Piecewise monotone estimation in one-parameter exponential family

Takeru Matsuda* Yuto Miyatake†

Abstract

The problem of estimating a piecewise monotone sequence of normal means is called the nearly isotonic regression. For this problem, an efficient algorithm has been devised by modifying the pool adjacent violators algorithm (PAVA). In this study, we investigate estimation of a piecewise monotone parameter sequence for general one-parameter exponential families such as binomial, Poisson and chi-square. We develop an efficient algorithm based on the modified PAVA, which utilizes the duality between the natural and expectation parameters. We also provide a method for selecting the regularization parameter by using an information criterion. Simulation results demonstrate that the proposed method detects change-points in piecewise monotone parameter sequences in a data-driven manner. Applications to spectrum estimation, causal inference and discretization error quantification of ODE solvers are also presented.

1 Introduction

There are many phenomena that involve monotonicity, such as the dose-response curve in medicine and the demand/supply curves in economics. Parameter estimation under such order constraints is a typical example of shape constrained inference (Barlow et al., 1972; Robertson et al., 1988; van Eeden, 2006; Groeneboom and Jongbloed, 2014). For example, suppose that we have $n$ normal observations $X_i \sim N(\mu_i, 1)$ for $i = 1, \ldots, n$, where $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_n$ is a monotone sequence of normal means. In this setting, the maximum likelihood estimate (MLE) of $\mu$ is the solution of the constrained optimization

$$\hat{\mu} = \text{argmin}_{\mu_1 \leq \cdots \leq \mu_n} \frac{1}{2} \sum_{i=1}^{n} (X_i - \mu_i)^2,$$

which coincides with the isotonic regression of $X_1, \ldots, X_n$ with uniform weights and efficiently solved by the pool adjacent violators algorithm (PAVA) (Robertson et al., 1988, Chapter 1). Statistical properties of isotonic regression estimators have been extensively studied such as the convergence rates and risk bounds (Bellec, 2018; Groeneboom and Jongbloed, 2014; Guntuboyina and Sen, 2018; Han et al., 2019).

Whereas isotonic regression is useful for estimating a monotone sequence of normal means, the order constraint may be violated at a few change-points in practice. In other words,

*Department of Mathematical Informatics, University of Tokyo & Statistical Mathematics Unit, RIKEN Center for Brain Science, e-mail: matsuda@mist.i.u-tokyo.ac.jp
†Cybermedia Center, Osaka University, e-mail: miyatake@cas.cmc.osaka-u.ac.jp
the parameter sequence may be only piecewise monotone. Thus, Tibshirani et al. (2011) investigated the problem of estimating a piecewise monotone sequence of normal means and called it the nearly isotonic regression. Specifically, for \( n \) (homoscedastic) normal observations \( X_i \sim N(\mu_i, 1) \) for \( i = 1, \ldots, n \), they formulated the problem as the regularized optimization given by

\[
\hat{\mu}_\lambda = \arg\min_{\mu} \frac{1}{2} \sum_{i=1}^{n} (X_i - \mu_i)^2 + \lambda \sum_{i=1}^{n-1} (\mu_i - \mu_{i+1})_+, \tag{2}
\]

where \((a)_+ = \max(a, 0)\) and \( \lambda > 0 \) is the regularization parameter. Then, they developed an efficient algorithm for this problem by modifying the PAVA. They also showed that the number of joined pieces provides an unbiased estimate of the degrees of freedom, which enables data-driven selection of the regularization parameter \( \lambda \).

In this study, we investigate estimation of a piecewise monotone parameter sequence for general one-parameter exponential families (Efron, 2022) including (heteroscedastic) normal, binomial, Poisson and (scaled) chi-square. Suppose that we have \( n \) observations \( X_i \sim p_i(x_i \mid \theta_i) \) for \( i = 1, \ldots, n \), where each \( p_i(x_i \mid \theta_i) \) is a one-parameter exponential family defined by

\[
p_i(x_i \mid \theta_i) = h_i(x_i) \exp(\theta_i x_i - w_i \psi(\theta_i)).
\]

For example, the binomial distribution \( \text{Bi}(N_i, r_i) \) with \( N_i \) (fixed) trials of success probability \( r_i \) corresponds to \( x_i \in \{0, 1, \ldots, N_i\} \), \( h_i(x_i) = N_i!/(x_i!(N_i - x_i)!) \), \( w_i = N_i \) and \( \psi(\theta_i) = \log(1 + e^{\theta_i}) \), where \( r_i = e^{\theta_i}/(1 + e^{\theta_i}) \). The Poisson distribution \( \text{Po}(\lambda_i) \) with mean \( \lambda_i \) corresponds to \( x_i \in \{0, 1, \ldots\} \), \( h_i(x_i) = 1/(x_i!) \), \( w_i = 1 \) and \( \psi(\theta_i) = e^{\theta_i} \), where \( \lambda_i = e^{\theta_i} \). The scaled chi-square distribution \( s_i \chi^2(d_i) \) with scale \( s_i \) and \( d_i \) degrees of freedom corresponds to \( x_i \geq 0 \), \( h_i(x_i) = x_i^{d_i/2-1}/\Gamma(d_i/2) \), \( w_i = d_i/2 \) and \( \psi(\theta_i) = -\log(-\theta_i) \), where \( s_i = -1/(2\theta_i) \). To estimate the piecewise monotone sequence \( \theta = (\theta_1, \ldots, \theta_n) \), we consider the regularized estimator defined by

\[
\hat{\theta}_\lambda = \arg\min_{\theta} -\sum_{i=1}^{n} \log p_i(x_i \mid \theta_i) + \lambda \sum_{i=1}^{n-1} (\theta_i - \theta_{i+1})_+
\]

\[
= \arg\min_{\theta} \sum_{i=1}^{n} (-\theta_i x_i + w_i \psi(\theta_i)) + \lambda \sum_{i=1}^{n-1} (\theta_i - \theta_{i+1})_+,
\]

where \( \lambda > 0 \) is the regularization parameter. We develop an efficient algorithm for this optimization problem by extending the modified PAVA and utilizing the duality between the natural parameters \( \theta_i \) and expectation parameters \( \eta_i = \mathbb{E}_{\theta_i}[X_i] = w_i \psi'(\theta_i) \). We also provide a method for selecting the regularization parameter \( \lambda \) by using an information criterion. Simulation results demonstrate that the proposed method successfully detects change-points of \( \theta \) in a data-driven manner. We present applications to spectrum estimation, causal inference and discretization error quantification of ODE solvers.

This paper is organized as follows. In Section 2 we develop a method for piecewise monotone estimation in general one-parameter exponential families. In Section 3 simulation results are presented. In Section 4 applications to spectrum estimation, causal inference and discretization error quantification are presented. In Section 5 concluding remarks are given. In Appendix, a brief review on (nearly) isotonic regression, technical proofs, and additional experiments are provided. A Julia package of the proposed method is available online at https://github.com/yutomiyatake/IsoFuns.jl.
2 Proposed method

2.1 Estimation algorithm

We propose the following algorithm for computing the regularization path of the estimator \( \lambda \). This algorithm outputs the set of critical points (knots) \( \lambda_0 = 0, \lambda_1, \ldots, \lambda_T \) and the estimate \( \hat{\eta}_{\lambda_t} = \psi'(\hat{\theta}_{\lambda_t}) \) at each critical point. Note that \( \psi' \) is monotonically increasing because \( \psi \) is strictly convex for exponential families (Efron, 2022). Since the solution \( \hat{\eta}_\lambda = \psi'(\hat{\theta}_\lambda) \) is piecewise linear with respect to \( \lambda \) as shown below (Theorem 1), the solution for general \( \lambda \) is readily obtained by linear interpolation.

Algorithm 1.

- **Input:** \( z \in \mathbb{R}^n \) (observation), \( w \in \mathbb{R}^n \) (weight)
- **Output:** \( \lambda_1, \ldots, \lambda_T \) (knot), \( \hat{\eta}_{\lambda_1}, \ldots, \hat{\eta}_{\lambda_T} \in \mathbb{R}^n \) (estimate)
- **Start with** \( t = 0, \lambda_0 = 0, \hat{\eta}_{\lambda_0} = z \) and \( K = n \) clusters \( A_j = \{j\} \) with value \( y_{A_j} = z_j \) for \( j = 1, \ldots, n \).
- **Repeat:**
  - Set \( s_0 = s_K = 0 \) and \( s_j = I(\hat{\eta}_{\lambda_{j-1}, \min_{A_j}} - \hat{\eta}_{\lambda_{j-1}, \max_{A_j}} > 0) \) for \( j = 1, \ldots, K - 1 \).
  - Compute \( m_j = (s_{j-1} - s_j)/\sum_{i \in A_j} w_i \) for \( j = 1, \ldots, K \).
  - Compute \( t_{j,j+1} = \lambda_t + (y_{A_{j+1}} - y_{A_j})/(m_j - m_{j+1}) \) for \( j = 1, \ldots, K - 1 \).
  - If \( t_{j,j+1} \leq \lambda_t \) for every \( j \), then terminate.
  - Set \( j_* = \arg\min_j \{t_{j,j+1} \mid t_{j,j+1} > \lambda_t\} \) and \( \lambda_{t+1} = t_{j_*, j_*+1} \).
  - Update \( y_{A_j} \) to \( y_{A_j} + m_j(\lambda_{t+1} - \lambda_t) \) and set \( \hat{\eta}_{\lambda_{t+1}, i} = y_{A_j} \) for \( i \in A_j \).
  - Merge \( A_{j_*+1} \) into \( A_{j_*} \) and renumber \( A_{j_*+2}, \ldots, A_K \) to \( A_{j_*+1}, \ldots, A_{K-1} \).
  - Decrease \( K \) by one and increase \( t \) by one.

Algorithm 1 can be viewed as a weighted version of the modified PAVA by Tibshirani et al. (2011), where the total weight \( \sum_{i \in A_j} w_i \) replaces the cardinality \( |A_j| \) for each \( A_j \).

Remark 1. Algorithm 1 can be intuitively understood by using a physical model of inelastic collisions (cf. Sibuya et al., 1999). Suppose that there are \( n \) free particles of mass 1 moving on the one-dimensional line, which are numbered 1, \ldots, \( n \) from the left, and the \( i \)th particle has mass \( w_i \) and velocity \( z_i \), whose sign represents the direction of the motion. The particles form clusters by perfectly inelastic collisions. For example, if the first and second particles collide \( (z_1 > z_2) \), then they stick together and become a cluster of mass \( w_1 + w_2 \) and velocity \( (w_1 z_1 + w_2 z_2)/(w_1 + w_2) \). In general, if a cluster of mass \( m_1 \) and velocity \( y_1 \) collides with another cluster of mass \( m_2 \) and velocity \( y_2 < y_1 \), then they form a cluster of mass \( m_1 + m_2 \) and velocity \( (m_1 y_1 + m_2 y_2)/(m_1 + m_2) \). Then, collisions cease within a finite time and eventually the particles are grouped into several clusters. Algorithm 1 can be viewed as simulating these collisions, where the regularization parameter \( \lambda \) specifies the elapsed time from the beginning and each critical point \( \lambda_t \) corresponds to the moment of collision.
From the initial condition of Algorithm 1, it coincides with (1) with $z_i$ for $i$ since the objective function of the optimization in (1) is strictly convex, it has a unique solution satisfying the subgradient condition (Bertsekas, 1997):

\[ (\hat{\theta}_\lambda)_i = (\psi')^{-1}(\lambda_{i+1} - \lambda_i)(\hat{\psi}_\lambda)_i + \frac{\lambda - \lambda_i}{\lambda_{i+1} - \lambda_i}(\hat{\psi}_{i+1})_i \]

for $i = 1, \ldots, n$.

Proof. Since the objective function of the optimization in (1) is strictly convex, it has a unique solution satisfying the subgradient condition (Bertsekas, 1997):

\[ -x_i + w_i\psi'((\hat{\theta}_\lambda)_i) + \lambda(\xi_i - \xi_{i-1}) = 0 \]

for $i = 1, \ldots, n$, where $\xi_0 = \xi_n = 0$ and

\[ \xi_i = \begin{cases} 1 & (\hat{\theta}_\lambda)_i > (\hat{\theta}_\lambda)_{i+1} \\ 0 & (\hat{\theta}_\lambda)_i < (\hat{\theta}_\lambda)_{i+1} \\ \in [0,1] & (\hat{\theta}_\lambda)_i = (\hat{\theta}_\lambda)_{i+1} \end{cases} \]

for $i = 1, \ldots, n - 1$. We show that (1) satisfies (2.1) in the following.

At $\lambda = 0$, the solution of (2.1) is clearly given by $(\hat{\theta}_0)_i = (\psi')^{-1}(x_i/w_i)$ for $i = 1, \ldots, n$. From the initial condition of Algorithm 1, it coincides with (1) with $\lambda = 0$ and $t = 0$.

Suppose that $\hat{\theta}_\lambda$ is clustered into $A_1, \ldots, A_K$ at $\lambda \geq 0$: $(\hat{\theta}_\lambda)_i = (\hat{\theta}_\lambda)_{A_j}$ for $i \in A_j$ and $j = 1, \ldots, K$, where $(\hat{\theta}_\lambda)_{A_j} \neq (\hat{\theta}_\lambda)_{A_{j+1}}$ for $j = 1, \ldots, K - 1$. We consider the change of $\hat{\theta}_\lambda$ as $\lambda$ increases from $\bar{\lambda}$. From Lemma 1, the clustering structure of $\hat{\theta}_\lambda$ remains the same and thus $x_i$ for $i = 1, \ldots, n$ are constant until some neighboring clusters merge. Thus, by summing up (2.1) for $i \in A_j$, we find that $\hat{\theta}_\lambda$ changes linearly with respect to $\lambda$ as long as the clustering structure remains the same:

\[ \psi'((\hat{\theta}_\lambda)_{A_j}) = \left( \sum_{i \in A_j} w_i \right)^{-1} \left( \sum_{i \in A_j} x_i - \lambda(\xi_{\max A_j} - \xi_{\min A_j - 1}) \right) \]

which yields

\[ \psi'((\hat{\theta}_\lambda)_{A_j}) - \psi'((\hat{\theta}_\lambda)_{A_j}) = \left( \sum_{i \in A_j} w_i \right)^{-1} (\lambda - \bar{\lambda})(\xi_{\min A_j - 1} - \xi_{\max A_j}). \]
Therefore, two clusters $A_j$ and $A_{j+1}$ merge \((\hat{\theta}_\lambda)_{A_j} = (\hat{\theta}_\lambda)_{A_{j+1}}\) at
\[
\lambda = \bar{\lambda} + \frac{\psi'((\hat{\theta}_\lambda)_{A_{j+1}}) - \psi'((\hat{\theta}_\lambda)_{A_j})}{m_j - m_{j+1}},
\]
with the merged value
\[
(\hat{\theta}_\lambda)_{A_j} = (\hat{\theta}_\lambda)_{A_{j+1}} = (\psi')^{-1}\left(\psi'((\hat{\theta}_\lambda)_{A_j}) + m_j(\lambda - \bar{\lambda})\right),
\]
where
\[
m_j = \frac{\xi_{\text{min} A_j} - \xi_{\text{max} A_j}}{\sum_{i \in A_j} w_i}.
\]
By putting $y_{A_j} = \psi'((\hat{\theta}_\lambda)_{A_j})$ and $s_j = \xi_{\text{max} A_j}$, the second term in (2.1) coincides with \((y_{A_{j+1}} - y_{A_j})/(m_j - m_{j+1})\) in Algorithm 1 and (2.1) coincides with the updated value of $y_{A_j}$ in Algorithm 1. Hence, Algorithm 1 computes the change-points $\lambda_1, \ldots, \lambda_T$ of the clustering structure and the solution of (2.1) for general $\lambda \in [\lambda_t, \lambda_{t+1}]$ correctly. From the linear interpolation property (2.1), the solution of (2.1) for general $\lambda \in [\lambda_t, \lambda_{t+1}]$ is given by (1).

Here, we summarize the specializations of Theorem 1 to the heteroscedastic normal, binomial, Poisson and chi-square for convenience.

**Corollary 1.** Let $X_i \sim N(\mu_i, \sigma_i^2)$ for $i = 1, \ldots, n$. Then, the estimator
\[
\hat{\mu}_\lambda = \text{argmin}_\mu \sum_{i=1}^n \log p_i(X_i \mid \mu_i) + \lambda \sum_{i=1}^{n-1} (\mu_i - \mu_{i+1})_+
\]
is given by the output of Algorithm 1 on $z = (x_1, \ldots, x_n)$ and $w = (\sigma_1^{-2}, \ldots, \sigma_n^{-2})$.

**Proof.** The optimization (1) is rewritten as
\[
\hat{\mu}_\lambda = \text{argmin}_\mu \sum_{i=1}^n \frac{(X_i - \mu_i)^2}{2\sigma_i^2} + \lambda \sum_{i=1}^{n-1} (\mu_i - \mu_{i+1})_+
\]
\[= \text{argmin}_\mu \sum_{i=1}^n \left(-\mu_i + \frac{X_i}{\sigma_i^2} + \frac{\lambda}{2}\sigma_i^{-2}\mu_i^2\right) + \sum_{i=1}^{n-1} (\mu_i - \mu_{i+1})_+,
\]
which has the form of (1) with $X_i$ replace by $\sigma_i^{-2}X_i$ and $\theta_i = \mu_i$, $\psi(\theta) = \theta^2/2$ and $w_i = \sigma_i^{-2}$. Thus, from Theorem 1 its solution is given by the output of Algorithm 1 on $z = (\sigma_1^{-2}x_1/\sigma_1^{-2}, \ldots, \sigma_n^{-2}x_n/\sigma_n^{-2}) = (x_1, \ldots, x_n)$ and $w = (\sigma_1^{-2}, \ldots, \sigma_n^{-2})$. □

**Corollary 2.** Let $X_i \sim \text{Bi}(N_i, r_i)$ for $i = 1, \ldots, n$. Then, the estimator (1) is given by the output of Algorithm 1 on $z = (x_1/N_1, \ldots, x_n/N_n)$ and $w = (N_1, \ldots, N_n)$.

**Corollary 3.** Let $X_i \sim \text{Po}(\lambda_i)$ for $i = 1, \ldots, n$. Then, the estimator (1) is given by the output of Algorithm 1 on $z = (x_1, \ldots, x_n)$ and $w = (1, \ldots, 1)$.

**Corollary 4.** Let $X_i \sim \sigma_i^2 \chi^2(d_i)$ for $i = 1, \ldots, n$. Then, the estimator (1) is given by the output of Algorithm 1 on $z = (x_1/d_1, \ldots, x_n/d_n)$ and $w = (d_1/2, \ldots, d_n/2)$.
In some situations, we may have bound constraints on \( \theta \) (e.g. Section 4.3). Such cases can be solved by simply thresholding the original solution as follows. Its proof is given in Appendix.

**Proposition 1.** Let

\[
\hat{\theta}_{\lambda, \alpha, \beta} = \arg\min_{\theta \in [\alpha, \beta]^n} - \sum_{i=1}^{n} \log p(X_i \mid \theta_i) + \lambda \sum_{i=1}^{n-1} (\theta_i - \theta_{i+1})_+.
\]  

Then,

\[
(\hat{\theta}_{\lambda, \alpha, \beta})_i = \min(\max((\hat{\theta}_\lambda)_i, \alpha), \beta)
\]

for \( i = 1, \ldots, n \), where \( \hat{\theta}_\lambda \) is given by (1).

### 2.2 Information criterion

In practice, the selection of the regularization parameter \( \lambda \) is a crucial issue like other regularized estimators such as LASSO. Here, we propose a method for selecting \( \lambda \) based on data by using an information criterion (Burnham and Anderson, 2002; Konishi and Kitagawa, 2008).

First, we recall the following result by Tibshirani et al. (2011) for nearly isotonic regression (1).

**Proposition 2.** (Tibshirani et al., 2011) For the nearly isotonic regression \( \hat{\mu}_\lambda \) in (1), let \( K_\lambda \) be the number of joined pieces in \( \hat{\mu}_\lambda \). Then, the quantity

\[
\hat{C}_p(\lambda) = \|\hat{\mu}_\lambda - X\|^2 + 2\sigma^2 K_\lambda - n\sigma^2
\]

is an unbiased estimate of the mean squared error of \( \hat{\mu}_\lambda \):

\[
E_\mu[\hat{C}_p(\lambda)] = E_\mu[\|\hat{\mu}_\lambda - \mu\|^2].
\]

Proposition 3 indicates that the number of joined pieces \( K_\lambda \) is an unbiased estimate of the degrees of freedom (Efron, 2004) of the nearly isotonic regression (1). Based on this result, Tibshirani et al. (2011) selected the regularization parameter \( \lambda \) by minimizing \( \hat{C}_p(\lambda) \) among the knots obtained from the modified PAVA. Note that a similar result on the degrees of freedom has been obtained for other estimators such as isotonic regression (Meyer and Woodroofe, 2000) and LASSO (Zou et al., 2007). In particular, Zou et al. (2007) showed that the number of nonzero regression coefficients is an unbiased estimate of the degrees of freedom for LASSO, and proposed to use it as the penalty term of AIC and BIC.

Now, we propose an information criterion for the estimator (1). Following the convention of information criteria (Konishi and Kitagawa, 2008, Chapter 3), we interpret each \( X_i \) as the sufficient statistic \( X_{i1} + \cdots + X_{im_i} \) for \( \theta_i \) from independent samples \( X_{ij} \sim \tilde{p}_i(x_i \mid \theta_i) \) for \( j = 1, \ldots, m_i \), and consider the asymptotics \( m_i \to \infty \) for every \( i \). For example, when each \( X_i \sim \text{Bi}(N_i, r_i) \) is a binomial random variable, \( m_i \) is set to \( N_i \) and each \( X_{ij} \) is taken to be the Bernoulli random variable with success probability \( r_i \). The asymptotics \( m_i \to \infty \) corresponds to \( N_i \to \infty, \lambda_i \to \infty \) and \( a_i \to \infty \) in the binomial, Poisson and gamma models, respectively.
Then, we consider prediction of $Y_i \sim p_i(y_i | \theta_i)$ for $i = 1, \ldots, n$ by using the estimator $\hat{\theta}_\lambda$ in (1). The prediction error is evaluated by the Kullback–Leibler discrepancy defined as

$$D(\theta, \hat{\theta}_\lambda) = E_\theta \left[ -\sum_{i=1}^{n} \log p_i(Y_i | (\hat{\theta}_\lambda)_i) \right],$$

which is equivalent to the Kullback–Leibler divergence between $p(y | \theta)$ and $p(y | \hat{\theta})$ up to an additive constant. By using the unbiased estimate of the degrees of freedom in Proposition 3, we adopt

$$AIC(\lambda) = -2 \sum_{i=1}^{n} \log p_i(X_i | (\hat{\theta}_\lambda)_i) + 2K\lambda$$

as an approximately unbiased estimator of the expected Kullback–Leibler discrepancy. From the same argument with the usual derivation of information criteria, the bias evaluation reduces to that for the Gaussian model up to $O(m_i^{-1})$ as $m_i \to \infty$ (Konishi and Kitagawa, 2008). Therefore, by using Proposition 3,

$$E_{\theta}[AIC(\lambda)] = 2E_{\theta}[D(\theta, \hat{\theta}_\lambda)] + O(m^{-1})$$

as $m = \min_i m_i \to \infty$. Thus, we select the regularization parameter by minimizing $AIC(\lambda)$ among knots:

$$\hat{\lambda} = \lambda_{\hat{k}}, \quad \hat{k} = \arg\min_k AIC(\lambda_k).$$

We will show the validity of this method by simulation in Section 3.

Remark 2. Ninomiya and Kawano (2016) derived an information criterion for $l_1$-regularized estimators in generalized linear models, which can be viewed as an extension of the result of Zou et al. (2007) on the degrees of freedom of LASSO in Gaussian linear models. Their criterion is an approximately unbiased estimator of the expected Kullback–Leibler discrepancy and its bias correction term does not admit a simple closed-form solution, which is similar to TIC and GIC (Konishi and Kitagawa, 2008). However, their simulation results imply that the bias correction term can be approximated well by twice the number of non-zero regression coefficients, which is shown to be an unbiased estimate of the degrees of freedom in the case of Gaussian linear models (Zou et al., 2007), especially when the sample size is large. Similarly, our simulation results below indicate that the unbiased estimate of the degrees of freedom in Gaussian nearly isotonic regression (Proposition 3) works well as a bias correction term of information criterion as long as the distribution is not very far from Gaussian. It is an interesting future problem to develop a more rigorous theory for this.

3 Simulation results

We check the performance of the proposed method for the binomial distribution. For $i = 1, \ldots, 100$, let $X_i$ be a sample from the binomial distribution with $N_i$ trials and success probability $r_i$, where $r_1, \ldots, r_{100}$ is a piecewise monotone sequence defined by

$$r_i = \begin{cases} 0.2 + 0.6 \cdot \frac{i-1}{49} & (i = 1, \ldots, 50) \\ 0.2 + 0.6 \cdot \frac{i-51}{49} & (i = 51, \ldots, 100) \end{cases}.$$
We apply the proposed method to estimate $r_1, \ldots, r_{100}$ from $X_1, \ldots, X_{100}$.

First, we set $N_i = 10$ for $i = 1, \ldots, 100$. Figure 1 shows $\hat{r}_\lambda$ for several knot values of $\lambda$. Similarly to the original nearly isotonic regression, the estimate is piecewise monotone and the number of joined pieces decreases as $\lambda$ increases. In this case, $\hat{r}_\lambda$ becomes monotone at the final knot $\lambda = 50.5$ and it coincides with the result of the proposed method. Figure 2 plots $\text{AIC}(\lambda)$ with respect to $\lambda$. It takes minimum at $\hat{\lambda} = 6.04$, which corresponds to the third panel of Figure 1. In this way, the proposed information criterion enables us to detect change-points in the parameter sequence of exponential families in a data-driven manner.

Next, we set $N_i = N$ for $i = 1, \ldots, 100$ with $N \in \{10, 20, 30, 50\}$. Figure 3 plots $\mathbb{E}_\theta[\text{AIC}(\lambda)]$ and $2\mathbb{E}_\theta[D(\theta, \hat{\theta}_\lambda)]$ with respect to $\lambda$ for each value of $N$, where we used 10000 repetitions. They show similar behaviors and take minimum at similar values of $\lambda$. Thus, the proposed information criterion is approximately unbiased. The absolute bias $|\mathbb{E}_\theta[\text{AIC}(\lambda)] - 2\mathbb{E}_\theta[D(\theta, \hat{\theta}_\lambda)]|$ decreases as $N$ increases, which is compatible with the fact that the binomial distribution becomes closer to the normal distribution for larger $N$. 

![Figure 1: Generalized nearly isotonic regression for the binomial distribution ($N = 10$) with several values of $\lambda$. black: samples $x_1/10, \ldots, x_{100}/10$, gray: true value $r_1, \ldots, r_{100}$, blue: estimate $\hat{r}_1, \ldots, \hat{r}_{100}$.](image)
Figure 2: AIC for the binomial distribution ($N = 10$).

Figure 3: Expected Kullback–Leibler discrepancy $2E_\theta[D(\theta, \hat{\theta}_\lambda)]$ (black) and $E_\theta[AIC(\lambda)]$ (blue, with standard deviation) for the binomial distribution.
Finally, we examine the case where the number of trials is not constant:

\[ N_i = \begin{cases} 30 & (i = 1, 4, \ldots, 100) \\ 40 & (i = 2, 5, \ldots, 98) \\ 50 & (i = 3, 6, \ldots, 99) \end{cases} \]

Figure 4 plots \( E_\theta[AIC(\lambda)] \) and \( 2E_\theta[D(\theta, \hat{\theta}_\lambda)] \) with respect to \( \lambda \), where we used 10000 repetitions. The bias of the proposed information criterion is sufficiently small. Thus, this criterion works well for determining the regularization parameter \( \lambda \) even when the number of trials is heterogeneous among samples.

Figure 4: Expected Kullback–Leibler discrepancy \( 2E_\theta[D(\theta, \hat{\theta}_\lambda)] \) (black) and \( E_\theta[AIC(\lambda)] \) (blue, with standard deviation) for the binomial distribution when the number of trials is heterogeneous.

See Appendix for a similar experiment on the chi-square distribution.

4 Applications

4.1 Spectrum estimation

Spectrum analysis is an important step in time series analysis that reveals periodicities in time series data (Brillinger, 2001; Brockwell and Davis, 2009). Specifically, the spectral density function of a Gaussian stationary time series \( X = (X_t \mid t \in \mathbb{Z}) \) is defined as

\[ p(f) = \sum_{k=-\infty}^{\infty} C_k \exp(-2\pi ikf), \quad -\frac{1}{2} \leq f \leq \frac{1}{2}, \]

where \( C_k = \text{Cov}[X_t X_{t+k}] \) is the autocovariance. Let

\[ p_j = \frac{1}{2\pi T} \left| \sum_{t=1}^{T} x_t \exp\left(-\frac{2\pi ij t}{T}\right) \right|^2, \quad j = 1, \ldots, T, \]

be the periodogram of the observation \( x_1, \ldots, x_T \). Then, from the theory of the Whittle likelihood (Whittle, 1953), the distribution of the periodogram is well approximated by the independent chi-square distributions:

\[ p_j \sim \frac{p(j/T)}{2} \chi^2(2), \quad j = 1, \ldots, T. \]
Based on this property, many methods have been developed to estimate the spectral density function by smoothing the periodogram (Brillinger, 2001).

The spectral density function of real time series data often tends to be decreasing (Anevski and Soulier, 2011) such as 1/f fluctuation (power law), possibly with a few peaks corresponding to characteristic periodicities or dominant frequencies. Thus, the proposed method is considered to be useful for estimating such nearly monotone spectral density functions. Figure 5 shows the result on the Wolfer sunspot data, which is the annual number of recorded sunspots on the sun’s surface for the period 1770-1869 (Brockwell and Davis, 2009). Note that the result is shown in log-scale following the convention of spectrum analysis, whereas we applied the proposed method to the raw periodogram. This figure indicates one dominant frequency around 0.1 cycle per year. This frequency corresponds well to the well-known characteristic period of approximately 11 years in the sunspot number.

![Figure 5: Result on the Wolfer sunspot data. black: log-periodogram, blue: generalized nearly isotonic regression.](image)

Estimation of a monotone spectral density has been studied in Anevski and Soulier (2011). They proposed two estimators given by the isotonic regression of the periodogram and log-periodogram. They derived their asymptotic distributions and showed that they are rate optimal. While the isotonic regression of the periodogram has smaller asymptotic variance than that of the log-periodogram, the latter has the advantage of being applicable to both short-memory and long-memory processes. Note that these estimators were defined as the solutions of the least squares problems, not the maximizer of the Whittle likelihood. It is an interesting future work to extend the result of Anevski and Soulier (2011) to estimation of a piecewise monotone spectral density.

### 4.2 Causal inference

Regression discontinuity design (RDD) is a statistical method for causal inference in econometrics (Angrist and Pischke, 2014, Chapter 4). It focuses on natural experiment situations where the assignment of a treatment is determined by some threshold of a covariate. One example is a scholarship that is given to all students above a threshold grade. Then, the (local) treatment effect is estimated by taking the difference of the average outcomes of the treatment and control groups at the threshold, which are estimated by applying parametric or nonparametric regression to each group separately.
Here, we explore a possibility of applying the proposed method to RDD. We use the minimum legal drinking age data, which is a well-known example of RDD (Angrist and Pischke, 2014, Chapter 4). This data consists of the number of fatalities (per one-hundred thousands) for several causes of death by age in months. We applied the proposed method with the Poisson distribution to the number of fatalities induced by motor vehicle accidents in 19-23 years old. Since the mortality has decreasing trend as a whole, we employed the regularization term \((\theta_{i+1} - \theta_i)_{+}\) instead of \((\theta_i - \theta_{i+1})_{+}\). Figure 6 shows the result. There is a sudden increase at 21 years old, which coincides with the minimum legal drinking age. Thus, it can be interpreted as the effect of drunk driving on the number of fatalities induced by motor vehicle accidents. In this way, the proposed method may be useful for RDD in some cases, especially when the threshold of treatment assignments is not known a priori and has to be estimated simultaneously with the treatment effect (Porter and Yu, 2015). Note that this method is applicable to RDD with categorical outcomes as well (Xu, 2017). Recently, Babii and Kumar (2021) proposed an application of isotonic regression to RDD.

Recently, RDD has been applied to situations where the treatment assignment is based on geographic boundaries (Keele and Titiunik, 2015) and it is called the spatial RDD. From our viewpoint, some of spatial RDD can be viewed as piecewise monotone estimation under partial orders induced from the geographic boundaries. It is an interesting future work to extend the proposed method to such partially ordered cases. Note that the isotonic regression is applicable to partial orders as well (Robertson et al., 1988, Chapter 1), such as multi-dimensional lattices (Anevski and Pastukhov, 2018, Beran and Dühngen, 2010) and graphs (Minami, 2020).

Figure 6: Result on the minimum legal drinking age data. black: data, blue: generalized nearly isotonic regression.

4.3 Discretization error quantification of ODE solvers

Numerical integration of ordinary differential equations (ODEs) plays an essential role in many research fields. It is used not only for the future prediction but also for estimating the past states and/or system parameters in data assimilation. The theory of numerical analysis tells us how the error induced by the discretization (e.g., Euler, Runge–Kutta) propagates, but standard discussion focuses on asymptotic behavior as the discretization stepsize goes
The expense of sufficiently accurate numerical integration is often prohibitive. Thus, in such cases, quantifying the reliability of numerical integration is essential. In the last few years, several approaches to quantifying the discretization error of ODE solvers have been developed (see, for example, Abdiul et al. (2020); Conrad et al. (2017); Chkrebtii et al. (2016); Cockayne et al. (2019); Lie et al. (2019); Oates et al. (2019); Tronarp et al. (2019, 2021)). Here, we apply the proposed method to discretization error quantification of ODE solvers.

Consider the ordinary differential equation
\[
d\frac{dx}{dt}(t) = f(x(t)), \quad x(0) = x_0 \in \mathbb{R}^m,
\]
(12)
where the vector field \( f : \mathbb{R}^m \to \mathbb{R}^m \) is assumed to be sufficiently differentiable. For time points \( t_1, \ldots, t_n \), let \( x_i \) be an approximation to \( x(t_i) \) obtained by applying an ODE solver such as Runge–Kutta to (4.3). Also, we assume that we have noisy observations \( y_1, \ldots, y_n \) of \( x(t_1), \ldots, x(t_n) \):
\[
y_i = x_k(t_i) + \varepsilon_i, \quad \varepsilon_i \sim N(0, \gamma^2), \quad i = 1, \ldots, n,
\]
(13)
where we focus on a specific element \( x_k \) to simplify the notation. We consider quantifying the discretization error \( \xi_i := (x_i)_k - x_k(t_i) \) for \( i = 1, \ldots, n \) based on \( x_1, \ldots, x_n \) and \( y_1, \ldots, y_n \). Note that we do not necessarily intend to estimate the discretization error as precisely as possible; instead, we aim to capture the scale of the discretization error and its qualitative behavior such as periodicity.

Building on our previous study (Matsuda and Miyatake, 2021), we model the discretization error as independent Gaussian random variables:
\[
\xi_i \sim N(0, \sigma_i^2), \quad i = 1, \ldots, n,
\]
(14)
where the variance \( \sigma_i^2 \) quantifies the magnitude of \( \xi_i \). By substituting (13) into (13), we obtain
\[
y_i = (x_i)_k + \varepsilon_i; \quad e_i \sim N(0, \gamma^2 + \sigma_i^2), \quad i = 1, \ldots, n,
\]
where \( e_i := -\xi_i + \varepsilon_i \). Thus, the square of the residual \( r_i = y_i - (x_i)_k \) follows the chi-square distribution with one degree of freedom:
\[
r_i^2 \sim (\gamma^2 + \sigma_i^2) \chi^2(1), \quad i = 1, \ldots, n.
\]
In the following, we introduce a block constraint on \( \sigma_1^2, \ldots, \sigma_n^2 \) with block size \( d \geq 1 \):
\[
\sigma_{(j-1)d+1}^2 = \cdots = \sigma_j^2 = \tilde{\sigma}_j^2, \quad j = 1, \ldots, \frac{n}{d},
\]
where the block size \( d \) controls the smoothness of \( \sigma_1^2, \ldots, \sigma_n^2 \) and \( n \) is assumed to be divisible by \( d \) for simplicity.\(^2\) Then, by putting \( s_j = r_{(j-1)d+1}^2 + \cdots + r_{jd}^2 \), we have
\[
s_j \sim (\gamma^2 + \tilde{\sigma}_j^2) \chi^2(d), \quad j = 1, \ldots, \frac{n}{d}.
\]
We apply the proposed method to estimate \( \tilde{\sigma}_1^2, \ldots, \tilde{\sigma}_{n/d}^2 \) from \( s_1, \ldots, s_{n/d} \), where we employ Theorem \( \text{l} \) to guarantee \( \tilde{\sigma}_j^2 \geq 0 \) for \( j = 1, \ldots, n/d \). Note that the sequence \( \tilde{\sigma}_1^2, \ldots, \tilde{\sigma}_{n/d}^2 \) is

\(^2\)If \( n \) is indivisible by \( d \), we simply ignore the data for the remaining indices.
expected to be piecewise monotone increasing, since the discretization error basically accumulates in every step of numerical integration, with possible drops if the ODE has periodicity (see Figure 7). From simulation results in Appendix, $d \geq 3$ is recommended to avoid large bias of AIC. This method can be viewed as an extension of our previous approach with the generalized isotonic regression (Matsuda and Miyatake, 2021).

The rest of the subsection checks how the above formulation works for quantifying the discretization error of ODE solvers. The idea of the proposed method leads to an intuition that the formulation suits a problem for which the discretization error gets large as time passes but exhibits periodic nature locally. Thus, we employ the FitzHugh–Nagumo (FN) model (FitzHugh, 1961; Nagumo et al., 1962):

$$\frac{dV}{dt} = c\left(V - \frac{V^3}{3} + R\right), \quad \frac{dR}{dt} = -\frac{1}{c}(V - a + bR)$$

as a toy problem. Since the solution to the FN model is almost periodic, the discretization error also varies periodically as long as the numerical solution is stable and captures the periodic nature.

We set the initial state and parameters to $V(0) = -1$, $R(0) = 1$ and $(a, b, c) = (0.2, 0.2, 3.0)$. We apply the explicit Euler method with the step size $\Delta t = 0.025$ to (4.3), and compare the numerical solution with the exact solution in Figure 7. It is observed that while the numerical approximations well capture the periodicity of the exact flow in a qualitative manner, its phase speed is slower than the exact flow, and the difference between the exact and numerical flows becomes significant as time passes.

**Remark 3.** Undoubtedly, it is easy to obtain much more accurate numerical solutions to the FN model. Nevertheless, we even employ the explicit Euler method with a relatively large step size as an example for which sufficiently accurate numerical integration is hard to attain.

Figure 8 shows the result of discretization error quantification on $V$, where $V$ is observed with observation noise variance 0.01 at $t_i = (i - 1)h$ with $i = 201, 202, \ldots, 1200$ and $h = 0.05$
(i.e., $V$ is observed for $t \in [10, 60]$) and $d = 3$. The top panel plots AIC($\lambda$) with respect to $\lambda$. In this case, AIC($\lambda$) is minimized at $\lambda_{\text{opt}} = 0.1134$. The bottom panel plots the estimated discretization error $\sigma_i$ with the actual error $|V_i - V(t_i)|$, where the result of the generalized isotonic regression (i.e., sufficiently large $\lambda$) is also shown for comparison. It indicates that the proposed method with $\lambda_{\text{opt}}$ captures the fluctuation of the discretization error in a more conformable manner than generalized isotonic regression. We conducted similar experiments for $d = 5, 10$ and obtained almost the same discretization error quantification results.

Figure 9 shows the result for $R$, where the observation noise variance was set to 0.004. The discussion for $V$ remains valid for $R$, although the error behavior for $R$ is different from that for $V$. For $V$, the error gets large moderately and then decreases quite sharply; for $R$, the error decreases moderately after a sharp increase.

In summary, the proposed method can capture the periodicity and scale of the actual discretization error well compared with the previous one using the generalized isotonic regression. The new method seems beneficial in that, for example, we may be able to understand how the error propagates in a more accurate way and further detect recovery of the numerical reliability. This method is expected to be useful in the inverse problem framework, and we leave further discussions to our future work.

![Figure 8](image_url)

**Figure 8:** Left: AIC($\lambda$) for the discretization error quantification for the state variable $V$. The degrees of freedom for the chi-square distribution is set to $d = 3$. Right: Discretization error quantification for the state variable $V$. The results with the optimal $\lambda$ that minimizes AIC and with PAVA (i.e., sufficiently large $\lambda$) are plotted. As a reference, the actual error is also displayed.

## 5 Conclusion

In this study, we extended nearly isotonic regression to general one-parameter exponential families such as binomial, Poisson and chi-square. We developed an efficient algorithm based on the modified PAVA and provided a method for selecting the regularization parameter by using an information criterion. Simulation results demonstrated that the proposed method detects change-points in piecewise monotone parameter sequences in a data-driven manner. We presented applications to spectrum estimation, causal inference and discretization error quantification of ODE solvers.

While we focused on simply ordered cases in this study, isotonic regression is also applicable
Figure 9: Left: AIC(\(\lambda\)) for the discretization error quantification for the state variable \(R\). The degrees of freedom for the chi-square distribution is set to \(d = 3\). Right: Discretization error quantification for the state variable \(R\). The results with the optimal \(\lambda\) that minimizes AIC and with PAVA (i.e., sufficiently large \(\lambda\)) are plotted. As a reference, the actual error is also displayed.

to partially ordered cases (Robertson et al., 1988, Chapter 1). Recent studies considered multidimensional lattices (Anevski and Pastukhov, 2018; Beran and Dümbgen, 2010) and graphs (Minami, 2020). It is an interesting future work to extend the proposed method to such settings. Such a generalization may be applicable to spatial regression discontinuity design as well as discretization error quantification of PDE solvers, which would be useful for reliable simulation as well as large-scale data assimilation.

We proposed an information criterion for selecting the regularization parameter based on a rather heuristic argument. Although it works practically well as long as the model is not very far from Gaussian, the bias is non-negligible in several cases such as the chi-square with a few degrees of freedom. It is a future problem to derive a more accurate information criterion like the one in Ninomiya and Kawano (2016). Note that the number of parameters grows with the sample size here, and thus the usual argument of Akaike information criterion is not directly applicable. Derivation of risk bounds like the one in Minami (2020) is another interesting direction for future work.

Acknowledgements

We thank Yuya Shimizu and Koki Fusejima for helpful comments. We thank Grace Chen for finding a bug of our code. Takeru Matsuda was supported by JSPS KAKENHI Grant Numbers 19K20220, 21H05205 and 22K17865, and JST Moonshot Grant Number JPMJMS2024. Yuto Miyatake was supported by JSPS KAKENHI Grant Numbers 20H01822, 20H00581 and 21K18301, and JST ACT-I Grant Number JPMJPR18US.

References

Abdulle, A. and G. Garegnani (2020). Random time step probabilistic methods for uncertainty quantification in chaotic and geometric numerical integration. *Stat. Comput.* 30, 907–932.
Amari, S.-i. (2016). *Information Geometry and Its Applications*, Volume 194 of *Applied Mathematical Sciences*. Springer, Tokyo.

Anevski, D. and V. Pastukhov (2018). The asymptotic distribution of the isotonic regression estimator over a general countable pre-ordered set. *Electronic Journal of Statistics* 12(2), 4180–4208.

Anevski, D. and P. Soulier (2011). Monotone spectral density estimation. *Ann. Statist.* 39(1), 418–438.

Angrist, J. D. and J.-S. Pischke (2014). *Mastering 'Metrics: The Path From Cause to Effect*. Princeton University Press.

Babii, A. and R. Kumar (2021). Isotonic regression discontinuity designs. *Journal of Econometrics*.

Barlow, R. E., D. J. Bartholomew, J. M. Bremner, and H. D. Brunk (1972). *Statistical Inference Under Order Restrictions. The Theory and Application of Isotonic Regression*. John Wiley & Sons, London-New York-Sydney.

Bellec, P. C. (2018). Sharp oracle inequalities for least squares estimators in shape restricted regression. *Ann. Statist.* 46(2), 745–780.

Beran, R. and L. Dümbgen (2010). Least squares and shrinkage estimation under bimonotonicity constraints. *Statistics and computing* 20(2), 177–189.

Bertsekas, D. P. (1997). Nonlinear programming. *Journal of the Operational Research Society* 48(3), 334–334.

Boyd, S. and L. Vandenberghe (2004). *Convex Optimization*. Cambridge University Press.

Brillinger, D. R. (2001). *Time Series: Data Analysis and Theory*. SIAM, Philadelphia, PA.

Brockwell, P. J. and R. A. Davis (2009). *Time Series: Theory and Methods* (Second ed.). Springer, New York.

Burnham, K. P. and D. R. Anderson (2002). *Model selection and multi-model inference*. Springer, New York.

Chkrebtii, O. A., D. A. Campbell, B. Calderhead, and M. A. Girolami (2016). Bayesian solution uncertainty quantification for differential equations. *Bayesian Anal.* 11(4), 1239–1267.

Cockayne, J., C. J. Oates, T. Sullivan, and M. Girolami (2019). Bayesian probabilistic numerical methods. *SIAM Rev.* 61, 756–789.

Conrad, P. R., M. Girolami, S. Särkkä, A. Stuart, and K. Zygalakis (2017). Statistical analysis of differential equations: introducing probability measures on numerical solutions. *Stat. Comput.* 27(4), 1065–1082.

Efron, B. (2004). The estimation of prediction error: covariance penalties and cross-validation. *J. Amer. Statist. Assoc.* 99(467), 619–632.

Efron, B. (2022). *Exponential Families in Theory and Practice*. Cambridge University Press.
FitzHugh, R. (1961). Impulses and physiological states in models of nerve membrane. *Biophys. J.* 1, 445–466.

Friedman, J., T. Hastie, H. Höfling, and R. Tibshirani (2007). Pathwise coordinate optimization.

Groeneboom, P. and G. Jongbloed (2014). *Nonparametric Estimation Under Shape Constraints*, Volume 38. Cambridge University Press, New York.

Guntuboyina, A. and B. Sen (2018). Nonparametric shape-restricted regression. *Statist. Sci.* 33(4), 568–594.

Hairer, E., S. P. Nørsett, and G. Wanner (1993). *Solving Ordinary Differential Equations I. Nonstiff Problems* (Second ed.). Springer-Verlag, Berlin.

Hairer, E. and G. Wanner (1996). *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems* (Second ed.). Springer-Verlag, Berlin.

Han, Q., T. Wang, S. Chatterjee, and R. J. Samworth (2019). Isotonic regression in general dimensions. *Ann. Statist.* 47(5), 2440–2471.

Keele, L. J. and R. Titiunik (2015). Geographic boundaries as regression discontinuities. *Political Analysis* 23(1), 127–155.

Konishi, S. and G. Kitagawa (2008). *Information Criteria and Statistical Modeling*. Springer Series in Statistics. Springer, New York.

Lehmann, E. L. and G. Casella (2006). *Theory of point estimation*. Springer Science & Business Media.

Lie, H. C., T. J. Sullivan, and A. Stuart (2019). Strong convergence rates of probabilistic integrators for ordinary differential equations. *Stat. Comput.* 29, 1265–1283.

Matsuda, T. and Y. Miyatake (2021). Estimation of ordinary differential equation models with discretization error quantification. *SIAM/ASA J. Uncertain. Quantif.* 9(1), 302–331.

Meyer, M. and M. Woodroofe (2000). On the degrees of freedom in shape-restricted regression. *Ann. Statist.* 28(4), 1083–1104.

Minami, K. (2020). Estimating piecewise monotone signals. *Electron. J. Stat.* 14(1), 1508–1576.

Nagumo, J. S., S. Arimoto, and S. Yoshizawa (1962). An active pulse transmission line simulating a nerve axon. *Proc. Inst. Radio Engrs* 50, 2061–2070.

Ninomiya, Y. and S. Kawano (2016). Aic for the lasso in generalized linear models. *Electron. J. Stat.* 10(2), 2537–2560.

Oates, C. J., J. Cockayne, R. G. Aykroyd, and M. Girolami (2019). Bayesian probabilistic numerical methods in time-dependent state estimation for industrial hydrocyclone equipment. *J. Am. Stat. Assoc.* 114, 1518–1531.
Porter, J. and P. Yu (2015). Regression discontinuity designs with unknown discontinuity points: testing and estimation. *J. Econometrics* 189(1), 132–147.

Robertson, T., F. T. Wright, and R. L. Dykstra (1988). *Order Restricted Statistical Inference*. Wiley Series in Probability and Mathematical Statistics: Probability and Mathematical Statistics. John Wiley & Sons, Ltd., Chichester.

Sibuya, M., T. Kawai, and K. Shida (1990). Equipartition of particles forming clusters by inelastic collisions. *Phys. A* 167(3), 676–689.

Tibshirani, R. J., H. Hoefling, and R. Tibshirani (2011). Nearly-isotonic regression. *Technometrics* 53(1), 54–61.

Tronarp, F., H. Kersting, S. Särkkä, and P. Hennig (2019). Probabilistic solutions to ordinary differential equations as non-linear Bayesian filtering: A new perspective. *Stat. Comput.* 29, 1297–1315.

Tronarp, F., S. Särkkä, and P. Hennig (2021). Bayesian ODE solvers: the maximum a posteriori estimate. *Stat. Comput.* 31(3), Paper No. 23, 18.

van Eeden, C. (2006). *Restricted Parameter Space Estimation Problems*. Springer, New York.

Whittle, P. (1953). Estimation and information in stationary time series. *Ark. Mat.* 2(5), 423–434.

Xu, K.-L. (2017). Regression discontinuity with categorical outcomes. *J. Econometrics* 201(1), 1–18.

Zou, H., T. Hastie, and R. Tibshirani (2007). On the “degrees of freedom” of the lasso. *Ann. Statist.* 35(5), 2173–2192.

A Background

A.1 Order restricted MLE of normal means

As discussed in the Introduction, order restricted MLE of normal means is reduced to the isotonic regression problem (1). Since this is a convex optimization over the closed set of points $(\mu_1, \ldots, \mu_n)$ that satisfy $\mu_1 \leq \cdots \leq \mu_n$, the maximum likelihood estimator uniquely exists. Figure 10 presents an example. This problem is efficiently solved by the pool adjacent violators algorithm (PAVA) given in Algorithm 2. See Chapter 1 of [Robertson et al. (1988)] for details.

**Algorithm 2** (Pool adjacent violators algorithm, PAVA).

- **Start with** $K = n$ clusters $A_i = \{i\}$ with values $y_{A_i} = x_i$ for $i = 1, \ldots, n$.
- **Repeat:**
  
  - If $y_{A_{j-1}} > y_{A_j}$ for some $j$, then merge $A_j$ into $A_{j-1}$, set its value to $(|A_{j-1}| y_{A_{j-1}} + |A_j| y_{A_j}) / (|A_{j-1}| + |A_j|)$, renumber $A_{j+1}, \ldots, A_K$ to $A_j, \ldots, A_{K-1}$ and decrease $K$ by one.
- **Return** $\hat{\mu}$ with $\hat{\mu}_i = y_{A_j}$ for $i \in A_j$
Figure 10: Example of nearly isotonic regression ($n = 200$). Black dots: sample $x_1, \ldots, x_n$, blue line: maximum likelihood estimate $\hat{\mu}_1, \ldots, \hat{\mu}_n$, red line: estimate $(\hat{\mu}_\lambda)_1, \ldots, (\hat{\mu}_\lambda)_n$ with $\lambda = 3.68$. Note that the two lines overlap in the corners.

A.2 Piecewise monotone estimation of normal means

As discussed in the Introduction, piecewise monotone estimation of normal means (nearly isotonic regression) is formulated as (1). Each of the regularization term $(\mu_i - \mu_{i+1})_+$ is piecewise linear and non-differentiable at $\mu_i = \mu_{i+1}$. This property leads to $(\hat{\mu}_\lambda)_i \leq (\hat{\mu}_\lambda)_{i+1}$ for sufficiently large $\lambda$ in the same way that the $l_1$ regularization term provides a sparse solution in LASSO. Figure 10 plots this estimator with $\lambda = 3.68$. Compared to the solution of isotonic regression, this estimator successfully captures the drop of $\mu_i$ around $i = 100$. Note that nearly isotonic regression coincides with isotonic regression when the regularization parameter $\lambda$ is sufficiently large. Recently, Minami (2020) investigated the risk bound of nearly isotonic regression.

The nearly isotonic regression is efficiently solved by a modification of PAVA (Algorithm 1 in the next Section with $w_1 = \cdots = w_n = 1$). This algorithm outputs the regularization path by computing the set of critical points (knots) $\lambda_0 = 0, \lambda_1, \ldots, \lambda_T$ and the estimate $\hat{\mu}_\lambda$ at each critical point. Since the solution path is piecewise linear between the critical points, the solution for general $\lambda$ is readily obtained by linear interpolation.

Remark 4. For isotonic regression, several algorithms other than PAVA have been developed, such as the minimum lower set algorithm (Robertson et al., 1988, Section 1.4). It is an interesting future work to extend these algorithms to nearly isotonic regression.

In practice, it is important to select an appropriate value of the regularization parameter $\lambda$ based on data. For this aim, Tibshirani et al. (2011) derived an unbiased estimate of the degrees of freedom (Efron, 2004) of nearly isotonic regression. Here, we briefly review this result. Suppose that we have an observation $X \sim N_n(\mu, \sigma^2 I)$ and estimate $\mu$ by an estimator $\hat{\mu} = \hat{\mu}(X)$, where $\sigma^2$ is known. From Stein’s lemma, the mean squared error of $\hat{\mu}$ is given by

$$E \mu \left[ \| \hat{\mu} - \mu \|^2 \right] = E \mu \left[ \| \hat{\mu} - X \|^2 \right] + 2\sigma^2 df\mu(\hat{\mu}) - n\sigma^2,$$

where

$$df\mu(\hat{\mu}) = E \mu \left[ \sum_{i=1}^n \frac{\partial \hat{\mu}}{\partial x_i}(X) \right]$$
is called the degrees of freedom of $\hat{\mu}$. For example, the degrees of freedom of a linear estimator $\hat{\mu} = AX$ do not depend on $\mu$ and is equal to $\text{tr}A$. In general, the degrees of freedom depend on $\mu$ and unbiased estimates of them have been derived, which can be used for the penalty term of model selection criteria such as Mallows’ $C_p$, AIC and BIC. For isotonic regression, Meyer and Woodroofe (2000) showed that the number of joined pieces is an unbiased estimate of the degrees of freedom. For LASSO, Zou et al. (2007) showed that the number of nonzero regression coefficients is an unbiased estimate of the degrees of freedom. Tibshirani et al. (2011) proved a similar result for nearly isotonic regression as follows.

**Proposition 3.** (Tibshirani et al., 2011) Let $K_\lambda$ be the number of joined pieces in $\hat{\mu}_\lambda$. Then,

$$E_\mu[K_\lambda] = \text{df}_\mu(\hat{\mu}_\lambda).$$

Therefore, the quantity

$$\hat{C}_p(\lambda) = \|\hat{\mu}_\lambda - X\|^2 + 2\sigma^2 K_\lambda - n\sigma^2$$

is an unbiased estimate of the mean squared error of $\hat{\mu}_\lambda$:

$$E_\mu[\hat{C}_p(\lambda)] = E_\mu[\|\hat{\mu}_\lambda - \mu\|^2].$$

Thus, Tibshirani et al. (2011) selected the regularization parameter $\lambda$ by minimizing $\hat{C}_p(\lambda)$ among the knots:

$$\hat{\lambda} = \lambda_k, \quad \hat{k} = \arg\min_k \hat{C}_p(\lambda_k).$$

The value of $\lambda$ in Figure 10 was selected by this method.

### A.3 Order restricted MLE in one-parameter exponential families

Consider a one-parameter exponential family

$$p(x \mid \theta) = h(x) \exp(\theta x - \psi(\theta)),$$

where $\psi$ is a smooth convex function. This class includes many standard distributions such as binomial, Poisson and gamma (Lehmann and Casella, 2006; Efron, 2022). The binomial distribution $\text{Bi}(N, r)$ with $N$ (fixed) trials of success probability $r$ corresponds to $x \in \{0, 1, \ldots, N\}$, $h(x) = N!/(x!(N - x)!)$ and $\psi(\theta) = N \log(1 + e^\theta)$, where $r = e^\theta/(1 + e^\theta)$. The Poisson distribution $\text{Po}(\lambda)$ with mean $\lambda$ corresponds to $x \in \{0, 1, \ldots\}$, $h(x) = 1/(x!)$ and $\psi(\theta) = e^\theta$, where $\lambda = e^\theta$. The gamma distribution $\text{Ga}(a, b)$ with shape $a$ (fixed) and scale $b$ corresponds to $x \geq 0$, $h(x) = x^{a-1}/\Gamma(a)$ and $\psi(\theta) = -a \log(-\theta)$, where $b = -1/\theta$, and it reduces to the chi-square distribution $\chi^2(d)$ with $d$ degrees of freedom when $a = d/2$ and $b = 2$. Also, the normal distribution $\text{N}(\theta, 1)$ with mean $\theta$ and variance one corresponds to $x \in \mathbb{R}$, $h(x) = (2\pi)^{-1/2} \exp(-x^2/2)$ and $\psi(\theta) = \theta^2/2$.

Exponential families have two canonical parametrizations called the natural parameter $\theta$ and the expectation parameter $\eta = E_\theta[X]$. They are dual in the sense that they have one-to-one correspondence given by $\eta = \psi'(\theta)$, which is related to the Legendre transform of the convex function $\psi$. This duality plays a central role in information geometry and $\theta$ and $\eta$ are called the e-coordinate and m-coordinate, respectively (Amari, 2016). Note that the normal
model is self-dual: \( \theta = \eta \). The relation \( \eta = \psi'(\theta) \) appears in the derivation of the first moment from the moment generating function. See (5.14) in Lehmann and Casella (2006).

For one-parameter exponential families, maximum likelihood estimation under order constraints reduces to a problem called the generalized isotonic regression and it is efficiently solved by PAVA as well (Robertson et al., 1988, Section 1.5). Suppose that we have \( n \) observations \( X_i \sim p(x \mid \theta_i) \) for \( i = 1, \ldots, n \) where \( \theta_1 \leq \cdots \leq \theta_n \). Then, the maximum likelihood estimate of \( \theta \) under the order constraint is given by

\[
\hat{\theta} = \arg\max_{\theta_1 \leq \cdots \leq \theta_n} \sum_{i=1}^{n} \log p(X_i \mid \theta_i) = \arg\min_{\theta_1 \leq \cdots \leq \theta_n} \sum_{i=1}^{n} (-\theta_i X_i + \psi(\theta_i)).
\]

This constrained optimization is solved by PAVA as follows.

**Proposition 4.** [Robertson et al., 1988, Theorem 1.5.2] Let \( \tilde{\eta} = (\tilde{\eta}_1, \ldots, \tilde{\eta}_n) \) be the output of PAVA on the realization \((x_1, \ldots, x_n)\) of \((X_1, \ldots, X_n)\). Then, the maximum likelihood estimate of \( \theta \) is given by \( \hat{\theta} = (\hat{\theta}_1, \ldots, \hat{\theta}_n) \) where \( \hat{\theta}_i = (\psi')^{-1}(\tilde{\eta}_i) \) for \( i = 1, \ldots, n \).

### B Proof of Lemma 1

**Proof.** We follow a similar discussion to Tibshirani et al. (2011). The KKT condition (Boyd and Vandenberghe, 2004, Section 5.5.3) for (11) is

\[
w_i \psi'(\hat{\theta}_{\lambda,i}) - X_i + \lambda (s_{\lambda,i} - s_{\lambda,i-1}) = 0 \quad \text{for } i = 1, \ldots, n,
\]

where

\[
s_{\lambda,i} \begin{cases} 
= 1 & (\hat{\eta}_{\lambda,i} - \hat{\eta}_{\lambda,i+1} > 0) \\
= 0 & (\hat{\eta}_{\lambda,i} - \hat{\eta}_{\lambda,i+1} < 0) \\
in [0,1] & (\hat{\eta}_{\lambda,i} - \hat{\eta}_{\lambda,i+1} = 0)
\end{cases}
\]

Suppose that

\[
(\hat{\mu}_{\lambda,j-1} \neq \hat{\mu}_{\lambda,j}) \hat{\mu}_{\lambda,j} = \hat{\mu}_{\lambda,j+1} = \cdots = \hat{\mu}_{\lambda,j+k}(\neq \hat{\mu}_{\lambda,j+k+1})
\]

for some \( \lambda = \bar{\lambda}(\geq 0) \). Then, we have \( s_{\lambda,j-1}, s_{\lambda,j+k} \in \{0,1\} \) and these values remain constant as \( \lambda \) increases as long as \( \hat{\mu}_{\lambda,j-1} \neq \hat{\mu}_{\lambda,j} \) and \( \hat{\mu}_{\lambda,j+k} \neq \hat{\mu}_{\lambda,j+k+1} \). We need to show that the KKT condition (13) admits the solution

\[
\hat{\mu}_{\lambda,j} = \hat{\mu}_{\lambda,j+1} = \cdots = \hat{\mu}_{\lambda,j+k},
\]

\[
s_{\lambda,j}, s_{\lambda,j+1}, \ldots, s_{\lambda,j+k-1} \in [0,1]
\]

for \( \lambda \geq \lambda_0 \). Below, assuming (13) for \( \lambda \geq \bar{\lambda} \) and (13) for \( \lambda = \bar{\lambda} \), we show that the corresponding \( s_{\lambda,i} \) satisfy (13) for \( \lambda > \bar{\lambda} \).

From the KKT condition (13), we have \( w_i (\hat{\mu}_{\lambda,i} - x_i) + \lambda (s_i - s_{i-1}) = 0 \) for \( i = j, \ldots, j+k \), and this relation can be rewritten as \( w_{i+1} (\hat{\mu}_{\lambda,i+1} - x_{i+1}) + \lambda (s_{i+1} - s_i) = 0 \) for \( i = j-1, \ldots, j+k-1 \). For \( \lambda \geq \bar{\lambda} \), multiplying these two expressions by \( w_{i+1} \) and \( w_i \), respectively, and considering the
are positive; thus, we have

where the assumption (B) is used. It is easy to show that

\[ A | \cdot | A \]

is positive, which can be proved by induction. Thus, every

... element of the first and last columns of \( A \) and subtraction lead to

\[
\begin{bmatrix}
  w_j + w_{j+1} & -w_j & -w_{j+1} \\
  -w_j + w_{j+2} & w_{j+1} + w_{j+2} & -w_j + w_{j+1} \\
  -w_{j+3} & w_{j+2} + w_{j+3} & -w_{j+2} \\
  \vdots & \vdots & \vdots \\
  -w_{j+k} & w_{j+k-1} + w_j & w_{j+k-1}
\end{bmatrix} = A \in \mathbb{R}^{k \times k}
\]

\[
\begin{bmatrix}
  s_{\lambda,j} \\
  s_{\lambda,j+1} \\
  \vdots \\
  s_{\lambda,j+k-1}
\end{bmatrix} = s_{\lambda} \in \mathbb{R}^k
\]

\[
= \frac{1}{\lambda}
\begin{bmatrix}
  w_j w_{j+1} & -w_j w_{j+1} & w_j w_{j+2} & -w_j w_{j+2} \\
  w_{j+1} w_{j+2} & w_{j+1} w_{j+2} & -w_{j+1} w_{j+2} & w_{j+1} w_{j+2} \\
  \vdots & \vdots & \vdots & \vdots \\
  w_{j+k-1} w_j & w_{j+k-1} w_j & -w_{j+k-1} w_{j+k} & w_{j+k-1} w_{j+k}
\end{bmatrix} = D \in \mathbb{R}^{k \times (k+1)}
\]

\[
\begin{bmatrix}
  s_{\lambda,j} - 1 \\
  s_{\lambda,j+1} \\
  \vdots \\
  s_{\lambda,j+k}
\end{bmatrix} = c_{\lambda} \in \mathbb{R}^k
\]

\[
+ \begin{bmatrix}
  w_j + 1 \\
  \vdots \\
  0
\end{bmatrix} = E \in \mathbb{R}^{k \times k}
\]

where the assumption (B) is used. It is easy to show that \( A \) is non-singular when all weights
are positive; thus, we have

\[
s_{\lambda} = \frac{1}{\lambda} A^{-1} D y + A^{-1} E c_{\lambda}.
\]

Since we have assumed (B) for \( \lambda = \tilde{\lambda} \), all elements of \( s_{\lambda} \) are in \([0, 1]\) when \( \lambda = \tilde{\lambda} \). It remains to show that all elements of \( s_{\lambda} \) remain in \([0, 1]\) when \( \lambda \geq \tilde{\lambda} \). As \( \lambda \) increases, the first term of the right-hand-side gets smaller in magnitude. Therefore, if \( A^{-1} E c_{\lambda} \) is in \([0, 1]\) coordinate-wise, then the right-hand-side will stay in \([0, 1]\) for increasing \( \lambda \). Below we show that every element of \( A^{-1} E c_{\lambda} \) is in \([0, 1]\).

Note that the first and last elements of \( c_{\lambda} \) is either 0 or 1, and all elements of \( A^{-1} E \) except for the first and last \((k-1)\)-th columns are zero. We will check that every element of the first and last columns of \( A^{-1} E \) is positive, and \((A^{-1} E)_{i1} + (A^{-1} E)_{i(k)} = 1\), which readily indicates that \( A^{-1} E c_{\lambda} \) is in \([0, 1]\). By Cramer’s rule, we have

\[
(A^{-1} E)_{i1} = \begin{bmatrix}
  w_{j+1} \\
  \vdots \\
  a_1 & a_2 & \cdots & \cdots & a_k \\
  0 & 0 & \cdots & \cdots & 0
\end{bmatrix}, \quad (A^{-1} E)_{ik} = \begin{bmatrix}
  0 & \cdots & \cdots & \cdots & 0 \\
  0 & \cdots & \cdots & \cdots & 0
\end{bmatrix}
\]

where \( | \cdot | \) denotes the determinant of a matrix, and \( a_i \) denotes the \( i \)-th column of \( A \). Here, the numerators and denominator \( | A | \) are positive, which can be proved by induction. Thus, every element of the first and last columns of \( A^{-1} E \) is positive. Further, since \((w_{j+1}, 0, \ldots, 0, w_{j+k})^\top = \ldots \)
\[
\sum_{i=1}^{k} a_k, \text{ it follows that } (A^{-1}E)_{i1} + (A^{-1}E)_{ik} = \begin{bmatrix}
\begin{array}{cccc}
w_{j+1} \\
0 \\
a_1 & a_2 & \cdots & \cdots & a_k \\
0 \\
w_{j+k} \\
|A|
\end{array}
\end{bmatrix} = |A| = 1.
\]

### C Proof of Proposition 1

**Proof.** We consider the case of \( \beta = \infty \) without loss of generality. Since (1) is a convex program, the necessary and sufficient condition for its optimal solution is given by the KKT condition (Boyd and Vandenberghe, 2004, Section 5.5.3):

\[
-x_i + \psi'(\theta_i) + \lambda(\rho_i - \rho_{i-1}) + \nu_i = 0, \\
\nu_i(\theta_i - \alpha) = 0,
\]

\[
\rho_i \begin{cases}
1 & (\theta_i > \theta_{i+1}) \\
0 & (\theta_i < \theta_{i+1}) \\
\in [0,1] & (\theta_i = \theta_{i+1})
\end{cases}
\]

\[
\theta_i \geq \alpha, \\
\nu_i \geq 0
\]

for \( i = 1, \ldots, n \). From (2.1) and (2.1), it is satisfied by taking \( \theta_i = \max((\hat{\theta}_\lambda)_i, \alpha) \), \( \rho_i = \xi_i \) and

\[
\nu_i = \begin{cases}
0 & (\theta_i > \alpha) \\
\psi'((\hat{\theta}_\lambda)_i) - \psi'(\alpha) & (\theta_i = \alpha)
\end{cases}
\]

for \( i = 1, \ldots, n \). Note that \( \nu_i \geq 0 \) since \( \psi \) is convex and thus \( \psi' \) is monotone increasing. □

### D Simulation result for chi-square

We check the performance of the proposed method for the chi-square distribution. For \( i = 1, \ldots, 100 \), let \( X_i \sim s_i \chi^2(d_i) \) be a sample from the chi-square distribution with \( d_i \) degrees of freedom, where \( s_1, \ldots, s_{100} \) is a piecewise monotone sequence defined by

\[
s_i = \begin{cases}
1 + 9 \cdot \frac{i-1}{49} & (i = 1, \ldots, 50) \\
1 + 9 \cdot \frac{i-51}{49} & (i = 51, \ldots, 100)
\end{cases}
\]

We apply the proposed method to estimate \( s_1, \ldots, s_{100} \) from \( X_1, \ldots, X_{100} \).

First, we set \( d_i = 5 \) for \( i = 1, \ldots, 100 \). Figure [1] shows \( \hat{s}_\lambda \) for several knot values of \( \lambda \). Similarly to the original nearly isotonic regression, the estimate is piecewise monotone and the number of joined pieces decreases as \( \lambda \) increases. In this case, \( \hat{s}_\lambda \) becomes monotone at
the final knot $\lambda = 270.04$ and it coincides with the result of the proposed method. Figure 12 plots $\text{AIC}(\lambda)$ with respect to $\lambda$. It takes minimum at $\hat{\lambda} = 80.68$, which corresponds to the third panel of Figure 11. In this way, the proposed information criterion enables to detect change-points in the parameter sequence in a data-driven manner.

Next, we set $d_i = d$ for $i = 1, \ldots, 100$ with $d \in \{2, 3, 5, 10\}$. Figure 13 plots $\mathbb{E}_\theta [\text{AIC}(\lambda)]$ and $2\mathbb{E}_\theta [L(\theta, \hat{\theta}_\lambda)]$ with respect to $\lambda$ for each value of $d$, where we used 10000 repetitions. They take minimum at similar values of $\lambda$. The absolute bias $|\mathbb{E}_\theta [\text{AIC}(\lambda)] - 2\mathbb{E}_\theta [D(\theta, \hat{\theta}_\lambda)]|$ decreases as $d$ increases, which is compatible with the fact that the chi-square distribution becomes closer to the normal distribution for larger $d$.

Finally, we examine the case where the degrees of freedom are not constant:

$$
\begin{align*}
    d_i &= \begin{cases} 
        6 & (i = 1, 6, \ldots, 96) \\
        7 & (i = 2, 7, \ldots, 97) \\
        8 & (i = 3, 8, \ldots, 98) \\
        9 & (i = 4, 9, \ldots, 99) \\
        10 & (i = 5, 10, \ldots, 100)
    \end{cases}
\end{align*}
$$

Figure 11: Generalized nearly isotonic regression for the chi-square distribution ($d = 5$) with several values of $\lambda$. black: samples $x_1/5, \ldots, x_{100}/5$, gray: true value $s_1, \ldots, s_{100}$, blue: estimate $\hat{s}_1, \ldots, \hat{s}_{100}$.

Next, we set $d_i = d$ for $i = 1, \ldots, 100$ with $d \in \{2, 3, 5, 10\}$. Figure 13 plots $\mathbb{E}_\theta [\text{AIC}(\lambda)]$ and $2\mathbb{E}_\theta [L(\theta, \hat{\theta}_\lambda)]$ with respect to $\lambda$ for each value of $d$, where we used 10000 repetitions. They take minimum at similar values of $\lambda$. The absolute bias $|\mathbb{E}_\theta [\text{AIC}(\lambda)] - 2\mathbb{E}_\theta [D(\theta, \hat{\theta}_\lambda)]|$ decreases as $d$ increases, which is compatible with the fact that the chi-square distribution becomes closer to the normal distribution for larger $d$.

Finally, we examine the case where the degrees of freedom are not constant:

$$
\begin{align*}
    d_i &= \begin{cases} 
        6 & (i = 1, 6, \ldots, 96) \\
        7 & (i = 2, 7, \ldots, 97) \\
        8 & (i = 3, 8, \ldots, 98) \\
        9 & (i = 4, 9, \ldots, 99) \\
        10 & (i = 5, 10, \ldots, 100)
    \end{cases}
\end{align*}
$$

Finally, we examine the case where the degrees of freedom are not constant:
Figure 12: AIC for the chi-square distribution \((d = 5)\).

Figure 13: Expected Kullback–Leibler discrepancy \(2E_\theta[D(\theta, \hat{\theta}_\lambda)]\) (black) and \(E_\theta[AIC(\lambda)]\) (blue, with standard deviation) for the chi-square distribution.
Figure 14 plots $E_{\theta}[\text{AIC}(\lambda)]$ and $2E_{\theta}[D(\theta, \hat{\theta}_{\lambda})]$ with respect to $\lambda$, where we used 10000 repetitions. The bias of the proposed information criterion is sufficiently small. Thus, this criterion works well for determining the regularization parameter $\lambda$ even when the degrees of freedom are heterogeneous among samples.

Figure 14: Expected Kullback–Leibler discrepancy $2E_{\theta}[D(\theta, \hat{\theta}_{\lambda})]$ (black) and $E_{\theta}[\text{AIC}(\lambda)]$ (blue, with standard deviation) for the chi-square distribution when the degrees of freedom are heterogeneous.