Problems of interpolation, classification, and clustering are considered. In the tenets of Radon–Nikodym approach \( \langle f(x)\psi^2 \rangle / \langle \psi^2 \rangle \), where the \( \psi(x) \) is a linear function on input attributes, all the answers are obtained from a generalized eigenproblem \( |f|\psi^{[i]}\rangle = \lambda^{[i]} |\psi^{[i]}\rangle \). The solution to the interpolation problem is a regular Radon–Nikodym derivative. The solution to the classification problem requires prior and posterior probabilities that are obtained using the Lebesgue quadrature \[^1\] technique. Whereas in a Bayesian approach new observations change only outcome probabilities, in the Radon–Nikodym approach not only outcome probabilities but also the probability space \( |\psi^{[i]}\rangle \) change with new observations. This is a remarkable feature of the approach: both the probabilities and the probability space are constructed from the data. The Lebesgue quadrature technique can be also applied to the optimal clustering problem. The problem is solved by constructing a Gaussian quadrature on the Lebesgue measure. A distinguishing feature of the Radon–Nikodym approach is the knowledge of the invariant group: all the answers are invariant relatively any non–degenerated linear transform of input vector \( x \) components. A software product implementing the algorithms of interpolation, classification, and optimal clustering is available from the authors.
I. INTRODUCTION

In our previous work\[1\] the concept of Lebesgue Integral Quadrature was introduced and subsequently applied to the problem of joint probability estimation\[2\]. In this paper a different application of the Lebesgue Integral Quadrature is developed. Consider a problem where attributes vector $\mathbf{x}$ of $n$ components is mapped to a single outcome $f$ (class label in ML) for $l = [1..M]$ observations.

$$ (x_0, x_1, \ldots, x_k, \ldots, x_{n-1})^{(l)} \rightarrow f^{(l)} \quad \text{weight } \omega^{(l)} $$

The data of this format is commonly available in practice. There is a number of problems of interest, e.g.:

- For a continuous attribute $f$ build optimal $\lambda_f^{[m]}$, $m = 0 \ldots D - 1$ discretization levels, the discretization of continuous features problem.

- For a discrete $f$: construct a $f$–predictor for a given $\mathbf{x}$ input vector, statistical classification problem, that arise in ML, statistics, etc. For a continuous $f$: predict its value for a given $\mathbf{x}$.

- For a given $\mathbf{x}$ estimate support of the measure in $\psi$ problem, in the simplistic formulation it is: find the number of observations that are “close enough” to a given $\mathbf{x}$. Find the $\text{Coverage}(\mathbf{x})$. The Christoffel function is often used as a proxy for the coverage\[3–5\], however a genuine $\text{Coverage}(\mathbf{x})$ is a very important characteristics in ML.

- Cluster the $\psi$ dataset according to $f$ separability (allocate $D \leq n$ linear combinations $\psi_G^{[m]}(\mathbf{x}) = \sum_{k=0}^{n-1} \alpha_k^{[m]} x_k$, $m = 0 \ldots D - 1$, that optimally separate the $f$ in terms of $\langle f \psi^2 \rangle / \langle \psi^2 \rangle$). For a given $\mathbf{x}$ construct the probability distribution of $f$ to fall into the found $D$ clusters.

Currently used techniques typically construct a norm, loss function, penalty function, metric, distance function, etc. on $f$, then perform optimization minimizing the $f$–error according to the norm chosen, such as backpropagation. The simplest approach of this type is the linear regression, $L^2$ norm minimization:

$$ \langle [f(\mathbf{x}) - f_{LS}(\mathbf{x})]^2 \rangle \rightarrow \min $$

(2)
\[ f_{LS}(x) = \sum_{k=0}^{n-1} \beta_k x_k \]  

As we have shown in [6, 7] the major drawback of the approaches of this type is a difficulty to select a “good” norm, this is especially the case for non–Gaussian data with spikes [8, 9].

II. RADON–NIKODYM SPECTRAL APPROACH

The Lebesgue integral quadrature [11] is an extension of Radon–Nikodym concept of constructing a classifier of \[ \langle f \psi^2 \rangle / \langle \psi^2 \rangle \] form, where the \( \psi(x) \) is a linear function on input attributes, to build support weight as a quadratic function on \( x_k \). It allows to approach many ML problems in a completely new, norm–free way, this greatly increase practical applicability. The main idea is to convert (1), a sample of \( M \) observations, to a set of \( n \) eigenvalue/eigenvector pairs, subject to the generalized eigenvalue problem:

\[
\left| f \right| \psi[i] = \lambda[i] \left| \psi[i] \right|
\]

\[
\sum_{k=0}^{n-1} \langle x_j | f | x_k \rangle \alpha_k[i] = \lambda[i] \sum_{k=0}^{n-1} \langle x_j | x_k \rangle \alpha_k[i]
\]

\[
\psi[i](x) = \sum_{k=0}^{n-1} \alpha_k[i] x_k
\]

Here and below the \( \langle \cdot \rangle \) is \( M \) observations sample averaging, in the case of observation with equal weights \( \omega[l] = 1 \). This is a plain sum:

\[
\langle 1 \rangle = \sum_{l=1}^{M} \omega[l]
\]

\[
F_{jk} = \langle x_j | f | x_k \rangle = \sum_{l=1}^{M} x_j[l] f[l] x_k[l] \omega[l]
\]

\[
G_{jk} = \langle x_j | x_k \rangle = \sum_{l=1}^{M} x_j[l] x_k[l] \omega[l]
\]

Here and below we assume that Gram matrix \( G_{jk} \) is a non–singular. In case of a degenerated \( G_{jk} \), e.g. in case of data redundancy in (1), for example the situation when two input attributes are identical \( x_k = x_{k+1} \) for all \( l \), a regularization procedure is required. A regularization algorithm is presented in the Appendix A. Below we consider the matrix \( G_{jk} \) to be positively defined (a regularization is already applied).
Familiar $L^2$ least squares minimization (2) regression answer to (3) is a linear system solution:

$$f_{LS}(y) = \sum_{j,k=0}^{n-1} y_j G^{-1}_{jk} \langle f x_k \rangle$$  \hfill (8)

The Radon–Nikodym answer[7] is:

$$f_{RN}(y) = \frac{\sum_{j,k,l,m=0}^{n-1} y_j G^{-1}_{jk} F_{kl} G^{-1}_{lm} y_m}{\sum_{j,k=0}^{n-1} y_j G^{-1}_{jk} y_k}$$  \hfill (9)

$$1/K(y) = \sum_{j,k=0}^{n-1} y_j G^{-1}_{jk} y_k$$  \hfill (10)

Here $G^{-1}_{kj}$ is Gram matrix inverse, the $K(y)$ is a Christoffel–like function. In case $x_k = Q_k(x)$, where $x$ is a continuous attribute and $Q_k(x)$ is a polynomial of the degree $k$, the $G_{jk}$ and $F_{jk}$ matrices from (7) are the $\langle Q_j | Q_k \rangle$ and $\langle Q_j | f | Q_k \rangle$ matrices of Refs. [1, 7], and the Christoffel function is $1/K(y) = \sum_{j,k=0}^{n-1} Q_j(y) G^{-1}_{jk} Q_k(y)$. The (1) is a more general data form, the $x_k$ now can be of arbitrary origin, an important generalization of previously considered a polynomial function of a continuous attribute.

The (5) solution is $n$ pairs $(\lambda[i], \psi[i](x))$. For positively defined $G_{jk} = \langle x_j | x_k \rangle$ the solution exists and is unique. For normalized $\psi[i]$ we have:

$$\delta_{ij} = \langle \psi[i] \mid \psi[j] \rangle = \sum_{m,k=0}^{n-1} \alpha_{m}^{[i]} \langle x_m \mid x_k \rangle \alpha_{k}^{[j]}$$  \hfill (11a)

$$\lambda[i] \delta_{ij} = \langle \psi[i] \mid f \mid \psi[j] \rangle = \sum_{m,k=0}^{n-1} \alpha_{m}^{[i]} \langle x_m \mid f \mid x_k \rangle \alpha_{k}^{[j]}$$  \hfill (11b)

Familiar $L^2$ least squares minimization (2) regression answer and Radon–Nikodym answers can be written in $\psi[i]$ basis. The (12), (13), and (14) are the (8), (9), and (10) written in the $\psi[i]$ basis:

$$f_{LS}(y) = \sum_{i=0}^{n-1} \lambda[i] \langle \psi[i] \rangle \psi[i](y)$$  \hfill (12)

$$f_{RN}(y) = \frac{\sum_{i=0}^{n-1} \lambda[i] \left[ \psi[i](y) \right]^2}{\sum_{i=0}^{n-1} \left[ \psi[i](y) \right]^2}$$  \hfill (13)
\[
\frac{1}{K(y)} = \sum_{i=0}^{n-1} [\psi^i(y)]^2 \tag{14}
\]

The main result of [1] is a constriction of the Lebesgue integral quadrature:

\[
f^i = \lambda^i \tag{15a}
\]

\[
w^i = \langle \psi^i \rangle^2 \tag{15b}
\]

\[
\langle 1 \rangle = \sum_{i=0}^{n-1} w^i \tag{15c}
\]

\[
n = \sum_{i=0}^{n-1} \langle [\psi^i]^2 \rangle \tag{15d}
\]

The Gaussian quadrature groups sums by function argument; it can be viewed as a \(n\)-point discrete measure, producing the Riemann integral. The Lebesgue quadrature groups sums by function value; it can be viewed as a \(n\)-point discrete distribution with \(f^i\) support points (15a) and the weights \(w^i\) (15b), producing the Lebesgue integral. Obtained discrete distribution has the number of support points equals to the rank of \(\langle x_j \mid x_k \rangle\) matrix, for non-degenerated basis it is equal to the dimension \(n\) of vector \(x\). The Lebesgue quadrature is unique, hence the principal component spectral decomposition is also unique when written in the Lebesgue quadrature basis. Substituting (12) to (2) obtain PCA variation expansion:

\[
\langle [f(x) - f_{LS}(x)]^2 \rangle = \langle f^2 \rangle - \sum_{i=0}^{n-1} (f^i)^2 w^i = \langle (f - \bar{f})^2 \rangle - \sum_{i=0}^{n-1} (f^i - \bar{f})^2 w^i \tag{16}
\]

Here \(\bar{f} = \langle f \rangle / \langle 1 \rangle\). The difference between (16) and regular principal components is that the basis \(|\psi^i\rangle\) (5) of the Lebesgue quadrature is unique. This removes the major limitation of a principal components method: it’s dependence on the scale of \(x\) attributes. The (16) does not require scaling and normalizing of input \(x\), e.g. if \(x_k\) attribute is a temperature in Fahrenheit, when it is converted to Celsius or Kelvin — the (16) expansion will be identical. Due to (5) invariance the variation expansion (16) will be the same for arbitrary non-degenerated linear transform of \(x\) components: \(x_j' = \sum_{k=0}^{n-1} T_{jk} x_k\).

In the basis of the Lebesgue quadrature Radon–Nikodym derivative expression (13) is the eigenvalues weighted with (20) weights. Such a solution is natural for interpolation type of problem, however for a classification problem the different weights should be used.
A. Prior and Posterior Probabilities

Assume that in (13) for some $x$ only a single eigenfunction $\psi^{i}(x)$ is non-zero, then (13) gives the corresponding $f^{[i]}$ regardless the weigh $w^{[i]}$. This is the right approach to interpolation problem, where the $f$ is known to be a deterministic function on $x$, but when considering $f$ as a random variable, a more reasonable approach is to classify the outcomes according to overall weight. Assume no information on $x$ is available, what is the best answer for estimation the outcomes of $f$? The answer is given by the prior probabilities (17a) that correspond to unconditional distribution of $f$ according to (15b) weights.

Prior weight for $f^{[i]}$: $w^{[i]}$\hspace{2cm} \text{(17a)}

Posterior weight for $f^{[i]}$: $w^{[i]}\text{Proj}^{[i]}(x) = w^{[i]} \frac{[\psi^{i}(x)]^2}{\sum_{j=0}^{n-1} [\psi^{j}(x)]^2}$ \hspace{1cm} \text{(17b)}

The posterior distribution uses the same $[\psi^{i}(x)]^2$ probability as (13) adjusted to $f^{[i]}$ outcome prior weight $w^{[i]}$. The corresponding average

$$f_{RNW}(y) = \frac{\sum_{i=0}^{n-1} \lambda^{[i]} w^{[i]} \text{Proj}^{[i]}(y)}{\sum_{i=0}^{n-1} w^{[i]} \text{Proj}^{[i]}(y)} = \frac{\sum_{i=0}^{n-1} \lambda^{[i]} w^{[i]} [\psi^{i}(y)]^2}{\sum_{i=0}^{n-1} w^{[i]} [\psi^{i}(y)]^2}$$ \hspace{1cm} \text{(18)}

is similar to (13), but uses the posterior weights (17b). These examples demonstrate two distinctive cases of $f$ on $x$ inference:

- If $f$ is a deterministic function on $x$, such as in the interpolation problem, then the probabilities of $f$ outcomes are not important, the only important characteristic is: how large is $|\psi^{[i]}\rangle$ eigenvector at given $x$; the weight is the $i$–th eigenvector projection (20). The best interpolation answer is then (13) $f_{RN}(x)$: the eigenvalues $\lambda^{[i]}$ weighted with the projections $\text{Proj}^{[i]}(x)$ as the weights.

- If $f$ (or some $x_k$) is a random variable, then inference answer depends on the distribution of $f$. The classification answer should include not only what the outcome $\lambda^{[i]}$ corresponds to a given $x$, but also how often the outcome $\lambda^{[i]}$ occurs; this is determined by the $w^{[i]}$. The best answer is then (18) $f_{RNW}(x)$: the eigenvalues $\lambda^{[i]}$ weighted with the posterior
weights \( w^{[i]} \text{Proj}^{[i]}(x) \). An important characteristic is

\[
\text{Coverage}(x) = \sum_{i=0}^{n-1} w^{[i]} \text{Proj}^{[i]}(x)
\]

that is equals to Lebesgue quadrature weights \( w^{[i]} \) weighted with projections. For \( \text{(15)} \) the probability space is \( n \) vectors \( |\psi^{[i]}\rangle \) with the probabilities \( w^{[i]} \). The coverage is a characteristic of how often given \( x \) occurs in the observations (here we assume that total sample space is projected to \( |\psi^{[i]}\rangle \) states).

The \( f_{RNW} \) can be interpreted as a Bayes style of answer. An observation \( x \) changes the outcome probabilities from \( \text{(17a)} \) to \( \text{(17b)} \). Despite all the similarity there is a very important difference between Bayesian inference and Radon–Nikodym approach. In the Bayesian inference\([10]\) the probability space is fixed, new observations can adjust only the probabilities of pre–set states. In Radon–Nikodym approach, the probability space is the Lebesgue quadrature \( \text{(15)} \) states \( |\psi^{[i]}\rangle \), the solution to \( \text{(4)} \) eigenproblem. This problem is determined by two matrices \( \langle x_j \mid f \mid x_k \rangle \) and \( \langle x_j \mid x_k \rangle \), that depend on the observation sample themselves. The key difference is that new observations coming to \( \text{(1)} \) change not only outcome probabilities, but also the probability space \( |\psi^{[i]}\rangle \). This is a remarkable feature of the approach: both the probabilities and the probability space are constructed from the data. For probability space of the Lebesgue quadrature \( \text{(15)} \) this flexibility allows us to solve the problem of optimal clustering.

III. OPTIMAL CLUSTERING

Considered in previous section two inference answers \( \text{(13)} \) and \( \text{(18)} \) use vector \( x \) of \( n \) components as input attributes \( x_k \). In a typical ML setup the number of attributes can grow quite substantially, and for a large enough \( n \) the problem of data overfitting is starting to rise. This is especially the case for norm–minimization approaches such as \( \text{(12)} \), and is much less so for Radon–Nikodym type of answer \( \text{(13)} \), where the answer is a linear superposition of the observed \( f \) with positive weight \( \psi^2(x) \) (the least squares answer is also a superposition of the observed \( f \), but the weight is not always positive). However, for large enough \( n \) the overfitting problem also arises in \( f_{RN} \). The Lebesgue quadrature \( \text{(15)} \) builds \( n \) cluster centers,
for large enough \( n \) the (13) finds the closest cluster in terms of \( \mathbf{x} \) to \( \psi[i] \) distance,

\[
\text{Proj}[i](\mathbf{x}) = \frac{[\psi[i](\mathbf{x})]^2}{\sum_{j=0}^{n-1} [\psi[j](\mathbf{x})]^2}
\]

and then uses corresponding \( f[i] \) as the result. Such a special cluster always exists for large enough \( n \), with \( n \) increase the Lebesgue quadrature (15) separates the \( \mathbf{x} \) space on smaller and smaller clusters in terms of (20) distance as the square of wavefunction projection.

In practical applications a hierarchy of dimensions is required. The number of sample observations \( M \) is typically in a \( 1,000 - 100,000 \) range. The dimension \( n \) of the attributes vector \( \mathbf{x} \) is at least ten times lower than the \( M \), \( n \) is typically \( 5 - 100 \). The number of clusters \( D \), required to identify the data is several times lower than the \( n \), \( D \) is typically \( 2 - 10 \); the \( D \leq n \leq M \) hierarchy must be always held.

The Lebesgue quadrature (15) gives us \( n \) cluster centers, the number of input attributes. We need to construct \( D \leq n \) clusters out of them, that provide “the best” classification for a given \( D \). Even the attributes selection problem (select \( D \) “best” attributes out of \( n \) available \( x_k \)) is of combinatorial complexity [11], and can be solved only heuristically with a various degree of success. The problem to construct \( D \) attributes out of \( n \) is even more complex. The problem is typically reduced to some optimization problem, but the difficulty to chose a norm and computational complexity make it impractical.

In this paper an original approach is used. The reason for our success is the very specific form for the Lebesgue quadrature weights (15b) \( w[i] = (\psi[i])^2 \) that allows us to construct a Gaussian quadrature in \( f \)-space of the dimension \( D \), providing the best \( D \)-dimensional separation of \( f \), and then to convert the solution to \( \mathbf{x} \) space!

A Gaussian quadrature constructs a set of nodes \( f_G[m] \) and weights \( w_G[m] \) such that

\[
\langle g(f) \rangle \approx \sum_{m=0}^{D-1} g(f_G[m])w_G[m]
\]

is exact when \( g \) is a polynomial of a degree \( 2D - 1 \) or less. The Gaussian quadrature can be considered as the optimal approximation of the distribution of \( f \) by \( D \)-point discrete

\[1\] This corresponds to the projection \( \text{Proj}[i](\mathbf{y}) = \langle \psi_{\mathbf{y}} | \psi[i] \rangle^2 \), where \( \psi_{\mathbf{y}}(\mathbf{x}) = \frac{\sum_{\mathbf{x}_{\mathbf{y}}} \psi[i](\mathbf{y}) \psi[i](\mathbf{x})}{\sqrt{\sum_{\mathbf{y}} [\psi[i](\mathbf{y})]^2}} \)
measure. With the measure $\langle \cdot \rangle$ in the form of $M$ terms sample sum (7) no inference of $f$ on $x$ can be obtained, we can only estimate the distribution of $f$.

Now consider $D$–point Gaussian quadrature built on $n$ point discrete measure of the Lebesgue quadrature (15), $D \leq n$. Introduce the measure $\langle \cdot \rangle_L$

$$\langle g(f) \rangle_L = \sum_{i=0}^{n-1} g(f[i])w[i]$$  \hspace{1cm} (23)

$$\langle 1 \rangle_L = \langle 1 \rangle$$  \hspace{1cm} (24)

and build Gaussian quadrature (22) on the Lebesgue measure $\langle \cdot \rangle_L$. Select some polynomials $Q_k(f)$, providing sufficient numerical stability, the result is invariant with respect to basis choice, $Q_m(f) = f^m$ and $Q_m = T_m(f)$ give identical results, but numerical stability can be drastically different [12, 13]. Then construct two matrices $\mathcal{F}_{st}$ and $\mathcal{G}_{st}$ (in (25a) and (25b) the $f[i]$ and $w[i]$ are (15a) and (15b)), solve generalized eigenvalue problem (25c), the $D$ nodes are $f_G^m = \lambda_G^m$ eigenvalues, the weights $w_G^m$, $m = 0 \ldots D - 1$, are:

$$\mathcal{F}_{st} = \langle Q_s | f | Q_t \rangle_L = \sum_{i=0}^{n-1} Q_s(f[i])Q_t(f[i])f[i]w[i]$$  \hspace{1cm} (25a)

$$\mathcal{G}_{st} = \langle Q_s | Q_t \rangle_L = \sum_{i=0}^{n-1} Q_s(f[i])Q_t(f[i])w[i]$$  \hspace{1cm} (25b)

$$\left| \mathcal{F} \right| \psi_G^m \left\rangle_L = \lambda_G^m \left| \mathcal{G} \right| \psi_G^m \left\rangle_L$$  \hspace{1cm} (25c)

$$\sum_{t=0}^{D-1} \mathcal{F}_{st} \alpha_t^m = \lambda_G^m \sum_{t=0}^{D-1} \mathcal{G}_{st} \alpha_t^m$$  \hspace{1cm} (25d)

$$\psi_G^m(f) = \sum_{t=0}^{D-1} \alpha_t^m Q_t(f)$$  \hspace{1cm} (25e)

$$f_G^m = \lambda_G^m$$  \hspace{1cm} (25f)

$$w_G^m = \frac{1}{\left\langle \psi_G^m \right\rangle L \left( \lambda_G^m \right)^2}$$  \hspace{1cm} (25g)

$$\langle 1 \rangle_L = \langle 1 \rangle = \sum_{m=0}^{D-1} w_G^m = \sum_{i=0}^{n-1} w[i]$$  \hspace{1cm} (25h)

The eigenfunctions $\psi_G^m(f)$ are polynomials of $D - 1$ degree that are equal (within a constant)
to Lagrange interpolating polynomials $L^{[m]}(f)$

$$\begin{align*}
L^{[m]}(f) &= \frac{\psi^{[m]}_G(f)}{\psi^{[m]}_G(f_G^{[m]})} = \begin{cases} 
1 & \text{if } f = f_G^{[m]} \\
0 & \text{if } f = f_G^{[s]}; s \neq m
\end{cases}
\end{align*}$$

(26)

Obtained $D$ clusters in $f$–space are optimal in a sense they, as the Gaussian quadrature, optimally approximate the distribution of $f$ among all $D$–points discrete distributions. The greatest advantage of this approach is that attributes selection problem of combinatorial complexity is now reduced to the generalized eigenvalue problem (25d) of dimension $D$!

Obtained solution is more generic than typically used disjunctive conjunction or conjunctive disjunction forms[11] because it is invariant with respect to arbitrary non–degenerated linear transform of the input attribute components $x_k$.

The eigenfunctions $\psi^{[m]}_G(f)$ (25d) are obtained in $f$–space. Because the measure $\langle \cdot \rangle_L$ (23) was chosen with the Lebesgue quadratures weights $w^{[i]} = \langle \psi^{[i]} \rangle$, the $\psi^{[m]}_G(f)$ (25e) can be converted to $x$ basis, $m, s = 0 \ldots D - 1$:

$$\psi^{[m]}_G(x) = \sum_{i=0}^{n-1} \psi^{[m]}_G(f^{[i]}) \langle \psi^{[i]} \rangle \psi^{[i]}(x)$$

(27)

$$\delta_{ms} = \langle \psi^{[m]}_G(x) \mid \psi^{[s]}_G(x) \rangle$$

(28)

$$\chi^{[m]}_G \delta_{ms} = \langle \psi^{[m]}_G(x) \mid f \mid \psi^{[s]}_G(x) \rangle$$

(29)

$$w^{[m]}_G = \langle \psi^{[m]}_G(x) \rangle^2 = \langle \psi^{[m]}_G(f) \rangle^2_L$$

(30)

The $\psi^{[m]}_G(x)$ is a function on $x$, it is obtained from $\psi^{[m]}_G(f)$ basis conversion [27]. This became possible only because the Lebesgue quadratures weights $w^{[i]} = \langle \psi^{[i]} \rangle^2$ have been used to construct the $\psi^{[m]}_G(f)$ in (25c). The $\psi^{[m]}_G(x)$ satisfies the same orthogonality conditions (28) and (29) for the measure $\langle \cdot \rangle$, as the $\psi^{[m]}_G(f)$ for the measure $\langle \cdot \rangle_L$. Lebesgue quadrature weight for $\psi^{[m]}_G(x)$ is the same as Gaussian quadrature weight for $\psi^{[m]}_G(f)$, Eq. (30).

The (27) is the solution to clustering problem. This solution optimally separates $f$–space relatively $D$ linear combinations of $x_k$ to construct the separation weights $\psi^2(x)$ of $\langle f \psi^2 \rangle / \langle \psi^2 \rangle$ form (note, this is not a problem of selecting optimal attributes for interpolation by basis functions, such as (3)). In the Appendix A a regularization procedure was described, and the $1 + \dim S^d$ linear combinations of $x_k$ were constructed to have a non–degenerated

\footnote{The (27) defines $D$ clusters. If 1) $D = n$, 2) all Lebesgue quadrature nodes $f^{[i]}$ are distinct and 3) no weigh $w^{[i]}$ is equal to zero, then $\lambda^{[m]}_G = f^{[m]}$ and $\psi^{[m]}_G(x) = \psi^{[m]}(x)$.}
$G_{jk}$ matrix. No information on $f$ have been used for that regularization. In contrast, the functions (27) select $D \leq n$ linear combinations of $x_k$, that optimally partition the $f$–space. The partitioning is performed according to the distribution of $f$, the eigenvalue problem (25c) of the dimension $D$ has been solved to obtain the optimal clustering. Obtained $\psi_{G}^{[m]}(x)$ (they are linear combination of $x_k$) should be used as input attributes in the approach considered in the Section II above, the (13) is directly applicable. The sums now to contain $D$ terms, the number of clusters.

IV. SELECTION OF THE ANSWER: $f_{RN}$ VS. $f_{RNW}$

For a given input attributes vector we now have two answers: interpolation $f_{RN}$ (13) and classification $f_{RNW}$ (18). Both are the answers of Radon–Nikodym $\langle f \psi^2 \rangle / \langle \psi^2 \rangle$ form, that can be reduced to weighted eigenvalues with $\text{Proj}^{[i]}$ and $w^{[i]} \text{Proj}^{[i]}$ weights respectively.

The question arise which one to apply. For a deterministic function $f(x)$, the $\text{Proj}^{[i]}$ weights from (20) constructs the state in $|\psi^{[i]}\rangle$ basis that is the most close to a given observation $x$. The $f_{RN}$ is regular Radon–Nikodym derivative of the measures $fd\mu$ and $d\mu$, see Section II.C of [1]. This is a solution of interpolatory type, see Appendix C below for demonstration. For a probabilistic $f$ the $w^{[i]} \text{Proj}^{[i]}$ weights, that include the prior probability of $f$ outcomes, is preferable form of outcome probabilities estimation, see Appendix B2 below for demonstration. The $w^{[i]} \text{Proj}^{[i]}$ posterior weights typically produce a good classification even without optimal clustering algorithm of Section III.

V. A FIRST ORDER LOGIC ANSWER TO THE CLASSIFICATION PROBLEM.

PRODUCT ATTRIBUTES.

Obtained solutions to interpolation (13) and classification (17b) problems are more general than a propositional logic type of answer. A regular basis function expansion (3) is a local function of arguments, thus it can be considered as a “propositional logic” type of answer. Consider the formulas including a quantor operator, e.g. for a binary $x_k$ and $f$ in (1) the

3 One can also consider a “hierarchical” clustering similar to “hidden layers” of the neural networks. The simplest approach is to take $n$ input $x_k$ and cluster them to $D_1$, then cluster obtained result to $D_2$, then to $D_3$, etc., $n \leq D_1 \leq D_2 \leq D_3 \ldots$. Another option is to initially group the $x_k$ attributes (e.g. by temporal or spatial closeness), perform Section III optimal clustering for every group to some (possibly different for different groups) $D$, then use obtained $\psi_{G}^{[m]}(x)$ for all groups as input attributes for the “next layer”.
expressions like these:

\[
\begin{align*}
&\text{if } \exists x_k = 1 \text{ then } f = 1 \\
&\text{if } \forall x_k = 0 \text{ then } f = 1
\end{align*}
\]

Similar expressions can be written for continuous \(x_k\) and \(f\), the main difference from the propositional logic is that these expressions include a quantor–like operator that is a function of several \(x_k\) attributes. The \(\psi^2(x)\) expansion includes the products of \(x_j x_k\), thus the Radon–Nikodym representation can be viewed as a more general form than a propositional logic. The most straightforward approach to obtain a “true” [first order logic] answer from a propositional logic model is to add all possible \(Q_{k_0}(x_0)Q_{k_1}(x_1) \ldots Q_{k_{n-1}}(x_{n-1})\) products to the list of input attributes. For a large enough \(D\) [33] we obtain a model with properties that are very similar to the first order logic. The attributes \(x_k\) are now polynomials of \(n\) variables with multi–index \(k\) of degree \(D\); they are constructed from initial attributes \(x_k\) with regular index \(k\). Multi–index degree [33] is invariant relatively any linear transform of the attributes: \(x'_j = \sum_{k=0}^{n-1} T_{jk} x_k\). This is very important, because in the Radon–Nikodym approach all the answers are invariant relatively any non–degenerated linear transform of the basis, thus we can construct similar to the first order logic knowledge representation with known invariant group! The situation was different with the logical formulas of disjunctive conjunction or conjunctive disjunction, where a basis transform change a formula index [11], and the invariant group is either completely unknown or poorly understood; a typical solution in this situation is to introduce a “formula complexity” concept to limit the formulas to be considered, the mutli–index constraint [33] can be viewed as a complexity of the formulas allowed. The terms

\[
\begin{align*}
x_k &= x_0^{k_0} x_1^{k_1} \ldots x_{n-1}^{k_{n-1}} \\
k &= (k_0, k_1, \ldots, k_{n-1}) \\
D &= \sum_{j=0}^{n-1} k_j \\
N(n, D) &= C_n^D_{n+D-1}
\end{align*}
\]
are now identified by a multi-index $k$ and added to $\{1\}$ as attributes. We will call them the “product” attributes. The number $\mathcal{N}(n, D)$ of “product” attributes is the number of possible polynomial distinct terms with multi-index not higher than $D$, it can be estimated as $(34)$. A few exact values: $\mathcal{N}(n, 1) = n$, $\mathcal{N}(n, 2) = (n + 1)n/2$, $\mathcal{N}(7, 7) = 1716$, $\mathcal{N}(8, 7) = 3432$, etc.

In a typical ML setup such a transform to “product” attributes is not a good idea because of:

- A linear transform of input attributes produces a different solution.
- Attributes offset and normalizing difficulty.
- Data overfitting, as we now have a much bigger number of input attributes $\mathcal{N}(n, D)$. A complexity criteria of constructed attributes is typically introduced to limit the number of input attributes. For example, a neural network topology can be considered as a variant of a complexity criteria.

The approach developed in this paper has these difficulties solved. The invariant group is a non–degenerated linear transform $T_{jk}$ of input attributes components, what makes using the products $x_jx_k$ and $\sum_{j', k'=0}^{n-1} T_{j'k'}x_j x_{k'}$ as attributes to produce identical solutions; for the same reason the terms $(31)$ $Q_{k_0}(x_0)Q_{k_1}(x_1) \ldots Q_{k_{n-1}}(x_{n-1})$ are $Q_k$ invariant, e.g. $Q_k(x) = x^k$ and $Q_k(x) = T_k(x)$ produce identical solutions. The attributes offset and normalizing are not important since $(5)$ is invariant relatively any non–degenerated linear transform of $\mathbf{x}$ components. The problem of data overfitting is not an issue since Section III optimal clustering answer $(27)$ allows to reduce $\mathcal{N}(n, D)$ input attributes to a given number $D$ of their linear combinations that optimally separate the $f$. The only cost to pay is that the Lebesgue quadrature now requires a generalized eigenproblem of $\mathcal{N}(n, D)$ dimension to be solved, but this is purely a computational complexity issue. Critically important, that we are now limited not by the data overfitting, but by the computational complexity. Regardless the input attributes number the optimal clustering solution $(27)$ selects given number $D \ll \mathcal{N}(n, D)$ of input attributes linear combinations that optimally separate $f$ in terms of $\langle f \psi^2 \rangle / \langle \psi^2 \rangle$.

In the Appendix C a simple example of usage of polynomial function of a single attribute $x$ as input attributes was demonstrated $(C1)$. Similarly, a polynomial of several variables $(31)$

4 Note, that since the constant does always present in the original $x_k$ attributes $\{1\}$ linear combinations, the $x_jx_k$ (and high order) products always include the $x_k$ (lower order products), what may produce a degenerated basis. The degeneracy can be removed either manually or by applying any regularization algorithm, such as the one from Appendix A. Unlike polynomials in a single variable, multidimensional polynomials cannot, in general, be factored $[14, 15]$. 
identified by the multi–index (32) can be used to construct input attributes. An increase of attributes number from \(n\) to \(\mathcal{N}(n, \mathcal{D})\) using “product” attributes (31) combined with subsequent attributes number decrease to \(D\) by the clustering solution (27) is a path to ML answers of the first order logic type: \(n\) original attributes (1) → \(\mathcal{N}(n, \mathcal{D})\) “product” attributes (31) → \(D\) cluster attributes (27).

A. Lenna Image Interpolation Example. Multi–index Constraints Comparison.

In [16] a two–dimensional image interpolation problem was considered with multi–index \(j\) constraint

\[
(x, y)^{(l)} \rightarrow f^{(l)} \quad \text{weight } \omega^{(l)} = 1
\]

\[
j = (j_x, j_y)
\]

\[
0 \leq j_x \leq n_x - 1
\]

\[
0 \leq j_y \leq n_y - 1
\]

basis: \(x^{j_x}y^{j_y}\)

\[
dim(\text{basis}) = n_xn_y
\]

of each multi–index component being in the \([0 \ldots n_{\{x,y\}} - 1]\) range; total number of basis functions is then \(n_xn_y\) (39). This is different from the constraint (33), where the sum of all multi–index components is equal to \(\mathcal{D}\); total number of basis functions is then (43). Different basis functions produce different interpolation, let us compare the interpolation in these two bases. Transform \(d_x \times d_y\) image pixel coordinates \((x, y)\) \((x = 0 \ldots d_x - 1; y = 0 \ldots d_y - 1)\) and gray intensity \(f\) to the data of (1) form:

\[
(x, y, 1)^{(l)} \rightarrow f^{(l)} \quad \text{weight } \omega^{(l)} = 1
\]

\[
j = (j_x, j_y, j_c)
\]

\[
\mathcal{D} = j_x + j_y + j_c
\]

See numerical implementation of multi–index recursive processing in com/polytechnik/utils/AttributesProductsMultiIndexed.java. The invariant group of the Radon–Nikodym approach allows the “product” attributes (31) to be calculated in any basis. For example these two solutions are identical:

- Take original basis, perform basis regularization of Appendix A obtain “product” attributes (31) from \(X_k\), then solve (5) of \(\mathcal{N}(n, \mathcal{D})\) dimension. Obtain the Lebesgue quadrature (15).

- In the previous step, after \(X_k\) calculation, solve (5) of dimension \(n\) to find \(\psi[i][x]\) (6), obtain “product” attributes (31) from these \(\psi[i][x]\), then solve (5) of \(\mathcal{N}(n, \mathcal{D})\) dimension. Obtain (15).

See com/polytechnik/utils/TestDataReadObservationXVectorF.java: testAttributesProducts()
basis : $x^j y^j = x^j_y^j 1^j$  \quad \dim(\text{basis}) = \mathcal{N}(n, D) \quad (43)

Input attributes vector $x$ is of dimension $n = 3$: pixel coordinates and const, this way the “product” attributes with the constraint (42) include all $x^j y^j$ terms with lower than $D$ degree $j_x + j_y \leq D$. Observation index $l$ run from 1 to total number of pixels $M = d_x \times d_y$.

Let us compare $n = n_y = 50; \dim(\text{basis}) = n_n y = 2500$ of basis (39) with $n = 3; D = 69; \dim(\text{basis}) = \mathcal{N}(n, D) = 2485$ of basis (43). The value of $D = 69$ is selected to have approximately the same total number of basis functions. The bases are different: $x^{67} y^2$, $x^{66} y^2$, etc. are among “product” attributes (43), but they are not among the (39) where the maximal degree for $x$ and $y$ is 49; similarly the $x^{49} y^{49}$ is in (39), but it is not in (43). As in [16] we choose 512x512 Lenna grayscale image as a testbed. If you have scala installed run

```
scala com.polytechnik.algorithms.ExampleImageInterpolation \
file:dataexamples/lena512.bmp 50 50 chebyshev
```

to reproduce [16] results using (8) and (9) for least squares and Radon–Nikodym. Then run (note: this code is unoptimized and slow):

```
java com/polytechnik/algorithms/ExampleImageInterpolation2 \
file:dataexamples/lena512.bmp 50 50 69
```

To obtain 4 files. The files `lena512.bmp.LS.50.50.bs2500.png` and `lena512.bmp.RN.50.50.bs2500.png` are obtained as (12) and (13) using (39) basis with $n_x = n_y = 50$, the result is identical to [16]. The files `lena512.bmp.LS.D.69.bs2485.png` and `lena512.bmp.RN.D.69.bs2485.png` are obtained from (12) and (13) using (43) basis with $D = 69$. The images are presented in Fig. 1. It was shown [16] that the Radon–Nikodym interpolation produces a sfumato type of picture because it averages with always positive weight $\psi^2(x)$; the (13) preserves the bounds of $f$: if original gray intensity is $[0 : 1]$ bounded then interpolated gray intensity is $[0 : 1]$ bounded as well; this is an important difference from positive polynomials interpolation [17] where only a low bound (zero) is preserved. In contradistinction to Radon–Nikodym the least squares interpolation strongly oscillates near image edges and may not preserve the bounds of gray intensity $f$. In this section we compare not least squares vs. Radon–Nikodym as we did in [16] but the bases: (39) vs. (43) as they have a different multi–index constraint. We observe that:
FIG. 1. Top: original image. Middle: least squares in (39) basis (left) and (43) basis (right). Bottom: Radon–Nikodym in (39) basis (left) and (43) basis (right). The bases (39) and (43) are of 2500 elements ($n_x = n_y = 50$) and 2485 elements ($n = 3, D = 69$) respectively.

- The bases produce similar results. Basis differences in LS are more pronounced, than in RN; always positive weight makes the RN less sensitive to basis choice.

- In RN a small difference is observed near image edges. With (39) RN still has small oscillations near edges, and with (43) RN has oscillations completely suppressed.
• The multi-index constraint (39) is not invariant relatively a linear transform of input attributes, for example $x^{n_x-1}y^{n_y-1}$ relatively $x = x' - y'$, $y = x' + y'$, but the (43) is invariant.

This makes us to conclude that the specific multi-index constraint is not very important, the results are similar. Whereas in the interpolation problem an explosion of basis functions number increases interpolation precision, in the classification problem an explosion of basis functions number leads to data overfitting. The optimal clustering solution (27) reduces the number of basis functions to a given $D$ thus it solves the problem of data overfitting. This reduction makes the multi-index constraint used for initial basis construction even less important.

VI. CONCLUSION

In this work the support weight of Radon–Nikodym form $\psi^2(x)$, with $\psi(x)$ function to be a linear function on $x_k$ components, was considered and applied to interpolation, classification, and optimal clustering problems. The most remarkable feature of the Radon–Nikodym approach is that input attributes $x_k$ are used not for constructing the $f$, but for constructing the probability density (support weight) $\psi^2(x)$, that is then used for evaluation of $f = \langle f(x)\psi^2 \rangle / \langle \psi^2 \rangle$. This way we can avoid using a norm in $f$–space, thus greatly increase the applicability of the approach.

A distinguishing feature of the developed approach is the knowledge of the predictor’s invariant group. Given a dataset, what $x$ basis transform does not change the answer? Typically in ML (neural networks, decision tree, SVM, etc.) the answer is either completely unknown or poorly understood. The answer is known for linear regression (and a few other linear models), but linear regression has an unsatisfactory knowledge representation. The developed in this paper Radon–Nikodym approach has 1) known invariant group (non-degenerated linear transform of $x$ components) and 2) advanced knowledge representation in the form of matrix spectrum; even an answer of the first order logic type becomes feasible. The knowledge is extracted by applying projection operators, thus completely avoiding using a norm in the solution to interpolation (13), classification (18), and optimal clustering (27) problems.

The developed approach, while being very advanced in dealing with input attributes $x_k$,
always assumes that the output class label \( f \) is a one-dimensional scalar. When \( f \) is a vector, the most straightforward approach is to build an individual Radon–Nikodym model for every \( f \) component. However, the constructed Lebesgue quadratures \( [15] \) will now be different for every \( f \) component and obtained quadratures set cannot be viewed as a probability space. The situation is similar to the one of our previous works \([3, 18]\), where the distribution regression problem can be directly approached by the Radon–Nikodym technique, however the distribution to distribution regression problem is a much more difficult case. As a perspective direction of our future research we see an application of joint distribution analysis \([2]\) to the problems with \( f \) of vector type, for example to a distribution to distribution regression problem.

**Appendix A: Regularization Example**

The input vector \( \mathbf{x} = (x_0, x_1, \ldots, x_k, \ldots, x_{n-1})^{(l)} \) from \([1]\) often has a redundant data, often highly redundant. An example of a redundant data is the situation when two attribute components are equal e.g. \( x_k = x_{k+1} \) for all \( l \). In this case the \( G_{jk} = \langle x_j | x_k \rangle \) matrix becomes degenerated and the generalized eigenvalue problem \([5]\) cannot be solved directly, thus a regularization is required. A regularization process consists in selection of such \( x_k \) linear combinations that remove the redundancy, mathematically the problem is equivalent to finding the rank of a symmetric matrix.

All the theory of this paper is invariant with respect to any non-degenerated linear transform of \( \mathbf{x} \) components. For this reason we may consider the vector \( \tilde{\mathbf{x}} \) with equal to zero average, as this transform improves the numerical stability of \( \langle x_j | x_k \rangle \) calculation. Obtain \( \langle \tilde{x}_j | \tilde{x}_k \rangle \) matrix (it is just plain covariance matrix):

\[
\tilde{\mathbf{x}} = (x_0 - \bar{x}_0, x_1 - \bar{x}_1, \ldots, x_k - \bar{x}_k, \ldots, x_{n-1} - \bar{x}_{n-1})
\]

\[\bar{x}_k = \frac{\langle x_k \rangle}{\langle 1 \rangle}\]  

\[\tilde{G}_{jk} = \langle \tilde{x}_j | \tilde{x}_k \rangle\]

\[\sigma_k = \sqrt{\frac{\tilde{G}_{kk}}{\langle 1 \rangle}}\]

For each \( k = 0 \ldots n - 1 \) consider the standard deviation \( \sigma_k \) of \( x_k \), select the set \( S \) of indexes \( k \), that have the standard deviation greater that a given \( \varepsilon \), determined by the computer’s
numerical precision. Then construct the matrix \( \tilde{G}_{jk} \) with the indexes in the set obtained: \( j, k \in S \). The new matrix \( \tilde{G}_{jk} \) is obtained by removing \( x_k \) components that are equal to a constant, but it still can be degenerated.

We need to regularize the problem by removing the redundancy. The criteria is like a condition number in the linear system problem, but because we deploy generalized eigenproblem anyway, we can do it straightforward. Consider generalized eigenproblem (A7) with the right hand side matrix equals to the diagonal components of \( \tilde{G}_{jk} \).

\[
\begin{align*}
  j, k & \in S \\
  \tilde{G}^d_{jk} & = \delta_{jk} \tilde{G}_{kk} \\
  \sum_{k \in S} \tilde{G}_{jk} \alpha_k^{[i]} & = \lambda^{[i]} \sum_{k \in S} \tilde{G}^d_{jk} \alpha_k^{[i]} \\
  S^d & : a \text{ set of } i, \text{ such that: } \lambda^{[i]} > \varepsilon \\
  X_{S^d} & = \sum_{k \in S} \alpha_k^{[S^d]} (x_k - \bar{x}_k)
\end{align*}
\]

By construction of the \( S \) set the right hand side diagonal matrix \( \tilde{G}^d_{jk} \) has only positive terms, that are not small, hence the (A7) has a unique solution. The eigenvalues \( \lambda^{[i]} \) of the problem (A7) have the meaning of a “normalized standard deviation”. Select (A8) set: the indexes \( i \), such that \( \lambda^{[i]} > \varepsilon \), determined by the computer’s numerical precision. Obtained \( S^d \) set determines regularized basis (A9). The matrix \( \langle X_i \mid X_m \rangle \) with \( i, m \in S^d \) is non–degenerated. After the constant component \( X = 1 \) is added to the basis (A9) the \( X = (\ldots X_i, \ldots, 1) \) can be used in (1) instead of the \( \mathbf{x} = (\ldots x_k \ldots) \). Alternatively to (A8) a regularization can be performed without solving the eigenproblem (A7), in a manner similar to Gaussian elimination with pivoting in a linear system problem, but these are the details.

Note, that for non–degenerated input data in the basis \( x_k \) the output basis \( X_i \) has the same number of components, and the inference results will be identical for these two bases. It is important to stress that

- No any information on \( f \) have been uses in the regularization of \( G_{jk} = \langle x_j \mid x_k \rangle \).

- All “standard deviation“ type of thresholds were compared with a given \( \varepsilon \), determined by the computer’s numerical precision. No “standard deviation“ is used in solving the problem itself.
The result of this appendix is a new basis $\mathbf{X} = (\ldots X_i \ldots, 1)$ of $1 + \dim S^d$ elements (A9) and const, that can be used in (1). This basis provides a non-degenerated Gram matrix $\langle X_i | X_m \rangle$ (7c).

Appendix B: RN Software Usage Description

The provided software is java written. The source code files of interest are com/polytech
nik/utils/{RN, RadonNikodymSpectralModel, DataReadObservationXVectorF, AttributesProductsMultiIndexed}.java. The class DataReadObservationXVectorF reads input data (1) from a comma-separated file and stores the observations. The method getDataRegularized() of it performs Appendix A data regularization and returns an object of DataReadObservationXVectorF.DataRegularized type that contains the matrices $\langle X_j | X_k \rangle$ and $\langle X_j | f | X_k \rangle$ (in the regularized basis $X_k$). The method getRadonNikodymSpectralModel() of this object creates Radon–Nikodym spectral model of Section II, it returns an object of RadonNikodymSpectralModel class. The method getRNatXoriginal(double [] xorig) of this object evaluates an observation at a point xorig in the original basis (1) and returns an object of RadonNikodymSpectralModel.RNPointEvaluation type; this object has the methods getRN(), getRNW(), and getPsikAtX() that, for the xorig given, calculate the (13), (18), and $\psi[i](xorig)$ components. An object of RadonNikodymSpectralModel type has a method reduceBasisSize(int D) that performs optimal clustering of Section III and returns RadonNikodymSpectralModel object with the basis, chosen as the optimal dimension D clustering f.

The com/polytechnik/utils/RN.java is a driver to be called from a command line. The driver’s arguments are:

- --data_file_to_build_model_from= The input file name to read (1) data and build Radon–Nikodym model from it. The file is comma-separated, if the first line starts with the |# — it considered to be the column’s headers. Empty lines and the lines starting with the | are considered as comments. All non-comment lines must have identical number of columns.

- --data_file_evaluation= The input files (multiple files possible) to evaluate the model built. The same format.
• **--data_cols**= The description of the input files data columns. The format is **--data_cols=numcols:xstart,xend:f:w**, where *numcols* is the number of columns in the input file, *xstart*, *xend* are the columns to be used for $x_k$, e.g. the columns $(x_{\text{start}}, x_{\text{start}+1}, \ldots, x_{\text{xend}-1}, x_{\text{xend}})$ are used as the $(x_0, x_1, \ldots, x_k, \ldots, x_{n-1})$ in (1) input. The *f* and *w* are the columns for $f$ and the weight $\omega$, if weight column index *w* is set to negative, then all weights $\omega$ are set to 1. Column identifiers are integers, base 0 column index. For example input file dataexamples/runge_function.csv of Appendix [C](#) has 9 columns, the $x_k$ are in the first 7 columns, then $f$ and $\omega$ columns follow, this corresponds to **--data_cols=9:0,6:7:8**

• **--clusters_number**= The value of $D$. If presents Section [III](#) optimal clustering is performed with this $D$ and the output is of this dimension. Otherwise all $n$ input components are used to construct the $\psi[i](x)$ from (6) and the dimension of the output is the rank of $\langle x_j \mid x_k \rangle$ matrix.

• **--max_multiindex**= The value of $D$. If presents then $\mathcal{N}(n,D)$ “product” attributes $X_{0}^{k_{0}}X_{1}^{k_{1}}\ldots X_{n-1}^{k_{n-1}}$ are constructed (31) in regularized basis (using recursive algorithm) with the multi-index $k$ lower or equal than the $D$, these “product” attributes are then used instead of $n$ original attributes $x_k$, see Section [V](#) above. For a large enough $D$ the problem may become numerically unstable. For $\mathcal{N}(n,D) \geq 500$ used eigenvalue routines may be very slow[6](#). The option is intended to be deployed together with **--clusters_number**= with the goal to obtain a model of the first order logic type.

• **--flag_print_internal_psik**= By default is true. Set **--flag_print_internal_psik=false** to suppress the output of $\psi[i](x)$ components.

• **--output_files_prefix**= If set all output files will be prefixed by this string. A typical usage is to save output to some other directory, such as **--output_files_prefix=/tmp**.

The program reads the data, builds Radon–Nikodym model from **--data_file_to_build_model_from** then evaluates it on itself and on all **--data_file_evaluation**= files. The output file has the same filename with the .RN.csv extension added. In comment section it

[6](#) For eigenproblem routines one can use [JNI](#) interface [com/polytechnik/lapack/Eigenvalues_JNI_lapacke.java](#) to LAPACK instead of java code, see [com/polytechnik/utils/EVSolver.java](#) for selection.
prints data statistics (filename, observations number, and the Lebesgue quadrature (15)). Each row corresponds to input file row. Calculated data is added to the same row. Data description is presented in the columns header. The first \( n + 2 \) columns are: the \( x_k \) (original input attributes), the observation \( f \), and the observation weight \( \omega \). Then the columns follow: \( f_{\text{RN}} \) (13), Christoffel (14), \( f_{\text{RNW}} \) (18) Coverage (19), and, unless the \(--\text{flag\_print\_internal\_psik}=false\), the \( \psi^i[x] \) (6) \( D \) components. Here the \( D \) is either the rank of \( \langle x_j \mid x_k \rangle \) matrix, or the parameter \(--\text{clusters\_number}=\) if it is specified. For all output files the following relations hold for the columns:

\[
f_{\text{RN}}^{(l)} = \frac{\sum_{i=0}^{D-1} f[i] \left[ \psi^i(x(l)) \right]^2}{\sum_{i=0}^{D-1} \left[ \psi^i(x(l)) \right]^2}
\]

(B1)

\[
\text{Christoffel}^{(l)} = \frac{1}{\sum_{i=0}^{D-1} \left[ \psi^i(x(l)) \right]^2}
\]

(B2)

\[
f_{\text{RNW}}^{(l)} = \frac{\sum_{i=0}^{D-1} f[i] w[i] \left[ \psi^i(x(l)) \right]^2}{\sum_{i=0}^{D-1} w[i] \left[ \psi^i(x(l)) \right]^2}
\]

(B3)

\[
\text{Coverage}^{(l)} = \frac{\sum_{i=0}^{D-1} w[i] \left[ \psi^i(x(l)) \right]^2}{\sum_{i=0}^{D-1} \left[ \psi^i(x(l)) \right]^2}
\]

(B4)

For the file the model is built from a few additional relations hold \((i, m = 0 \ldots D - 1)\):

\[
w^{[m]} = \left[ \sum_{l=1}^{M} \psi^m(x(l)) \omega^{(l)} \right]^2
\]

(B5)

\[
f^{[m]} \delta_{im} = \sum_{l=1}^{M} \psi^i(x(l)) \psi^m(x(l)) f^{(l)} \omega^{(l)}
\]

(B6)

\[
\delta_{im} = \sum_{l=1}^{M} \psi^i(x(l)) \psi^m(x(l)) \omega^{(l)}
\]

(B7)

Obtained \( D \) states \( \psi^m(x) \) (for \( D < \text{rank of } \langle x_j \mid x_k \rangle \) these are the \( \psi^m_G(x) \) from (27), \( w^{[m]} = w^{[m]}_G \) from (30), and \( f^{[m]} = \lambda^{[m]}_G \)) provide the optimal clustering of \( f \) among all \( D \)-point discrete measures.
1. Software Installation And Testing

- Install java 1.8 or later.

- Download the source code `code_polynomials_quadratures.zip` from [19].

- Decompress and recompile the program. Run a setf test.

  ```
  unzip code_polynomials_quadratures.zip
  javac -g com/polytechnik/*/*java
  java com/polytechnik/utils/TestDataReadObservationXVectorF
  ```

- Run the program with bundled deterministic data file (Runge function [C2]).

  ```
  java com/polytechnik/utils/RN --data_cols=9:0,6:7:8 \
  --data_file_to_build_model_from=dataexamples/runge_function.csv \
  --data_file_evaluation=dataexamples/runge_function.csv
  ```

  Here, for usage demonstration, we evaluate the model twice. The file `runge_function.csv.RN.csv` will be created (the same file is written twice, because the built model is then test–evaluated on the same input `dataexamples/runge_function.csv`). See Appendix [C] below for interpolation results obtained from the output.

- Run the program with the constructed $\psi^i(x^{(l)})$ as input. They are in the columns with the index 13 to 19 of the file `runge_function.csv.RN.csv` (20 columns total).

  ```
  java com/polytechnik/utils/RN --data_cols=20:13,19:7:8 \
  --data_file_to_build_model_from=runge_function.csv.RN.csv
  ```

  The file `runge_function.csv.RN.csv.RN.csv` will be created. Because the input $x_k$ are now selected as $\psi^k(x)$, with this input, the Radon–Nikodym approach of Section [II] produce exactly the input $x_k$ as the result $\psi^k(x)$, possibly with $\pm 1$ factor. There are 7 nodes/weights of the Lebesgue quadrature [15] for input data file `dataexamples`
Some of the Lebesgue weights are 0. This may happen with \((15b)\) definition. The weights sum is equal to total measure, for \((C3)\) it is equal to 2.

- The dimension of the Lebesgue quadrature is \(n\), it is the number of input attributes \(x_k\).
  When we start to increase the \(n\), the Lebesgue quadrature starts to partition the \(x\) space on smaller and smaller elements. The \((I3)\) type of answer will eventually start to exhibit data overfitting effect. Radon–Nikodym is much less prone to it than a direct expansion of \(f\) in \(x_k\), a \((3)\) type of answers, but for a large enough \(n\) even the \(\langle f\psi^2 \rangle / \langle \psi^2 \rangle\) type of answer is starting to overfit the data. We need to select \(D \leq n\) linear combinations of \(x_k\) that optimally separate the \(f\). Optimal clustering is described in Section III. Run the program

```
java com/polytechnik/utils/RN --data_cols=9:0,6:7:8 \\
 --data_file_to_build_model_from=dataexamples/runge_function.csv \\
 --clusters_number=4
```

Running with \(--clusters_number\) equals to 5, 6, or 7 may fail to construct a Gaussian quadrature \((25c)\) as the number of the measure \((23)\) support points should be greater or equal than the dimension of Gaussian quadrature built on this measure. For \(--clusters_number=4\) the obtained quadrature gives exactly the \((B8)\) nodes with zero weights removed: an optimal approximation of the measure with four support points
by four points discrete measure is the measure itself.

\[ f[0] = 0.04229340238324669 \quad w[0] = 0.2453611587651926 \]
\[ f[1] = 0.06535351052064764 \quad w[1] = 0.5222926033797383 \]
\[ f[2] = 0.1646927391304583 \quad w[2] = 0.671034340007315 \]
\[ f[3] = 0.702523874736917 \quad w[3] = 0.5613118978475647 \] (B9)

A more interesting case is to set --clusters_number=3

```
java com/polytechnik/utils/RN --data_cols=9:0,6:7:8 \
   --data_file_to_build_model_from=dataexamples/runge_function.csv \
   --clusters_number=3
```

\[ f[0] = 0.0553329558917538 \quad w[0] = 0.7374543901309345 \]
\[ f[1] = 0.1628540299041175 \quad w[1] = 0.7011836153811847 \] (B10)
\[ f[2] = 0.702513758981318 \quad w[2] = 0.5613619944876921 \]

The (B10) is the optimal approximation of the measure (B8) with 4 support points by a 3–point discrete distribution. This is typical application of a Gaussian quadrature; the \( n \)–point Gaussian quadrature requires \( 0 \ldots 2n – 1 \) distribution moments for calculation, the measure must have at least \( n \) support points. The distribution moments of \( f \) can be obtained using different measures, for example using the sample sum (7) directly.

A remarkable feature of the Lebesgue integral measure (23) is that the obtained eigenvectors (25e) can be converted from \( f \) to \( x \) space. The conversion formula is (27).

The \( \psi^m_G(x) \), \( m = 0 \ldots D – 1 \) create the weights, that optimally separate \( f \) in terms of \( \langle f\psi^2 \rangle / \langle \psi^2 \rangle \) separation. This is a typical setup of the technique we developed:

- For a large number \( n \) of input attributes create the Lebesgue integral quadrature (15).
- Select the number of clusters \( D \leq n \). Using Lebesgue measure (23) build Gaussian quadrature (25) in \( f \) space. It provides the optimal clustering of the dimension \( D \).
- Convert obtained results from \( f \) to \( x \) space using (27), obtain the \( \psi^m_G(x) \) classifiers.
- One can also entertain a first order logic –like model using the attributes of Section V.
• The three function $\psi^m_G(x)$, corresponding to (B10) nodes, are presented in Fig. 2. The $\text{Proj}^i(x)$ (this is squared and normalized $\psi^m_G(x)$ as (20)). One can clearly see that the states $\psi^m_G(x)$ are localized exactly near the $f^m$ nodes (B10). This technique is a much more powerful one, than, say, support–vector machine linear separation. In Radon–Nikodym approach the separation weights are the $\left[\psi^m_G(x)\right]^2$ that are obtained without an introduction of a norm with subsequent minimization the difference between the result and a prediction with respect to the norm. The separation by the functions $\psi^m_G(x)$ is optimal among all $D$– dimensional separations of $[\psi(x)]^2$ type. The cost is that the solution is now two–step[3]. On the first step the Lebesgue quadrature is built and the measure (23) is obtained. On the second step the Gaussian quadrature (25) is built on this measure; the result is then converted to $x$ space (27). The $\left[\psi^m_G(x)\right]^2$ are the optimal separation weights.
2. Nominal Attributes Example

In ML applications the attributes can be nominal. They may be of orderable (low, medium, high) or unorderable (apple, orange, tomato) type. A nominal attribute taking two values can be converted to \{0, 1\} binary attribute. Orderable attributes (low, medium, high) can be converted to \{1, 2, 3\}, or, say, \{1, 2, 10\} this depends on the problem. For unorderable attributes the conversion is more difficult, however in some situations it is straightforward: a “country” attribute taking the value: “country name from a list of eight countries”, can be converted to three binary attributes.

The \( f \), predicted by a ML system, is called a class label. It is often a binary attribute. This leads to the nodes of the Lebesgue quadrature to be grouped near two values of the class label. We have tested a number of datasets from [UC Irvine Machine Learning Repository](http://archive.ics.uci.edu/ml) and other sources. For direct comparison with the existing software such as [C5.0](http://ida.ics.uci.edu/research/air/SOFTWARE/c5.html) or [Weka 3: Machine Learning Software in Java](http://www.cs.waikato.ac.nz/ml/weka/) a care should be taken of nominal attributes conversion and class label representation. We are going to discuss the details in a separate publication, here we present only qualitative aspects of Radon–Nikodym application to ML problem with the binary class label. Take [breast-cancer-wisconsin](http://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+Data+Set) database, the breast-cancer-wisconsin.data dataset is of 699 records, we removed 16 records with unknown (“?”) attributes and split the dataset as 500:183 for training:testing. Obtained files are

\[
\begin{array}{lll}
\text{wc breast-cancer-wisconsin_S.names} \ \\
\text{breast-cancer-wisconsin_S.data} \ \\
\text{breast-cancer-wisconsin_S.test}
\end{array}
\]

\[
\begin{array}{lll}
139 & 938 & 6234 \text{ breast-cancer-wisconsin_S.names} \\
500 & 500 & 14266 \text{ breast-cancer-wisconsin_S.data} \\
183 & 183 & 5182 \text{ breast-cancer-wisconsin_S.test} \\
822 & 1621 & 25682 \text{ total}
\end{array}
\]

This data has nominal class label 2:Benign, 4:Malignant. The [C5.0](http://ida.ics.uci.edu/research/air/SOFTWARE/c5.html), when run on this dataset produces a very good classifier:

\[
c5.0 \text{-f mldata/breast-cancer-wisconsin_S}
\]

Evaluation on training data (500 cases):
(a) (b) <-classified as
---- ----
293 10  (a): class 2
3 194  (b): class 4

Evaluation on test data (183 cases):
(a) (b) <-classified as
---- ----
139 2  (a): class 2
4 38  (b): class 4

Now let us run the RN program to obtain the Lebesgue quadrature

```
java com/polytechnik/utils/RN --data_cols=11:1,9:10:-1 \
    --data_file_to_build_model_from=mldata/breast-cancer-wisconsin_S.data \
    --data_file_evaluation=mldata/breast-cancer-wisconsin_S.test
```

The number of the nodes is 10, it is equal to the number of input attributes $x_k$.

\[
\begin{align*}
    f^0 &= 2.090917684500027 & w^0 &= 308.30166232236996 \\
    f^1 &= 3.198032991602546 & w^1 &= 5.307371268658678 \\
    f^2 &= 3.344418191526764 & w^2 &= 0.0189894231470068 \\
    f^3 &= 3.5619620739712725 & w^3 &= 0.3341989402039986 \\
    f^4 &= 3.6221628167395497 & w^4 &= 0.254958854552573 \\
    f^5 &= 3.7509806530824346 & w^5 &= 1.2339290581894928 \\
    f^6 &= 3.7939096228600513 & w^6 &= 5.146789024450902 \\
    f^7 &= 3.8081118648848045 & w^7 &= 0.16082536035874645 \\
    f^8 &= 3.8799894340830727 & w^8 &= 50.25004460556501 \\
    f^9 &= 3.9574710127612613 & w^9 &= 128.99123411160124
\end{align*}
\]  

(B11)

Then we calculate a joint distribution of realization/prediction for $f_{RN}$ and $f_{RNW}$. The continuous to nominal conversion for $f_{RN}$ and $f_{RNW}$ was performed by comparing predicted value with the average. Evaluation without clustering on training data (B12) (500 cases), and on test data (B13) (183 cases) is:

\[
\begin{align*}
    \text{Distribution}(f_{RN}) : & \quad 183 \quad 120 \\
    & \quad 0 \quad 197
\end{align*}
\]

\[
\begin{align*}
    \text{Distribution}(f_{RNW}) : & \quad 294 \quad 9 \\
    & \quad 13 \quad 184
\end{align*}
\]  

(B12)
We see that $f_{RN}$ that equally treats the states with low and high prior probability often gives spurious misclassifications. In the same time the $f_{RNW}$ that uses the projections adjusted to prior probability gives the superior prediction.

When we cluster to $D = 2$:

\[
\begin{align*}
\text{java com/polytechnik/utils/RN --data_cols=11:1,9:10:-1} & \backslash \\
\text{--data_file_to_build_model_from=mldata/breast-cancer-wisconsin_S.data} & \backslash \\
\text{--data_file_evaluation=mldata/breast-cancer-wisconsin_S.test} & \backslash \\
\text{--clusters_number=2} & \\
\end{align*}
\]

\[
\begin{align*}
&f[0] = 2.0946398432689 \quad w[0] = 310.52326905818705 \\
&f[1] = 3.924320437715293 \quad w[1] = 189.47673094181317
\end{align*}
\]

The evaluation with $D = 2$ clustering on training data (B15) (500 cases) and on test data (B16) (183 cases) gives the joint distribution of realization/prediction for $f_{RN}$ and $f_{RNW}$:

\[
\begin{align*}
\text{Distribution}(f_{RN}) : & 292 \quad 11 \\
& 7 \quad 190
\end{align*}
\]

\[
\begin{align*}
\text{Distribution}(f_{RNW}) : & 295 \quad 8 \\
& 13 \quad 184
\end{align*}
\]

\[
\begin{align*}
\text{Distribution}(f_{RN}) : & 141 \quad 0 \\
& 0 \quad 42
\end{align*}
\]

\[
\begin{align*}
\text{Distribution}(f_{RNW}) : & 141 \quad 0 \\
& 1 \quad 41
\end{align*}
\]

Now, after the states with low prior probabilities (17a) are removed, both $f_{RN}$ and $f_{RNW}$ exhibit a good classification. For $D = 3$, however, we still get a type of (B12) and (B13) behavior of spurious misclassifications by $f_{RN}$ and no such behavior in $f_{RNW}$.

This makes us to conclude that the $f_{RNW}$ answer is the superior answer for predicting the probabilistic $f$. The posterior distribution (17b) is Radon–Nikodym alternative to Bayes.

**Appendix C: RN Program Application With A Different Definition Of The Probability**

Besides a typical ML classification problem the RN Program can be used for a number of different tasks, e.g. it can be applied to the interpolation problem. The reason is simple: as an input Radon–Nikodym only needs the $F_{jk}$ and $G_{jk}$ matrices [7] which are calculated
FIG. 3. Runge function (C2) interpolation result for \( n = 7 \). The input data (1) was prepared (C1) in a way the classification problem solver from Appendix B to reproduce interpolation results of the Appendix D of [13]. The \( f_{RNW}(x) \) (18) (olive), Christoffel function (blue) (14), and the Coverage(x) (sky) (19) for the measure \( \langle g \rangle = \int_{-1}^{1} g(x)dx \) (C3) are also calculated.

from (1) sample that is a file of \( M \) rows and \( n + 2 \) columns (\( n \) for \( x_k \) and two for \( f \) and the weight \( \omega \)). In the Appendix B the probabilities (7) were obtained as an ensemble average calculated from the data, what is typical for ML classification problem.

Input file can be constructed in a way that calculated averages represent a probability of different kind, such as time average probability. Consider function interpolation problem, the \( \langle \cdot \rangle \) now has a meaning of time–average \( \langle g \rangle = \int g(x) \omega(x)dx \), see Section II of [13]. A one–dimensional interpolation problem[7] can be reduced to (1) data by converting a two–columns sequence \( x^{(l)} \to f^{(l)} \), \( l = 1 \ldots M \) to:

\[
(1, x, x^2, \ldots, x^{n-1})^{(l)} \to f^{(l)} \quad \text{weight } \omega^{(l)} \quad \text{(C1)}
\]

Because the result is invariant relatively any non–degenerated basis components linear transform any polynomials (e.g. \( P_m(x) \), \( T_m(x) \), etc.) can be used instead of the \( x^n \) in (C1).
For example: to reproduce Runge function $d = 1$ interpolation problem

$$f(x) = \frac{1}{1 + 25x^2} \quad (C2)$$

$$d\mu = dx \quad (C3)$$

$$x \in [-1:1]$$

for $n = 7$, the result of the Appendix D of [13], take $x$ sequence with a small step about $dx = 10^{-4}$, it will be about $M = 1 + 2/dx$ total points $x \in [-1, -1 + dx, -1 + 2dx, \ldots, 1 - 2dx, 1 - dx, 1]$ and create a comma–separated file of $M$ rows and $n + 2$ columns: $1, x, x^2, \ldots, x^{n-1}, f(x), \omega$. First $n$ columns are the $x$ from (C1), then $f(x)$ from (C2) follows, and the last column is the observation weight $\omega = dx$ for all points except the $dx/2$ for the edges. This file \texttt{dataexamples/runge\_function.csv} is bundled with \texttt{provided software}.

Run the program

```
java com/polytechnik/utils/RN --data_cols=9:0,6:7:8 \\
   --data_file_to_build_model_from=dataexamples/runge\_function.csv
```

The output file \texttt{runge\_function.csv.RN.csv} has a few more columns, four of them are: the $f_{RN}$ from [13], the Christoffel function (14), the $f_{RNW}$ from (18), and the Coverage($x$) (19). The result is presented in Fig. 3. With the data prepared as (C1) the Christoffel–like function (14) is the regular Christoffel function for the measure (C3). The $f_{RNW}(x)$ is also presented in Fig. 3. The $f_{RNW}(x)$, same as the $f_{RN}(x)$, is a weighted superposition (18) of the eigenvalues, but the weights are the posterior weights (17b), that are a product of prior weights by the $\psi^{[i]}$ projections: $w^{[i]} \text{Proj}^{[i]}$. For Runge function in $n = 7$ case only four prior weights (B8) are non–zero, thus in Fig. 3 the $f_{RNW}(x)$ is a superposition of four eigenvalues. As we discussed above in the Section II A, the $f_{RN}(x)$ should be used for a deterministic functions, and the $f_{RNW}(x)$ is the answer for classification of a probabilistic $f$, it uses the posterior weights (17b). Same result can be also obtained using multi–index multiplications of Section V, take a single $x$ attribute and multiply it by itself 6 times. The quadrature will be identical, but the $x$ attribute is now scaled, it should be scaled back to the original basis for plotting Fig. 3.

```
java com/polytechnik/utils/RN --data_cols=9:1,1:7:8 \\
   --max_multiindex=6 \\
   --data_file_to_build_model_from=dataexamples/runge\_function.csv
```
For simplicity it is easier to use all 7 input columns of provided `dataexamples/runge_function.csv` directly, without the `--max_multiindex=6` option.

Radon–Nikodym interpolation [16] of an image (\(d = 2\) problem), can be performed in a similar way. Create a file of \(M = d_x \times d_y\) rows and \(n = n_x \times n_y + 2\) columns. Each row corresponds to a single pixel. The last two columns are: pixel gray intensity and the weight (equals to 1). The first \(n = n_x \times n_y\) columns are a function of pixel coordinate \((x_l \in 0 \ldots d_x - 1, y_l \in 0 \ldots d_y - 1)\) as \(T_{j_x}(2 \frac{x_l}{d_x - 1} - 1)T_{j_y}(2 \frac{y_l}{d_y - 1} - 1)\), \(j_x = 0 \ldots n_x - 1, j_y = 0 \ldots n_y - 1\). The \(T_m(x)\) is Chebyshev polynomial \(T_0 = 1; T_1 = x; \ldots\) chosen for numerical stability. In [16] the multi–index \(j = (j_x, j_y)\) has (37) and (38) constraints. After running the RN Program interpolated \(f_{RN}\) and Christoffel function columns are added, the \(f_{RN}(x_l,y_l)\) provides required interpolation. While the Gaussian quadrature cannot be obtained for \(d = 2\), the Christoffel function (14) can be easily calculated not only in \(d > 1\) case, but also for an arbitrary \(x\) space with a measure \(\langle \cdot \rangle\).

The input file can be also constructed for \(x\) vector to represent a random variable. For example a distribution regression problem where a “bag” of observations is mapped to a single outcome \(f\) can be approached[18] by using the moments of the distribution of a single “observations bag” as an input \(x\). For every “bag”, calculate it’s distribution moments (one can use any choice of polynomials), then put these moments as \(x\) (now the \(x_k\) components are the moments of the distribution of a bag’s instance), and use the \(f\) as the outcome.

Similarly, the temporal dependencies can be converted to (1) type of data. Assume \(f\) has a \(f(x(t))\) form. Then each \(x_k(t)\) can be converted to the moments \(\langle Q_s(x_k)\rangle_t, s = 0 \ldots n_t\), relatively some time–averaging \(\langle \cdot \rangle_t\) measure, such as in the Section II of [13]. Then the \(n \times n_t\) input attributes \(\langle Q_s(x_k)\rangle_t, k = 0 \ldots n_1; s = 0 \ldots n_t - 1\), are “mixed” moments: time averaged \(\langle \cdot \rangle_t\) first and then ensemble averaged in (7). They can be used in (1) data input. Note, that “combined” averaging in (7) as \(\langle \langle Q_s(x_j(t)) | Q_u(x_k(t)) \rangle_t \rangle_t\) produces different result than the “mixed” one: \(\langle \langle Q_s(x_j(t)) | Q_u(x_k(t)) \rangle_t \rangle\). Numerical experiments show that \(\langle Q_s(x_k)\rangle_t\) attributes typically show a better result than using \((x_k(t), x_k(t - \delta), x_k(t - 2\delta), \ldots)\) as a “vectorish” \(x_k\). With the temporal (and spatial) attributes the dimension of (1) input can grow very fast. In such a situation Section III optimal clustering is of critical importance: this way we can select only a few combinations of input attributes, that optimally separate the \(f\).

The strength of the Radon–Nikodym approach is that it requires only two matrices (7)
as an input, and the average $\langle \cdot \rangle$, used to calculate the $F_{jk}$ and $G_{jk}$, can be chosen with a different definition of the probability. The input file (\texttt{--data_file_to_build_model_from} parameter) can be prepared in a form to represent any probability space in any basis of any dimension. One row corresponds to a single realization, all rows correspond to the entire sample. After the input datafile is prepared for the chosen probability space — the features introduced in this paper $f_{RN}(x)$, $K(x)$, $f_{RNW}(x)$, Coverage$(x)$, along with $\psi_{G}^{[m]}(x)$ clusters\cite{27} are calculated by the provided software.

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