Data-Driven Anomaly Detection based on a Bias Change ⋆

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Abstract: This paper proposes off-line and on-line data-driven approaches to anomaly detection based on generalized likelihood ratio tests for a bias change. The procedure is divided into two steps. Assuming availability of a nominal dataset, a nonparametric density estimate is obtained in the first step, prior to the test. Second, the unknown bias change is estimated from test data. Based on the expectation maximization (EM) algorithm, batch and sequential maximum likelihood estimators of the bias change are derived for the case where the density estimate is given by a Gaussian mixture. Approximate asymptotic expressions for the probabilities of error are suggested based on available results. Real world experiments illustrate the approach.

Keywords: Fault detection and diagnosis; Nonparametric methods; Estimation and filtering

1. INTRODUCTION

In anomaly detection, the main objective is to determine whether observations conform to expected (normal) behavior or not (i.e. an anomaly). Anomaly detection appears in a variety of applications, such as condition monitoring of machines, fraud detection, intrusion detection, etc. Chandola et al. (2009) provide a survey of anomaly detection. A factor that distinguishes anomaly detection to related detection problems is the lack of knowledge of the anomaly. This is a rather common situation, e.g. in condition monitoring and fault detection. A mathematical model is a common description of the available knowledge. However, it may be difficult to determine such a model a priori in some applications. A more common situation is perhaps that it is possible to collect measurements (data) under normal conditions. This nominal dataset contains relevant information about the conforming behavior and it is possible to infer the presence of an anomaly based only on nominal data.

Examples of data-driven approaches to anomaly detection are one-class classification algorithms, e.g. Devroye and Wise (1980); Schölkopf et al. (2001), where a boundary region in the observation space is determined from a nominal dataset. Fresh observations falling outside this region are classified as anomalies. A shortcoming with such an approach is that all knowledge about the normal behavior is summarized by a region in the observation space. For instance, this approach would fail to recognize that if observations consistently fall in a low probability region of the support, it is more likely that an anomaly is present. An alternative is to estimate a model of the measurements density based on the nominal data. In this case, anomalies can be detected based on the probability that test data has under the estimated density model. Since it is often difficult to determine the family of distributions, mixture models are commonly used, e.g. Agarwal (2007), as well as nonparametric estimates (Desforges et al., 1998; Yeung and Chow, 2002). A shortcoming with approaches based on a model solely for the normal behavior is that it is not possible to provide an estimate of how certain the test is of the presence of an anomaly. This type of information is however often important in practice to support decisions of recovery actions.

With the possibility of determining probabilistic models for both the normal and abnormal behaviors, anomaly detection can be seen as a hypothesis testing problem (HTP). In a HTP, it is possible to quantify the decision uncertainties since probabilistic models are defined for the entire problem. In a binary HTP, the null hypothesis $\mathcal{H}^0$ describes the nominal behavior and the alternative hypothesis $\mathcal{H}^1$ describes the abnormal behavior. The hypotheses are described by the statistical behavior of the measurements $\mathbf{y} \in \mathbb{R}^d$ under each hypothesis,

$$\mathcal{H}^0 : \mathbf{y} \sim p^0(\mathbf{y}), \quad \mathcal{H}^1 : \mathbf{y} \sim p^1(\mathbf{y}). \tag{1}$$

When the hypotheses densities, $p^0(\mathbf{y})$ and $p^1(\mathbf{y})$, are given or when their family of parametric distributions are known, there are well-established statistical tests based on *likelihood ratios*, i.e. $\Lambda(\mathbf{y}) \triangleq p^1(\mathbf{y})/p^0(\mathbf{y})$, (Neyman and Pearson, 1933; Wald, 1945).

An approach to overcome the lack of knowledge for the anomaly is to define it as a change *relative to nominal*. In this manner, the available knowledge about the nominal behavior can be used to test for an anomaly. Here, a **bias** (location) change is considered, i.e. the density for the alternative hypothesis is written as $p^1(\mathbf{y}) = p^0(\mathbf{y} - \boldsymbol{\Delta})$, for a bias change $\boldsymbol{\Delta}$. Using this model, this article aims at providing an approach for anomaly detection that without

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requiring specification of a density function and based only on availability of a nominal dataset,

- is flexible and can be used for different problems,
- can provide estimates of the decision uncertainties,
- requires only minimal and meaningful specification parameters from the user.

This is achieved via a two step approach. First, the nominal dataset is used to find a nonparametric estimate of the density function for $\mathcal{H}^0$, denoted $\widehat{p}^0(\mathbf{y})$. In the second step, incoming test measurements are used to find a maximum likelihood estimate $\widehat{\mathbf{\Delta}}$ of the unknown bias change. These estimates are used to define the approximate model

$$\mathcal{H}^0 : \mathbf{y}_i \sim \widehat{p}^0(\mathbf{y}), \quad \mathcal{H}^1 : \mathbf{y}_i \sim \widehat{p}^1(\mathbf{y}|\widehat{\mathbf{\Delta}}) = \widehat{p}^0(\mathbf{y} - \widehat{\mathbf{\Delta}}), \quad (2)$$

which is tested based on a generalized likelihood ratio (GLR) assuming this model to be true. Both on-line and off-line tests are devised.

The presentation is organized as follows, Sec. 2 presents the bias change model and reviews the GLR test. Sec. 3 presents the approaches used to find the estimate $\widehat{p}^0(\mathbf{y})$ based on a nominal dataset. The resulting density model will be a finite mixture distribution. Sec. 4 defines maximum likelihood estimators for $\mathbf{\Delta}$ based on the Expectation Maximization algorithm. Algorithms are derived for mixtures of multivariate Gaussian distributions. The use of GLR tests based on the approximate models (2) is illustrated in Sec. 5 through real data examples followed by concluding remarks.

2. THE BIAS CHANGE MODEL AND GLR TEST

The assumption that an anomaly will appear as a bias change from nominal gives the following hypotheses

$$\mathcal{H}^0 : \mathbf{y} \sim p^0(\mathbf{y}), \quad \mathcal{H}^1 : \mathbf{y} \sim p^1(\mathbf{y}|\mathbf{\Delta}) = p^0(\mathbf{y} - \mathbf{\Delta}), \quad (3)$$

for the unknown bias vector $\mathbf{\Delta}$. The expected value of $\mathbf{y}$ under $\mathcal{H}^1$ can be written as

$$\mathbb{E}_{p^1}[\mathbf{y}] = \mathbb{E}_{p^0}[\mathbf{y}] + \mathbf{\Delta}, \quad (4)$$

i.e., it changes the mean of $\mathbf{y}$ by $\mathbf{\Delta}$. This model is easy to interpret and bias changes are often considered when detecting anomalies, e.g. in the literature of fault diagnosis (Isermann, 2006). The model describes situations where the data is shifted in the observation space. The parameter $\mathbf{\Delta}$ also carries valuable information about the problem. E.g. if Σ is the density covariance, then $\mathbf{\Delta}\Sigma^{-1}\mathbf{\Delta}^T$ measures the significance of the change relative to the density volume, similar to a signal to noise ratio.

Introducing the notation $\mathbf{Y}_{i:j} = [\mathbf{y}_i, \cdots, \mathbf{y}_j]$ $(j > i)$, for N independent and identically distributed (i.i.d.) measurements, $\mathbf{Y}_N \triangleq \mathbf{Y}_{1:N}$, the objective is to decide whether $\mathbf{Y}_N$ belongs to $\mathcal{H}^0$ or $\mathcal{H}^1$ in (3). This can be done with a generalized (log-) likelihood ratio (GLR),

$$\begin{aligned} \widehat{S}_N &\triangleq \log \widehat{\Lambda}_N(\mathbf{Y}_N) = \max_{\mathbf{\Delta}} \log \frac{p_N^1(\mathbf{Y}_N|\mathbf{\Delta})}{p_N^0(\mathbf{Y}_N)} \\ &= \log \frac{p_N^1(\mathbf{Y}_N|\widehat{\mathbf{\Delta}}_N)}{p_N^0(\mathbf{Y}_N)} = \sum_{j=1}^{N} \log \frac{p^0(\mathbf{y}_j - \widehat{\mathbf{\Delta}}_N)}{p^0(\mathbf{y}_j)}, \end{aligned} \quad (5)$$

where $\widehat{\mathbf{\Delta}}_N$ is a maximum likelihood (ML) estimate of the unknown bias. Batch estimation of $\mathbf{\Delta}$ is discussed in Sec. 4.1. The GLR is tested based on a threshold check

$$\widehat{S}_N \underset{\mathcal{H}^0}{\overset{\mathcal{H}^1}{\gtrless}} \eta, \quad (6)$$

the above notation means that $\mathcal{H}_0$ is chosen if the test statistic $\widehat{S}_N$ is smaller than the threshold η otherwise $\mathcal{H}_1$ is chosen.

2.1 Unknown Change Time

The GLR quantity used in (5) assumes that the entire batch $\mathbf{Y}_N$ was collected under either $\mathcal{H}_0$ or $\mathcal{H}_1$, i.e. the change time is known. In many practical situations, the change time is unknown. For a batch $\mathbf{Y}_N$, there are $N+1$ possibilities, either no change was present or a change appeared at any $t \in \{1, \ldots, N\}$. A hypothesis test for this problem can be defined according to (Basseville and Nikiforov, 1993, Sec. 2.6.1)

$$\mathcal{H}^0 : \mathbf{y}_i \sim p^0(\mathbf{y}), \ 1 \le i \le N, \quad (7a)$$

$$\mathcal{H}^1 : \begin{cases} \mathbf{y}_i \sim p^0(\mathbf{y}), & 1 \le i \le t-1, \\ \mathbf{y}_i \sim p^1(\mathbf{y}|\mathbf{\Delta}) = p^0(\mathbf{y} - \mathbf{\Delta}), & t \le i \le N, \end{cases} \quad (7b)$$

where both t and $\mathbf{\Delta}$ are unknown in $\mathcal{H}^1$. The resulting GLR is based on a joint maximization of the unknowns as

$$\begin{aligned} \widetilde{S}_N &\triangleq \max_{1 \le t \le N} \max_{\mathbf{\Delta}} \log \frac{p_{1:t-1}^0(\mathbf{Y}_{1:t-1}) p_{t:N}^1(\mathbf{Y}_{t:N}|\mathbf{\Delta})}{p_n^0(\mathbf{Y}_N)} \\ &= \max_{1 \le t \le N} \log \frac{p_{t:N}^1(\mathbf{Y}_{t:N}|\widehat{\mathbf{\Delta}}_{t:N})}{p_{t:N}^0(\mathbf{Y}_{t:N})} = \max_{1 \le t \le N} \widehat{S}_{t:N}. \end{aligned} \quad (8)$$

the hypotheses are chosen as in (6) with $\widehat{S}_N$ replaced by $\widetilde{S}_N$, an estimate of the change time is

$$\widehat{t}_N = \arg\max_t \widehat{S}_{t:N} \quad (9)$$

and the estimate for the change is $\widehat{\mathbf{\Delta}}_{\widehat{t}_N:N}$. The statistic $\widetilde{S}_N$ requires finding the ML estimate of the change $\widehat{\mathbf{\Delta}}_{t:N}$ for N possible splits $t \in \{1, \ldots, N\}$ and evaluation of the related log-likelihood ratio $\widehat{S}_{t:N}$.

2.2 On-line Solution

The formulation in (7) and (8) is essentially offline. An on-line approach is however possible by repeating the procedure for the sequence $\{\mathbf{y}_n\}$ for each incoming measurement (Gustafsson, 2000, Sec. 3.5.3). Every time a new data $\mathbf{y}_n$ is received, n estimates $\widehat{\mathbf{\Delta}}_{t:n}$, $t \in \{1, \ldots, n\}$, should be found and the associated $\widehat{S}_{t:n}$ evaluated. The complexity therefore increases with n. The estimate $\widehat{\mathbf{\Delta}}_{t:n}$ requires solution of an optimization problem and is more computationally demanding than the evaluation of $\widehat{S}_{t:n}$. To reduce complexity, the estimates $\widehat{\mathbf{\Delta}}_{t:n}$ can be found sequentially in the data, i.e. $\widehat{\mathbf{\Delta}}_{t:n}$ is found based only on the previous value $\widehat{\mathbf{\Delta}}_{t:n-1}$ and current measurement $\mathbf{y}_n$. Sequential estimation of $\mathbf{\Delta}$ is discussed in Sec. 4.2.

The denominator for $\widehat{S}_{t:n}$ in (5), i.e. the log-likelihood function for $\mathcal{H}_0$, can be computed sequentially under the i.i.d. assumption. Given the previous value $\log p_{t:n-1}^0(\mathbf{Y}_{t:n-1})$ and $\mathbf{y}_n$, it can be updated as

$$\log p_{t:n}^0(\mathbf{Y}_{t:n}) = \log p_{t:n-1}^0(\mathbf{Y}_{t:n-1}) + \log p^0(\mathbf{y}_n). \quad (10)$$

The numerator for $\widehat{S}_{t:n}$, i.e. the log-likelihood function for $\mathcal{H}_1$, must however be evaluated for the entire $\mathbf{Y}_{t:n}$ based on $\widehat{\mathbf{\Delta}}_{t:n}$ and, in general, cannot be found sequentially.

2.3 Asymptotic Performance

Associated to any test is the probability of deciding incorrectly for $\mathcal{H}^0$, denoted β, and the probability of deciding incorrectly for $\mathcal{H}^1$, denoted α. For a GLR test they are given by $\beta = \Pr\left(\widehat{S}_N|\mathcal{H}^1 < \eta\right)$ and $\alpha = \Pr\left(\widehat{S}_N|\mathcal{H}^0 \geq \eta\right)$. While in general no analytical solution is available, they can in principle be found based on Monte Carlo techniques. An alternative is to find α and β based on the asymptotic behavior of the GLR statistic. The asymptotic behavior of the test statistic is given by (Mackay, 2003, App. 6A-C)

$$2\widehat{S}_N|\mathcal{H}^0 \overset{\text{as.}}{\sim} \mathcal{X}^2_d, \tag{11a}$$

$$2\widehat{S}_N|\mathcal{H}^1 \overset{\text{as.}}{\sim} \mathcal{X}'^2_d\left(\lambda(\boldsymbol{\Delta}^1)\right),\ \lambda(\boldsymbol{\Delta}) \triangleq \boldsymbol{\Delta}^T\mathbf{F}(\mathbf{0})\boldsymbol{\Delta}, \tag{11b}$$

where $\boldsymbol{\Delta}^1$ is the true parameter under $\mathcal{H}^1$, $\mathcal{X}^2_d$ is the chi-square distribution with d degrees of freedom, $\mathcal{X}'^2_d(\lambda)$ is the non-central chi-square with non-centrality parameter λ and $\mathbf{F}(\mathbf{0})$ is the Fisher information for $\boldsymbol{\Delta}$ evaluated at zero. This result is valid whenever the correct models are used and $\widehat{\boldsymbol{\Delta}}_N$ tends to the true value $\boldsymbol{\Delta}^1$. Since under $\mathcal{H}^0$ the asymptotic behavior of the test statistic does not depend on unknowns, a threshold can be found from (11a) for a desired error level α'. An estimate of β can also be computed based on the maximum likelihood estimate $\widehat{\boldsymbol{\Delta}}$. This is summarized as follows

$$\eta(\alpha') = \inf\left\{\eta \in \mathbb{R} : \textstyle\int_\eta^\infty \mathcal{X}^2_d(z)\,\mathrm{d}z \geq \alpha'\right\}, \tag{12a}$$

$$\beta(\alpha') = \textstyle\int_{-\infty}^{\eta(\alpha')} \mathcal{X}'^2_d\left(z; \lambda(\widehat{\boldsymbol{\Delta}})\right)\,\mathrm{d}z. \tag{12b}$$

To apply the GLR test for the bias change model, the unknown density $p^0(\mathbf{y})$ is needed. In a practical setup, it is often common to introduce assumptions on the data distribution, the Gaussian model being a common choice. Although the Gaussian model gives statistical tests that can be conveniently described by sufficient statistics (Trees and Bell, 2013), it is clear that there will be situations where this model is a poor description of $\mathcal{H}^0$. In this paper, no assumption is forced about $\mathcal{H}^0$, instead, all knowledge is considered to be contained in a nominal dataset and the approximate model (2) is used as an approximation.

3. NONPARAMETRIC DENSITY ESTIMATORS

A nominal dataset $\mathbf{Y}^0_{N_0}$ with N_0 i.i.d. observations from $\mathcal{H}^0$ is used to find a nonparametric density estimate $\widehat{p}^0(\mathbf{y})$. The density model will take the form of a finite mixture

$$\widehat{p}^0(\mathbf{y}) = \sum_{k\in\mathcal{K}} \pi_k\,\kappa(\mathbf{y}; \mathbf{y}^0_k, \mathbf{h}),\ \sum_{k\in\mathcal{K}} \pi_k = 1,\ \pi_k > 0, \tag{13}$$

where $\mathcal{K}$ is an index set with cardinality $|\mathcal{K}| = K \leq N_0$, $\kappa(\cdot)$ is a kernel function satisfying $\kappa(\mathbf{y}) \geq 0$ and $\int \kappa(\mathbf{y})\,\mathrm{d}\mathbf{y} = 1$. The bandwidth $\mathbf{h} \in \mathbb{R}^d$ is fixed and the weighting coefficients $\{\pi_k\}$ are found according to the chosen density estimator. Two nonparametric density estimators are presented next.

3.1 Kernel Density Estimator

The first type of estimator considered is a so called kernel density estimator (KDE), or Parzen estimator. The KDE based on the nominal dataset $\mathbf{Y}^0_{N_0}$ is given by a finite mixture model (13) with

$$\mathcal{K} = \{1, 2, \ldots, N_0\}, \quad \pi_k = \tfrac{|(\mathbf{h})|^{-1/2}}{N_0}, \tag{14a}$$

$$\kappa(\mathbf{y}; \mathbf{y}^0_k, \mathbf{h}) = \kappa\left(S(\mathbf{h})^{-1/2}\left(\mathbf{y} - \mathbf{y}^0_k\right)\right), \tag{14b}$$

where $S(\mathbf{h})$ is a positive definite scaling matrix. The KDE model has as many components as data points and the coefficients $\{\pi_k\}$ are fixed and identical. As shown by Parzen (1962); Cacoullos (1966), this estimator is consistent and asymptotically unbiased. The KDE method requires specification of the bandwidth $\mathbf{h}$. There are several approaches reported in the literature for bandwidth selection (Jones et al., 1996b,a). Here, a diagonal $S(\mathbf{h})$ will be considered with bandwidth elements chosen using Silverman's rule of thumb (Silverman, 1986),

$$S(\mathbf{h}) = \mathrm{diag}(\mathbf{h}), \quad \sqrt{h_j} = \tfrac{4}{d+2}^{\frac{1}{d+4}} N_0^{\frac{-1}{d+4}} \widehat{\sigma}_j, \tag{15}$$

for $j = \{1, \ldots, d\}$ and where $\widehat{\sigma}_j$ is an estimate of the data standard deviation over the jth dimension.

Besides requiring storage of the entire dataset, performing inference with a KDE will become computationally intensive when N_0 is large. An alternative is to consider reduced mixture models, with $K \ll N_0$ components. When the number of components K is fixed, it is possible to find maximum likelihood estimates for the parameters using, e.g., the EM algorithm (Dempster et al., 1977). A disadvantage with such an approach is that the number of components K must be pre-specified.

3.2 A Sparse Density Estimator

An alternative will be considered here based on the generalized cross entropy (GCE) method presented by Botev and Kroese (2011), which does not require specification of K or $\mathbf{h}$. For a dataset $\mathbf{Y}^0_{N_0}$, the estimate is given as

$$\widehat{p}^0(\mathbf{y}) = \sum_{k\in\mathcal{K}} \lambda^*_k \kappa(\mathbf{y}; \mathbf{y}^0_k, \mathbf{h}^*), \tag{16}$$

with $\mathcal{K} = \{1, \ldots, N_0\}$ and where the bandwidth $\mathbf{h}^*$ and weights λ^*_k are given by

$$(\mathbf{h}^*, \boldsymbol{\lambda}^*) = \Big\{(\mathbf{h}, \boldsymbol{\lambda}) : \mathbf{1}^T\boldsymbol{\lambda}(\mathbf{h}) = 1,$$
$$\boldsymbol{\lambda}(\mathbf{h}) = \arg\min_{\boldsymbol{\lambda}\geq 0}\ \boldsymbol{\lambda}^T C(\mathbf{h})\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\widehat{\boldsymbol{\phi}}(\mathbf{h})\Big\}. \tag{17a}$$

The quadratic program (QP) for $\boldsymbol{\lambda}(\mathbf{h})$ is defined by

$$\widehat{\phi}_i(\mathbf{h}) = \frac{1}{N_0 - 1}\sum_{j\neq i} \kappa(\mathbf{y}^0_j; \mathbf{y}^0_i, \mathbf{h}),\ i = 1, \ldots, N_0, \tag{17b}$$

$$C_{ij}(\mathbf{h}) = \int_{\mathbb{R}^d} \kappa(\mathbf{y}; \mathbf{y}^0_i, \mathbf{h})\kappa(\mathbf{y}; \mathbf{y}^0_j, \mathbf{h})\,\mathrm{d}\mathbf{y}, \tag{17c}$$

and $C(\mathbf{h}) \in \mathbb{R}^{N_0\times N_0}$ is positive definite by construction.

This approach is algorithmically similar to the support vector density estimator by Vapnik and Mukherjee (2000), in which the condition $\mathbf{1}^T\boldsymbol{\lambda}(\mathbf{h}) = 1$ is included as a constraint in the QP and $\mathbf{h}$ is pre-specified. As noted by Botev and Kroese (2011), the QP in (17a) is closely related to the support vector regression problem with an ϵ-insensitive error function, see e.g. (Bishop, 2006, Sec. 7.1.4), and most elements in $\boldsymbol{\lambda}^*$ will be close to zero.

Computing the estimate To avoid solving (17a) for a d-dimensional $\mathbf{h}$, a simplification is made which considers a scalar bandwidth h applied to a diagonal covariance estimate, i.e.

$$S(h) = h\widehat{\Sigma}, \quad \text{where } \widehat{\Sigma}_{ij} = \begin{cases} 0, \text{if } i \neq j \\ \widehat{\sigma}_i^2, \text{if } i = j \end{cases} \tag{18}$$

where $i, j \in \{1, \ldots, d\}$. In this manner, only one bandwidth parameter needs to be found and different scaling is allowed for the different dimensions. The resulting problem (17a) is solved by addressing the nonlinear least squares

$$h^* = \arg\min_h \left(\mathbf{1}^T \boldsymbol{\lambda}(h) - 1\right)^2, \tag{19}$$

where $\boldsymbol{\lambda}(h)$ is the solution to the QP (17a) and $\boldsymbol{\lambda}^* = \boldsymbol{\lambda}(h^*)$.

To remove small components in $\boldsymbol{\lambda}^*$, a pruning approach is suggested here. Let $\boldsymbol{\lambda}^*$ be ordered as $\lambda_1^* \leq \lambda_2^* \leq \ldots \lambda_{N_0}^*$, the ϵ approximation of (16) is written by replacing $\mathcal{K}$ and λ_k^* in (16) with $\mathcal{K}_\epsilon$ and π_k^* respectively, where

$$\mathcal{K}_\epsilon : \left\{k : \sum_{j=1}^{k} \lambda_j^* \geq \epsilon, 1 \leq k \leq N_0\right\}, \; \pi_k^* \triangleq \frac{\lambda_k^*}{\sum_{j \in \mathcal{K}_\epsilon} \lambda_j^*}, \tag{20}$$

and $|\mathcal{K}_\epsilon| = K$ will typically be much smaller than the number of data samples N_0.

Multivariate Gaussian kernel The GCE method requires solution of $C_{ij}(\mathbf{h})$ in (17c), which is not always analytically tractable. For the Gaussian case, i.e. $\kappa(\mathbf{y}; \mathbf{y}_k^0, \mathbf{h}) = \mathcal{N}(\mathbf{y}; \mathbf{y}_k^0, S(\mathbf{h}))$, it can be shown from completion of the squares that

$$C_{ij}(\mathbf{h}) = \mathcal{N}(\mathbf{y}_i^0; \mathbf{y}_j^0, 2S(\mathbf{h})), \tag{21}$$

see the Appendix for a proof.

4. ESTIMATING THE BIAS CHANGE

For $\widehat{p}^0(\mathbf{y})$ achieved using either the KDE or the GCE methods, the model for the alternative hypothesis in (2) can be written as the finite mixture

$$\widehat{p}^1(\mathbf{y}|\boldsymbol{\Delta}) = \widehat{p}^0(\mathbf{y} - \boldsymbol{\Delta}) = \sum_{k=1}^{K} \pi_k \kappa_k(\mathbf{y} - \boldsymbol{\Delta}), \tag{22}$$

where $\kappa_k(\mathbf{y}) \triangleq \kappa(\mathbf{y}; \mathbf{y}_k^0, \mathbf{h})$. The objective of this section is to derive batch and sequential maximum likelihood estimators of $\boldsymbol{\Delta}$ in (22). First, notice that for a mixture density $p(\mathbf{y})$, $\mathbb{E}_p[\mathbf{y}] = \sum_{k=1}^{K} \pi_k \mathbb{E}_{\kappa_k}[\mathbf{y}]$. Using this relation with (4), an estimate of Δ can be computed based on $\mathbf{Y}_N$ from the sample estimate

$$\widehat{\boldsymbol{\Delta}}_N^{\mathrm{S}} = \frac{1}{N}\sum_{i=1}^{N} \mathbf{y}_i - E_{\widehat{p}^0}[\mathbf{y}] = \frac{1}{N}\sum_{i=1}^{N} \mathbf{y}_i - \sum_{k=1}^{K} \pi_k \mathbb{E}_{\kappa_k}[\mathbf{y}]. \tag{23}$$

This estimate is asymptotically unbiased. However, for a given sample $\mathbf{Y}_N$, it does not necessarily maximizes the likelihood function (e.g. if the density has multiple modes) and an alternative is needed. It is well known that direct optimization of the likelihood function in mixture models is problematic (Bishop, 2006, Sec. 9.2.1). For mixtures, the EM algorithm can be used to compute maximum likelihood estimates.

4.1 Batch Estimation using EM

The EM algorithm (Dempster et al., 1977), is a two step iterative procedure for finding maximum likelihood parameter estimates in probabilistic models involving latent variables. Let $\mathbf{X}$ and $\mathbf{Y}$ denote latent and measured variables, with joint distribution $p(\mathbf{Y}, \mathbf{X}|\boldsymbol{\theta})$ governed by the parameter vector $\boldsymbol{\theta}$ and let

$$\begin{aligned} \mathcal{Q}\left(\boldsymbol{\theta}, \boldsymbol{\theta}'\right) &\triangleq \int \ln p(\mathbf{Y}, \mathbf{X}|\boldsymbol{\theta}) p(\mathbf{X}|\mathbf{Y}, \boldsymbol{\theta}') \, \mathrm{d}\mathbf{X} \\ &= \mathbb{E}_{\boldsymbol{\theta}'}[\ln p(\mathbf{Y}, \mathbf{X}|\boldsymbol{\theta})|\mathbf{Y}]. \end{aligned} \tag{24}$$

For iterates $\boldsymbol{\theta}^{(i)}$, the expectation (24) is computed for $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{(i-1)})$ in the E-step. In the M-step, the resulting $\mathcal{Q}$-function is maximized w.r.t. $\boldsymbol{\theta}$ to update the iterate $\boldsymbol{\theta}^{(i)}$. The steps are repeated until a convergence criterion is satisfied. The EM algorithm guarantees that the iterates satisfy $p(\mathbf{Y}|\boldsymbol{\theta}^{(i)}) \geq p(\mathbf{Y}|\boldsymbol{\theta}^{(i-1)})$ and therefore they eventually converge to a stationary point of the likelihood function. For a measurement batch $\mathbf{Y}_N$, the estimate achieved after convergence of the algorithm is denoted as $\widehat{\boldsymbol{\theta}}_N$.

As previously noted, the model (22) can be interpreted as a mixture model, where the parameter $\boldsymbol{\theta} = \boldsymbol{\Delta}$ is common to all mixture components. Hence, the model (22) can be written as $\widehat{p}^1(\mathbf{y}|\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k \kappa_k(\mathbf{y}|\boldsymbol{\theta})$. Introducing a discrete latent variable to denote which of the K components that generated a certain measurement $\mathbf{y}_n$, it is possible to show that the E-step amounts to (Bishop, 2006, Sec. 9.3.1)

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta'}) = \sum_{n=1}^{N}\sum_{k=1}^{K} \zeta_{nk}(\boldsymbol{\theta}') \log \pi_k \kappa_k(\mathbf{y}_n|\boldsymbol{\theta}), \tag{25a}$$

$$\zeta_{nk}(\boldsymbol{\theta}') \triangleq \frac{\pi_k \kappa_k(\mathbf{y}_n|\boldsymbol{\theta}')}{\sum_{j=1}^{K} \pi_j \kappa_j(\mathbf{y}_n|\boldsymbol{\theta}')}. \tag{25b}$$

The solution to the M-step depends on the form of the kernel function and on how the unknown parameters enter this function. Explicit solutions are given next for the Gaussian mixture model (GMM) based on $\mathbf{Y}_N$ and with

$$\boldsymbol{\theta} = \boldsymbol{\Delta}, \quad \kappa_k(\mathbf{y}|\boldsymbol{\theta}) = \kappa_k(\mathbf{y} - \boldsymbol{\Delta}) = \mathcal{N}(\mathbf{y} - \boldsymbol{\Delta}; \mathbf{y}_k^0, S). \tag{26}$$

The M-step can be found explicitly by finding the solution to $\frac{\partial}{\partial \boldsymbol{\Delta}} \mathcal{Q}\left(\boldsymbol{\Delta}, \boldsymbol{\Delta}'\right) = 0$. This gradient is given by

$$\sum_{n=1}^{N}\sum_{k=1}^{K} \zeta_{nk}(\boldsymbol{\Delta}') \left[\frac{\partial}{\partial \boldsymbol{\Delta}} \log \kappa_k(\boldsymbol{y}_n - \boldsymbol{\Delta})\right]$$

the term in brackets simplifies to $S^{-1}[(\mathbf{y}_n - \mathbf{y}_k^0) - \boldsymbol{\Delta}]$ giving

$$\begin{aligned} \boldsymbol{\Delta} &= \frac{\sum_{n=1}^{N}\sum_{k=1}^{K} \zeta_{nk}(\boldsymbol{\Delta}') \left(\mathbf{y}_n - \mathbf{y}_k^0\right)}{\sum_{n=1}^{N}\sum_{k=1}^{K} \zeta_{nk}(\boldsymbol{\Delta}')} \\ &= \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K} \zeta_{nk}(\boldsymbol{\Delta}') \left(\mathbf{y}_n - \mathbf{y}_k^0\right), \end{aligned} \tag{27}$$

where the last step follows since $\sum_{k=1}^{K} \zeta_{nk}(\boldsymbol{\Delta}') = 1$. The resulting iterates $\boldsymbol{\Delta}^{(i)}$ produced from the EM algorithm are given in Algorithm 1 for a convergence criterion based on $\|\boldsymbol{\Delta}^{(i)} - \boldsymbol{\Delta}^{(i-1)}\|_2^2$. The algorithm can be initialized using (23), which for the GMM gives

$$\boldsymbol{\Delta}^{(0)} = \frac{1}{N}\sum_{n=1}^{N} \mathbf{y}_n - \sum_{k=1}^{K} \pi_k \mathbf{y}_k^0. \tag{28}$$

4.2 Sequential Estimation using Stochastic Approximation

To evaluate the E-step in the EM algorithm, all measurements in $\mathbf{Y}$ must be available and the EM algorithm is

Algorithm 1 Batch EM for bias change in GMM

Set $i=1$, $\boldsymbol{\Delta}^{(i-1)}$ as (23) and $\epsilon > 0$.
repeat
  E-Step: compute $\zeta_{nk}(\boldsymbol{\Delta}^{(i-1)})$ as in (25b)
  M-step: compute $\boldsymbol{\Delta}^{(i)}$ according to (27)
until $\|\boldsymbol{\Delta}^{(i)}-\boldsymbol{\Delta}^{(i-1)}\|_2^2 \leq \epsilon$
return $\widehat{\boldsymbol{\Delta}}_N = \boldsymbol{\Delta}^{(i)}$ {Return the estimate}

Algorithm 2 Sequential EM for bias change in GMM

Set $n=t$, $\widehat{\boldsymbol{\Delta}}_{t:n-1}=\mathbf{0}$, $\gamma_0 \in (0,1)$ and $\rho \in (\frac{1}{2}, 1]$
for all incoming $\mathbf{y}_n$ **do**
  E-Step: compute $\zeta_{nk}(\widehat{\boldsymbol{\Delta}}_{t:n-1})$ as in (25b) and set $\tilde{n}=n-t+1$.
  M-step: set $\gamma_{\tilde{n}}=\gamma_0\tilde{n}^{-\rho}$ and compute $\widehat{\boldsymbol{\Delta}}_{t:n}$ as in (32)
end for

therefore a batch approach. A sequential version of EM was suggested by Cappé and Moulines (2009), based on a stochastic approximation of the E-step according to,

$$\widetilde{\mathcal{Q}}_n(\boldsymbol{\theta}) = \gamma_n \mathbb{E}_{\widehat{\boldsymbol{\theta}}_{n-1}}[\ln p(\mathbf{y},\mathbf{z}|\boldsymbol{\theta})|\mathbf{y}_n] + (1-\gamma_n)\widetilde{\mathcal{Q}}_{n-1}(\boldsymbol{\theta}), \quad (29)$$

where γ_n is the step-size, controlling the adaptation rate to incoming measurements. The M-step is unchanged and the estimate $\widehat{\boldsymbol{\theta}}_n$ is taken as the maximum of the $\widetilde{\mathcal{Q}}$-function. Consistency and convergence rate for the estimator (29) are studied in Cappé and Moulines (2009). For consistency, γ_n must be chosen such that $0<\gamma_n<1$, $\sum_{j=1}^{\infty}\gamma_j=\infty$ and $\sum_{j=1}^{\infty}\gamma_j^2 < \infty$. To satisfy these conditions, the authors suggest the use of $\gamma_n=\gamma_0 n^{-\rho}$ for $\gamma_0 \in (0,1)$ and $\rho \in (\frac{1}{2}, 1]$. The particular choice $\gamma_0 = \rho = 1$ is equivalent to the recursion of Equation 12 in Titterington (1984).

For mixture models, (29) follows as

$$\widetilde{\mathcal{Q}}_n(\boldsymbol{\theta}) = \gamma_n \sum_{k=1}^{K} \zeta_{nk}(\widehat{\boldsymbol{\theta}}_{n-1}) \log \pi_k \kappa_k(\mathbf{y}_n|\boldsymbol{\theta}) + (1-\gamma_n)\widetilde{\mathcal{Q}}_{n-1}(\boldsymbol{\theta}) \quad (30)$$

where $\zeta_{nk}(\cdot)$ is evaluated at the previous estimate $\widehat{\boldsymbol{\theta}}_{n-1}$. For a GMM as in (26), a recursive solution to the M-step can be found. Starting with $\widetilde{\mathcal{Q}}_0(\boldsymbol{\Delta}) = -\frac{1}{2}\boldsymbol{\Delta}^T S^{-1}\boldsymbol{\Delta}$ and $\widehat{\boldsymbol{\Delta}}_0=\mathbf{0}$ (no change), direct maximization of $\widetilde{\mathcal{Q}}_1(\boldsymbol{\Delta})$, $\widetilde{\mathcal{Q}}_2(\boldsymbol{\Delta})$, $\ldots$, $\widetilde{\mathcal{Q}}_n(\boldsymbol{\Delta})$, for a sequence $\{\mathbf{y}_n\}$ gives

$$\widehat{\boldsymbol{\Delta}}_n = \gamma_n \sum_{k=1}^{K} \zeta_{nk}(\widehat{\boldsymbol{\Delta}}_{n-1})(\mathbf{y}_n - \mathbf{y}_k^0) + (1-\gamma_n)\widehat{\boldsymbol{\Delta}}_{n-1}, \quad (31)$$

see the Appendix for a proof. Similarly, to find $\widehat{\boldsymbol{\Delta}}_{t:n}$ sequentially as described in Sec. 2.2, the recursion is

$$\widehat{\boldsymbol{\Delta}}_{t:n} = \gamma_{\tilde{n}} \sum_{k=1}^{K} \zeta_{nk}(\widehat{\boldsymbol{\Delta}}_{t:n-1})(\mathbf{y}_n - \mathbf{y}_k^0) + (1-\gamma_{\tilde{n}})\widehat{\boldsymbol{\Delta}}_{t:n-1}, \quad (32)$$

where $\tilde{n}=n-t+1$. Recursion (32) gives rise to Algorithm 2, which produces an estimate $\widehat{\boldsymbol{\Delta}}_{t:n}$ sequentially at each new measurement $\mathbf{y}_n$.

Notice that the computational complexities of Algorithms 1 and 2 are directly proportional to the number of kernels K. Therefore, the use of sparse models, such as the ones given by the GCE method, gives the advantage of a reduced computation load.

5. ILLUSTRATIVE EXAMPLES

5.1 Detection of Eruption Increase

The Old Faithful geyser dataset (Azzalini and Bowman, 1990) is considered here to illustrate the methods for the batch multivariate case with known change time. The dataset contains 272 measurements with $d=2$ dimensions representing the registered length of the geyser's eruptions and the time in between them (both in minutes). A fraction $N_0=222$ of the measurements are used to estimate a density for the nominal model $\widehat{p}^0(\mathbf{y})$. Three different models of $p^0(\mathbf{y})$ are considered:

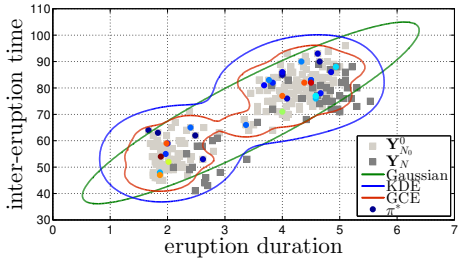
- a Gaussian with parameters given from the standard maximum likelihood equations,
- a nonparametric model given by the KDE with a Gaussian kernel and bandwidth found using (15),
- a nonparametric model given by the GCE with a Gaussian kernel and an $\epsilon=10^{-8}$ approximation.

The measurements $\mathbf{Y}_{N_0}$ are shown in Fig. 1(a) together with contour lines for the density models. The components chosen for the GCE model are also shown in Fig. 1(a) with a colormap relating to the weights π^*. With $K=32$, the GCE requires 86% less data to represent the density compared to the KDE. The GCE is also richer in details and with a tighter support compared to the KDE and Gaussian models.

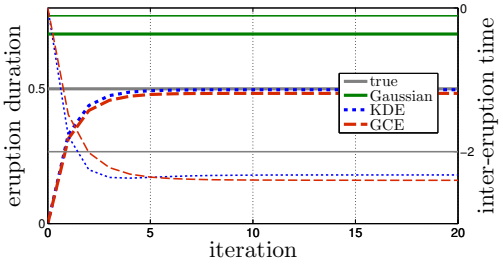
A bias change is considered to illustrate the situation where the length of eruptions is increased by half a minute and the interval between them is reduced by 2 minutes, i.e. $\boldsymbol{\Delta}=[0.5,\ -2]^T$. These values are added to the $N=50$ remaining measurements, which can be seen in Fig.1(a). Using these abnormal measurements $\mathbf{Y}_N$, $\boldsymbol{\Delta}$ is estimated for the three different models. For the Gaussian model, a standard maximum likelihood estimate is used. The estimates for the GCE and KDE models are based on Algorithm 1 with initial values chosen $\boldsymbol{\Delta}_0 = [0,0]^T$ for a comparison. Notice the large bias for the estimate given by the Gaussian model. The iterates $\boldsymbol{\Delta}^{(i)}$ are shown in Fig. 1(b) as a function of iterations. Due to the sparsity of the GCE, $\widehat{\boldsymbol{\Delta}}_N$ is computed 40 times faster compared to the one given by the KDE. After convergence of the iterates, the GLR statistic $\widehat{S}_N$ is computed for the different models, the values are 9.18, 21.71 and 83.71 for the Gaussian, KDE and GCE models, respectively. Based on the asymptotic expression (12a), a threshold $\eta(0.01)=4.60$ is found. All tests can detect the change, although the one based on the GCE gives a much clearer response.

5.2 On-line Wear Detection in an Industrial Robot

By processing torque measurements collected from an industrial robot joint, a scalar quantity y is generated to infer the mechanical condition of the joint gearbox (Bittencourt et al., 2014). The generated quantity y is positive and remains close to zero under normal conditions, deviating otherwise to indicate an anomaly. The data processing used in the generation of y makes it difficult to determine its distribution function. From this application, it is however possible to collect nominal measurements before the application of the test. Based on $N_0 = 66$

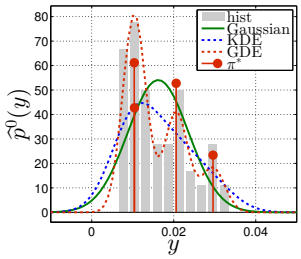


(a) Estimates of $p^0(\mathbf{y})$ and measurements.

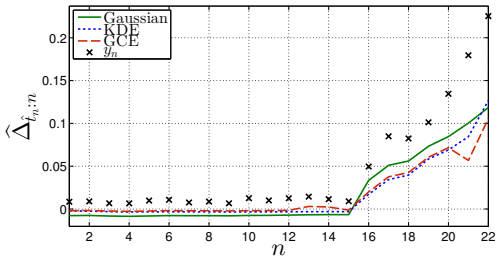


(b) Estimates of eruption duration (thick) and inter-eruption interval (thin). Notice the different axes.

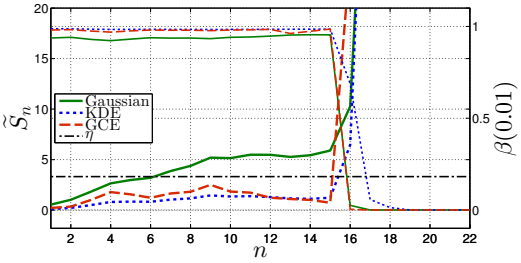
Fig. 1. GLR test for detection of eruptions increase in a geyser dataset. Notice how the test measurements $\mathbf{Y}_N$ in Fig. 1(a) overlap with the support for the nominal models. Despite this, a detection is achieved with any of the models.



(a) Estimation of $p^0(y)$.



(b) Test data sequence y_n and estimates $\widehat{\Delta}_{\hat{t}_n:n}$.



(c) GLR statistic $\widetilde{S}_n$ (thick) and $\beta(0.01)$ (thin). Notice the different axes.

Fig. 2. GLR test for detection of abnormalities in the gearbox of a robot joint. Notice the false alarms triggered with the use of a Gaussian model.

nominal samples, the three models from Sec. 5.1 are considered. The resulting models and histogram of $Y^0_{N_0}$ can be seen in Fig. 2(a). The measurements distribution is multimodal and asymmetric, which makes the Gaussian model a poor representation of the measurements and its mean falls in a region of the support with little data. The KDE estimate captures the asymmetry in the data, but not the multiple modes and presents a wide support. Perhaps a more sophisticated choice of bandwidth would have improved the KDE estimate. The GCE estimate uses only four components, a reduction of 96% compared to the KDE. It also captures the multiple modes, asymmetry and has a tighter support.

Using these models, the objective is to detect a wear fault appearing around $t=16$ in a sequence $\{y_n\}$ with $1\leq n\leq 22$. The change time is unknown and an online solution is sought as described in Secs. 2.1 and 2.2. To reduce the computational complexity, sequential maximum likelihood estimates $\widehat{\Delta}_{t:n}$ are found for $1\leq t\leq n$. For the Gaussian model, the standard maximum likelihood estimate is used. Algorithm 2 is used for the KDE and GCE models with $\gamma_0=0.6$ and $\rho=1$. The data $\{y_n\}$ and the different estimates $\widehat{\Delta}_{\hat{t}_n:n}$, with $\widehat{t}_n$ given in (9), are shown in Fig. 2(b). Up to $n=16$, y_n has values smaller than the mean for the Gaussian model making the estimate to deviate towards negative values.

The resulting models are used to find the GLR statistics $\widetilde{S}_n$ as given in (8), these are shown in Fig. 2(c) together with the threshold $\eta(0.01)=3.32$ found according to (12a). The Gaussian model generates false alarms from $n=7$ and the KDE and GCE based tests detect a change from $n=16$. The error probabilities $\beta(0.01)$ given by (12b) are found based on numerical evaluation of the Fisher information, the values are also shown in Fig. 2(c) as a function of n. As can be seen, there is a sharp decay of β for the Gaussian and GCE models, although the Gaussian model gives smaller values of β for $n<16$. The value for β achieved with the KDE decays more slowly compared to the others, with a value of 0.73 at $n=16$.

In this application, an early detection is very important to allow for condition based maintenance, giving enough time to perform maintenance. To decide for maintenance actions, it is also critical to have few false alarms and that the detection error β can be used to support service decisions. In this application, the test obtained using the GCE model presented the best compromise for these requirements.

6. CONCLUSIONS

This paper proposed a two step approach for anomaly detection using a bias change model and GLR tests. In the first step, a model for the normality is found based on a nominal dataset. Nonparametric density estimates are used which give high flexibility since specification of a density function is not needed. In the second step, maximum likelihood estimates of a bias change are computed using the EM algorithm. The use of a sparse density model can considerably reduce the computations needed for the estimators. The density model and bias change estimate are then used in GLR tests to decide if an abnormality is

present or not. Both off-line and on-line cases are considered and the approach only requires availability of nominal data and minimal/meaningful specification in terms of a desired probability of false alarm (to find a threshold). Using asymptotic expressions for the GLR statistic, it is also possible to give estimates of the uncertainties associated with the decision, which are important to support higher level decisions. The efficacy of the approaches was illustrated in real data examples to detect an increase of eruptions in a geyser and a wear fault in an industrial robot joint. The results achieved show clear improvements compared to tests based on a Gaussian assumption.

Currently, the decision errors are estimated based on asymptotic expressions which may differ for a finite number of measurements. In this direction, it would be interesting to study approaches to provide estimates for the finite sample behavior of the error probabilities. This could possibly lead to the derivation of adaptive thresholds and more accurate error estimates.

APPENDIX

Proof of (21). Let $C_{ij} \triangleq \int_{\mathbb{R}^d} \mathcal{N}(\mathbf{y};\mathbf{y}_i,S)\mathcal{N}(\mathbf{y};\mathbf{y}_i,S)\,\mathrm{d}\mathbf{y}$, $P \triangleq S^{-1}$ and $c=(2\pi)^{-d/2}|S|^{-1/2}$ then

$$C_{ij} = c\int e^{-\frac{1}{2}\{[\mathbf{y}-\mathbf{y}_i]^T P[\mathbf{y}-\mathbf{y}_i]+[\mathbf{y}-\mathbf{y}_j]^T P[\mathbf{y}-\mathbf{y}_j]\}}\,\mathrm{d}\mathbf{y}.$$

Using weighted inner product notation, the term in curly brackets is written as $\langle \mathbf{y}-\mathbf{y}_i,\mathbf{y}-\mathbf{y}_i\rangle_P + \langle \mathbf{y}-\mathbf{y}_j,\mathbf{y}-\mathbf{y}_j\rangle_P$ and simplifies to

$$\begin{aligned}&2\langle \mathbf{y},\mathbf{y}\rangle_P - 2\langle \mathbf{y},\mathbf{y}_i+\mathbf{y}_j\rangle_P + \langle \mathbf{y}_i,\mathbf{y}_i\rangle_P + \langle \mathbf{y}_j,\mathbf{y}_j\rangle_P + \\ &\quad + \left(\tfrac{1}{2}\langle \mathbf{y}_i+\mathbf{y}_j,\mathbf{y}_i+\mathbf{y}_j\rangle_P - \tfrac{1}{2}\langle \mathbf{y}_i+\mathbf{y}_j,\mathbf{y}_i+\mathbf{y}_j\rangle_P\right)\\ &\quad = \langle \mathbf{y}-\tfrac{\mathbf{y}_i+\mathbf{y}_j}{2}, y-\tfrac{\mathbf{y}_i+\mathbf{y}_j}{2}\rangle_{2P} + \langle \mathbf{y}_i-\mathbf{y}_j,\mathbf{y}_i-\mathbf{y}_j\rangle_{P/2}.\end{aligned}$$

Rearranging c and taking the integral gives the result

$$C_{ij} = \mathcal{N}(\mathbf{y}_i;\mathbf{y}_j,2S)\int \mathcal{N}(\mathbf{y};\tfrac{\mathbf{y}_i+\mathbf{y}_j}{2},S/2)\,\mathrm{d}\mathbf{y} = \mathcal{N}(\mathbf{y}_i;\mathbf{y}_j,2S).$$

Proof of (31). We show the results for $n=1$ and $n=2$, the remaining follows by induction. Let $P \triangleq S^{-1}$, $\widetilde{\mathcal{Q}}_0(\boldsymbol{\Delta}) = -\frac{1}{2}\boldsymbol{\Delta}^T P\boldsymbol{\Delta} = -\frac{1}{2}\|\boldsymbol{\Delta}\|_P^2$, $\widehat{\boldsymbol{\Delta}}_0 = \mathbf{0}$, and (26), then (30) gives

$$\widetilde{Q}_1(\boldsymbol{\Delta}) \propto -\tfrac{1}{2}\gamma_1\sum_{k=1}^{K}\zeta_{1k}(\widehat{\boldsymbol{\Delta}}_0)\|(\mathbf{y}_1-\mathbf{y}_k)-\boldsymbol{\Delta}\|_P^2 - \tfrac{1}{2}(1-\gamma_1)\|\boldsymbol{\Delta}\|_P^2$$

$$\frac{\partial}{\partial\boldsymbol{\Delta}}\widetilde{Q}_1(\boldsymbol{\Delta}) = \gamma_1\sum_{k=1}^{K}\zeta_{1k}(\widehat{\boldsymbol{\Delta}}_0)P[(\mathbf{y}_1-\mathbf{y}_k)-\boldsymbol{\Delta}] - (1-\gamma_1)P\boldsymbol{\Delta}$$

and therefore $\widehat{\boldsymbol{\Delta}}_1 = \gamma_1\sum_{k=1}^{K}\zeta_{1k}(\widehat{\boldsymbol{\Delta}}_0)(\mathbf{y}_1-\mathbf{y}_k)$. Similarly, for $n=2$

$$\begin{aligned}\frac{\partial}{\partial\boldsymbol{\Delta}}\widetilde{Q}_2(\boldsymbol{\Delta}) &= \gamma_2\sum_{k=1}^{K}\zeta_{2k}(\widehat{\boldsymbol{\Delta}}_1)P\left[(\mathbf{y}_2-\mathbf{y}_k)-\boldsymbol{\Delta}\right]\\ &+ (1-\gamma_1)\left[\gamma_1\sum_{k=1}^{K}\zeta_{1k}(\widehat{\boldsymbol{\Delta}}_0)P\left[(\mathbf{y}_1-\mathbf{y}_k)-\boldsymbol{\Delta}\right] - (1-\gamma_1)P\boldsymbol{\Delta}\right]\end{aligned}$$

which gives $\widehat{\boldsymbol{\Delta}}_2 = \gamma_2\sum_{k=1}^{K}\zeta_{2k}(\widehat{\boldsymbol{\Delta}}_1)(\mathbf{y}_2-\mathbf{y}_k^0) + (1-\gamma_2)\widehat{\boldsymbol{\Delta}}_1$.

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