# Kernel Learning for Novelty Detection 

John Shawe-Taylor<br>University College London

NIPS Workshop Kernel Learning: Automatic Selection of Optimal Kernels, December 2008

Joint work with Zakria Hussain

## Outline

(9) Introduction

- Motivating problem
- 1-class SVMs


## Outline

(9) Introduction

- Motivating problem
- 1-class SVMs
(2) Multiple Kernel Learning
- Method 1: constraining the 1-norm of the weight vectors
- Method 2: constraining a convex combination of the 1-norm and 2-norm of the weight vectors


## Outline

(9) Introduction

- Motivating problem
- 1-class SVMs
(2) Multiple Kernel Learning
- Method 1: constraining the 1-norm of the weight vectors
- Method 2: constraining a convex combination of the 1-norm and 2-norm of the weight vectors
(3) Experiments
- Assessing impact of $\mu$
- Including negative examples


## Outline

(9) Introduction

- Motivating problem
- 1-class SVMs
(2) Multiple Kernel Learning
- Method 1: constraining the 1-norm of the weight vectors
- Method 2: constraining a convex combination of the 1-norm and 2-norm of the weight vectors
(3) Experiments
- Assessing impact of $\mu$
- Including negative examples

4 Conclusions

## Outline

(9) Introduction

- Motivating problem
- 1-class SVMs
(2) Multiple Kernel Learning
- Method 1: constraining the 1-norm of the weight vectors
- Method 2: constraining a convex combination of the 1-norm and 2-norm of the weight vectors
(3) Experiments
- Assessing impact of $\mu$
- Including negative examplesConclusions


## Content based image retrieval

- Consider problem of content based image retrieval (CBIR) using relevance feedback.


## Content based image retrieval

- Consider problem of content based image retrieval (CBIR) using relevance feedback.
- There are many metrics under which we can compare images: colour, texture, objects included, etc.



## Content based image retrieval

- Consider problem of content based image retrieval (CBIR) using relevance feedback.
- There are many metrics under which we can compare images: colour, texture, objects included, etc.
- Learning to identify the target of the search is improved if we can identify the metric that best characterises the type of search: eg
- sunset scene $\Rightarrow$ colour,
- Sunset over waterfall $\Rightarrow$ colour \& texture, etc.

weight the vertices of each SOM


## Content based image retrieval

- Consider problem of content based image retrieval (CBIR) using relevance feedback.
- There are many metrics under which we can compare images: colour, texture, objects included, etc.
- Learning to identify the target of the search is improved if we can identify the metric that best characterises the type of search: eg
- sunset scene $\Rightarrow$ colour,
- Sunset over waterfall $\Rightarrow$ colour \& texture, etc.
- Baseline system is PicSOM - uses 11 self-organising maps (SOMs) to represent database of images in 11 metrics - estimates a density of relevant vs irrelevant to weight the vertices of each SOM.


## Content based image retrieval

- Consider problem of content based image retrieval (CBIR) using relevance feedback.
- There are many metrics under which we can compare images: colour, texture, objects included, etc.
- Learning to identify the target of the search is improved if we can identify the metric that best characterises the type of search: eg
- sunset scene $\Rightarrow$ colour,
- Sunset over waterfall $\Rightarrow$ colour \& texture, etc.
- Baseline system is PicSOM - uses 11 self-organising maps (SOMs) to represent database of images in 11 metrics - estimates a density of relevant vs irrelevant to weight the vertices of each SOM.
- Implicitly reweights the metrics via the density.


## 1-class SVMs

- Negative data is sparse so consider 1-class learning initially.
Vetrics correspond to kernels: so task is about using combination of kernels to solve a retrieval task If we include 'Inarning the Lernol', wen enn autometically identify the relevant metrics for the particular search.


## 1-class SVMs

- Negative data is sparse so consider 1-class learning initially.
- Metrics correspond to kernels: so task is about using combination of kernels to solve a retrieval task.

If we include 'learning the kernel', we can automatical
identify the relevant metrics for the particular search.
Potential to scale to very large numbers of metrics/submetrics.

## 1-class SVMs

- Negative data is sparse so consider 1-class learning initially.
- Metrics correspond to kernels: so task is about using combination of kernels to solve a retrieval task.
- If we include 'learning the kernel', we can automatically identify the relevant metrics for the particular search.
Potential to scale to very large numbers of
metrics/submetrics.


## 1-class SVMs

- Negative data is sparse so consider 1-class learning initially.
- Metrics correspond to kernels: so task is about using combination of kernels to solve a retrieval task.
- If we include 'learning the kernel', we can automatically identify the relevant metrics for the particular search.
- Potential to scale to very large numbers of metrics/submetrics.


## Optimisation problem

$$
\begin{array}{ll}
\min _{\mathbf{w}, \xi} & \frac{1}{2}\|\mathbf{w}\|_{2}^{2}+C\|\xi\|_{1} \\
\text { subject to } & \left\langle\mathbf{w}, \phi\left(\mathbf{x}_{i}\right)\right\rangle \geq 1-\xi_{i} \\
& \xi_{i} \geq 0, \quad i=1, \ldots, m
\end{array}
$$

## Outline

(1)
Introduction

- Motivating problem
- 1-class SVMs
(2) Multiple Kernel Learning
- Method 1: constraining the 1-norm of the weight vectors
- Method 2: constraining a convex combination of the 1-norm and 2-norm of the weight vectorsExperiments
- Assessing impact of $\mu$
- Including negative examplesConclusions


## A linear combination of kernels

Let $\kappa_{k}$ denote the $k$ th kernel from a set $\mathbb{K}=\left\{\kappa_{1}, \ldots, \kappa_{|\mathbb{K}|}\right\}$ of kernels. We define a weighted combination of kernels like so:

$$
\kappa_{\mathbf{z}}=\sum_{k=1}^{|\mathbb{K}|} z_{k} \kappa_{k}
$$

where $\mathbf{z}=\left(z_{1}, \ldots, z_{|\mathbb{K}|}\right), z_{i} \in \mathbb{R}^{+}$.

## MKL Optimisation: Constraining the 1-norm (Recap)

Let $K=|\mathbb{K}|$, then we have the following 1 -class SVM for MKL when regularising over the weight vector using the 1-norm (primal):

$$
\begin{array}{ll}
\min _{\mathbf{w}_{k}, \xi} & \frac{1}{2}\left(\sum_{k=1}^{K}\left\|\mathbf{w}_{k}\right\|_{2}\right)^{2}+C\|\xi\|_{1} \\
\text { subject to } & \sum_{k=1}^{K}\left\langle\mathbf{w}_{k}, \phi_{k}\left(\mathbf{x}_{i}\right)\right\rangle \geq 1-\xi_{i} \\
& \xi_{i} \geq 0, \quad i=1, \ldots, m
\end{array}
$$

## Constraining the 1-norm continued

## The dual becomes:

$\min _{\beta} \max _{\alpha}$
$\beta$
subject to

$$
\begin{aligned}
& \sum_{i, j=1}^{m} \alpha_{i} \alpha_{j} \kappa_{k}\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) \leq \beta \\
& \sum_{i=1}^{m} \alpha_{i}=1 \\
& 0 \leq \alpha_{i} \leq C, i=1, \ldots, m
\end{aligned}
$$

## Experimental issues

- We ran experiments with a set of Gaussian kernels composed of different width parameters.

choose 1 kernel


## Experimental issues

- We ran experiments with a set of Gaussian kernels composed of different width parameters.
- Problem: only chose 1 kernel for learning, namely the Gaussian kernel with the largest width parameter. This is also true for experiments conducted with the VOC data sets (cat, cow, dog).

choose 1 kernel.

and 2 -norm in the optimisation problem


## Experimental issues

- We ran experiments with a set of Gaussian kernels composed of different width parameters.
- Problem: only chose 1 kernel for learning, namely the Gaussian kernel with the largest width parameter. This is also true for experiments conducted with the VOC data sets (cat, cow, dog).
- Our conjecture: except in degenerate cases will only choose 1 kernel.



## Experimental issues

- We ran experiments with a set of Gaussian kernels composed of different width parameters.
- Problem: only chose 1 kernel for learning, namely the Gaussian kernel with the largest width parameter. This is also true for experiments conducted with the VOC data sets (cat, cow, dog).
- Our conjecture: except in degenerate cases will only choose 1 kernel.
- A solution: Constrain a convex combination of the 1-norm and 2-norm in the optimisation problem.


## MKL Optimisation: Constraining a combination of the 1-norm and 2-norm

Constraining using both these norms gives us the following primal problem, with $\mu$ controlling the sparsity trade-off,

$$
\begin{array}{ll}
\min _{\mathbf{w}_{k}, \xi} & \frac{\mu}{2}\left(\sum_{k=1}^{K}\left\|\mathbf{w}_{k}\right\|_{2}\right)^{2}+\frac{1-\mu}{2} \sum_{k=1}^{K}\left\|\mathbf{w}_{k}\right\|_{2}^{2}+C\|\xi\|_{1} \\
\text { subject to } & \sum_{k=1}^{K}\left\langle\mathbf{w}_{k}, \phi_{k}\left(\mathbf{x}_{i}\right)\right\rangle \geq 1-\xi_{i} \\
& \xi_{i} \geq 0, \quad i=1, \ldots, m
\end{array}
$$

## Constraining a combination of the 1-norm and 2-norm continued

Let $D=\sum_{k=1}^{K}\left\|\mathbf{w}_{k}\right\|_{2}$, then the dual is:
$\max _{\alpha}$

$$
W(\boldsymbol{\alpha})=\sum_{i=1}^{m} \alpha_{i}-\frac{A}{2} \sum_{k=1}^{K} \beta_{k}+\frac{B}{2}\left(\sum_{k \in J} \sqrt{\beta_{k}}\right)^{2}
$$

subject to

$$
\begin{aligned}
& \beta_{k}=\sum_{i, j=1}^{m} \alpha_{i} \alpha_{j} \kappa_{k}\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) \\
& 0 \leq \alpha_{i} \leq C, i=1, \ldots, m
\end{aligned}
$$

where $A=1 /(1-\mu)$ and
$B=\left((|J|-1) \mu^{2}+\mu\right) /\left((1-\mu)(1-\mu+\mu|J|)^{2}\right)$, where $J=\left\{k: z_{k} \neq 0\right\}$, is the set of indices $k$, for which

$$
\beta_{k}>\mu^{2} D^{2}
$$

## Combination of 1- and 2-norm continued

From the Lagrangian we get,

$$
z_{k}=\max \left\{0, \frac{1}{1-\mu}\left(\frac{\sqrt{\beta_{k}}}{D}-\mu\right)\right\},
$$

Also,

$$
D=\frac{\sum_{k \in J} \sqrt{\beta_{k}}}{1-\mu+\mu|J|}
$$

## Algorithm for combination of 1- and 2-norm

We perform coordinate-wise descent in the $\alpha$ vector. Writing

$$
g_{i}\left(\alpha_{i}\right)=\frac{\partial W(\boldsymbol{\alpha})}{\partial \alpha_{i}},
$$

where $\alpha_{i}$ is the $i$-th coordinate of $\alpha$ in the argument of $W(\cdot)$, we seek the solution of $g_{i}\left(\alpha_{i}\right)=0$ as the new value for $\alpha_{i}$.

## Algorithm for combination of 1- and 2-norm

We expand $g_{i}\left(\alpha_{i}\right)$ in a Taylor series around the current values $\alpha^{0}$ :

$$
g_{i}\left(\alpha_{i}\right) \approx \frac{\partial W\left(\alpha^{0}\right)}{\partial \alpha_{i}}+\frac{\partial W^{2}\left(\alpha^{0}\right)}{\partial \alpha_{i}^{2}}\left(\alpha_{i}-\alpha_{i}^{0}\right)=0
$$

and solve for $\alpha_{i}$. Hence our update rule for each $\alpha_{i}$ becomes:

$$
\alpha_{i}=\alpha_{i}^{0}-\frac{\frac{\partial W\left(\alpha^{0}\right)}{\partial \alpha_{i}}}{\frac{\partial W^{2}\left(\alpha^{0}\right)}{\partial \alpha_{i}^{2}}}
$$

## Algorithm for combination of 1- and 2-norm

Initialise $\boldsymbol{\alpha}^{0}$ vector to zero with one element, say $\alpha_{1}^{0}>0$.

- Repeat until KKT conditions satisfied or $\left\|\boldsymbol{\alpha}^{n}-\boldsymbol{\alpha}^{n-1}\right\|_{2}<\epsilon$, where $\epsilon$ is a small positive real number
- Compute update rule for each component of $\alpha$ using:

$$
\alpha_{i}=\alpha_{i}^{0}-\frac{\frac{\partial W\left(\alpha^{0}\right)}{\partial \alpha_{i}}}{\frac{\partial W^{2}\left(\alpha^{0}\right)}{\partial \alpha_{i}^{2}}}
$$

- update $\mathbf{z}$ and $D$

Decision function:

$$
f(\mathbf{x})=\sum_{i=1}^{m} \alpha_{i} \sum_{k \in J} \frac{z_{k}}{\mu+(1-\mu) z_{k}} \kappa_{k}\left(\mathbf{x}_{i}, \mathbf{x}\right)
$$

## Outline



## Introduction

- Motivatina problem
- 1-class SVMsMultiple Kernel Learning
- Method 1: constraining the 1-norm of the weight vectors
- Method 2: constraining a convex combination of the 1 -norm and 2-norm of the weight vectors
(3) Experiments
- Assessing impact of $\mu$
- Including negative examplesConclusions


## Datasets considered

- Considered the PASCAL VOC data: cat, cow, dog


## Datasets considered

- Considered the PASCAL VOC data: cat, cow, dog
- 11 feature sets extracted for PICSOM

| Feature | dimensions |
| :--- | :---: |
| DCT coefficients of average colour in rectangular grid | 12 |
| CIE L*a*b* colour of two dominant colour clusters | 6 |
| Histogram of local edge statistics | 80 |
| Haar transform of quantized HSV colour histogram | 256 |
| Histogram of interest point SIFT features | 256 |
| Average CIE L*a*b* colour | 15 |
| Three central moments of CIE L*a*b* colour distribution | 45 |
| Histogram of four Sobel edge directions | 20 |
| Co-occurrence matrix of four Sobel edge directions | 80 |
| Magnitude of the $16 \times 16$ FFT of Sobel edge image | 128 |
| Histogram of relative brightness of neighboring pixels | 40 |

## Effect of $\mu$ on sparsity



Figure: Sparsity as function of $\mu$ for cats

Introduction

## Effect of $\mu$ on retrieval



Figure: Average precision 20 against $\mu$ for cats

Introduction

## Effect of $\mu$ on retrieval



Figure: Average precision 20 against $\mu$ for cats

- Note that PicSOM uses negative examples

Introduction

## Including negative examples

- Included negatives by negating features, i.e. negating kernel entries between differently labelled images


Figure: Average precision 20 against $\mu$ for cats

## Complete precision/recall curves



Figure: Precision/recall curve for cats

Introduction

## Average Precision scores

| Obj. | MKL 2-class $(\mu: 0.5)$ |  |  | MKL 1-class $(\mu: 0.5)$ |  | 1-class SVM |  | PicSOM |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | AP20 | AP50 | \#ker | AP20 | AP50 | \#ker | AP20 | AP50 | AP20 | AP50 |
| Cat | $\mathbf{0 . 5 2}$ | $\mathbf{0 . 4 6}$ | 3 | 0.34 | 0.24 | 2 | 0.14 | 0.13 | 0.25 | 0.25 |
| Cow | $\mathbf{0 . 2 9}$ | $\mathbf{0 . 2 0}$ | 5 | 0.17 | 0.14 | 3 | 0.14 | 0.12 | 0.25 | $\mathbf{0 . 2 0}$ |
| Dog | $\mathbf{0 . 3 7}$ | $\mathbf{0 . 3 6}$ | 11 | 0.11 | 0.13 | 2 | 0.11 | 0.12 | 0.28 | 0.28 |

## Outline

(7) Introduction

- Motivating problem
- 1-class SVMs
(2) Multiple Kernel Learning
- Method 1: constraining the 1-norm of the weight vectors
- Method 2: constraining a convex combination of the 1-norm and 2-norm of the weight vectors
(3) Experiments
- Assessing impact of $\mu$
- Including negative examples

4 Conclusions

## Conclusions

- Considered CBIR task in which learning the search metric corresponds to learning the kernel


## Conclusions

- Considered CBIR task in which learning the search metric corresponds to learning the kernel
- In 1-class MKL don't get variable sparsity by varying $C$


## Conclusions

- Considered CBIR task in which learning the search metric corresponds to learning the kernel
- In 1-class MKL don't get variable sparsity by varying $C$
- Flexible mix of 1-norm and 2-norm regularisation gives natural control of sparsity with good performance against PicSOM and 1-class SVM on VOC cats



## Conclusions

- Considered CBIR task in which learning the search metric corresponds to learning the kernel
- In 1-class MKL don't get variable sparsity by varying $C$
- Flexible mix of 1-norm and 2-norm regularisation gives natural control of sparsity with good performance against PicSOM and 1-class SVM on VOC cats
- Using negative (non-relevant) examples improves performance.



## Conclusions

- Considered CBIR task in which learning the search metric corresponds to learning the kernel
- In 1-class MKL don't get variable sparsity by varying $C$
- Flexible mix of 1-norm and 2-norm regularisation gives natural control of sparsity with good performance against PicSOM and 1-class SVM on VOC cats
- Using negative (non-relevant) examples improves performance.
- SOM uses density learning to weight metrics - should compare with same approach in kernel methods

