Extrapolating prediction error for ‘extreme’ multi-class classification

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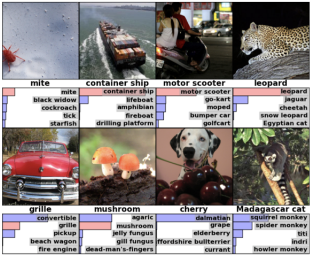
(Joint work with Rakesh Achanta and Yuval Benjamini.)

Multi-class classification



from Krizhevsky et al. 2012

- MNIST digit recognition: 10 categories
- Human motion database: 51 categories
- ImageNet: 22,000 categories
- Wikipedia: 325,000 categories

Facial recognition

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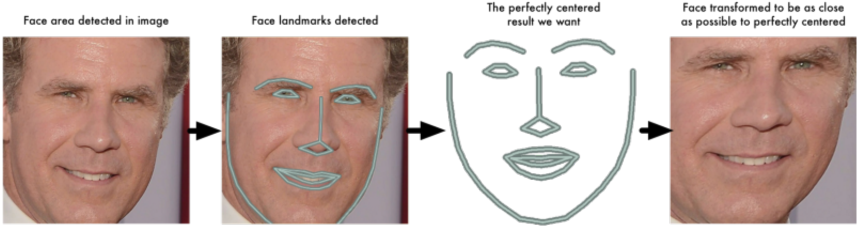

Facial recognition

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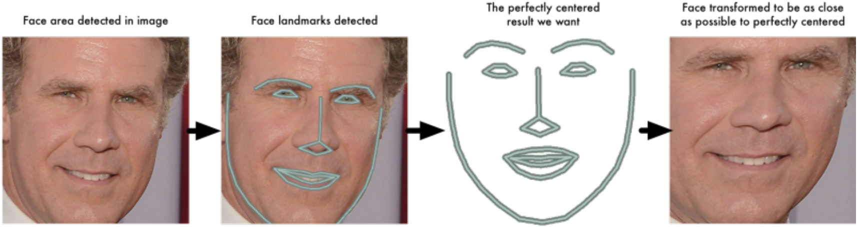
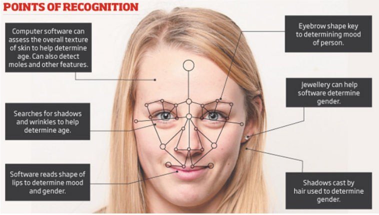
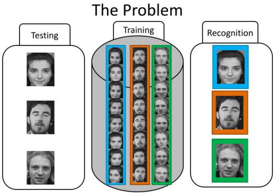


- Feature extraction



Accuracy vs. number of classes



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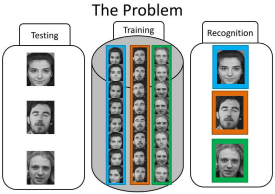

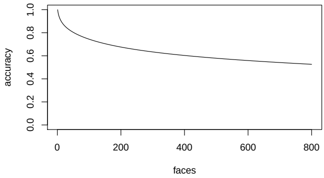

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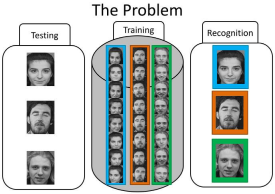
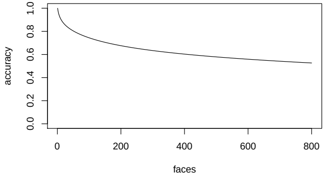
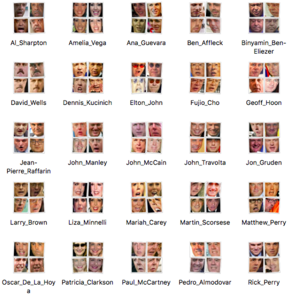




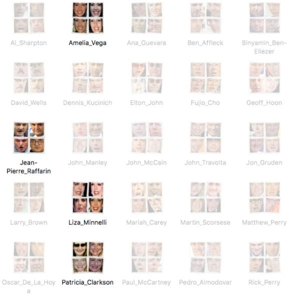
How does the accuracy scale with the number of classes (faces)?

Setup

1. Population of categories $\pi(y)$

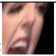
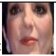


2. Subsample k labels, $y_1, \ldots, y_k$



Setup

3. Collect training and test data $x_j^{(i)}$ (faces) for labels (people) $\{y_1, \ldots, y_k\}$.

Label	Training			Test
y_1=Amelia	$x_1^{(1)} =$ 	$x_1^{(2)} =$ 	$x_1^{(3)} =$ 	$x_1^* =$ 
y_2=Jean-Pierre	$x_2^{(1)} =$ 	$x_2^{(2)} =$ 	$x_2^{(3)} =$ 	$x_2^* =$ 
y_3=Liza	$x_3^{(1)} =$ 	$x_3^{(2)} =$ 	$x_3^{(3)} =$ 	$x_3^* =$ 
y_4=Patricia	$x_4^{(1)} =$ 	$x_4^{(2)} =$ 	$x_4^{(3)} =$ 	$x_4^* =$ 

4. Train a classifier and compute test error.

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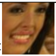
y_1=Amelia	$x_1^{(1)} =$ 	$x_1^{(2)} =$ 	$x_1^{(3)} =$ 	$x_1^* =$ 
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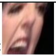
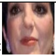
y_3=Liza	$x_3^{(1)} =$ 	$x_3^{(2)} =$ 	$x_3^{(3)} =$ 	$x_3^* =$ 
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Can we analyze how error depends on k?

Key assumption: marginal classifier

- The classifier is *marginal* if it learns a model *independently* for each class.

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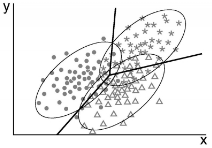
- Examples: LDA/QDA 

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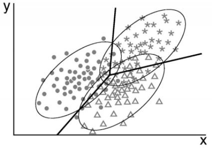
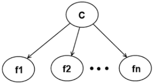
- Examples: LDA/QDA 

, naïve Bayes 

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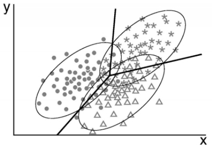
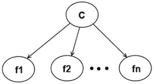
- Examples: LDA/QDA 

, naïve Bayes 

- Non-marginal classifiers: Multinomial logistic, multilayer neural networks, k-nearest neighbors

Definitions

$\hat{F}_{y^{(i)}}$ is the empirical distribution obtained from the training data for label $y^{(i)}$.

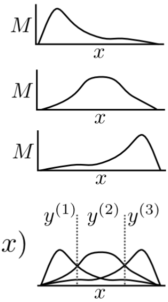
Classification Rule

$$M_{y^{(1)}}(x) = \mathcal{M}(\hat{F}_{y^{(1)}})(x)$$

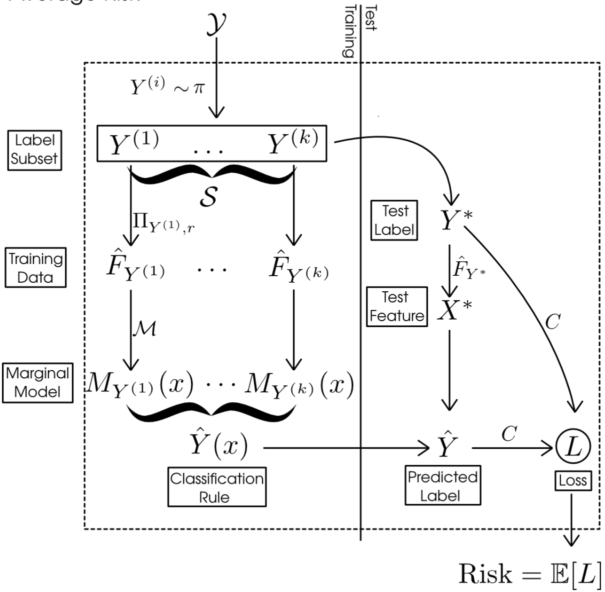
$$M_{y^{(2)}}(x) = \mathcal{M}(\hat{F}_{y^{(2)}})(x)$$

$$M_{y^{(3)}}(x) = \mathcal{M}(\hat{F}_{y^{(3)}})(x)$$

$$\hat{Y}(x) = \text{argmax}_{y \in \mathcal{S}} M_y(x)$$



Average Risk



Theoretical Result

Theorem. **(Z.**, Achanta, Benjamini.) Suppose π, $\{F_y\}_{y\in\mathcal{Y}}$ and marginal classifier $\mathcal{F}$ satisfy *(some regularity condition)*. Then, there exists some function $\bar{D}(u)$ on $[0,1] \to [0,1]$ such that the k-class average risk is given by

$$\text{AvRisk}_k = (k-1)\int \bar{D}(u)u^{k-2}du.$$

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What is this $\bar{D}(u)$ function? We will explain in the following toy example...

Toy example

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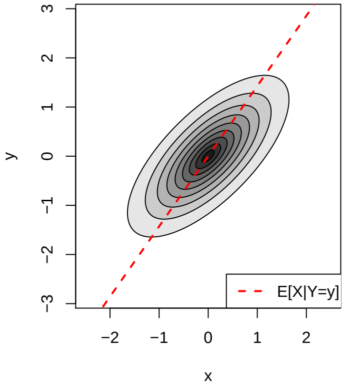
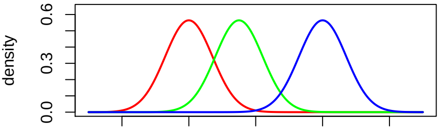
$X|Y \sim N(\rho Y, 1-\rho^2)$ i.e. $(Y,X) \sim N(0, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix})$.

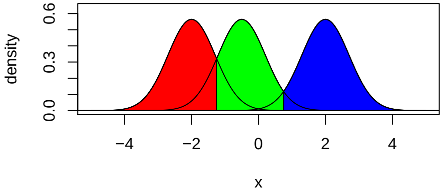


Toy example



- Suppose $k = 3$, and we draw Y_1, Y_2, Y_3.
- The *Bayes rule* is the optimal classifier and depends on knowing the true densities:
$$\hat{y}(x) = \text{argmax}_{y_i} p(x|y_i)$$
- The *Bayes Risk*, which is the misclassification rate of the optimal classifier.

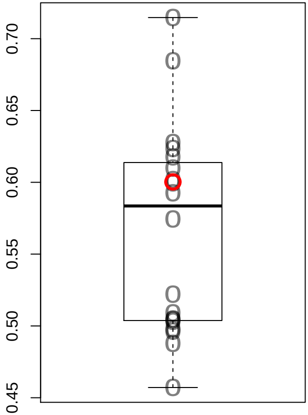
Toy example

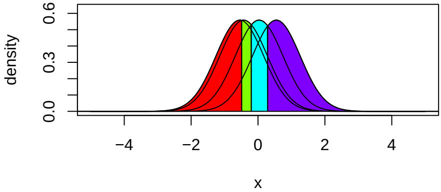


- The *Bayes Risk* is the expected test error of the Bayes rule,

$$\frac{1}{k}\sum_{i=1}^{k}\Pr[\hat{y}(x) \neq Y | Y = y_i]$$

Toy example





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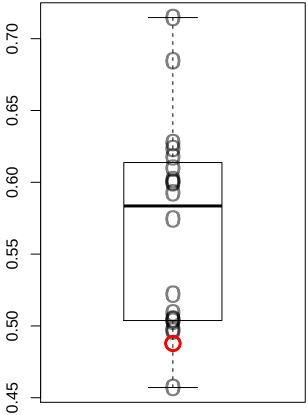

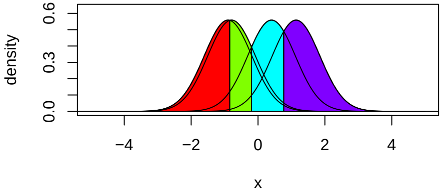

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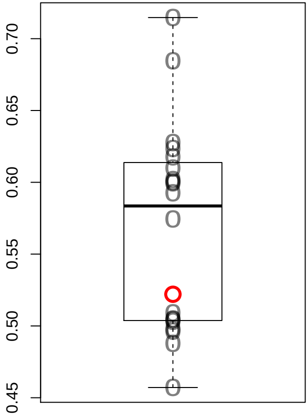

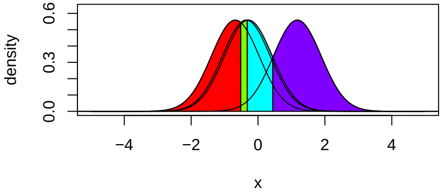

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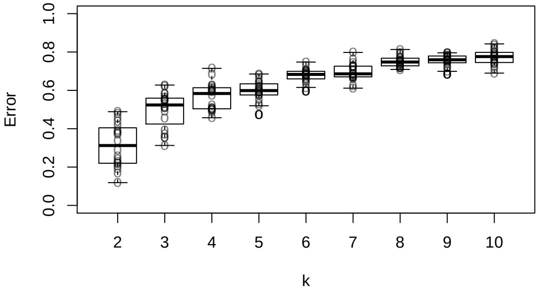

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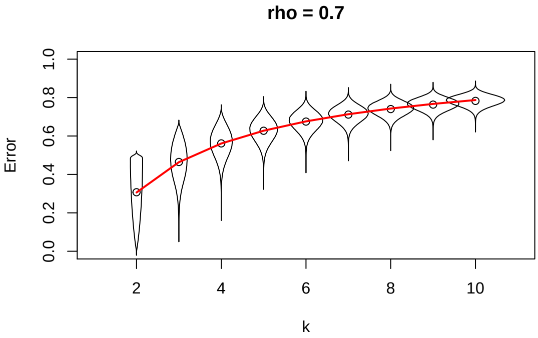
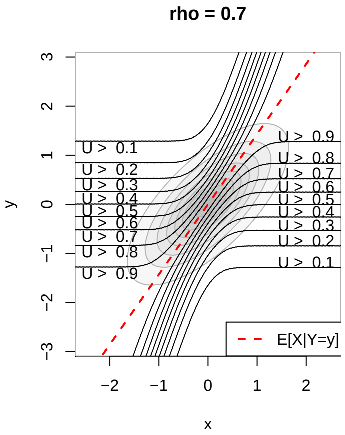


Defining the U-function

Define $U_x(y)$ as follows:

- Suppose we have test instance (face) x whose true label (person) is y.
- Let Y' be a random *incorrect* label (person).
- Use the classifier to guess whether x belongs to y or Y'.
- Define $U_x(y)$ as the probabilility of success (randomizing over training data).

Toy example



$$U_y(x) = \Pr[d(x, \rho Y') > d(x, \rho y)], \text{ for } Y' \sim N(0, 1).$$

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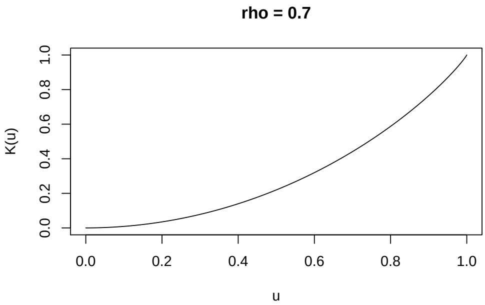
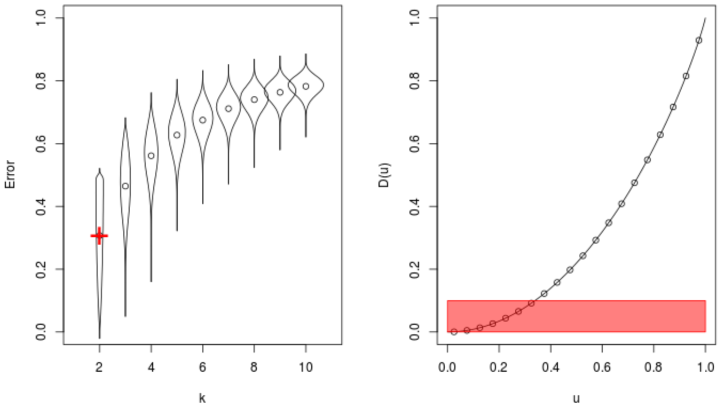


Computing average risk

$$\text{AvRisk}_k = (k-1) \int \bar{D}(u) u^{k-2} du.$$



$(k = 2)$

Computing average risk

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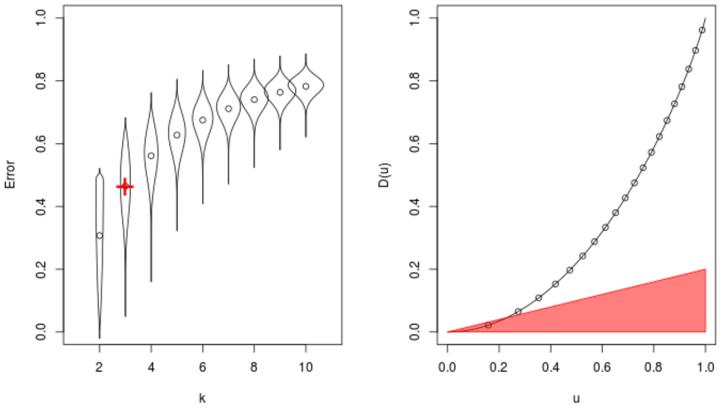

$(k = 3)$

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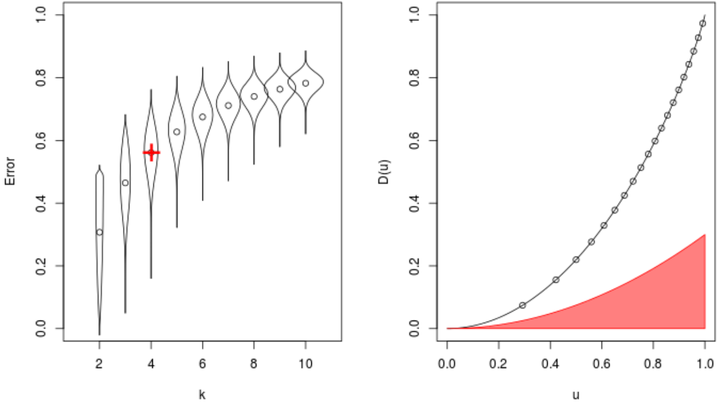

$(k = 4)$

Computing average risk

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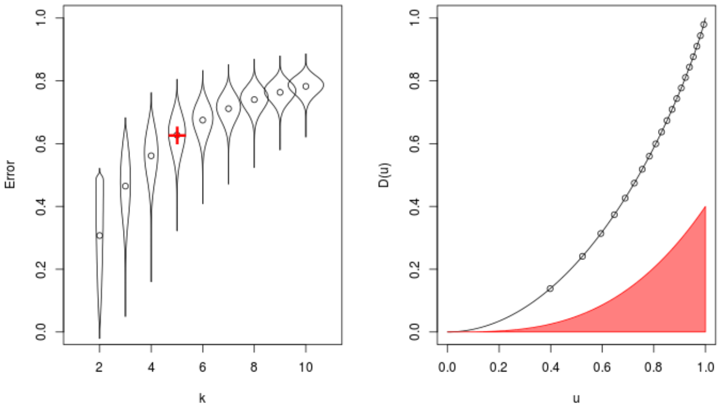

$(k = 5)$

Computing average risk

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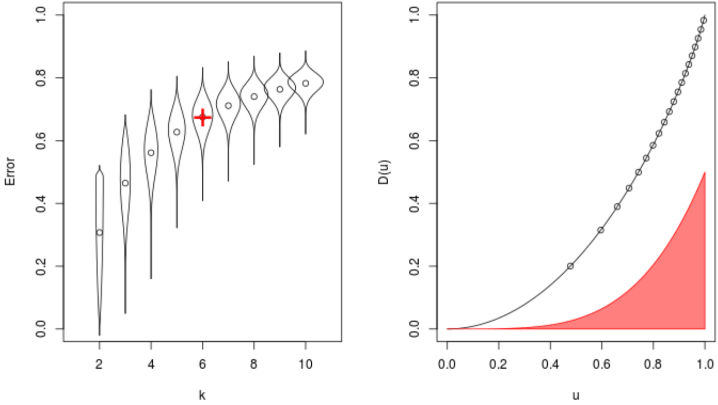

$(k = 6)$

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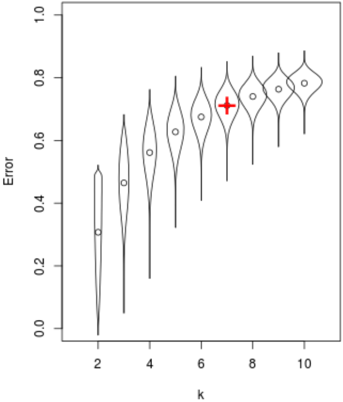

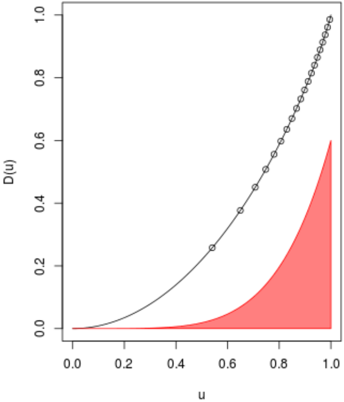

$(k = 7)$

Computing average risk

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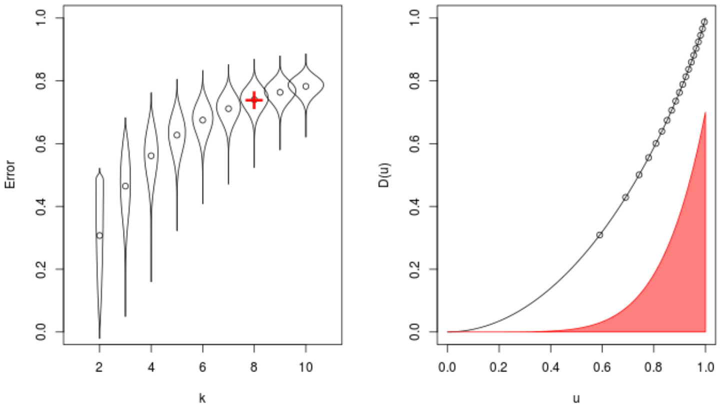

$(k = 8)$

Computing average risk

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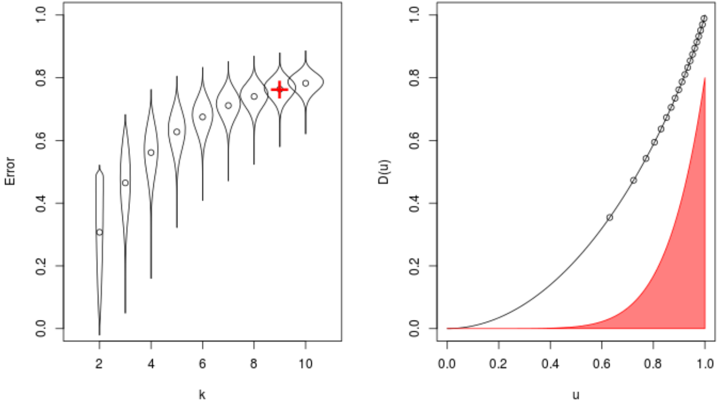

$(k = 9)$

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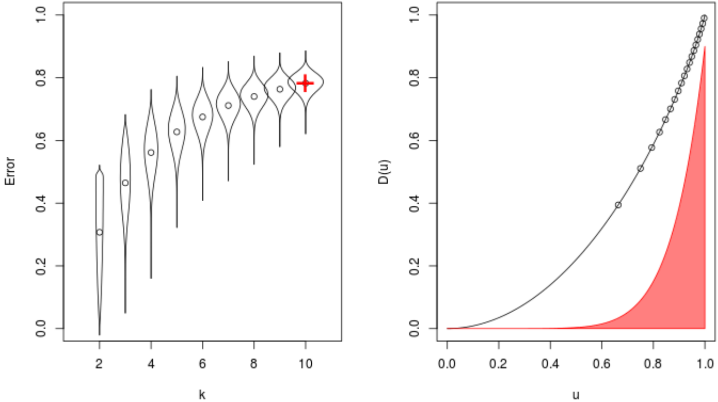
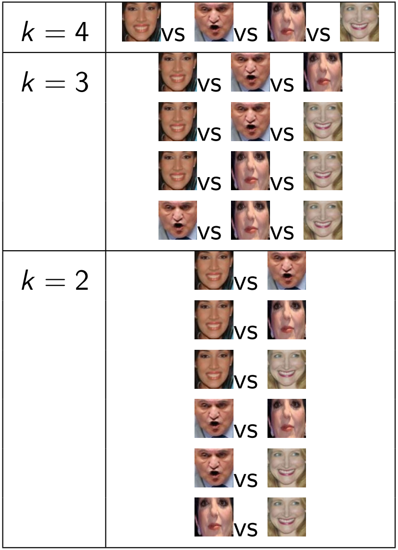


$(k = 10)$

Implication: estimate $\bar{D}(u)$ to predict risk

- Theoretical result links k-class average risk to $\bar{D}(u)$ function
- In real data, we do not know $\bar{D}(u)$ since it depends on the unknown joint distribution
- However, given a model, we can estimate $\bar{D}(u)$

Subsampled risk estimates



- Suppose we have data for k classes (subsampled from π)
- The test error TestErr_k is an unbiased estimate for AvRisk_k
- For any $\ell < k$, we can estimate AvRisk_ℓ by *subsampling* the k classes, and taking the average test risk, AvTestErr_ℓ.

Parametric modelling approach

Assume that for set of basis functions $h_1, \ldots, h_\ell$, we have

$$\bar{D}(u) = \sum_{\ell=1}^{m} \beta_\ell h_\ell(u).$$

Then

$$\text{AvRisk}_k = \sum_{\ell=1}^{m} \beta_\ell H_{\ell,k} = \beta^T \vec{H}_k$$

where

$$H_{\ell,k} = (k-2) \int_0^1 h_\ell(u) u^{k-2} du.$$

and $\vec{H}_k = (H_{1,k}, \ldots, H_{\ell,k})$

Prediction extrapolation as regression

1. Choose basis $h_1, \ldots, h_\ell$

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2. Obtain subsampled test errors $\text{AvTestErr}_2, \ldots, \text{AvTestErr}_k$.
3. Fit regression model

$$\hat{\beta} = \text{argmin}_\beta \sum_{i=2}^{k} \left(\text{AvTestErr}_i - \vec{H}_i^T \beta_\ell\right)^2$$

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4. For $K > k$, predict AvRisk_K as

$$\widehat{\text{AvRisk}}_K = \vec{H}_K^T \beta_\ell.$$

Examples of basis functions

- Polynomials, $1, x, x^2, \ldots$
- Cubic splines
- Linear splines, $[x - t_\ell]_+$

Optional constraint: assume β is *non-negative*. In the case of linear splines, this results in a *convex* fit.