

Homework

- Project: [CoNLL 2004 shared task](#)
- Homework for next week from today:
 - ★ Write a program which calculates the probability of each verb sense from the training data
 - ★ Don't rely on the verb sense tags, though you can use them for debugging
 - ★ Turn in program, plus sense probabilities for *exchange* and *feel*
- Item read chapter 1 of *Learning with kernels* at <http://www.learning-with-kernels.org/>

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Perceptron

- Rosenblatt's perceptron algorithm constructs a linear decision boundary (*separating hyperplane*)
- For each misclassified training example, update weights (primal form):
$$w \leftarrow w + \eta(y_i - \hat{y}_i)x_i$$
- This is a form of gradient descent to minimize the negative margin of misclassified points:

$$\hat{w} = \operatorname{argmin}_w - \sum_{i \in \mathcal{M}} y_i (x_i \cdot w)$$

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Perceptron

- The functional margin γ :

$$\gamma = \min_i y_i (x_i \cdot w)$$

is non-negative if the data is separated by the hyperplane w , and the larger γ is, the greater the separation

- Novikoff (1962): Suppose some weight vector w_0 (where $\|w\| = 1$) correctly classifies all examples in the training set with margin γ , and $R = \max_i \|x_i\|$. Then the number of corrections made by the perceptron algorithm is at most:

$$\left(\frac{2R}{\gamma}\right)^2$$

- The difficulty of learning a concept depends on the pattern length divided by the margin

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Perceptron

- The perceptron algorithm suffers from a few serious problems
- If the training data is not separable (i.e., $\gamma < 0$), it will not converge to a solution
- If the margin γ is very small, convergence will be very slow
- When the margin is large, the solution is not unique and will depend on the starting conditions
- The first two problems can be addressed by increasing the dimensionality of the feature space to improve separation

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Feature spaces

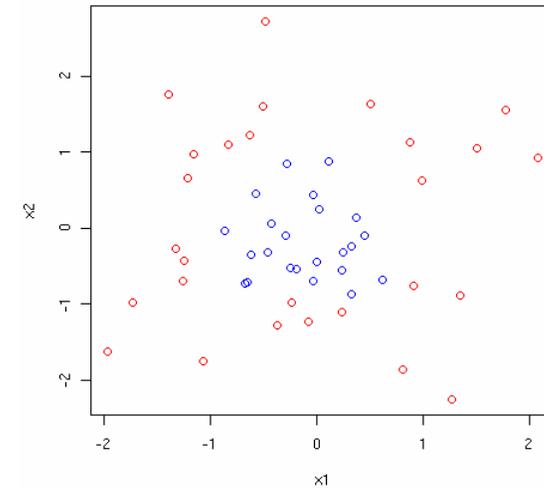
- For example, we could expand a two dimensional input space to a six-dimensional polynomial feature space:

$$\Phi : (x_1, x_2) \rightarrow (x_1, x_2, x_1 x_2, x_2 x_1, x_1^2, x_2^2)$$

- A separating hyperplane in this feature space corresponds to a 2nd degree polynomial decision boundary in the input space
- By using the perceptron algorithm in this derived feature space, we can find a non-linear boundary in the input space
- While increasing the dimensionality generally improves separation, it can also introduce it's own problems

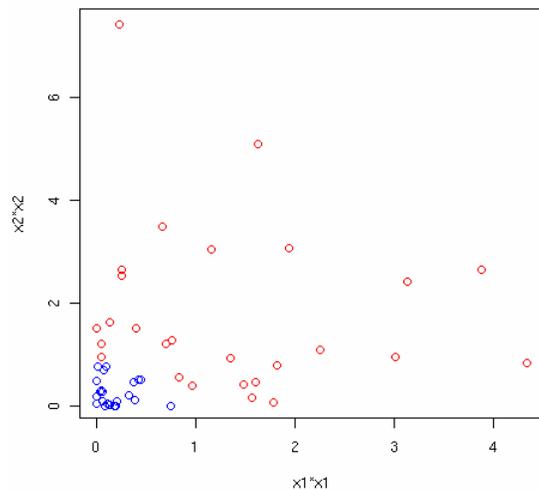
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Feature spaces



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Feature space



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Feature spaces

- One drawback to this is computational: our feature vectors and weight will get very long in a hurry
- A solution is to use the *dual form* of the perceptron algorithm, which represents the decision boundary by the embedding strength of the training examples:

$$w = \sum_i \alpha_i y_i x_i$$

and the decision boundary is:

$$\hat{y} = \text{sign}\left(\sum \alpha_i y_i (x_i \cdot x)\right)$$

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Kernel functions

- Now the training data only enters into our calculations via dot products $(x_i \cdot x_j)$
- For certain feature spaces, the dot product can be computed efficiently without actually constructing the complete feature vectors
- And, it turns out that a broad class of *kernel functions* $K(x_i, x_j)$ are dot products in some (possibly ∞ -dimensional) feature space
- Representing kernel Hilbert spaces (RKHS)
- The dual form of the perceptron algorithm can use any of these kernel functions in place of the dot product:

$$\hat{y} = \text{sign}\left(\sum \alpha_i y_i K(x_i, x)\right)$$

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Kernel functions

- Linear kernel

$$K(x_i, x_j) = (x_i \cdot x_j)$$

- Polynomial kernel

$$K(x_i, x_j) = (x_i \cdot x_j)^d$$

- Radial basis function (RBF) kernel

$$K(x_i, x_j) = \exp\left(\frac{-|x_i - x_j|^2}{\sigma^2}\right)$$

- Kernels are a kind of similarity measure

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Kernel functions

- Other kernel functions are used occasionally, but these are the most important
- Linear kernels are very useful when feature vectors are sparse (e.g., texts represented as a bag of words)
- Polynomial kernels fit curves
- RBFs are Gaussian blobs centered on training examples (k nearest neighbors?)
- Using a kernel function, the inputs need not even be in a vector space (string kernels, tree kernels)
- 'Kernelizing' the perceptron can improve performance on inseparable or poorly separated training data, with the risk of overtraining

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Perceptron

- We still don't have a unique solution from the perceptron algorithm for separable problems
- We can fix this by imposing a stronger constraint
- Rather than minimizing the negative margin of misclassified points:

$$\hat{w} = \underset{w}{\text{argmin}} - \sum_{i \in \mathcal{M}} y_i (x_i \cdot w)$$

we can instead maximize the functional margin:

$$\gamma = \min_i y_i (x_i \cdot w)$$

- Recall how increasing the margin improved things with boosting

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Canonical hyperplane

- A problem: many weight vectors represent the same hyperplane, so we can rescale the weights (and increase the functional margin) without changing the classification decisions

- We define the *geometric margin*:

$$\rho = \frac{\gamma}{\|w\|}$$

and we say that a separating hyperplane w is *canonical* if the functional margin $\gamma = 1$

- For a canonical hyperplane, the distance to the closest data point is $1/\|w\|$

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Optimal margin classifier

- We've already seen plenty of evidence that large margins are good
- Here's a theoretical bound on the generalization error of a separating hyperplane
- Suppose $\|w\| \leq \Lambda$ and $\|x\| \leq R$ for $\Lambda, R > 0$, and the *margin error* ν is the fraction of the m training examples with margin smaller than $\frac{\rho}{\|w\|}$ for $\rho > 0$. Then, with probability at least $1 - \delta$, the probability of misclassifying a test example is bounded by:

$$\nu + \sqrt{\frac{c}{m} \left(\frac{R^2 \Lambda^2}{\rho^2} (\log m)^2 + \log \frac{1}{\delta} \right)}$$

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Optimal margin classifier

- Some observations about this:

$$\nu + \sqrt{\frac{c}{m} \left(\frac{R^2 \Lambda^2}{\rho^2} (\log m)^2 + \log \frac{1}{\delta} \right)}$$

- The error is the sum of the margin error ν (i.e., training error) and a capacity term ($\sqrt{\dots}$)
- As m gets large, the capacity term gets small
- The capacity term gets larger as Λ and R (which are more or less fixed by the training data) increase
- Increasing the margin ρ will decrease the capacity term, but increase the margin error

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Optimal margin classifier

- This bound suggests we want to find a separating hyperplane that maximizes the margin ρ without increasing the margin error ν
- For a canonical hyperplane, $\gamma = 1$ and:

$$\rho = \frac{1}{\|w\|}$$

Thus maximizing ρ is the same as minimizing $\|w\|$

- In other words, we want to find a canonical hyperplane where $\|w\|$ is small and no training points have margin less than $1/\|w\|$
- In other other words, we want no points where $y(w \cdot x) < 1$

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Optimal margin classifier

- We can frame this a *quadratic programming* problem:

$$\begin{aligned} \text{find:} \quad & \min_w \frac{1}{2} \|w\|^2 \\ \text{such that:} \quad & y_i (x_i \cdot w) \geq 1, \text{ for all } i = 1, \dots, m \end{aligned}$$

- To solve this, we introduce the Lagrangian:

$$L(w, \alpha) = \frac{1}{2} \|w\|^2 - \sum_i \alpha_i (y_i (x_i \cdot w) - 1)$$

where $\alpha_i \geq 0$

- We minimize L with respect to w by setting the derivatives to zero, which gives us:

$$w = \sum_i \alpha_i y_i x_i$$

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Optimal margin classifier

- The decision boundary is given by:

$$\hat{y} = \text{sign}\left(\sum \alpha_i y_i (x_i \cdot x)\right)$$

- At the solution, $\alpha_i (y_i (x_i \cdot w) - 1) = 0$ for all i
- So, if $\alpha_i > 0$, then $y_i (x_i \cdot w) = 1$ and x_i is right on the margin
- If $y_i (x_i \cdot w) > 1$ and x_i is not on the margin, then $\alpha_i = 0$
- Thus, the decision boundary is a linear combination of training points which lie precisely on the margin (*support vectors*). The other training points are irrelevant.

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Optimal margin classifier

- With some substitutions and tinkering, we get the dual problem:

$$\begin{aligned} \text{find:} \quad & \max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j (x_i \cdot x_j) \\ \text{such that:} \quad & \alpha_i \geq 0 \end{aligned}$$

- This can be solved using standard convex optimization techniques
- Because this is stated in terms of the dual parameters α_i , it is easily kernelized

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Support vector machines

- By directly controlling capacity, optimal margin classifiers reduce the dangers of overtraining
- Because most training points don't lie right on the margin, the dual solution will tend to be sparse
- Optimal margin classifiers improve on the perceptron, but still fail for non-separable problems
- Support Vector Machines (SVM) extend optimal margin classifiers to non-linear decision boundaries (using kernel functions) and non-separable problems (using slack variables)

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Support vector machines

- A *slack variable* ξ_i reflects the extent to which a point fails to satisfy the margin

- Now the quadratic program is:

$$\text{find: } \min_w \frac{1}{2} \|w\|^2 + \frac{C}{m} \sum_i \xi_i$$

$$\text{such that: } y_i (x_i \cdot w) \geq 1 - \xi_i, \text{ for all } i = 1, \dots, m$$

- The dual problem is:

$$\text{find: } \max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j (x_i \cdot x_j)$$

$$\text{such that: } 0 \leq \alpha_i \leq \frac{C}{m} \text{ and } \sum_i \alpha_i y_i = 0$$

- The constant C reflects the trade-off between our conflicting goals: to maximize the margin and to minimize the margin error

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Support vector machines

- Soft margin SVMs will find a solution even for non-separable problems
- The support vectors (for which $\alpha_i \neq 0$) are either on the margin, with $\alpha_i < \frac{C}{m}$ and $\xi_i = 0$, or they are training errors, with $\alpha_i = \frac{C}{m}$ and $\xi_i > 0$
- There's no obvious way to set the constant C , other than cross-validation, etc. (but: ν -SVMs)
- demo, demo, demo

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Support vector machines

- The hype about SVMs claimed that the combination of the kernel trick with capacity control makes them transcend the curse of dimensionality
- Not so: SVMs will overtrain given the right circumstances
- Choice of kernel function is crucial, and a bit of an art

Method	Error (4+0 feats)	Error (4+6 feats)
SVM (linear)	0.450	0.472
SVM (poly 2)	0.078	0.152
SVM (poly 5)	0.180	0.370
SVM (poly 10)	0.230	0.434
BRUTO	0.084	0.090
MARS	0.156	0.173
Bayes optimal	0.029	0.029

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