SIMFEAT: A Simple Feature Extraction Toolbox

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Motivation

- Feature selection/extraction is essential before classification or regression
- High number of correlated features gives rise to:
  - Collinearity
  - Overfitting
- Linear methods offer interpretability $\sim$ knowledge discovery
- Linear algorithms are commonly used: PCA, PLS, CCA, ...
- Linear algorithms fail when data distributions are curved

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- Linear algorithms are commonly used: PCA, PLS, CCA, ...
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Outline

- PCA is widely used
- PCA is not optimal for supervised problems
- PLS is a good alternative to PCA, yet *suboptimal* in MSE sense
- Orthonormalized PLS (OPLS) is optimal in MSE sense
- Real problems typically show non-linear relations

Notation preliminaries

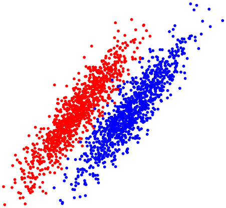
Data	$\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{l}$, $\mathbf{x}_i \in \mathbb{R}^N$, $\mathbf{y}_i \in \mathbb{R}^M$.
Input Data Matrix	$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_l]^\top$
Label Matrix	$\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_l]^\top$
Number of projections	n_p
Projected Inputs	$\mathbf{X}' = \mathbf{X}\mathbf{U}$
Projected Outputs	$\mathbf{Y}' = \mathbf{Y}\mathbf{V}$
Projection matrices	$\mathbf{U}$ $(N \times n_p)$, and $\mathbf{V}$ $(M \times n_p)$
Covariance	$\mathbf{C}_{xy} = E\{(\mathbf{x} - \boldsymbol{\mu}_x)(\mathbf{y} - \boldsymbol{\mu}_y)\} \sim \frac{1}{l}\mathbf{X}^\top\mathbf{Y}$
Frobenius norm of a matrix	$\|A\|_F^2 = \sum_{ij} a_{ij}^2$

Notation preliminaries

1. $tr(\mathbf{AB}) = tr(\mathbf{BA})$
2. $(\mathbf{AB})^\top = \mathbf{B}^\top \mathbf{A}^\top$, $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$
3. $\frac{\partial(\mathbf{a}^\top \mathbf{b})}{\partial \mathbf{a}} = \mathbf{b}$, $\frac{\partial(\mathbf{b}^\top \mathbf{a})}{\partial \mathbf{a}} = \mathbf{b}^\top$
4. $\mathbf{CV} = \mathbf{VD} \longrightarrow$ `[V D] = eig(C);`
5. $\mathbf{C} = \mathbf{UAV}^\top \longrightarrow$ `[U A V] = svd(C);`
6. Orthogonal transform = rotation $\rightarrow \mathbf{U}^{-1} = \mathbf{U}^\top$
7. Download `matrixcookbook.pdf` !

Notation preliminaries

- Imagine a classification problem in which labels matter (a lot!)
- "Blind" feature extraction is not a good choice.
- Let's see what happens with different methods ...



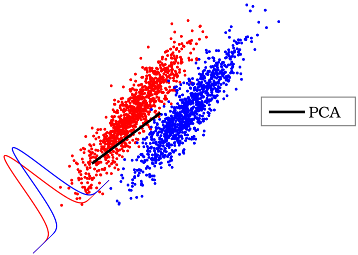
Principal Component Analysis (PCA)

"Find projections that maximize the variance of the projected data"

PCA: maximize: $\mathrm{Tr}\{\|\mathbf{XU}\|_F^2\} = \mathrm{Tr}\{(\mathbf{XU})^\top(\mathbf{XU})\} = \mathrm{Tr}\{\mathbf{U}^\top\mathbf{C}_{xx}\mathbf{U}\}$

subject to: $\mathbf{U}^\top\mathbf{U} = \mathbf{I}$

```
» Cxx = X'*X;
» [U D] = eigs(Cxx,np);
» Xproj = X*U;
```

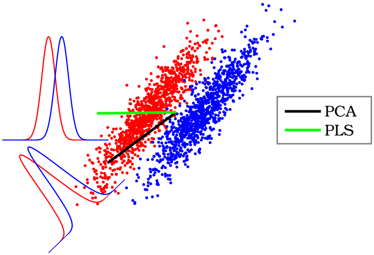


Partial Least Squares (PLS)

"Find directions of maximum input-output cross-covariance"

$$\text{PLS:} \quad \text{maximize:} \quad \mathrm{Tr}\{(\mathbf{XU})^\top(\mathbf{YV})\} = \mathrm{Tr}\{\mathbf{U}^\top \mathbf{C}_{xy}\mathbf{V}\}$$
$$\text{subject to:} \quad \mathbf{U}^\top\mathbf{U} = \mathbf{V}^\top\mathbf{V} = \mathbf{I}$$

```
» Cxy=X'*Y;
» [U D V] = svds(Cxy,np);
» Xproj = X*U;
```



Orthonormalized Partial Least Squares (OPLS)

"Choose the projection matrix **U** *that minimizes the MSE error ..."*

OPLS: find: $\mathbf{U} = \arg\min\{\|\mathbf{Y} - \mathbf{X}'\mathbf{W}\|_F^2\}$

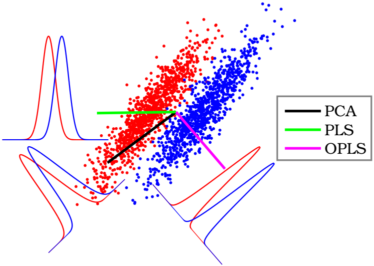
where: $\mathbf{X}' = \mathbf{X}\mathbf{U}, \qquad \mathbf{W} = (\mathbf{X}'^\top \mathbf{X}')^{-1}\mathbf{X}'\mathbf{Y}$

Orthonormalized Partial Least Squares (OPLS)

"... which can be rewritten as **[Worsley98]***:"*

$$\text{OPLS:} \quad \text{maximize:} \quad \mathrm{Tr}\{\mathbf{U}^\top \mathbf{C}_{xy}\mathbf{C}_{xy}^\top \mathbf{U}\}$$
$$\text{subject to:} \quad \mathbf{U}^\top \mathbf{C}_{xx}\mathbf{U} = \mathbf{I}$$

```
» Cxy=X'*Y;Cxx=X'*X;
» [U,D] = eigs((Cxy)*(Cxy'),Cxx,np);
» [U,D] = eigs(inv(Cxx)*(Cxy)*(Cxy'),np);
» Xproj = X*U;
```



Canonical Correlation Analysis (CCA)

Unlike PCA or PLS, CCA looks for directions of max I/O correlation:

CCA: $$\mathbf{u}, \mathbf{v} = \arg\max_{\mathbf{u},\mathbf{v}} \frac{(\mathbf{u}^\top \mathbf{C}_{xy} \mathbf{v})^2}{\mathbf{u}^\top \mathbf{C}_{xx} \mathbf{u} \; \mathbf{v}^\top \mathbf{C}_{yy} \mathbf{v}}$$

CCA(2): $$\mathbf{u}, \mathbf{v} = \arg\max_{\mathbf{u},\mathbf{v}} \; \mathbf{u}^\top \mathbf{C}_{xy} \mathbf{v}$$

$$\text{subject to: } \mathbf{u}^\top \mathbf{C}_{xx} \mathbf{u} = \mathbf{v}^\top \mathbf{C}_{yy} \mathbf{v} = 1$$

CCA(3): $$\mathbf{U}, \mathbf{V} = \arg\max_{\mathbf{U},\mathbf{V}} \; \mathrm{Tr}\{\mathbf{U}^\top \mathbf{C}_{xy} \mathbf{V}\}$$

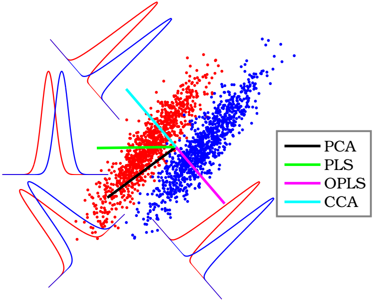
$$\text{subject to: } \mathbf{U}^\top \mathbf{C}_{xx} \mathbf{U} = \mathbf{V}^\top \mathbf{C}_{yy} \mathbf{V} = \mathbf{I}$$

Canonical Correlation Analysis (CCA)

Unlike PCA or PLS, CCA looks for directions of max I/O correlation:

$$\begin{pmatrix} \mathbf{0} & \mathbf{C}_{xy} \\ \mathbf{C}_{xy}^{\top} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{C}_{xx} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_{yy} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}$$

```
» A = [0 Cxy; Cxy' 0];   B = [Cxx 0; 0 Cyy];
» [UV D] = eigs(A,B,np); u = UV(1:d/2,:);
» Xproj = X*u;
```



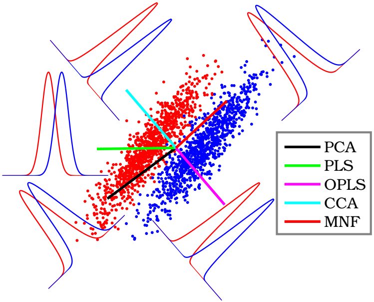
Minimum Noise Fraction (MNF)

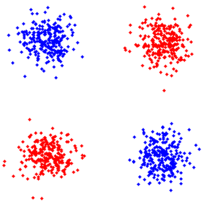
"Maximize the signal-to-noise ratio of the projections:"

$$\text{MNF:} \qquad \text{maximize:} \quad \mathrm{Tr}\left\{\frac{(\mathbf{XU})^\top(\mathbf{XU})}{(\mathbf{NU})^\top(\mathbf{NU})}\right\}$$

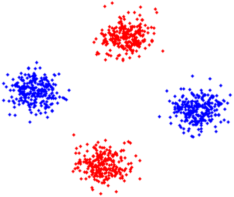
$$\text{subject to:} \quad \mathbf{X} = \mathbf{S} + \mathbf{N}, \qquad \mathbf{S}^\top\mathbf{N} = \mathbf{S}\mathbf{N}^\top = \mathbf{0}$$

```
» N=noise(X,10);
» [U,D] = eigs(X'*X,N'*N,np);
» Xproj = X*U;
```

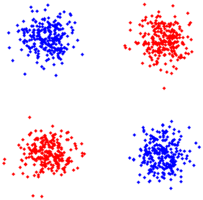




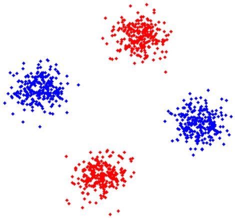
Original data



PCA



Original data



OPLS

Kernel methods for non-linear feature extraction

1. Map the points in $\mathcal{X}$ to a higher dimensional space $\mathcal{H}$:

$$\mathbf{X} \rightarrow \mathbf{\Phi}$$

2. Express projection matrix $\mathbf{U}$ in $\mathcal{H}$ as a linear combination of mapped data

$$\mathbf{U} = \mathbf{\Phi}^\top \mathbf{A}$$

3. Replace the dot (scalar) products by a kernel function:

$$\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^\top$$

4. Express your new algorithm as a function of $\mathbf{K}$ and solve it for $\mathbf{A}$
5. Compute projections

$$\mathcal{P}(\mathbf{X}^*) = \mathbf{\Phi}^*\mathbf{U} = \mathbf{\Phi}^*\ \mathbf{\Phi}^\top\mathbf{A} = \mathbf{K}(\mathbf{X}^*, \mathbf{X})\mathbf{A}$$

Kernel Principal Component Analysis (KPCA)

- *"Find projections maximizing the variance of the projected data in $\mathcal{H}$"*
- Apply the representer's theorem: $\mathbf{U} = \mathbf{\Phi}^\top \mathbf{A}$ where $\mathbf{A} = [\alpha_1, \ldots, \alpha_n]^\top$

$$\text{KPCA:} \qquad \begin{aligned} \text{maximize:} \quad & \text{Tr}\{\mathbf{A}^\top \mathbf{K}\mathbf{K}\mathbf{A}\} \\ \text{subject to:} \quad & \mathbf{A}^\top \mathbf{K}\mathbf{A} = \mathbf{I} \end{aligned}$$

- Including Lagrange multipliers $\mathbf{\Lambda}$, this problem is equivalent to

$$\mathbf{K}\mathbf{K}\mathbf{A} = \mathbf{K}\mathbf{\Lambda}\mathbf{A} \quad \rightarrow \quad \mathbf{K}\mathbf{A} = \mathbf{\Lambda}\mathbf{A}$$

```
» [A,L] = eigs(K,np);
» Xtestproj = K(Xtest,Xtrain)*A;
```

Kernel Partial Least Squares (KPLS)

- *"Find projections for maximum input-output cross-covariance"*
- Apply the representer's theorem: $\mathbf{U} = \mathbf{\Phi}^\top \mathbf{A}$ where $\mathbf{A} = [\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_n]^\top$

$$\text{KPLS:} \qquad \begin{array}{ll} \text{maximize:} & \text{Tr}\{\mathbf{U}^\top \mathbf{\Phi}^\top \mathbf{Y} \mathbf{V}\} \\ \text{subject to:} & \mathbf{U}^\top \mathbf{U} = \mathbf{V}^\top \mathbf{V} = \mathbf{I} \end{array}$$

- Including Lagrange multipliers $\mathbf{\Lambda}$, this problem is equivalent to

$$\left(\begin{array}{cc} \mathbf{0} & \mathbf{K}_x \mathbf{Y} \\ \mathbf{Y} \mathbf{K}_x & \mathbf{0} \end{array} \right) \left(\begin{array}{c} \boldsymbol{\alpha} \\ \mathbf{v} \end{array} \right) = \lambda \left(\begin{array}{c} \boldsymbol{\alpha} \\ \mathbf{v} \end{array} \right)$$

» $[\alpha \;\; V \;\; D] = svds(K * Y, np)$;

» `Xtestproj = K(Xtest,Xtrain) *` α;

Kernel Orthonormalized Partial Least Squares (KOPLS)

- *"Find optimal projections in MSE terms"*
- Apply the representer's theorem: $\mathbf{U} = \mathbf{\Phi}^\top \mathbf{A}$ where $\mathbf{A} = [\alpha_1, \ldots, \alpha_n]^\top$

$$\text{KOPLS:} \quad \begin{array}{ll} \text{maximize:} & \text{Tr}\{\mathbf{U}^\top \mathbf{\Phi}^\top \mathbf{Y}\mathbf{Y}^\top \mathbf{\Phi}\mathbf{U}\} \\ \text{subject to:} & \mathbf{U}^\top \mathbf{\Phi}^\top \mathbf{\Phi}\mathbf{U} = \mathbf{I} \end{array}$$

- Including Lagrange multipliers $\mathbf{\Lambda}$, this problem is equivalent to

$$\text{KOPLS:} \quad \begin{array}{ll} \text{maximize:} & \text{Tr}\{\mathbf{A}^\top \mathbf{K}_x \mathbf{K}_y \mathbf{K}_x \mathbf{A}\} \\ \text{subject to:} & \mathbf{A}^\top \mathbf{K}_x \mathbf{K}_x \mathbf{A} = \mathbf{I} \end{array}$$

```
» M = Kx*Y*Y'*Kx;   N = Kx*Kx;
» [A D] = eigs(M,N,np);
» Xtestproj = K(Xtest,Xtrain) * A;
```

Kernel Canonical Correlation Analysis (KCCA)

- *"Find projections that maximize input-output correlation"*
- Apply the representer's theorem: $\mathbf{U} = \mathbf{\Phi}^\top \mathbf{A}$ where $\mathbf{A} = [\alpha_1, \ldots, \alpha_n]^\top$
- Including Lagrange multipliers $\mathbf{\Lambda}$, this problem is equivalent to

$$\begin{pmatrix} \mathbf{0} & \mathbf{K}_x\mathbf{Y} \\ \mathbf{Y}\mathbf{K}_x & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{K}_x\mathbf{K}_x & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_y \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{v} \end{pmatrix}$$

```
» M = [0 Kx*Y;Y*Kx 0];     N = [Kx*Kx 0;0 Cyy];
» [AV D] = eigs(M,N,np);
» a = AV(1:n/2,:);
» Xtestproj = K(Xtest,Xtrain) * a;
```

Kernel Minimum Noise Fraction (KMNF)

- *"Find projections that maximize SNR in $\mathcal{H}$"*
- Apply the representer's theorem: $\mathbf{U} = \mathbf{\Phi}^\top \mathbf{A}$ where $\mathbf{A} = [\alpha_1, \ldots, \alpha_n]^\top$
- Including Lagrange multipliers $\mathbf{\Lambda}$, this problem is equivalent to

$$\text{KMNF:} \qquad \text{maximize:} \quad \mathrm{Tr}\left\{ \frac{\mathbf{A}^\top \mathbf{K}^2 \mathbf{A}}{\mathbf{A}^\top \mathbf{K}_{xn} \mathbf{K}_{xn} \mathbf{A}} \right\}$$

$$\text{subject to:} \quad \mathbf{A}^\top \mathbf{K}_{xn} \mathbf{K}_{xn} \mathbf{A} = \mathbf{I}$$

```
» Kxx=kernel('rbf',X,X,sigma);
» Kxx=kernelcentering(Kxx);
» N=noise(X,10);
» Kxn=kernel('rbf',X,N,sigma);
» Kxn=kernelcentering(Kxn);
» [A D] = eigs(Kxx*Kxx',Kxn*Kxn',np);
» Xtestproj = K(Xtest,Xtrain) * A;
```

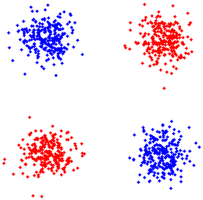
Kernel Entropy Components Analysis (KECA)

- *"Find projections with maximum entropy in $\mathcal{H}$"*
- Apply the representer's theorem: $\mathbf{U} = \mathbf{\Phi}^\top \mathbf{A}$ where $\mathbf{A} = [\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_n]^\top$
- Including Lagrange multipliers $\mathbf{\Lambda}$, this problem is equivalent to

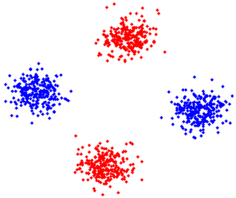
$$\text{KECA:} \qquad \mathbf{K} = \mathbf{A}\mathbf{D}\mathbf{A}^\top \quad \text{s.t. maximum Rényi entropy of } \mathbf{\Phi}\mathbf{U}$$

```
» K = kernel('rbf',X,X,sigma);
» [A,D] = eigs(K);
» lambda = diag(D);
» d=size(A,1);
» for t=1:size(A,2)
      m(t)=lambda(t)*(A(:,t)'*ones(d,1))^2;
  end
» [val,ind] = sort(m,'descend');
» A = A(:,ind);
» Xtestproj = K(Xtest,Xtrain) * A;
```

An illustrative example (cont'd)

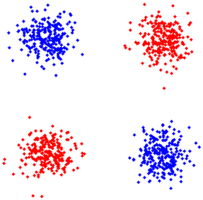


Original data

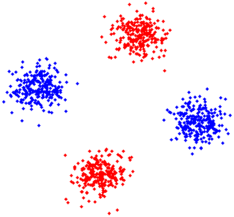


PCA

An illustrative example (cont'd)

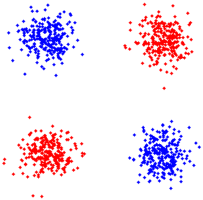


Original data



OPLS

An illustrative example (cont'd)



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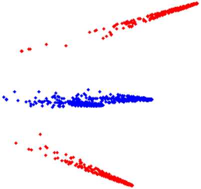
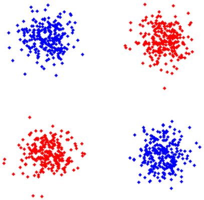


KPCA

An illustrative example (cont'd)



Original data

KOPLS

Method	Maximized Function	Constraints	Solved Problem	Features
PCA	$\mathrm{Tr}\{\mathbf{U}^\top \mathbf{C}_{xx}\mathbf{U}\}$	$\mathbf{U}^\top\mathbf{U}=\mathbf{I}$	$\mathbf{C}_{xx}\mathbf{U}=\mathbf{U}\boldsymbol{\Lambda}$	$\tilde{\mathbf{X}}\mathbf{U}$
	PCA projects linearly the input data onto the directions of largest input variance.			
MNF	$\mathrm{Tr}\{(\mathbf{U}^\top \mathbf{C}_{xx}\mathbf{U})/(\mathbf{U}^\top \mathbf{C}_{nn}\mathbf{U})\}$	$\mathbf{U}^\top\mathbf{C}_{nn}\mathbf{U}=\mathbf{I}$	$\mathbf{C}_{xx}\mathbf{U}=\mathbf{C}_{nn}\mathbf{U}\boldsymbol{\Lambda}$	$\tilde{\mathbf{X}}\mathbf{U}$
	MNF maximizes the ratio between the signal and the noise variances for all the features.			
PLS	$\mathrm{Tr}\{\mathbf{U}^\top \mathbf{C}_{xy}\mathbf{V}\}$	$\mathbf{U}^\top\mathbf{U}=\mathbf{V}^\top\mathbf{V}=\mathbf{I}$	$\mathbf{C}_{xy}=\mathbf{U}\boldsymbol{\Lambda}\mathbf{V}^\top$	$\tilde{\mathbf{X}}\mathbf{U}$
	PLS finds directions of maximum covariance between the projected input and desired output $\mathbf{Y}$.			
OPLS	$\mathrm{Tr}\{\mathbf{U}^\top \mathbf{C}_{xy}\mathbf{C}_{xy}^\top\mathbf{U}\}$	$\mathbf{U}^\top\mathbf{C}_{xx}\mathbf{U}=\mathbf{I}$	$\mathbf{C}_{xy}\mathbf{C}_{xy}^\top\mathbf{U}=\mathbf{C}_{xx}\mathbf{U}\boldsymbol{\Lambda}$	$\tilde{\mathbf{X}}\mathbf{U}$
	OPLS finds optimal directions for performing linear regression of $\tilde{\mathbf{Y}}$ on the projected input data.			
CCA	$\mathrm{Tr}\{\mathbf{U}^\top \mathbf{C}_{xy}\mathbf{V}\}$	$\mathbf{U}^\top\mathbf{C}_{xx}\mathbf{U}=\mathbf{I}\ \mathbf{V}^\top\mathbf{C}_{yy}\mathbf{V}=\mathbf{I}$	$\begin{pmatrix}\mathbf{0} & \mathbf{C}_{xy}\\ \mathbf{C}_{xy}^\top & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{U}\\ \mathbf{V}\end{pmatrix}=\begin{pmatrix}\mathbf{C}_{xx} & \mathbf{0}\\ \mathbf{0} & \mathbf{C}_{yy}\end{pmatrix}\begin{pmatrix}\mathbf{U}\\ \mathbf{V}\end{pmatrix}\boldsymbol{\Lambda}$	$\tilde{\mathbf{X}}\mathbf{U}$
	CCA finds projections of the input and output data matrices such that each column of $\tilde{\mathbf{Y}}$ can be reconstructed from the corresponding column of $\tilde{\mathbf{X}}$ with minimum square loss.			
KPCA	$\mathrm{Tr}\{\mathbf{A}^\top \tilde{\mathbf{K}}_{xx}\tilde{\mathbf{K}}_{xx}\mathbf{A}\}$	$\mathbf{A}^\top\tilde{\mathbf{K}}_{xx}\mathbf{A}=\mathbf{I}$	$\tilde{\mathbf{K}}_{xx}\mathbf{A}=\mathbf{A}\boldsymbol{\Lambda}$	$\tilde{\mathbf{K}}_{xx}\mathbf{A}$
	KPCA finds directions of maximum variance of the input data in $\mathcal{H}$.			
KMNF	$\mathrm{Tr}\{(\mathbf{A}^\top \tilde{\mathbf{K}}_{xx}^2\mathbf{A})/(\mathbf{A}^\top\tilde{\mathbf{K}}_{xn}\tilde{\mathbf{K}}_{nx}\mathbf{A})\}$	$\mathbf{A}^\top\tilde{\mathbf{K}}_{xn}\tilde{\mathbf{K}}_{nx}\mathbf{A}=\mathbf{I}$	$\tilde{\mathbf{K}}_{xx}^2\mathbf{A}=\tilde{\mathbf{K}}_{xn}\tilde{\mathbf{K}}_{xn}^\top\mathbf{A}\boldsymbol{\Lambda}$	$\tilde{\mathbf{K}}_{xx}\mathbf{A}$
	KMNF finds directions of maximum signal to noise ratio of the projected data in $\mathcal{H}$.			
KPLS	$\mathrm{Tr}\{\mathbf{A}^\top \tilde{\mathbf{K}}_{xx}\tilde{\mathbf{Y}}\mathbf{V}\}$	$\mathbf{A}^\top\tilde{\mathbf{K}}_{xx}\mathbf{A}=\mathbf{V}^\top\mathbf{V}=\mathbf{I}$	$\tilde{\mathbf{K}}_{xx}\tilde{\mathbf{Y}}=\mathbf{A}\boldsymbol{\Lambda}\mathbf{V}^\top$	$\tilde{\mathbf{K}}_{xx}\mathbf{A}$
	KPLS finds directions of maximum covariance between the input data in $\mathcal{H}$ and the output $\mathbf{Y}$.			
KOPLS	$\mathrm{Tr}\{\mathbf{A}^\top \mathbf{K}_{xx}\mathbf{K}_{yy}\mathbf{K}_{xx}\mathbf{A}\}$	$\mathbf{A}^\top\mathbf{K}_{xx}^2\mathbf{A}=\mathbf{I}$	$\mathbf{K}_{yy}\mathbf{K}_{xx}\mathbf{A}=\mathbf{K}_{xx}\mathbf{A}\boldsymbol{\Lambda}$	$\tilde{\mathbf{K}}_{xx}\mathbf{A}$
	KOPLS extracts features that minimize the residuals of a multiregression approximating $\tilde{\mathbf{Y}}$.			
KCCA	$\mathrm{Tr}\{\mathbf{A}^\top \mathbf{K}_{xx}\tilde{\mathbf{Y}}\mathbf{V}\}$	$\mathbf{A}^\top\mathbf{K}_{xx}^2\mathbf{A}=\mathbf{I}\ \mathbf{V}^\top\mathbf{C}_{yy}\mathbf{V}=\mathbf{I}$	$\begin{pmatrix}\mathbf{0} & \mathbf{K}_{xx}\tilde{\mathbf{Y}}\\ \tilde{\mathbf{Y}}^\top\mathbf{K}_{xx} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{A}\\ \mathbf{V}\end{pmatrix}=\begin{pmatrix}\mathbf{K}_{xx}^2 & \mathbf{0}\\ \mathbf{0} & \mathbf{C}_{yy}\end{pmatrix}\begin{pmatrix}\mathbf{A}\\ \mathbf{V}\end{pmatrix}\boldsymbol{\Lambda}$	$\tilde{\mathbf{K}}_{xx}\mathbf{A}$
	KCCA finds directions in feature space of maximum correlation with a certain projection of $\tilde{\mathbf{Y}}$.			

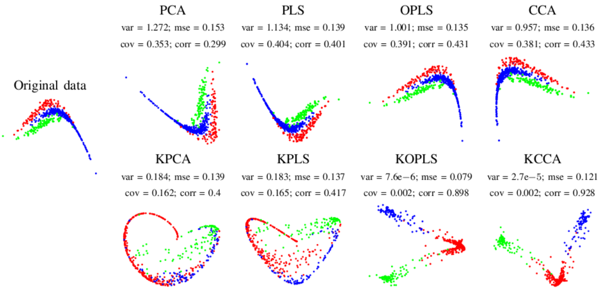


Figura: Projections by different methods in a three-class problem. For the first projection of each method, we show its variance (var), the mean-square-error when the projected data **XU** are used to approximate **Y** (mse), and the largest covariance (cov) and correlation (corr) that can be achieved with any linear projection of the target data.

Conclusions

- Defined the most useful linear and kernel methods for feature extraction
- KPCA is useful in unsupervised learning or as pre-processor
- An excellent alternative to supervised methods is KPLS
- KOPLS is optimal in the MSE sense
- KCCA optimizes correlation but strong regularization needed
- Major problem: non-sparse computationally demanding methods

References

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Notes on kernel methods ...

- Centering data in kernel feature spaces is typically assumed

$$\mathbf{K} \leftarrow \mathbf{HKH}$$

where $H_{ij} = \delta_{ij} - \frac{1}{l}$, $\delta_{ij} = 1$ if $i = j$, and zero otherwise.

```
» H = eye(l)-1/l*ones(l,l);
» K = H*K*H;
```

- Estimate the sigma value for the RBF kernel

```
» sigma = mean(pdist(X));
» sigma = median(pdist(X));
```

- Plot the empirical mapping

```
» K = kernel('rbf',X,X,sigma);
» [V D] = eig(K);    % K=PHI*PHI'=V*D*V';
» PHI = V*D^(1/2);
» plot(PHI(:,1),PHI(:,2),'ko');
» plot3(PHI(:,1),PHI(:,2),PHI(:,3),'ko');
```

Nom	Mida	Tipus
gpml-matlab	4 elements	carpeta
methods	11 elements	carpeta
tools	14 elements	carpeta
Contents.m	2,5 KB	script/funció MATLAB
COPYING.txt	1,4 KB	document de text pla
lecture.pdf	1,7 MB	Adobe Acrobat Document
README.txt	5,1 KB	document de text pla
simfeat.m	8,1 KB	script/funció MATLAB

```
» cd methods
» ls
     cca.m kcca.m keca.m kmnf.m kopls.m
     kpca.m kpls.m mnf.m opls.m pca.m pls.m
» help kcca
» np = 10;
» U = pca(X,np);      % a linear unsupervised method
» U = pls(X,Y,np);    % a linear supervised method
» A = kpca(X,np);     % a kernel unsupervised method
» A = kopls(X,Y,np);% a kernel supervised method
» U,A: struct!
```

```
» Xprojtest = Xtest*U.basis;
» Xprojtest = kernel('rbf',Xtest,X,sigma) * A.basis;
» cd ..
» Ypred = predict(Y,Xtest,U,np);
» Ypred = predict(Y,Xtest,A,np);
» cd tools
» ls
» binarize.m gen_eig.m kernel.m
» plotFeatures.m plotKernelFeatures.m figures.m
     estimateSigma.m generate_toydata.m noise.m
     kernelcentering.m predict.m
» simfeat
```