Probabilistic Outputs for SVMs and Comparisons to Regularized Likelihood Methods

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Outline

- Background.
- Related Work.
- Platt's Method.
- Results and Conclusions.

SVM and Probabilities

- In many settings we want to give an input to a classifier and we are more interested in the degree of its belief that the output should be +1.
- Typical examples include combining individual predictions and the "reject" option.
- In such cases it is useful to produce a probability $P(y = 1|x)$.
- However SVMs don't do that.

SVM and Probabilities (2)

- Tradiotional SVM training:

$$\min \frac{1}{2}||w||^2 + C\sum_i \xi_i$$

  s.t. $y_i(w \cdot x_i) \geq 1 - \xi_i$, $\xi_i \geq 0$
- Classification of a point x: $f(x) = w \cdot x$.
- Focus on accuracy. Zero/one loss.
- When the loss function is not symmetric probabilities can help.

(Not so) Recent Work (1)

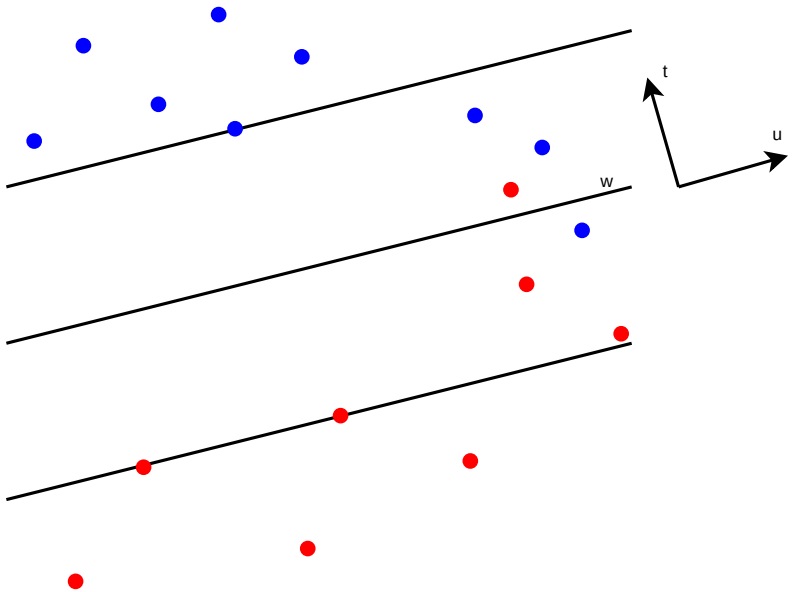
- Wahba's Approach: Train an SVM to minimize the negative log likelihood

$$\min \sum_i -y_i f(x_i) + \log(1 + e^{f(x_i)})$$

  Can add a regularization term to control the complexity of f versus fit to the data.
- In this case $P(y = 1|x) = \frac{1}{1+e^{-f(x)}}$.
- This fomulation gives solutions with many support vectors.

(Not so) Recent Work (2)

- Vapnik's Approach: Fit a function $P(y = 1|t, u)$ on the data.



- Vapnik uses a linear combination of basis functions (cosines) to fit $P(y = 1|t, u)$.
- Need to solve a linear system for every new input x.
- Issues with monotonicity and outputs outside $[0, 1]$?

(Not so) Recent Work (3)

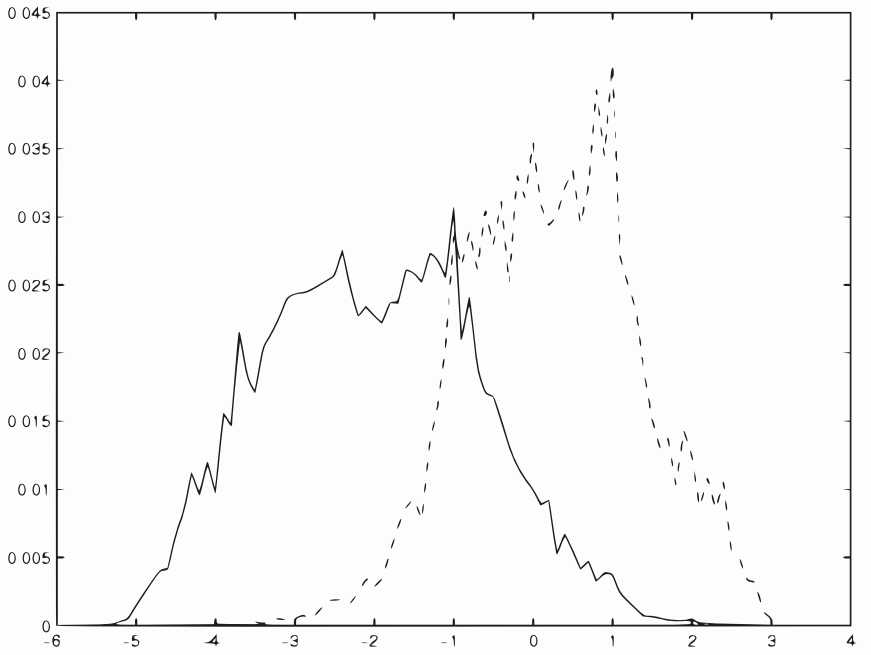
- Hastie & Tibshirani: Fit gaussians(?) to $p(f|y=\pm 1)$.

$$\begin{aligned} P(y=1|f) &= \frac{p(f|y=1)P(y=1)}{\sum_{i=\pm 1} P(y=i)p(f|y=i)} \\ &= \frac{q\exp(\frac{-(f-\mu_1)^2}{\sigma^2})}{q\exp(\frac{-(f-\mu_1)^2}{\sigma^2}) + (1-q)\exp(\frac{-(f-\mu_2)^2}{\sigma^2})} \\ &= \frac{1}{1+\frac{1-q}{q}\exp(\frac{-(f-\mu_2)^2}{\sigma^2} + \frac{(f-\mu_1)^2}{\sigma^2})} \\ &= \frac{1}{1+\exp(2\frac{\mu_2-\mu_1}{\sigma^2}f + \frac{\mu_1^2-\mu_2^2}{\sigma^2} + \ln\frac{1-q}{q})} \end{aligned}$$

- With unequal variances we get $P(y=1|f) = \frac{1}{1+e^{af^2+bf+c}}$ where $a = \frac{\sigma_2^2-\sigma_1^2}{\sigma_2^2\sigma_1^2}$
- Non monotonic.

Platt's Method (1)

- Idea: Look at the data! (but not Vapnik's u)



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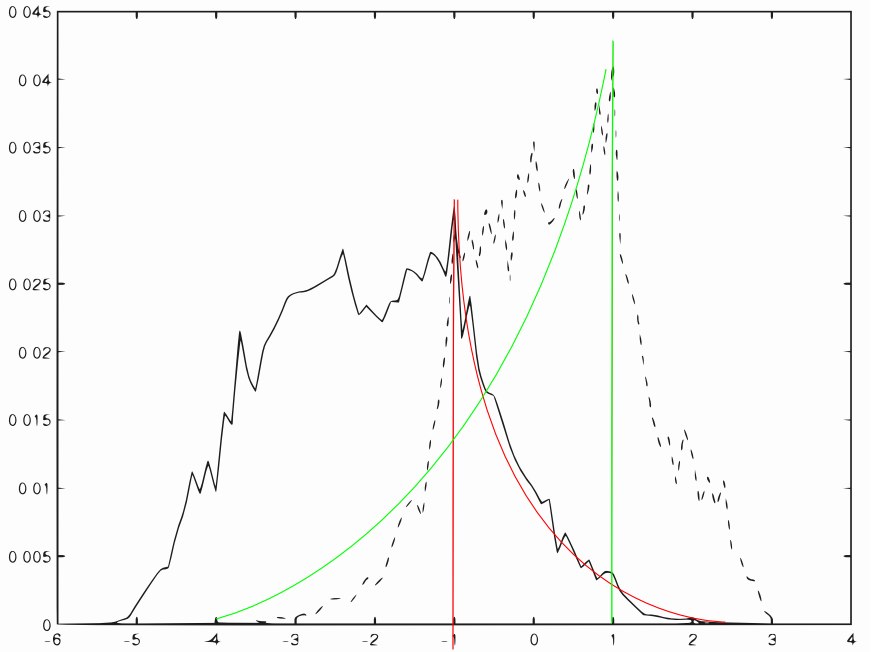

- $p(f|y=i)$ seems to be exponentially ditributed when f is in the wrong side of the margin. E.g. $p(f|y=1) = r_1 e^{-r_1(1-f)}, \ f \leq 1$
- If we use Bayes' rule we get

$$p(y=1|f) = \frac{1}{1+\exp(Af+B)}$$

where $A = -(r_1 + r_2)$ and $B = r_1 - r_2 + \ln \frac{P(y=-1)}{P(y=1)}$

Platt's Method (2)

- Platt's sigmoid vs. Hastie & Tibshirani's sigmoid. (number of parameters, training procedure)
- Using the previous histogram we can compute estimates of $p(f \in \text{bin}_i)$ and $p(f \in \text{bin}_i | y = 1)$. Then by Bayes' rule:

$$P(y = 1 | f \in \text{bin}_i) = \frac{p(f \in \text{bin}_i | y = 1) P(y = 1)}{p(f \in \text{bin}_i)}$$

- Plotting these probabilities and the fitted sigmoid we see that Platt's sigmoid is doing well in practice.
- The reliability diagrams we saw are also sigmoid shaped.

Platt's Method (3)

- Training data: (p_i, t_i). p_i sigmoid's response to f_i, $t_i = \frac{y_i+1}{2}$.
- Parameters are fit by minimizing: $-\log \prod p_i^{t_i}(1-p_i)^{1-t_i}$

$$\min -\sum_i t_i \log(p_i) + (1-t_i)\log(1-p_i)$$

- Issue: How to choose the training set?
- Using the output of the SVM for the training set.
- Biased estimate both for linear and non linear SVMs.
- (Re)using a hold out set. Using cross-validation.

Platt's Method (4)

- Another issue: How to avoid overfitting?
- Overfitting occurs when there are very few examples from one class which are seperable from the other class.
- Then the learned sigmoid is essentially a step function.
- We are back to bad probabilities.
- Add some regularization by changing t_i ($0 \rightarrow \epsilon_-$, $1 \rightarrow 1 - \epsilon_+$).
- Minimizing the same function is still valid.
- Similar trick is used in neural net training when there is no error propagated back if the difference between the target and the output is small.

Platt's Method (5)

- MAP estimate

$$t_i = \begin{cases} \frac{N_+ + 1}{N_+ + 2} & \text{if } y_i = 1 \\ \\ \frac{1}{N_- + 2} & \text{if } y_i = -1 \end{cases}$$

Platt's Method (5)

- MAP estimate

$$t_i = \begin{cases} \frac{N_+ + 1}{N_+ + 2} & \text{if } y_i = 1 \\ \\ \frac{1}{N_- + 2} & \text{if } y_i = -1 \end{cases}$$

- These are derived in the same way as class probabilities in the leaves of a decision tree when we use Laplacian smoothing.
- We start with two examples one positive and one negative. Then we get N_+ positives (N_- negatives).

Experiments

- Three models: raw SVM, SVM+sigmoid and SVM trained for maximizing log likelihood.
- Reuters, Adult and Web data sets.
- Linear and quadratic kernels.
- Accuracy of Raw SVM ($f(x) = 0$) vs. SVM+sigmoid ($P(y = 1) = 0.5$)
- Quality of probabilities of log likelihood SVM vs. SVM+sigmoid

Results

- Zero threshold is not always optimal (we knew that from 578). Sigmoid threshold is significantly better for unbalanced problems.
- Produced probabilities are not worse than those of regularized likelihood SVM. Solution is sparser and fitting the sigmoid is much simpler than implementing a kernel machine.
- SVM with sigmoid and regularized likelihood SVM are trained to optimize one measure but they preform similarly for both accuracy and log likelihood. For a particular set of hypotheses (e.g. SVMs with quadratic kernels) it is hard to know in advance which training method will perform better.

More Recent Results

- Beware of the pseudocode! A recent paper by Chih-Jen Lin points out bugs and numerical difficulties.
- Platt's method is not specific to SVMs.
- Any model that predicts poor probabilities should be calibrated but already well calibrated models such as neural nets cannot benefit from any type of calibration.
- Reliability diagrams in the latter case are very close to straight lines and a sigmoid is not a good model for fitting straight lines.