Variational Bayesian Inference for Hidden Markov Models With Multivariate Gaussian Output Distributions

Christian Gruhl, Bernhard Sick

Abstract—Hidden Markov Models (HMM) have been used for several years in many time series analysis or pattern recognitions tasks. HMM are often trained by means of the Baum-Welch algorithm which can be seen as a special variant of an expectation maximization (EM) algorithm. Second-order training techniques such as Variational Bayesian Inference (VI) for probabilistic models regard the parameters of the probabilistic models as random variables and define distributions over these distribution parameters, hence the name of this technique. VI can also bee regarded as a special case of an EM algorithm. In this article, we bring both together and train HMM with multivariate Gaussian output distributions with VI. The article defines the new training technique for HMM. An evaluation based on some case studies and a comparison to related approaches is part of our ongoing work.

Index Terms—Variational Bayesian Inference, Hidden Markov Model, Gaussian-Wishart distribution

1 INTRODUCTION

Hidden Markov Models (HMM) are a standard technique in time series analysis or data mining. Given a (set of) time series sample data, they are typically trained by means of a special variant of an expectation maximization (EM) algorithm, the Baum-Welch algorithm. HMM are used for gesture recognition, machine tool monitoring, or speech recognition, for instance.

Second-order techniques are used to find values for parameters of probabilistic models from sample data. The parameters are regarded as random variables, and distributions are defined over these variables. These type of these second-order distributions depends on the type of the underlying probabilistic models. Typically, so called conjugate distributions are chosen, e.g., a Gaussian-Wishart distribution for an underlying Gaussian for which mean and covariance matrix have to be determined. Second-order techniques have some advantages over conventional approaches, e.g.,

- the uncertainty associated with the determination of the parameters can be numerically expressed and used later,
- prior knowledge about parameters can be considered in the parameter estimation process, and
- the parameter estimation (i.e., training) process can more easily be controlled (e.g., to avoid singularities),
- the training process can easily be extended to automate the search for an appropriate number of model components in a mixture density model (e.g., a Gaussian mixture model).

If point estimates for parameters are needed, they can be derived from the second-order distributions in a maximum posterior (MAP) approach or by taking the expectation of the second-order distributions. Variational Bayesian Inference (VI), which can also be seen as a special variant of an expectation maximization (EM) algorithm, is a typical second-order approach [1].

Although the idea to combine VI and HMM is not completely new and there were already approaches to perform the HMM training in a variational framework (cf. [2]), typically only models with univariate output distributions (i.e., scalar values) are considered.

In this article, we bring these two ideas together and propose VI for HMM with multivariate Gaussian output distributions. The article defines the algorithm. An in-depth analysis of its properties, an experimental evaluation, and a comparison to related work a are part of our current research.

Section 2 introduces the model and the notation we use in our work. Section 3 introduces VI for HMM. Finally, Section 4 concludes the article with a summary of the key results and a brief outlook.

2 MODEL AND NOTATION

We assume a GMM where each Gaussian is the output distribution of a hidden state. This is not so simple as it seems on first sight, especially when the Gaussians are overlapping. Thus it is not clear which observation was generated by which Gaussian (or by which state).

The GMM can be interpreted as a special instance of a HMM, namely a HMM that consists of a transition matrix with the same transition probabilities from each state to every other state that is similar to the initial state distribution.
Fig. 1. Graphical Model. Observations \( x_n \), are depending on latent variables \( z_n \), which are the estimate of the state, as well as the GMM parameters \( \Lambda \) (precision matrices) and \( \mu \) (mean vector, which also depends on the precision matrix) for the \( J \) components. The latent variables \( z_n \) have an additional dependency on the transition matrix \( \Pi \).

The mixing coefficients estimated for the GMM are similar to the starting probabilities of the HMM.

In the remainder of the article, we use the following notation:

- \( E[x] \) is the expectation of the random variable \( x \),
- vectors are denoted with a bold, lowercase symbol e.g., \( x \),
- matrices are denoted with a bold, uppercase symbol e.g., \( X \),
- \( X \) is the sequence of observations \( x_n \), with \( 1 \leq n \leq N \) and \( N = |X| \),
- \( Z \) is the set of latent variables \( z_{n,j} \), with \( 1 \leq n \leq N \) and \( N = |X| \), \( 1 \leq j \leq J \) and \( J \) being the number of states (which is equal to the number of components of the GMM) (Here we use a 1-out-of-\( K \) coding.),
- \( \Theta \) is the parameter vector/matrix containing all model parameters (including transition probabilities \( \pi \), as well as output parameters \( \mu, \Lambda \)),
- \( \mathcal{L} \) is the likelihood or its lower bound approximation,
- \( \Pi \) is the transition matrix with rows \( \pi_i \),
- \( \pi_i \) are the transition probabilities for state \( i \), with \( 1 \leq i \leq J \) and elements \( \pi_{i,j} \),
- \( \pi_{i,j} \) is the transition probability to move from state \( i \) to state \( j \), with \( 1 \leq i, j \leq J \), and
- \( \pi_j \) is the probability to start in state \( j \).

2.1 Hidden Markov Model

A Hidden Markov Model (HMM)

3 Variational Inference

The direct optimization of \( p(X|\Theta) \) is difficult, but the optimization of the complete-data likelihood function \( p(X,Z|\Theta) \) is significantly easier. We introduce a distribution \( q(Z) \) defined over the latent variables, and we observe that, for any choice of \( q(Z) \), the following decomposition holds

\[
\ln p(X|\Theta) = \mathcal{L}(q, \Theta) + KL(q||p) \tag{1}
\]

where we define

\[
\mathcal{L}(q, \Theta) = \int q(Z) \ln \left\{ \frac{p(X,Z|\Theta)}{q(Z)} \right\} \, dZ \tag{2}
\]

\[
KL(q||p) = -\int q(Z) \ln \left\{ \frac{p(Z|X, \Theta)}{q(Z)} \right\} \, dZ \tag{3}
\]

The latent variables \( Z \) absorbed the model parameters \( \Theta \), which are also random variables in this setup. To obtain an optimal model we are interested in maximizing the lower bound with respect to our variational distribution \( q \):

\[
\arg\max_q \mathcal{L}(q) \tag{4}
\]

Which is the same as minimizing Eq. (3). Therefore optimum is reached when the variational distribution \( q(Z) \) matches the conditional (posterior) distribution \( p(Z|X) \). In that case the \( KL(q||p) \) divergence vanishes since \( \ln(1) = 0 \).

Factorization of the real distribution \( p \) (see Fig. 1). N. B., only the values of samples \( x_n \), are observed.

\[
p(X, Z, \Pi, \mu, \Sigma) = p(X|Z, \mu, \Lambda)p(Z|\Pi)p(\Pi)p(\mu|\Lambda)p(\Lambda) \tag{5}
\]

We assume, that a factorization of the variational distribution \( q \) is possible as follows:

\[
q(Z, \Pi, \mu, \Lambda) = q(Z) q(\Pi) q(\mu, \Lambda) \tag{6}
\]

\[
q(Z) = q(\sum_{i=1}^J q(\pi_i) \prod_{j=1}^J q(\mu_j, \Lambda_j) \tag{7}
\]

3.1 Choice of Distributions

For each state \( j \), we assign an independent Dirichlet prior distribution for the transition probabilities, so that

\[
p(\Pi) = \prod_{j=1}^J Dir(\pi_{j,0}) \tag{9}
\]

\[
\alpha_{j,0} = \{\alpha_{j,1}, \ldots, \alpha_{j,0}\} \tag{10}
\]

The variational posterior distributions for the model parameters turn out to have the following form:

\[
q(\Pi) = \prod_{j=1}^J Dir(\pi_j|\alpha_j) \tag{11}
\]

\[
\alpha_j = \{\alpha_{j,1}, \ldots, \alpha_{j,J}\} \tag{12}
\]

The means are assigned independent univariate Gaussian conjugate prior distributions, conditional on the
precisions. The precisions themselves are assigned independent Wishart prior distributions:

\[ p(\mu, \Lambda) = p(\mu|\Lambda)p(\Lambda) \]  \hspace{1cm} (13)

\[ = \prod_{j=1}^{J} N(\mu_j|m_0,(\beta_0\Lambda_j)^{-1}) \cdot \mathcal{W}(\Lambda_j|W_0,\nu_0) \]  \hspace{1cm} (14)

The variational posterior distributions for the model parameters are as follows (application of Bayes theorem):

\[ q(\mu_j, \Lambda_j) = \mathcal{N}(\mu_j|m_j, (\beta_j\Lambda_j)^{-1}) \cdot \mathcal{W}(\Lambda_j|W_j,\nu_j) \]  \hspace{1cm} (15)

The variational posterior for \( q(Z) \) will have the form:

\[ q(Z) \propto \prod_{n=1}^{N} \prod_{j=1}^{J} (b_{n,j})^{z_{n,j}} \prod_{n=1}^{N} \prod_{j=1}^{J} \prod_{s=1}^{M} (a_{j,s})^{z_{n,j},z_{n,s}} \]  \hspace{1cm} (16)

Which is identical to the one given by McGrory et al. in [2]. The expected logarithm for Eq. (16) can be derived to:

\[ \mathbb{E}[\ln q(Z)] = \sum_{n=1}^{N} \sum_{j=1}^{J} \gamma(z_{n,j}) \mathbb{E}[\ln p(x_n|\mu_j, \Lambda_j^{-1})] \]

\[ + \sum_{n=1}^{N-1} \sum_{j=1}^{J} \sum_{s=1}^{M} \xi(z_{n,j}, z_{n+1,s}) \mathbb{E}[\ln \pi_{j,s}] \]  \hspace{1cm} (17)

The distribution over \( Z \) given the transition table \( \Pi \) expands to:

\[ p(Z|\Pi) = p(z_1|\pi) \prod_{n=2}^{N} (p(z_n|z_{n-1}, \omega)) \]  \hspace{1cm} (18)

\[ = \pi \prod_{n=2}^{N} (a_{n-1,n})^{z_{n-1,j}, z_{n,s}} \]  \hspace{1cm} (19)

and its expected value to:

\[ \mathbb{E}[\ln p(Z|\Pi)] = \sum_{j=1}^{J} \pi_j \]

\[ + \sum_{n=2}^{N} \sum_{j=1}^{J} \sum_{s=1}^{M} \xi(z_{n-1,j}, z_{n,s}) \cdot \mathbb{E}[\ln \pi_{j,s}] \]  \hspace{1cm} (20)

For Eq. (19) confer Eq. (26) and Eq. (36).

### 3.2 E-Step

The expectation step (E-Step) uses the Baum Welch algorithm to estimate the latent variables for all observations in the sequence.

The latent variables \( \gamma(z_{n,j}, \omega) \) denotes the probability that the observation at time step \( n \) was generated by the \( j \)-th component of the model.

\[ \gamma(z_n) = \mathbb{E}[z_n] = p(z_n|X) = \frac{v(z_n|\omega(z_n))}{\sum_{z \in Z} v(z|\omega(z))} \]  \hspace{1cm} (21)

\[ \gamma(z_{n,j}) = \mathbb{E}[z_{n,j}] = \frac{v(z_{n,j}|\omega(z_{n,j}))}{\sum_{k=1}^{J} v(z_{n,k}|\omega(z_{n,k}))} \]  \hspace{1cm} (22)

The transition probabilities \( \xi(z_{n-1,j}, z_{n,s}) \) express the uncertainty how likely it is, that a transition from state \( j \) to \( s \) has happened if observation \( x_{n-1} \) was generated by the \( j \)-th component and the \( n \)-th observation by the \( s \)-th component.

\[ \xi(z_{n-1,j}, z_{n,s}) = \frac{v(z_{n-1,j}|a_{j,s}b_{n,s}\omega(z_{n,s}))}{\sum_{k=1}^{J} \sum_{l=1}^{J} v(z_{n-1,k}|a_{k,l}b_{n,l}\omega(z_{n,l}))} \]  \hspace{1cm} (25)

with

\[ a_{j,s} = \exp \left\{ \mathbb{E}[\ln \pi_{j,s}] \right\} \]  \hspace{1cm} (26)

\[ b_{n,j} = \exp \left\{ \mathbb{E}[\ln p(x_n|\mu_j, \Lambda_j)] \right\} \]  \hspace{1cm} (27)

and the popular Baum Welch algorithm:

\[ v(z_{1,j}) = \pi_j b_{1,j} \]  \hspace{1cm} (28)

\[ v(z_{n,j}) = b_{n,j} \sum_{k=1}^{J} v(z_{n-1,k}) \]  \hspace{1cm} (29)

\[ \omega(z_{N,j}) = 1 \]  \hspace{1cm} (30)

\[ \omega(z_{n,j}) = \sum_{s=1}^{J} \omega(z_{n+1,s}) \cdot a_{j,s} \cdot b_{n+1,s} \]  \hspace{1cm} (31)

Note that we substituted the common function names to \( \alpha \rightarrow \nu \) and \( \beta \rightarrow \omega \), since those symbols are already occupied by other definitions.

\[ \mathbb{E}[\ln p(x_n|\mu_j, \Lambda_j^{-1})] = \frac{1}{2} \mathbb{E}_{\Lambda_j}[\ln |\Lambda_j|] - \ln \left( \frac{(2\pi)^D}{2} \right) \]

\[ - \frac{1}{2} \mathbb{E}_{\mu,\Lambda_j}[(x_n - \mu_j)^T A_j(x_n - \mu_j)] \]  \hspace{1cm} (32)

\[ \mathbb{E}_{\Lambda_j}[\ln |\Lambda_j|] = \sum_{d=1}^{D} \psi(d + 1 - \frac{d}{2}) + D \ln 2 + \ln |W_j| \]  \hspace{1cm} (33)

\[ \mathbb{E}_{\mu_j,\Lambda_j}[(x_n - \mu_j)^T A_j(x_n - \mu_j)] = D \beta^{-1}_j + \nu_j (x_n - m_j)^T W_j (x_n - m_j) \]  \hspace{1cm} (34)
The conditional probability that a given observation $x_n$ is generated by the $j$th state (that means the probability of $z_{n,j} = 1$) is given by:

$$\gamma(z_{n,j}) = E[z_{n,j}] = \sum_z \gamma(z) \cdot z_{n,j} \quad (35)$$

Estimating the initial probabilities $\pi$ that the model starts in state $j$.

$$\pi_j = \frac{\gamma(z_{1,j})}{\sum_{k=1}^{J} \gamma(z_{1,k})} = \gamma(z_{1,j} = 1) \quad (36)$$

At the beginning of the sequence there is no predecessor state, thus we can directly use the estimated latent variable as prior probability for the $j$-th state.

### 3.3 M-Step

The Maximization step:

$$N_j = \sum_{n=1}^{N} \gamma(z_{n,j}) \quad (37)$$

$$\bar{x}_j = \frac{1}{N_j} \sum_{n=1}^{N} \gamma(z_{n,j})x_n \quad (38)$$

$$S_j = \frac{1}{N_j} \sum_{n=1}^{N} \gamma(z_{n,j})(x_n - \bar{x}_j)(x_n - \bar{x}_j)^T \quad (39)$$

$$\beta_j = \beta_0 + N_j \quad (40)$$

$$\nu_j = \nu_0 + N_j \quad (41)$$

$$m_j = \frac{1}{\beta_j} (\beta_0 m_0 + \bar{x}_j N_j) \quad (42)$$

$$W_j^{-1} = W_0^{-1} + N_j S_j$$

$$+ \frac{\beta_0 N_j}{\beta_0 + N_j} (\bar{x}_j - m_0)(\bar{x}_j - m_0)^T \quad (43)$$

All equations are based on the Variational Mixture of Gaussians and adjusted for our hidden Markov model.

Maximizing the hyper distribution for the transition matrix:

$$\alpha_{j,s} = \alpha_{j,s}^{(0)} + \sum_{n=1}^{N-1} \xi(z_{n,j}, z_{(n+1),s}) \quad (44)$$

for $1 \leq j, s \leq J$ and $\alpha_{j}^{(0)}$ being the prior values for state $j$.

The hyper parameters for the initial starting probabilities are maximized as follows:

$$\alpha_j = \alpha_0 + N_j \quad (45)$$

### 3.4 Variational LowerBound

To decide whether the model has converged we consult the change of the likelihood function of the model. If the model does not change anymore (or only in very small steps) the likelihood of multiple successive training iterations will be nearly identical. The calculation of the actual likelihood is too hard (is it even possible?) to be practicable, to cumbersome, this we use a lower bound approximation for the likelihood.

For the variational mixture of Gaussians, the lower bound is given by

$$\mathcal{L} = \sum_{z} \int \int \int q(Z|X, \Pi, \mu, \Lambda) \ln \left\{ \frac{p(X, Z|\Pi, \mu, \Lambda)}{q(Z|\Pi, \mu, \Lambda)} \right\} \, d\Pi d\mu d\Lambda \quad (46)$$

Wich is in our case:

$$\mathcal{L} = E[\ln p(X|Z, \Pi, \mu, \Lambda)] - E[\ln q(Z|\Pi, \mu, \Lambda)] \quad (47)$$

$$= E[\ln p(X|Z, \mu, \Lambda)] + E[\ln p(Z|\Pi)]$$

$$+ E[\ln p(\Pi)] + E[\ln p(\mu, \Lambda)] - E[\ln q(\Pi)]$$

$$- E[\ln q(\mu)] - E[\ln q(\mu, \Lambda)] \quad (48)$$

The lower bound $\mathcal{L}$ is used to detect convergence of the model, i.e., approaching of the best (real) parameters of the underlying distribution.
\[ E \left[ \ln p(\mathbf{I}) \right] = \sum_{j=1}^{J} \left( \ln \left( C(\alpha_{j}^{(0)}) \right) + \sum_{s=1}^{J} (\alpha_{j,s}^{(0)} - 1) \cdot E \left[ \ln \tilde{\pi}_{j,s} \right] \right) \quad (49) \]

\[ E \left[ \ln q(\mathbf{I}) \right] = \sum_{j=1}^{J} \left( \ln \left( C(\alpha_{j}) \right) + \sum_{s=1}^{J} (\alpha_{j,s} - 1) \cdot E \left[ \ln \tilde{\pi}_{j,s} \right] \right) \quad (50) \]

\[ E \left[ \ln \tilde{\pi}_{j,s} \right] = \psi(\alpha_{j,s}) - \sum_{k=1}^{J} \psi(\alpha_{j,k}) \quad (51) \]

\[ E \left[ \ln p(\mathbf{X}|\mathbf{Z}, \mathbf{\mu}, \mathbf{\Lambda}) \right] = \frac{1}{2} \sum_{j=1}^{J} N_{j} \left\{ D \ln (\beta_{0}/2\pi) + E \left[ \ln |\mathbf{A}_{j}| \right] \right\} - D \beta_{j}^{-1} - \nu_{j} \text{Tr} \left( \mathbf{S}_{j} \mathbf{W}_{j} \right) - \nu_{j} (\bar{x}_{j} - \mathbf{m}_{j})^{T} \mathbf{W}_{j} (\bar{x}_{j} - \mathbf{m}_{j}) - D \ln (2\pi) \quad (52) \]

\[ E \left[ \ln q(\mathbf{\mu}, \mathbf{\Lambda}) \right] = \frac{1}{2} \sum_{j=1}^{J} \left\{ D \ln (\beta_{0}/2\pi) + E \left[ \ln |\mathbf{A}_{j}| \right] \right\} - D \beta_{0} - \beta_{0} \nu_{j}(\mathbf{m}_{j} - \mathbf{m}_{0})^{T} \mathbf{W}_{j} (\mathbf{m}_{j} - \mathbf{m}_{0}) + J \ln B(\mathbf{W}_{0}, \nu_{0}) + \frac{\nu_{0} - D - 1}{2} \sum_{j=1}^{J} E \left[ \ln |\mathbf{A}_{j}| \right] \]

\[ E \left[ \ln q(\mathbf{\mu}, \mathbf{\Lambda}) \right] = \frac{1}{2} \sum_{j=1}^{J} \left\{ D \ln (\beta_{0}/2\pi) + E \left[ \ln |\mathbf{A}_{j}| \right] \right\} - D \beta_{0} - H [q(\mathbf{A}_{j})] \quad (54) \]

\[ H [q(\mathbf{A}_{j})] = \ln B(\mathbf{W}_{j}, \nu_{j}) - \frac{\nu_{j} - D - 1}{2} E \left[ \ln |\mathbf{A}_{j}| \right] + \frac{\nu_{j} D}{2} \quad (55) \]

### 3.5 Choice of Hyper Parameters

We can either choose the priors \( \alpha_{j,s}^{0} \) for the transitions on random (with a seed) or make some assumptions and use that for initialization e.g.:

\[ \alpha_{j,s}^{0} \begin{cases} 0.5, \quad \text{if } j = s \\ \frac{1}{27}, \quad \text{otherwise} \end{cases} \quad (56) \]

Which means that the probability to stay in a state is always .5 and transitions to the other states is equally likely.

The prior for the starting states \( \alpha_{j}^{0} = \alpha^{0} \) is the same for all states.

Do we need to include actual prior knowledge when using VI approaches? No, the main advantage in relying on a training that is based on variational Bayesian inference is, that the introduction of the distributions over the model parameters prevents us from running into local minima. Especially those that arise when a component (or a state) collapses over a single observation (or multiple observations with identical characteristics). In that case the variance approaches 0 (and the mean \( \infty \) since \( \int p(x)dx = 1 \) and would normally dramatically increase the likelihood for the model – this is also known as singularity (and one of the known drawbacks of normal EM). Using the 2nd order approaches prevents this by a low density in the parameter space where the variance approaches 0 (Therefore \( p(x|\sigma) \to \infty \) is attenuated by a low density for \( p(\sigma) \)).

### 4 Conclusion and Outlook

In this article, we adapted the concept of second-order training techniques to Hidden Markov Models. A training algorithm has been defined following the ideas of Variational Bayesian Inference and the Baum-Welch algorithm.

Part of our ongoing research is the evaluation of the new training algorithm using various benchmark data, the analysis of the computational complexity of the algorithm as well as the actual run-times on these benchmark data, and a comparison to a standard Baum-Welch approach.

In our future work we will extend the approach further by allowing different discrete and continuous distributions in different dimensions of an output distribution. We will also used the HMM trained with the new algorithm for anomaly detection (in particular for the detection of temporal anomalies). For that purpose, we will extend the technique we have proposed for GMM in [3].

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### Appendix

**Dirichlet**

\[ Dir(\mathbf{\mu}|\alpha) = C(\alpha) \prod_{k=1}^{K} \mu_{k}^{\alpha_{k}-1} \quad (57) \]

with constraints

\[ \sum_{k=1}^{K} \mu_{k} = 1 \quad (58) \]

\[ 0 \leq \mu_{k} \leq 1 \quad (59) \]

\[ ||\mathbf{\mu}|| = ||\alpha|| = K \quad (60) \]
\[ \hat{\alpha} = \sum_{k=1}^{K} \alpha_k \]  

\[ C(\alpha) = \frac{\Gamma(\hat{\alpha})}{\prod_{k=1}^{K} \Gamma(\alpha_k)} \]  

\[ H[\mu] = -\sum_{k=1}^{K} (\alpha_k - 1) \{ \psi(\alpha_k) - \psi(\hat{\alpha}) \} - \ln C(\alpha) \]  

Digamma function:
\[ \Psi(a) \equiv \frac{d}{da} \ln \Gamma(a) \]  

Gamma function:
\[ \Gamma(x) \equiv \int_{0}^{\infty} u^{x-1} e^{-u} du \]  

Normal and Wishart
\[ \mathcal{N}(x|\mu, \Lambda) = \frac{1}{(2\pi)^{D/2} \left| \Lambda^{-1} \right|^{1/2}} \cdot \exp \left\{ \frac{1}{2} (x - \mu)^T \Lambda (x - \mu) \right\} \]  

\[ \mathcal{W}(\Lambda|W, \nu) = B(W, \nu)|\Lambda|^{\frac{1}{2}D(\nu-D-1)} \cdot \exp \left\{ \frac{1}{2} \text{Tr}(W^{-1}\Lambda) \right\} \]  

where
\[ B(W, \nu) = |W|^{-\nu/2} \cdot \left( 2^{\nu D/2} \pi^{D(D-1)/4} \prod_{i=1}^{D} \Gamma \left( \frac{\nu + 1 - i}{2} \right) \right)^{-1} \]  

Gaussian-Wishart
\[ p(\mu, \Lambda|\mu_0, \beta, W, \nu) = \mathcal{N}(\mu|\mu_0, (\beta \Lambda)^{-1}) \mathcal{W}(\Lambda|W, \nu) \]  

This is the conjugate prior distribution for a multivariate Gaussian \( \mathcal{N}(x|\mu, \Lambda) \) in which both the mean \( \mu \) and precision matrix \( \Lambda \) are unknown, and is also called the Normal-Wishart distribution.

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Christian Gruhl received his M.Sc. in Computer Science in 2014 at the University of Kassel with Honors. Currently he is working towards his Ph.D. as a research assistant at the Intelligent Embedded Systems lab of Prof. Sick. His research interests focus on 2nd order training algorithms for machine learning and its applications in cyber physical systems.

Bernhard Sick received a diploma (1992, M.Sc. equivalent), a Ph.D. degree (1999), and a “Habilitation” degree (2004), all in computer science, from the University of Passau, Germany. Currently, he is full professor for Intelligent Embedded Systems at the Faculty for Electrical Engineering and Computer Science of the University of Kassel, Germany. There, he is conducting research in the areas Autonomic and Organic Computing and Technical Data Analytics with applications in biometrics, intrusion detection, energy management, automotive engineering, and others. Bernhard Sick authored more than 100 peer-reviewed publications in these areas. He is a member of IEEE (Systems, Man, and Cybernetics Society, Computer Society, and Computational Intelligence Society) and GI (Gesellschaft fuer Informatik). Bernhard Sick is associate editor of the IEEE Transactions on Cybernetics; he holds one patent and received several thesis, best paper, teaching, and inventor awards.