Optimization (Wrap-up), and Hyperplane based Classifiers (Perceptron and Support Vector Machines)

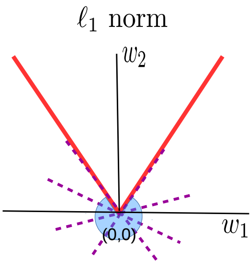
Piyush Rai

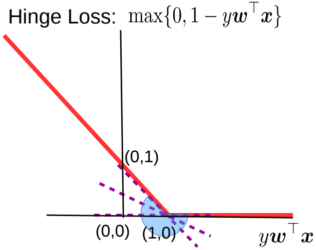
Introduction to Machine Learning (CS771A)

August 30, 2018

Recap: Subgradient Descent

- Use subgradient at non-differentiable points, use gradient elsewhere





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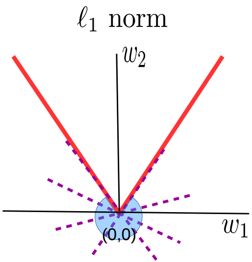

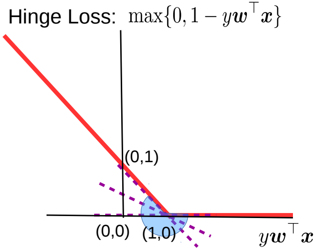

- Left: each entry of (sub)gradient vector for $||\boldsymbol{w}||_1$, Right: (sub)gradient vector for hinge loss

$$t_d = \begin{cases} -1, & \text{for } w_d < 0 \\ [-1, +1] & \text{for } w_d = 0 \\ +1 & \text{for } w_d > 0 \end{cases} \qquad \boldsymbol{t} = \begin{cases} 0, & \text{for } y_n \boldsymbol{w}^\top \boldsymbol{x}_n > 1 \\ -y_n \boldsymbol{x}_n & \text{for } y_n \boldsymbol{w}^\top \boldsymbol{x}_n < 1 \\ k y_n \boldsymbol{x}_n & \text{for } y_n \boldsymbol{w}^\top \boldsymbol{x}_n = 1 \quad (\text{where } k \in [-1, 0]) \end{cases}$$

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Lagrangian: $\mathcal{L}(\boldsymbol{w}, \alpha) = f(\boldsymbol{w}) + \alpha g(\boldsymbol{w})$

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- Multiple constraints (inequality/equality) can also be handled likewise

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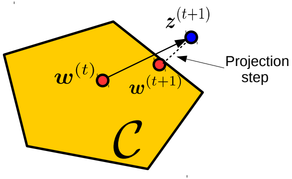

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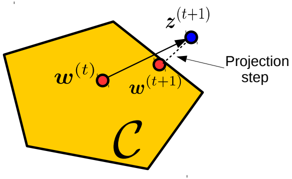
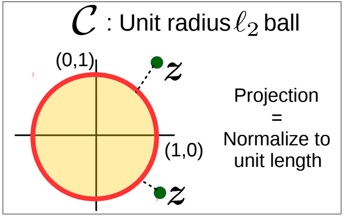
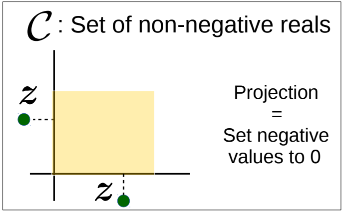


- In some cases, the projection step is very easy





Co-ordinate Descent (CD)

- Standard GD update for $\boldsymbol{w} \in \mathbb{R}^D$ at each step

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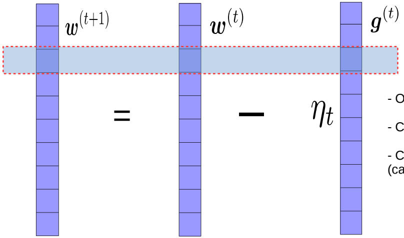

- Order: Random/cyclic

- Can also update in "blocks"

- Cost of update independent of D
(caching previous computations helps)

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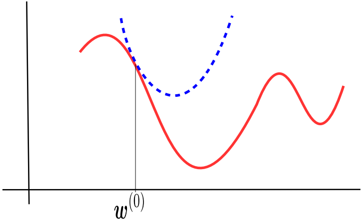

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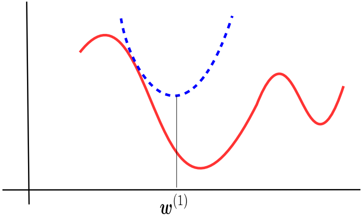

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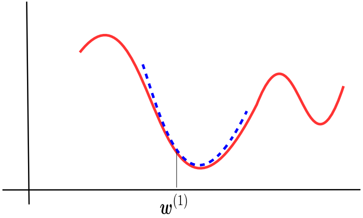

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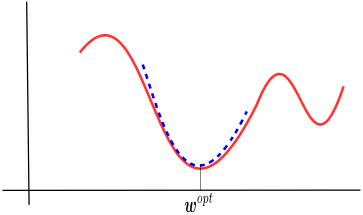

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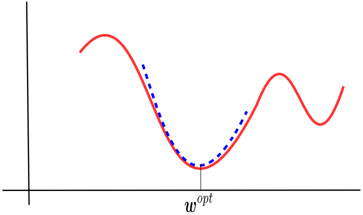

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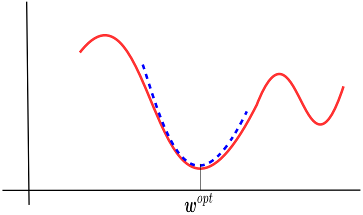

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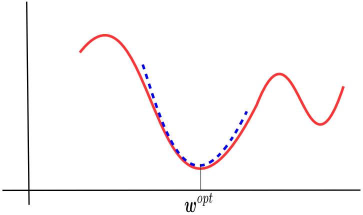

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- Many ways to approximate the Hessian (e.g., using previous gradients); also look at L-BFGS etc.

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- Gradient methods are simple to understand and implement
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  - Backpropagation algorithm used in deep neural nets is GD + chain rule of differentiation
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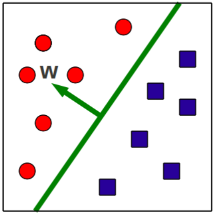
Hyperplane based Classification



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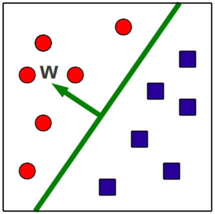

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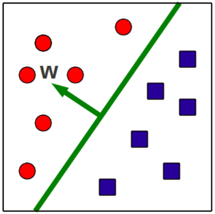

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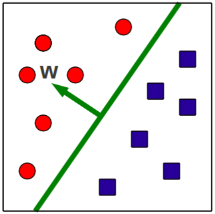

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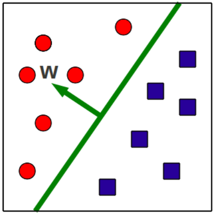

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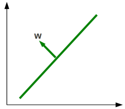

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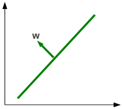

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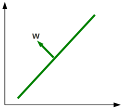

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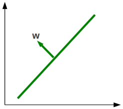

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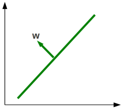

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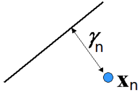

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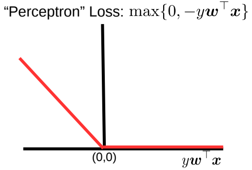

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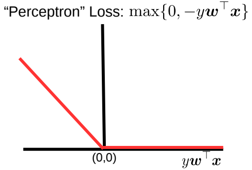

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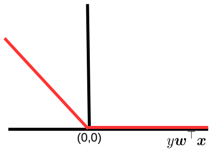

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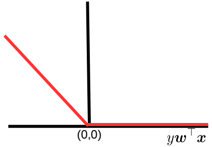

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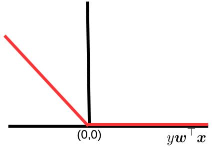

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  - As we'll see, many other models will also lead to $\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n$ (for some suitable α_n's)

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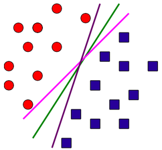
  - Note: In practice, we might want to stop sooner (to avoid overfitting)

Perceptron and (Lack of) Margins

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



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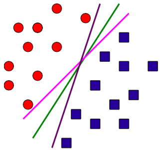

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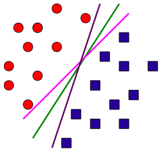

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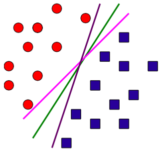

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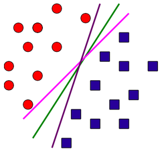

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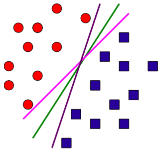

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  - **Support Vector Machine (SVM)** does this directly by learning the maximum margin hyperplane

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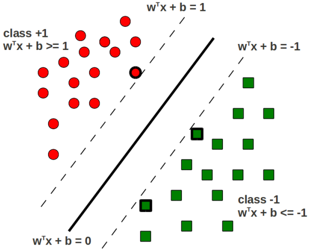

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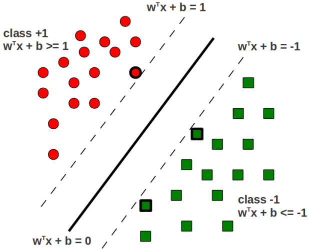

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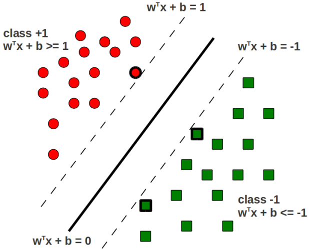

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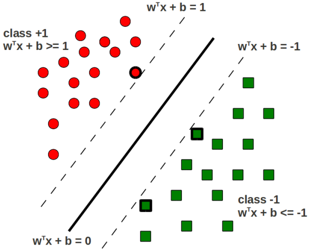

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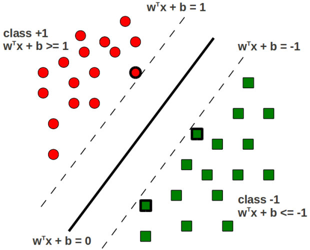

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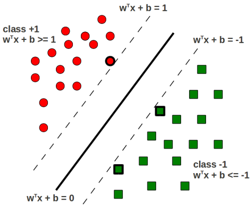
Learning a Maximum Margin Hyperplane



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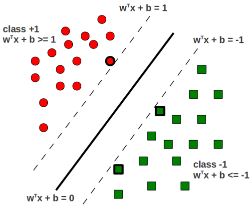

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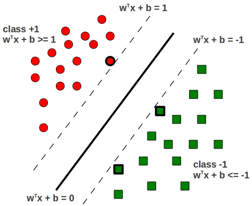

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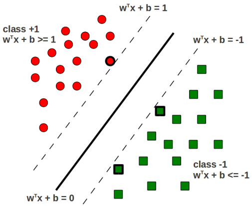

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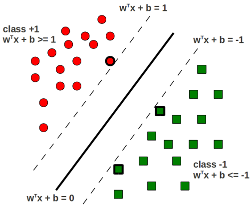

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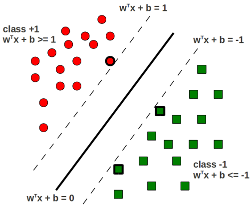

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- **Note:** Can replace $y_n(\boldsymbol{w}^T \boldsymbol{x}_n + b) \geq 1$ by $y_n(\boldsymbol{w}^T \boldsymbol{x}_n + b) \geq m$ for some $m > 0$. It won't change the solution for $\boldsymbol{w}$, will just scale it by a constant, without changing the direction of $\boldsymbol{w}$ (exercise)

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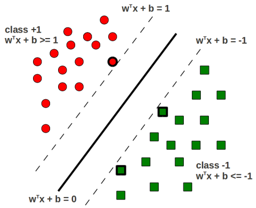

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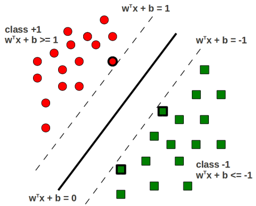

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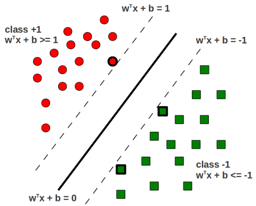

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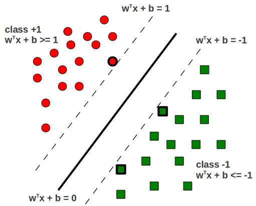

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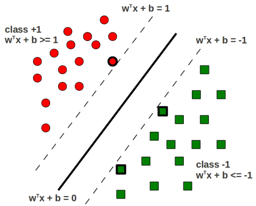

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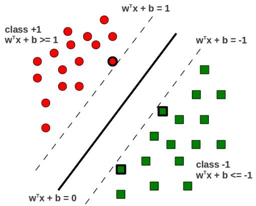

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- Constrained optimization with N inequality constraints (note: function and constraints are convex)

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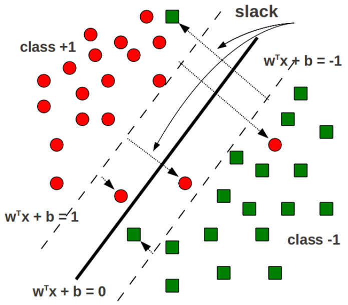

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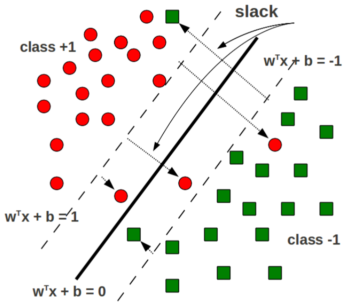

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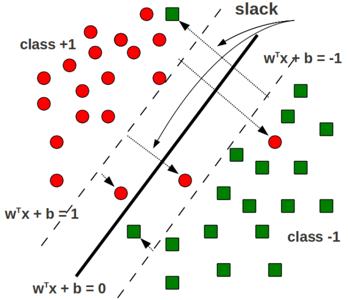

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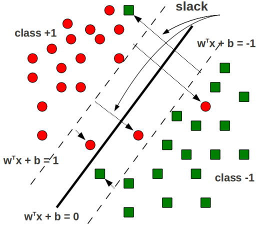
  - Basically, we want a soft-margin condition: $y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \geq 1 - \xi_n, \quad \xi_n \geq 0$

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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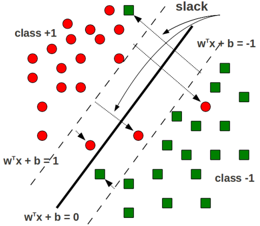

- The primal objective for soft-margin SVM can thus be written as

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

$$\text{subject to} \quad y_n(\boldsymbol{w}^T \boldsymbol{x}_n + b) \geq 1 - \xi_n, \quad \xi_n \geq 0 \qquad n = 1, \ldots, N$$

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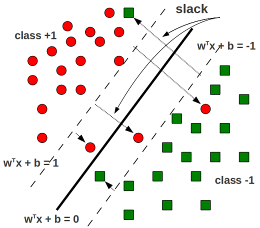

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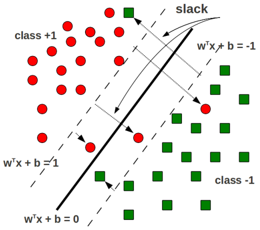

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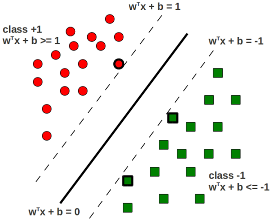
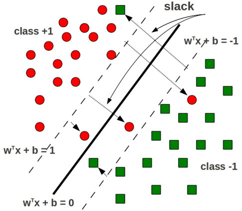
- Constrained optimization with $2N$ inequality constraints
- Parameter C controls the trade-off between large margin vs small training error





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

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

Solving Hard-Margin SVM

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

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

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- 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

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

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

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- Substituting $\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n$ in Lagrangian, we get the dual problem as (verify)

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

Solving Hard-Margin SVM

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

$$\max_{\boldsymbol{\alpha} \geq 0} \quad \mathcal{L}_D(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{G}\boldsymbol{\alpha}$$

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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Hard-Margin SVM: The Solution

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

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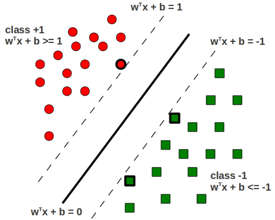

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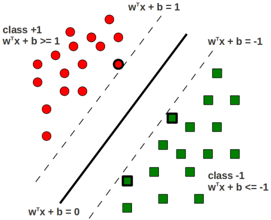

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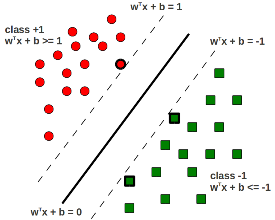

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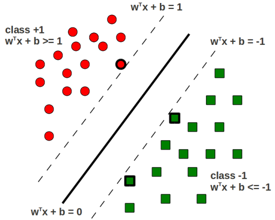

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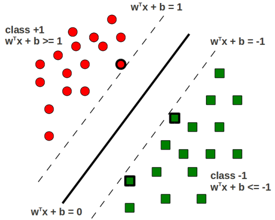

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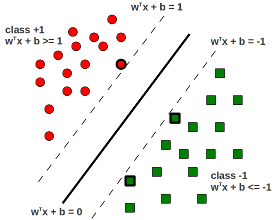

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- Recall the support vectors "support" the margin boundaries

Solving Soft-Margin SVM

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- Note: The terms in red above were not present in the hard-margin SVM

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- Recall the soft-margin SVM optimization problem:

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$$\text{subject to} \quad 1 \leq y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) + \xi_n, \quad -\xi_n \leq 0 \qquad n = 1,\ldots,N$$

- 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:

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

- 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

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

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

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = 0 \Rightarrow \boxed{\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n}, \quad \frac{\partial \mathcal{L}}{\partial b} = 0 \Rightarrow \sum_{n=1}^{N} \alpha_n y_n = 0, \quad \frac{\partial \mathcal{L}}{\partial \xi_n} = 0 \Rightarrow C - \alpha_n - \beta_n = 0$$

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

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

Solving Soft-Margin SVM

- Interestingly, the dual variables β don't appear in the objective!

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

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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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Support Vectors in Soft-Margin SVM

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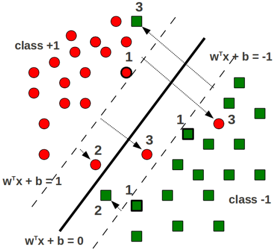

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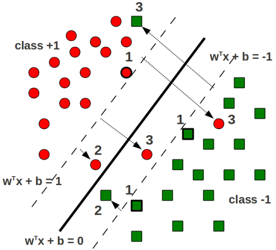

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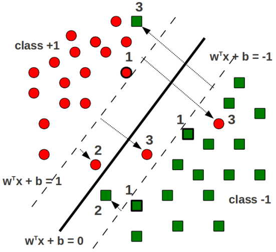

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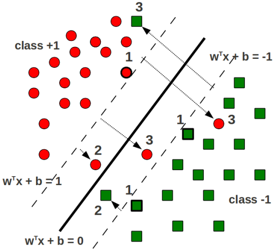

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3. Lying on the wrong side of the hyperplane ($\xi_n \geq 1$)

SVMs via Dual Formulation: Some Comments

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

$$\text{Hard-Margin SVM:} \quad \max_{\boldsymbol{\alpha} \geq 0} \; \mathcal{L}_D(\alpha) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{G} \boldsymbol{\alpha}$$

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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: 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, sklearn also provides SVM
- 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

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