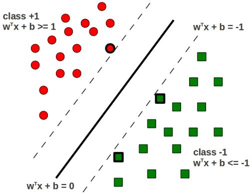

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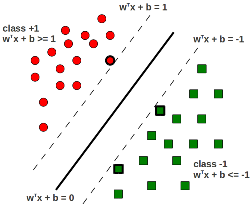

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- Want the hyperplane $(\boldsymbol{w}, b)$ to have the largest possible margin

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  - Wait until we cover Learning Theory!

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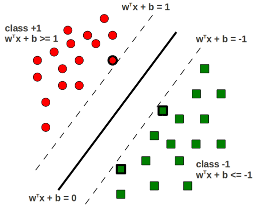

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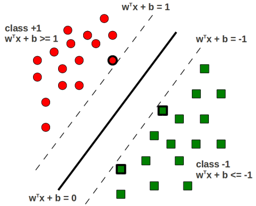

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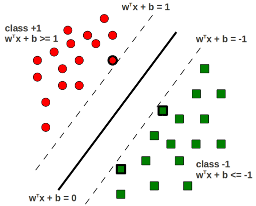

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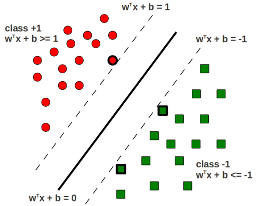

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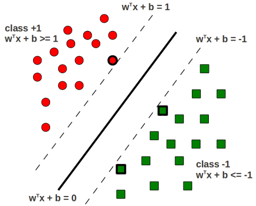

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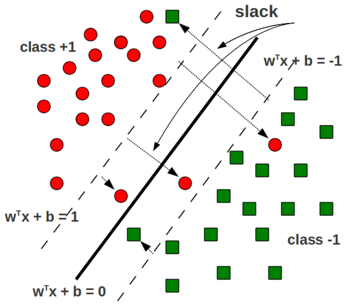
- Thus the hard-margin SVM minimizes a convex objective function which is a Quadratic Program (QP) with N linear inequality constraints

Soft-Margin SVM (More Commonly Used)

- Allow some training examples to fall **within** the margin region, or be even misclassified (i.e., fall on the wrong side). Preferable if training data is noisy



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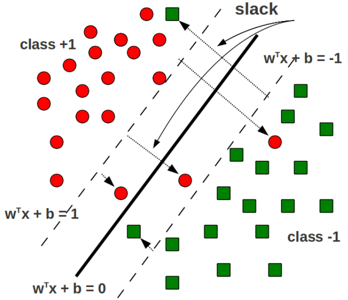

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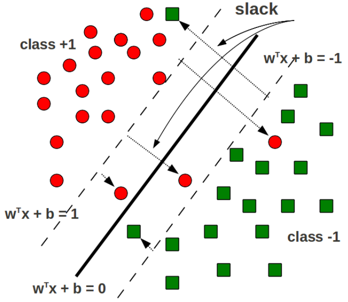

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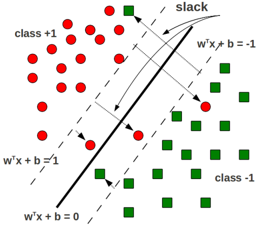
  - Basically, we want a soft-margin condition: $y_n(\boldsymbol{w}^T \boldsymbol{x}_n + b) \geq 1 - \xi_n, \quad \xi_n \geq 0$

Soft-Margin SVM (More Commonly Used)

- Goal: Maximize the margin, while also minimizing the sum of slacks (don't want too many training examples violating the margin condition)



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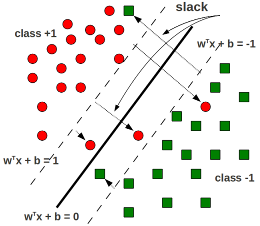

- The primal objective for soft-margin SVM can thus be written as

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

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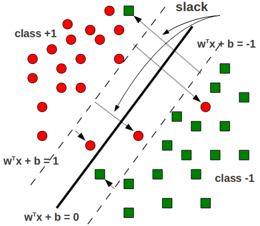

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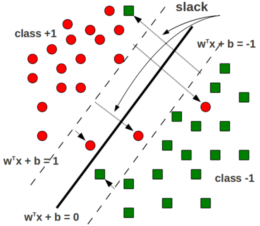

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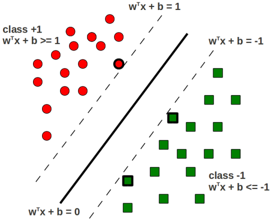
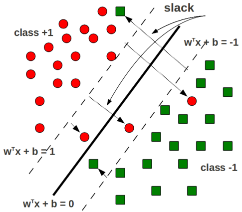
- Thus the soft-margin SVM also minimizes a convex objective function which is a Quadratic Program (QP) with $2N$ linear inequality constraints
- Param. C controls the trade-off between large margin vs small training error

Summary: Hard-Margin SVM vs Soft-Margin SVM





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

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

Brief Detour: Solving Constrained Optimization Problems

Constrained Optimization via Lagrangian

- Consider optimizing the following objective, subject to some constraints

$$\begin{aligned} \min_{\boldsymbol{w}} \quad & f(\boldsymbol{w}) \\ \text{s.t} \quad & g_n(\boldsymbol{w}) \leq 0, \quad n = 1, \ldots, N \\ & h_m(\boldsymbol{w}) = 0, \quad m = 1, \ldots, M \end{aligned}$$

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- Introduce Lagrange multipliers $\boldsymbol{\alpha} = \{\alpha_n\}_{n=1}^N$, $\alpha_n \geq 0$, and $\boldsymbol{\beta} = \{\beta_m\}_{m=1}^M$, one for each constraint, and construct the following Lagrangian

$$\mathcal{L}(\boldsymbol{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\boldsymbol{w}) + \sum_{n=1}^{N} \alpha_n g_n(\boldsymbol{w}) + \sum_{m=1}^{N} \beta_n h_n(\boldsymbol{w})$$

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- Thus $\min_{\boldsymbol{w}} \mathcal{L}_P(\boldsymbol{w}) = \min_{\boldsymbol{w}} \max_{\boldsymbol{\alpha} \geq 0, \boldsymbol{\beta}} \mathcal{L}(\boldsymbol{w}, \boldsymbol{\alpha}, \boldsymbol{\beta})$ solves the same problem as the original problem and will have the same solution. For convex f, g, h, the order of min and max is interchangeable.

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- Karush-Kuhn-Tucker (KKT) Conditions: At the optimal solution, $\alpha_n g_n(\boldsymbol{w}) = 0$ (note the $\max_\alpha$)

Solving Hard-Margin SVM

Solving Hard-Margin SVM

- The hard-margin SVM optimization problem is:

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

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

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

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- We will solve this Lagrangian by solving a dual problem (eliminate $\boldsymbol{w}$ and b and solve for the "dual variables" $\boldsymbol{\alpha}$)

Solving Hard-Margin SVM

- The original Lagrangian is

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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 $\boldsymbol{x}_n$)
- Substituting $\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n$ in Lagrangian and also using $\sum_{n=1}^{N} \alpha_n y_n = 0$

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

Solving Hard-Margin SVM

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

$$\boxed{\max_{\boldsymbol{\alpha} \geq 0} \mathcal{L}_D(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{G}\boldsymbol{\alpha} \qquad \text{s.t.} \quad \sum_{n=1}^{N} \alpha_n y_n = 0}$$

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

† If interested in more details of the solver, see: "Support Vector Machine Solvers" by Bottou and Lin

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  - Using (projected) gradient methods (projection needed because the α's are constrained). Gradient methods will usually be much faster than QP methods.

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Hard-Margin SVM: The Solution

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

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n$$

$$b = -\frac{1}{2}\left(\min_{n:y_n=+1} \boldsymbol{w}^T \boldsymbol{x}_n + \max_{n:y_n=-1} \boldsymbol{w}^T \boldsymbol{x}_n\right)$$

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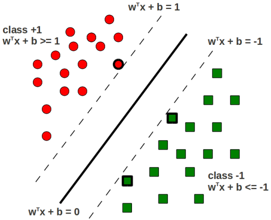
- **A nice property:** Most α_n's in the solution will be zero (sparse solution)



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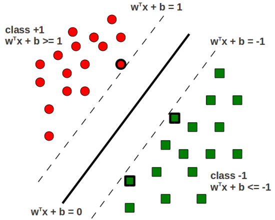

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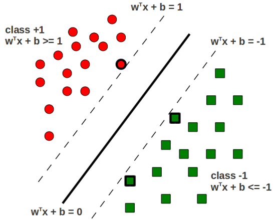

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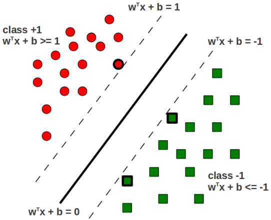

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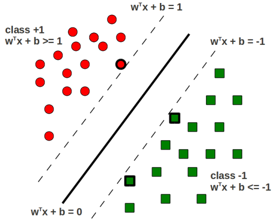

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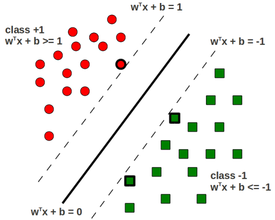

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- These examples are called support vectors
- Recall the support vectors "support" the margin boundaries

Solving Soft-Margin SVM

Solving Soft-Margin SVM

- Recall the soft-margin SVM optimization problem:

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

- Note: $\boldsymbol{\xi} = [\xi_1, \ldots, \xi_N]$ is the vector of slack variables

Solving Soft-Margin SVM

- Recall the soft-margin SVM optimization problem:

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- Note: $\boldsymbol{\xi} = [\xi_1,\ldots,\xi_N]$ is the vector of slack variables
- Introduce Lagrange Multipliers α_n, β_n $(n = \{1,\ldots,N\})$, for constraints, and solve the Lagrangian:

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

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- Note: The terms in red above were not present in the hard-margin SVM
- Two sets of dual variables $\boldsymbol{\alpha} = [\alpha_1,\ldots,\alpha_N]$ and $\boldsymbol{\beta} = [\beta_1,\ldots,\beta_N]$. 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

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

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- **Note:** $\boldsymbol{\alpha}$ is again sparse. Nonzero α_n's correspond to the support vectors

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Support Vectors in Soft-Margin SVM

- The hard-margin SVM solution had only one type of support vectors
  - .. ones that lie on the margin boundaries $\boldsymbol{w}^T\boldsymbol{x} + b = -1$ and $\boldsymbol{w}^T\boldsymbol{x} + b = +1$

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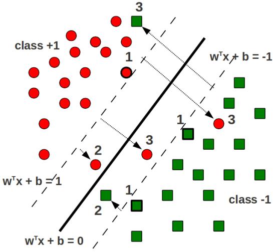

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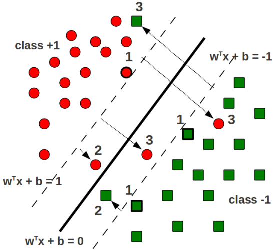

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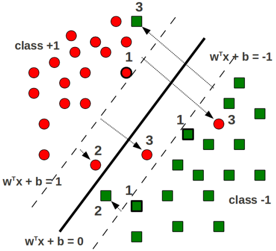

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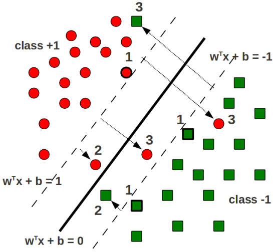

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3. Lying on the wrong side of the hyperplane ($\xi_n \geq 1$)

SVMs via Dual Formulation: Some Comments

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

$$\text{Hard-Margin SVM:} \quad \max_{\boldsymbol{\alpha} \geq 0} \mathcal{L}_D(\alpha) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{G}\boldsymbol{\alpha} \quad \text{s.t.} \quad \sum_{n=1}^{N} \alpha_n y_n = 0$$

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- A lot of work[†] has gone into speeding up optimization in these settings

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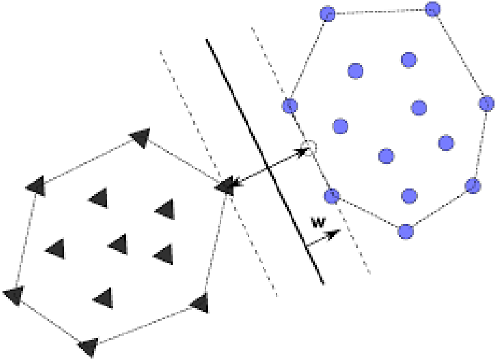
SVM Dual Formulation: A Geometric View

- Convex Hull Interpretation[†]: Solving the SVM dual is equivalent to finding the shortest line connecting the convex hulls of both classes (the SVM's hyperplane will be the perpendicular bisector of this line)



[†] See: "Duality and Geometry in SVM Classifiers" by Bennett and Bredensteiner

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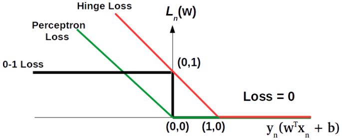
- This is called **"Hinge Loss"**. Can also learn SVMs by minimizing this loss via stochastic sub-gradient descent (can also add a regularizer on $\boldsymbol{w}$, e.g., ℓ_2)



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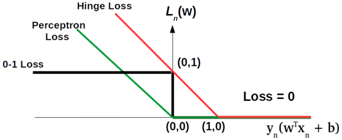
- Can think of our loss as basically the sum of the slacks $\xi_n \geq 0$, which is

$$\boxed{\ell(\boldsymbol{w}, b) = \sum_{n=1}^{N} \ell_n(\boldsymbol{w}, b) = \sum_{n=1}^{N} \xi_n = \sum_{n=1}^{N} \max\{0, 1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b)\}}$$

- This is called **"Hinge Loss"**. Can also learn SVMs by minimizing this loss via stochastic sub-gradient descent (can also add a regularizer on $\boldsymbol{w}$, e.g., ℓ_2)



- Recall that, Perceptron also minimizes a sort of similar loss function

$$\ell(\boldsymbol{w}, b) = \sum_{n=1}^{N} \ell_n(\boldsymbol{w}, b) = \sum_{n=1}^{N} \max\{0, -y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b)\}$$

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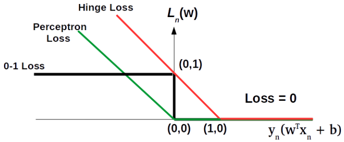

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- Perceptron, SVM, Logistic Reg., all minimize convex approximations of the 0-1 loss (optimizing which is NP-hard; moreover it's non-convex/non-smooth)

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, SVMStruct, Vowpal Wabbit, etc.
- Lots of work on scaling up SVMs† (both large N and large D)
- Extensions beyond binary classification (e.g., multiclass, structured outputs)
- Can even be used for regression problems (Support Vector Regression)
- Nonlinear extensions possible via kernels

† See: "Support Vector Machine Solvers" by Bottou and Lin