Decision and regression tree ensemble methods and their applications in automatic learning

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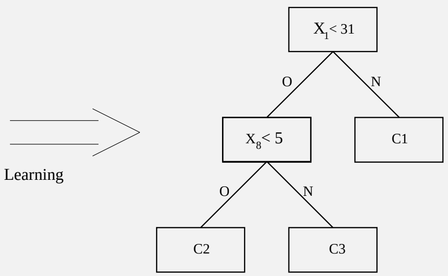
Part I

Supervised learning algorithm (Batch Mode)

- Inputs: learning sample ls of (x, y) observations ($ls \in (X \times Y)^*$)
- Output: a model $f_A^{ls} \in \mathcal{F}_A \subset Y^X$ (decision tree, MLP, ...)

X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	Y
60	19	18	17	0	1	1	1	C1
60	3	22	23	1	29	11	23	C1
75	9	2	1	3	77	46	3	C1
2	10	10	2	234	0	0	0	C2
3	7	9	18	5	0	0	0	C2
2	14	5	10	8	10	8	10	C3
65	3	20	21	2	0	1	1	?



- Objectives:
  - maximise accuracy on independent observations
  - interpretability, scalability

Induction of single decision/regression trees (Reminder)

- Algorithm development (1960-1995)
  - Top-down growing of trees by recursive partitioning
    - local optimisation of split score (variance, entropy)
  - Bottom-up pruning to prevent over-fitting
    - global optimisation of complexity vs accuracy (B/V tradeoff)
- Characterisation
  - Highly scalable algorithm
  - Interpretable models (rules)
  - Robustness: irrelevant variables, scaling, outliers
  - Expected accuracy often low (high variance)
- Many variants and extensions
  - C4.5, CART, ID3 ...
  - oblique, fuzzy, hybrid ...

Bias/variance decomposition (of average error)

Accuracy of models produced by an algorithm in a given context

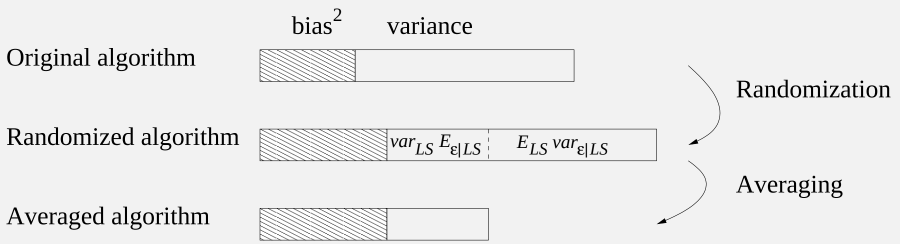
- Assume problem (inputs X, outputs Y, relation $P(X,Y)$)
  and sampling scheme (e.g. fixed size $LS \sim P^N(X,Y)$).
- Take model error function (e.g. $Err_{f,Y} \equiv E_{X,Y}\{(f(X)-Y)^2\}$)
  and evaluate *expected* error of algo A (i.e. $\overline{Err}_{A,Y} \equiv E_{LS}\{Err_{f_A^{ls},Y}\}$)
- We have $\overline{Err}_{A,Y} - Err_{B,Y} = Bias_A^2 + Var_A$
  where
  - B is the best possible model (here, $B(\cdot) \equiv E_{Y|\cdot}$)
  - $Bias_A^2 = Err_{\bar{f}_A,B}$ ($\bar{f}_A$ is the average model)
  - $Var_A = \overline{Err}_{A,\bar{f}_A}$ (dependence of model on sample)

Ensembles of trees (How?/Why?)

- Perturb and Combine paradigm (1990-2005)
  - Build several trees (e.g. 100, by randomisation)
  - Combine trees by voting, averaging... (i.e. aggregation)
- Characterisation
  - Can preserve scalability (+ trivially parallel)
  - Does not preserve interpretability
  - Can preserve robustness (irrelevant variables, scaling, outliers)
  - Can improve accuracy significantly
- Many generic variants (Bagging, Stacking, Boosting, ...)
- Non-generic variants: (Random Forests, Random Subspace, ...)

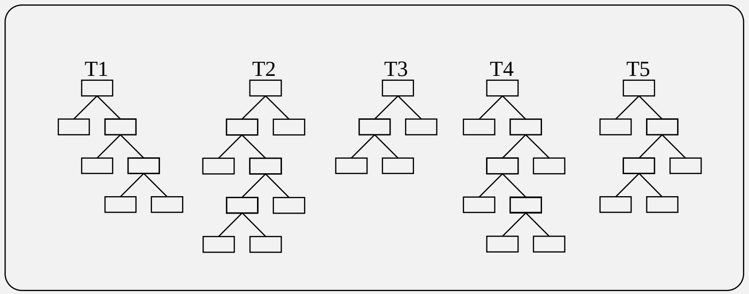
Variance reduction by randomisation and averaging

Denote by $f_{A,\varepsilon}^{ls}$ randomised version of A (where $\varepsilon \sim U[0,1)$)
Averaged model: $f_{A,\varepsilon}^{T,ls} = T^{-1}\sum_{i=1}^{T} f_{A,\epsilon_i}^{ls}$ (in the limit $f_{A,\varepsilon}^{\infty,ls}$)



Can reduce *Variance* strongly, without increasing too much *Bias*.

Extra-Trees: learning algorithm

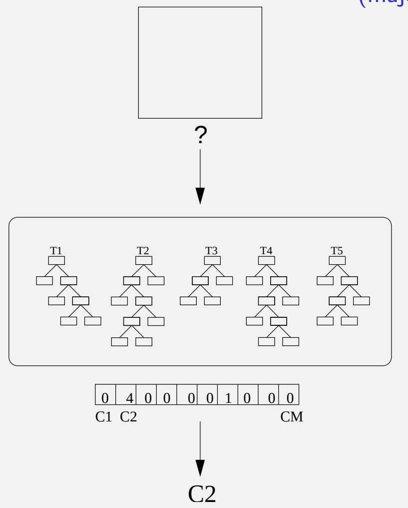


- Ensemble of trees $T_1, T_2, \ldots T_T$ (generated independently)
- Random splitting (choice of variable and cut-point)
- Trees are fully developed (perfect fit on ls)
- Ultra-fast ($\sqrt{n}N\log N$)

(Presentation based on [Geu02, GEW04])

Extra-Trees: prediction algorithm

- Aggregation (majority vote or averaging)



Extra-Trees splitting algorithm (for numerical attributes)

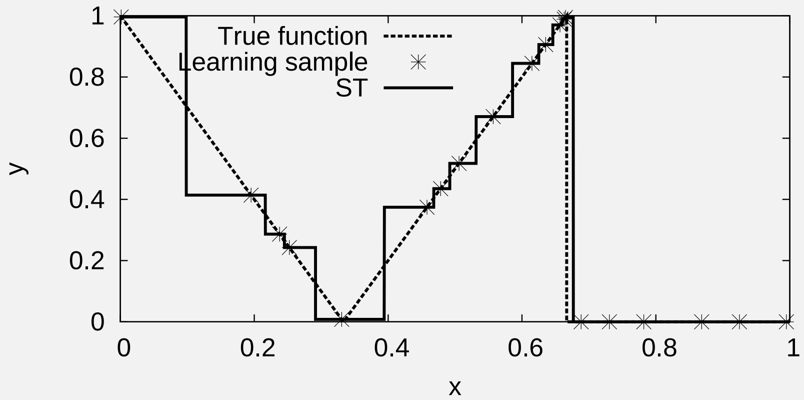
Given a node of a tree and a sample S corresponding to it

- Select K attributes $\{X_1, \ldots, X_K\}$ at random;
- For each X_i (draw a split at random)
  - Let $x^S_{i,\min}$ and $x^S_{i,\max}$ be the min and max values of X_i in S;
  - Draw a cut-point $x_{i,c}$ uniformly in $]x^S_{i,\min}, x^S_{i,\max}]$;
  - Let $t_i = [X_i < x_{i,c}]$.
- Return a split $t_i = \arg\max_{t_i} \text{Score}(t_i, S)$.

NB: the node becomes a LEAF

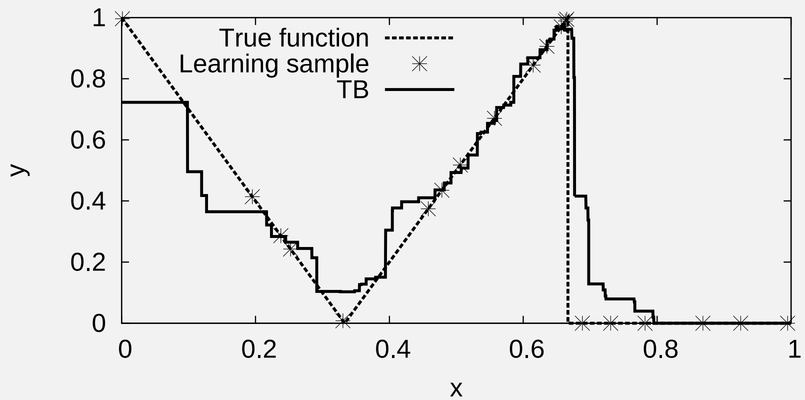
- if $|S| < n_{\min}$;
- if all attributes are constant in S;
- if the output is constant in S;

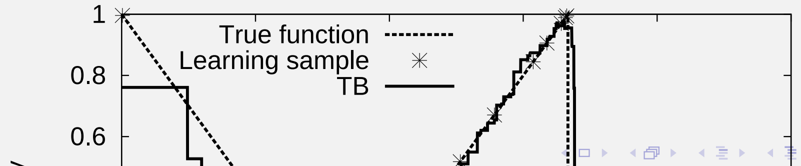
Geometric properties (of Single Trees)



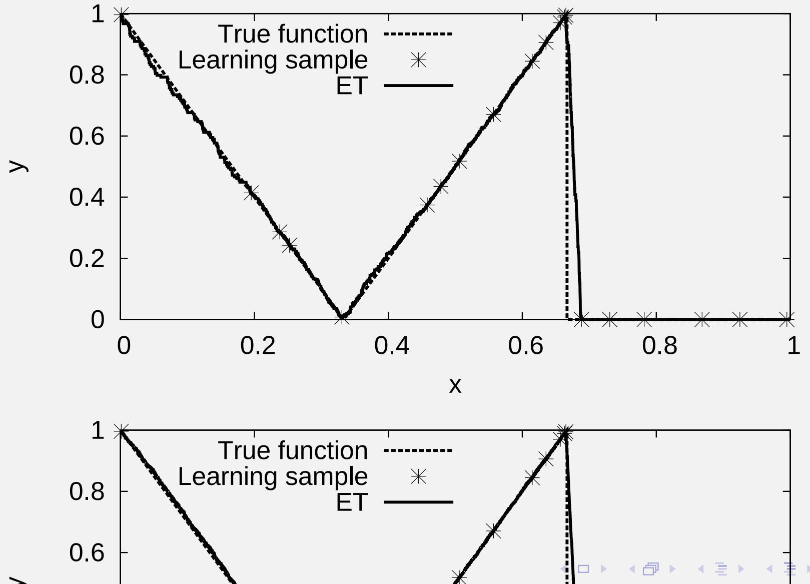
A single fully developed CART tree.

Geometric properties (of Tree Bagging models)



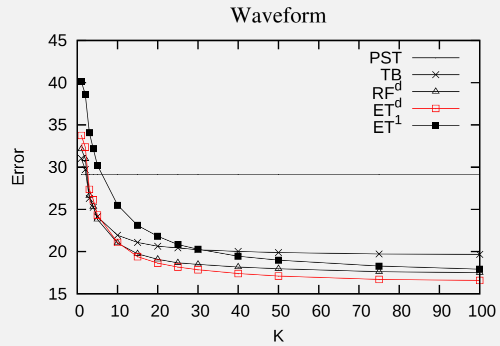


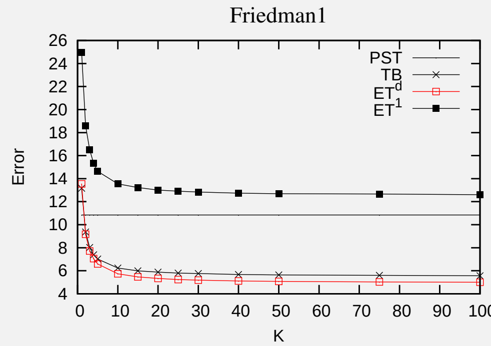
Geometric properties (of Extra-Trees models)



Parameters (of the Extra-Trees learning algorithm)

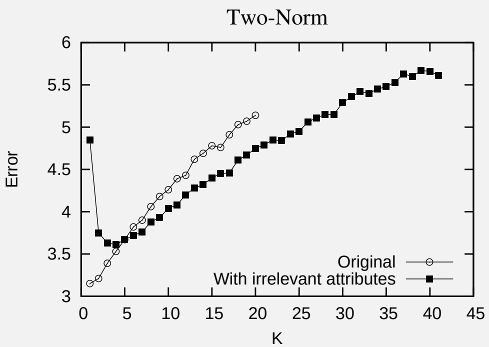
Averaging strength T

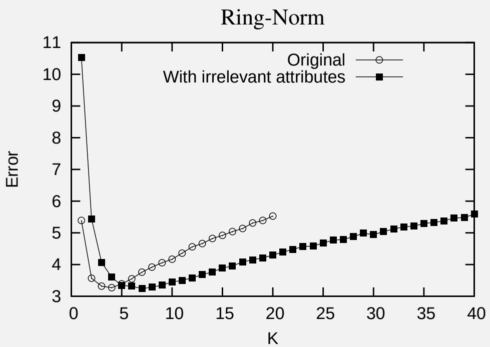




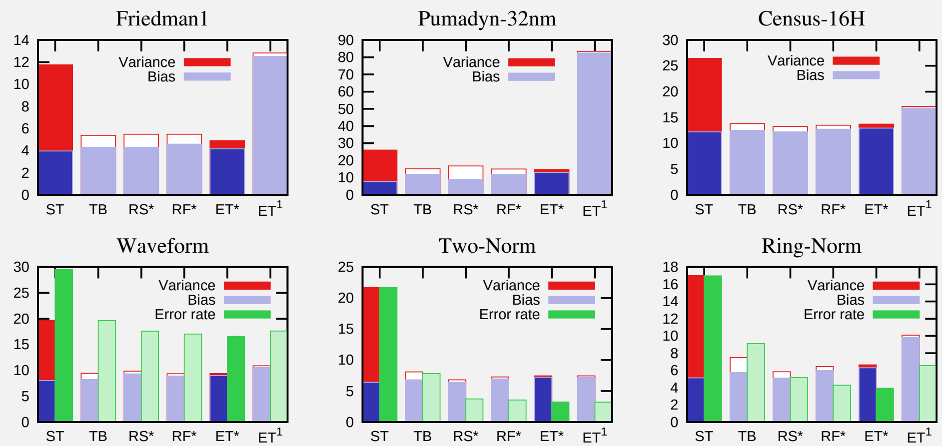
Parameters (of the Extra-Trees learning algorithm)

Attribute selection strength K (w.r.t. irrelevant variables)





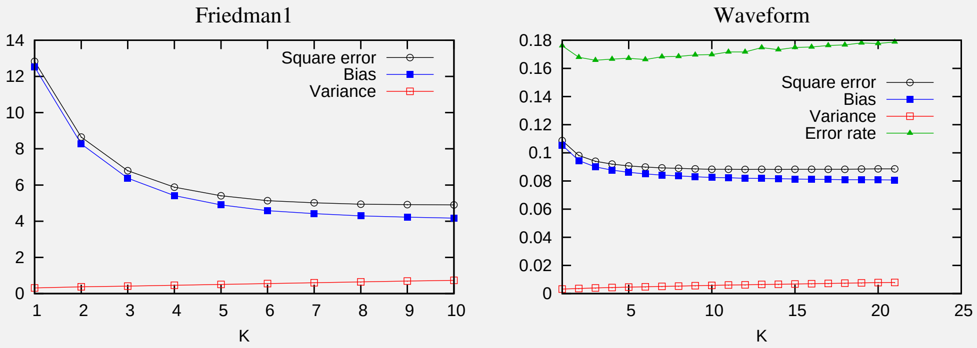
Bias/variance tradeoff (of the Extra-Trees models)



Bias/variance tradeoff

(of the Extra-Trees learning algorithm)

Effect of attribute selection strength K



Extra-Trees: variants of setting K

Automatic tuning of K

- by (10-fold) cross-validation
- on (large enough) independent test sample

Default settings

- $K = \sqrt{n}$, in classification
- $K = n$, in regression (*n* =number of variables)

Totally randomised trees

- correspond to $K = 1$
- splits (attribute and cut-point) totally at random
- ultra-fast "non-supervised" learning algorithm
- tree structures independent of output values
- akin to KNN, or kernel-based method

Optimal control problem

(stochastic, discrete-time, infinite horizon)

$x_{t+1} = f(x_t, u_t, w_t)$ (stochastic dynamics, $w_t \sim P_w(w_t|x_t, u_t)$)

$r_t = r(x_t, u_t, w_t)$ (real valued reward signal bounded over $X \times U \times W$)

γ (discount factor $\in [0, 1)$)

$\mu(\cdot) : X \to U$ (closed-loop, stationary control policy)

$J_h^\mu(x) = E\left\{\sum_{t=0}^{h-1} \gamma^t r(x_t, \mu(x_t), w_t)|x_0 = x\right\}$ (finite horizon return)

$J_\infty^\mu(x) = \lim_{h\to\infty} J_h^\mu(x)$ (infinite horizon return)

Optimal *infinite* horizon control policy

$\mu_\infty^*(\cdot)$ that maximises $J_\infty^\mu(x)$ for all x.

(Presentation based on [EGW03, EGW05])

Batch mode reinforcement learning problem

Suppose that instead of system model $(f(\cdot,\cdot,\cdot), r(\cdot,\cdot,\cdot), P_w(\cdot|\cdot,\cdot))$, the only information we have is a (finite) sample F of four-tuples:

$$F = \{(x_{t^i}, u_{t^i}, r_{t^i}, x_{t^i+1}), i = 1, \cdots, \#F\}.$$

Each four-tuple corresponds to a system transition

The objective of batch mode RL is to determine an approximation $\hat{\mu}(\cdot)$ of $\mu^*_\infty(\cdot)$ from the sole knowledge of F

(Many one-step episodes: x_{t^f} distributed independently)

(One single episode: $x_{t^{f+1}} = x_{t^f+1}$)

(In general: several multi-step episodes)

Q-function iteration to solve Bellman equation

Idea: $\mu^*_\infty(\cdot) \equiv$ can be obtained as the limit of a sequence of optimal finite horizon (time-varying) policies.

Define sequence of value-functions Q_h and policies by $\mu^*_h(t,x)$:
$Q_0(x,u) \equiv 0$
$Q_h(x,u) = E_{w|x,u}\{r(x,u,w) + \gamma \max_{u'} Q_{h-1}(f(x,u,w),u')\}$ $(\forall h \in \mathbb{N})$
$\mu^*_h(t,x) = \arg\max_u Q_{h-t}(x,u)$ $(\forall h \in \mathbb{N}, \forall t = 0,\ldots,h-1)$

NB: these sequences converge $(Q_h \xrightarrow{\sup} Q_\infty$ and $\mu^*_h(t,x) \xrightarrow{J^\mu_\infty} \mu^*_\infty(x))$

Alternative view: (Bellman equation)
$Q_\infty(x,u) = E_{w|x,u}\{r(x,u,w) + \gamma \max_{u'} Q_\infty(f(x,u,w),u')\}$
$\mu^*_\infty(x) = \arg\max_u Q_\infty(x,u)$

Fitted Q iteration algorithm

Idea1: replace expectation operator $E_{w|x,u}$ by average over sample
Idea2: represent Q_h by model to interpolate from samples
Supervised learning (regression): does the two in a single step

- Inputs:
  - a set F of four-tuples $((x_{t^i}, u_{t^i}, r_{t^i}, x_{t^i+1}), i = 1, \cdots, \#F)$
  - a regression algorithm A $(A : ls \rightarrow f^{ls}_A)$
- Initialisation: $\hat{Q}_0(x,u) \equiv 0$
- Iteration: (for $h = 1, 2, \ldots$)
  - Training set construction: $(\forall i = 1, \ldots \#F)$
    $x_i = (x_{t^i}, u_{t^i})$;
    $y_i = r_{t^i} + \gamma \max_u \hat{Q}_{h-1}(x_{t^i+1}, u)$,
  - Q-function fitting:
    $\hat{Q}_h = A(ls)$ where $ls = ((x_1,y_1),\ldots,(x_{\#F}, y_{\#F}))$

Coupling with tree-based models

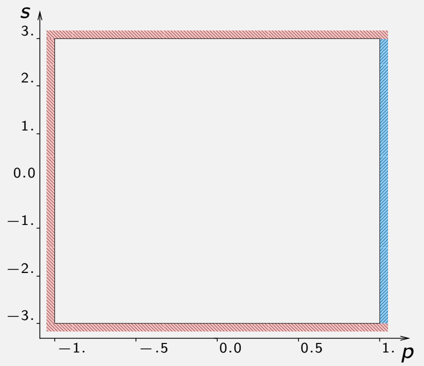
Use tree-based regression as supervised learning algorithm
NB: many tree-based methods: 'non-divergence' to infinity
NB: ET^∞_1: guarantee 'convergence' (when $h \rightarrow \infty$)
NB: Tree structures can be frozen for $h > h_0$: 'convergence'

Generality of framework
X, U discrete or continuous, high-dimensional; no strong hypothesis on f, r, etc
Minimum-time problem: define $r(x,u,w) = 1_{Goal}(f(x,u,w))$.
Stabilisation, tracking: define $r(x,u,w) = ||f(x,u,w) - x_{ref}||$

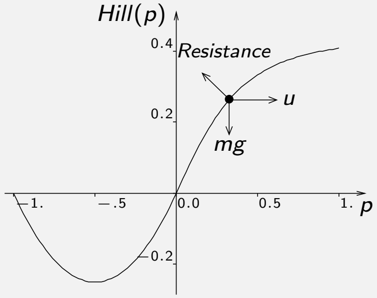
Solves at the same time: system identification, state-space discretisation, curse-of-dimensionality, Bellman equation

Car on the hill problem

(problem description)



State space X : ($position \times speed$)



$Hill(p)$ and forces on the car:

Car on the hill problem

(problem description)

Deterministic problem
$u = -4$: full deceleration
$u = +4$: full acceleration
$r(goal) = 1$
$r(lost) = -1$
$r = 0$, otherwise

F: 1000 episodes
Random walk starting from $(p, s) = (-0.50, 0)$ until goal or lost
$\Rightarrow$ 58090 four-tuples

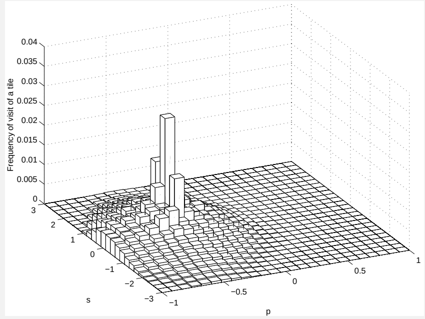
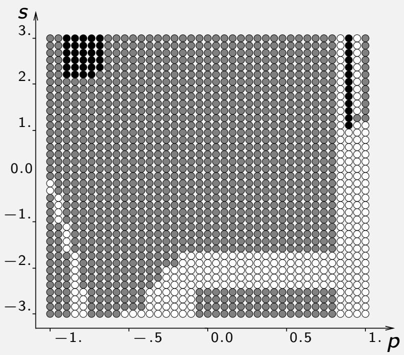


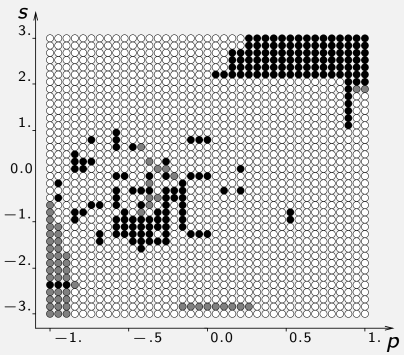
Figure: Distribution of four-tuples (coordinates of x_{t^i})

Illustration: sequence of $\hat{Q}_h$-functions

(on car on the hill problem)



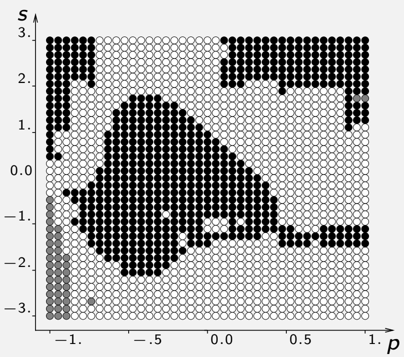
(a) $\arg\max_{u \in U} \hat{Q}_1(x, u)$



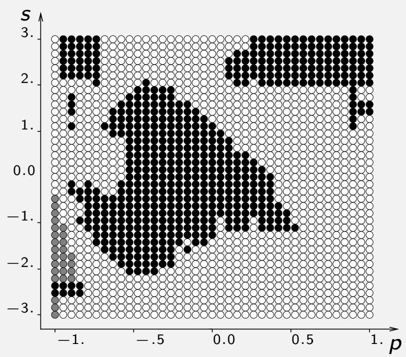
(b) $\arg\max_{u \in U} \hat{Q}_{10}(x, u)$

Illustration: sequence of $\hat{Q}_h$-functions

(on car on the hill problem)

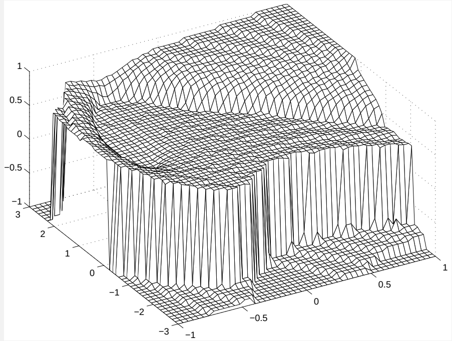


(c) $\arg\max_{u \in U} \hat{Q}_{20}(x, u)$

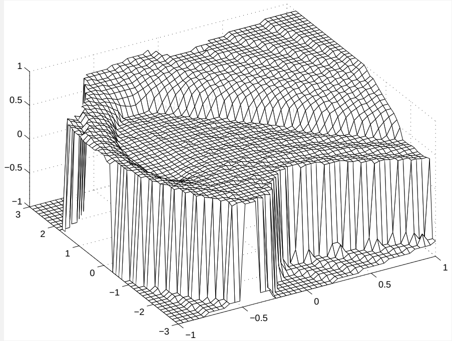


(d) $\arg\max_{u \in U} \hat{Q}_{50}(x, u)$

Illustration: true Q-function (on car on the hill problem)

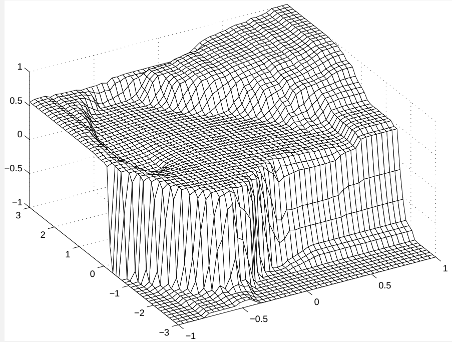


(a) $Q(., -4)$

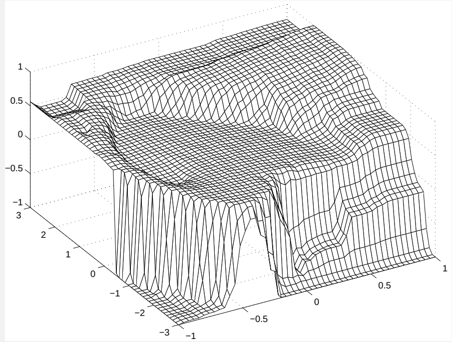


(b) $Q(., 4)$

Illustration: fitted $\hat{Q}_{50}$-function (on car on the hill problem)

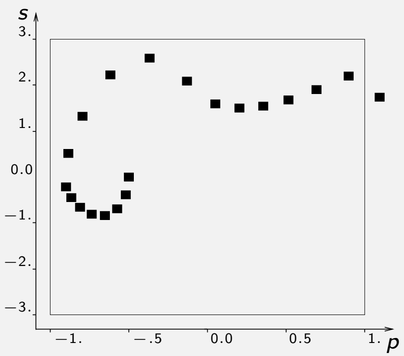


(c) $\hat{Q}_{50}(., -4)$



(d) $\hat{Q}_{50}(., 4)$

Illustration: an optimal trajectory (on car on the hill problem)



Electric power system stabilisation

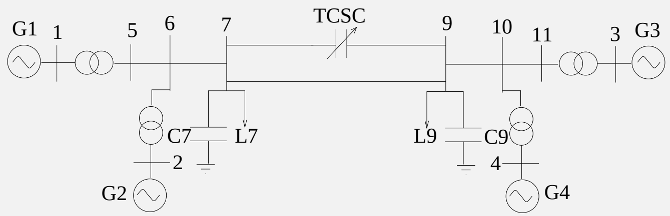


Figure: Four-machine test system

Use of simulator + fitted Q iteration (Extra-Trees),
5-dimensional $X \times U$ space; 1,1000,000 four-tuples.

Electric power system stabilisation

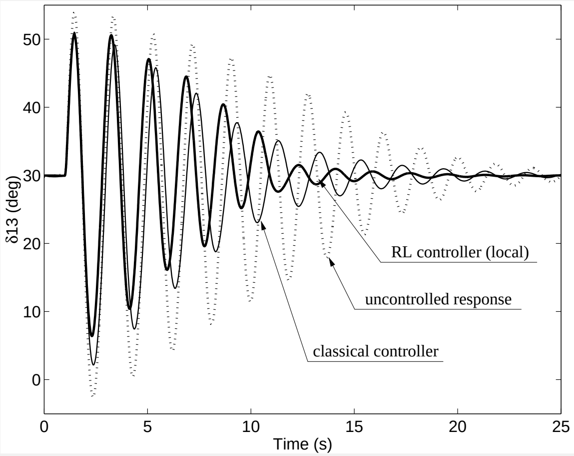


Figure: The system responses to 100 ms, self-clearing, short circuit

Electric power system stabilisation

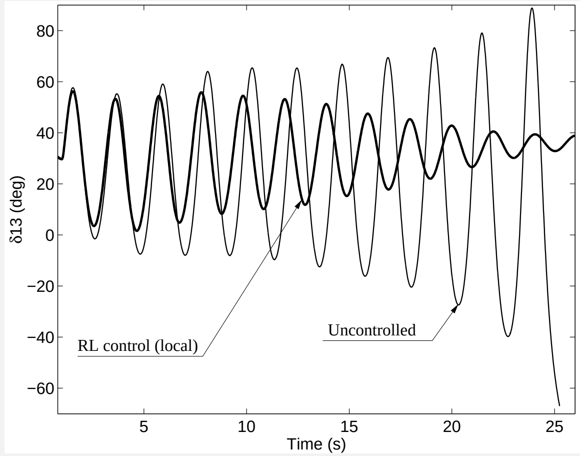


Figure: 100 ms short circuit cleared by opening line

Electric power system stabilisation

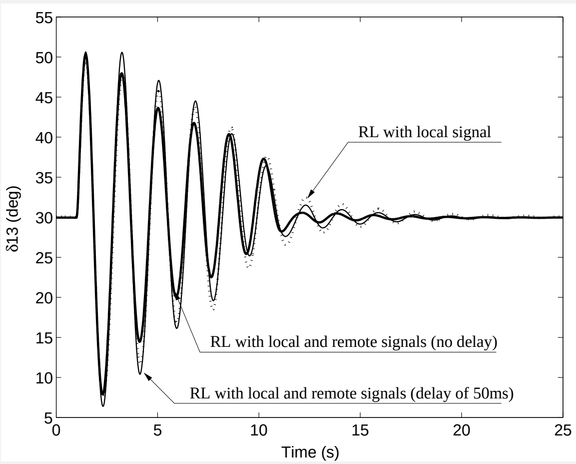


Figure: Local vs remote signals with/without communication delay

Generic pixel-based image classification

Idea: investigate whether it is possible to create a robust image classification algorithm by the sole use of supervised learning on the low-level pixel-based representation of the images.

Question: how to inject invariance in a generic way into a supervised learning algorithm ?

NB: work used mainly on Extra-Trees, but other supervised learners could also be used (e.g. SVMs, K*NN*...).

(Presentation based on [MGPW04, MGPW05])

Examples

- Hand written digit recognition *(0, 1, 2, ..., 9)*

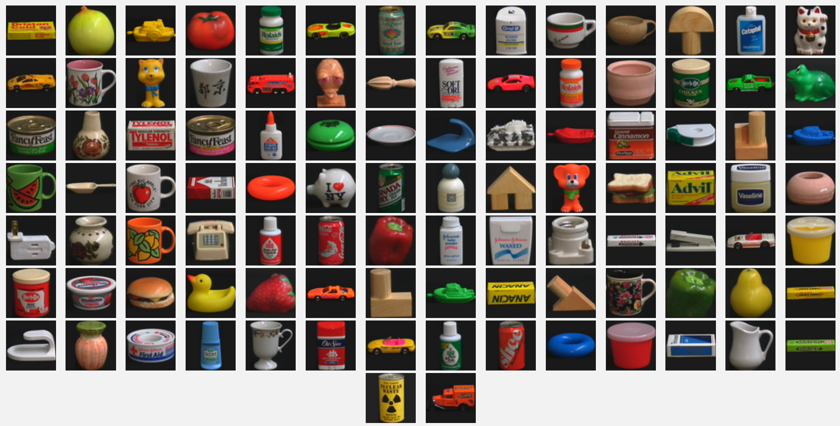
- Face classification *(Jim, Jane, John, ...)*

Examples

- Texture classification *(Metal, Bricks, Flowers, Seeds, ...)*

Examples

- Object recognition *(Cup X, Bottle Y, Fruit Z, ...)*

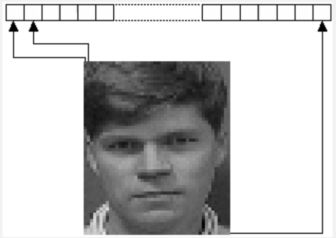


Principle of proposed solution (global)

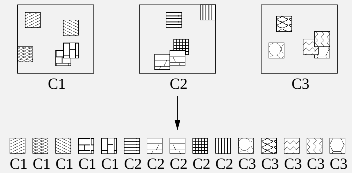
- Learning sample of N pre-classified images,

$$ls = \{(\mathbf{a}^i, c^i), i = 1, \ldots, N\}$$

$\mathbf{a}^i$: vector of pixel values of the entire image
c^i: image class



Principle of solution (local)

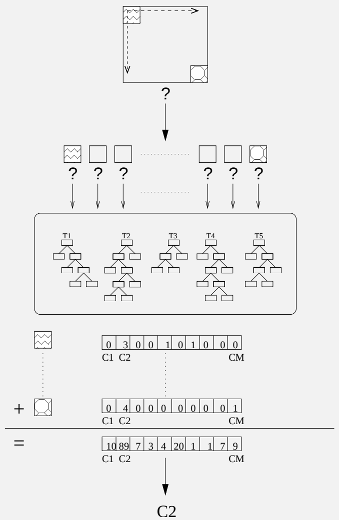


Learning sample of N_w sub-windows (size $w \times w$, pre-classified),

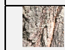
$$ls = \{(\mathbf{a}^i, c^i), i = 1, \ldots, N_w\}$$

$\mathbf{a}^i$: vector of pixel-values of the sub-window
c^i: class of mother image (from which the window was extracted)

Local approach: prediction



Datasets and protocols

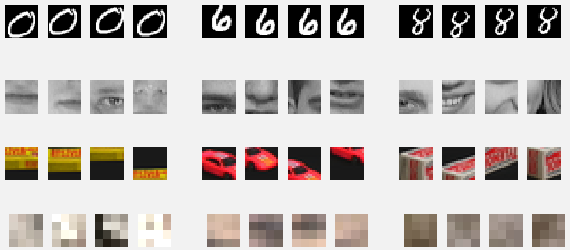
Datasets	# images	# base attributes	# classes	N_w	w
 MNIST	70000	784 ($28 * 28 * 1$)	10	300,000	24
 ORL	400	10304 ($92 * 112 * 1$)	40	120,000	20
 COIL-100	7200	3072 ($32 * 32 * 3$)	100	120,000	16
 OUTEX	864	49152 ($128 * 128 * 3$)	54	120,000	4

- MNIST: LS = 60000 images ; TS = 10000 images
- ORL: Stratified cross-validation: 10 random splits LS = 360; TS = 40
- COIL-100: LS = 1800 images ; TS = 5400 images (36 images per object)
- OUTEX: LS = 432 images (8 images per texture) ; TS = 432 images (8 images per texture)

A few results: accuracy

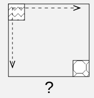
DBs	Extra-Trees	Extra-Trees with sub-windows	State-of-the-art
MNIST	3.26%	2.63%	0.5% [DKN04]
ORL	4.56% ± 1.43	1.66% ± 1.08	2% [Rav04]
COIL-100	1.96%	0.37%	0.1% [OM02]
OUTEX	65.05%	2.78%	0.2% [MPV02]

24 × 24:
20 × 20:
16 × 16:
4 × 4 :

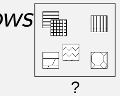


A few results: CPU times

- Learning stage: depends on parameters
  MNIST: 6h, ORL: 37s, COIL-100: 1h, OUTEX: 11m
- Prediction: depends on parameters and sub-window sampling
  - *Exhaustive (all sub-windows)*



    MNIST: 2msec, ORL: 354msec
    COIL-100: 14msec, OUTEX: 800msec
  - *Random subset of sub-windows*

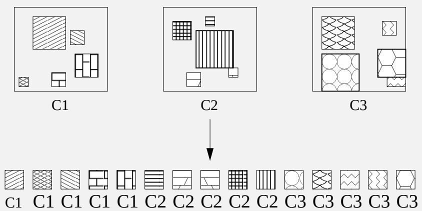


    MNIST: 1msec, ORL: 10msec
    COIL-100: 5msec, OUTEX: 33msec

Sub-windows of random size

(robustness w.r.t. scale)

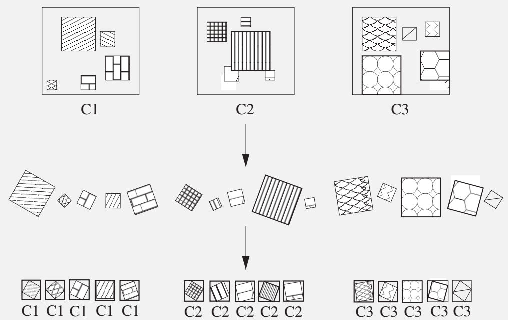
- Extraction of sub-windows of random size
- Rescaling to standard size



Sub-windows of random size and orientation

(more robustness)

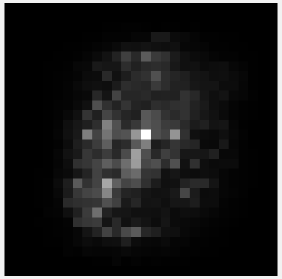
- Extraction of sub-windows of random size
- + Random rotation
- Rescaling to standard size

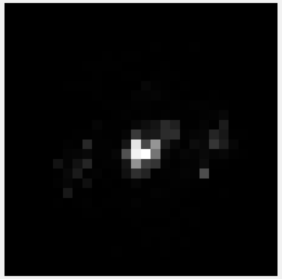


Attribute importance measures (global approach)

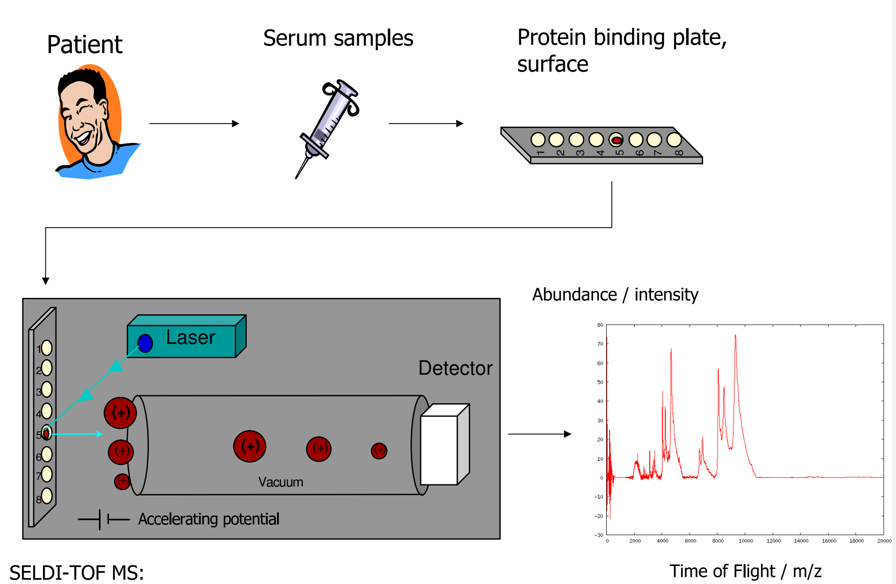
Compute information quantity (Shannon) brought by each pixel in each tree, and average over the trees.


ORL (faces)


MNIST (all digits)

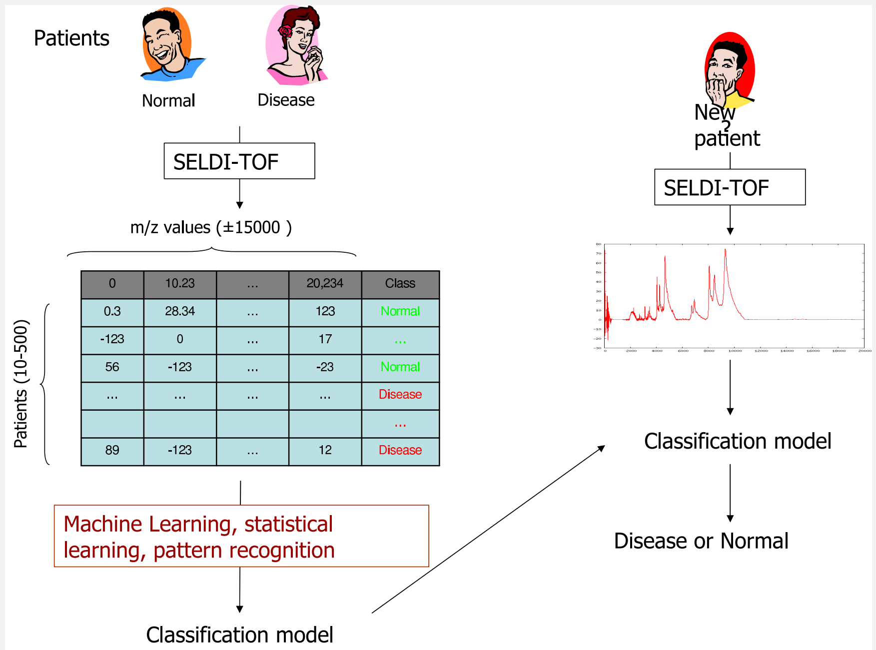

MNIST (0 vs 8)

Part II



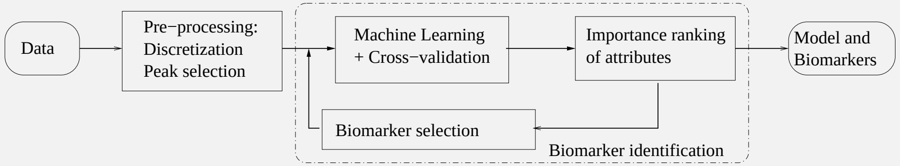
SELDI-TOF MS:

Surface Enhanced Laser Desorption/ Ionisation Time of Flight Mass Spectrometry



0	10.23	...	20,234	Class
0.3	28.34	...	123	Normal
-123	0	...	17	...
56	-123	...	-23	Normal
...	...	...	...	Disease
				...
89	-123	...	12	Disease

Supervised learning based methodology



(Presentation based on [GFd+04])

RA and IBD

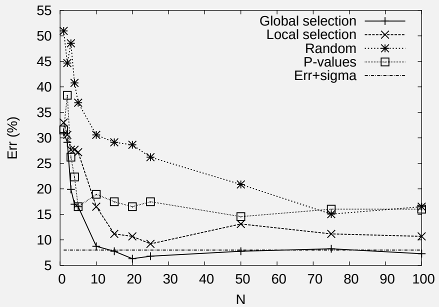
- RA Early diagnosis of Rhumatoid Arthritis
- IBD Better understanding of Inflammatory Bowel Diseases

Datasets collected at University Hospital of Liège.

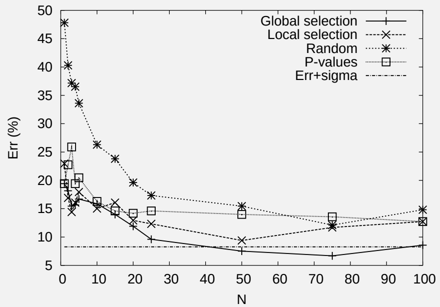
Patients			Number of attributes				
Dataset	#target	#others	Raw	$p = .3\%$	$p = .5\%$	$p = 1\%$	Peaks
RA	68	138	15445	1026	626	319	136
IBD	240	240	13799	1086	664	338	152

Toolbox: Single trees, Tree Bagging, Tree Boosting, Random Forests, Extra-Trees

Biomarker identification



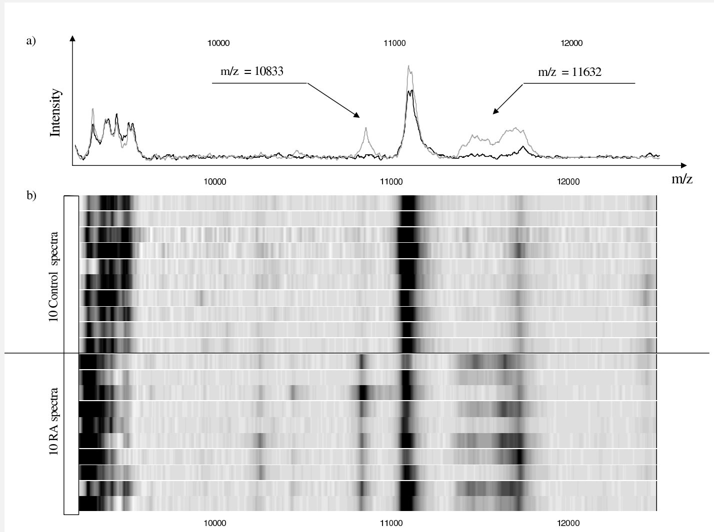
RA dataset



IBD dataset

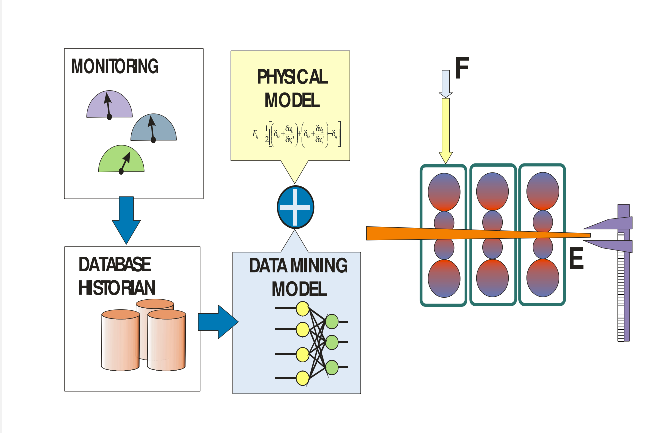
Figure: Variation of accuracy with number of biomarkers (Tree Boosting)

Graphical visualisation of biomarker identification (RA)



Steal-mill control

(ULg, PEPITe, ARCELOR)



- Development of a friction model, taking into account steel quality and temperature.
- Improve pre-setting of steel-mill controller
- Reduce waste

Wide area control of power systems

(ULg, PEPITe, Hydro-Québec)

- Improve generation shedding scheme of the Churchill-Falls power plant
- Reduce probability of blackout
- At the same time improve selectivity of control scheme
- New automaton in operation
- Application to other control schemes undergoing

Failure analysis of manufacturing process

(PEPITe, Valéo)

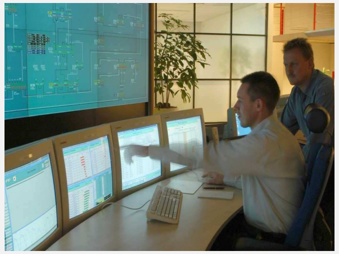
Problem

- Car reflector manufacturing line
- High, unexplained defect rate
- 40 process parameters (T,H, pH, flow...) measured every 5 minutes

Approach

- Two-month period data collection
- Database of 400,000 measurements
- Database analysis using PEPITo software
- Identification of the root cause
- Default rate reduced by 20%

SCADA system data mining (PEPITe, AREVA, TENNET)



Challenges faced by TENNET

- Minimise exchanges of reactive power
  - Formalise operators actions
  - Discover optimal network states
  - Optimise forecasting of industrial loads
- Decide of network upgrades effectively
  - Objective decision-making process for long-term planning
  - Validate state estimators

Goal of this project: show the value of Data Mining with respect to these challenges

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