Support Vector Machines (Contd.), Classification Loss Functions and Regularizers

Piyush Rai

CS5350/6350: Machine Learning

September 13, 2011

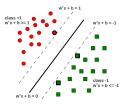
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SVMs, Loss Functions and Regularization

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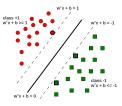
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• SVM finds the maximum margin hyperplane that separates the classes



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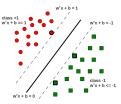
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• Margin
$$\gamma = \frac{1}{||\mathbf{w}||}$$

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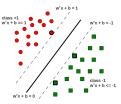
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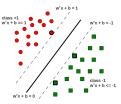


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• The optimization problem for the separable case (no misclassified training example)

• This is a Quadratic Program (QP) with N linear inequality constraints

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• Our optimization problem is:

$$\begin{array}{ll} \text{Minimize} & f(\mathbf{w}, b) = \frac{||\mathbf{w}||^2}{2} \\ \text{subject to} & 1 \le y_n(\mathbf{w}^T \mathbf{x}_n + b), \qquad n = 1, \dots, N \end{array}$$

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Introducing Lagrange Multipliers α_n (n = {1,..., N}), one for each constraint, leads to the Primal Lagrangian:

$$\begin{array}{ll} \text{Minimize} \quad L_P(\mathbf{w}, b, \alpha) = \frac{||\mathbf{w}||^2}{2} + \sum_{n=1}^N \alpha_n \{1 - y_n(\mathbf{w}^T \mathbf{x}_n + b)\} \\ \text{subject to} \quad \alpha_n \geq 0; \quad n = 1, \dots, N \end{array}$$

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- We can now solve this Lagrangian
 - i.e., optimize $L(\mathbf{w}, b, \alpha)$ w.r.t. \mathbf{w} , b, and α
 - .. making use of the Lagrangian Duality theory..

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SVMs, Loss Functions and Regularization

• Take (partial) derivatives of L_P w.r.t. w, b and set them to zero

$$\frac{\partial L_P}{\partial \mathbf{w}} = \mathbf{0} \Rightarrow \mathbf{w} = \sum_{n=1}^N \alpha_n y_n \mathbf{x}_n,$$

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• Substituting these in the Primal Lagrangian L_P gives the Dual Lagrangian

$$\begin{aligned} \text{Maximize } & L_D(\mathbf{w}, b, \alpha) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n(\mathbf{x}_m^T \mathbf{x}_n) \\ \text{subject to } & \sum_{n=1}^{N} \alpha_n y_n = 0, \quad \alpha_n \geq 0; \quad n = 1, \dots, N \end{aligned}$$

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- Several off-the-shelf solvers exist to solve such QPs
- Some examples: quadprog (MATLAB), CVXOPT, CPLEX, IPOPT, etc.

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SVMs, Loss Functions and Regularization

• Once we have the α_n 's, w and b can be computed as:

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

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$$\alpha_n\{1-y_n(\mathbf{w}^T\mathbf{x}_n+b)\}=0$$

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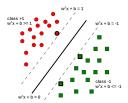
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- α_n is non-zero only if x_n lies on one of the two margin boundaries, i.e., for which y_n(w^Tx_n + b) = 1
- These examples are called support vectors
- Support vectors "support" the margin boundaries



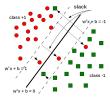
• Non-separable case: No hyperplane can separate the classes perfectly

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- Still want to find the maximum margin hyperplane but this time:

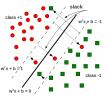
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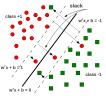
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• Recall: For the separable case (training loss = 0), the constraints were:

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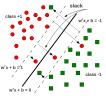
• For the non-separable case, we relax the above constraints as:

$$y_n(\mathbf{w}^T\mathbf{x}_n+b) \geq 1-\xi_n \quad \forall n$$

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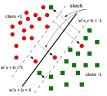
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• ξ_n is called slack variable (distance \mathbf{x}_n goes past the margin boundary)

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• $\xi_n \ge 0, \forall n$, misclassification when $\xi_n > 1$

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- The optimization problem for the non-separable case

Minimize
$$f(\mathbf{w}, b) = \frac{||\mathbf{w}||^2}{2} + C \sum_{n=1}^{N} \xi_n$$

subject to $y_n(\mathbf{w}^T \mathbf{x}_n + b) \ge 1 - \xi_n, \quad \xi_n \ge 0 \qquad n = 1, \dots, N$

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• C dictates which term $(\frac{||\mathbf{w}||^2}{2} \text{ or } C \sum_{n=1}^N \xi_n)$ will dominate the minimization

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C dictates which term (^{||w||²}/₂ or C Σ^N_{n=1} ξ_n) will dominate the minimization
 Small C ⇒ ^{||w||²}/₂ dominates ⇒ prefer large margins

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 - Large $C \Rightarrow C \sum_{n=1}^{N} \xi_n$ dominates \Rightarrow prefer small # of misclassified examples

(a)

SVM - Non-separable case

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 Small C ⇒ ^{||w||²}/₂ dominates ⇒ prefer large margins
 - ... but allow potentially large # of misclassified training examples
 - Large C ⇒ C ∑^N_{n=1} ξ_n dominates ⇒ prefer small # of misclassified examples
 .. at the expense of having a small margin

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(a)

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subject to $1 \le y_n(\mathbf{w}^T \mathbf{x}_n + b) + \xi_n, \quad 0 \le \xi_n \qquad n = 1, \dots, N$

Introducing Lagrange Multipliers α_n, β_n (n = {1,..., N}), for the constraints, leads to the Primal Lagrangian:

$$\begin{array}{ll} \text{Minimize} \quad L_P(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{||\mathbf{w}||^2}{2} + +C\sum_{n=1}^N \xi_n + \sum_{n=1}^N \alpha_n \{1 - y_n(\mathbf{w}^T \mathbf{x}_n + b) - \xi_n\} - \sum_{n=1}^N \beta_n \xi_n \\ \text{subject to} \quad \alpha_n, \beta_n \ge 0; \quad n = 1, \dots, N \end{array}$$

• Our optimization problem is:

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

subject to $1 \le y_n(\mathbf{w}^T \mathbf{x}_n + b) + \xi_n, \quad 0 \le \xi_n \qquad n = 1, \dots, N$

Introducing Lagrange Multipliers α_n, β_n (n = {1,..., N}), for the constraints, leads to the Primal Lagrangian:

$$\begin{array}{ll} \text{Minimize} \quad L_P(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{||\mathbf{w}||^2}{2} + C\sum_{n=1}^N \xi_n + \sum_{n=1}^N \alpha_n \{1 - y_n(\mathbf{w}^T \mathbf{x}_n + b) - \xi_n\} - \sum_{n=1}^N \beta_n \xi_n \\ \text{subject to} \quad \alpha_n, \beta_n \ge 0; \quad n = 1, \dots, N \end{array}$$

• Comparison note: Terms in red font were not there in the separable case

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• Take (partial) derivatives of L_P w.r.t. **w**, b, ξ_n and set them to zero

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• Take (partial) derivatives of L_P w.r.t. **w**, b, ξ_n and set them to zero

$$\frac{\partial L_{\mathsf{P}}}{\partial \mathsf{w}} = \mathbf{0} \Rightarrow \mathsf{w} = \sum_{n=1}^{\mathsf{N}} \alpha_n y_n \mathsf{x}_n,$$

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• Take (partial) derivatives of L_P w.r.t. **w**, b, ξ_n and set them to zero

$$\frac{\partial L_{P}}{\partial \mathbf{w}} = \mathbf{0} \Rightarrow \mathbf{w} = \sum_{n=1}^{N} \alpha_{n} y_{n} \mathbf{x}_{n}, \quad \frac{\partial L_{P}}{\partial b} = \mathbf{0} \Rightarrow \sum_{n=1}^{N} \alpha_{n} y_{n} = \mathbf{0},$$

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• Using $C - \alpha_n - \beta_n = 0$ and $\beta_n \ge 0$

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• Using $C - \alpha_n - \beta_n = 0$ and $\beta_n \ge 0 \Rightarrow \alpha_n \le C$

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- Using $C \alpha_n \beta_n = 0$ and $\beta_n \ge 0 \Rightarrow \alpha_n \le C$
- Substituting these in the Primal Lagrangian L_P gives the Dual Lagrangian

$$\begin{aligned} \text{Maximize} \quad & L_D(\mathbf{w}, b, \boldsymbol{\xi}, \alpha, \beta) = \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_{m,n=1}^N \alpha_m \alpha_n y_m y_n(\mathbf{x}_m^T \mathbf{x}_n) \\ \text{subject to} \quad & \sum_{n=1}^N \alpha_n y_n = 0, \quad 0 \leq \alpha_n \leq C; \quad n = 1, \dots, N \end{aligned}$$

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• Take (partial) derivatives of L_P w.r.t. w, b, ξ_n and set them to zero

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

- Using $C \alpha_n \beta_n = 0$ and $\beta_n \ge 0 \Rightarrow \alpha_n \le C$
- Substituting these in the Primal Lagrangian L_P gives the Dual Lagrangian

Maximize
$$L_D(\mathbf{w}, b, \boldsymbol{\xi}, \alpha, \beta) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n(\mathbf{x}_m^T \mathbf{x}_n)$$

subject to $\sum_{n=1}^{N} \alpha_n y_n = 0$, $0 \le \alpha_n \le C$; $n = 1, \dots, N$

• Again a Quadratic Programming problem in α

• • • • • • • • • • • •

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subject to $\sum_{n=1}^{N} \alpha_n y_n = 0$, $0 \le \alpha_n \le C$; $n = 1, \dots, N$

- Again a Quadratic Programming problem in α
- Given α, the solution for w, b has the same form as the separable case
- Note: α is again sparse. Nonzero α_n 's correspond to the support vectors

(CS5350/6350)

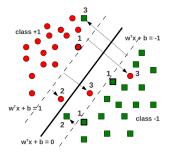
SVMs, Loss Functions and Regularization

• The separable case has only one type of support vectors

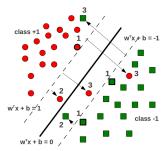
• .. ones that lie on the margin boundaries $\mathbf{w}^T \mathbf{x} + b = -1$ and $\mathbf{w}^T \mathbf{x} + b = +1$

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- The separable case has only one type of support vectors
 - .. ones that lie on the margin boundaries $\mathbf{w}^T \mathbf{x} + b = -1$ and $\mathbf{w}^T \mathbf{x} + b = +1$
- The non-separable case has three types of support vectors

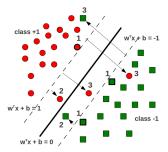


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Q Lying on the margin boundaries $\mathbf{w}^T \mathbf{x} + b = -1$ and $\mathbf{w}^T \mathbf{x} + b = +1$ ($\xi_n = 0$)

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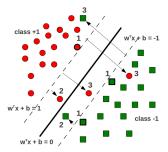


Lying on the margin boundaries w^Tx + b = -1 and w^Tx + b = +1 (ξ_n = 0)
 Lying within the margin region (0 < ξ_n < 1) but still on the correct side

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- The separable case has only one type of support vectors
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Q Lying on the margin boundaries $\mathbf{w}^T \mathbf{x} + b = -1$ and $\mathbf{w}^T \mathbf{x} + b = +1$ ($\xi_n = 0$)

- 2 Lying within the margin region $(0 < \xi_n < 1)$ but still on the correct side
- Solution Using on the wrong side of the hyperplane $(\xi_n \ge 1)$

(CS5350/6350)

SVMs, Loss Functions and Regularization

- Training time of the standard SVM is $O(N^3)$ (have to solve the QP)
 - Can be prohibitive for large datasets

- Training time of the standard SVM is $O(N^3)$ (have to solve the QP)
 - Can be prohibitive for large datasets
- Lots of research has gone into speeding up the SVMs
 - Many approximate QP solvers are used to speed up SVMs
 - Online training (e.g., using stochastic gradient descent)

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- Popular SVM implementations: libSVM, SVMLight, SVM-struct, etc.
 - Also http://www.kernel-machines.org/software

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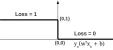
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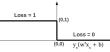
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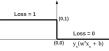


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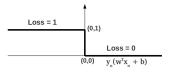
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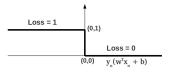
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- Different loss function approximations and regularizers lead to specific algorithms (e.g., Perceptron, SVM, Logistic Regression, etc.).

(CS5350/6350)

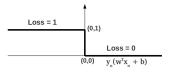
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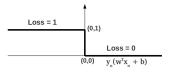


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(CS5350/6350)

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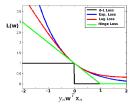
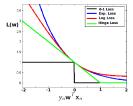


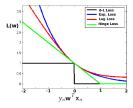
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 - Note: hinge loss is not smooth at (1,0) but subgradient descent can be used

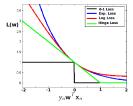
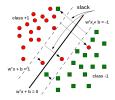


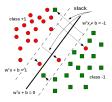
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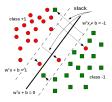
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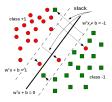
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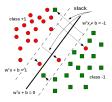
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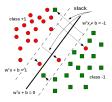
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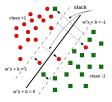
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(CS5350/6350)

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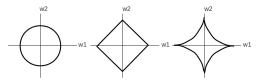


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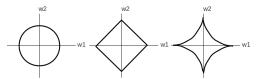


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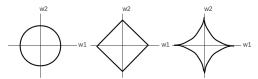


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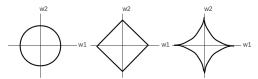


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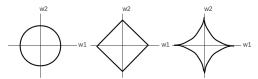


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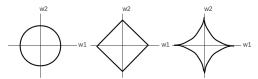


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- ℓ_p norm: $||\mathbf{w}||_p = (\sum_{d=1}^D w_d^p)^{1/p}$

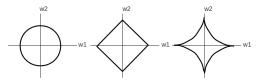


Figure: Contour plots. Left: ℓ_2 norm, Center: ℓ_1 norm, Right: ℓ_p norm (for p < 1)

- Smaller p favors sparser vector w (most entries of w close/equal to 0)
 - But the norm becomes non-convex for p < 1 and is hard to optimize
- The ℓ_1 norm is the most preferred regularizer for sparse **w** (many w_d 's zero)
 - Convex, but it's not smooth at the axis points
 - .. but several methods exists to deal with it, e.g., subgradient descent
- The ℓ_2 squared norm tries to keep the individual w_d 's small

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• Norm based regularizers are used as approximations to $R^{cnt}(\mathbf{w}, b)$

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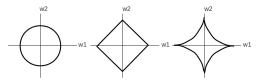


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- The ℓ_2 squared norm tries to keep the individual w_d 's small
 - Convex, smooth, and the easiest to deal with

(CS5350/6350)

SVMs, Loss Functions and Regularization

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- Introduction to Kernels
- Nonlinear classification algorithms
 - Kernelized Perceptron
 - Kernelized Support Vector Machines

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