Prediction in kernelized output spaces: output kernel trees and ensemble methods

Pierre Geurts Florence d'Alché–Buc

IBISC CNRS, Université d'Evry, GENOPOLE, Evry, France
Department of EE and CS, University of Liège, Belgium

25 janvier 2007

Motivation

- In many domains (e.g. text, computational biology), we want to predict complex or structured outputs. e.g. graphs, time series, classes with hierarchical relations, position in a graph, images...
- The main goal of our research team is to develop machine learning tools to extract structures:
- We try to address this issue by several ways and through text and systems biology applications :
  - learning structure of BN (Bayesian networks) and DBN (Dynamic bayesian network) : unsupervised approaches
  - learning interactions as a classification concept : supervised and semi-supervised approaches
  - learning mapping between structures when input and output are strongly dependent : supervised approaches
  - learning mapping between input feature vectors and structured outputs (this talk)

Supervised learning with structured outputs

- **Example 1**: Image reconstruction
- **Example 2** : Find the position of a gene/protein/enzyme in a biological network from various biological descriptors (function of the protein, localization, expression data)
- Very few solutions exist for these tasks (one precursor: KDE), none are explanatory
- We present a set of methods for handling complex outputs that have some explanatory power and illustrate it on these two problems with a main focus on the biological network completion
  - Output Kernel Tree: an extension of regression tree to kernelized output spaces
  - Ensemble methods devoted to regressors in kernelized output spaces

Outline

Supervised learning with complex outputs

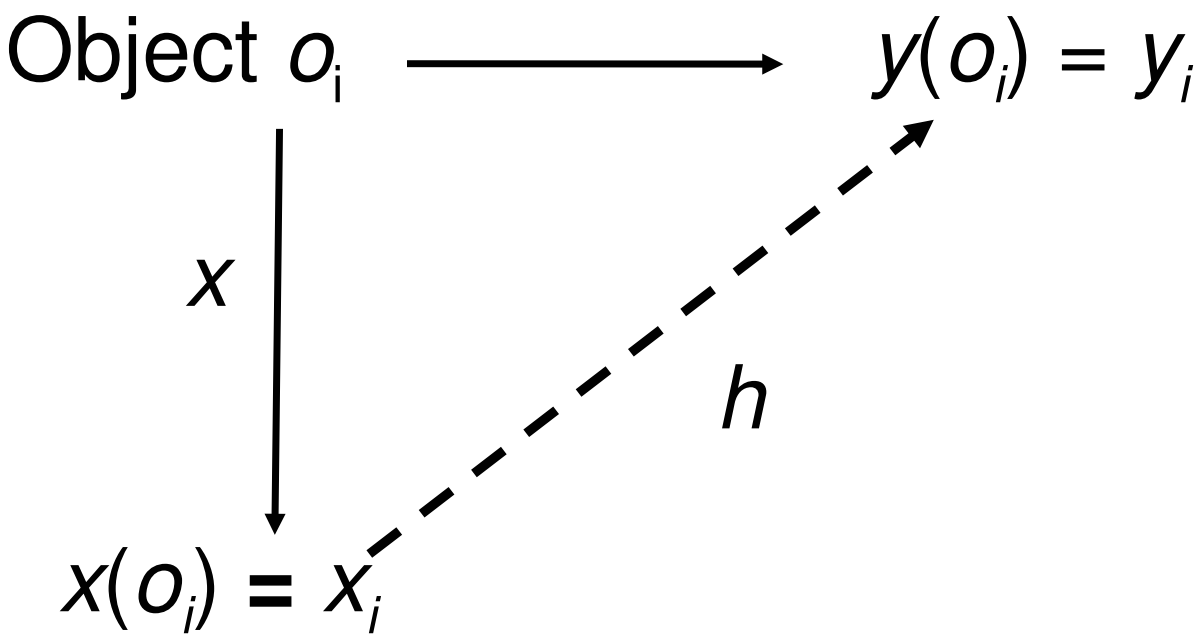
- Suppose we have a sample of objects $\{o_i, i = 1, \ldots, N\}$ drawn from a fixed but unknown probability distribution
- Suppose we have two representations of the objects:
  - an input feature vector representation: $x_i = x(o_i) \in \mathcal{X}$
  - an output representation : $y_i = y(o_i) \in \mathcal{Y}$ where $\mathcal{Y}$ is not necessary a vectorial space (it can be a finite set with complex relations between elements)

From a learning sample $\{(x_i, y_i)|i = 1, \ldots, N\}$ *with* $x_i \in \mathcal{X}$ *and* $y_i \in \mathcal{Y}$*, find a function* $h : \mathcal{X} \to \mathcal{Y}$ *that minimizes the expectation of some loss function* $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ *over the joint distribution of input/output pairs:*

$$E_{x,y}\{\ell(h(x), y)\}$$

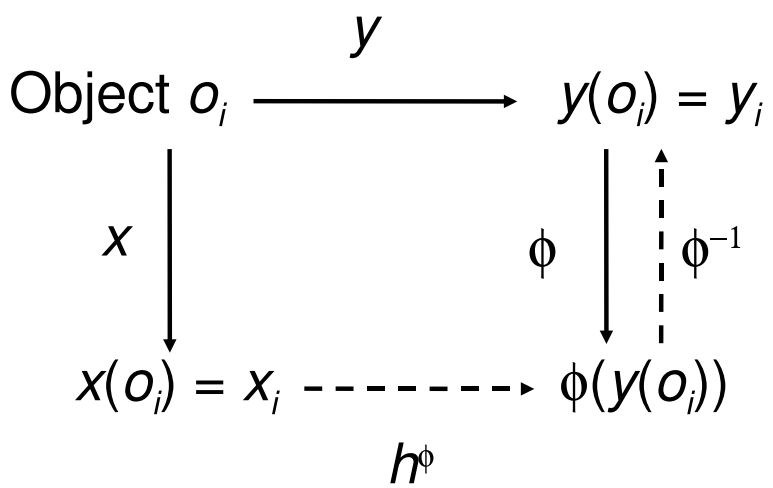
- Complex outputs: no constraint (for the moment) on the nature of $\mathcal{Y}$

General approach



Use the kernel trick for the outputs

- Additional information to the training set:
  - A Gram matrix $K = (k_{ij})$, with $k_{ij} = k(y_i, y_j)$ and k a Mercer Kernel with the corresponding mapping ϕ such that $k(y, y') =< \phi(y), \phi(y') >$.
- Approach:
  1. Approximate the feature map ϕ with a function $h^{\phi} : \mathcal{X} \rightarrow \mathcal{H}$ defined on the input space
  2. Get a prediction in the original output space by approximating the function ϕ^{-1} (pre-image problem)



Possible applications

- Learning a mapping from an input vector into a structured output (graphs, sequences, trees, time series...)
- Learning with alternative loss functions (hierarchical classification for instance)
- Learning a kernel as a function of some inputs

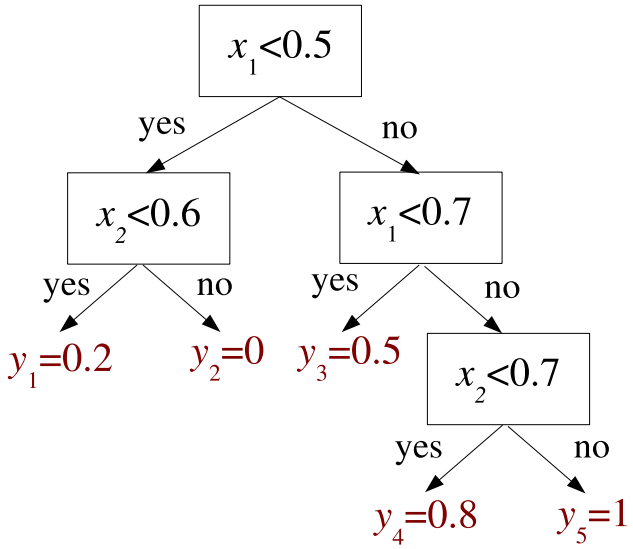
Learning a kernel as a function of some inputs

- In some applications, we want to learn a relationship between objects rather than an output (e.g. network completion problem)
- Learning data set: $\{x_i | i = 1, K = (k_{ij}), i, j = 1 \ldots, N\}$
- In this case, we can make kernel predictions from predictions in $\mathcal{H}$ (without needing pre-images)

$$g(x, x') = \langle h^{\phi}(x), h^{\phi}(x') \rangle.$$

Outline

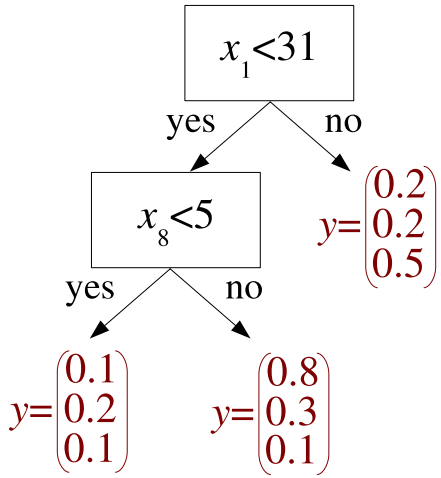
Standard regression trees



- A learning algorithm that solves the regression problem ($\mathcal{Y} = I\!R$ and $\ell(y_1, y_2) = (y_1 - y_2)^2$) with a tree structured model
- Basic idea of the learning procedure:
  - Recursively split the learning sample with tests based on the inputs trying to reduce as much as possible the variance of the output
  - Stop when the output is constant in the leaf (or some stopping criterion is met)

Focus on regression trees on multiple outputs

$\mathcal{Y} = I\!R^n$ and $\ell(y_1, y_2) = ||y_1 - y_2||^2$



The algorithm is the same but:

- The best split is the one that maximizes the variance reduction:

$$\text{Score}_R(Test, S) = \text{var}\{y|S\} - \frac{N_l}{N}\text{var}\{y|S_l\} - \frac{N_r}{N}\text{var}\{y|S_r\},$$

  where N is the size of S, N_l (resp. N_r) the size of S_l (resp. S_r), and $\text{var}\{Y|S\}$ denotes the variance of the output Y in the subset S:

- $$\text{var}\{y|S\} = \frac{1}{N}\sum_{i=1}^{N} ||y_i - \overline{y}||^2 \text{ with } \overline{y} = \frac{1}{N}\sum_{i=1} y_i$$

Regression trees in output feature space

- Let us suppose we have access to an output Gram matrix $k(y_i, y_j)$ with k a kernel defined on $\mathcal{Y} \times \mathcal{Y}$ (with corresponding feature map $\phi : \mathcal{Y} \rightarrow \mathcal{F}$ such that $k(y_i, y_j) = \langle \phi(y_i), \phi(y_j) \rangle$)
- The idea is to grow a multiple output regression tree in the output feature space:
  - The variance becomes:

$$\text{var}\{\phi(y)|S\} = \frac{1}{N} \sum_{i=1}^{N} ||\phi(y_i) - \frac{1}{N} \sum_{i=1} \phi(y_i)||^2$$

  - Predictions at leaf nodes become pre-images of the centers of mass

$$\hat{y}_L = \phi^{-1}(\frac{1}{N_L} \sum_{i=1}^{N_L} \phi(y_i))$$

- We need to express everything in terms of kernel values only and return to the original output space $\mathcal{Y}$

Kernelization

- The variance may be written:

$$\begin{aligned} \text{var}\{\phi(y)|S\} &= \frac{1}{N}\sum_{i=1}^{N}||\phi(y_i) - \frac{1}{N}\sum_{i=1}\phi(y_i)||^2 \\ &= \frac{1}{N}\sum_{i=1}^{N} < \phi(y_i), \phi(y_i) > - \frac{1}{N^2}\sum_{i,j=1}^{N} < \phi(y_i), \phi(y_j) >, \end{aligned}$$

  which makes use only of dot products between vectors in the output feature space

- We can use the kernel trick and replace these dot-products by kernels:

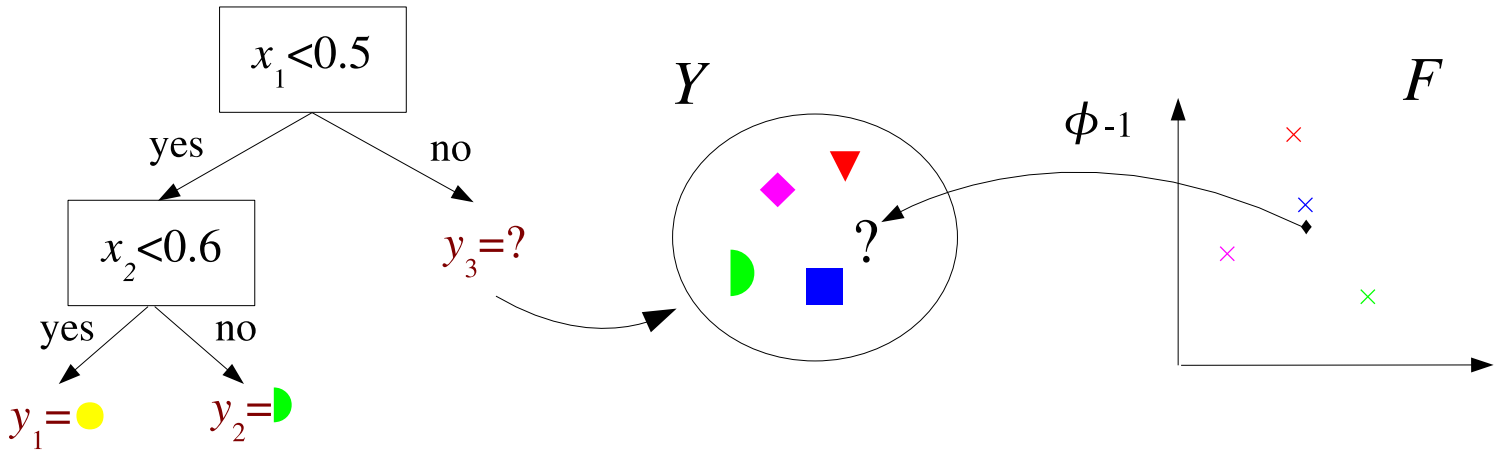
$$\text{var}\{\phi(y)|S\} = \frac{1}{N}\sum_{i=1}^{N} k(y_i, y_i) - \frac{1}{N^2}\sum_{i,j=1}^{N} k(y_i, y_j)$$

- From kernel values only, we can thus grow a regression tree that minimizes output feature space variance

Prediction in the original output space

- Each leaf is associated with a subset of outputs from the learning sample

$$\hat{y}_L = \phi^{-1}\left(\frac{1}{N_L}\sum_{i=1}^{N_L}\phi(y_i)\right)$$



- Generic proposal for the pre-image problem: Find the output in the leaf closest to the center of mass:

$$\hat{y}_L = \arg\min_{y' \in \{y_1,\ldots,y_{N_L}\}} ||\phi(y') - \frac{1}{N_L}\sum_{i=1}^{N_L}\phi(y_i)||^2 = \arg\min_{y' \in \{y_1,\ldots,y_{N_L}\}} k(y',y') - \frac{2}{N_L}\sum_{i=1}^{N_L} k(y_i,y')$$

Outline

Ensemble methods

- Parallel ensemble methods based on randomization:
  - Grow several models in parallel and average their predictions
  - Greatly improve accuracy of single regressors by reducing their variance
  - Usually, they can be applied directly (e.g., bagging, random forests, extra-trees)
- Boosting algorithms:
  - Grow the models in sequence by focusing on “difficult” examples
  - Need to be extended to regressors with kernelized outputs
  - We propose a kernelization of gradient boosting approaches (Friedman, 2001).

Parallel ensemble methods

- To make a prediction, we need to compute:

$$\hat{y}_{\mathcal{T}}(x) = \phi^{-1}\left(\frac{1}{M}\sum_{m=1}^{M} h^{\phi}(x; a_m)\right).$$

- With output kernel trees as base regressors, ensemble predictions in the output feature space may be written:

$$\frac{1}{M}\sum_{m=1}^{M} h^{\phi}(x; a_m) = \sum_{i=1}^{N_{LS}} k_{\mathcal{T}}(x_i, x)\phi(y_i), \text{ with } k_{\mathcal{T}}(x, x') = M^{-1}\sum_{m=1}^{M} k_{t_m}(x, x'),$$

where $k_{t_m}(x, x') = N_L^{-1}$ if x and x' reach the same leaf L in the mth tree, t_m, and 0 otherwise.

- Predictions can then be computed by:

$$\hat{y}_{\mathcal{T}}(x) = \arg \min_{y' \in LS | k_{\mathcal{T}}(x', x) \neq 0} k(y', y') - 2\sum_{i=1}^{N_{LS}} k_{\mathcal{T}}(x_i, x) k(y_i, y').$$

Generic gradient boosting (1/3)

- General supervised learning problem:

  From a learning sample $\{(x_i, y_i)|i = 1, \ldots, N\}$ *with* $x_i \in \mathcal{X}$ *and* $y_i \in \mathcal{Y}$*, find a function* $F : \mathcal{X} \rightarrow \mathcal{Y}$ *that minimizes the expectation of some loss function* ℓ *over the joint distribution of input/output pairs:*

$$E_{x,y}\{\ell(F(x), y)\}$$

- Boosting tries to find an approximation $F(x)$ of the form:

$$F(x) = F_0(x) + \sum_{m=1}^{M} \beta_m h(x; a_m),$$

where $h(x; a)$ is a simple parametrized function of the input variables x, characterized by a vector of parameters a.

Generic gradient boosting (2/3)

- "Greedy-stagewise" approach: From some starting function $F_0(x)$, for $m = 1, 2, \ldots, M$:

$$\begin{aligned}(\beta_m, a_m) &= \arg\min_{\beta,a} \sum_{i=1}^{N} \ell(y_i, F_{m-1}(x_i) + \beta h(x_i; a)) \\ F_m(x) &= F_{m-1}(x) + \beta_m h(x; a_m)\end{aligned}$$

- $\min_{\beta,a}$ may be difficult to compute $\Rightarrow$ find the function that is the closest to the steepest-descent direction in the N-dimensional data space at $F_{m-1}(x)$:

$$-g_m(x_i) = -[\frac{\delta \ell(y_i, F(x_i))}{\delta F(x_i)}]_{F(x)=F_{m-1}(x)}$$

- To generalize, find the function $h(x; a_m)$ that produces $\{h(x_i; a_m)\}_1^N$ most parallel to $-g_m$, e.g. obtained from:

$$a_m = \arg\min_{\beta,a} \sum_{i=1}^{N} (-g_m(x_i) - \beta h(x_i; a))^2.$$

Generic gradient boosting (3/3)

Gradient Boost

1. $F_0(x) = \arg\min_\rho \sum_{i=1}^N \ell(y_i, \rho)$
2. For $m = 1$ to M do:
   1. $y_i^m = -[\frac{\delta \ell(y_i, F(x_i))}{\delta F(x_i)}]_{F(x)=F_{m-1}(x)}, i = 1, \ldots, N$
   2. $a_m = \arg\min_{a,\beta} \sum_{i=1}^N (y_i^m - \beta h(x_i; a))^2$
   3. $\rho_m = \arg\min_\rho \sum_{i=1}^N \ell(y_i, F_{m-1}(x_i) + \rho h(x_i; a_m))$
   4. $F_m(x) = F_{m-1}(x) + \rho_m h(x; a_m)$

- Replace a minimization over any (differentiable) loss ℓ by a least-squares function minimization (2.2) and only a single parameter optimization based on ℓ (2.3)
- Can take benefit of any $h(x; a)$ for which a feasible least-squares algorithm exists

Gradient boosting with square loss

- If $\ell(y_1, y_2) = (y_1 - y_2)^2/2$, the algorithm becomes:

LS Boost

1. $F_0(x) = \frac{1}{N}\sum_{i=1}^{N} y_i$
2. For $m = 1$ to M do:
   1. $y_i^m = y_i - F_{m-1}(x_i), i = 1, \ldots, N$
   2. $a_m = \arg\min_a \sum_{i=1}^{N} (y_i^m - h(x_i; a))^2$
   3. $F_m(x) = F_{m-1}(x) + h(x; a_m)$

- e.g., $h(x; a)$ are small regression trees (Friedman's Multiple Additive Regression Trees, MART).

Gradient boosting with square loss

- If $\ell(y_1, y_2) = (y_1 - y_2)^2/2$, the algorithm becomes:

LS Boost

1. $F_0(x) = \frac{1}{N}\sum_{i=1}^{N} y_i$
2. For $m = 1$ to M do:
   1. $y_i^m = y_i - F_{m-1}(x_i), i = 1, \ldots, N$
   2. $a_m = \arg\min_a \sum_{i=1}^{N} (y_i^m - h(x_i; a))^2$
   3. $F_m(x) = F_{m-1}(x) + \mu h(x; a_m)$

- e.g., $h(x; a)$ are small regression trees (Friedman's Multiple Additive Regression Trees, MART).
- In practice, it is very useful to regularize ($\mu << 1$)

Kernelizing the output (1/2)

LS Boost in a kernelized output space

1. $F_0^\phi(x) = \frac{1}{N}\sum_{i=1}^N \phi(y_i)$
2. For $m = 1$ to M do:
   1. $\phi_i^m = \phi(y_i) - F_{m-1}^\phi(x_i), i = 1, \ldots, N$
   2. $a_m = \arg\min_a \sum_{i=1}^N ||\phi_i^m - h^\phi(x_i; a)||^2$
   3. $F_m^\phi(x) = F_{m-1}^\phi(x) + h^\phi(x; a_m)$

- Replace y by a vector $\phi(y)$ from some feature space $\mathcal{H}$ (in which we only assume it is possible to compute dot-products)
- F^ϕ and h^ϕ are now functions from $\mathcal{X}$ to $\mathcal{H}$

Kernelizing the output (2/2)

LS Boost in a kernelized output space

1. $F_0^{\phi}(x) = \frac{1}{N}\sum_{i=1}^{N}\phi(y_i)$
2. For $m = 1$ to M do:
   1. $\phi_i^m = \phi(y_i) - F_{m-1}^{\phi}(x_i),\ i = 1,\ldots,N$
   2. $a_m = \arg\min_a \sum_{i=1}^{N} ||\phi_i^m - h^{\phi}(x_i;a)||^2$
   3. $F_m^{\phi}(x) = F_{m-1}^{\phi}(x) + h^{\phi}(x;a_m)$

- To be a feasible solution, we need to be able to compute from kernel only:
  - the output Gram matrix K^m at step m, i.e. $K_{i,j}^m = \langle \phi_i^m, \phi_j^m \rangle$ (*to compute 2.2*)
  - $\langle F_M^{\phi}(x), \phi(y) \rangle$, $\forall x, y$ (*to compute predictions, pre-images*)
- This is possible when $h^{\phi}(x;a_m)$ at step m may be written

$$h^{\phi}(x;a_m) = \sum_{i=1}^{N} w_i(x;a_m)\phi_i^m$$

Kernelizing the output: learning stage (1/2)

$$
\begin{aligned}
K^m_{i,j} &\triangleq \langle \phi^m_i, \phi^m_j \rangle = \langle \phi(y_i) - F^{\phi}_{m-1}(x_i), \phi(y_j) - F^{\phi}_{m-1}(x_j) \rangle \\
&= \langle \phi(y_i) - F^{\phi}_{m-2}(x_i) - h^{\phi}(x_i; a_{m-1}), \phi(y_j) - F^{\phi}_{m-2}(x_j) - h^{\phi}(x_j; a_{m-1}) \rangle \\
&= \langle \phi^{m-1}_i, \phi^{m-1}_j \rangle - \langle \phi^{m-1}_i, h^{\phi}(x_j; a_{m-1}) \rangle - \langle h^{\phi}(x_i; a_{m-1}), \phi^{m-1}_j \rangle \\
&\quad + \langle h^{\phi}(x_i; a_{m-1}), h^{\phi}(x_j; a_{m-1}) \rangle .
\end{aligned}
$$

Using $h^{\phi}(x; a_{m-1}) = \sum_{i=1}^{N} w_i(x; a_{m-1}) \phi^{m-1}_i$ and $K^{m-1}_{i,j} \triangleq \langle \phi^{m-1}_i, \phi^{m-1}_j \rangle$:

$$
\begin{aligned}
K^m_{i,j} &= K^{m-1}_{i,j} - \sum_{l=1}^{N} w_l(x_j; a_m) K^{m-1}_{i,l} - \sum_{l=1}^{N} w_l(x_i; a_m) K^{m-1}_{l,j} \\
&\quad + \sum_{k,l=1}^{N} w_k(x_i; a_m) w_l(x_j; a_m) K^{m-1}_{k,l},
\end{aligned}
$$

Kernelizing the output: learning stage (2/2)

Output kernel based boosting: learning

Input: a learning sample $\{(x_i, y_i)\}_{i=1}^N$ and an output Gram matrix K (with $K_{i,j} = k(y_i, y_j)$).

Output: an ensemble of weight functions $\left\{(w_i(x; a_m))_{i=1}^N\right\}_{m=0}^M$.

1. $w_i(x; a_0) \equiv 1/N$, $W_{i,j}^0 = 1/N, \forall i, j = 1, \ldots, N$, $K^0 = K$.
2. For $m = 1$ to M do:
   1. $K^m = (I - W^{m-1})' K^{m-1} (I - W^{m-1})$.
   2. Apply the base learner to the output Gram matrix K^m to get a model $(w_i(x; a_m))_{i=1}^N$.
   3. Compute $W_{i,j}^m = w_i(x_j; a_m), i, j = 1, \ldots, N$ from the resulting model.

(K^1 is the original output Gram matrix centered)

Kernelizing the output: prediction stage (1/3)

- In the output feature space, predictions are of the form:

$$F_M^{\phi}(x) = \sum_{i=1}^{N} w_i^F(x)\phi(y_i).$$

- Output and kernel predictions are then obtained from:

$$\begin{aligned} F(x) &= \arg\min_{y' \in \mathcal{Y}} ||\phi(y') - \sum_{i=1}^{N} w_i^F(x)\phi(y_i)||^2 \\ &= \arg\min_{y' \in \mathcal{Y}} k(y', y') - 2\sum_{i=1}^{N} w_i^F(x)k(y_i, y'). \\ \hat{k}(x_1, x_2) &= \sum_{i=1}^{N}\sum_{j=1}^{N} w_i^F(x_1)w_j^F(x_2)K_{i,j}. \end{aligned}$$

- A recursive algorithm may be devised to compute the weight vector $w^F(x) = (w_1^F(x), \ldots, w_N^F(x))$.

Kernelizing the output: prediction stage (2/3)

- For the m^{th} model, we have:

$$h^{\phi}(x; a_m) = \sum_{i=1}^{N} w_i(x; a_m)\phi_i^m$$

where each output feature vector ϕ_i^m may be further written:

$$\phi_i^m = \sum_{j=1}^{N} O_{i,j}^m \phi(y_j)$$

- The following recursion computes the $N \times N$ matrices O^m:
  - $O^0 = I$
  - $O^m = O^{m-1} - W^{m-1\prime} O^{m-1}, \forall m = 1, \ldots, M$
- Denoting by $p^m(x)$ the (line) vector $(w_1(x; a_m), \ldots, w_N(x; a_m))$, we thus have:

$$w^F(x) = \sum_{m=0}^{M} p^m(x) O^m$$

Kernelizing the output: prediction stage (3/3)

Output kernel based boosting: predictions

Input: a test sample of Q input vectors, $\{x'_1, \ldots, x'_Q\}$.

Output: a prediction $F_M^{\mathcal{Y}}(x'_i) \in \mathcal{Y}$ for each input $x'_i, i = 1, \ldots, Q$ and an output kernel matrix prediction $\hat{K}$ with $\hat{K}_{i,j} = \langle F_M^{\phi}(x'_i), F_M^{\phi}(x'_j) \rangle, i, j = 1, \ldots, Q$.

1. $O^0 = I$, $W^0_{i,j} = 1/N, \forall i, j = 1, \ldots, N$, $W^F_{i,j} = \frac{1}{N}, \forall i = 1, \ldots, Q, j = 1, \ldots, N$
2. For $m = 1$ to M do:
   1. $O^m = O^{m-1} - W^{m-1\prime} O^{m-1}$.
   2. Compute the $Q \times N$ matrix P^m with $P^m_{i,j} = w_j(x'_i; a_m), \forall i = 1, \ldots, Q, \forall j = 1, \ldots, N$.
   3. Set W^F to $W^F + P^m O^m$.
   4. Compute $W^m_{i,j} = w_i(x_j; a_m), \forall i, j = 1, \ldots, N$ from the mth model.

Kernelizing the output: prediction stage (3/3)

Output kernel based boosting: predictions

Input: a test sample of Q input vectors, $\{x'_1, \ldots, x'_Q\}$.

Output: a prediction $F_M^{\mathcal{Y}}(x'_i) \in \mathcal{Y}$ for each input $x'_i, i = 1, \ldots, Q$ and an output kernel matrix prediction $\hat{K}$ with $\hat{K}_{i,j} = \langle F_M^{\phi}(x'_i), F_M^{\phi}(x'_j) \rangle, i, j = 1, \ldots, Q$.

1. $O^0 = I$, $W^0_{i,j} = 1/N, \forall i, j = 1, \ldots, N$, $W^F_{i,j} = \frac{1}{N}, \forall i = 1, \ldots, Q, j = 1, \ldots, N$
2. For $m = 1$ to M do:
   1. $O^m = O^{m-1} - W^{m-1\prime} O^{m-1}$.
   2. Compute the $Q \times N$ matrix P^m with $P^m_{i,j} = w_j(x'_i; a_m), \forall i = 1, \ldots, Q, \forall j = 1, \ldots, N$.
   3. Set W^F to $W^F + P^m O^m$.
   4. Compute $W^m_{i,j} = w_i(x_j; a_m), \forall i, j = 1, \ldots, N$ from the mth model.
3. To compute predictions in the output space:
   1. Compute $S = 1_{Q \times 1} diag(K)' - 2W^F K$.
   2. $F_M^{\mathcal{Y}}(x'_i) = y_k$ with $k = \arg\min_{j=1,\ldots,N} S_{i,j}, \forall i = 1, \ldots, Q$.

Kernelizing the output: prediction stage (3/3)

Output kernel based boosting: predictions

Input: a test sample of Q input vectors, $\{x'_1, \ldots, x'_Q\}$.

Output: a prediction $F_M^{\mathcal{Y}}(x'_i) \in \mathcal{Y}$ for each input $x'_i, i = 1, \ldots, Q$ and an output kernel matrix prediction $\hat{K}$ with $\hat{K}_{i,j} = \langle F_M^{\phi}(x'_i), F_M^{\phi}(x'_j) \rangle, i, j = 1, \ldots, Q$.

1. $O^0 = I$, $W^0_{i,j} = 1/N, \forall i, j = 1, \ldots, N$, $W^F_{i,j} = \frac{1}{N}, \forall i = 1, \ldots, Q, j = 1, \ldots, N$
2. For $m = 1$ to M do:
   1. $O^m = O^{m-1} - W^{m-1\prime} O^{m-1}$.
   2. Compute the $Q \times N$ matrix P^m with $P^m_{i,j} = w_j(x'_i; a_m), \forall i = 1, \ldots, Q, \forall j = 1, \ldots, N$.
   3. Set W^F to $W^F + P^m O^m$.
   4. Compute $W^m_{i,j} = w_i(x_j; a_m), \forall i, j = 1, \ldots, N$ from the mth model.
3. To compute predictions in the output space:
   1. Compute $S = 1_{Q \times 1} diag(K)' - 2W^F K$.
   2. $F_M^{\mathcal{Y}}(x'_i) = y_k$ with $k = \arg\min_{j=1,\ldots,N} S_{i,j}, \forall i = 1, \ldots, Q$.
4. To compute kernel predictions:
   1. $\hat{K} = W^F K W^{F\prime}$.

With OK3 as base learner

- The prediction of the mth tree at some point x is given by:

$$h^{\phi}(x; a_m) = \sum_{i=1}^{N} w_i(x; a_m)\phi_i^m,$$

  with $w_i(x; a_m) = \frac{1}{N_L}$ if x and x_i reach the same leaf of size N_L, 0 otherwise.
- The matrices W^m are symmetric and positive definite.
  - $\phi(x)$ is an N-dimensional vector whose i-th component is equal to $1/\sqrt{N_L}$ when x reaches the leaf of size N_L that contains x_i, 0 otherwise.
- To constrain the tree complexity, we fix the number of splits to a small number J (using a best first strategy to grow the tree).
- When $\mathcal{Y} = I\!R$ and $k(y_1, y_2) = y_1 y_2$, we get MART.

Direct features from tree based methods

- Interpretability:
  - Single tree: a single tree provides a rule-based model that is directly interpretable
  - Ensemble of trees: a ranking of the features according to their relevance can be obtained by summing the total variance reduction over all nodes where the feature appears and normalizing over all variables

- Computational efficiency:
  - Learning stage: node splitting goes from $O(N)$ for standard trees to $O(N^2)$ for OK3. Matrix updates for gradient boosting are also quadratic in N with output kernel trees.
  - Prediction stage: pre-image computation is $O(N_L^2)$, where N_L is the size of the leaf for a single tree and the support of $k_{\mathcal{T}}(x, .)$ for an ensemble.

Outline

First application: image reconstruction (Weston et al., NIPS 2002)

- Predict the bottom half of an image representing a handwritten digit from its top half
- Subset of the USPS dataset: 1000 images, 16×16 pixels
  - Input variables: 8×16(=128) continuous variables
  - Output kernel: radial basis-function (RBF) kernel: $k(y, y') = \exp(-||y - y'||^2/2\sigma^2)$
- Protocol
  - Estimation of the average RBF loss by 5-fold CV
  - Comparison with k-NN and Kernel Dependency Estimation (KDE, a full kernel-based method for structured output prediction fitting a ridge regression model on each direction found by kernel PCA)

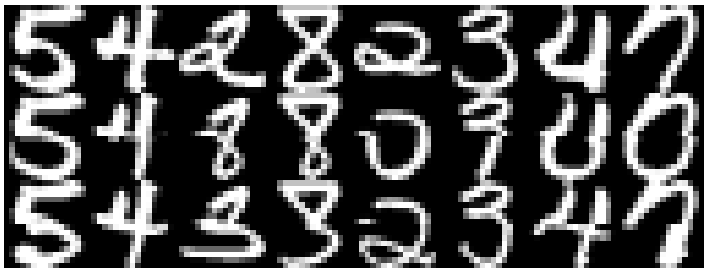
Illustration: accuracy results

Method	RBF error
Baseline	1.0853
Best achievable	0.3584
k-NN	0.7501
KDE linear	0.7990
KDE RBF	0.6778
OK3+Single trees	0.9013
OK3+Bagging	0.7337
OK3+Extra-trees	0.6949

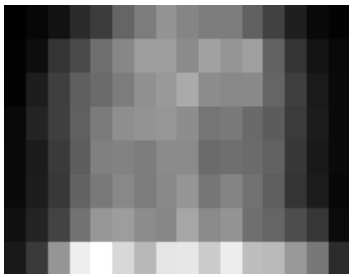
Examples of predictions

OK3+ET

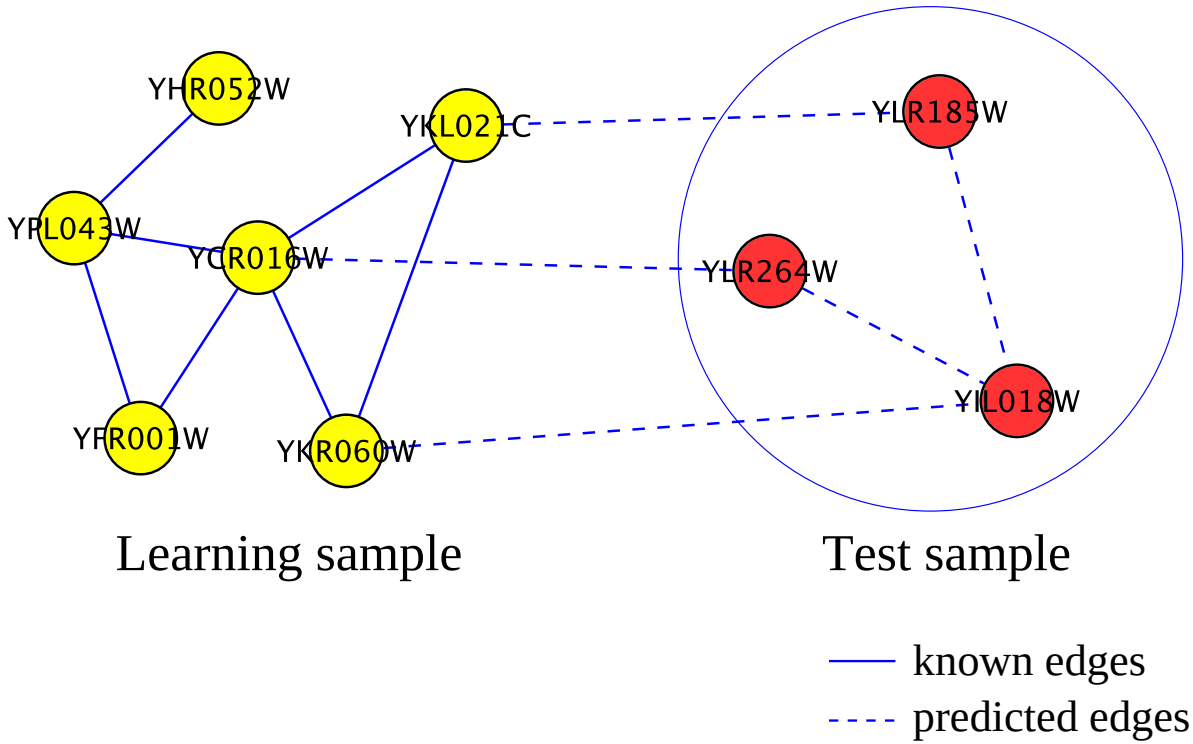
KDE RBF



Feature ranking

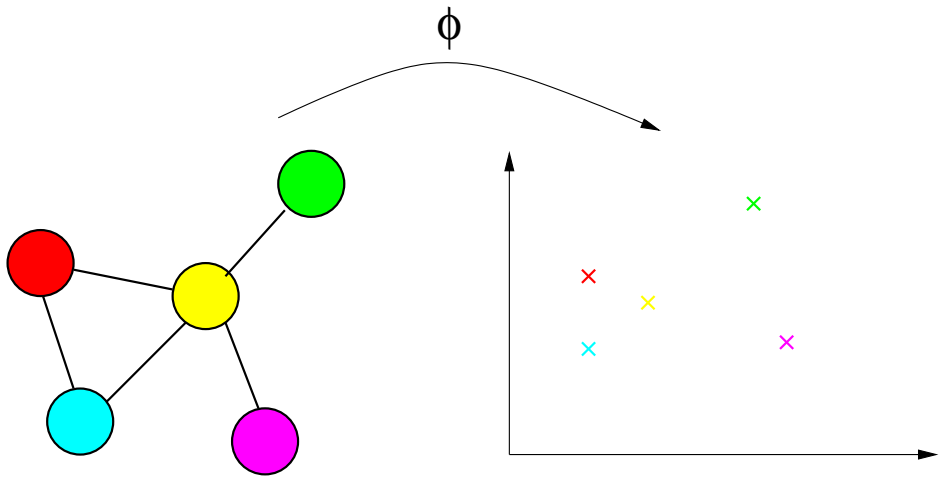


Supervised graph inference (Yamanishi et al., 2004)



- From a known network where each vertex is described by some input feature vector x, predict the edges involving new vertices described by their input feature vector

A general solution based on a kernelized output space



- Define a kernel k on pairs of vertices such that $k(v, v')$ encodes the proximity of vertices in the graph.
- Use a machine learning method that can handle a kernelized output space to get an approximation $g(x(v), x(v'))$ of the kernel value between v and v' described by their input feature vectors $x(v)$ and $x(v')$
- Connect these two vertices if $g(x(v), x(v')) > k_{th}$

(by varying k_{th} we get different tradeoffs between true positive and false positive rates)

A kernel on graph nodes

- Diffusion kernel (Kondor and Lafferty, 2002):
  The Gram matrix K with $K_{i,j} = k(v_i, v_j)$ is given by:

$$K = \exp(-\beta L)$$

  where the graph Laplacian L is defined by:

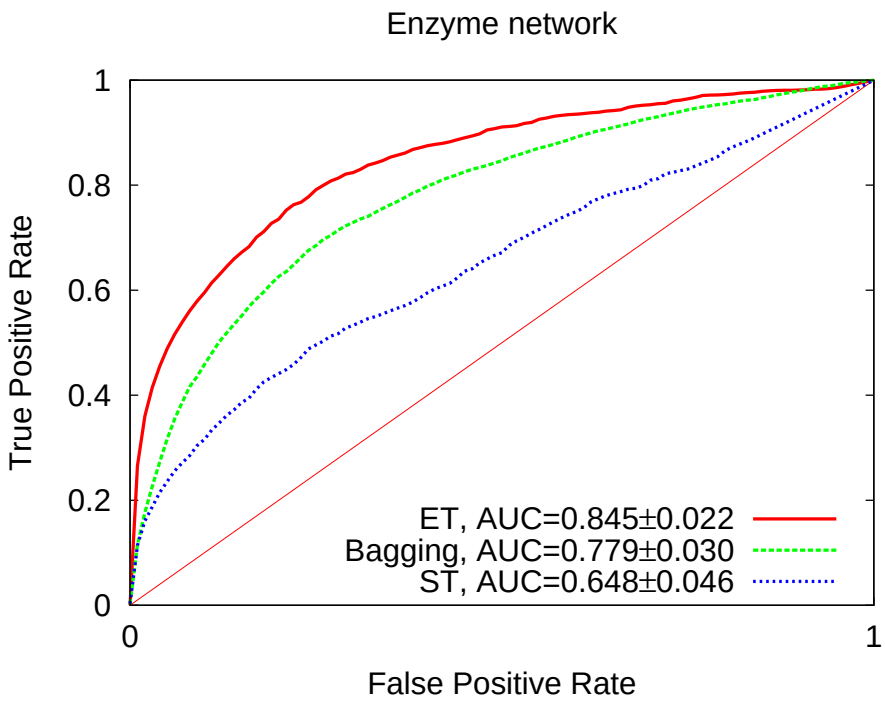
$$L_{i,j} = \begin{cases} d_i & \text{the degree of node } v_i \text{ if } i = j; \\ -1 & \text{if } y(v_i) \text{ and } y(v_j) \text{ are connected;} \\ 0 & \text{otherwise.} \end{cases}$$

- As the diffusion coefficient β increases, kernel values diffuse more completely through the graph

Biological networks

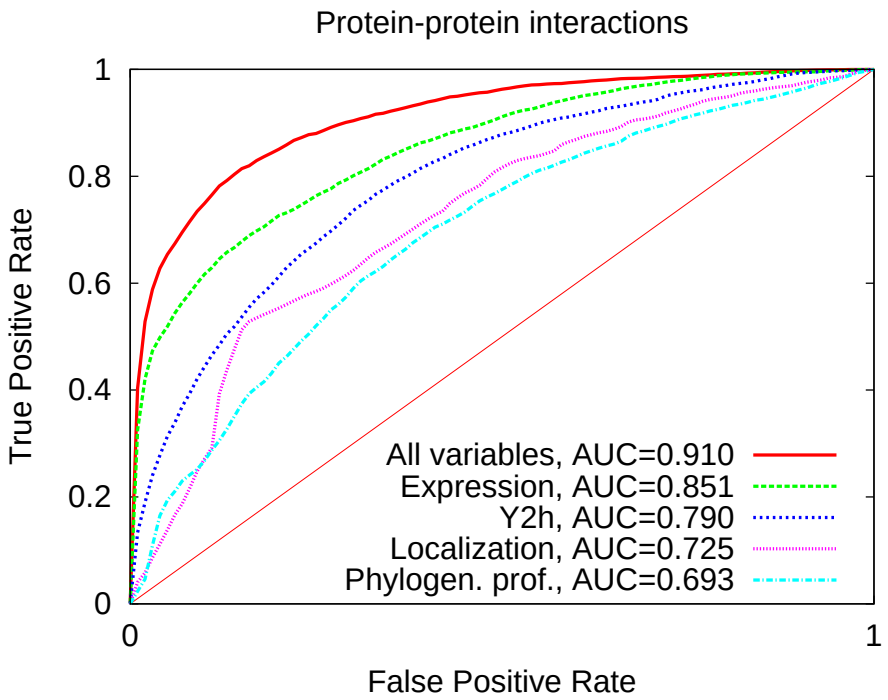
- Application to two networks in the Yeast:
  - Protein-protein interaction network: 984 proteins, 2478 edges (Kato et al., 2005)
  - Enzyme network: 668 enzymes and 2782 edges (Yamanishi et al., 2005)
- Input features:
  - Expression data: expression of the gene in 325 experiments
  - Phylogenetic profiles: presence or absence of an ortholog in 145 species
  - Localization data: presence or absence of the protein in 23 intracellular location
  - Yeast two hybrid data: data from a high-throughput experiment to detect protein-protein interactions

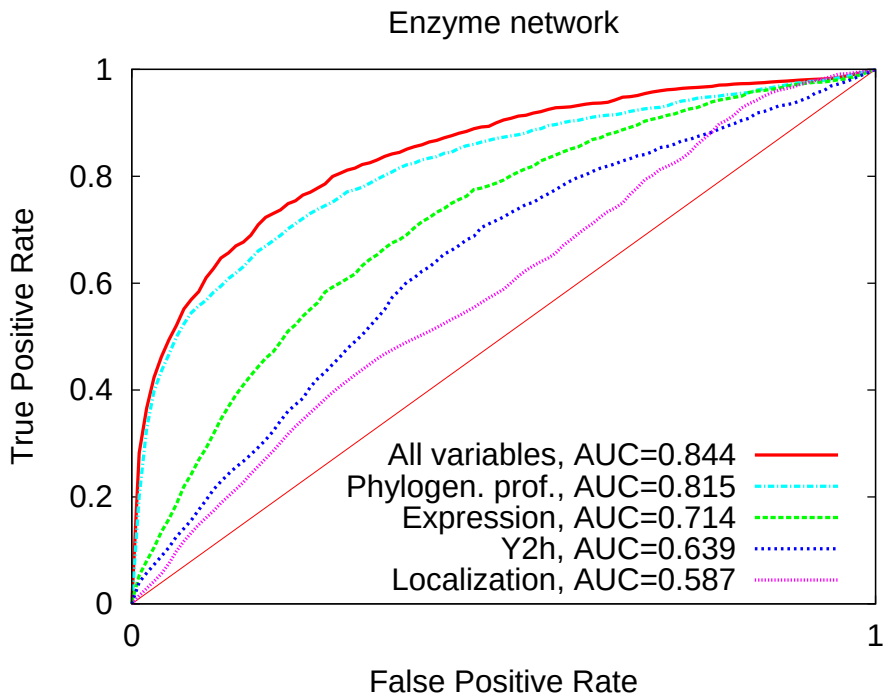
Comparison of different tree based methods



Diffusion kernel as a graph kernel, 10-fold cross-validation, ensembles of 100 output kernel trees

Comparison of different sets of features





Diffusion kernel as a graph kernel, 10-fold cross-validation, ensembles of 100 output kernel trees, extra-trees randomization method

Comparison with full kernel based methods

Protein network

Inputs	OK3+ET	[1]
expr	0.851	0.776
phy	0.693	0.767
loc	0.725	0.788
y2h	0.790	0.612
All	**0.910**	**0.939**

Enzyme network

Inputs	OK3+ET	[2]
expr	0.714	0.706
phy	0.815	0.747
loc	0.587	0.577
All	**0.847**	**0.804**

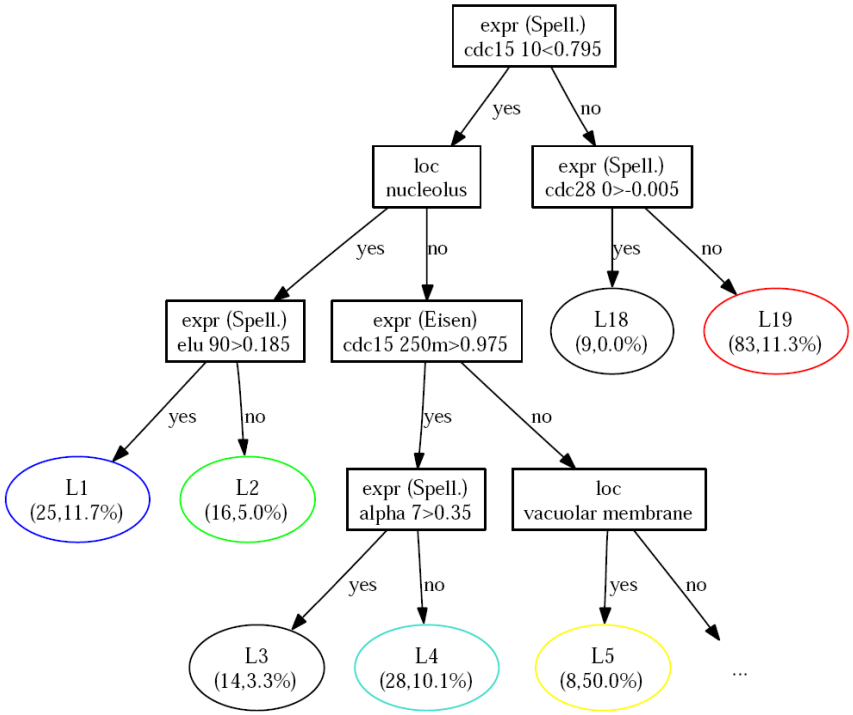
- [1] Kato et al., ISMB 2005: EM based algorithm for kernel matrix completion
- [2] Yamanishi et al., ISMB 2005: compare a kernel canonical correlation analysis based solution and a metric learning approach

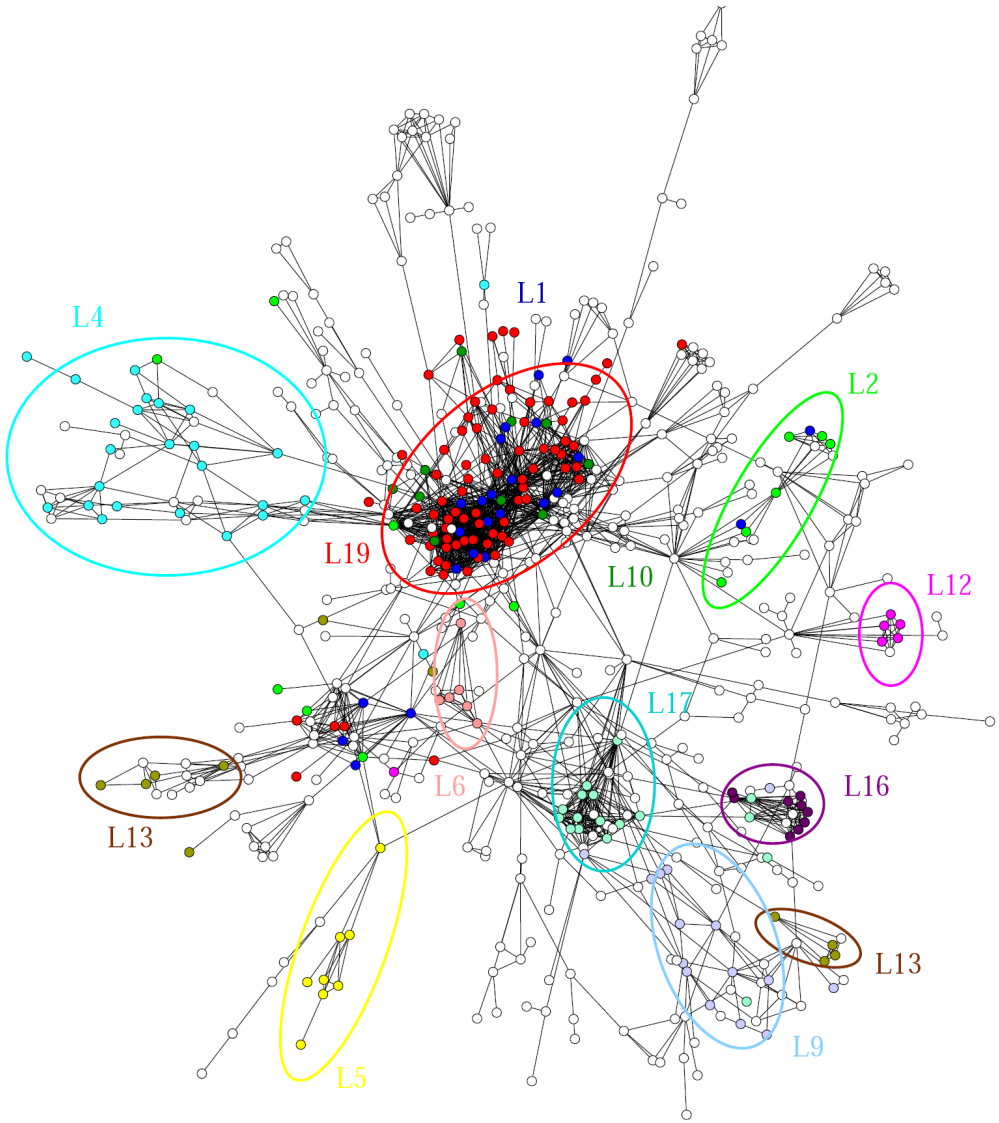
Robustness

Evolution of the AUC when x% of the edges are randomly deleted in the learning sample (OK3+ET, 100 trees)

	0%	20%	50%	80%
Protein network	0.910	0.906	0.896	0.883
Enzyme network	0.844	0.800	0.812	0.753

Interpretability: rules and clusters (an example with a protein-protein network)



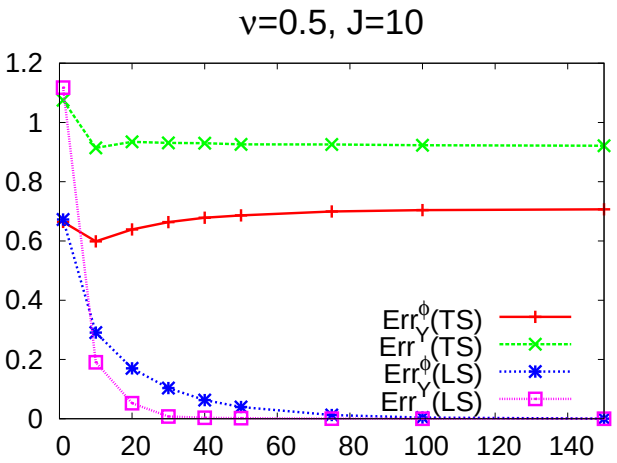


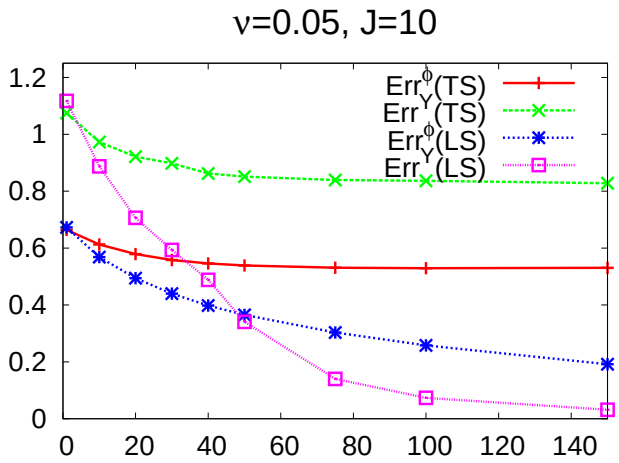
Interpretability: feature ranking

Protein-protein interactions			Enzyme network		
#	Att.	Imp	#	Att.	Imp
1	loc - nucleolus	0.021	1	phy - dre	0.011
2	expr (Spell.) - elu 120	0.013	2	phy - rno	0.009
3	loc - cytoplasm	0.012	3	expr (Eisen) - cdc15 120m	0.008
4	expr (Eisen) - sporulation ndt80 early	0.012	4	phy - ecu	0.008
5	loc - nucleus	0.012	5	expr (Eisen) - cdc15 160m	0.008
6	expr (Eisen) - sporulation 30m	0.011	6	phy - pfa	0.007
7	expr (Eisen) - sporulation ndt80 middle	0.010	7	phy - mmu	0.007
8	expr (Spell.) - alpha 14	0.010	8	loc - cytoplasm	0.006
9	expr (Spell.) - elu 150	0.010	9	expr (Eisen) - cdc15 30m	0.005
10	loc - mitochondrion	0.009	10	expr (Eisen) - elutriation 5.5hrs	0.005

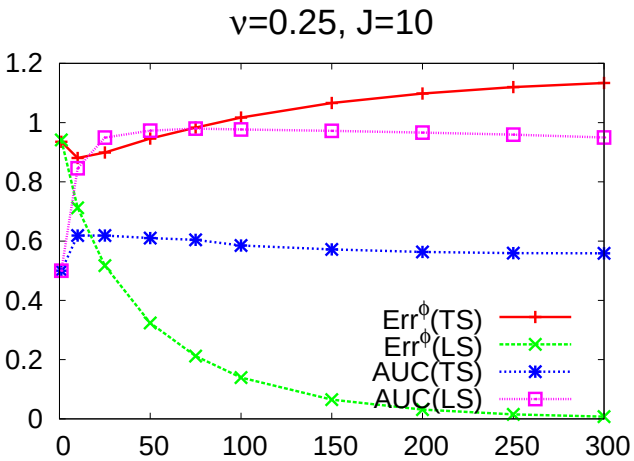
Experiments with boosting

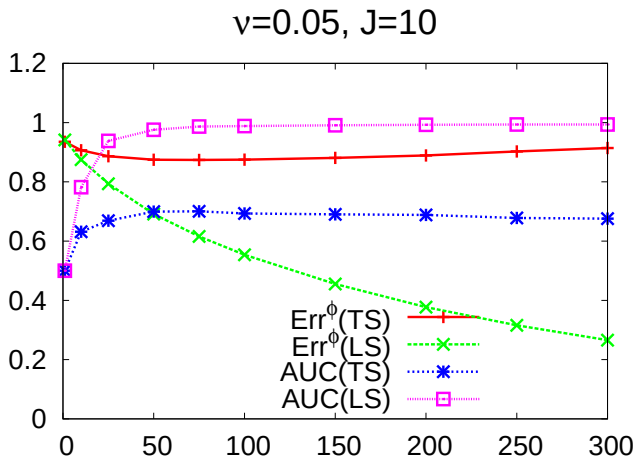
- On the image completion task (#LS=200,#TS=800):





- On the network completion problem (#LS=334,#TS=334):





(Err^{ϕ} is the error of $F^{\phi}_{M}(x)$ (i.e. in $\mathcal{H}$), Err^{Y} is the error of the pre-image)

Experiments with boosting

Image	
Method	$Err^{\mathcal{Y}}(TS)$
OK3 (single trees)	1.0399
OK3+Bagging	0.8643
OK3+ET	0.8169
OK3+OKBoost	0.8318
OK3+OKBoost+ET	<u>0.8071</u>

Network	
Method	AUC(TS)
OK3 (single trees)	0.6001
OK3+Bagging	0.7100
OK3+ET	<u>0.7884</u>
OK3+OKBoost	0.7033
OK3+OKBoost+ET	0.7811

($\mu = 0.01$, $M = 500$, Tree size J determined by 5-fold CV)

Conclusion and future works

- A new method for prediction in kernelized output spaces
  - When used in a single tree, it can provide interpretable results in the form of a rule based model.
  - When used in an ensemble of trees, it provide competitive accuracy and can rank the input features according to their relevance
- **Future works:**
  - Other frameworks : transduction (straightfoward), semi-supervised...
  - Other applications: hierarchical classification, sequence predictions,...
  - Analysis of the role played by the output kernel in the cost function (regularization, output kernel learning)
  - Improving gradient boosting by explicit regularization and use of other base learners
  - Study links between this approach and Taskar's approaches (features on input/outputs)

Another base learner for boosting (1/2)

- A simpler base learner:
  1. Find a direction $v = \sum_{i=1}^{N} v_i \phi(y_i^m), ||v|| = 1$, in the output feature space
  2. Project the data in this direction to obtain a training set:

     $$\{(x_i, \langle \phi(y_i^m), v \rangle) | i = 1, \ldots, N\}$$

     and use any regression method to find an approximation $f_m(x_i)$ of $\langle \phi(y_i^m), v \rangle$
  3. Output the function:

$$h^{\phi}(x; a_m) = f_m(x)v = \sum_{i=1}^{N} f_m(x) v_i \phi(y_i^m)$$

Another base learner for boosting (2/2)

- How to select the direction v ?
  - Choose the direction of maximum variance (kernel PCA)
  - Choose a direction at random
  - For computational efficiency reason, choose a direction among the outputs in the learning sample.
- Regression method:
  - Any regression method can be plugged
  - With regression trees, we get MART when $\mathcal{Y} = I\!R$ and $k(y_1, y_2) = y_1 y_2$