Statistics and Clustering with Kernels

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Overview

- Kernel Ridge Regression
- Kernel PCA
- Spectral Clustering
- Kernel Covariance and Canonical Correlation Analysis
- Kernel Measures of Independence

Kernel Ridge Regression

- Regularized least squares regression:

$$\min_{w} \sum_{i=1}^{n} \left(y_i - \langle w, x_i \rangle\right)^2 + \lambda \|w\|^2$$

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- Replace w with $\sum_{i=1}^{n} \alpha_i x_i$

$$\min_{\alpha} \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{n} \langle x_i, x_j \rangle \right)^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \langle x_i, x_j \rangle$$

- α^* can be solved in closed form solution

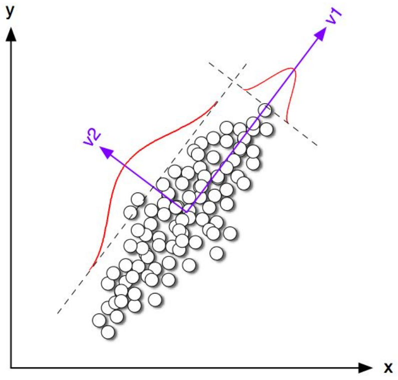
$$\alpha^* = \left(K + \lambda I\right)^{-1} y$$

PCA

Equivalent formulations:

- Minimize squared error between original data and a projection of our data into a lower dimensional subspace
- Maximize variance of projected data

Solutions: Eigenvectors of the empirical covariance matrix



(fig: Tristan Jehan)

PCA continued

- Empirical covariance matrix (biased):

$$\hat{C} = \frac{1}{n} \sum_i (x_i - \mu)(x_i - \mu)^T$$

  where μ is the sample mean.

- $\hat{C}$ is positive (semi-)definite symmetric

- PCA:

$$\max_w \frac{w^T \hat{C} w}{\|w\|^2}$$

Data Centering

- We use the notation X to denote the design matrix where every column of X is a data sample
- We can define a centering matrix

$$H = I - \frac{1}{n} e e^T$$

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- The design matrix of *centered* data can be written compactly in matrix form as XH
  - The ith column of XH is equal to $x_i - \mu$, where $\mu = \frac{1}{n}\sum_j x_j$ is the sample mean

Kernel PCA

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- Kernel PCA:
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$$\max_{w} \frac{w^T \hat{C} w}{\|w\|^2} = \max_{\alpha} \frac{1}{n} \frac{\alpha^T HKHKH\alpha}{\alpha^T HKH\alpha}$$

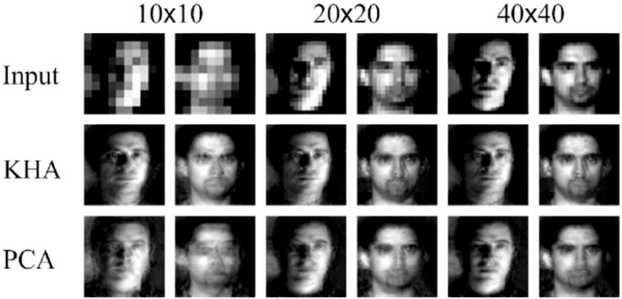
This is a Rayleigh quotient with known solution

$$HKH\beta_i = \lambda_i \beta_i$$

Kernel PCA

- Set β to be the eigenvectors of HKH, and λ the corresponding eigenvalues
- Set $\alpha = \beta\lambda^{-\frac{1}{2}}$

Example, image super-resolution:



(fig: Kim et al., PAMI 2005.)

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- **Spectral Clustering**
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Spectral Clustering

- Represent similarity of images by weights on a graph
- Normalized cuts optimizes the ratio of the cost of a cut and the volume of each cluster

$$Ncut(A_1, \ldots, A_k) = \sum_{i=1}^{k} \frac{cut(A_i, \bar{A}_i)}{vol(A_i)}$$

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- Exact optimization is NP-hard, but relaxed version can be solved by finding the eigenvalues of the *graph Laplacian*

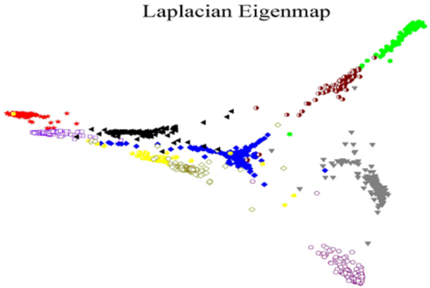
$$\mathcal{L} = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

where D is the diagonal matrix with entries equal to the row sums of similarity matrix, A.

Spectral Clustering (continued)

- Compute $\mathcal{L} = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$.
- Map data points based on the eigenvalues of $\mathcal{L}$

  Example, handwritten digits (0-9):



(fig: Xiaofei He)

- Cluster in mapped space using k-means

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Multimodal Data

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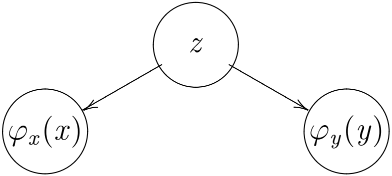
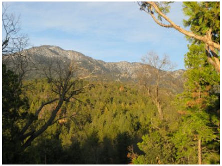
- e.g. images and text



x: 

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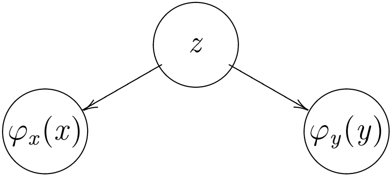
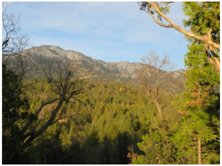


x: 

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- Learn kernelized projections that relate both spaces

Kernel Covariance

- KPCA is maximization of auto-covariance
- Instead maximize *cross*-covariance

$$\max_{w_x, w_y} \frac{w_x C_{xy} w_y}{||w_x|| \, ||w_y||}$$

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- Can also be kernelized (replace w_x by $\sum_i \alpha_i (x_i - \mu_x)$, etc.)

$$max_{\alpha,\beta} \frac{\alpha^T H K_x H K_y H \beta}{\sqrt{\alpha^T H K_x H \alpha \beta^T H K_y H \beta}}$$

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- Solution is given by (generalized) eigenproblem

$$\begin{pmatrix} \mathbf{0} & HK_xHK_yH \\ HK_yHK_xH & \mathbf{0} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \lambda \begin{pmatrix} HK_xH & \mathbf{0} \\ \mathbf{0} & HK_yH \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Kernel Canonical Correlation Analysis (KCCA)

- Alternately, maximize *correlation* instead of covariance

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- Kernelization is straightforward as before

$$\max_{\alpha, \beta} \frac{\alpha^T H K_x H K_y H \beta}{\sqrt{\alpha^T \left(H K_x H\right)^2 \alpha \beta^T \left(H K_y H\right)^2 \beta}}$$

KCCA (continued)

- Problem:
- If the data in either modality are linearly independent (as many dimensions as data points), there exists a projection of the data that respects any arbitrary ordering
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- Solution: Regularize

$$\max_{w_x, w_y} \frac{w_x^T C_{xy} w_y}{\sqrt{(w_x^T C_{xx} w_x + \varepsilon_x \|w_x\|^2) \left(w_y^T C_{yy} w_y + \varepsilon_y \|w_y\|^2\right)}}$$

- As $\varepsilon_x \to \infty$, $\varepsilon_x \to \infty$, solution approaches maximum covariance

KCCA Algorithm

- Compute K_x, K_y
- Solve for α and β as the eigenvectors of

$$\begin{pmatrix} \mathbf{0} & HK_xHK_yH \\ HK_yHK_xH & \mathbf{0} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \lambda \begin{pmatrix} (HK_xH)^2 + \varepsilon_x HK_xH & \mathbf{0} \\ \mathbf{0} & (HK_yH)^2 + \varepsilon_y HK_yH \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Content Based Image Retrieval with KCCA

- Hardoon et al., 2004
- Training data consists of images with text captions
- Learn embeddings of both spaces using KCCA and appropriately chosen image and text kernels
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- A kind of multi-variate regression

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- Different kernels encode different statistical properties of the data
- Use an appropriate kernel such that zero correlation in the Hilbert space implies independence

Example: Polynomial Kernel

- First degree polynomial kernel (i.e. linear) captures correlation only
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Hilbert-Schmidt Independence Criterion

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- (Biased) empirical HSIC:

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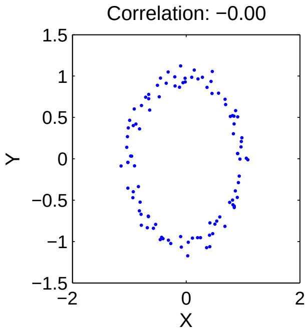
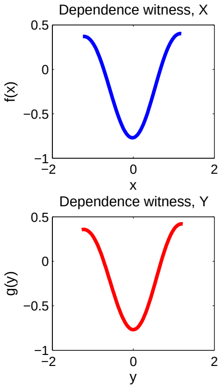
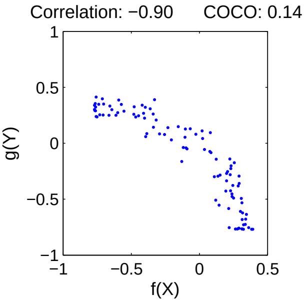
Hilbert-Schmidt Independence Criterion (continued)

- Ring-shaped density, correlation approx. zero
- Maximum singular vectors (functions) of C_{xy}







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- Use norm of V_{xy} instead of the norm of C_{xy}

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- If the kernels on x and y are characteristic (e.g. Gaussian kernels, see Fukumizu et al., 2008) $\| C_{xy} \|^2_{HS} = \| V_{xy} \|^2_{HS} = 0$ iff x and y are independent!

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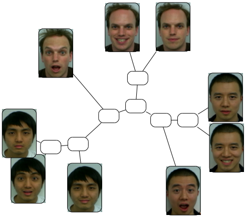
  - Taxonomy discovery (Blaschko & Gretton, 2008)



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- Questions?

Structured Output Learning

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- Structured output learning extends this concept to more complex and interdependent output spaces

Examples of Structured Output Problems in Computer Vision

- Multi-class classification (Crammer & Singer, 2001)
- Hierarchical classification (Cai & Hofmann, 2004)
- Segmentation of 3d scan data (Anguelov et al., 2005)
- Learning a CRF model for stereo vision (Li & Huttenlocher, 2008)
- Object localization (Blaschko & Lampert, 2008)
- Segmentation with a learned CRF model (Szummer et al., 2008)
- ...
- More examples at CVPR 2009

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  - linear w.r.t. *joint* kernel

$$f(x, y) = \langle w, \varphi(x, y) \rangle$$

Multi-Class Joint Feature Map

- Simple joint kernel map:
- define $\varphi_y(y_i)$ to be the vector with 1 in place of the current class, and 0 elsewhere

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Multiclass Perceptron

- Reminder: we want

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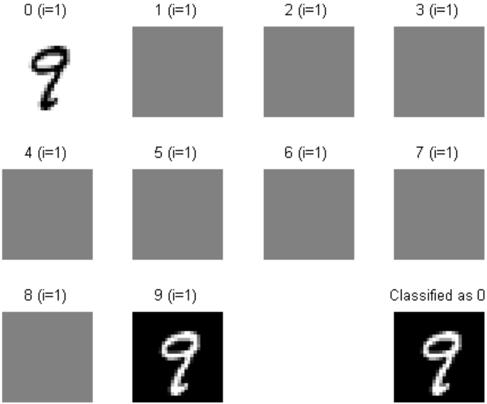
- Example: perceptron training with a multiclass joint feature map
- Gradient of loss for example i is

$$\partial_w \ell(x_i, y_i, w) = \begin{cases} 0 & \text{if } \langle w, \varphi(x_i, y_i)\rangle \geq \langle w, \varphi(x_i, y)\rangle \forall y \neq y_i \\ \max_{y \neq y_i} \varphi(x_i, y_i) - \varphi(x_i, y) & \text{otherwise} \end{cases}$$

Perceptron Training with Multiclass Joint Feature Map



(Credit: Lyndsey Pickup)

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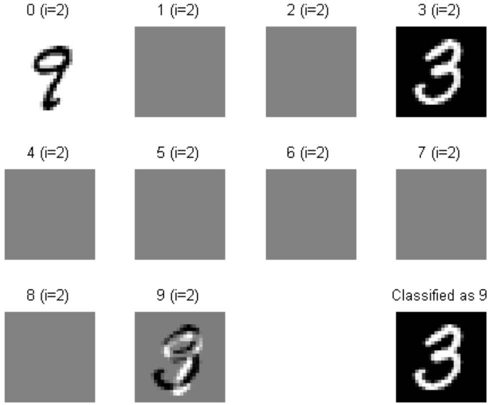

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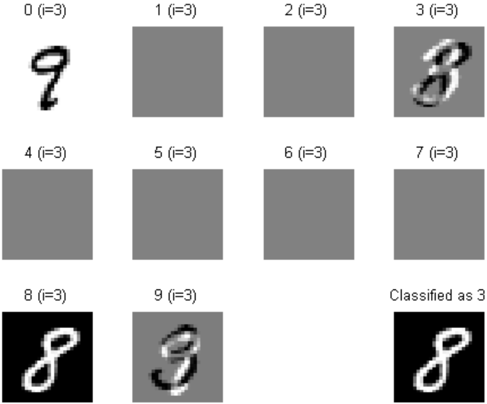

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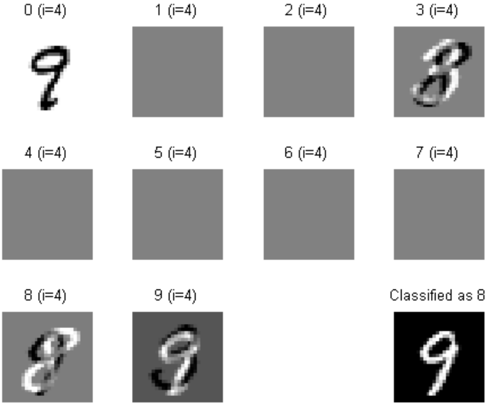

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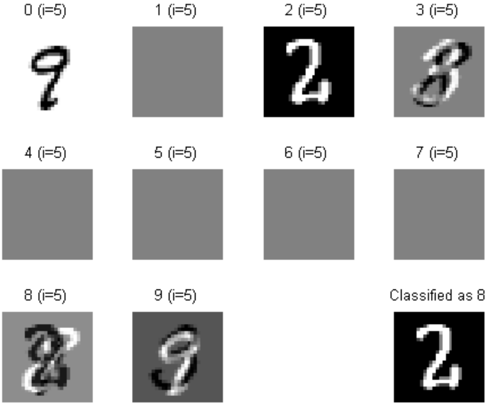

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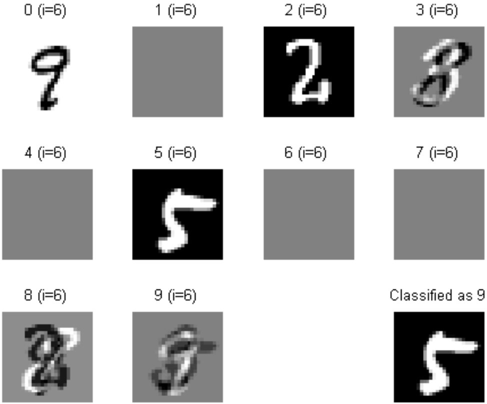

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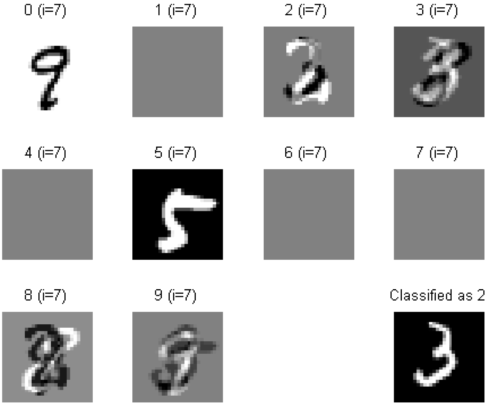

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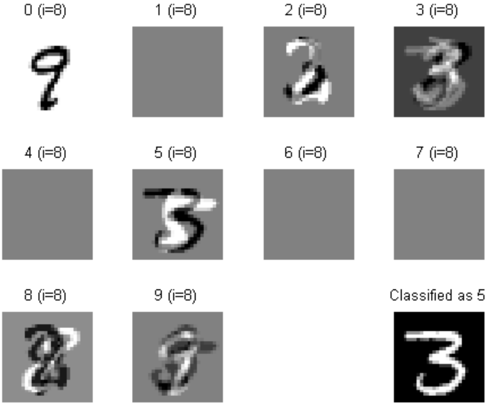

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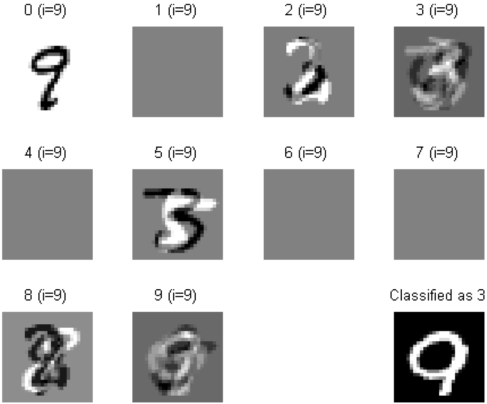

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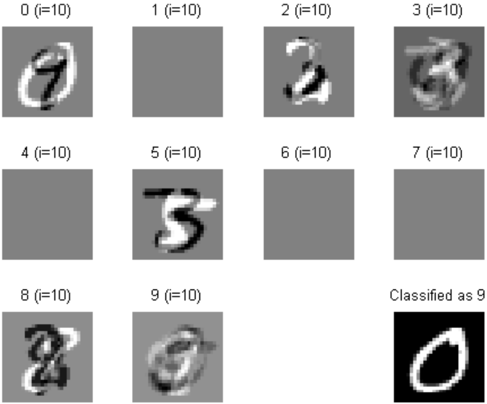

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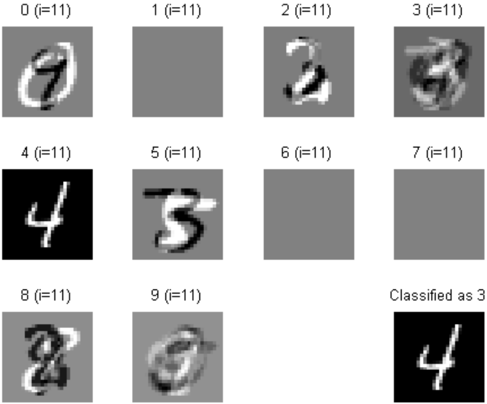

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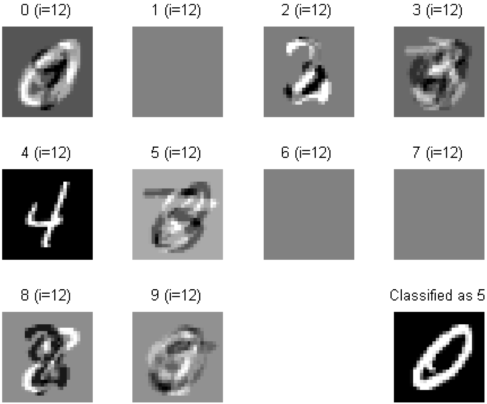

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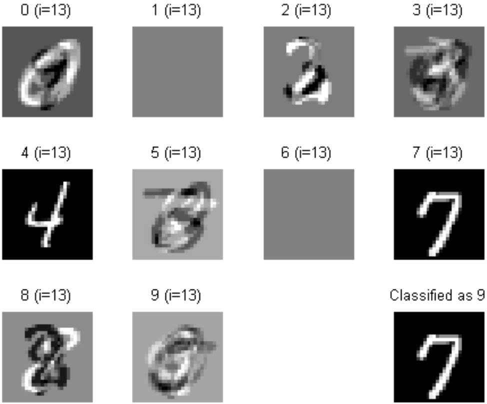

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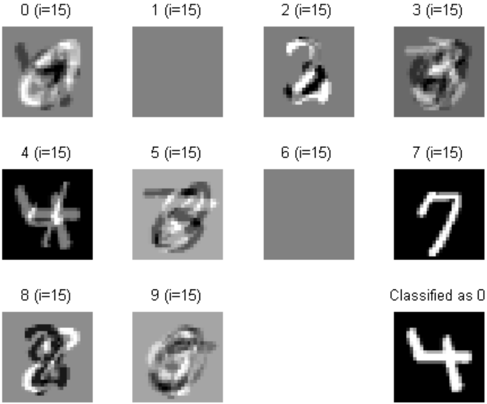

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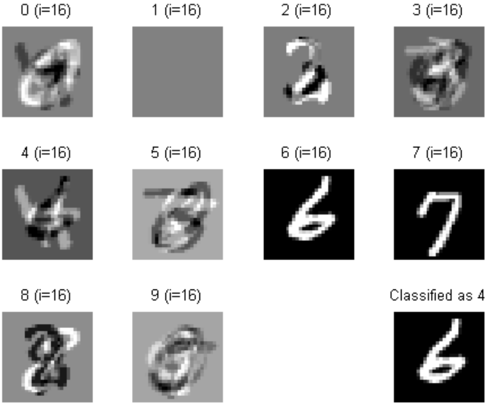

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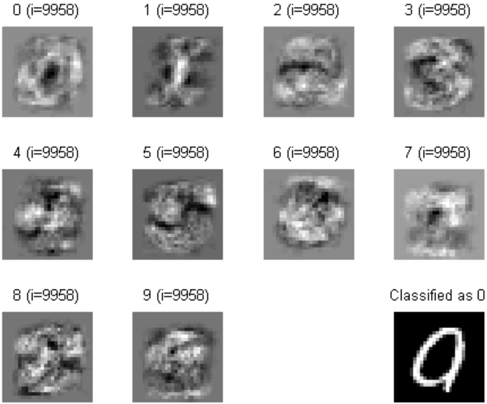

Final result
(Credit: Lyndsey Pickup)

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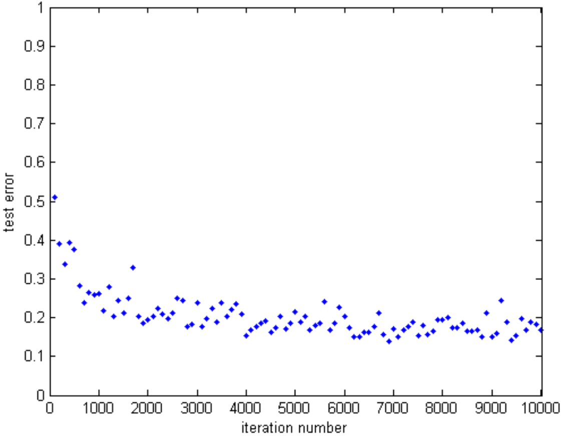

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Crammer & Singer Multi-Class SVM

- Instead of training using a perceptron, we can enforce a large margin and do a batch convex optimization:

$$\begin{aligned} \min_{w} \quad & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i \\ \text{s.t.} \quad & \langle w, \varphi(x_i, y_i)\rangle - \langle w, \varphi(x_i, y)\rangle \geq 1 - \xi_i \qquad \forall y \neq y_i \end{aligned}$$

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- Can also be written only in terms of kernels

$$
w = \sum_{x}\sum_{y} \alpha_{xy}\varphi(x, y)
$$

- Can use a *joint kernel*

$$
k : \mathcal{X} \times \mathcal{Y} \times \mathcal{X} \times \mathcal{Y} \to \mathbb{R}
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$$
k(x_i, y_i, x_j, y_j) = \langle \varphi(x_i, y_i), \varphi(x_j, y_j)\rangle
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Structured Output Support Vector Machines (SO-SVM)

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- Pay a loss proportional to the difference between true and predicted error (task dependent)

$$\Delta(y_i, y)$$

Margin Rescaling

Variant: Margin-Rescaled Joint-Kernel SVM for output space $\mathcal{Y}$ (Tsochantaridis et al., 2005)

- Idea: some *wrong* labels are *worse* than others: loss $\Delta(y_i, y)$
- Solve

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- Another variant is *slack* rescaling (see Tsochantaridis et al., 2005)

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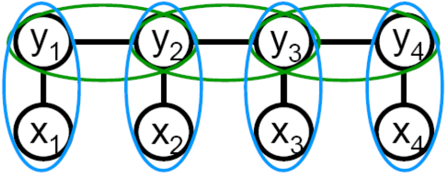
- As a simple example take an HMM
- We need to model emission probabilities and transition probabilities
    - Learn these discriminatively

A Joint Kernel Map for Label Sequence Learning



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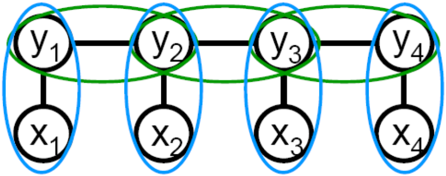

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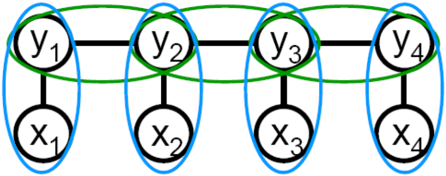

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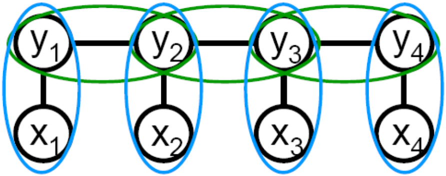

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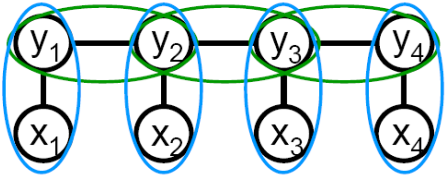

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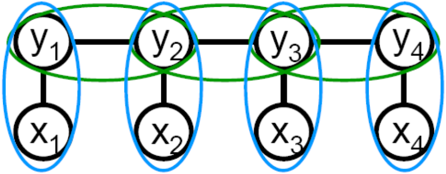
  - $f_t(x_i, y_i) = \langle w_t, \varphi_t(y_i, y_{i+1}) \rangle$
  - Can use $\varphi_t(y_i, y_{i+1}) = \varphi_y(y_i) \otimes \varphi_y(y_{i+1})$

A Joint Kernel Map for Label Sequence Learning (continued)



$$p(x, y) \quad \propto \quad \prod_i e^{f_e(x_i, y_i)} \prod_i e^{f_t(y_i, y_{i+1})} \quad \text{for an HMM}$$

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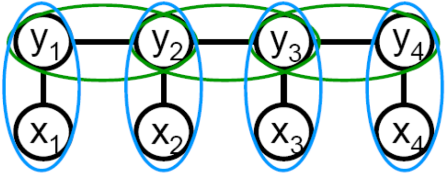

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f(x, y) &= \sum_i f_e(x_i, y_i) + \sum_i f_t(y_i, y_{i+1}) \\
&= \langle w_e, \sum_i \varphi_e(x_i, y_i) \rangle + \langle w_t, \sum_i \varphi_t(y_i, y_{i+1}) \rangle
\end{aligned}
$$

Constraint Generation

$$\min_{w} \quad \|w\|^2 + C\sum_{i=1}^{n} \xi_i$$

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- Initialize constraint set to be empty
- Iterate until convergence:
  - Solve optimization using current constraint set
  - Add maximially violated constraint for current solution

Constraint Generation with the Viterbi Algorithm

- To find the maximially violated constraint, we need to maximize w.r.t. y

$$\langle w, \varphi(x_i, y) \rangle + \Delta(y_i, y)$$

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- For HMMs, $\max_y \langle w, \varphi(x_i, y)\rangle$ can be found using the Viterbi algorithm
- It is a simple modification of this procedure to incorporate $\Delta(y_i, y)$ (Tsochantaridis et al., 2004)

Discriminative Training of Object Localization

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- Structured output learning is not restricted to outputs specified by graphical models
- We can formulate object localization as a regression from an image to a bounding box

$$g : \mathcal{X} \rightarrow \mathcal{Y}$$

- $\mathcal{X}$ is the space of all images
- $\mathcal{Y}$ is the space of all bounding boxes

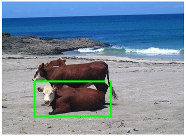
Joint Kernel between Images and Boxes: Restriction Kernel

- Note: $x|_y$ (the image restricted to the box region) is again an image.
- Compare two images with boxes by comparing the images within the boxes:

$$k_{joint}((x,y),(x',y')\ ) = k_{image}(x|_y, x'|_{y'},)$$

- Any common image kernel is applicable:
  - linear on cluster histograms: $k(h,h') = \sum_i h_i h'_i$,
  - χ^2-kernel: $k_{\chi^2}(h,h') = \exp\left(-\frac{1}{\gamma}\sum_i \frac{(h_i-h'_i)^2}{h_i+h'_i}\right)$
  - pyramid matching kernel, ...
- The resulting joint kernel is positive definite.

Restriction Kernel: Examples

$k_{joint}\Big($  ,  $\Big) = k\Big($  ,  $\Big)$

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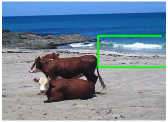
$k_{joint}\Big($  ,  $\Big) = k\Big($  ,  $\Big)$

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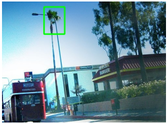
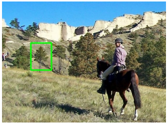
$k_{joint}\Big($  ,  $\Big) = k\Big($  ,  $\Big)$

could also be large.

- Note: This behaves differently from the common tensor products

$$k_{joint}(\ (x,y),(x',y')\ ) \neq k(x,x')k(y,y'))\ !$$

Constraint Generation with Branch and Bound

- As before, we must solve

$$\max_{y \in \mathcal{Y}} \langle w, \varphi(x_i, y) \rangle + \Delta(y_i, y)$$

where

$$\Delta(y_i, y) = \begin{cases} 1 - \frac{\text{Area}(y_i \bigcap y)}{\text{Area}(y_i \bigcup y)} & \text{if } y_{i\omega} = y_\omega = 1 \\ 1 - \left(\frac{1}{2}(y_{i\omega} y_\omega + 1) \right) & \text{otherwise} \end{cases}$$

and $y_{i\omega}$ specifies whether there is an instance of the object at all present in the image

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- Solution: use branch-and-bound over the space of all rectangles in the image (Blaschko & Lampert, 2008)

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- Set the loss to the number of incorrect pixels

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Constraint Generation with Graph Cuts

- As the graph is loopy, we cannot use Viterbi
- Loopy belief propagation is approximate and can lead to poor learning performance for structured output learning of graphical models (Finley & Joachims, 2008)
- Solution: use graph cuts (Szummer et al., 2008)
- $\Delta(y_i, y)$ can be easily incorporated into the energy function

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- Questions?