Lecture 24: Support vector machines

Reading: Chapter 9

STATS 202: Data mining and analysis

Jonathan Taylor
November 30, 2018
Slide credits: Sergio Bacallado

Support vector machines

- A **support vector machine** is a support vector classifier applied on an expanded set of predictors, e.g.

$$\Phi : (X_1, X_2) \to (X_1, X_2, X_1X_2, X_1^2, X_2^2).$$

- We expand the vector of predictors for each sample x_i and then perform the algorithm.
- We only need to know the dot products:

$$\langle \Phi(x_i), \Phi(x_k) \rangle \equiv K(x_i, x_k)$$

for every pair of samples (x_i, x_k).

The kernel trick

- Often, the dot product:

  $$\langle \Phi(x_i), \Phi(x_k) \rangle \equiv K(x_i, x_k)$$

  is a simple function $f(x_i, x_k)$ of the original vectors. Even if the mapping Φ significantly expands the space of predictors.

- **Example 1:** Polynomial kernel

  $$K(x_i, x_k) = (1 + \langle x_i, x_k \rangle)^2.$$

- With two predictors, this corresponds to the mapping:

  $$\Phi : (X_1, X_2) \to (\sqrt{2}X_1, \sqrt{2}X_2, \sqrt{2}X_1X_2, X_1^2, X_2^2).$$

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$$K(x_i, x_k) = \exp(-\gamma d(x_i, x_k)^2),$$

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- In this case, the mapping Φ is an expansion into an infinite number of transformations! We can apply the method even if we don't know what these transformations are.

The kernel trick

- **Fact:** if the matrix K is positive semi-definite, then there exists *some* mapping Φ to *some* feature space, such that $K(x_i, x_k) = \langle \Phi(x_i), \Phi(x_k) \rangle$ for every $\{x_1, \ldots, x_n\}$ in feature space.
- There are lots of known kernels out there.
- Q: If we don't know which transformations we are using, why would we expect the SVM to work?
  - The kernel $K(x_i, x_k)$ measures the similarity between samples x_i and x_k.
  - We can evaluate whether K is a good measure of similarity without understanding the feature expansion Φ.

Kernels for non-standard data types

- We can define families of kernels (with tuning parameters), which capture similarity between non-standard kinds of data:
  1. Text, strings
  2. Images
  3. Graphs
  4. Histograms

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- Other times, the expansion Φ is infinite-dimensional or simply not known.

Example. Kernels for strings

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- **Gap weight kernel:** For each word u of length p, we define a feature:

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with $0 < \lambda \leq 1$.

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- The number of features can be huge! However, this can be computed in $\mathcal{O}(Mp\log n)$ steps where M is the number of matches.

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  1. **One vs. one:** Construct $\binom{n}{2}$ SVMs comparing every pair of classes. Apply all SVMs to a test observation and classify to the class that wins the most one-on-one challenges.
  2. **One vs. all:** For each class k, construct an SVM $\beta^{(k)}$ coding class k as 1 and all other classes as -1. Assign a test observation to the class k^*, such that the distance from x_i to the hyperplane defined by $\beta^{(k^*)}$ is largest (the distance is negative if the sample is misclassified).

Relationship of SVM to logistic regression

Recall the Lagrange form of the problem.

$$\min_{\beta_0, w, \epsilon} \quad \frac{1}{2}\|w\|^2 + D\sum_{i=1}^{n} \epsilon_i$$

subject to

$$y_i(\beta_0 + w \cdot x_i) \geq (1 - \epsilon_i) \quad \text{for all } i = 1, \ldots, n,$$

$$\epsilon_i \geq 0 \quad \text{for all } i = 1, \ldots, n.$$

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$$\hat{\epsilon}_i = 1 - y_i(\beta_0 + w \cdot x_i).$$
- Or,
$$\hat{\epsilon} = \max(1 - y_i(\beta_0 + w \cdot x_i), 0).$$

Relationship of SVM to logistic regression

- Plugging this into the objective (and replacing w with β) yields

$$\min_{\beta} \quad \sum_{i=1}^{n} \max(1 - y_i(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}, 0) + \frac{\lambda}{2} \sum_{j=1}^{p} \|\beta_j\|^2 +$$

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- Loss for logistic regression is also a function of $y_i(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}$.

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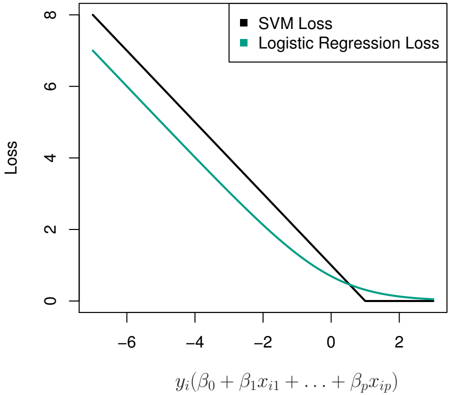
- Loss for logistic regression is also a function of $y_i(\beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}$.
- Large $\lambda \iff$ small $D \iff$ large C.

Comparing the losses



Flatness of SVM related to insensitivity to outliers. . .

The kernel trick can be applied beyond SVMs

Kernels and dot products:

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- Associated to K is a dot product. For x in the feature space $\mathbb{R}^p$, define $K_x : \mathbb{R}^p \to \mathbb{R}$ by

$$K_x(x_0) = K(x, x_0)$$

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- The kernel defines a dot product on linear combinations of the K_x's for different x's:

$$\langle \sum_j c_j K_{x_j}, \sum_i d_i K_{y_i} \rangle_K = \sum_{i,j} c_j d_i K(x_j, y_i)$$

and hence a length

$$\| \sum_j c_j K_{x_j} \|_K^2 = \sum_{i,j} c_i c_j K(x_i, x_j)$$

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Kernel regression:

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- For tuning parameter λ define

$$\hat{f}_\lambda = \mathsf{argmin}_f \sum_{i=1}^{n} (Y_i - f(X_i))^2 + \lambda \|f\|_K^2$$

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- Remarkably, it is known that

$$\hat{f} = \sum_{i=1}^{n} \hat{\alpha}_i K_{X_i}.$$

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- Problem reduces to finding

$$\hat{\alpha} = \mathsf{argmin}_{\alpha} \sum_{i=1}^{n} (Y_i - \sum_{j=1}^{n} \alpha_j K(X_i, X_j))^2 + \lambda \sum_{l,r=1}^{n} \alpha_l \alpha_r K(X_i, X_j)$$

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- Finding $\hat{\alpha}$ is just like ridge regression!
- Just like smoothing splines, we solved a problem over an big space of functions! Smoothing splines are a special case of the kernel trick...

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- Even if Φ expands the predictors to a very high dimensional space, we can do PCA!
- The cost only depends on the number of observations n.

Chapter summary

- Starting with idea of maximum margin classifier, we arrive at the support vector classifier.
- Introduction of kernel yields convenient nonlinear decision boundaries.
- Support vector classifier loss is not unrelated to logistic regression, piecewise linear loss instead of smooth loss.
- Kernel trick can also be used for logistic regression (even PCA).